Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:53 am BST

PDB ID	:	6O9D
Title	:	Structure of the IRAK4 kinase domain with compound 5
Authors	:	Yu, C.; Drobnick, J.; Bryan, M.C.; Kiefer, J.; Lupardus, P.J.
Deposited on	:	2019-03-13
Resolution	:	2.51 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 following versions of software and data (see references ⓘ) were used in the production of this report:

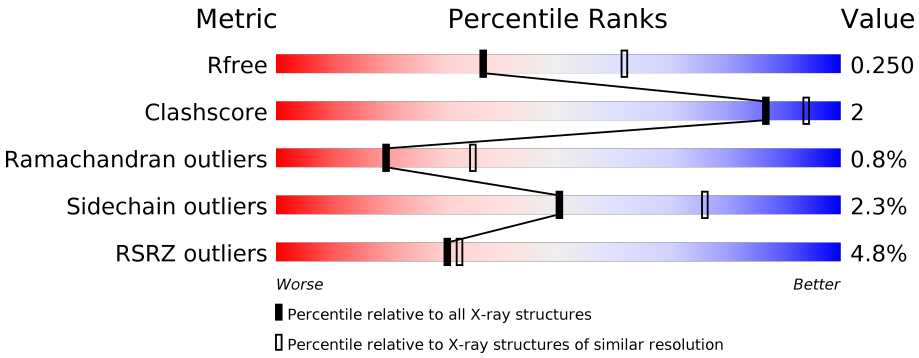
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	320	4% 82% 7% 11%
1	B	320	5% 82% 6% • 11%
1	C	320	3% 79% 9% 12%
1	D	320	5% 80% 8% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9296 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	286	Total	C	N	O	P	S	0	1	0
			2243	1407	373	445	3	15			
1	B	284	Total	C	N	O	P	S	0	0	0
			2248	1411	379	441	3	14			
1	C	283	Total	C	N	O	P	S	0	0	0
			2236	1401	375	443	3	14			
1	D	284	Total	C	N	O	P	S	0	0	0
			2231	1399	372	443	3	14			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	MET	-	initiating methionine	UNP Q9NWZ3
A	145	HIS	-	expression tag	UNP Q9NWZ3
A	146	HIS	-	expression tag	UNP Q9NWZ3
A	147	HIS	-	expression tag	UNP Q9NWZ3
A	148	HIS	-	expression tag	UNP Q9NWZ3
A	149	HIS	-	expression tag	UNP Q9NWZ3
A	150	HIS	-	expression tag	UNP Q9NWZ3
A	151	GLY	-	expression tag	UNP Q9NWZ3
A	152	GLU	-	expression tag	UNP Q9NWZ3
A	153	ASN	-	expression tag	UNP Q9NWZ3
A	154	LEU	-	expression tag	UNP Q9NWZ3
A	155	TYR	-	expression tag	UNP Q9NWZ3
A	156	PHE	-	expression tag	UNP Q9NWZ3
A	157	GLN	-	expression tag	UNP Q9NWZ3
A	158	GLY	-	expression tag	UNP Q9NWZ3
A	159	SER	-	expression tag	UNP Q9NWZ3
A	461	GLY	-	expression tag	UNP Q9NWZ3
A	462	ASN	-	expression tag	UNP Q9NWZ3
A	463	SER	-	expression tag	UNP Q9NWZ3
B	144	MET	-	initiating methionine	UNP Q9NWZ3
B	145	HIS	-	expression tag	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	146	HIS	-	expression tag	UNP Q9NWZ3
B	147	HIS	-	expression tag	UNP Q9NWZ3
B	148	HIS	-	expression tag	UNP Q9NWZ3
B	149	HIS	-	expression tag	UNP Q9NWZ3
B	150	HIS	-	expression tag	UNP Q9NWZ3
B	151	GLY	-	expression tag	UNP Q9NWZ3
B	152	GLU	-	expression tag	UNP Q9NWZ3
B	153	ASN	-	expression tag	UNP Q9NWZ3
B	154	LEU	-	expression tag	UNP Q9NWZ3
B	155	TYR	-	expression tag	UNP Q9NWZ3
B	156	PHE	-	expression tag	UNP Q9NWZ3
B	157	GLN	-	expression tag	UNP Q9NWZ3
B	158	GLY	-	expression tag	UNP Q9NWZ3
B	159	SER	-	expression tag	UNP Q9NWZ3
B	461	GLY	-	expression tag	UNP Q9NWZ3
B	462	ASN	-	expression tag	UNP Q9NWZ3
B	463	SER	-	expression tag	UNP Q9NWZ3
C	144	MET	-	initiating methionine	UNP Q9NWZ3
C	145	HIS	-	expression tag	UNP Q9NWZ3
C	146	HIS	-	expression tag	UNP Q9NWZ3
C	147	HIS	-	expression tag	UNP Q9NWZ3
C	148	HIS	-	expression tag	UNP Q9NWZ3
C	149	HIS	-	expression tag	UNP Q9NWZ3
C	150	HIS	-	expression tag	UNP Q9NWZ3
C	151	GLY	-	expression tag	UNP Q9NWZ3
C	152	GLU	-	expression tag	UNP Q9NWZ3
C	153	ASN	-	expression tag	UNP Q9NWZ3
C	154	LEU	-	expression tag	UNP Q9NWZ3
C	155	TYR	-	expression tag	UNP Q9NWZ3
C	156	PHE	-	expression tag	UNP Q9NWZ3
C	157	GLN	-	expression tag	UNP Q9NWZ3
C	158	GLY	-	expression tag	UNP Q9NWZ3
C	159	SER	-	expression tag	UNP Q9NWZ3
C	461	GLY	-	expression tag	UNP Q9NWZ3
C	462	ASN	-	expression tag	UNP Q9NWZ3
C	463	SER	-	expression tag	UNP Q9NWZ3
D	144	MET	-	initiating methionine	UNP Q9NWZ3
D	145	HIS	-	expression tag	UNP Q9NWZ3
D	146	HIS	-	expression tag	UNP Q9NWZ3
D	147	HIS	-	expression tag	UNP Q9NWZ3
D	148	HIS	-	expression tag	UNP Q9NWZ3
D	149	HIS	-	expression tag	UNP Q9NWZ3

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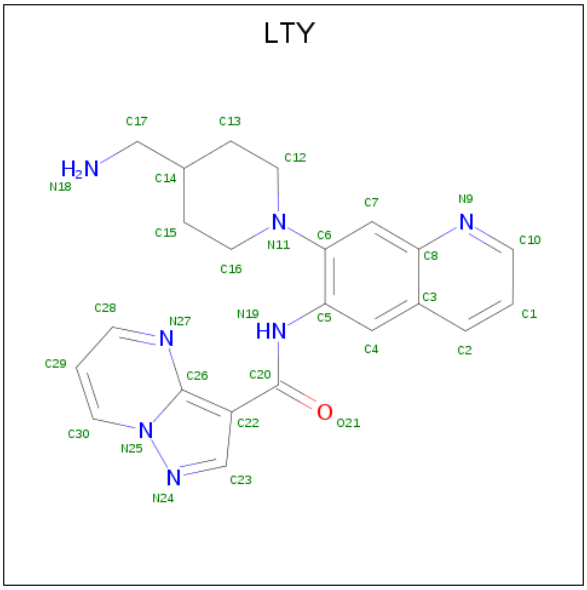
Chain	Residue	Modelled	Actual	Comment	Reference
D	150	HIS	-	expression tag	UNP Q9NWZ3
D	151	GLY	-	expression tag	UNP Q9NWZ3
D	152	GLU	-	expression tag	UNP Q9NWZ3
D	153	ASN	-	expression tag	UNP Q9NWZ3
D	154	LEU	-	expression tag	UNP Q9NWZ3
D	155	TYR	-	expression tag	UNP Q9NWZ3
D	156	PHE	-	expression tag	UNP Q9NWZ3
D	157	GLN	-	expression tag	UNP Q9NWZ3
D	158	GLY	-	expression tag	UNP Q9NWZ3
D	159	SER	-	expression tag	UNP Q9NWZ3
D	461	GLY	-	expression tag	UNP Q9NWZ3
D	462	ASN	-	expression tag	UNP Q9NWZ3
D	463	SER	-	expression tag	UNP Q9NWZ3

- Molecule 2 is N-{7-[4-(aminomethyl)piperidin-1-yl]quinolin-6-yl}pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: LTY) (formula: $C_{22}H_{23}N_7O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	22	7	1		
2	B	1	Total	C	N	O	0	0
			30	22	7	1		
2	C	1	Total	C	N	O	0	0
			30	22	7	1		
2	D	1	Total	C	N	O	0	0
			30	22	7	1		

- Molecule 3 is water.

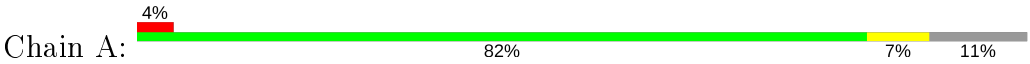
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	57	Total O 57 57	0	0
3	B	62	Total O 62 62	0	0
3	C	49	Total O 49 49	0	0
3	D	50	Total O 50 50	0	0

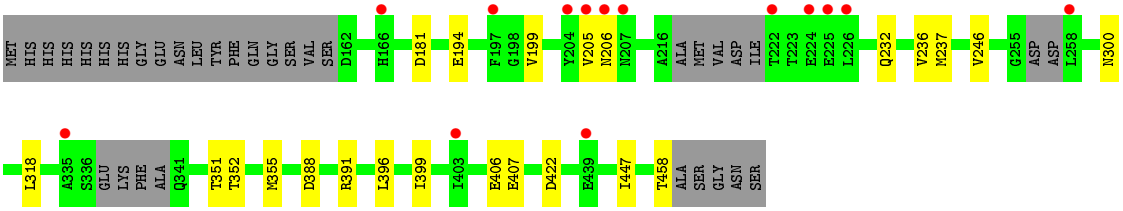
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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

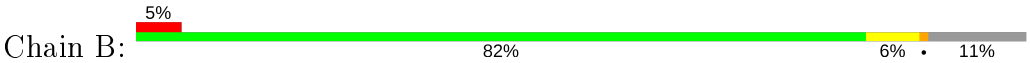
Chain A:

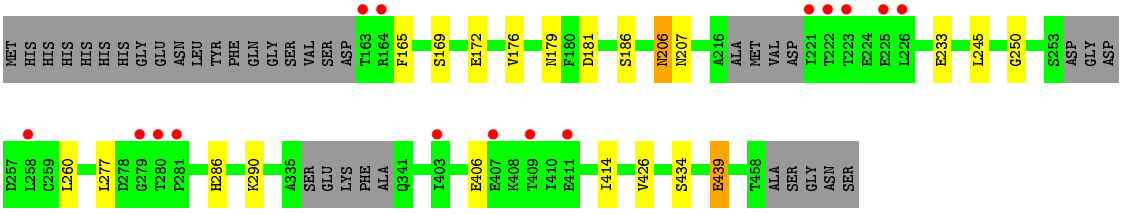




- Molecule 1: Interleukin-1 receptor-associated kinase 4

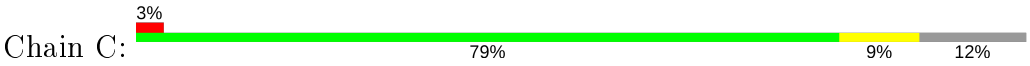
Chain B:

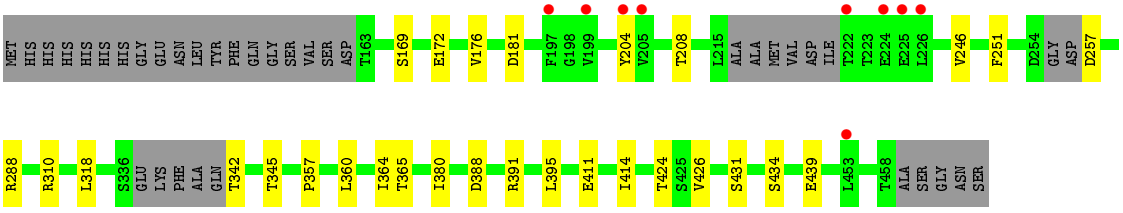




- Molecule 1: Interleukin-1 receptor-associated kinase 4

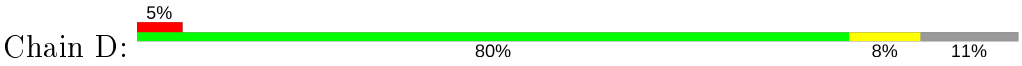
Chain C:

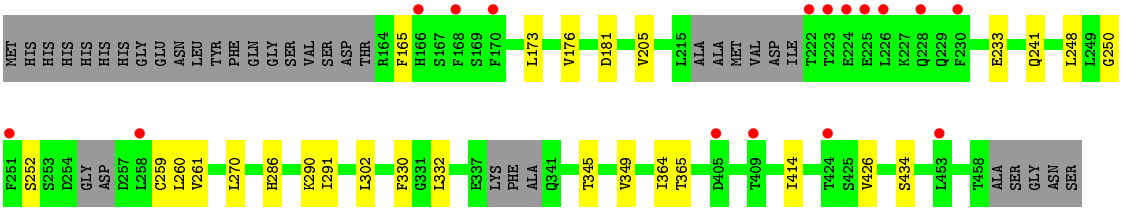




- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain D:




MET HIS HIS HIS HIS HIS GLY GLU ASN LEU TYR PHE GLN GLY SER VAL SER ASP THR R164 F165 H166 S167 F168 S169 F170 L173 V176 D181 V205 L215 ALA ALA MET VAL ASP ILE T222 T223 E224 E225 L226 K227 Q228 Q229 F230 E233 Q241 L248 L249 G250
F251 S252 S253 D254 GLY ASP D257 L258 C259 L260 V261 L270 H286 K290 I291 L302 F330 G331 L332 E337 LYS PHE ALA Q341 T345 V349 I364 T365 D405 T409 I414 T424 S425 V426 S434 L453 T458 ALA SER GLY ASN SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.34Å 139.10Å 87.83Å 90.00° 123.53° 90.00°	Depositor
Resolution (Å)	25.27 – 2.51 48.62 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.27-2.51) 99.3 (48.62-2.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.195 , 0.239 0.200 , 0.250	Depositor DCC
R_{free} test set	2455 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9296	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.69% 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, LTY, 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	0.52	0/2248	0.72	0/3028
1	B	0.52	0/2250	0.69	0/3028
1	C	0.51	0/2239	0.68	0/3016
1	D	0.50	0/2233	0.69	0/3008
All	All	0.51	0/8970	0.69	0/12080

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	2243	0	2185	7	0
1	B	2248	0	2219	8	0
1	C	2236	0	2193	12	0
1	D	2231	0	2173	12	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0
3	A	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	62	0	0	0	0
3	C	49	0	0	0	0
3	D	50	0	0	0	0
All	All	9296	0	8770	38	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 (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:TPO:HB	1:C:364:ILE:HD11	1.70	0.72
1:A:351:THR:O	1:A:355:MET:HG3	2.08	0.54
1:A:194:GLU:HG2	1:A:199:VAL:HG22	1.90	0.54
1:B:286:HIS:CE1	1:B:290:LYS:HE2	2.44	0.52
1:B:439:GLU:HG3	1:C:439:GLU:HB2	1.91	0.52
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.90	0.52
1:D:414:ILE:HG12	1:D:426:VAL:HG11	1.93	0.51
1:D:252:SER:HB3	1:D:259:CYS:HB2	1.93	0.51
1:D:173:LEU:HA	1:D:176:VAL:HG22	1.91	0.51
1:D:233:GLU:HG2	1:D:260:LEU:HD13	1.93	0.51
1:C:288:ARG:HB3	1:C:380:ILE:HG23	1.92	0.50
1:B:439:GLU:H	1:B:439:GLU:CD	2.16	0.50
1:D:286:HIS:CE1	1:D:290:LYS:HE2	2.48	0.49
1:D:165:PHE:HB3	1:D:250:GLY:HA2	1.94	0.49
1:C:176:VAL:HB	1:C:204:TYR:H	1.78	0.48
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.94	0.48
1:C:342:TPO:HG22	1:C:365:THR:HB	1.96	0.47
1:D:176:VAL:HG11	1:D:205:VAL:HG22	1.95	0.47
1:D:248:LEU:HD12	1:D:261:VAL:O	2.14	0.47
1:C:388:ASP:HB3	1:C:391:ARG:HB3	1.96	0.46
1:C:414:ILE:HG12	1:C:426:VAL:HG11	1.96	0.46
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.98	0.46
1:C:246:VAL:HG11	1:C:318:LEU:HD12	1.96	0.46
1:B:233:GLU:HG2	1:B:260:LEU:HD13	1.98	0.45
1:A:396:LEU:O	1:A:399:ILE:HG12	2.16	0.44
1:D:332:LEU:HD22	1:D:349:VAL:HG21	2.00	0.44
1:C:169:SER:HB3	1:C:172:GLU:HB2	2.01	0.43
1:D:270:LEU:HD13	1:D:291:ILE:HG21	2.01	0.43
1:C:310:ARG:HD3	1:C:364:ILE:HG23	2.02	0.42
1:A:232:GLN:O	1:A:236:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:SER:HB3	1:B:172:GLU:HG3	2.01	0.42
1:B:165:PHE:HB3	1:B:250:GLY:HA2	2.02	0.42
1:D:345:TPO:HB	1:D:364:ILE:HD11	2.02	0.42
1:A:388:ASP:HB3	1:A:391:ARG:HB3	2.01	0.42
1:C:357:PRO:HA	1:C:360:LEU:HD12	2.02	0.41
1:D:302:LEU:HD11	1:D:330:PHE:HE1	1.86	0.41
1:C:251:PHE:C	1:C:251:PHE:CD1	2.94	0.40
1:B:206:ASN:HB3	1:B:207:ASN:H	1.66	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	276/320 (86%)	265 (96%)	7 (2%)	4 (1%)	11	20
1	B	273/320 (85%)	257 (94%)	13 (5%)	3 (1%)	14	26
1	C	273/320 (85%)	262 (96%)	10 (4%)	1 (0%)	34	54
1	D	273/320 (85%)	263 (96%)	9 (3%)	1 (0%)	34	54
All	All	1095/1280 (86%)	1047 (96%)	39 (4%)	9 (1%)	19	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	B	406	GLU
1	A	205	VAL
1	A	181	ASP
1	C	181	ASP
1	A	206	ASN
1	B	181	ASP

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Mol	Chain	Res	Type
1	B	186	SER
1	D	181	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	242/275 (88%)	237 (98%)	5 (2%)	53 78
1	B	245/275 (89%)	238 (97%)	7 (3%)	42 69
1	C	244/275 (89%)	237 (97%)	7 (3%)	42 69
1	D	242/275 (88%)	239 (99%)	3 (1%)	71 88
All	All	973/1100 (88%)	951 (98%)	22 (2%)	50 76

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	MET
1	A	352	THR
1	A	407	GLU
1	A	422	ASP
1	A	458	THR
1	B	176	VAL
1	B	179	ASN
1	B	206	ASN
1	B	245	LEU
1	B	277	LEU
1	B	434	SER
1	B	439	GLU
1	C	208	THR
1	C	257	ASP
1	C	395	LEU
1	C	411	GLU
1	C	424	THR
1	C	431	SER
1	C	434	SER

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Mol	Chain	Res	Type
1	D	241	GLN
1	D	365	THR
1	D	434	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	394	GLN
1	B	178	ASN
1	B	241	GLN
1	B	286	HIS
1	B	307	HIS
1	B	394	GLN
1	C	166	HIS
1	C	451	GLN
1	C	455	GLN
1	D	166	HIS
1	D	286	HIS
1	D	293	GLN
1	D	390	HIS
1	D	394	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

12 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	D	346	1	8,9,10	0.95	0	8,12,14	2.77	2 (25%)
1	SEP	C	346	1	8,9,10	0.99	1 (12%)	8,12,14	1.65	2 (25%)
1	SEP	B	346	1	8,9,10	0.88	0	8,12,14	3.25	3 (37%)
1	SEP	A	346	1	8,9,10	0.91	0	8,12,14	2.27	2 (25%)
1	TPO	A	342	1	8,10,11	0.93	0	10,14,16	1.34	2 (20%)
1	TPO	B	342	1	8,10,11	1.18	1 (12%)	10,14,16	1.34	1 (10%)
1	TPO	B	345	1	8,10,11	1.30	1 (12%)	10,14,16	1.26	0
1	TPO	C	342	1	8,10,11	0.85	0	10,14,16	1.22	2 (20%)
1	TPO	C	345	1	8,10,11	1.43	1 (12%)	10,14,16	1.24	2 (20%)
1	TPO	A	345	1	8,10,11	1.43	2 (25%)	10,14,16	0.88	0
1	TPO	D	345	1	8,10,11	0.91	0	10,14,16	1.31	1 (10%)
1	TPO	D	342	1	8,10,11	1.47	1 (12%)	10,14,16	1.33	2 (20%)

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	D	346	1	-	1/5/8/10	-
1	SEP	C	346	1	-	0/5/8/10	-
1	SEP	B	346	1	-	1/5/8/10	-
1	SEP	A	346	1	-	1/5/8/10	-
1	TPO	A	342	1	-	1/9/11/13	-
1	TPO	B	342	1	-	1/9/11/13	-
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	C	342	1	-	1/9/11/13	-
1	TPO	C	345	1	-	4/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	TPO	D	342	1	-	1/9/11/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	TPO	P-OG1	-3.01	1.53	1.59
1	A	345	TPO	CB-CA	2.68	1.59	1.53
1	C	345	TPO	CB-CA	2.56	1.59	1.53
1	C	346	SEP	P-OG	-2.49	1.52	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	CG2-CB	2.32	1.57	1.51
1	B	345	TPO	CB-CA	2.26	1.58	1.53
1	B	342	TPO	P-OG1	-2.20	1.55	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	346	SEP	OG-CB-CA	7.85	115.78	108.14
1	D	346	SEP	OG-CB-CA	7.03	114.99	108.14
1	A	346	SEP	OG-CB-CA	5.35	113.36	108.14
1	B	346	SEP	P-OG-CB	-3.62	108.32	118.30
1	C	346	SEP	O2P-P-OG	3.45	115.93	106.73
1	C	346	SEP	P-OG-CB	-2.96	110.14	118.30
1	D	345	TPO	O2P-P-OG1	2.65	117.87	105.99
1	B	342	TPO	O2P-P-OG1	2.64	117.84	105.99
1	D	342	TPO	O2P-P-OG1	2.64	117.83	105.99
1	B	346	SEP	OG-P-O1P	2.64	113.88	106.47
1	A	342	TPO	O3P-P-OG1	2.62	117.73	105.99
1	D	346	SEP	P-OG-CB	-2.53	111.33	118.30
1	C	342	TPO	P-OG1-CB	-2.51	115.64	123.21
1	A	346	SEP	P-OG-CB	-2.48	111.46	118.30
1	A	342	TPO	P-OG1-CB	-2.35	116.11	123.21
1	C	345	TPO	O2P-P-O1P	-2.19	102.12	110.68
1	C	345	TPO	O3P-P-OG1	2.09	115.37	105.99
1	C	342	TPO	O3P-P-OG1	2.08	115.30	105.99
1	D	342	TPO	OG1-P-O1P	-2.04	101.51	109.39

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	346	SEP	N-CA-CB-OG
1	B	346	SEP	N-CA-CB-OG
1	A	346	SEP	N-CA-CB-OG
1	B	342	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	C	345	TPO	CA-CB-OG1-P
1	A	345	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	D	345	TPO	CA-CB-OG1-P
1	D	345	TPO	CB-OG1-P-O1P
1	A	342	TPO	CB-OG1-P-O1P
1	C	345	TPO	CB-OG1-P-O1P
1	D	342	TPO	CB-OG1-P-O3P
1	B	345	TPO	CA-CB-OG1-P
1	A	345	TPO	CA-CB-OG1-P
1	C	342	TPO	CB-OG1-P-O1P
1	A	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	342	TPO	1	0
1	C	345	TPO	1	0
1	D	345	TPO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	LTY	B	501	-	29,34,34	0.53	0	35,48,48	0.47	0
2	LTY	C	501	-	29,34,34	0.50	0	35,48,48	0.49	0
2	LTY	A	501	-	29,34,34	0.67	0	35,48,48	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LTY	D	501	-	29,34,34	0.55	0	35,48,48	0.84	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
2	LTY	B	501	-	-	2/12/24/24	0/5/5/5
2	LTY	C	501	-	-	4/12/24/24	0/5/5/5
2	LTY	A	501	-	-	2/12/24/24	0/5/5/5
2	LTY	D	501	-	-	6/12/24/24	0/5/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	LTY	C13-C14-C17-N18
2	C	501	LTY	C7-C6-N11-C12
2	C	501	LTY	C7-C6-N11-C16
2	D	501	LTY	C7-C6-N11-C12
2	D	501	LTY	C7-C6-N11-C16
2	B	501	LTY	C7-C6-N11-C12
2	A	501	LTY	C7-C6-N11-C16
2	A	501	LTY	C7-C6-N11-C12
2	D	501	LTY	C15-C14-C17-N18
2	B	501	LTY	C7-C6-N11-C16
2	C	501	LTY	C5-C6-N11-C12
2	C	501	LTY	C5-C6-N11-C16
2	D	501	LTY	C5-C6-N11-C16
2	D	501	LTY	C5-C6-N11-C12

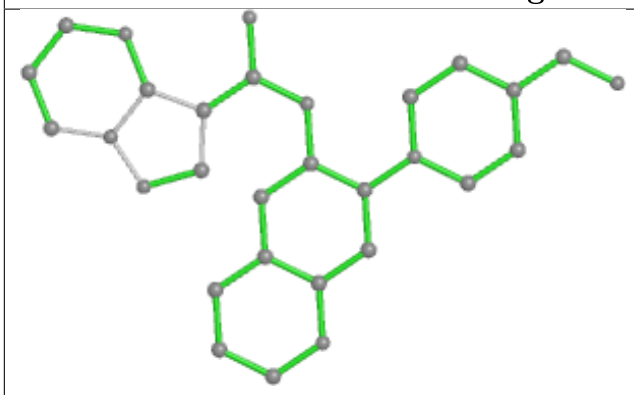
There are no ring outliers.

No monomer is involved in short contacts.

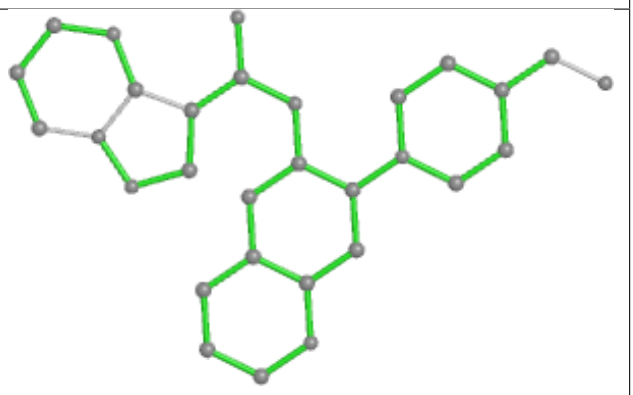
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

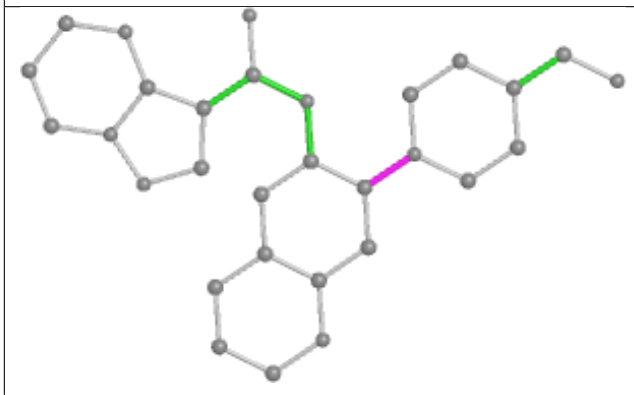
Ligand LTY B 501



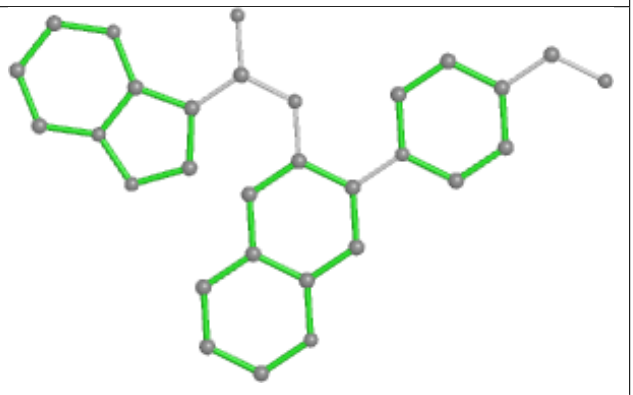
Bond lengths



Bond angles

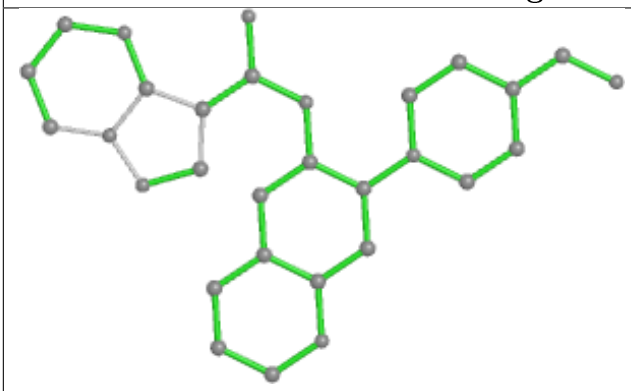


Torsions

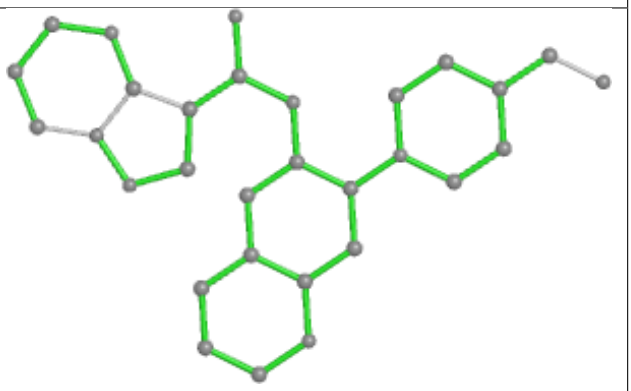


Rings

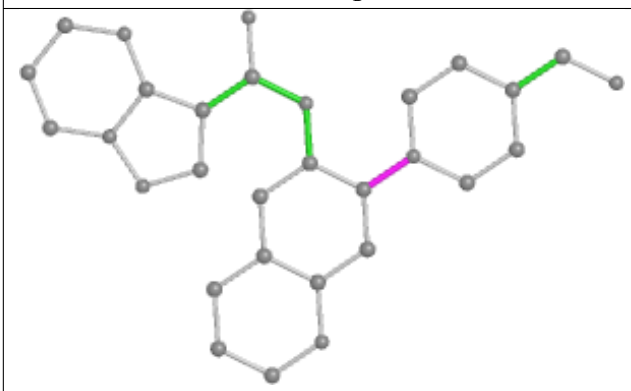
Ligand LTY C 501



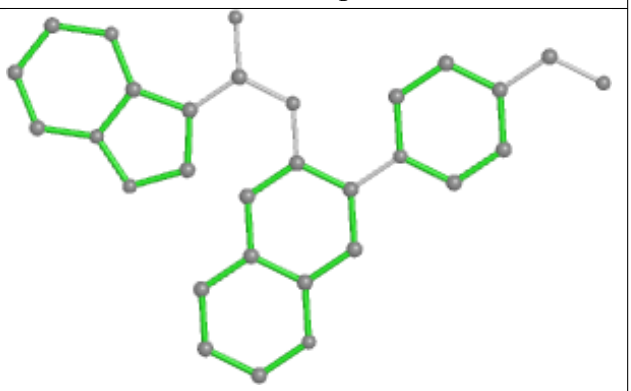
Bond lengths



Bond angles

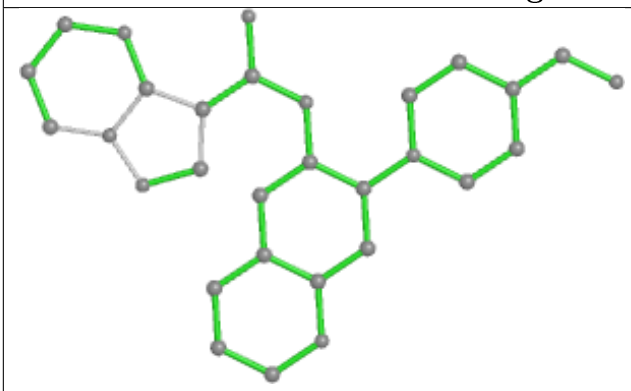


Torsions

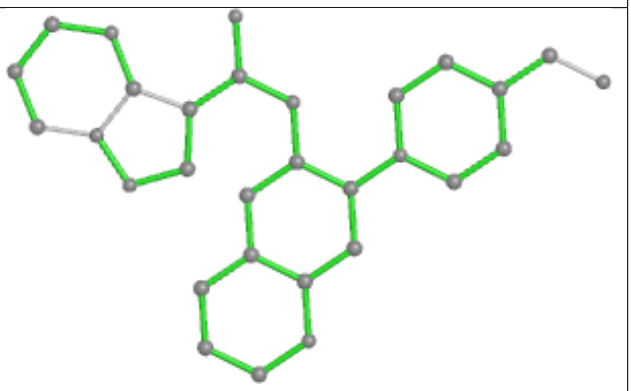


Rings

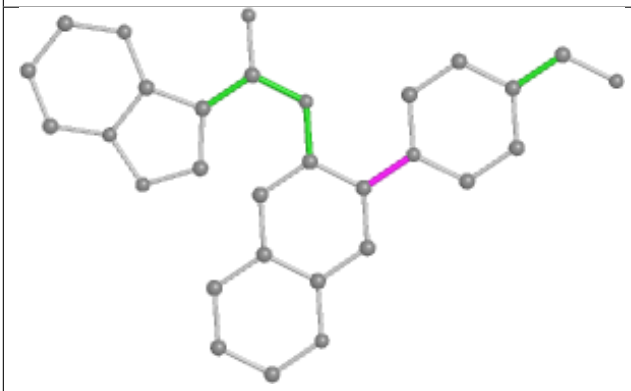
Ligand LTY A 501



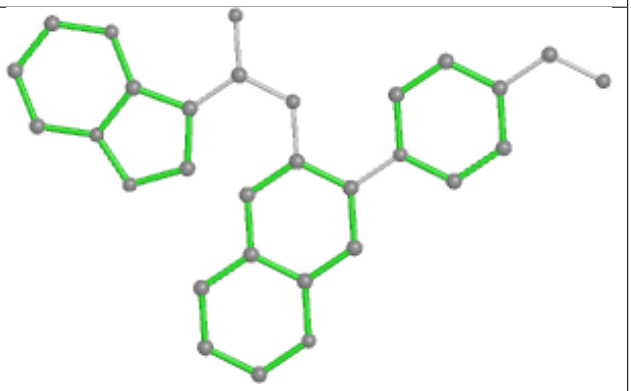
Bond lengths



Bond angles

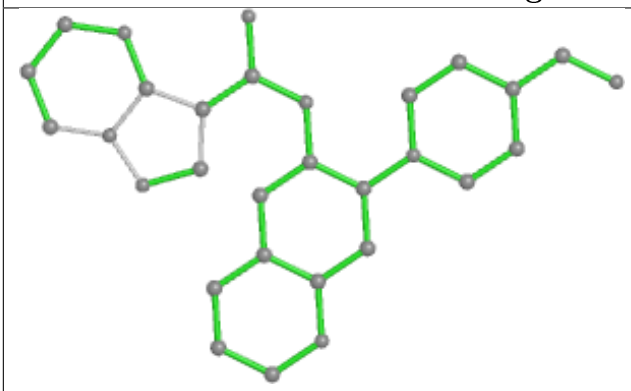


Torsions

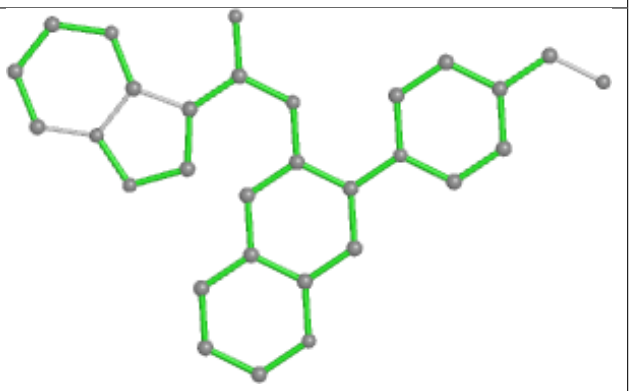


Rings

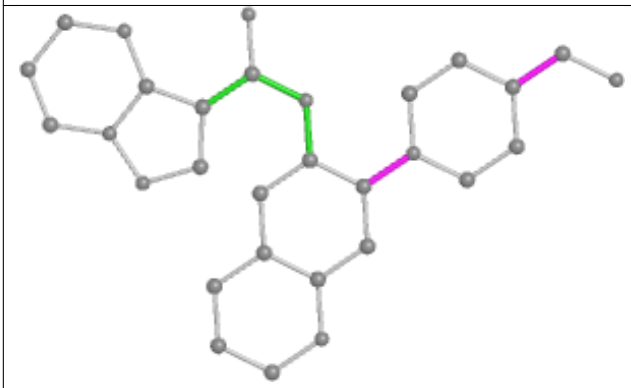
Ligand LTY D 501



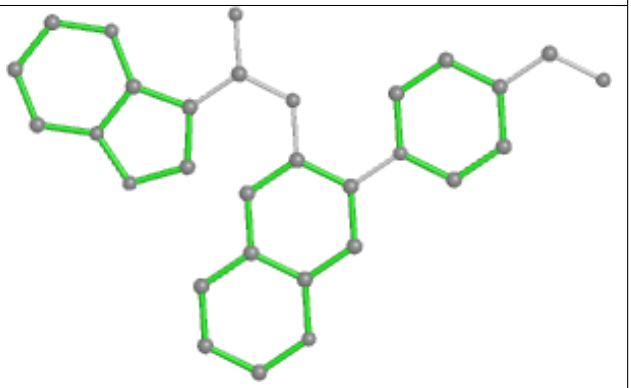
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	283/320 (88%)	0.37	14 (4%)	29	31	23, 43, 73, 89	0
1	B	281/320 (87%)	0.23	15 (5%)	26	28	21, 40, 72, 94	0
1	C	280/320 (87%)	0.21	9 (3%)	47	51	25, 44, 74, 87	0
1	D	281/320 (87%)	0.41	16 (5%)	23	25	23, 46, 74, 97	0
All	All	1125/1280 (87%)	0.31	54 (4%)	30	32	21, 43, 74, 97	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	LEU	7.2
1	C	204	TYR	6.6
1	D	222	THR	6.4
1	C	226	LEU	5.5
1	D	223	THR	5.2
1	D	224	GLU	5.0
1	B	222	THR	4.7
1	B	409	THR	4.6
1	B	163	THR	4.5
1	D	258	LEU	4.5
1	D	166	HIS	3.8
1	D	251	PHE	3.8
1	C	225	GLU	3.5
1	D	228	GLN	3.5
1	C	224	GLU	3.3
1	B	221	ILE	3.2
1	D	168	PHE	3.2
1	D	226	LEU	3.2
1	A	166	HIS	3.1
1	B	223	THR	3.1
1	A	204	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	206	ASN	2.9
1	A	205	VAL	2.9
1	A	222	THR	2.9
1	D	453	LEU	2.8
1	C	199	VAL	2.8
1	C	205	VAL	2.7
1	C	222	THR	2.6
1	B	258	LEU	2.6
1	A	207	ASN	2.5
1	B	225	GLU	2.5
1	C	453	LEU	2.4
1	B	280	THR	2.4
1	A	225	GLU	2.4
1	B	164	ARG	2.4
1	A	335	ALA	2.4
1	B	403	ILE	2.3
1	D	170	PHE	2.3
1	A	258	LEU	2.3
1	C	197	PHE	2.3
1	D	225	GLU	2.3
1	A	403	ILE	2.3
1	B	411	GLU	2.3
1	D	230	PHE	2.2
1	B	226	LEU	2.2
1	D	405	ASP	2.2
1	D	424	THR	2.2
1	A	224	GLU	2.2
1	A	439	GLU	2.2
1	D	409	THR	2.1
1	A	197	PHE	2.1
1	B	407	GLU	2.1
1	B	281	PRO	2.0
1	B	279	GLY	2.0

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	TPO	C	342	11/12	0.81	0.16	75,76,79,79	4
1	SEP	D	346	10/11	0.82	0.18	62,64,65,65	4
1	SEP	A	346	10/11	0.84	0.14	73,75,76,77	4
1	TPO	B	342	11/12	0.88	0.17	72,73,74,74	4
1	TPO	A	342	11/12	0.89	0.15	84,85,85,86	4
1	SEP	C	346	10/11	0.90	0.13	64,65,66,67	4
1	SEP	B	346	10/11	0.91	0.12	58,61,63,63	4
1	TPO	A	345	11/12	0.94	0.13	71,72,75,76	0
1	TPO	D	342	11/12	0.94	0.12	57,58,60,61	4
1	TPO	C	345	11/12	0.96	0.09	67,69,69,70	0
1	TPO	D	345	11/12	0.97	0.16	58,60,63,64	0
1	TPO	B	345	11/12	0.97	0.11	55,56,59,61	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

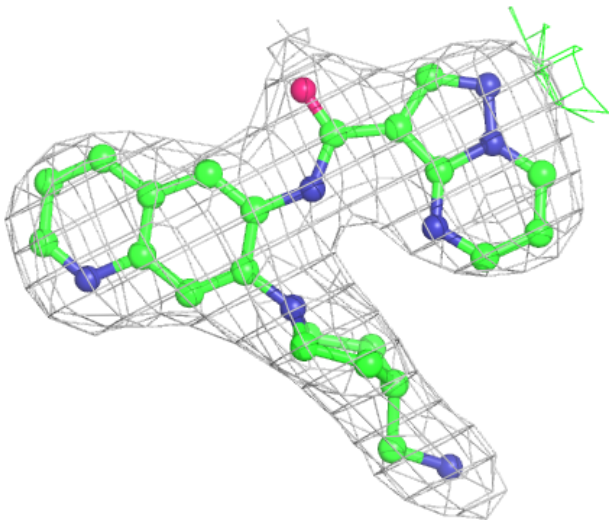
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

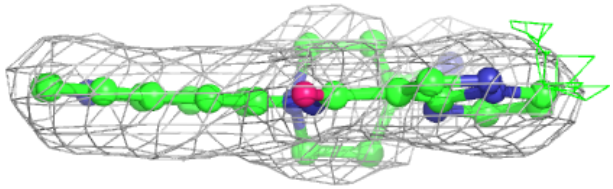
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LTY	D	501	30/30	0.95	0.17	26,34,38,39	0
2	LTY	C	501	30/30	0.96	0.13	24,31,36,37	0
2	LTY	A	501	30/30	0.97	0.14	15,23,30,35	0
2	LTY	B	501	30/30	0.97	0.14	23,27,37,38	0

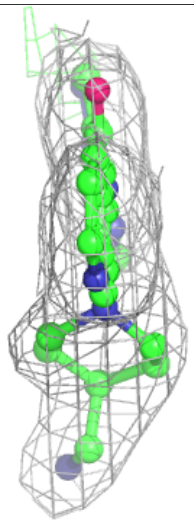
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LTY 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)

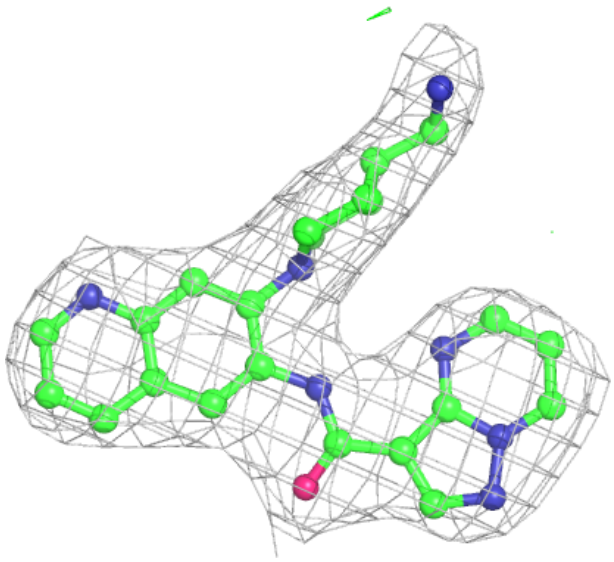


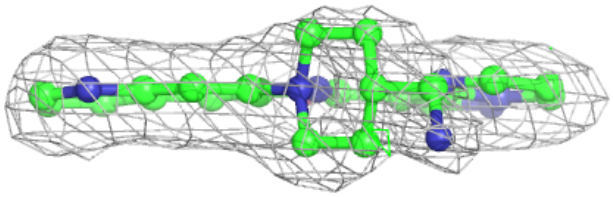


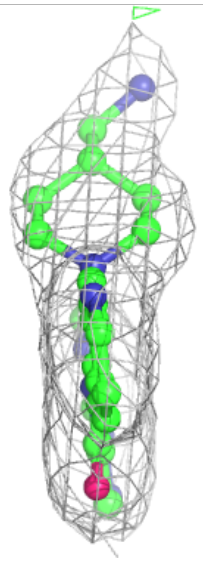


Electron density around LTY C 501:

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

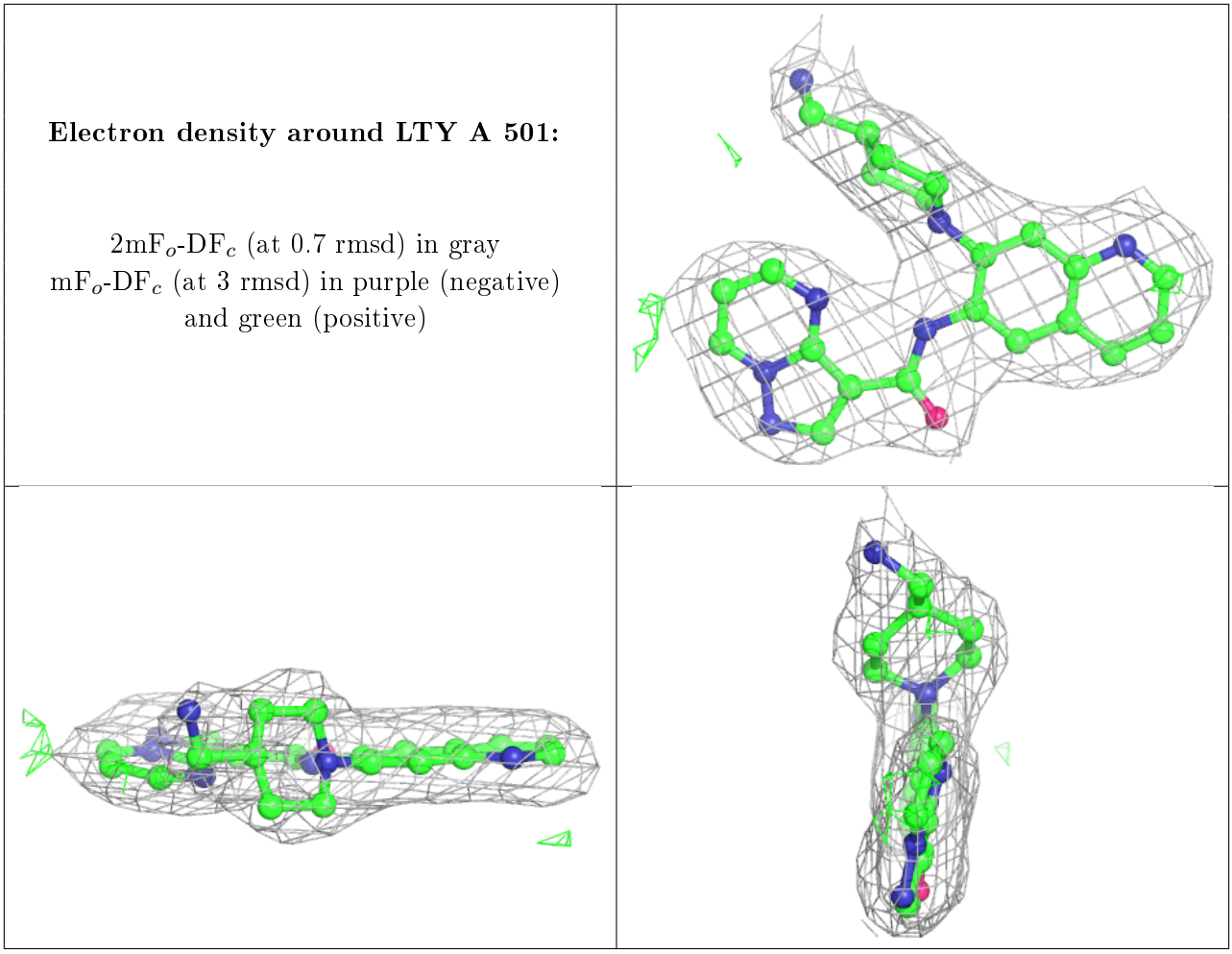






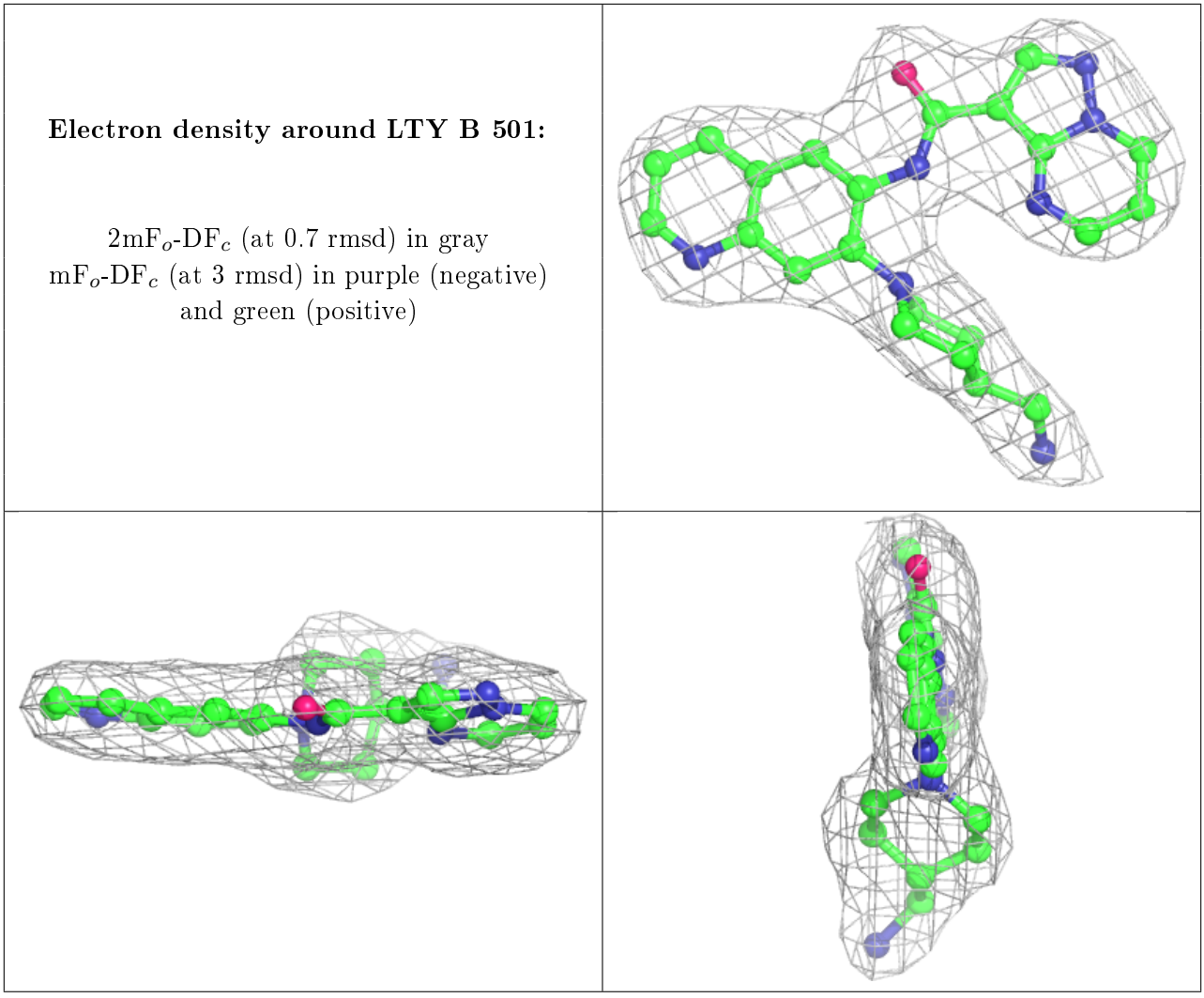
Electron density around LTY A 501:

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



Electron density around LTY 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)



6.5 Other polymers

There are no such residues in this entry.