



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:11 AM UTC

PDB ID : 6O9D / pdb_00006o9d
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

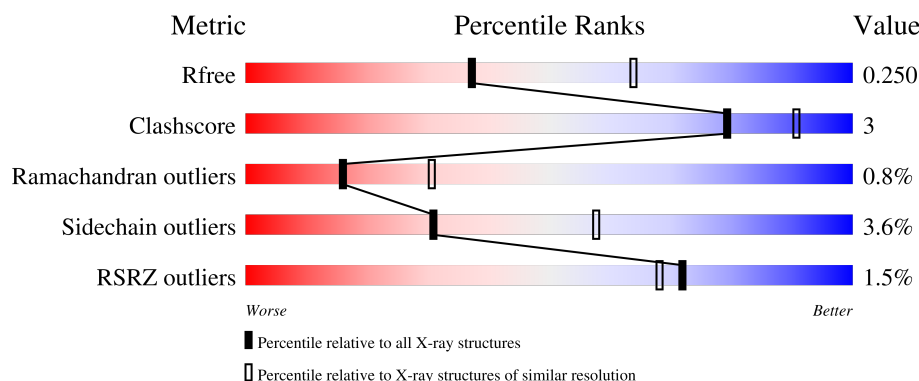
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	320	2% 76% 12% • 11%
1	B	320	2% 79% 9% • 11%
1	C	320	% 75% 12% • 12%
1	D	320	% 75% 12% • 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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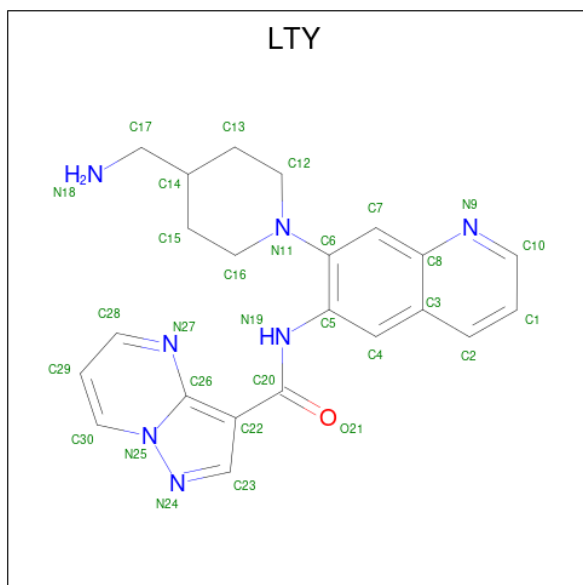
Chain	Residue	Modelled	Actual	Comment	Reference
B	146	HIS	-	expression tag	UNP Q9NWZ3
B	147	HIS	-	expression tag	UNP Q9NWZ3
B	148	HIS	-	expression tag	UNP Q9NWZ3
B	149	HIS	-	expression tag	UNP Q9NWZ3
B	150	HIS	-	expression tag	UNP Q9NWZ3
B	151	GLY	-	expression tag	UNP Q9NWZ3
B	152	GLU	-	expression tag	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 (CCD ID: LTY) (formula: C₂₂H₂₃N₇O).



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		

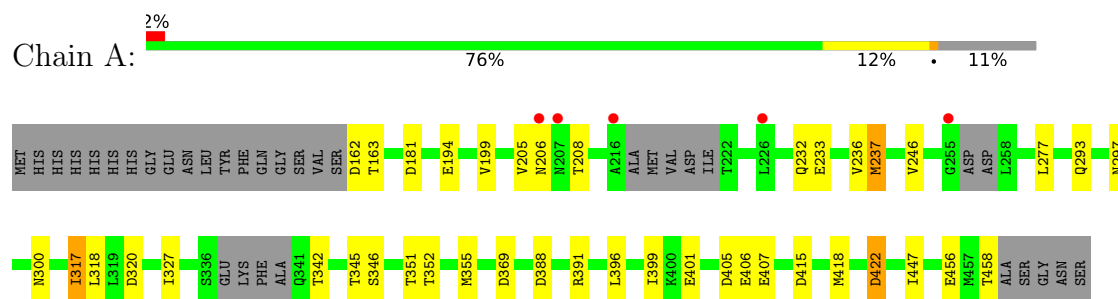
- Molecule 3 is water.

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

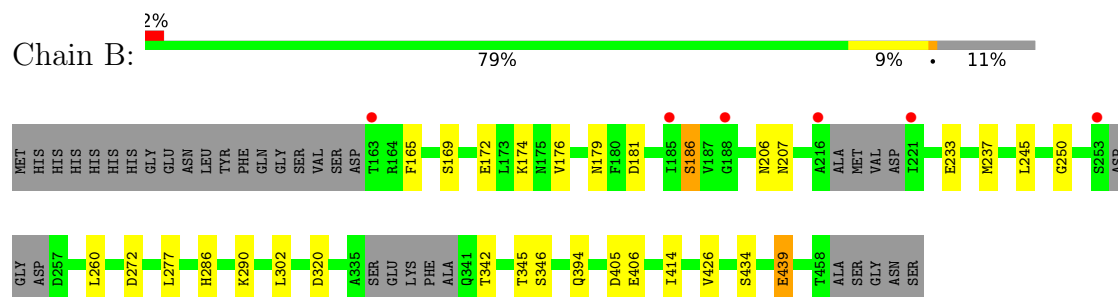
3 Residue-property plots [i](#)

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

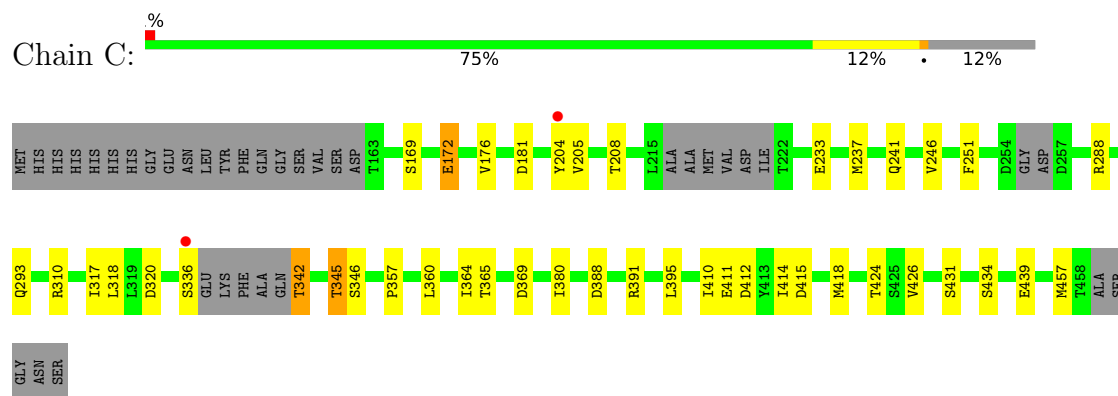
- Molecule 1: Interleukin-1 receptor-associated kinase 4



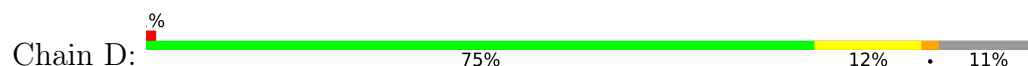
- Molecule 1: Interleukin-1 receptor-associated kinase 4

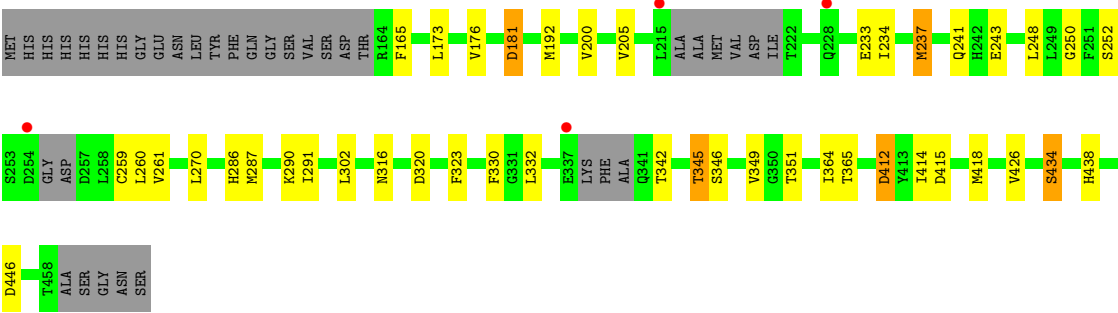


- Molecule 1: Interleukin-1 receptor-associated kinase 4



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





4 Data and refinement statistics

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 25.27 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.27-2.51) 99.5 (25.27-2.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.02%)	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)	0.35 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LTY, SEP, TPO

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	0.88	2/2248 (0.1%)	1.41	15/3028 (0.5%)
1	B	0.90	0/2250	1.32	5/3028 (0.2%)
1	C	0.87	0/2239	1.36	11/3016 (0.4%)
1	D	0.86	0/2233	1.39	11/3008 (0.4%)
All	All	0.88	2/8970 (0.0%)	1.37	42/12080 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	THR	CA-C	-6.76	1.44	1.52
1	A	208	THR	N-CA	-5.20	1.39	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	320	ASP	CA-CB-CG	6.83	119.43	112.60
1	D	320	ASP	CA-CB-CG	6.64	119.24	112.60
1	D	316	ASN	CA-CB-CG	6.50	119.09	112.60
1	A	320	ASP	CA-CB-CG	6.39	119.00	112.60
1	D	412	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	405	ASP	CA-C-N	6.18	133.34	121.54
1	A	405	ASP	C-N-CA	6.18	133.34	121.54
1	A	162	ASP	CA-C-N	6.15	130.73	120.70
1	A	162	ASP	C-N-CA	6.15	130.73	120.70
1	B	405	ASP	CA-C-N	6.07	133.14	121.54
1	B	405	ASP	C-N-CA	6.07	133.14	121.54
1	C	293	GLN	CA-C-N	5.93	126.70	119.99
1	C	293	GLN	C-N-CA	5.93	126.70	119.99
1	D	446	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	438	HIS	CA-C-N	5.67	127.88	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	438	HIS	C-N-CA	5.67	127.88	120.28
1	A	297	ASN	CA-C-N	5.65	126.10	119.94
1	A	297	ASN	C-N-CA	5.65	126.10	119.94
1	C	317	ILE	N-CA-C	-5.50	99.31	107.51
1	C	412	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	163	THR	N-CA-C	-5.49	106.03	114.16
1	A	317	ILE	N-CA-C	-5.44	99.31	107.37
1	B	320	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	181	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	369	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	369	ASP	CA-C-N	5.25	127.66	120.46
1	C	369	ASP	C-N-CA	5.25	127.66	120.46
1	C	172	GLU	N-CA-C	-5.24	105.24	111.69
1	A	293	GLN	CA-C-N	5.23	125.75	119.94
1	A	293	GLN	C-N-CA	5.23	125.75	119.94
1	A	422	ASP	CA-CB-CG	5.19	117.79	112.60
1	D	351	THR	CA-C-N	5.13	127.41	120.38
1	D	351	THR	C-N-CA	5.13	127.41	120.38
1	A	456	GLU	CA-C-N	5.11	127.63	120.28
1	A	456	GLU	C-N-CA	5.11	127.63	120.28
1	B	272	ASP	CA-CB-CG	5.11	117.70	112.60
1	C	205	VAL	N-CA-CB	5.10	118.18	111.25
1	D	434	SER	CA-C-N	5.09	127.52	120.29
1	D	434	SER	C-N-CA	5.09	127.52	120.29
1	C	410	ILE	CA-C-N	5.08	127.34	120.38
1	C	410	ILE	C-N-CA	5.08	127.34	120.38
1	B	174	LYS	N-CA-C	-5.06	105.67	111.14

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	9	0
1	B	2248	0	2219	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2236	0	2193	15	0
1	D	2231	0	2174	16	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
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	8771	48	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.

All (48) 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:B:237:MET:HA	1:B:237:MET:HE2	1.77	0.66
1:C:237:MET:HE2	1:C:237:MET:HA	1.78	0.65
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.84	0.59
1:D:237:MET:HA	1:D:237:MET:HE2	1.86	0.56
1:D:415:ASP:HB3	1:D:418:MET:HE2	1.88	0.55
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:439:GLU:CD	1:B:439:GLU:H	2.16	0.53
1:D:192:MET:HE3	1:D:200:VAL:HG12	1.91	0.53
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: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:D:287:MET:HE2	1:D:323:PHE:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:251:PHE:C	1:C:251:PHE:CD1	2.94	0.45
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
1:B:165:PHE:HB3	1:B:250:GLY:HA2	2.02	0.42
1:B:169:SER:HB3	1:B:172:GLU:HG3	2.01	0.42
1:D:345:TPO:HB	1:D:364:ILE:HD11	2.02	0.42
1:A:237:MET:HE1	1:A:246:VAL:HG23	2.02	0.42
1:A:388:ASP:HB3	1:A:391:ARG:HB3	2.01	0.42
1:C:457:MET:HE2	1:C:457:MET:HB3	1.95	0.41
1:A:415:ASP:HB3	1:A:418:MET:HE2	2.02	0.41
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:B:206:ASN:HB3	1:B:207:ASN:H	1.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	276/320 (86%)	265 (96%)	7 (2%)	4 (1%)	9 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	273/320 (85%)	257 (94%)	13 (5%)	3 (1%)	11	22
1	C	273/320 (85%)	262 (96%)	10 (4%)	1 (0%)	30	49
1	D	273/320 (85%)	263 (96%)	9 (3%)	1 (0%)	30	49
All	All	1095/1280 (86%)	1047 (96%)	39 (4%)	9 (1%)	16	31

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
1	B	186	SER
1	D	181	ASP

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	242/275 (88%)	232 (96%)	10 (4%)	27	53
1	B	245/275 (89%)	236 (96%)	9 (4%)	30	57
1	C	244/275 (89%)	235 (96%)	9 (4%)	30	57
1	D	242/275 (88%)	235 (97%)	7 (3%)	37	65
All	All	973/1100 (88%)	938 (96%)	35 (4%)	31	58

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	A	237	MET

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Mol	Chain	Res	Type
1	A	277	LEU
1	A	317	ILE
1	A	327	ILE
1	A	352	THR
1	A	401	GLU
1	A	407	GLU
1	A	422	ASP
1	A	458	THR
1	B	176	VAL
1	B	179	ASN
1	B	186	SER
1	B	245	LEU
1	B	277	LEU
1	B	302	LEU
1	B	394	GLN
1	B	434	SER
1	B	439	GLU
1	C	208	THR
1	C	233	GLU
1	C	241	GLN
1	C	336	SER
1	C	395	LEU
1	C	411	GLU
1	C	424	THR
1	C	431	SER
1	C	434	SER
1	D	234	ILE
1	D	237	MET
1	D	241	GLN
1	D	243	GLU
1	D	365	THR
1	D	412	ASP
1	D	434	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	190	ASN
1	A	244	ASN
1	A	286	HIS
1	A	394	GLN

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Mol	Chain	Res	Type
1	A	435	GLN
1	A	455	GLN
1	B	241	GLN
1	B	286	HIS
1	B	307	HIS
1	B	442	ASN
1	C	297	ASN
1	C	390	HIS
1	C	394	GLN
1	C	451	GLN
1	D	206	ASN
1	D	241	GLN
1	D	286	HIS
1	D	297	ASN
1	D	316	ASN
1	D	390	HIS
1	D	394	GLN
1	D	451	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	TPO	A	342	1	8,10,11	1.00	0	10,14,16	1.50	2 (20%)
1	SEP	C	346	1	8,9,10	1.02	1 (12%)	7,12,14	1.40	1 (14%)
1	TPO	C	342	1	8,10,11	0.90	0	10,14,16	1.37	2 (20%)
1	TPO	D	345	1	8,10,11	0.95	0	10,14,16	1.44	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	B	342	1	8,10,11	1.28	1 (12%)	10,14,16	1.49	1 (10%)
1	SEP	B	346	1	8,9,10	0.92	0	7,12,14	3.21	2 (28%)
1	TPO	C	345	1	8,10,11	1.52	2 (25%)	10,14,16	1.32	2 (20%)
1	SEP	D	346	1	8,9,10	0.99	0	7,12,14	2.81	1 (14%)
1	SEP	A	346	1	8,9,10	0.95	0	7,12,14	2.25	1 (14%)
1	TPO	A	345	1	8,10,11	1.50	2 (25%)	10,14,16	0.96	0
1	TPO	B	345	1	8,10,11	1.39	2 (25%)	10,14,16	1.35	1 (10%)
1	TPO	D	342	1	8,10,11	1.59	1 (12%)	10,14,16	1.48	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	TPO	A	342	1	-	1/9/11/13	-
1	SEP	C	346	1	-	0/6/8/10	-
1	TPO	C	342	1	-	0/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	TPO	B	342	1	-	1/9/11/13	-
1	SEP	B	346	1	-	2/6/8/10	-
1	TPO	C	345	1	-	3/9/11/13	-
1	SEP	D	346	1	-	2/6/8/10	-
1	SEP	A	346	1	-	2/6/8/10	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	D	342	1	-	1/9/11/13	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	TPO	P-OG1	-3.36	1.53	1.59
1	A	345	TPO	CB-CA	2.84	1.59	1.53
1	C	345	TPO	CB-CA	2.71	1.59	1.53
1	C	346	SEP	P-OG	-2.57	1.52	1.60
1	B	342	TPO	P-OG1	-2.49	1.55	1.59
1	B	345	TPO	CB-CA	2.40	1.58	1.53
1	A	345	TPO	CG2-CB	2.32	1.57	1.51
1	C	345	TPO	P-OG1	-2.25	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	P-OG1	-2.05	1.55	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C	346	SEP	O2P-P-OG	3.55	115.93	106.67
1	D	345	TPO	O2P-P-OG1	3.09	117.87	105.85
1	B	342	TPO	O2P-P-OG1	3.08	117.84	105.85
1	D	342	TPO	O2P-P-OG1	3.08	117.83	105.85
1	A	342	TPO	O3P-P-OG1	3.05	117.73	105.85
1	C	342	TPO	P-OG1-CB	-2.83	115.64	123.33
1	B	346	SEP	OG-P-O1P	2.75	113.88	106.44
1	A	342	TPO	P-OG1-CB	-2.66	116.11	123.33
1	C	345	TPO	O3P-P-OG1	2.44	115.37	105.85
1	C	342	TPO	O3P-P-OG1	2.43	115.30	105.85
1	C	345	TPO	O2P-P-O1P	-2.24	102.12	110.83
1	D	342	TPO	OG1-P-O1P	-2.20	101.51	109.33
1	B	345	TPO	O2P-P-OG1	2.02	113.73	105.85

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	A	342	TPO	CB-OG1-P-O1P
1	A	345	TPO	CA-CB-OG1-P
1	B	345	TPO	CA-CB-OG1-P
1	B	345	TPO	CB-OG1-P-O1P
1	D	345	TPO	CB-OG1-P-O1P
1	D	342	TPO	CB-OG1-P-O3P
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	D	345	TPO	1	0
1	C	345	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	C	501	-	33,34,34	0.63	0	43,48,48	0.72	1 (2%)
2	LTY	D	501	-	33,34,34	0.86	2 (6%)	43,48,48	0.88	0
2	LTY	A	501	-	33,34,34	0.98	1 (3%)	43,48,48	0.78	1 (2%)
2	LTY	B	501	-	33,34,34	0.66	0	43,48,48	0.71	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	C	501	-	-	4/14/24/24	0/5/5/5
2	LTY	D	501	-	-	5/14/24/24	0/5/5/5
2	LTY	A	501	-	-	2/14/24/24	0/5/5/5
2	LTY	B	501	-	-	2/14/24/24	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LTY	C23-N24	4.08	1.39	1.32
2	D	501	LTY	C23-N24	2.97	1.37	1.32
2	D	501	LTY	C22-C26	-2.20	1.39	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LTY	C22-C26-N27	-2.42	130.18	132.07
2	C	501	LTY	C28-N27-C26	2.25	117.30	115.55

There are no chirality outliers.

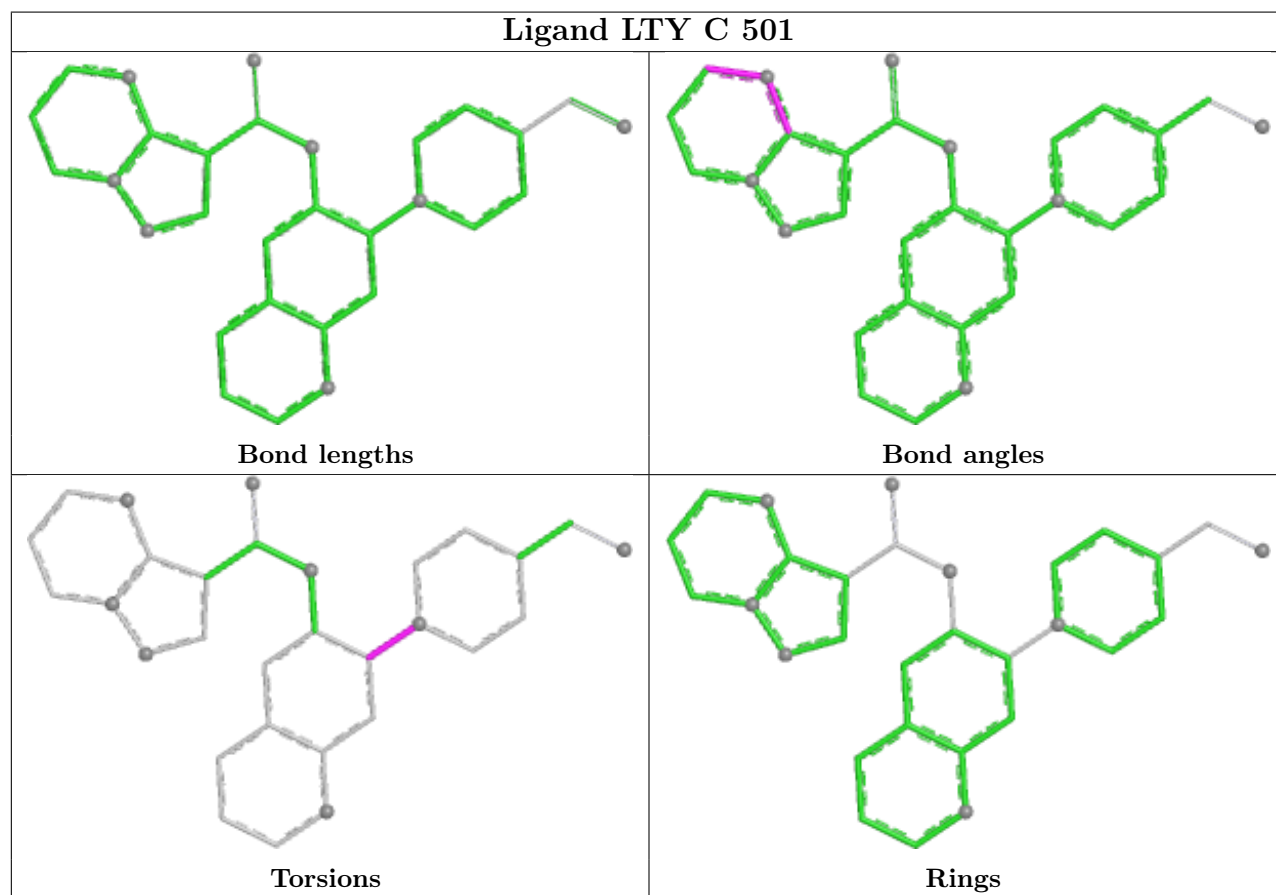
All (13) torsion outliers are listed below:

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	A	501	LTY	C7-C6-N11-C16
2	B	501	LTY	C7-C6-N11-C12
2	A	501	LTY	C7-C6-N11-C12
2	B	501	LTY	C7-C6-N11-C16
2	D	501	LTY	C15-C14-C17-N18
2	C	501	LTY	C5-C6-N11-C16
2	C	501	LTY	C5-C6-N11-C12
2	D	501	LTY	C5-C6-N11-C16

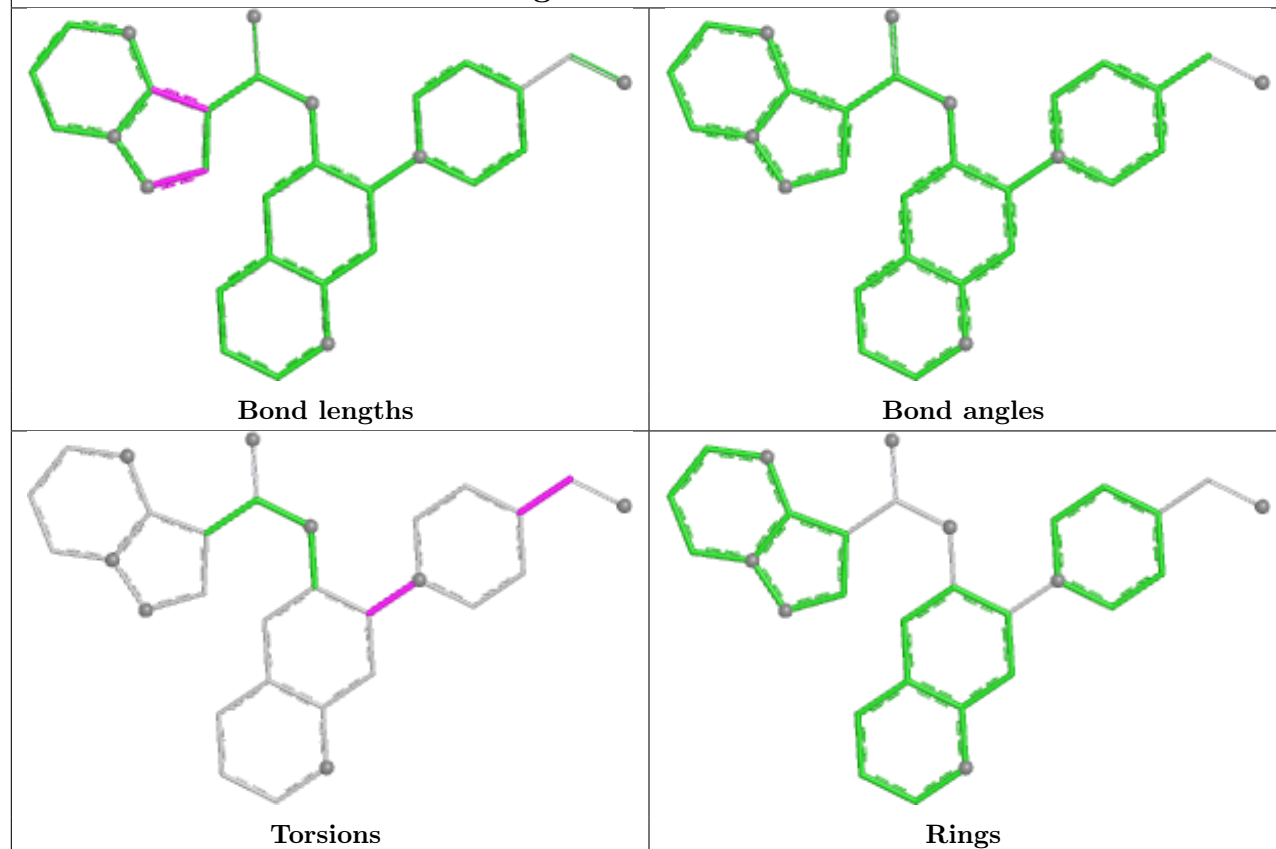
There are no ring outliers.

No monomer is involved in short contacts.

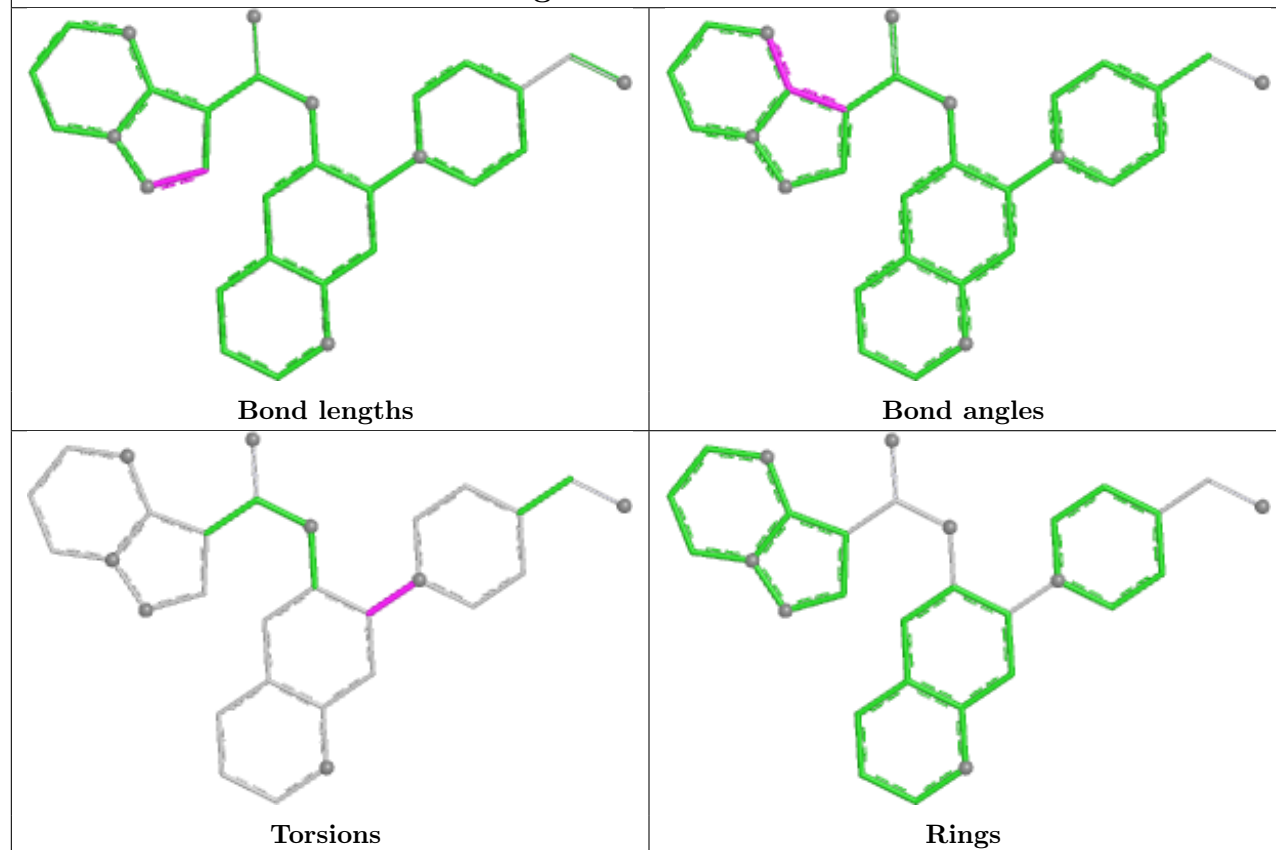
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

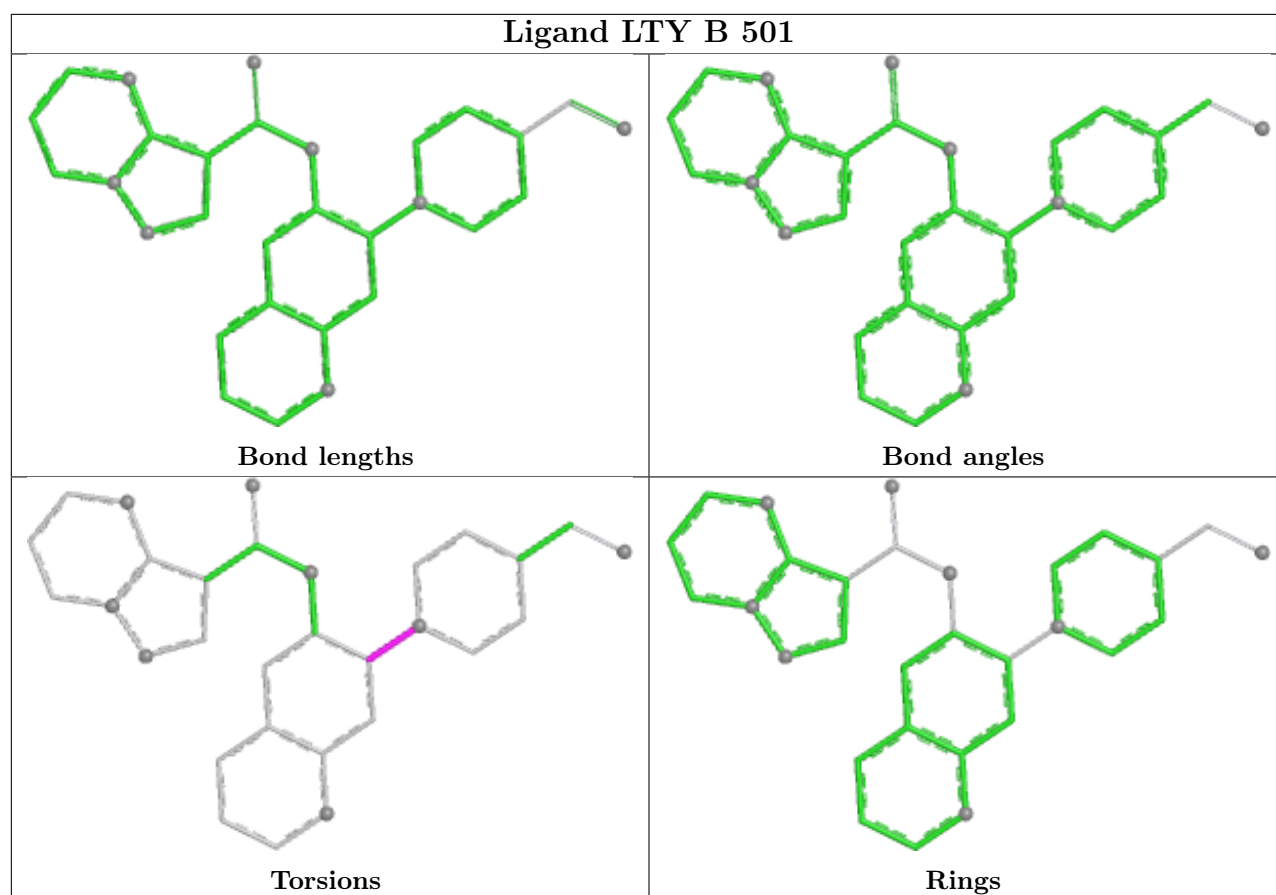


Ligand LTY D 501



Ligand LTY A 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	283/320 (88%)	-0.05	5 (1%) 67 64	19, 43, 73, 89	1 (0%)
1	B	281/320 (87%)	-0.15	6 (2%) 63 59	21, 40, 72, 94	0
1	C	280/320 (87%)	-0.10	2 (0%) 84 81	25, 44, 74, 87	0
1	D	281/320 (87%)	0.02	4 (1%) 73 70	23, 46, 74, 97	0
All	All	1125/1280 (87%)	-0.07	17 (1%) 72 68	19, 43, 74, 97	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	GLY	3.7
1	C	336	SER	3.4
1	B	216	ALA	3.0
1	C	204	TYR	3.0
1	A	226	LEU	2.8
1	A	206	ASN	2.5
1	A	216	ALA	2.5
1	B	163	THR	2.5
1	B	221	ILE	2.3
1	D	215	LEU	2.3
1	D	337	GLU	2.3
1	B	253	SER	2.2
1	D	228	GLN	2.2
1	B	188	GLY	2.2
1	A	207	ASN	2.1
1	B	185	ILE	2.0
1	D	254	ASP	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SEP	A	346	10/11	0.55	0.12	73,75,76,77	4
1	SEP	C	346	10/11	0.67	0.11	64,65,66,67	4
1	SEP	D	346	10/11	0.70	0.11	62,64,65,65	4
1	TPO	C	342	11/12	0.78	0.11	75,76,79,79	4
1	SEP	B	346	10/11	0.79	0.09	58,61,63,63	4
1	TPO	B	342	11/12	0.79	0.12	72,73,74,74	4
1	TPO	A	342	11/12	0.86	0.08	84,85,85,86	4
1	TPO	D	342	11/12	0.89	0.08	57,58,60,61	4
1	TPO	A	345	11/12	0.89	0.09	71,72,75,76	0
1	TPO	C	345	11/12	0.93	0.08	67,69,69,70	0
1	TPO	B	345	11/12	0.94	0.07	55,56,59,61	0
1	TPO	D	345	11/12	0.95	0.08	58,60,63,64	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

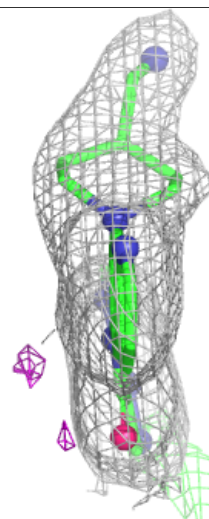
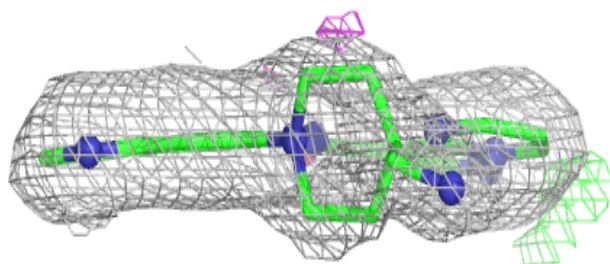
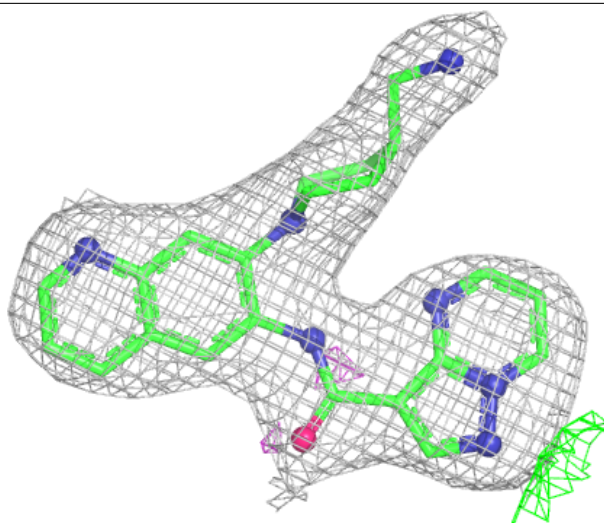
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LTY	D	501	30/30	0.94	0.07	26,34,38,39	0
2	LTY	B	501	30/30	0.96	0.07	23,27,37,38	0
2	LTY	C	501	30/30	0.96	0.06	24,31,36,37	0
2	LTY	A	501	30/30	0.96	0.06	15,23,30,35	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.

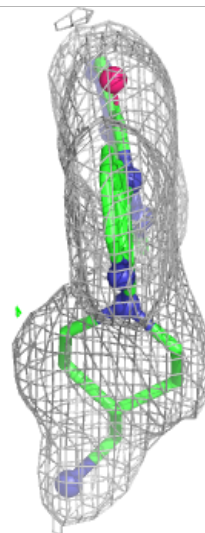
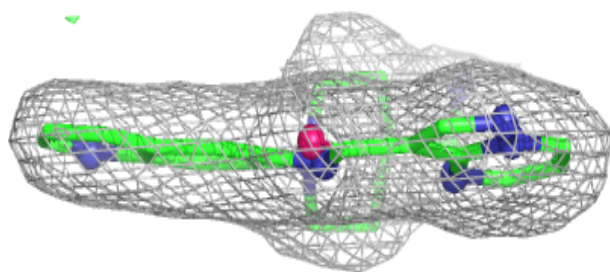
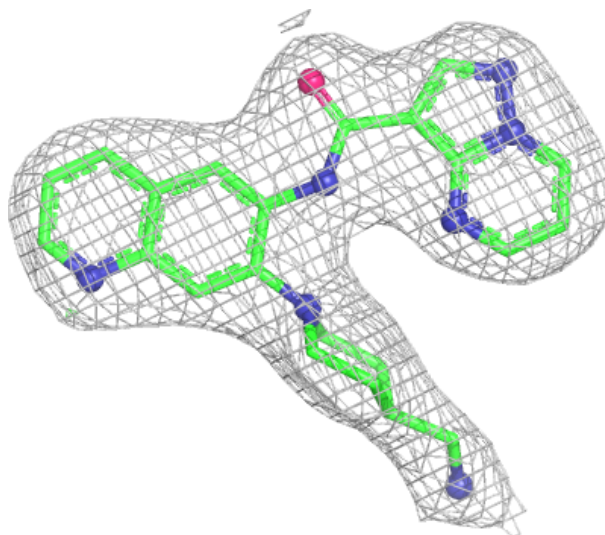
Electron density around LTY D 501:

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



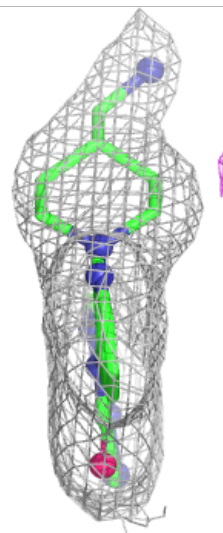
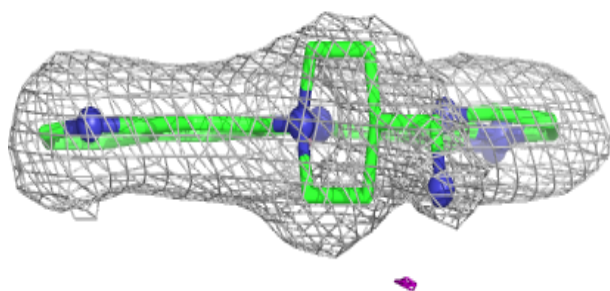
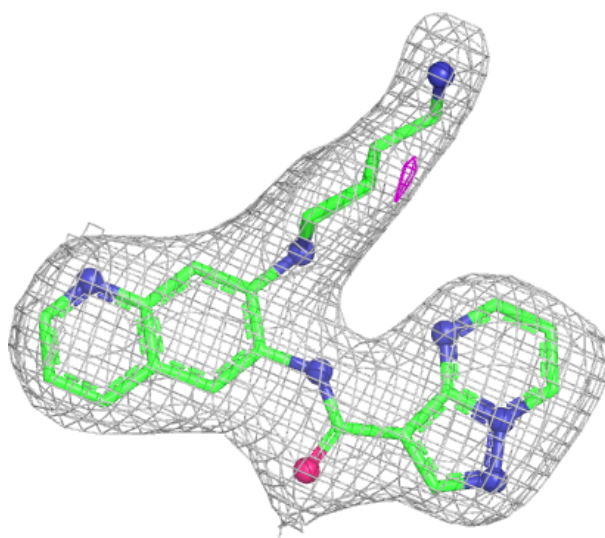
Electron density around LTY B 501:

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



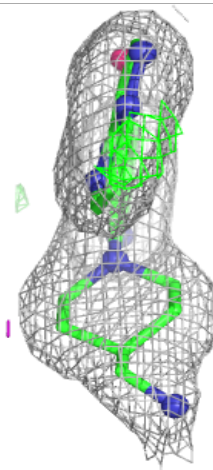
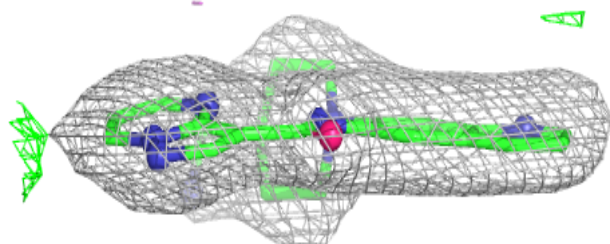
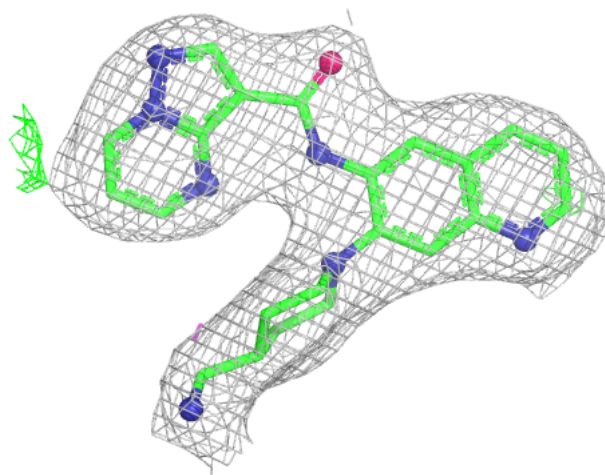
Electron density around LTY C 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.