



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 07:18 PM EST

PDB ID : 4GH6  
Title : Crystal structure of the PDE9A catalytic domain in complex with inhibitor 28  
Authors : Hou, J.; Ke, H.  
Deposited on : 2012-08-07  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

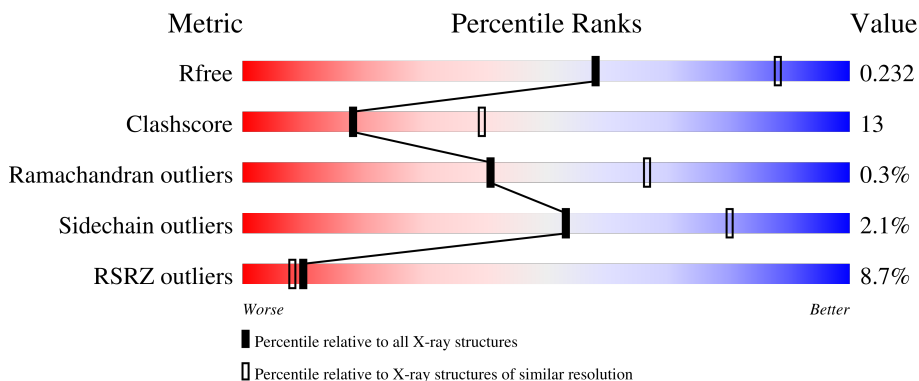
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	
1	B	326	

## 2 Entry composition [i](#)

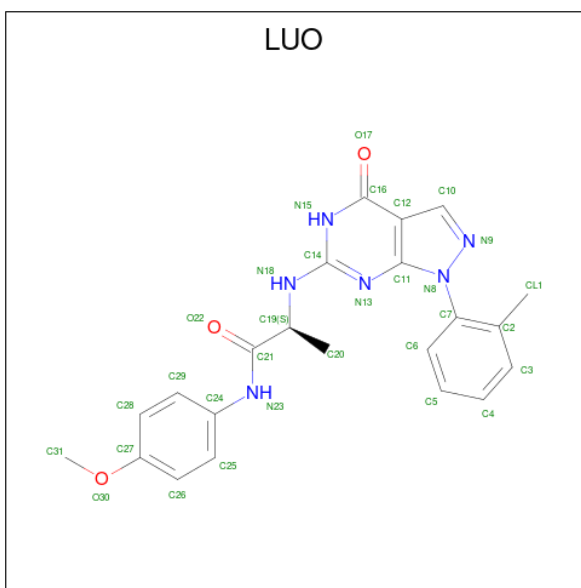
There are 5 unique types of molecules in this entry. The entry contains 5505 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	326	Total 2695	C 1727	N 446	O 492	S 30	0	0	0
1	B	326	Total 2695	C 1727	N 446	O 492	S 30	0	0	0

- Molecule 2 is N-(4-methoxyphenyl)-N 2 -[1-(2-methylphenyl)-4-oxo-4,5-dihydro-1H-pyrazol o[3,4-d]pyrimidin-6-yl]-L-alaninamide (three-letter code: LUO) (formula: C<sub>22</sub>H<sub>22</sub>N<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 31	C 22	N 6	O 3	0	0
2	B	1	Total 31	C 22	N 6	O 3	0	0
2	B	1	Total 31	C 22	N 6	O 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

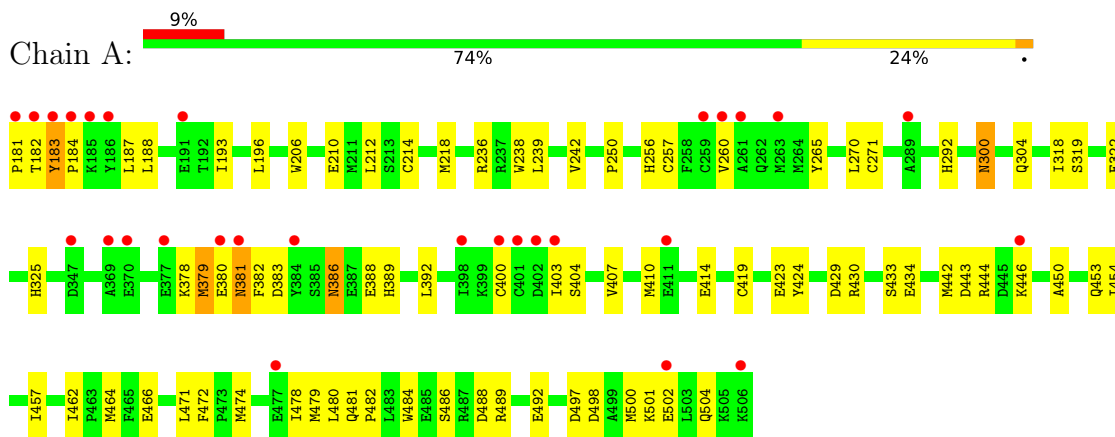
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	8	Total	O	0	0
			8	8		

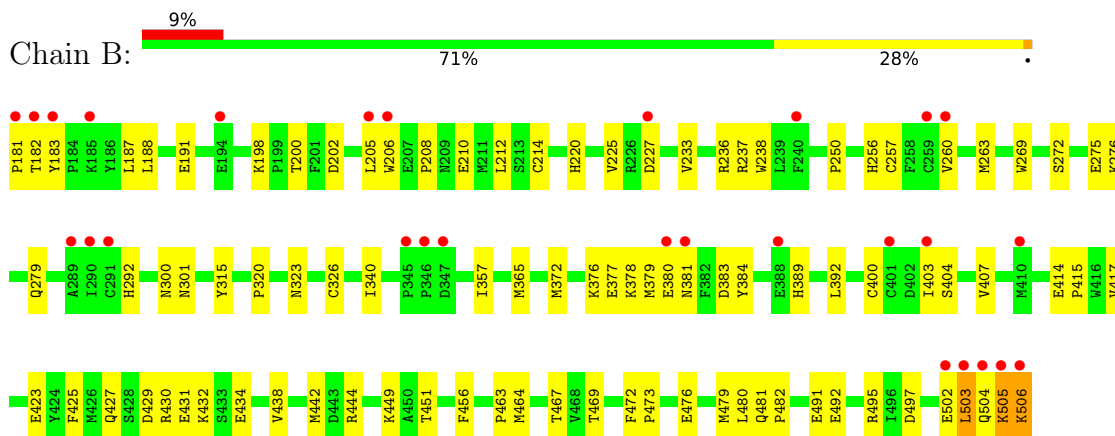
### 3 Residue-property plots i

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: High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A



- Molecule 1: High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.28Å 104.28Å 270.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.73 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 93.7 (29.73-2.71)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.26 (at 2.72Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.212 , 0.245 0.200 , 0.232	Depositor DCC
$R_{free}$ test set	4124 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtrriage
Anisotropy	0.506	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LUO, MG, ZN

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	0.41	0/2765	0.58	0/3743
1	B	0.38	0/2765	0.59	0/3743
All	All	0.39	0/5530	0.58	0/7486

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	2695	0	2640	70	0
1	B	2695	0	2640	71	0
2	A	31	0	22	3	0
2	B	62	0	44	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	0	0
5	B	8	0	0	0	0
All	All	5505	0	5346	145	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 13.

All (145) 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)
2:A:601:LUO:H22	2:A:601:LUO:O22	1.74	0.85
1:A:270:LEU:HD13	1:A:478:ILE:HD12	1.60	0.82
1:A:400:CYS:HA	1:A:464:MET:HE3	1.61	0.81
2:B:601:LUO:O22	2:B:601:LUO:H22	1.82	0.78
1:B:430:ARG:O	1:B:434:GLU:HG3	1.88	0.73
1:A:236:ARG:HD2	1:B:187:LEU:HD21	1.71	0.72
1:B:506:LYS:HE3	1:B:506:LYS:HA	1.73	0.70
2:B:602:LUO:H1	2:B:602:LUO:N9	2.06	0.70
1:A:386:ASN:ND2	1:A:389:HIS:H	1.89	0.70
1:B:183:TYR:HB3	1:B:187:LEU:HD12	1.74	0.69
1:B:378:LYS:HD2	1:B:392:LEU:HD12	1.74	0.69
1:A:379:MET:HE3	1:A:379:MET:HA	1.73	0.69
1:A:183:TYR:HB3	1:A:187:LEU:HD12	1.76	0.68
1:A:497:ASP:O	1:A:501:LYS:HG3	1.93	0.68
2:B:601:LUO:H12	2:B:602:LUO:H17	1.76	0.67
1:B:379:MET:HA	1:B:379:MET:HE2	1.76	0.67
1:B:260:VAL:HG21	1:B:292:HIS:CE1	2.30	0.66
1:B:417:VAL:HG11	1:B:449:LYS:HG3	1.76	0.66
1:B:372:MET:O	1:B:376:LYS:HG3	1.97	0.65
1:A:386:ASN:HD22	1:A:386:ASN:C	2.00	0.64
1:A:378:LYS:HG3	1:A:392:LEU:HD12	1.79	0.64
1:B:403:ILE:HD11	1:B:464:MET:CE	2.28	0.63
1:B:403:ILE:HD11	1:B:464:MET:HE1	1.80	0.63
1:A:407:VAL:HG11	1:A:479:MET:CE	2.31	0.61
1:A:300:ASN:C	1:A:300:ASN:HD22	2.03	0.61
2:B:601:LUO:O22	2:B:601:LUO:C25	2.47	0.60
1:A:498:ASP:O	1:A:502:GLU:HG3	2.02	0.60
1:A:500:MET:HG2	1:A:504:GLN:HE21	1.67	0.59
1:B:451:THR:HB	2:B:602:LUO:H7	1.85	0.58
1:A:386:ASN:HD22	1:A:389:HIS:H	1.51	0.58
2:A:601:LUO:C11	2:A:601:LUO:H1	2.33	0.58
1:A:212:LEU:HD22	1:A:239:LEU:HB3	1.86	0.57
1:B:301:ASN:OD1	1:B:320:PRO:HG2	2.03	0.57
1:A:300:ASN:O	1:A:304:GLN:HG2	2.05	0.57
1:A:236:ARG:HD2	1:B:187:LEU:CD2	2.33	0.57
1:B:227:ASP:OD2	1:B:279:GLN:HG3	2.07	0.55
2:B:602:LUO:O22	2:B:602:LUO:H22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:VAL:HG21	1:B:292:HIS:HE1	1.70	0.55
2:B:601:LUO:C11	2:B:601:LUO:H1	2.37	0.55
1:B:300:ASN:ND2	1:B:442:MET:HE3	2.22	0.54
1:A:379:MET:HA	1:A:379:MET:CE	2.38	0.54
1:A:379:MET:HE1	1:A:471:LEU:HD13	1.89	0.54
1:B:188:LEU:HD11	1:B:214:CYS:HA	1.90	0.54
1:B:429:ASP:CG	1:B:444:ARG:HH12	2.11	0.54
1:A:429:ASP:OD2	1:A:444:ARG:NH1	2.41	0.54
1:A:193:ILE:HD11	1:B:233:VAL:HG11	1.90	0.53
1:A:410:MET:CE	1:A:486:SER:HA	2.39	0.53
1:A:453:GLN:O	1:A:457:ILE:HG13	2.09	0.53
1:A:462:ILE:O	1:A:466:GLU:HB2	2.08	0.53
1:A:407:VAL:HG11	1:A:479:MET:HE3	1.91	0.52
1:B:383:ASP:H	1:B:389:HIS:HD2	1.56	0.52
1:A:407:VAL:HG11	1:A:479:MET:HE2	1.92	0.51
1:A:250:PRO:HG2	1:A:423:GLU:HB2	1.92	0.51
1:B:506:LYS:HE3	1:B:506:LYS:CA	2.38	0.51
1:A:196:LEU:HD21	1:A:214:CYS:HB3	1.92	0.51
1:A:386:ASN:HB3	1:A:389:HIS:HB2	1.92	0.51
1:B:300:ASN:ND2	1:B:442:MET:CE	2.74	0.50
1:A:430:ARG:O	1:A:434:GLU:HG3	2.12	0.50
1:B:429:ASP:OD1	1:B:444:ARG:NH1	2.45	0.50
1:A:386:ASN:ND2	1:A:386:ASN:C	2.65	0.50
1:B:250:PRO:HG2	1:B:423:GLU:HB2	1.94	0.50
1:A:471:LEU:HB3	1:A:472:PHE:CD1	2.47	0.50
1:B:492:GLU:OE1	1:B:495:ARG:HD2	2.12	0.50
1:A:188:LEU:O	1:B:237:ARG:NH1	2.45	0.49
1:B:198:LYS:HB2	1:B:200:THR:HG22	1.93	0.49
1:B:256:HIS:O	1:B:260:VAL:HG23	2.12	0.49
1:A:443:ASP:OD2	1:A:446:LYS:HG3	2.12	0.49
1:A:410:MET:HE3	1:A:486:SER:HA	1.96	0.48
1:A:206:TRP:HB3	1:A:210:GLU:HB2	1.95	0.48
1:A:500:MET:HG2	1:A:504:GLN:NE2	2.28	0.48
1:A:270:LEU:CD1	1:A:478:ILE:HD12	2.36	0.48
1:A:379:MET:CE	1:A:382:PHE:HB2	2.44	0.48
1:B:425:PHE:CE1	1:B:444:ARG:HA	2.48	0.48
1:A:400:CYS:CA	1:A:464:MET:HE3	2.39	0.48
1:B:365:MET:HB3	2:B:601:LUO:O30	2.13	0.48
1:B:432:LYS:HG3	1:B:438:VAL:HG21	1.95	0.48
2:A:601:LUO:O22	2:A:601:LUO:C25	2.44	0.48
1:B:400:CYS:O	1:B:404:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:HIS:CE1	1:B:225:VAL:HG11	2.49	0.47
1:A:403:ILE:HD11	1:A:464:MET:HE1	1.97	0.47
1:B:407:VAL:HG11	1:B:479:MET:CE	2.46	0.47
1:A:183:TYR:HB3	1:A:184:PRO:HD2	1.97	0.46
1:A:380:GLU:O	1:A:381:ASN:HB2	2.15	0.46
1:A:386:ASN:ND2	1:A:388:GLU:N	2.62	0.46
1:B:427:GLN:O	1:B:431:GLU:HG3	2.16	0.46
1:B:463:PRO:O	1:B:467:THR:HG23	2.16	0.46
1:A:236:ARG:NH2	1:B:236:ARG:HH21	2.14	0.46
1:B:208:PRO:O	1:B:212:LEU:HG	2.16	0.46
1:A:450:ALA:O	1:A:454:ILE:HG13	2.16	0.45
1:A:481:GLN:HB3	1:A:482:PRO:CD	2.47	0.45
1:B:315:TYR:CE1	1:B:323:ASN:HB3	2.52	0.45
1:A:187:LEU:CD2	1:B:236:ARG:HB3	2.47	0.45
1:A:181:PRO:HB2	1:A:182:THR:H	1.60	0.45
1:A:318:ILE:O	1:A:319:SER:C	2.55	0.45
1:A:424:TYR:CD2	1:A:442:MET:HG2	2.52	0.45
1:B:377:GLU:O	1:B:380:GLU:HG3	2.16	0.44
1:A:386:ASN:ND2	1:A:388:GLU:H	2.14	0.44
1:B:206:TRP:HB3	1:B:210:GLU:HB2	2.00	0.44
1:B:272:SER:O	1:B:275:GLU:HB2	2.17	0.44
1:A:238:TRP:O	1:A:242:VAL:HG23	2.17	0.44
2:B:602:LUO:C21	2:B:602:LUO:N13	2.78	0.44
1:A:250:PRO:O	1:A:419:CYS:HB3	2.17	0.44
1:A:400:CYS:O	1:A:404:SER:HB3	2.18	0.44
1:B:379:MET:HA	1:B:379:MET:CE	2.45	0.44
1:B:202:ASP:CG	1:B:205:LEU:HG	2.38	0.43
1:B:504:GLN:O	1:B:505:LYS:HB2	2.18	0.43
1:B:506:LYS:OXT	1:B:506:LYS:HG3	2.18	0.43
1:B:469:THR:HG21	1:B:476:GLU:HB2	2.00	0.43
2:B:602:LUO:O22	2:B:602:LUO:C25	2.64	0.43
1:B:191:GLU:H	1:B:191:GLU:CD	2.20	0.43
1:A:488:ASP:O	1:A:492:GLU:HG3	2.19	0.43
1:B:505:LYS:O	1:B:505:LYS:HG2	2.18	0.43
1:B:206:TRP:CD1	1:B:206:TRP:N	2.87	0.43
1:B:276:LYS:HD2	1:B:384:TYR:CE2	2.54	0.43
1:B:502:GLU:C	1:B:504:GLN:H	2.22	0.43
1:A:300:ASN:C	1:A:300:ASN:ND2	2.70	0.43
1:B:263:MET:SD	1:B:479:MET:HE1	2.58	0.42
1:B:481:GLN:HB3	1:B:482:PRO:CD	2.48	0.42
1:A:480:LEU:HD12	1:A:480:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:SER:O	1:A:407:VAL:HB	2.19	0.42
1:A:183:TYR:CB	1:A:187:LEU:HD12	2.47	0.42
1:B:181:PRO:HB2	1:B:182:THR:H	1.65	0.42
1:A:187:LEU:HD21	1:B:236:ARG:HB3	2.01	0.42
1:B:407:VAL:HG11	1:B:479:MET:HE2	2.02	0.42
1:B:476:GLU:HA	1:B:480:LEU:HB2	2.00	0.42
1:A:218:MET:HG2	1:A:265:TYR:CD1	2.55	0.42
1:B:202:ASP:C	1:B:202:ASP:OD2	2.57	0.42
1:A:322:GLU:HA	1:A:325:HIS:CD2	2.55	0.41
1:B:269:TRP:CE3	1:B:269:TRP:HA	2.55	0.41
1:B:451:THR:O	2:B:602:LUO:H16	2.20	0.41
1:A:271:CYS:HB3	1:A:472:PHE:CD2	2.55	0.41
1:B:456:PHE:HB2	2:B:601:LUO:H11	2.02	0.41
1:A:386:ASN:HD21	1:A:388:GLU:HB3	1.85	0.41
1:B:472:PHE:HA	1:B:473:PRO:HD2	1.88	0.41
1:B:326:CYS:SG	1:B:357:ILE:HA	2.61	0.41
1:B:503:LEU:CD2	1:B:503:LEU:O	2.69	0.41
1:A:260:VAL:HG21	1:A:292:HIS:CE1	2.56	0.40
1:A:383:ASP:H	1:A:389:HIS:HD2	1.67	0.40
1:A:414:GLU:OE1	1:A:489:ARG:NH2	2.54	0.40
1:A:256:HIS:O	1:A:260:VAL:HG23	2.21	0.40
1:B:383:ASP:H	1:B:389:HIS:CD2	2.37	0.40
1:B:403:ILE:HB	1:B:456:PHE:HZ	1.85	0.40
1:B:414:GLU:N	1:B:415:PRO:HD2	2.36	0.40
1:A:481:GLN:HA	1:A:484:TRP:CE3	2.57	0.40
1:B:238:TRP:CE3	1:B:340:ILE:HD13	2.57	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	324/326 (99%)	309 (95%)	14 (4%)	1 (0%)	41	66
1	B	324/326 (99%)	305 (94%)	18 (6%)	1 (0%)	41	66
All	All	648/652 (99%)	614 (95%)	32 (5%)	2 (0%)	41	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	ASN
1	B	505	LYS

### 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	303/303 (100%)	296 (98%)	7 (2%)	50	78
1	B	303/303 (100%)	297 (98%)	6 (2%)	55	81
All	All	606/606 (100%)	593 (98%)	13 (2%)	53	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	TYR
1	A	257	CYS
1	A	300	ASN
1	A	379	MET
1	A	386	ASN
1	A	433	SER
1	A	474	MET
1	B	257	CYS
1	B	381	ASN
1	B	491	GLU
1	B	497	ASP
1	B	503	LEU
1	B	506	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	304	GLN
1	A	351	GLN
1	A	381	ASN
1	A	386	ASN
1	A	389	HIS
1	A	504	GLN
1	B	243	HIS
1	B	245	ASN
1	B	304	GLN
1	B	389	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LUO	B	601	-	30,34,34	3.63	9 (30%)	30,48,48	2.20	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LUO	B	602	-	30,34,34	3.63	9 (30%)	30,48,48	2.23	6 (20%)
2	LUO	A	601	-	30,34,34	3.62	9 (30%)	30,48,48	2.11	6 (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
2	LUO	B	601	-	-	4/18/18/18	0/4/4/4
2	LUO	B	602	-	-	7/18/18/18	0/4/4/4
2	LUO	A	601	-	-	4/18/18/18	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	LUO	N9-N8	-13.55	1.13	1.39
2	B	601	LUO	N9-N8	-13.43	1.14	1.39
2	A	601	LUO	N9-N8	-13.41	1.14	1.39
2	B	601	LUO	C12-C16	-8.45	1.33	1.47
2	A	601	LUO	C12-C16	-8.44	1.33	1.47
2	B	602	LUO	C12-C16	-8.41	1.33	1.47
2	B	601	LUO	O17-C16	6.53	1.36	1.23
2	B	602	LUO	O17-C16	6.50	1.36	1.23
2	A	601	LUO	O17-C16	6.47	1.36	1.23
2	A	601	LUO	CL1-C2	-5.83	1.39	1.51
2	B	602	LUO	CL1-C2	-5.81	1.39	1.51
2	B	601	LUO	CL1-C2	-5.80	1.39	1.51
2	A	601	LUO	C12-C11	-5.53	1.33	1.41
2	B	601	LUO	C12-C11	-5.51	1.33	1.41
2	B	602	LUO	C12-C11	-5.50	1.33	1.41
2	B	601	LUO	C21-N23	3.54	1.43	1.35
2	A	601	LUO	C21-N23	3.46	1.43	1.35
2	B	602	LUO	C21-N23	3.45	1.43	1.35
2	A	601	LUO	C11-N8	-2.68	1.33	1.37
2	B	602	LUO	C11-N8	-2.64	1.33	1.37
2	B	601	LUO	C11-N8	-2.61	1.33	1.37
2	B	602	LUO	C24-N23	-2.50	1.36	1.41
2	B	601	LUO	C24-N23	-2.46	1.36	1.41
2	A	601	LUO	C24-N23	-2.43	1.36	1.41
2	A	601	LUO	C16-N15	-2.24	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	LUO	C16-N15	-2.24	1.34	1.37
2	B	601	LUO	C16-N15	-2.19	1.34	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	LUO	C10-N9-N8	6.21	112.07	103.93
2	B	602	LUO	C24-N23-C21	-6.13	112.73	127.40
2	B	601	LUO	C10-N9-N8	6.09	111.91	103.93
2	A	601	LUO	C10-N9-N8	5.99	111.78	103.93
2	B	601	LUO	C12-C16-N15	5.70	120.61	114.86
2	A	601	LUO	C12-C16-N15	5.69	120.61	114.86
2	B	602	LUO	C12-C16-N15	5.64	120.56	114.86
2	B	601	LUO	C24-N23-C21	-5.37	114.53	127.40
2	A	601	LUO	C24-N23-C21	-5.26	114.80	127.40
2	B	601	LUO	C31-O30-C27	-3.80	109.25	117.51
2	B	601	LUO	O17-C16-C12	-3.79	116.73	123.30
2	B	602	LUO	C31-O30-C27	-3.67	109.55	117.51
2	A	601	LUO	O17-C16-C12	-3.65	116.97	123.30
2	B	602	LUO	O17-C16-C12	-3.62	117.02	123.30
2	A	601	LUO	C31-O30-C27	-3.12	110.74	117.51
2	B	602	LUO	C2-C7-N8	2.56	120.57	118.25
2	B	601	LUO	C2-C7-N8	2.54	120.56	118.25
2	B	601	LUO	C3-C2-C7	2.07	120.13	116.00
2	A	601	LUO	C3-C2-C7	2.05	120.09	116.00

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	LUO	N13-C14-N18-C19
2	A	601	LUO	N15-C14-N18-C19
2	B	601	LUO	N13-C14-N18-C19
2	B	601	LUO	N15-C14-N18-C19
2	B	602	LUO	C19-C21-N23-C24
2	B	601	LUO	C28-C27-O30-C31
2	B	601	LUO	C26-C27-O30-C31
2	B	602	LUO	C28-C27-O30-C31
2	A	601	LUO	C28-C27-O30-C31
2	A	601	LUO	C26-C27-O30-C31
2	B	602	LUO	C26-C27-O30-C31
2	B	602	LUO	O22-C21-N23-C24

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Mol	Chain	Res	Type	Atoms
2	B	602	LUO	C20-C19-C21-O22
2	B	602	LUO	C20-C19-C21-N23
2	B	602	LUO	C2-C7-N8-N9

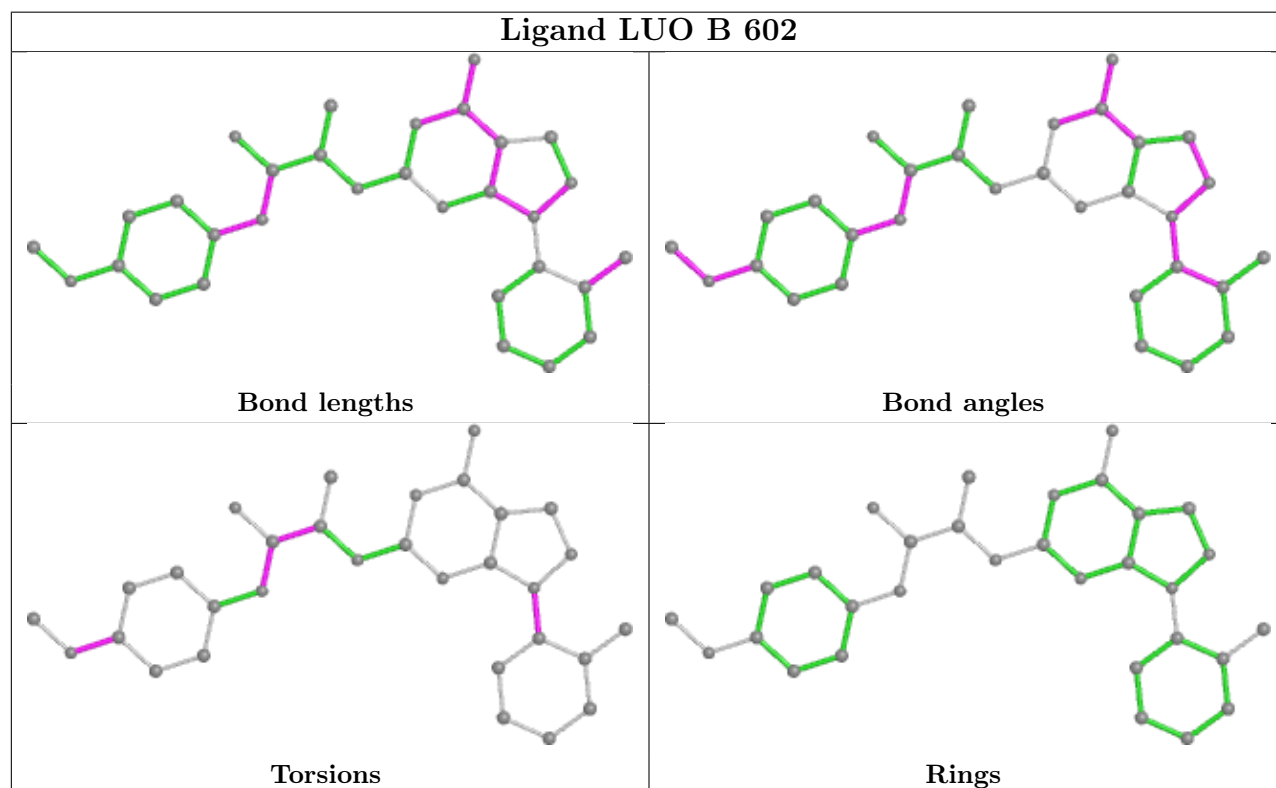
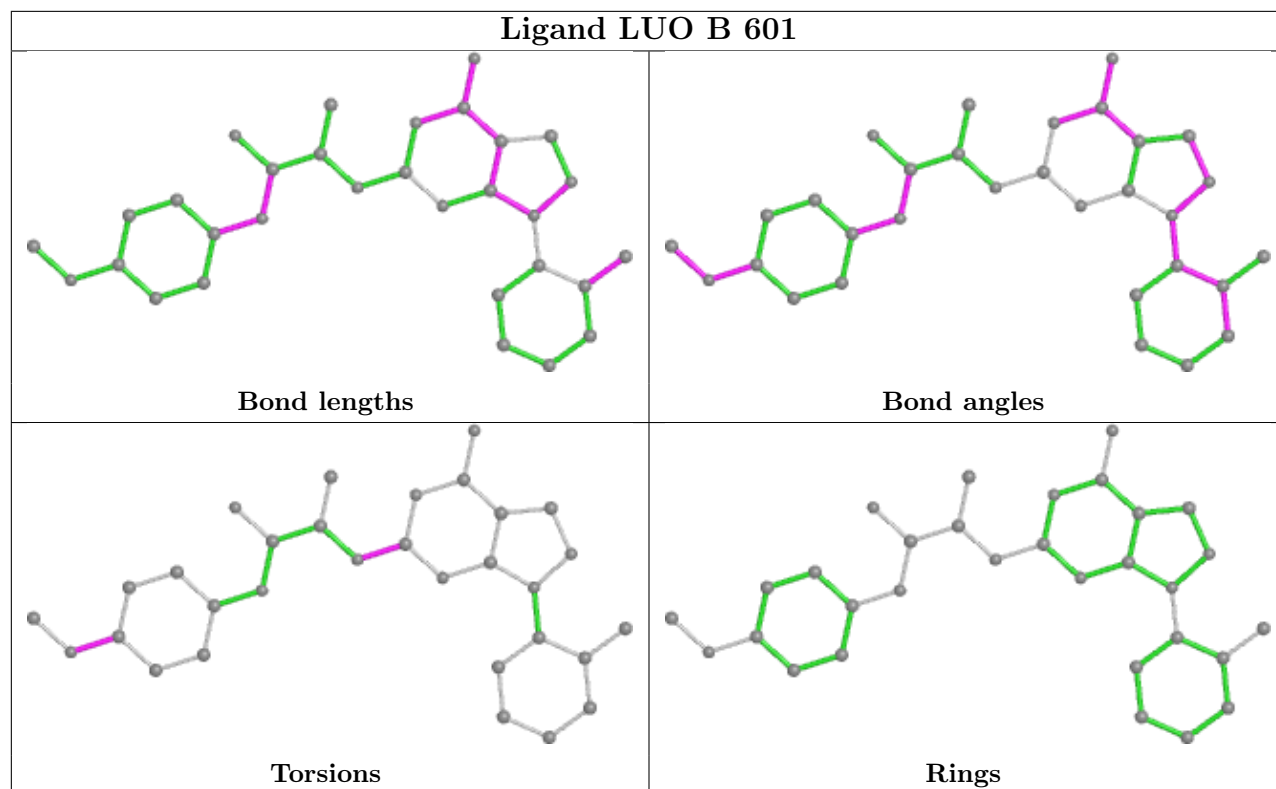
There are no ring outliers.

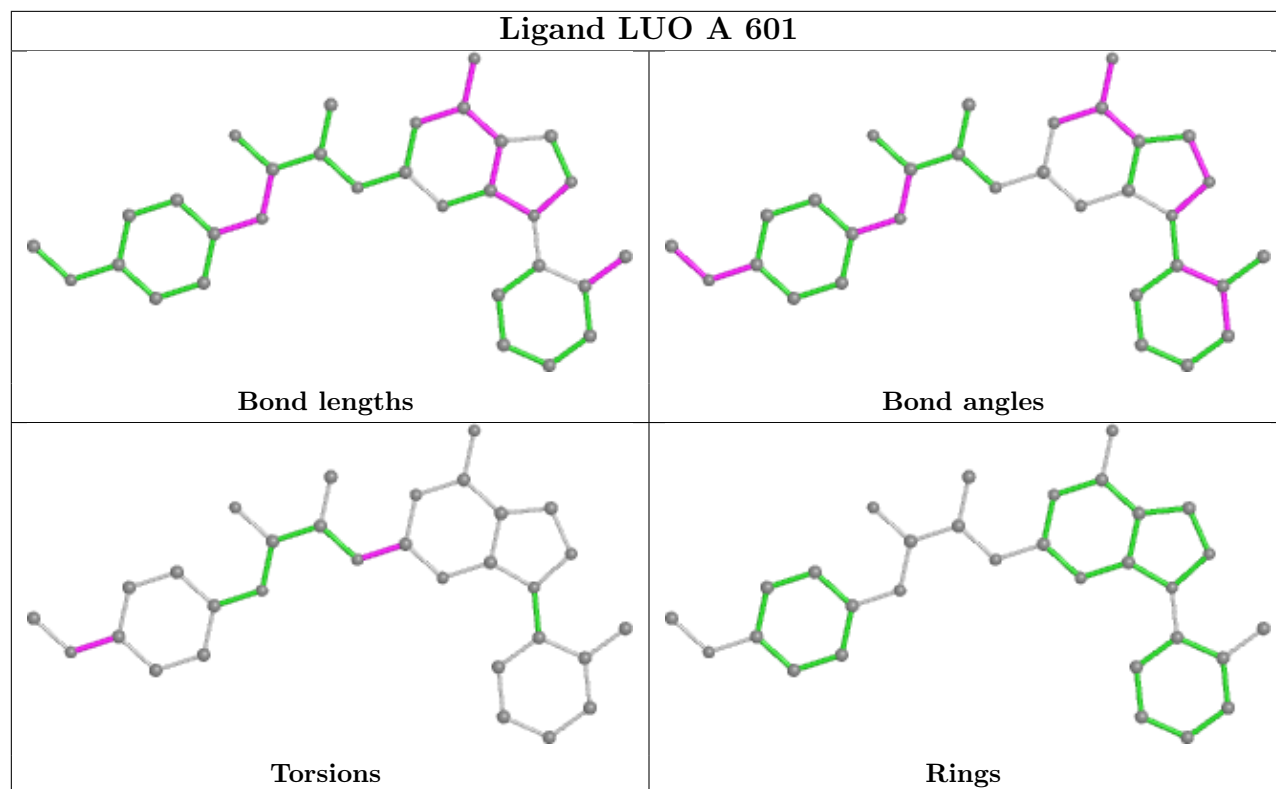
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	LUO	6	0
2	B	602	LUO	7	0
2	A	601	LUO	3	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	326/326 (100%)	0.35	29 (8%) <b>9</b> <b>7</b>	31, 49, 76, 102	0
1	B	326/326 (100%)	0.37	28 (8%) <b>10</b> <b>8</b>	28, 52, 75, 110	0
All	All	652/652 (100%)	0.36	57 (8%) <b>10</b> <b>8</b>	28, 51, 76, 110	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	506	LYS	7.1
1	B	505	LYS	6.4
1	B	182	THR	5.7
1	A	182	THR	5.2
1	B	380	GLU	4.9
1	A	401	CYS	4.0
1	A	506	LYS	3.9
1	A	181	PRO	3.9
1	B	345	PRO	3.6
1	B	346	PRO	3.6
1	A	380	GLU	3.5
1	A	502	GLU	3.5
1	A	186	TYR	3.4
1	B	181	PRO	3.3
1	B	289	ALA	3.2
1	A	261	ALA	3.1
1	B	504	GLN	3.1
1	B	185	LYS	3.0
1	A	183	TYR	3.0
1	B	194	GLU	2.9
1	B	290	ILE	2.9
1	A	377	GLU	2.9
1	A	400	CYS	2.8
1	A	403	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	260	VAL	2.8
1	A	347	ASP	2.6
1	B	502	GLU	2.6
1	B	347	ASP	2.6
1	B	401	CYS	2.6
1	A	259	CYS	2.5
1	B	240	PHE	2.5
1	B	205	LEU	2.4
1	A	381	ASN	2.4
1	A	446	LYS	2.3
1	B	403	ILE	2.3
1	A	260	VAL	2.3
1	A	191	GLU	2.3
1	B	381	ASN	2.3
1	A	402	ASP	2.3
1	A	398	ILE	2.3
1	A	370	GLU	2.2
1	A	369	ALA	2.2
1	A	263	MET	2.2
1	B	410	MET	2.2
1	B	183	TYR	2.1
1	A	411	GLU	2.1
1	A	184	PRO	2.1
1	B	291	CYS	2.1
1	A	289	ALA	2.1
1	B	388	GLU	2.1
1	A	384	TYR	2.1
1	A	477	GLU	2.1
1	A	185	LYS	2.0
1	B	206	TRP	2.0
1	B	227	ASP	2.0
1	B	259	CYS	2.0
1	B	503	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

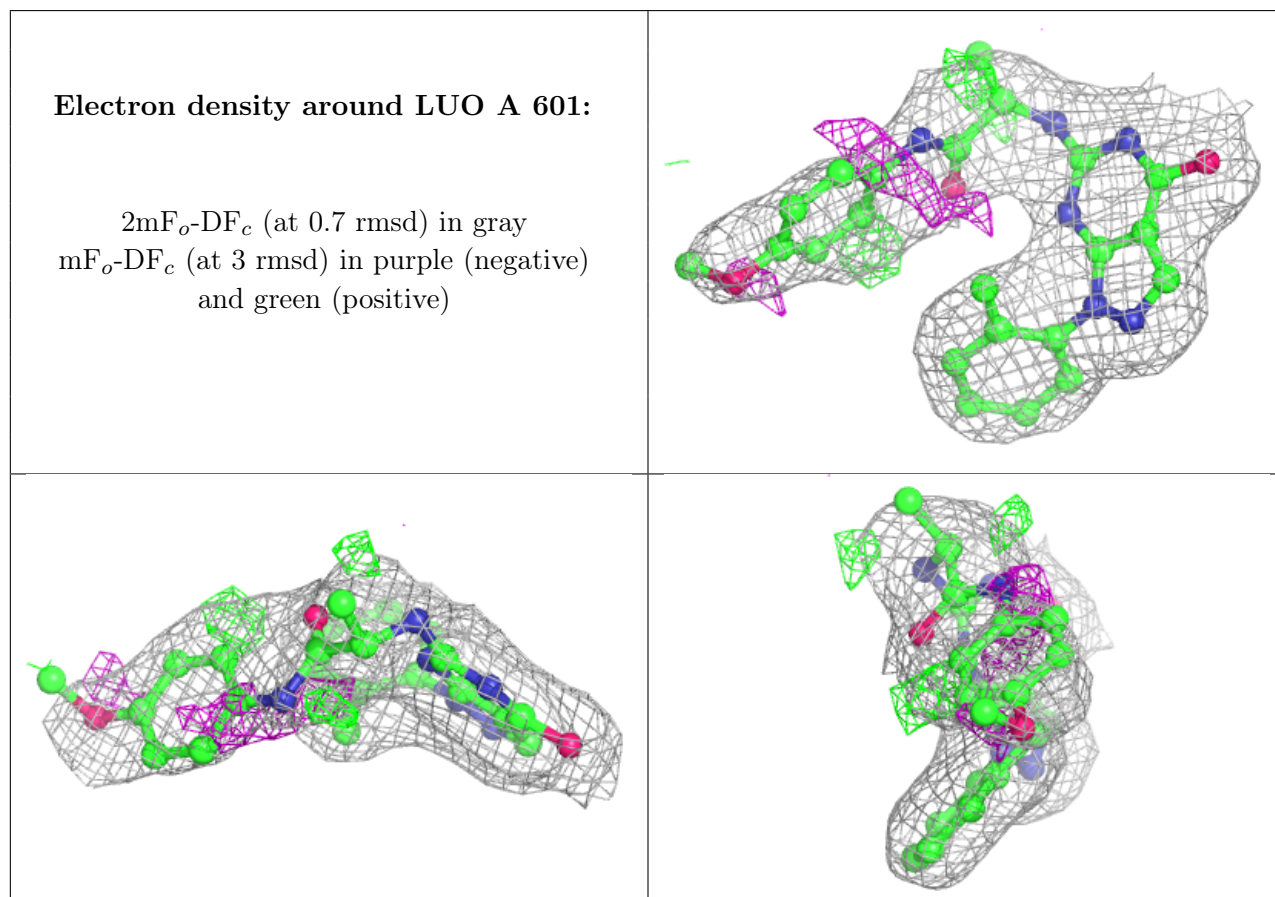
There are no monosaccharides in this entry.

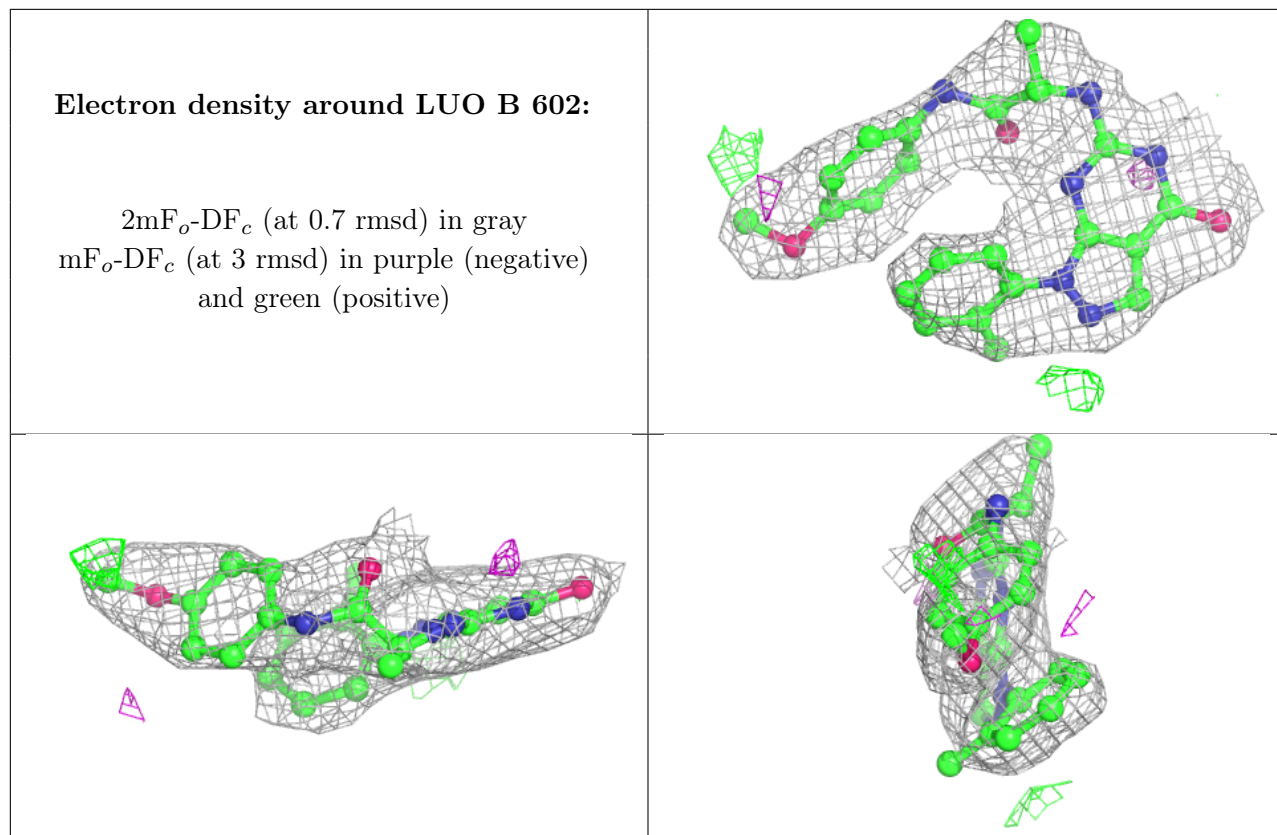
## 6.4 Ligands [i](#)

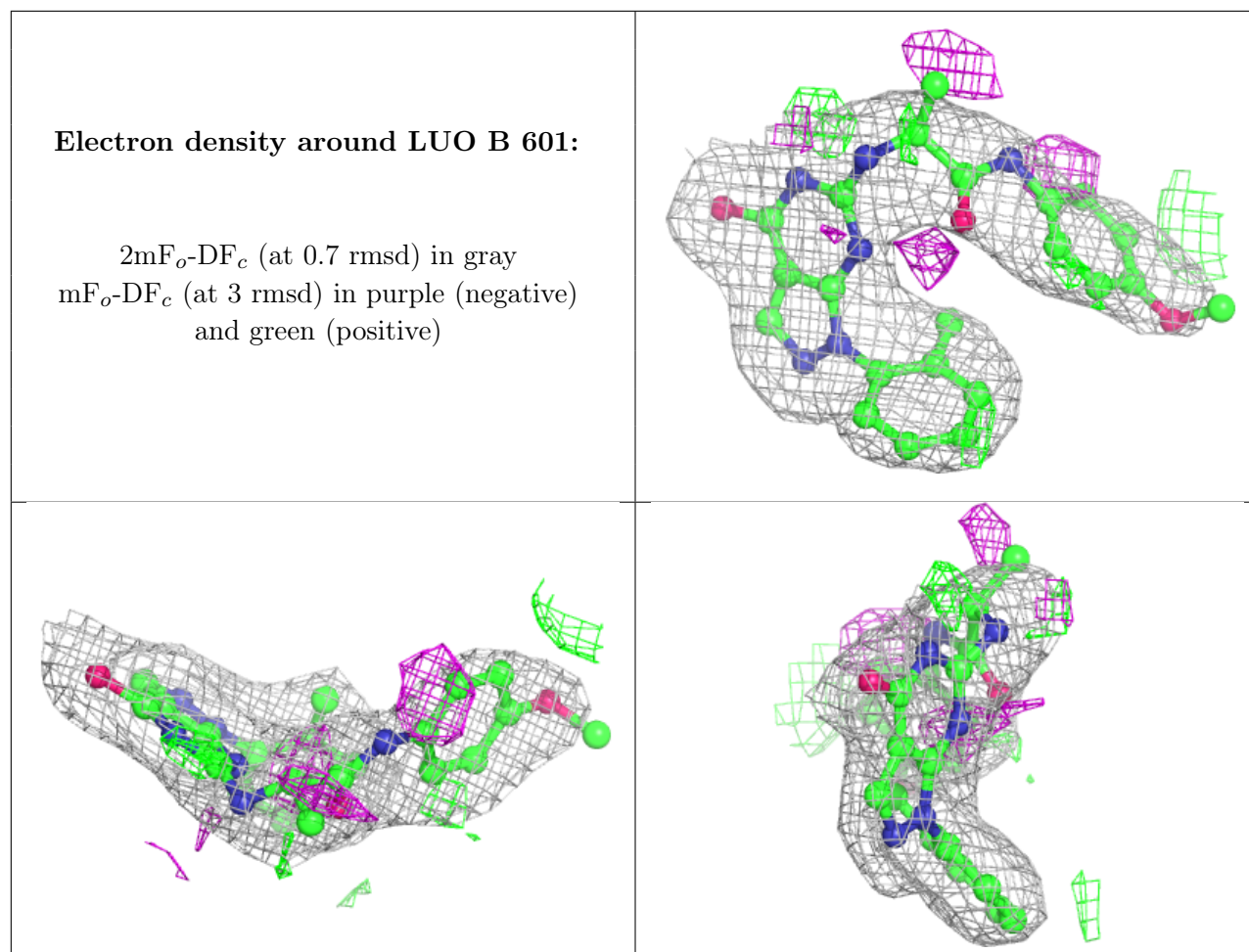
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	LUO	A	601	31/31	0.91	0.22	37,44,59,62	0
2	LUO	B	602	31/31	0.91	0.20	75,81,85,85	0
2	LUO	B	601	31/31	0.92	0.25	37,44,68,72	0
4	MG	A	603	1/1	0.95	0.24	43,43,43,43	0
3	ZN	B	603	1/1	0.96	0.06	61,61,61,61	0
3	ZN	A	602	1/1	0.97	0.06	60,60,60,60	0
4	MG	B	604	1/1	0.97	0.19	36,36,36,36	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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.