



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 08:03 PM EDT

PDB ID : 3RAW  
Title : Crystal Structure of human CDC-like kinase 3 isoform in complex with leucettine L41  
Authors : Filippakopoulos, P.; Fedorov, O.; King, O.; Debdab, M.; Carreaux, F.; Renault, S.; Bullock, A.; Muniz, J.R.C.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Meijer, L.; Bazureau, J.P.; Knapp, S.; Structural Genomics Consortium (SGC)  
Deposited on : 2011-03-28  
Resolution : 2.09 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 : 2.35  
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)

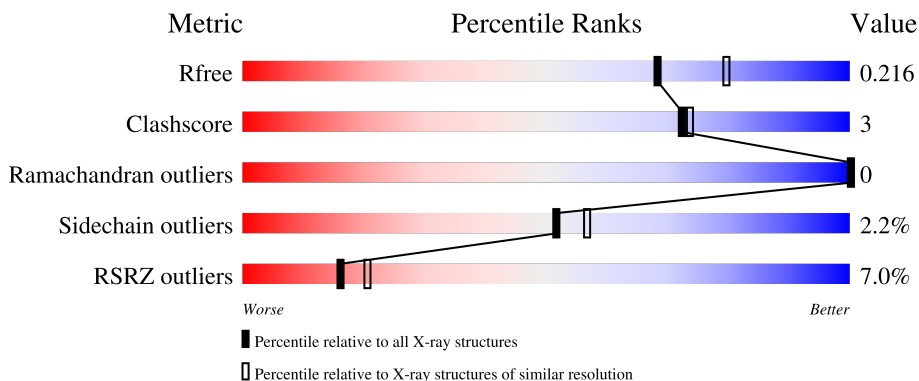
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	381	 7% 84% 8% 8%
1	B	381	 6% 83% 8% 8%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.35

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5928 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 CLK3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2839	1822	497	503	17	0	3	0
1	B	349	2797	1797	490	492	18	0	2	0

There are 46 discrepancies between the modelled and reference sequences:

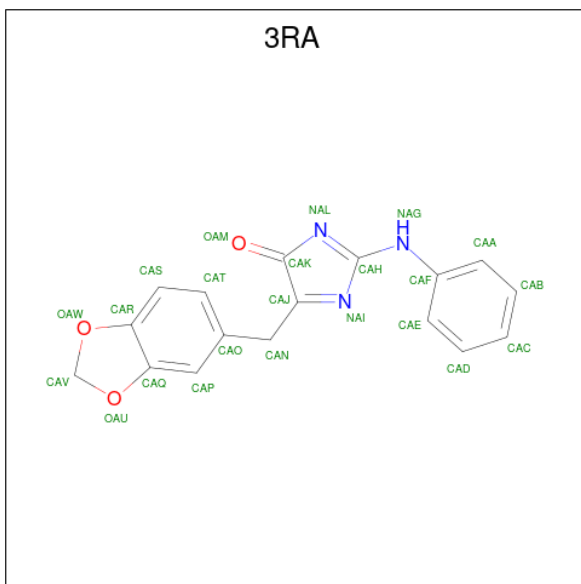
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	expression tag	UNP P49761
A	105	HIS	-	expression tag	UNP P49761
A	106	HIS	-	expression tag	UNP P49761
A	107	HIS	-	expression tag	UNP P49761
A	108	HIS	-	expression tag	UNP P49761
A	109	HIS	-	expression tag	UNP P49761
A	110	HIS	-	expression tag	UNP P49761
A	111	SER	-	expression tag	UNP P49761
A	112	SER	-	expression tag	UNP P49761
A	113	GLY	-	expression tag	UNP P49761
A	114	VAL	-	expression tag	UNP P49761
A	115	ASP	-	expression tag	UNP P49761
A	116	LEU	-	expression tag	UNP P49761
A	117	GLY	-	expression tag	UNP P49761
A	118	THR	-	expression tag	UNP P49761
A	119	GLU	-	expression tag	UNP P49761
A	120	ASN	-	expression tag	UNP P49761
A	121	LEU	-	expression tag	UNP P49761
A	122	TYR	-	expression tag	UNP P49761
A	123	PHE	-	expression tag	UNP P49761
A	124	GLN	-	expression tag	UNP P49761
A	125	SER	-	expression tag	UNP P49761
A	126	MET	-	expression tag	UNP P49761
B	104	MET	-	expression tag	UNP P49761
B	105	HIS	-	expression tag	UNP P49761

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Chain	Residue	Modelled	Actual	Comment	Reference
B	106	HIS	-	expression tag	UNP P49761
B	107	HIS	-	expression tag	UNP P49761
B	108	HIS	-	expression tag	UNP P49761
B	109	HIS	-	expression tag	UNP P49761
B	110	HIS	-	expression tag	UNP P49761
B	111	SER	-	expression tag	UNP P49761
B	112	SER	-	expression tag	UNP P49761
B	113	GLY	-	expression tag	UNP P49761
B	114	VAL	-	expression tag	UNP P49761
B	115	ASP	-	expression tag	UNP P49761
B	116	LEU	-	expression tag	UNP P49761
B	117	GLY	-	expression tag	UNP P49761
B	118	THR	-	expression tag	UNP P49761
B	119	GLU	-	expression tag	UNP P49761
B	120	ASN	-	expression tag	UNP P49761
B	121	LEU	-	expression tag	UNP P49761
B	122	TYR	-	expression tag	UNP P49761
B	123	PHE	-	expression tag	UNP P49761
B	124	GLN	-	expression tag	UNP P49761
B	125	SER	-	expression tag	UNP P49761
B	126	MET	-	expression tag	UNP P49761

- Molecule 2 is 5-(1,3-benzodioxol-5-ylmethyl)-2-(phenylamino)-4H-imidazol-4-one (three-letter code: 3RA) (formula: C<sub>17</sub>H<sub>13</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	17	3	3		
2	B	1	Total	C	N	O	0	0
			23	17	3	3		

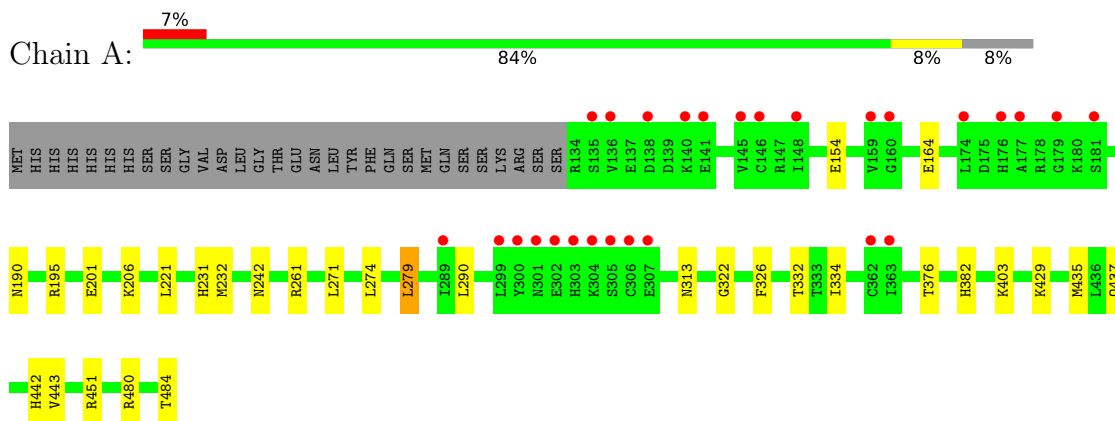
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	118	Total	O	0	0
			118	118		

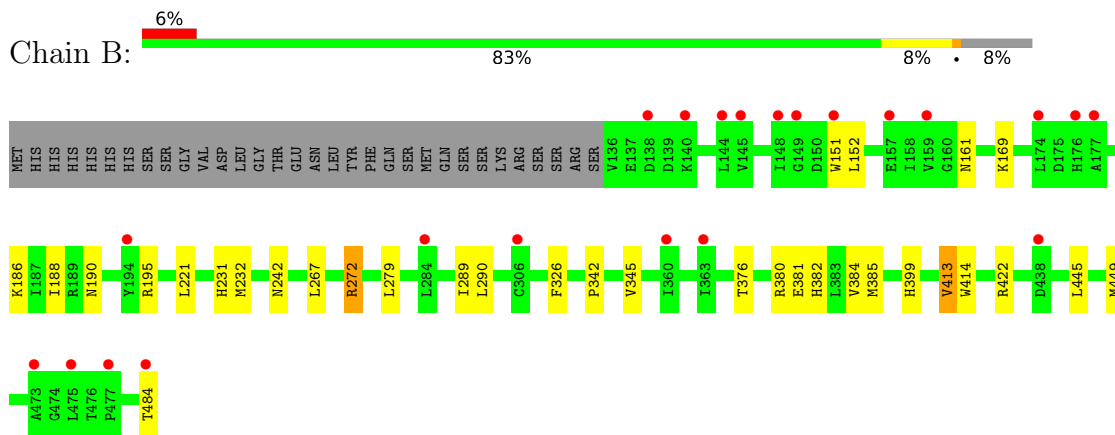
### 3 Residue-property plots [i](#)

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: Dual specificity protein kinase CLK3



- Molecule 1: Dual specificity protein kinase CLK3



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.67Å 122.42Å 69.28Å 90.00° 92.60° 90.00°	Depositor
Resolution (Å)	36.26 – 2.09 35.15 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.1 (36.26-2.09) 98.1 (35.15-2.09)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.08Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.181 , 0.219 0.181 , 0.216	Depositor DCC
$R_{free}$ test set	1988 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.058 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3RA

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	0.76	0/2926	0.75	2/3962 (0.1%)
1	B	0.71	0/2879	0.74	0/3900
All	All	0.74	0/5805	0.75	2/7862 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	261	ARG	NE-CZ-NH2	5.24	122.92	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2839	0	2707	15	0
1	B	2797	0	2662	21	0
2	A	23	0	13	1	0
2	B	23	0	13	1	0
3	A	128	0	0	3	0
3	B	118	0	0	3	0
All	All	5928	0	5395	38	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:NH2	3:B:84:HOH:O	2.16	0.68
1:B:272[B]:ARG:HD2	3:B:520:HOH:O	2.02	0.59
1:B:380:ARG:NH1	1:B:413:VAL:HG13	2.23	0.53
1:B:186:LYS:HE2	1:B:188:ILE:HD11	1.91	0.52
1:B:380:ARG:HD3	1:B:413:VAL:O	2.12	0.50
1:B:152:LEU:N	1:B:152:LEU:HD12	2.27	0.49
1:A:271:LEU:HD13	1:A:274:LEU:HD12	1.94	0.49
1:B:445:LEU:HD11	1:B:449:MET:HE1	1.94	0.49
1:A:451:ARG:NE	3:A:557:HOH:O	2.38	0.47
1:A:435:MET:HE3	1:A:443:VAL:HA	1.97	0.47
1:B:267:LEU:HD21	1:B:289:ILE:CD1	2.46	0.46
1:B:151:TRP:C	1:B:152:LEU:HD12	2.36	0.46
1:B:384:VAL:HG21	1:B:414:TRP:CG	2.51	0.46
1:B:381:GLU:O	1:B:385:MET:HG3	2.16	0.46
1:A:429:LYS:HE2	3:A:528:HOH:O	2.16	0.45
1:A:190:ASN:HB2	1:A:231:HIS:CE1	2.52	0.45
1:B:195:ARG:HG3	1:B:232:MET:HG2	1.96	0.45
2:A:1:3RA:NAI	2:A:1:3RA:HAE	2.32	0.45
1:A:195:ARG:HG3	1:A:232:MET:HG2	1.98	0.44
1:B:342:PRO:HG2	1:B:345:VAL:HG23	1.99	0.44
1:B:380:ARG:HH12	1:B:413:VAL:HG13	1.83	0.43
2:B:2:3RA:NAI	2:B:2:3RA:HAE	2.34	0.43
1:A:332:THR:HG22	1:A:334:ILE:H	1.84	0.43
1:B:272[A]:ARG:HD3	3:B:520:HOH:O	2.19	0.43
1:B:445:LEU:HD11	1:B:449:MET:CE	2.48	0.43
1:A:279:LEU:HD13	1:A:326:PHE:CD1	2.54	0.43
1:B:190:ASN:OD1	1:B:195:ARG:NH1	2.51	0.42
1:B:190:ASN:HB2	1:B:231:HIS:CE1	2.54	0.42
1:A:451:ARG:NH2	3:A:557:HOH:O	2.48	0.42
1:A:313:ASN:HD21	1:A:484:THR:C	2.22	0.42
1:A:201:GLU:HB2	1:A:322:GLY:HA2	2.02	0.42
1:B:376:THR:HG21	1:B:382:HIS:CG	2.55	0.41
1:B:279:LEU:HD13	1:B:326:PHE:CD1	2.56	0.41
1:A:437:GLN:HB2	1:A:442:HIS:CE1	2.56	0.41
1:A:376:THR:HG21	1:A:382:HIS:CG	2.56	0.40
1:A:403:LYS:HA	1:A:403:LYS:HD2	1.97	0.40
1:B:242:ASN:HA	1:B:290:LEU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASN:HA	1:A:290:LEU:HA	2.02	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	352/381 (92%)	343 (97%)	9 (3%)	0	100	100
1	B	349/381 (92%)	339 (97%)	10 (3%)	0	100	100
All	All	701/762 (92%)	682 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	296/345 (86%)	289 (98%)	7 (2%)	49	53
1	B	289/345 (84%)	281 (97%)	8 (3%)	43	47
All	All	585/690 (85%)	570 (97%)	15 (3%)	52	50

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	GLU
1	A	164	GLU
1	A	206	LYS
1	A	221	LEU
1	A	279	LEU
1	A	480[A]	ARG
1	A	480[B]	ARG
1	B	161	ASN
1	B	169	LYS
1	B	221	LEU
1	B	272[A]	ARG
1	B	272[B]	ARG
1	B	399	HIS
1	B	413	VAL
1	B	484	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	HIS
1	B	176	HIS
1	B	404	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

2 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	3RA	B	2	-	26,26,26	2.87	5 (19%)	29,36,36	2.08	9 (31%)
2	3RA	A	1	-	26,26,26	2.75	5 (19%)	29,36,36	2.13	9 (31%)

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	3RA	B	2	-	-	2/8/26/26	0/4/4/4
2	3RA	A	1	-	-	2/8/26/26	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	3RA	CAN-CAJ	-10.19	1.39	1.50
2	A	1	3RA	CAN-CAJ	-10.06	1.39	1.50
2	A	1	3RA	CAN-CAO	-6.74	1.40	1.51
2	B	2	3RA	CAN-CAO	-6.73	1.40	1.51
2	A	1	3RA	CAJ-CAK	-4.97	1.39	1.49
2	B	2	3RA	CAF-NAG	-4.48	1.32	1.41
2	B	2	3RA	CAK-NAL	-3.84	1.31	1.37
2	B	2	3RA	CAJ-CAK	-3.25	1.43	1.49
2	A	1	3RA	CAF-NAG	-2.70	1.36	1.41
2	A	1	3RA	CAK-NAL	-2.39	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	3RA	CAO-CAN-CAJ	5.47	126.62	113.58
2	A	1	3RA	CAK-CAJ-NAI	-5.22	105.25	111.58
2	A	1	3RA	CAN-CAJ-CAK	-4.89	120.27	129.44
2	A	1	3RA	CAO-CAN-CAJ	4.81	125.03	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	3RA	CAN-CAJ-CAK	-4.08	121.79	129.44
2	B	2	3RA	CAK-CAJ-NAI	-3.90	106.86	111.58
2	A	1	3RA	OAW-CAV-OAU	-3.00	103.28	108.08
2	B	2	3RA	OAU-CAQ-CAP	2.91	131.74	127.85
2	B	2	3RA	CAN-CAO-CAT	-2.90	116.75	120.89
2	B	2	3RA	NAG-CAH-NAI	2.72	128.13	119.86
2	A	1	3RA	OAU-CAQ-CAP	2.66	131.41	127.85
2	B	2	3RA	CAN-CAO-CAP	2.60	124.50	120.38
2	B	2	3RA	CAB-CAA-CAF	2.45	122.65	119.72
2	A	1	3RA	CAN-CAO-CAT	-2.44	117.40	120.89
2	B	2	3RA	CAP-CAQ-CAR	-2.37	119.01	122.02
2	A	1	3RA	NAG-CAH-NAI	2.31	126.88	119.86
2	A	1	3RA	OAW-CAR-CAS	2.27	131.94	127.81
2	A	1	3RA	CAN-CAO-CAP	2.26	123.96	120.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	3RA	NAL-CAH-NAG-CAF
2	A	1	3RA	CAK-CAJ-CAN-CAO
2	B	2	3RA	CAK-CAJ-CAN-CAO
2	A	1	3RA	NAL-CAH-NAG-CAF

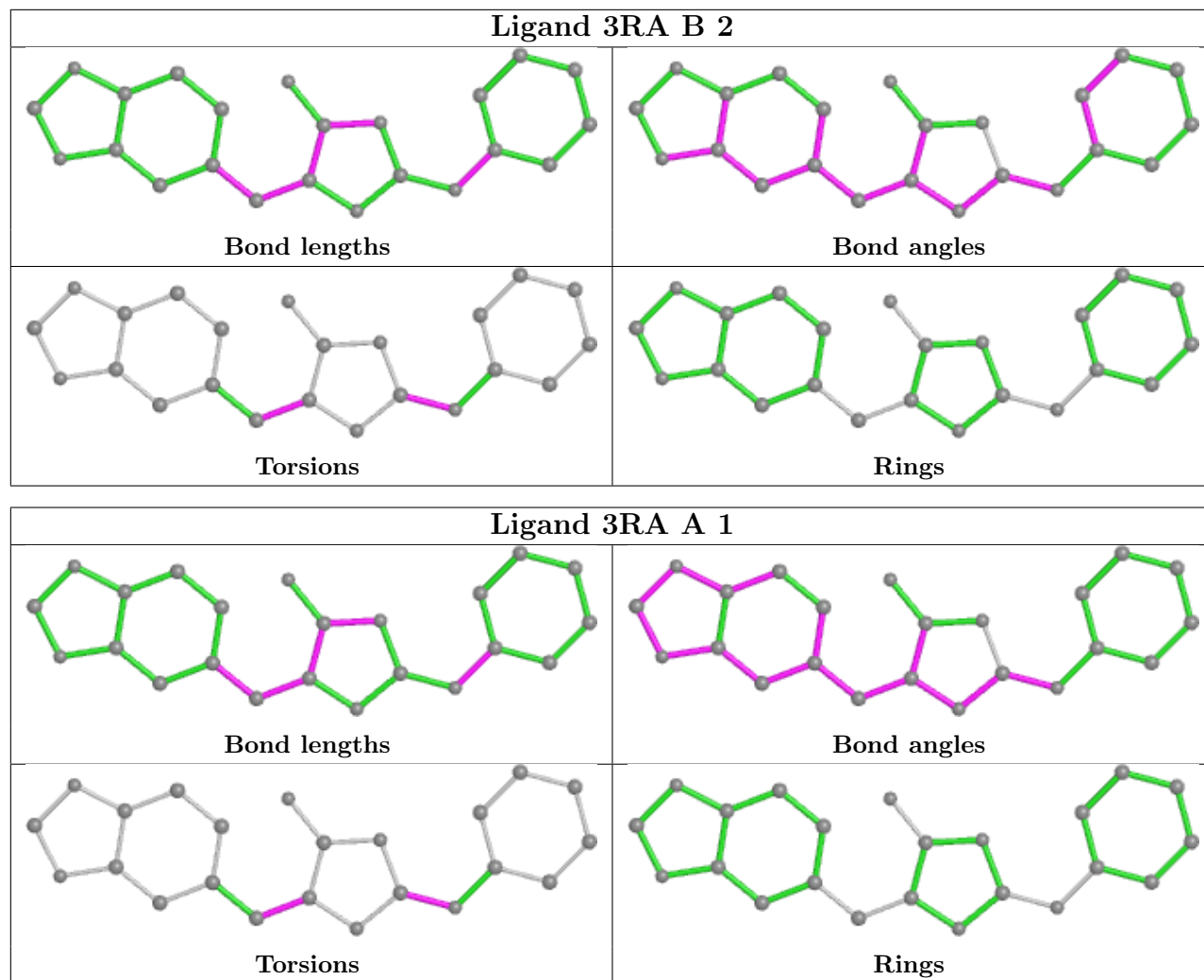
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	3RA	1	0
2	A	1	3RA	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	351/381 (92%)	0.17	27 (7%) <b>13</b> <b>17</b>	20, 42, 87, 120	0
1	B	349/381 (91%)	0.19	22 (6%) <b>20</b> <b>24</b>	22, 43, 87, 110	0
All	All	700/762 (91%)	0.18	49 (7%) <b>16</b> <b>20</b>	20, 42, 87, 120	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	CYS	5.8
1	B	176	HIS	4.2
1	B	477	PRO	4.0
1	B	148	ILE	3.7
1	A	305	SER	3.6
1	A	179	GLY	3.6
1	A	300	TYR	3.6
1	B	151	TRP	3.5
1	A	303	HIS	3.4
1	A	146	CYS	3.4
1	B	484	THR	3.3
1	A	136	VAL	3.3
1	A	304	LYS	3.3
1	A	145	VAL	3.1
1	B	145	VAL	3.1
1	A	140	LYS	3.1
1	B	140	LYS	3.0
1	B	363	ILE	3.0
1	A	177	ALA	2.9
1	B	144	LEU	2.8
1	B	174	LEU	2.8
1	B	473	ALA	2.8
1	A	138	ASP	2.8
1	B	159	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	157	GLU	2.7
1	A	174	LEU	2.7
1	A	148	ILE	2.7
1	A	302	GLU	2.7
1	B	284	LEU	2.6
1	A	299	LEU	2.6
1	B	475	LEU	2.6
1	A	135	SER	2.5
1	B	177	ALA	2.5
1	A	301	ASN	2.4
1	A	307	GLU	2.4
1	A	159	VAL	2.4
1	A	363	ILE	2.4
1	B	438	ASP	2.3
1	A	176	HIS	2.3
1	A	160	GLY	2.3
1	B	194	TYR	2.2
1	B	306	CYS	2.2
1	B	138	ASP	2.2
1	A	141	GLU	2.2
1	B	149	GLY	2.1
1	B	360	ILE	2.1
1	A	362	CYS	2.1
1	A	181	SER	2.1
1	A	289	ILE	2.1

## 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.

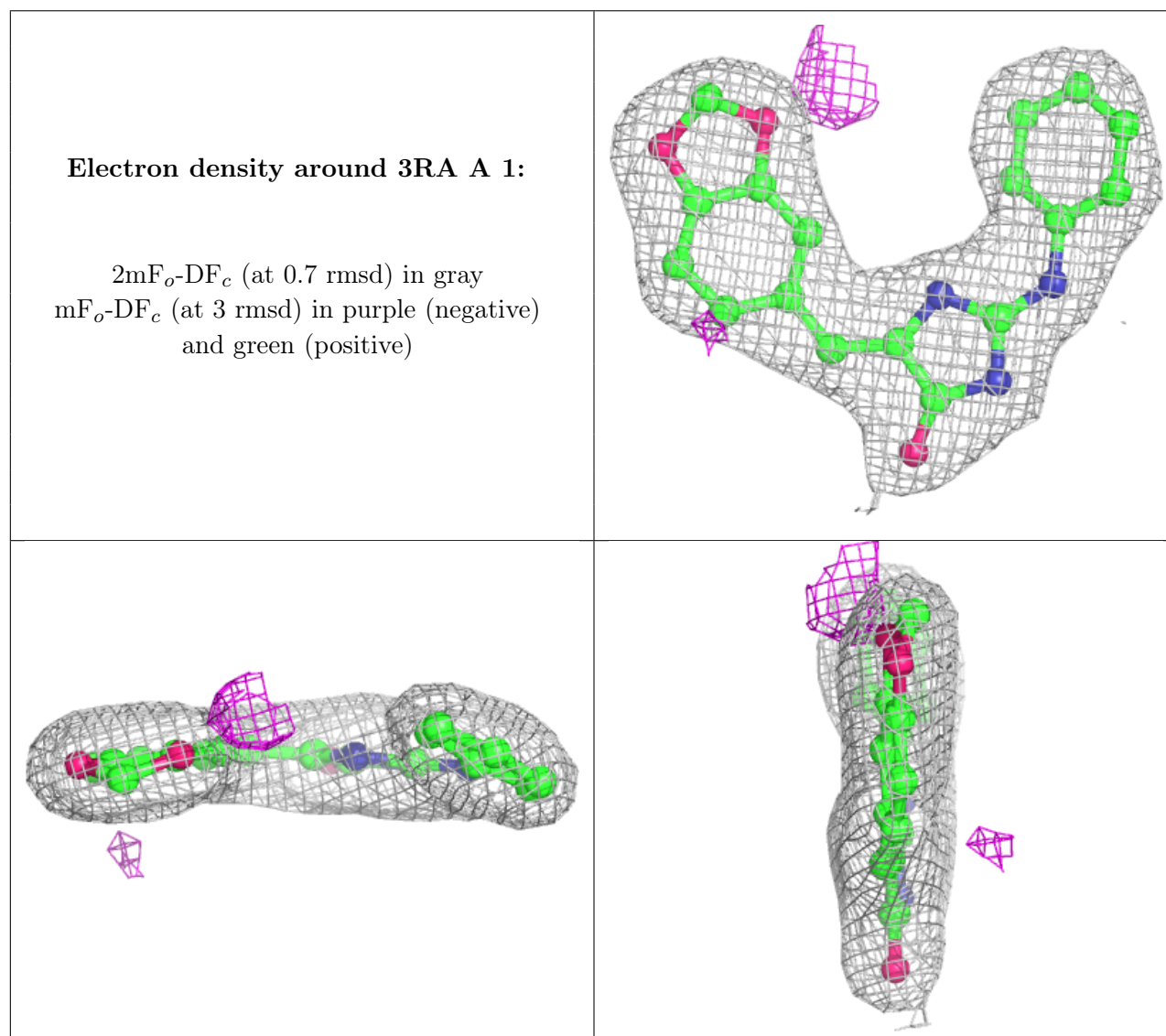
## 6.4 Ligands [i](#)

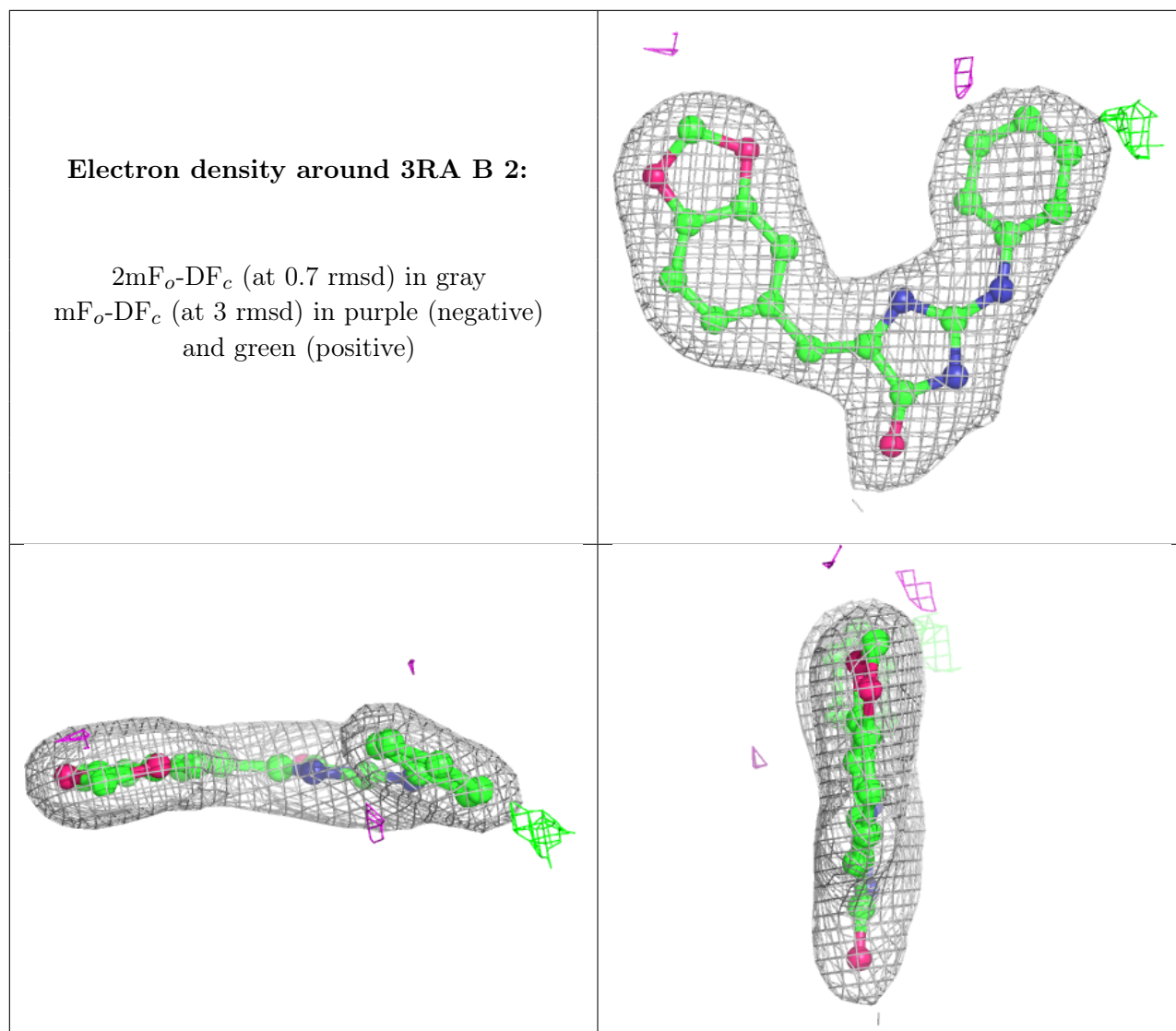
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	3RA	A	1	23/23	0.98	0.08	26,34,52,57	0
2	3RA	B	2	23/23	0.98	0.09	26,31,45,48	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.