



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 07:24 PM EDT

PDB ID : 6KHD  
Title : Crystal structure of CLK1 in complex with CX-4945  
Authors : Lee, J.Y.; Yun, J.S.; Jin, H.; Chang, J.H.  
Deposited on : 2019-07-15  
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>.

---

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

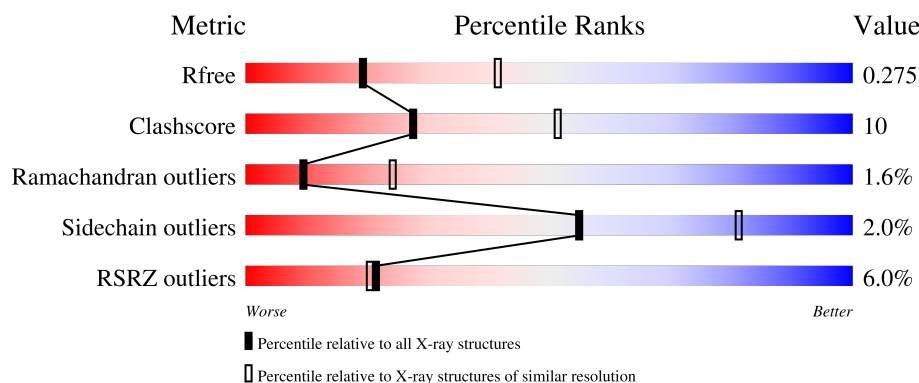
# 1 Overall quality at a glance

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	484	<div> <div>5%</div> <div> <div></div> <div>50%</div> <div>16%</div> <div>33%</div> </div> </div>
1	B	484	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>11%</div> <div>31%</div> </div> </div>
1	C	484	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>17%</div> <div>33%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7710 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.

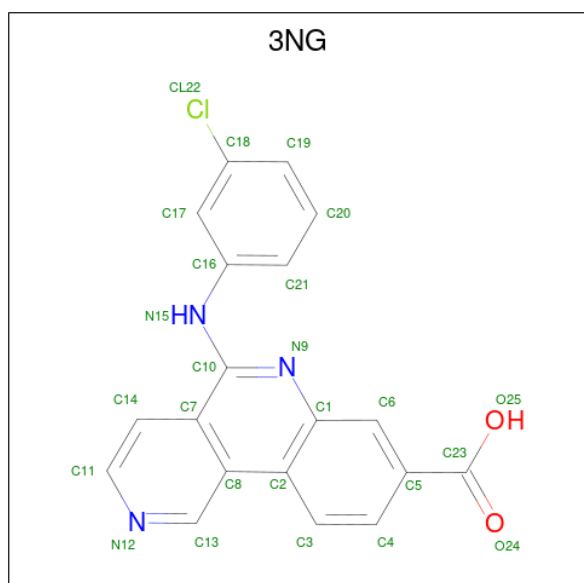
- Molecule 1 is a protein called Dual specificity protein kinase CLK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	1	0
			2497	1602	414	465	16			
1	B	332	Total	C	N	O	S	0	1	0
			2564	1650	421	477	16			
1	C	325	Total	C	N	O	S	0	0	0
			2552	1642	430	465	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	ALA	ARG	conflict	UNP P49759
B	432	ALA	ARG	conflict	UNP P49759
C	432	ALA	ARG	conflict	UNP P49759

- Molecule 2 is 5-[(3-chlorophenyl)amino]benzo[c][2,6]naphthyridine-8-carboxylic acid (three-letter code: 3NG) (formula: C<sub>19</sub>H<sub>12</sub>ClN<sub>3</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



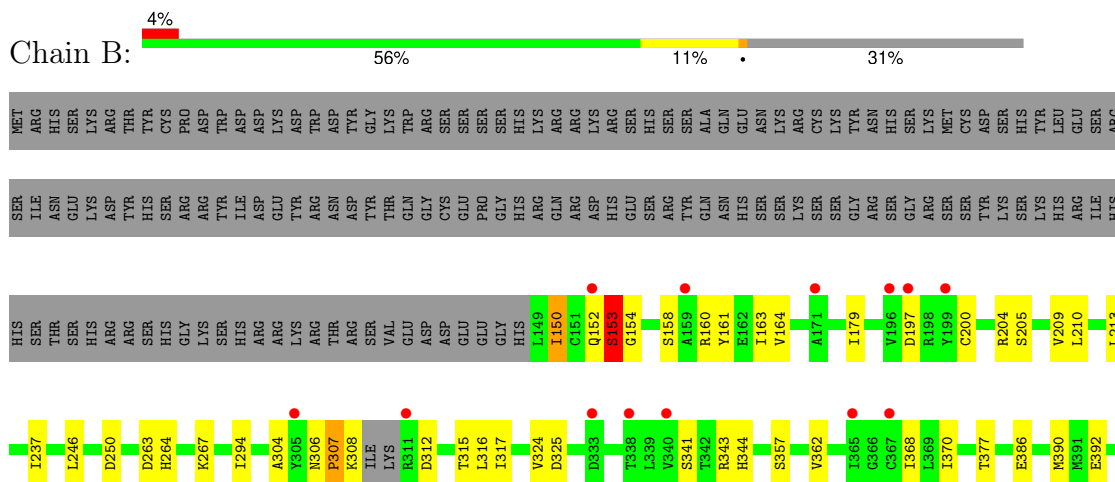
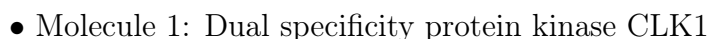
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		
2	B	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		
2	C	1	Total	C	Cl	N	O	0	0
			25	19	1	3	2		

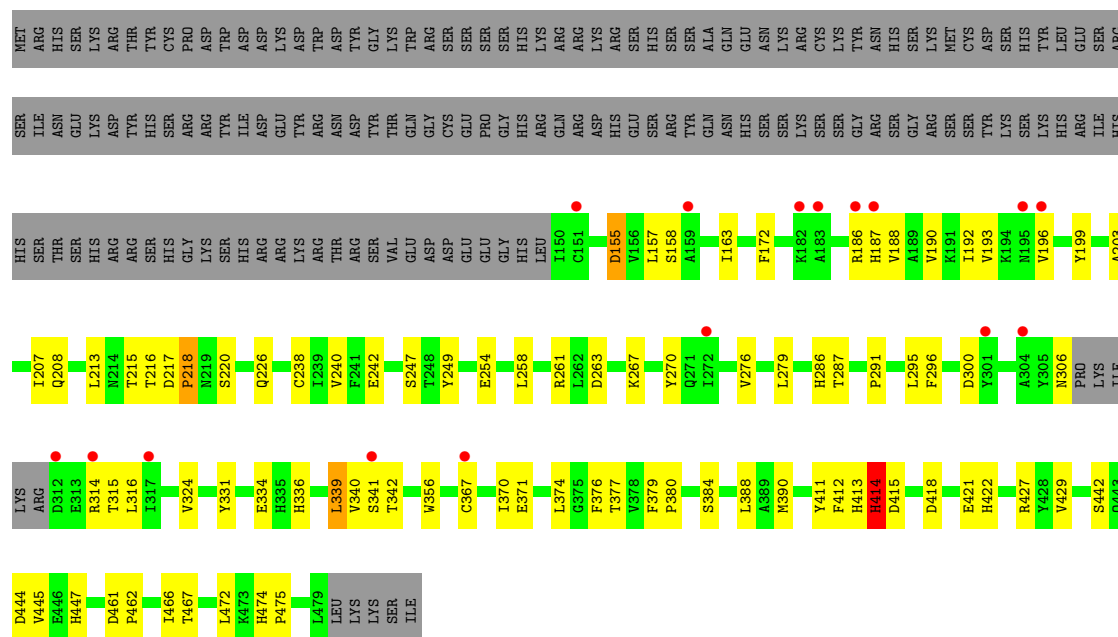
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	7	Total	O	0	0
			7	7		
3	C	5	Total	O	0	0
			5	5		



- Molecule 1: Dual specificity protein kinase CLK1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.53Å 115.67Å 90.61Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	31.93 – 2.70 31.94 – 2.67	Depositor EDS
% Data completeness (in resolution range)	98.6 (31.93-2.70) 98.6 (31.94-2.67)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.200 , 0.274 0.204 , 0.275	Depositor DCC
$R_{free}$ test set	1999 reflections (6.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: 3NG

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	0.49	1/2560 (0.0%)	0.64	1/3479 (0.0%)
1	B	0.46	0/2633	0.64	1/3584 (0.0%)
1	C	0.43	0/2618	0.59	1/3556 (0.0%)
All	All	0.46	1/7811 (0.0%)	0.63	3/10619 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	CYS	CB-SG	-5.24	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	339	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	149	LEU	CA-CB-CG	6.09	129.31	115.30
1	B	307	PRO	N-CA-CB	5.56	109.97	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	149	LEU	Peptide

## 5.2 Too-close contacts [i](#)

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	2497	0	2341	59	0
1	B	2564	0	2374	36	0
1	C	2552	0	2405	54	0
2	A	25	0	11	0	0
2	B	25	0	11	0	0
2	C	25	0	11	1	0
3	A	10	0	0	6	0
3	B	7	0	0	3	0
3	C	5	0	0	2	0
All	All	7710	0	7153	149	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 10.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:CYS:SG	1:A:152:GLN:N	2.46	0.89
1:B:419:TRP:NE1	3:B:1101:HOH:O	2.03	0.84
1:A:149:LEU:HB2	1:A:194:LYS:HG2	1.66	0.78
1:C:258:LEU:O	3:C:1101:HOH:O	2.04	0.76
1:C:331:TYR:HB2	1:C:334:GLU:HG3	1.69	0.74
1:A:339:LEU:O	3:A:1101:HOH:O	2.08	0.72
1:C:306:ASN:O	3:C:1102:HOH:O	2.08	0.71
1:C:286:HIS:O	1:C:287:THR:HB	1.91	0.71
1:C:442:SER:HB3	1:C:447:HIS:CE1	2.27	0.70
1:C:413:HIS:O	1:C:415:ASP:N	2.25	0.69
1:A:250:ASP:OD2	3:A:1102:HOH:O	2.11	0.69
1:A:155:ASP:HB2	1:A:163:ILE:HD12	1.74	0.68
1:B:153:SER:O	1:B:163:ILE:HB	1.92	0.68
1:C:422:HIS:O	1:C:427:ARG:NH1	2.28	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:GLU:O	1:C:422:HIS:ND1	2.29	0.66
1:B:390:MET:HG2	1:B:433:CYS:SG	2.36	0.65
1:C:377:THR:HG22	1:C:379:PHE:H	1.59	0.65
1:A:195:ASN:HB2	1:A:236:HIS:CD2	2.31	0.65
1:A:340:VAL:HA	1:A:346:ARG:NH2	2.12	0.64
1:C:249:TYR:HB2	1:C:291:PRO:HB2	1.78	0.64
1:A:205:SER:OG	3:A:1103:HOH:O	2.15	0.64
1:C:261:ARG:NH1	1:C:263:ASP:OD1	2.31	0.64
1:A:204:ARG:NH2	1:C:216:THR:HG23	2.13	0.64
1:A:339:LEU:CD2	1:A:340:VAL:H	2.11	0.63
1:B:246:LEU:HD22	1:B:250:ASP:HB3	1.81	0.62
1:B:197:ASP:O	1:B:200:CYS:N	2.32	0.62
1:C:276:VAL:HA	1:C:279:LEU:HD12	1.80	0.62
1:C:254:GLU:O	1:C:314:ARG:NH1	2.33	0.61
1:A:371:GLU:HG2	1:A:377:THR:HA	1.83	0.61
1:B:419:TRP:CH2	1:B:426:GLY:HA2	2.36	0.60
1:C:196:VAL:HB	1:C:199:TYR:HD2	1.66	0.60
1:A:339:LEU:HD22	1:A:340:VAL:H	1.68	0.59
1:B:440:MET:HE3	1:B:448:GLU:HG3	1.85	0.59
1:C:444:ASP:OD1	1:C:445:VAL:N	2.36	0.58
1:B:264:HIS:HD2	1:B:316:LEU:HD23	1.68	0.58
1:C:190:VAL:HG22	1:C:240:VAL:HG22	1.86	0.57
1:A:445:VAL:HG22	1:A:449:ARG:HE	1.70	0.56
1:A:150:ILE:H	1:A:150:ILE:HD13	1.71	0.56
1:A:220:SER:OG	1:A:322:LYS:NZ	2.25	0.56
1:C:374:LEU:HB3	1:C:376:PHE:CE2	2.41	0.55
1:B:204:ARG:NH1	1:B:237:ILE:HD11	2.22	0.55
1:C:295:LEU:HD22	1:C:324:VAL:HG11	1.89	0.55
1:B:324:VAL:HG23	1:B:325:ASP:HB2	1.89	0.55
1:B:440:MET:CE	1:B:448:GLU:HG3	2.36	0.54
1:B:264:HIS:CD2	1:B:316:LEU:HD23	2.42	0.54
1:B:386:GLU:HG2	3:B:1101:HOH:O	2.07	0.54
1:B:164:VAL:HG21	1:B:179:ILE:HG13	1.89	0.54
1:A:401:HIS:CE1	3:A:1105:HOH:O	2.60	0.54
1:B:306:ASN:O	1:B:308:LYS:N	2.41	0.54
1:C:193:VAL:HG21	1:C:203:ALA:HB2	1.90	0.53
1:B:153:SER:OG	1:B:154:GLY:N	2.40	0.53
1:C:390:MET:HG2	1:C:429:VAL:HG13	1.91	0.53
1:A:479:LEU:H	1:A:479:LEU:HD12	1.74	0.53
1:C:367:CYS:O	1:C:371:GLU:HG3	2.09	0.53
1:A:348:PRO:HD2	1:A:465:ARG:HH22	1.73	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASP:O	1:A:293:ASN:ND2	2.42	0.52
1:C:186:ARG:NH1	1:C:188:VAL:HG12	2.25	0.52
1:C:203:ALA:O	1:C:207:ILE:HG13	2.10	0.52
1:C:158:SER:O	1:C:158:SER:OG	2.26	0.52
1:B:392:GLU:HA	1:B:396:GLY:O	2.10	0.52
1:C:172:PHE:HA	1:C:199:TYR:CD1	2.45	0.52
1:C:157:LEU:HD21	1:C:163:ILE:HD11	1.90	0.52
1:A:215:THR:O	1:A:218:PRO:HD3	2.10	0.52
1:A:340:VAL:HA	1:A:346:ARG:HH22	1.74	0.52
1:A:434:LYS:HD2	1:A:438:GLU:HB3	1.91	0.51
1:B:267:LYS:HG2	1:B:480:LEU:HD21	1.92	0.51
1:C:220:SER:HB2	1:C:226:GLN:HG3	1.93	0.51
1:A:401:HIS:CE1	1:A:402:MET:HG3	2.46	0.51
1:A:324:VAL:HG23	1:A:325:ASP:H	1.76	0.51
1:B:294[A]:ILE:HD11	1:B:368:ILE:HD13	1.91	0.51
1:A:206:GLU:HB2	1:A:327:GLY:HA2	1.92	0.50
1:C:336:HIS:HB3	1:C:356:TRP:CZ2	2.46	0.50
1:A:267:LYS:O	1:A:271:GLN:HG3	2.11	0.50
1:A:197:ASP:HA	1:A:200:CYS:HB2	1.93	0.50
1:B:449:ARG:HD3	1:B:475:PRO:HB2	1.92	0.50
1:A:167:LEU:HD12	1:A:175:VAL:HG12	1.94	0.49
1:B:152:GLN:O	1:B:153:SER:HB3	2.12	0.49
1:A:358:GLN:OE1	1:A:358:GLN:N	2.37	0.49
1:A:392:GLU:OE2	1:A:398:LEU:HG	2.12	0.49
1:C:155:ASP:HB2	1:C:163:ILE:HD12	1.96	0.48
1:C:466:ILE:HG12	1:C:467:THR:O	2.14	0.48
1:A:419:TRP:CZ2	1:A:426:GLY:HA2	2.49	0.48
1:C:192:ILE:HG23	1:C:238:CYS:SG	2.54	0.47
1:A:150:ILE:HD13	1:A:150:ILE:N	2.29	0.47
1:B:317:ILE:HA	3:B:1104:HOH:O	2.13	0.47
1:C:208:GLN:HA	1:C:208:GLN:OE1	2.14	0.47
1:A:401:HIS:ND1	3:A:1105:HOH:O	2.36	0.47
1:B:200:CYS:O	1:B:204:ARG:HG3	2.15	0.46
1:B:158:SER:O	1:B:158:SER:OG	2.29	0.46
1:C:411:TYR:HB2	1:C:412:PHE:CE1	2.51	0.46
1:A:290:LYS:HD2	1:A:292:GLU:OE1	2.15	0.46
1:C:339:LEU:HD12	1:C:340:VAL:H	1.79	0.46
1:A:158:SER:H	1:A:233:HIS:CE1	2.33	0.46
1:B:205:SER:O	1:B:209:VAL:HG23	2.16	0.46
1:B:160:ARG:HD3	1:B:161:TYR:CZ	2.50	0.46
1:B:209:VAL:O	1:B:213:LEU:HG	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:PHE:CZ	1:C:316:LEU:HD11	2.51	0.46
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.79	0.45
1:C:384:SER:O	1:C:388:LEU:HG	2.16	0.45
1:C:341:SER:HA	1:C:342:THR:HA	1.66	0.45
1:A:195:ASN:HB2	1:A:236:HIS:HD2	1.79	0.45
1:A:401:HIS:NE2	1:A:402:MET:HG3	2.32	0.45
1:A:419:TRP:HZ2	1:A:426:GLY:HA2	1.82	0.45
1:B:434:LYS:HE3	1:B:439:PHE:CD1	2.52	0.44
1:A:214:ASN:OD1	1:A:226:GLN:HG3	2.17	0.44
1:C:270:TYR:CE1	1:C:472:LEU:HD22	2.52	0.44
1:A:149:LEU:HD23	1:A:236:HIS:NE2	2.33	0.44
1:A:151:CYS:SG	1:A:163:ILE:HD13	2.58	0.44
1:A:255:ASN:O	1:A:258:LEU:HG	2.17	0.44
1:B:210:LEU:HD23	1:B:210:LEU:HA	1.78	0.44
1:C:226:GLN:HB2	1:C:242:GLU:CD	2.38	0.44
1:C:263:ASP:O	1:C:267:LYS:HG3	2.18	0.44
1:C:413:HIS:CE1	1:C:414:HIS:CE1	3.06	0.44
1:A:157:LEU:HD11	1:A:163:ILE:HD11	1.99	0.43
1:B:263:ASP:OD1	1:B:263:ASP:N	2.47	0.43
1:A:266:ARG:HG2	1:A:480:LEU:HD11	2.01	0.43
1:A:474:HIS:HA	1:A:475:PRO:HD2	1.74	0.43
1:A:446:GLU:HA	1:A:449:ARG:HG3	2.00	0.43
1:C:247:SER:HA	1:C:295:LEU:HA	2.00	0.43
1:C:474:HIS:CG	1:C:475:PRO:HD2	2.54	0.43
1:B:150:ILE:HD12	1:B:150:ILE:O	2.19	0.43
1:B:304:ALA:O	1:B:312:ASP:HA	2.18	0.43
1:A:324:VAL:HG23	1:A:325:ASP:N	2.32	0.43
1:A:339:LEU:N	3:A:1101:HOH:O	2.51	0.43
1:C:215:THR:OG1	1:C:216:THR:N	2.52	0.43
1:A:157:LEU:HA	1:A:233:HIS:CE1	2.54	0.42
1:B:419:TRP:HH2	1:B:429:VAL:HB	1.84	0.42
1:B:421:GLU:O	1:B:426:GLY:HA3	2.19	0.42
1:A:290:LYS:HB2	1:A:292:GLU:OE1	2.20	0.42
1:A:394:ILE:HG12	1:A:434:LYS:O	2.20	0.42
1:A:267:LYS:HG2	1:A:480:LEU:HD21	2.00	0.42
1:A:471:ALA:O	1:A:477:PHE:HE2	2.03	0.41
1:C:411:TYR:HB2	1:C:412:PHE:CD1	2.56	0.41
1:C:217:ASP:HA	1:C:218:PRO:HD2	1.81	0.41
1:A:280:HIS:CD2	1:A:358:GLN:HG3	2.55	0.41
1:C:370:ILE:HD12	1:C:370:ILE:HA	1.88	0.41
1:C:213:LEU:HD21	1:C:279:LEU:CD2	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:HIS:CD2	1:C:336:HIS:N	2.87	0.41
1:B:362:VAL:HG11	1:B:466:ILE:O	2.20	0.41
2:C:1000:3NG:H3	2:C:1000:3NG:H13	1.79	0.41
1:A:378:VAL:C	1:A:380:PRO:HD3	2.42	0.40
1:B:197:ASP:C	1:B:200:CYS:H	2.23	0.40
1:A:275:SER:O	1:A:278:PHE:HB3	2.21	0.40
1:C:461:ASP:HA	1:C:462:PRO:HD2	1.97	0.40
1:A:450:LEU:HB2	1:A:476:PHE:CE1	2.56	0.40
1:C:380:PRO:HD2	1:C:390:MET:SD	2.61	0.40
1:C:442:SER:HB3	1:C:447:HIS:ND1	2.35	0.40
1:C:186:ARG:NH1	1:C:187:HIS:O	2.54	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	317/484 (66%)	297 (94%)	17 (5%)	3 (1%)	17	40
1	B	329/484 (68%)	296 (90%)	25 (8%)	8 (2%)	6	15
1	C	321/484 (66%)	280 (87%)	37 (12%)	4 (1%)	13	32
All	All	967/1452 (67%)	873 (90%)	79 (8%)	15 (2%)	9	24

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ILE
1	A	337	SER
1	B	341	SER
1	C	414	HIS
1	B	153	SER
1	B	307	PRO

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	419	TRP
1	C	418	ASP
1	B	357	SER
1	B	344	HIS
1	C	155	ASP
1	A	357	SER
1	B	150	ILE
1	C	218	PRO
1	B	343	ARG

### 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	259/445 (58%)	250 (96%)	9 (4%)	36	65
1	B	262/445 (59%)	258 (98%)	4 (2%)	65	86
1	C	264/445 (59%)	261 (99%)	3 (1%)	73	90
All	All	785/1335 (59%)	769 (98%)	16 (2%)	55	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	CYS
1	A	153	SER
1	A	201	GLU
1	A	247	SER
1	A	261	ARG
1	A	262	LEU
1	A	263	ASP
1	A	333	ASP
1	A	392	GLU
1	B	153	SER
1	B	315	THR
1	B	370	ILE
1	B	377	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	300	ASP
1	C	315	THR
1	C	414	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	264	HIS
1	C	413	HIS
1	C	414	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](#)

3 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	3NG	B	1000	-	28,28,28	1.81	6 (21%)	39,40,40	4.97	12 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	3NG	A	1000	-	28,28,28	1.74	6 (21%)	39,40,40	4.61	11 (28%)
2	3NG	C	1000	-	28,28,28	1.85	7 (25%)	39,40,40	5.00	12 (30%)

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	3NG	B	1000	-	-	4/8/8/8	0/4/4/4
2	3NG	A	1000	-	-	0/8/8/8	0/4/4/4
2	3NG	C	1000	-	-	0/8/8/8	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	3NG	C7-C8	-5.36	1.33	1.42
2	B	1000	3NG	C7-C8	-5.25	1.33	1.42
2	A	1000	3NG	C7-C8	-4.83	1.34	1.42
2	C	1000	3NG	C10-N15	4.15	1.42	1.36
2	B	1000	3NG	C10-C7	-4.11	1.39	1.44
2	A	1000	3NG	C10-N15	3.79	1.42	1.36
2	C	1000	3NG	C10-C7	-3.68	1.40	1.44
2	A	1000	3NG	C10-C7	-3.61	1.40	1.44
2	B	1000	3NG	C10-N15	3.58	1.41	1.36
2	B	1000	3NG	C10-N9	3.07	1.37	1.32
2	A	1000	3NG	C10-N9	2.91	1.37	1.32
2	A	1000	3NG	C13-N12	2.51	1.36	1.32
2	B	1000	3NG	C13-N12	2.48	1.36	1.32
2	C	1000	3NG	C2-C1	-2.46	1.37	1.41
2	C	1000	3NG	C10-N9	2.23	1.36	1.32
2	B	1000	3NG	C2-C1	-2.16	1.37	1.41
2	C	1000	3NG	C13-N12	2.09	1.36	1.32
2	A	1000	3NG	C2-C1	-2.04	1.37	1.41
2	C	1000	3NG	C14-C7	-2.03	1.38	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	3NG	N15-C10-N9	-20.99	99.91	118.55
2	C	1000	3NG	C7-C10-N15	20.54	140.56	119.77

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	3NG	N15-C10-N9	-20.49	100.35	118.55
2	B	1000	3NG	C7-C10-N15	20.04	140.05	119.77
2	A	1000	3NG	N15-C10-N9	-19.07	101.61	118.55
2	A	1000	3NG	C7-C10-N15	18.66	138.65	119.77
2	A	1000	3NG	C14-C7-C10	-4.71	117.37	124.16
2	B	1000	3NG	C14-C7-C10	-4.55	117.60	124.16
2	B	1000	3NG	C4-C5-C23	-3.97	112.52	120.37
2	C	1000	3NG	C14-C7-C10	-3.93	118.49	124.16
2	C	1000	3NG	C4-C5-C23	-3.73	112.99	120.37
2	B	1000	3NG	C14-C11-N12	-3.59	118.83	123.80
2	B	1000	3NG	C2-C1-N9	-3.43	119.78	122.98
2	A	1000	3NG	C14-C11-N12	-3.40	119.09	123.80
2	A	1000	3NG	C4-C5-C23	-3.21	114.03	120.37
2	C	1000	3NG	C10-C7-C8	3.17	121.33	117.58
2	B	1000	3NG	C6-C5-C23	3.00	126.72	120.59
2	C	1000	3NG	C16-N15-C10	2.92	135.72	128.22
2	A	1000	3NG	C10-C7-C8	2.85	120.95	117.58
2	C	1000	3NG	C6-C5-C23	2.75	126.21	120.59
2	A	1000	3NG	C16-N15-C10	2.64	134.99	128.22
2	C	1000	3NG	C13-C8-C7	2.64	120.86	117.61
2	C	1000	3NG	C3-C2-C1	2.61	121.25	117.58
2	C	1000	3NG	C2-C1-N9	-2.60	120.56	122.98
2	B	1000	3NG	C10-C7-C8	2.37	120.39	117.58
2	A	1000	3NG	C3-C2-C1	2.34	120.86	117.58
2	C	1000	3NG	C14-C11-N12	-2.33	120.56	123.80
2	A	1000	3NG	C2-C1-N9	-2.32	120.81	122.98
2	A	1000	3NG	C11-N12-C13	2.32	121.83	117.19
2	B	1000	3NG	C11-N12-C13	2.31	121.81	117.19
2	A	1000	3NG	C6-C5-C23	2.24	125.17	120.59
2	B	1000	3NG	O25-C23-C5	2.24	120.58	114.84
2	B	1000	3NG	O25-C23-O24	-2.20	118.63	123.35
2	B	1000	3NG	C14-C7-C8	2.19	122.01	119.32
2	C	1000	3NG	O25-C23-C5	2.05	120.10	114.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

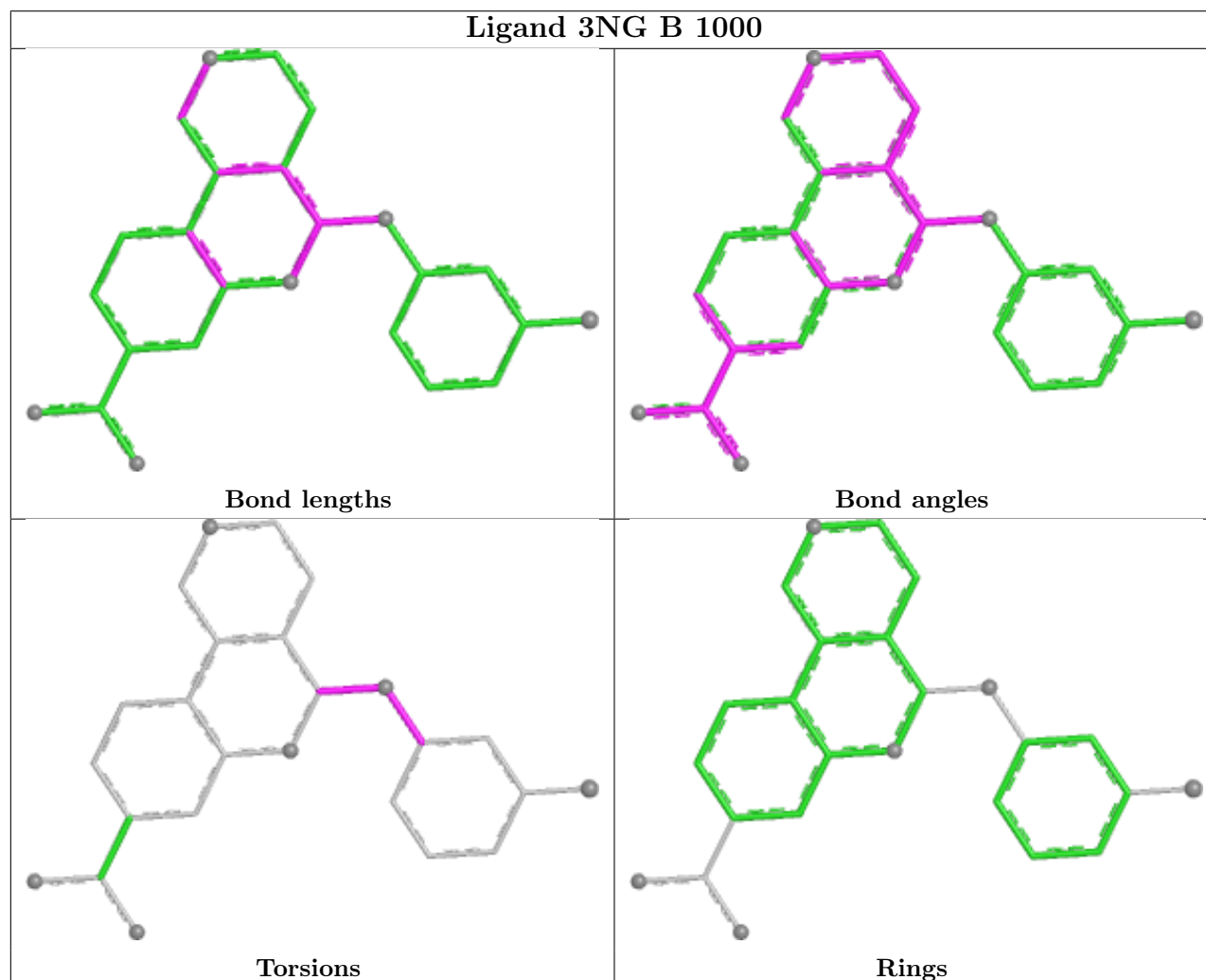
Mol	Chain	Res	Type	Atoms
2	B	1000	3NG	N9-C10-N15-C16
2	B	1000	3NG	C21-C16-N15-C10
2	B	1000	3NG	C17-C16-N15-C10
2	B	1000	3NG	C7-C10-N15-C16

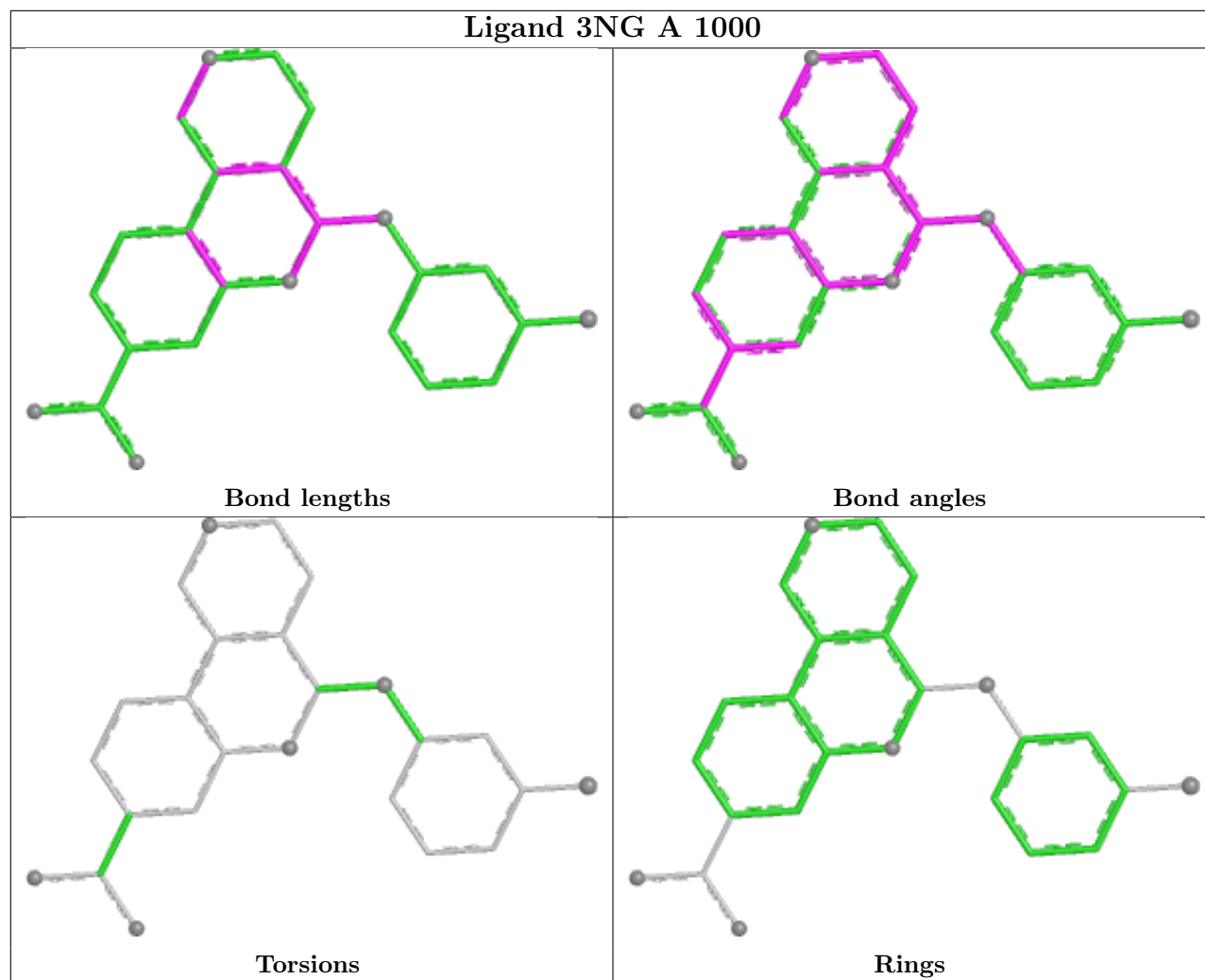
There are no ring outliers.

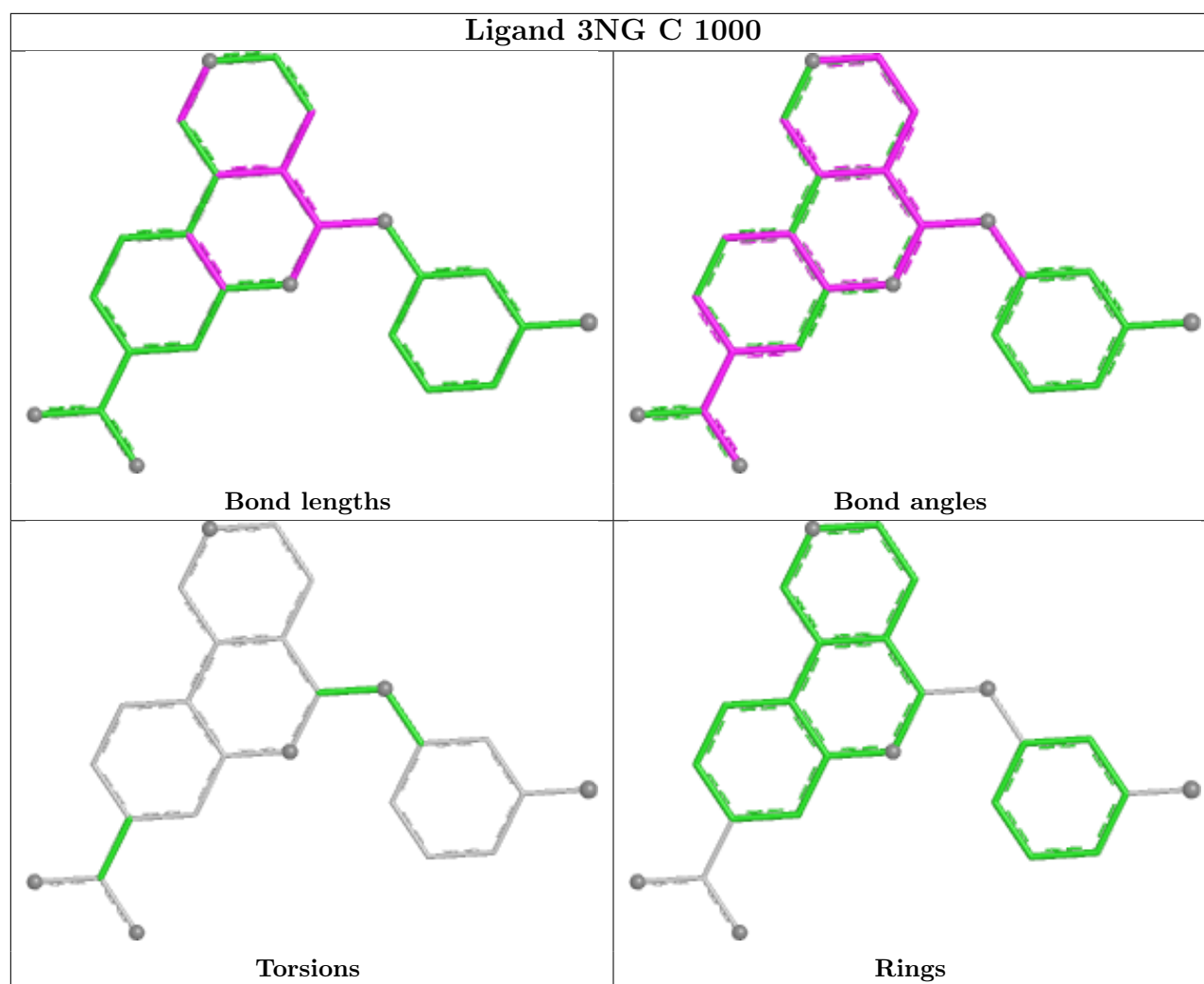
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1000	3NG	1	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	322/484 (66%)	0.27	23 (7%)	16 14	37, 58, 97, 107	0
1	B	332/484 (68%)	0.27	20 (6%)	21 20	40, 61, 87, 98	0
1	C	325/484 (67%)	0.27	16 (4%)	29 28	43, 65, 88, 104	0
All	All	979/1452 (67%)	0.27	59 (6%)	21 20	37, 62, 90, 107	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	ILE	8.2
1	B	340	VAL	5.3
1	A	402	MET	4.6
1	A	414	HIS	4.1
1	A	404	GLN	3.9
1	A	415	ASP	3.9
1	A	412	PHE	3.6
1	A	417	LEU	3.6
1	A	337	SER	3.4
1	C	341	SER	3.3
1	B	199	TYR	3.3
1	B	305	TYR	3.3
1	C	304	ALA	3.2
1	B	152	GLN	3.1
1	A	420	ASP	3.1
1	B	338	THR	3.0
1	C	183	ALA	3.0
1	A	419	TRP	2.9
1	A	335	HIS	2.9
1	B	311	ARG	2.9
1	C	182	LYS	2.8
1	A	413	HIS	2.6
1	C	159	ALA	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	333	ASP	2.6
1	A	411	TYR	2.6
1	B	367	CYS	2.6
1	A	338	THR	2.4
1	B	412	PHE	2.4
1	B	401	HIS	2.4
1	B	415	ASP	2.4
1	C	195	ASN	2.4
1	C	301	TYR	2.3
1	C	187	HIS	2.3
1	B	171	ALA	2.3
1	B	480	LEU	2.3
1	C	151	CYS	2.3
1	A	424	SER	2.3
1	A	302	THR	2.3
1	B	411	TYR	2.3
1	C	196	VAL	2.2
1	A	418	ASP	2.2
1	C	272	ILE	2.2
1	B	399	PRO	2.2
1	C	186	ARG	2.2
1	A	352	LEU	2.2
1	C	367	CYS	2.2
1	C	312	ASP	2.2
1	C	314	ARG	2.1
1	A	409	ARG	2.1
1	B	197	ASP	2.1
1	B	417	LEU	2.1
1	A	392	GLU	2.1
1	A	368	ILE	2.1
1	C	317	ILE	2.1
1	A	407	ARG	2.0
1	B	365	ILE	2.0
1	B	196	VAL	2.0
1	B	159	ALA	2.0
1	A	367	CYS	2.0

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

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](#)

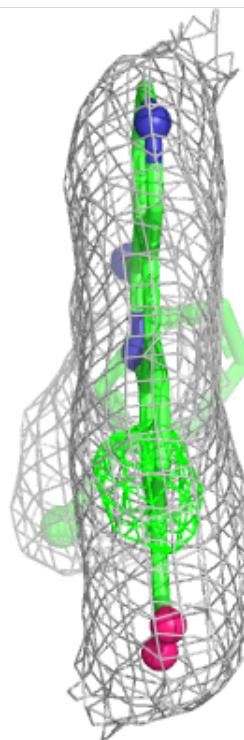
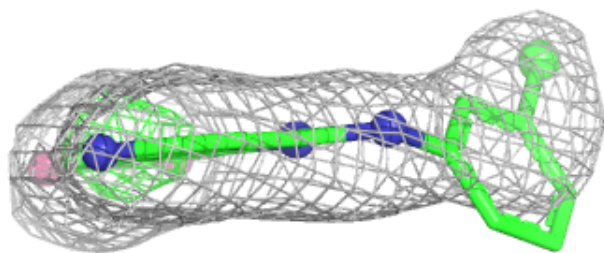
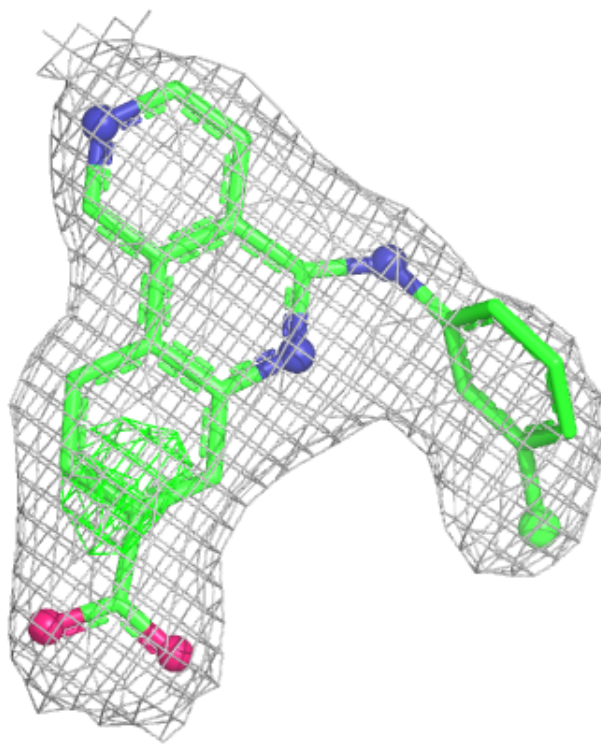
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	3NG	B	1000	25/25	0.88	0.30	74,78,97,116	0
2	3NG	A	1000	25/25	0.90	0.30	74,79,92,116	0
2	3NG	C	1000	25/25	0.93	0.26	72,78,92,116	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 3NG B 1000:**

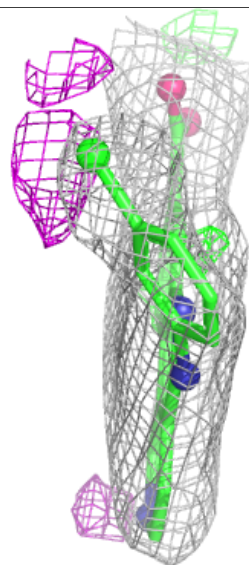
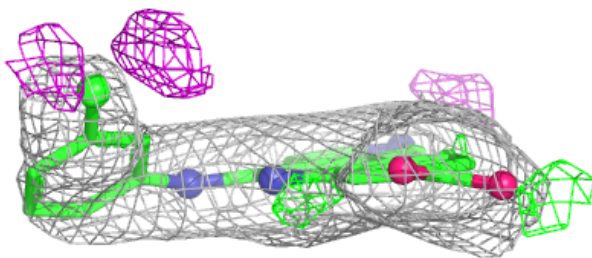
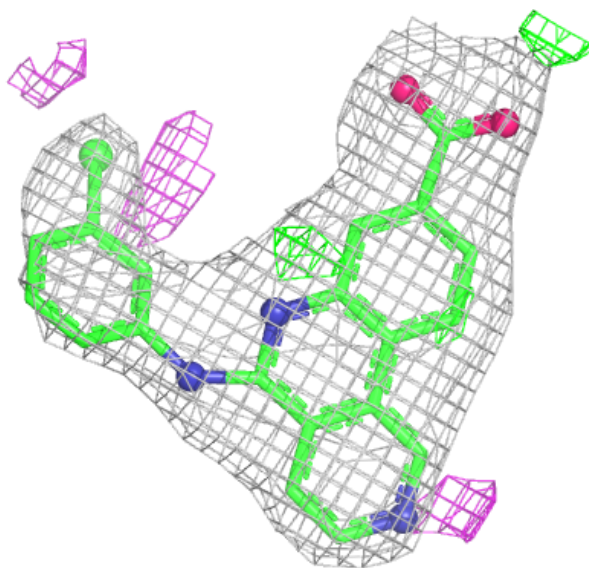
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

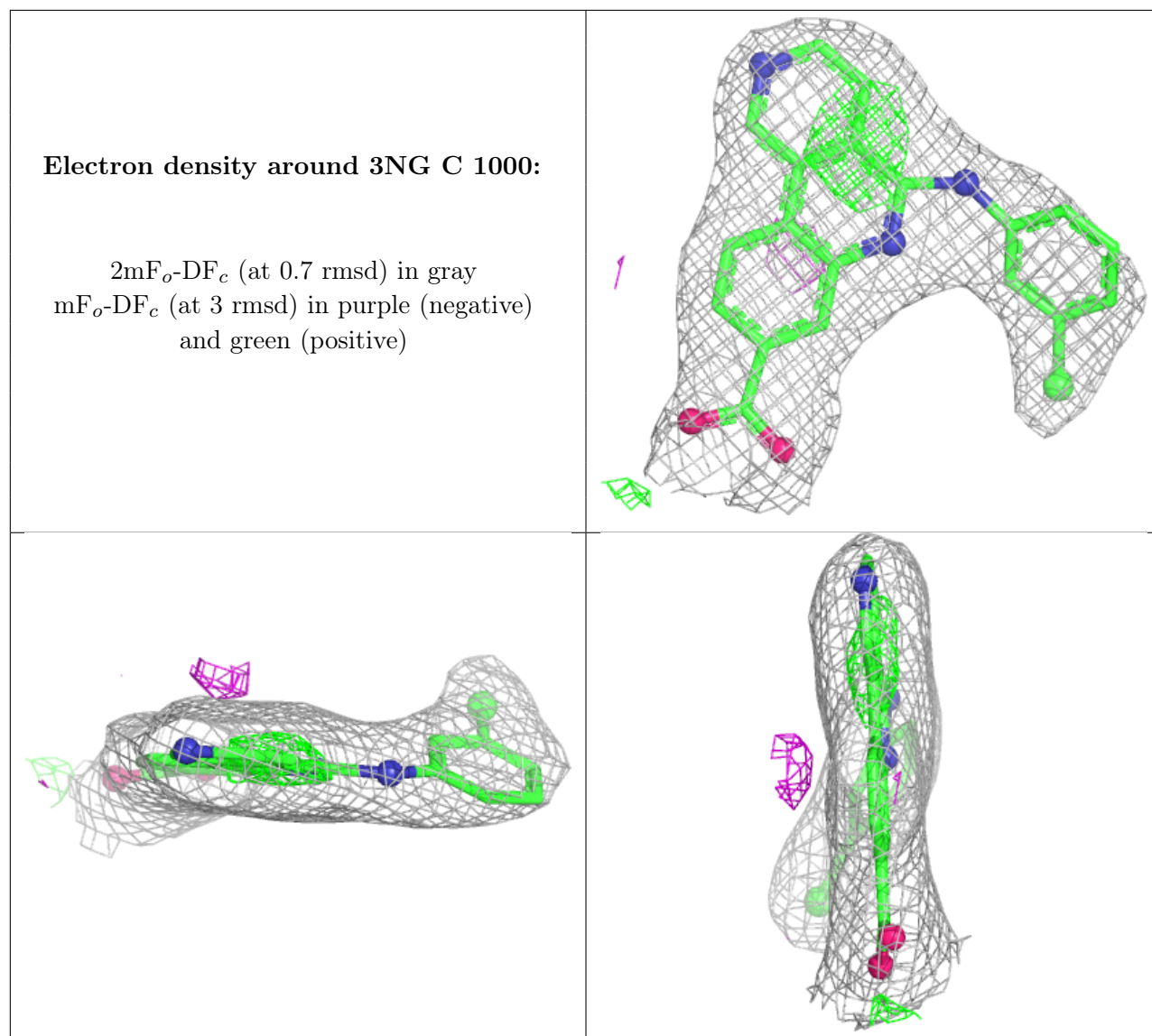




**Electron density around 3NG A 1000:**

$2mF_o-DF_c$  (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.