



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 06:02 PM EDT

PDB ID : 5SF6  
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN COMPLEX WITH N1(CCCC1)c2nn(c(n2)CCc4nn3c(nc(c3C)C)c(n4)NC(C)C)C, micromolar IC50=0.002775  
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Deposited on : 2022-01-21  
Resolution : 2.03 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

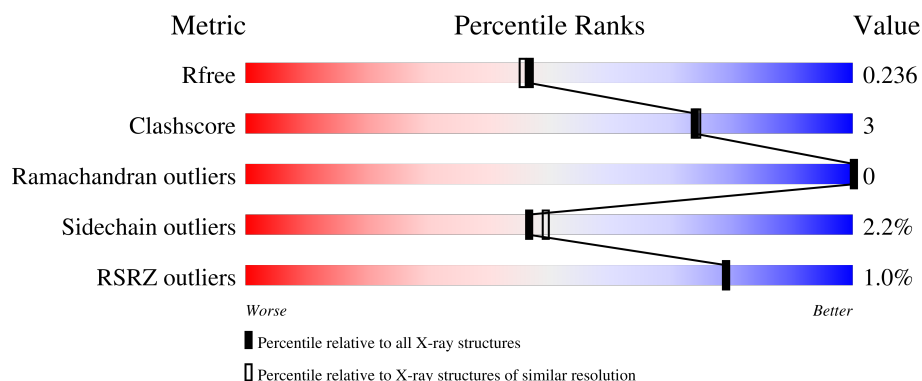
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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))
$R_{free}$	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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	343	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>9%</div> </div> </div>
1	B	343	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
1	C	343	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>9%</div> </div> </div>
1	D	343	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10807 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 cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	1	0
			2544	1626	432	462	24			
1	B	315	Total	C	N	O	S	0	2	0
			2559	1635	434	465	25			
1	C	313	Total	C	N	O	S	0	0	0
			2541	1624	432	461	24			
1	D	311	Total	C	N	O	S	0	0	0
			2523	1614	430	455	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	GLY	-	expression tag	UNP Q9Y233
A	448	SER	-	expression tag	UNP Q9Y233
B	447	GLY	-	expression tag	UNP Q9Y233
B	448	SER	-	expression tag	UNP Q9Y233
C	447	GLY	-	expression tag	UNP Q9Y233
C	448	SER	-	expression tag	UNP Q9Y233
D	447	GLY	-	expression tag	UNP Q9Y233
D	448	SER	-	expression tag	UNP Q9Y233

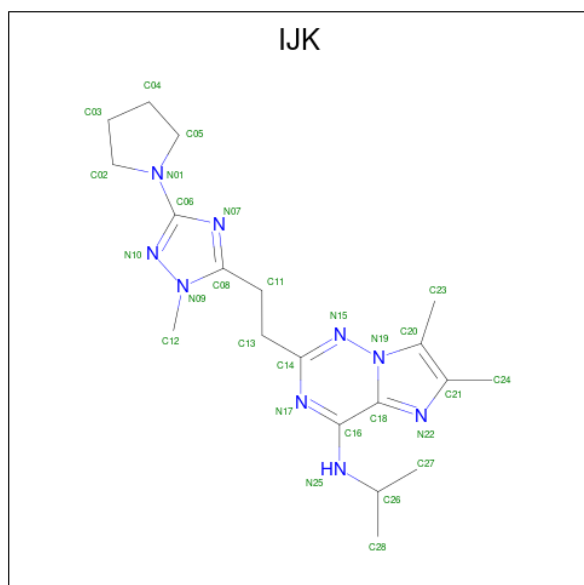
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (8S)-6,7-dimethyl-2-{2-[1-methyl-3-(pyrrolidin-1-yl)-1H-1,2,4-triazol-5-yl]ethyl}-N-(propan-2-yl)imidazo[2,1-f][1,2,4]triazin-4-amine (three-letter code: IJK) (formula: C<sub>19</sub>H<sub>29</sub>N<sub>9</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			28	19	9		
4	B	1	Total	C	N	0	0
			28	19	9		
4	C	1	Total	C	N	0	0
			28	19	9		
4	D	1	Total	C	N	0	0
			28	19	9		

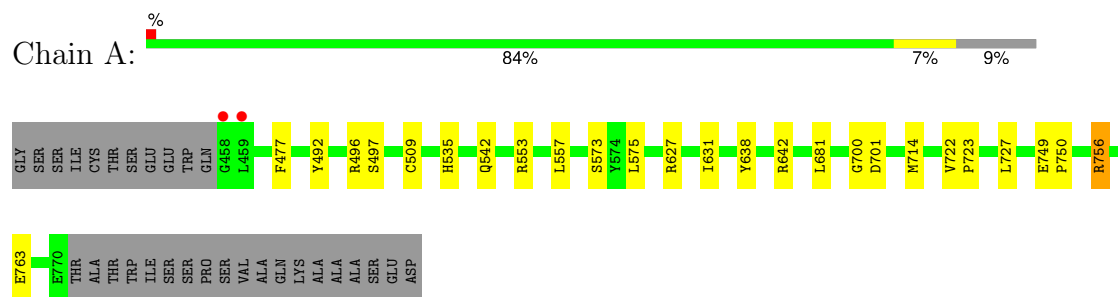
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	129	Total 129	O 129	0	0
5	B	155	Total 155	O 155	0	0
5	C	144	Total 144	O 144	0	0
5	D	92	Total 92	O 92	0	0

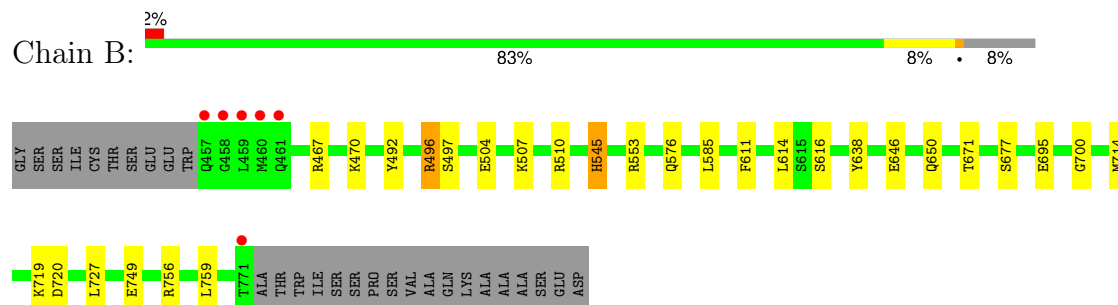
### 3 Residue-property plots

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.

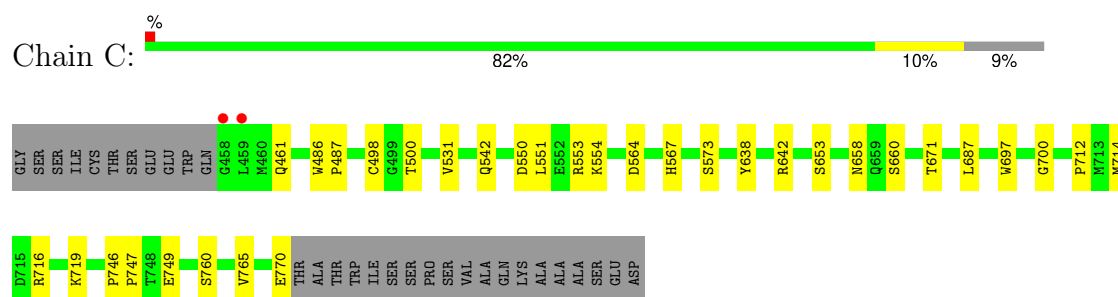
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



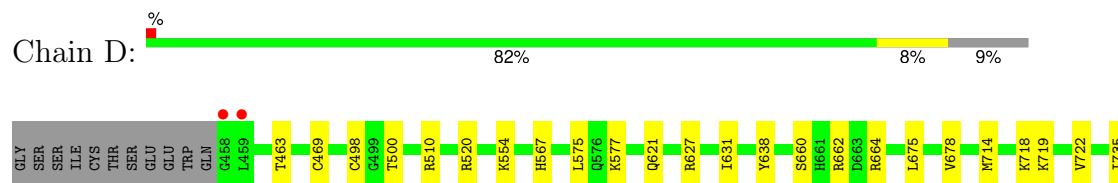
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

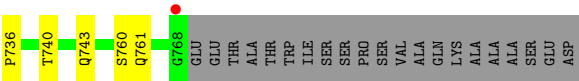


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.47Å 135.47Å 235.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.63 – 2.03 43.63 – 2.03	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.63-2.03) 96.0 (43.63-2.03)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.179 , 0.232 0.186 , 0.236	Depositor DCC
$R_{free}$ test set	5186 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: IJK, MG, CME, 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	0.92	0/2598	0.99	2/3515 (0.1%)
1	B	0.91	2/2616 (0.1%)	0.99	2/3540 (0.1%)
1	C	0.88	0/2592	0.97	1/3507 (0.0%)
1	D	0.87	0/2574	0.97	1/3483 (0.0%)
All	All	0.89	2/10380 (0.0%)	0.98	6/14045 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	695	GLU	CD-OE2	-8.24	1.16	1.25
1	B	695	GLU	CD-OE1	6.40	1.32	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	756	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	D	510	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	C	716	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	A	642	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	510	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	496	ARG	NE-CZ-NH1	5.01	122.81	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	2544	0	2516	13	0
1	B	2559	0	2524	14	0
1	C	2541	0	2511	23	0
1	D	2523	0	2499	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	28	0	0	0	0
4	B	28	0	0	0	0
4	C	28	0	0	0	0
4	D	28	0	0	0	0
5	A	129	0	0	1	0
5	B	155	0	0	1	0
5	C	144	0	0	6	0
5	D	92	0	0	1	0
All	All	10807	0	10050	61	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 (61) 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:497:SER:O	1:B:553:ARG:HD2	1.74	0.87
1:C:550:ASP:OD1	5:C:901:HOH:O	1.96	0.82
1:D:761:GLN:HE21	1:D:761:GLN:HA	1.61	0.65
1:C:749:GLU:HG3	5:C:1024:HOH:O	1.97	0.63
1:B:727:LEU:HD12	1:B:759:LEU:HD11	1.81	0.62
1:C:749:GLU:CG	5:C:1024:HOH:O	2.48	0.62
1:D:740:THR:HA	1:D:743:GLN:HE21	1.66	0.61
1:B:727:LEU:CD1	1:B:759:LEU:HD11	2.30	0.61
1:D:761:GLN:HA	1:D:761:GLN:NE2	2.16	0.59
1:A:700:GLY:HA3	1:A:714:MET:O	2.04	0.58
1:B:727:LEU:HD12	1:B:759:LEU:CD1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:GLN:HE21	1:C:500:THR:HG21	1.70	0.56
1:D:627:ARG:O	1:D:631:ILE:HG12	2.06	0.56
1:C:770:GLU:O	1:C:770:GLU:HG3	2.05	0.54
1:C:498:CYS:SG	1:C:554:LYS:HG2	2.47	0.54
1:A:749:GLU:N	1:A:750:PRO:CD	2.71	0.53
1:C:542:GLN:NE2	1:C:542:GLN:HA	2.23	0.53
1:C:653:SER:O	5:C:902:HOH:O	2.19	0.53
1:B:700:GLY:HA3	1:B:714:MET:O	2.09	0.53
1:A:756:ARG:NE	5:A:901:HOH:O	2.23	0.51
1:B:611:PHE:HB3	1:B:614:LEU:HD22	1.93	0.50
1:A:497:SER:OG	1:A:557:LEU:HD11	2.13	0.49
1:D:719:LYS:O	1:D:722:VAL:HG23	2.13	0.49
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.48	0.48
1:B:646:GLU:O	1:B:650:GLN:HB2	2.14	0.47
1:C:697:TRP:CH2	1:C:719:LYS:HG2	2.49	0.47
1:A:701:ASP:HB3	1:C:687:LEU:HD13	1.98	0.47
1:C:700:GLY:HA3	1:C:714:MET:O	2.15	0.46
1:B:545:HIS:HE1	1:D:760:SER:HB2	1.81	0.46
1:D:498:CYS:SG	1:D:554:LYS:HG2	2.55	0.46
1:B:492:TYR:CZ	1:B:496:ARG:HD2	2.51	0.46
1:C:765:VAL:HG22	1:C:770:GLU:HG2	1.97	0.45
1:A:497:SER:O	1:A:553:ARG:HD2	2.16	0.45
1:C:638:TYR:OH	1:C:642:ARG:HD3	2.16	0.45
1:B:756:ARG:HD2	5:B:907:HOH:O	2.17	0.45
1:C:749:GLU:HG2	5:C:1024:HOH:O	2.15	0.44
1:A:542:GLN:NE2	1:A:542:GLN:HA	2.33	0.44
1:A:627:ARG:O	1:A:631:ILE:HG12	2.18	0.44
1:A:722:VAL:N	1:A:723:PRO:CD	2.81	0.44
1:D:675:LEU:O	1:D:678:VAL:HG22	2.17	0.43
1:B:638:TYR:CD1	1:B:671:THR:HG21	2.53	0.43
1:C:564:ASP:O	1:C:567:HIS:HB2	2.19	0.43
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.54	0.43
1:D:735:ILE:HB	1:D:736:PRO:HD3	2.01	0.42
1:D:718:LYS:O	1:D:719:LYS:C	2.57	0.42
1:D:714:MET:HE2	5:D:929:HOH:O	2.18	0.42
1:A:727:LEU:HD23	1:A:727:LEU:HA	1.84	0.42
1:B:504:GLU:HB3	1:B:507:LYS:HD2	2.01	0.42
1:B:545:HIS:CE1	1:D:760:SER:HB2	2.55	0.42
1:B:727:LEU:CD1	1:B:759:LEU:CD1	2.96	0.41
1:A:727:LEU:HD21	1:A:763:GLU:HG3	2.01	0.41
1:C:486:TRP:N	1:C:487:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:TYR:CD1	1:C:671:THR:HG21	2.56	0.41
1:C:553:ARG:NH1	5:C:901:HOH:O	2.53	0.41
1:C:658:ASN:OD1	1:C:660:SER:HB3	2.20	0.41
1:D:520:ARG:HD2	1:D:567:HIS:O	2.20	0.41
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.97	0.41
1:C:746:PRO:N	1:C:747:PRO:CD	2.84	0.40
1:C:486:TRP:HB3	1:C:531:VAL:HG21	2.02	0.40
1:D:660:SER:O	1:D:664:ARG:HG3	2.21	0.40
1:C:542:GLN:HA	1:C:542:GLN:HE21	1.85	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	311/343 (91%)	304 (98%)	7 (2%)	0	100	100
1	B	314/343 (92%)	306 (98%)	8 (2%)	0	100	100
1	C	310/343 (90%)	304 (98%)	6 (2%)	0	100	100
1	D	308/343 (90%)	299 (97%)	9 (3%)	0	100	100
All	All	1243/1372 (91%)	1213 (98%)	30 (2%)	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	282/305 (92%)	278 (99%)	4 (1%)	62	67
1	B	283/305 (93%)	272 (96%)	11 (4%)	27	26
1	C	281/305 (92%)	278 (99%)	3 (1%)	70	75
1	D	279/305 (92%)	271 (97%)	8 (3%)	37	37
All	All	1125/1220 (92%)	1099 (98%)	26 (2%)	47	47

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	SER
1	A	575	LEU
1	A	638	TYR
1	A	681	LEU
1	B	467	ARG
1	B	470	LYS
1	B	545	HIS
1	B	576	GLN
1	B	585	LEU
1	B	616	SER
1	B	677	SER
1	B	719	LYS
1	B	720[A]	ASP
1	B	720[B]	ASP
1	B	749	GLU
1	C	573	SER
1	C	712	PRO
1	C	760	SER
1	D	463	THR
1	D	469	CYS
1	D	500	THR
1	D	575	LEU
1	D	577	LYS
1	D	621	GLN
1	D	638	TYR
1	D	662	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	542	GLN

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Mol	Chain	Res	Type
1	A	604	GLN
1	A	743	GLN
1	A	761	GLN
1	B	495	HIS
1	B	542	GLN
1	B	604	GLN
1	C	461	GLN
1	C	542	GLN
1	C	604	GLN
1	C	709	GLN
1	C	743	GLN
1	D	644	GLN
1	D	650	GLN
1	D	724	GLN
1	D	743	GLN
1	D	761	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	CME	A	509	1	8,9,10	0.40	0	6,9,11	1.23	1 (16%)
1	CME	B	509	1	8,9,10	0.41	0	6,9,11	0.57	0
1	CME	D	509	1	8,9,10	0.78	0	6,9,11	0.76	0
1	CME	C	509	1	8,9,10	0.52	0	6,9,11	0.53	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
1	CME	A	509	1	-	1/5/8/10	-
1	CME	B	509	1	-	0/5/8/10	-
1	CME	D	509	1	-	2/5/8/10	-
1	CME	C	509	1	-	2/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	CME	CZ-CE-SD	-2.21	105.99	113.39

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	509	CME	SD-CE-CZ-OH
1	C	509	CME	SD-CE-CZ-OH
1	A	509	CME	SD-CE-CZ-OH
1	C	509	CME	CE-SD-SG-CB
1	D	509	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z  > 2$
4	IJK	D	803	-	21,31,31	2.38	5 (23%)	22,45,45	2.05	7 (31%)
4	IJK	C	803	-	21,31,31	3.14	7 (33%)	22,45,45	1.26	3 (13%)
4	IJK	B	803	-	21,31,31	2.21	5 (23%)	22,45,45	1.72	4 (18%)
4	IJK	A	803	-	21,31,31	2.86	9 (42%)	22,45,45	1.67	5 (22%)

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
4	IJK	D	803	-	-	0/9/20/20	0/4/4/4
4	IJK	C	803	-	-	0/9/20/20	0/4/4/4
4	IJK	B	803	-	-	1/9/20/20	0/4/4/4
4	IJK	A	803	-	-	0/9/20/20	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	IJK	C14-N15	8.32	1.42	1.34
4	D	803	IJK	C18-N22	7.08	1.40	1.33
4	C	803	IJK	C18-N22	6.64	1.39	1.33
4	A	803	IJK	C14-N17	5.91	1.41	1.33
4	C	803	IJK	C14-N17	5.45	1.40	1.33
4	B	803	IJK	C26-N25	5.14	1.54	1.46
4	A	803	IJK	C02-N01	-5.06	1.38	1.46
4	A	803	IJK	C26-N25	4.95	1.54	1.46
4	B	803	IJK	C14-N15	4.90	1.39	1.34
4	D	803	IJK	C14-N15	4.73	1.39	1.34
4	A	803	IJK	C18-N22	4.71	1.37	1.33
4	A	803	IJK	C13-C14	-4.49	1.45	1.50
4	A	803	IJK	C14-N15	4.29	1.38	1.34
4	C	803	IJK	C16-N17	4.26	1.38	1.33
4	B	803	IJK	C02-N01	-4.04	1.40	1.46
4	C	803	IJK	C26-N25	3.81	1.52	1.46
4	D	803	IJK	C26-N25	3.57	1.52	1.46
4	D	803	IJK	C16-C18	-3.51	1.39	1.44
4	C	803	IJK	C13-C14	-3.12	1.46	1.50
4	C	803	IJK	C06-N01	2.88	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	IJK	C16-N17	2.86	1.36	1.33
4	B	803	IJK	C16-C18	-2.85	1.40	1.44
4	A	803	IJK	C24-C21	-2.70	1.46	1.50
4	B	803	IJK	C13-C14	-2.61	1.47	1.50
4	A	803	IJK	C16-C18	-2.15	1.41	1.44
4	D	803	IJK	C14-N17	2.15	1.36	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	803	IJK	N15-C14-N17	-4.56	119.43	125.91
4	B	803	IJK	C27-C26-N25	-4.03	102.04	109.95
4	D	803	IJK	C23-C20-C21	3.88	135.96	129.31
4	A	803	IJK	C11-C13-C14	-3.61	106.37	112.48
4	A	803	IJK	C28-C26-N25	3.46	116.74	109.95
4	C	803	IJK	C08-N07-C06	-3.29	102.02	103.90
4	B	803	IJK	C28-C26-N25	3.24	116.30	109.95
4	D	803	IJK	C05-N01-C06	3.23	128.97	123.49
4	D	803	IJK	C12-N09-C08	-3.10	125.71	128.87
4	B	803	IJK	C11-C13-C14	-2.78	107.77	112.48
4	D	803	IJK	C02-N01-C06	-2.59	119.10	123.49
4	B	803	IJK	N15-C14-N17	-2.57	122.26	125.91
4	C	803	IJK	C28-C26-N25	2.55	114.96	109.95
4	A	803	IJK	C27-C26-N25	-2.50	105.03	109.95
4	A	803	IJK	N25-C16-N17	2.41	123.16	118.56
4	A	803	IJK	N15-C14-N17	-2.38	122.52	125.91
4	D	803	IJK	C13-C14-N15	2.38	120.68	116.89
4	D	803	IJK	C13-C14-N17	2.07	119.84	116.73
4	C	803	IJK	C02-N01-C06	-2.00	120.10	123.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

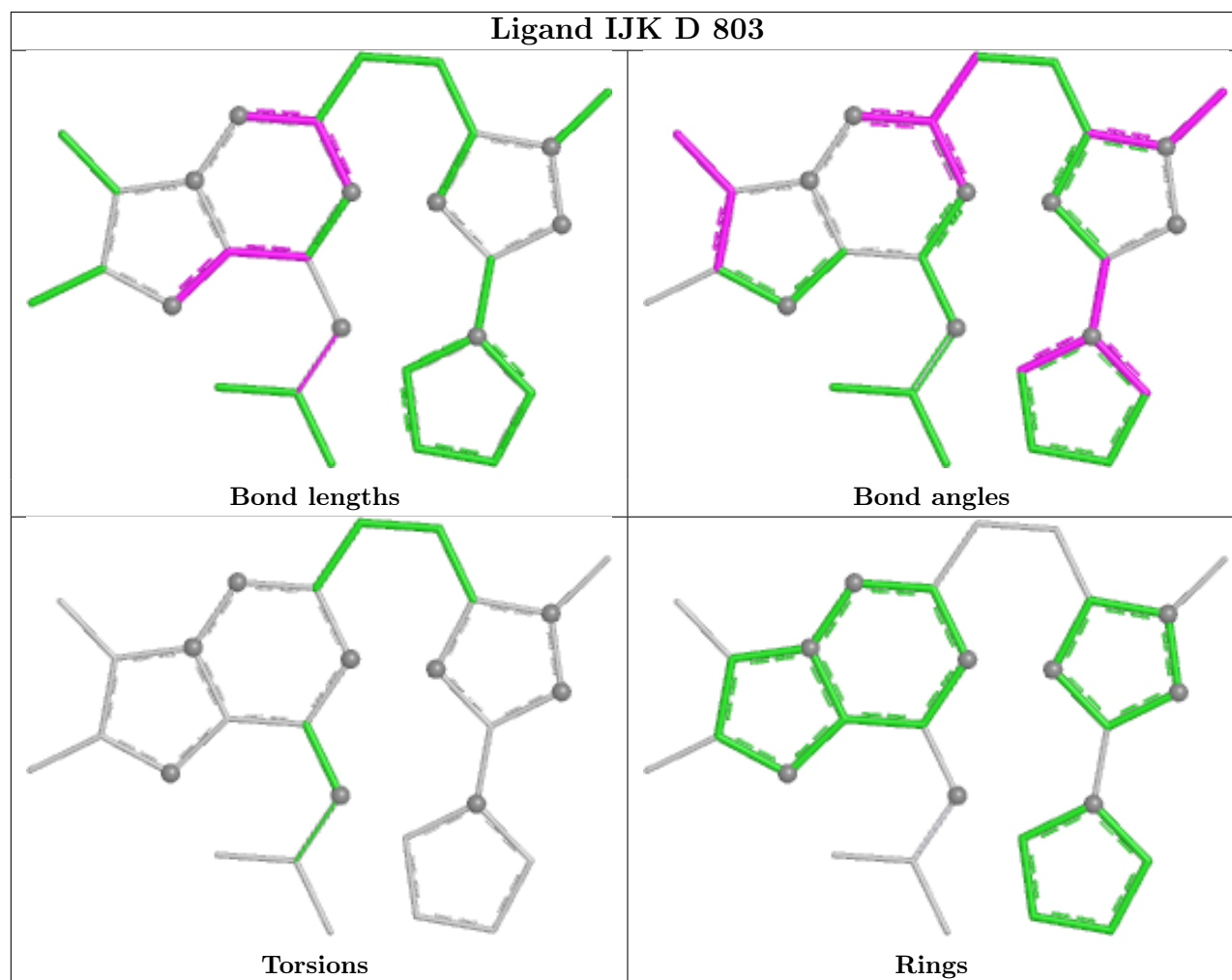
Mol	Chain	Res	Type	Atoms
4	B	803	IJK	N09-C08-C11-C13

There are no ring outliers.

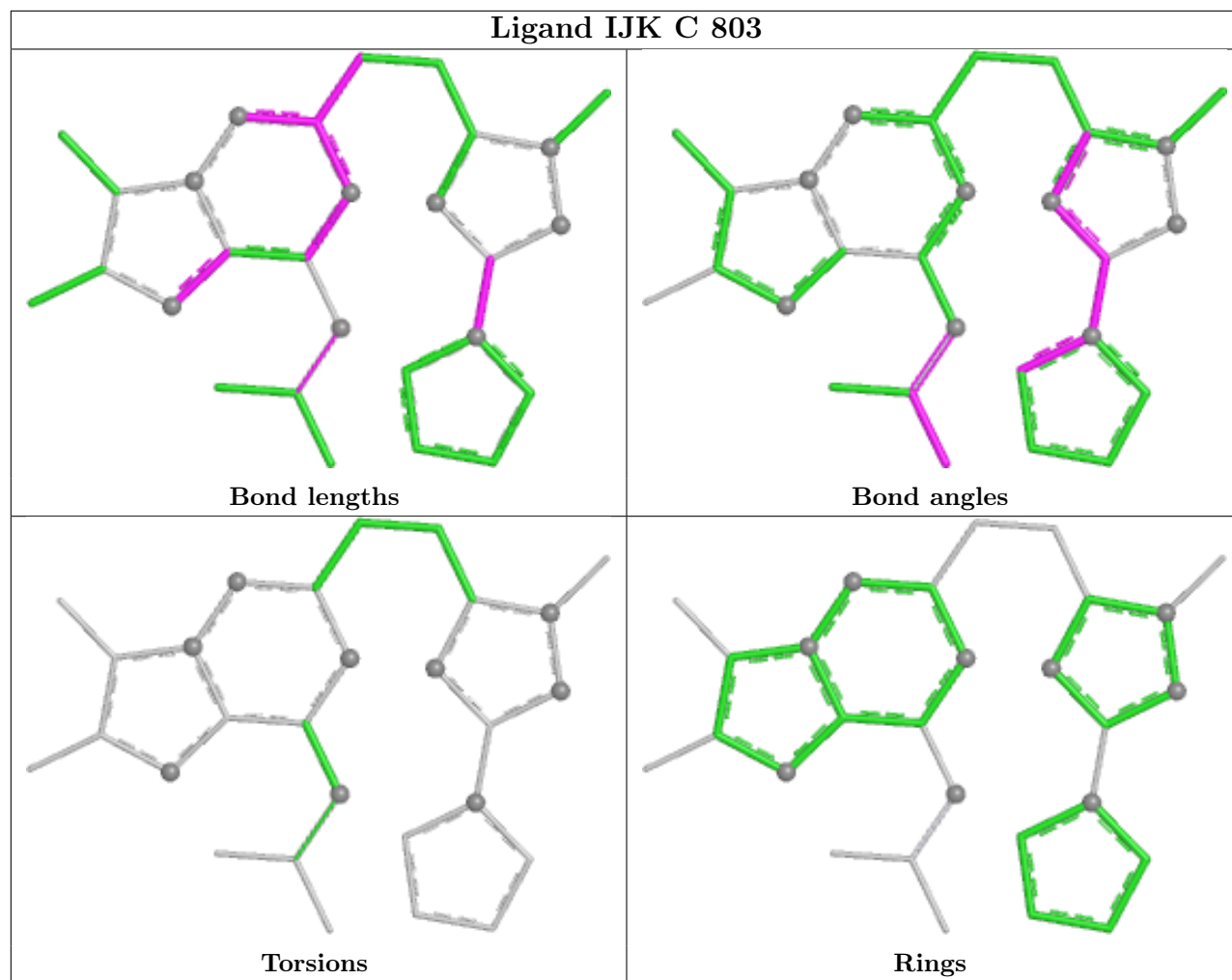
No monomer is involved in short contacts.

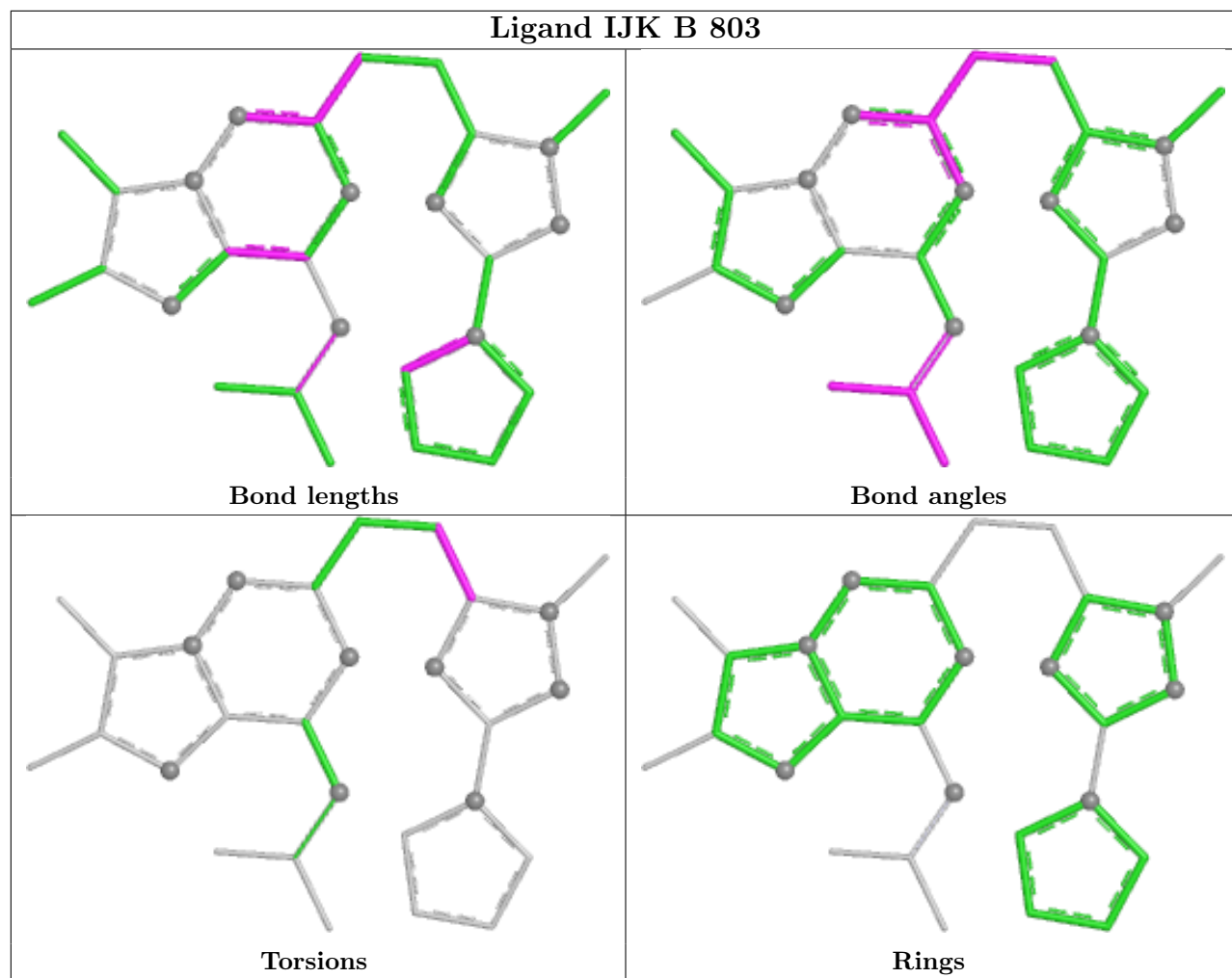
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

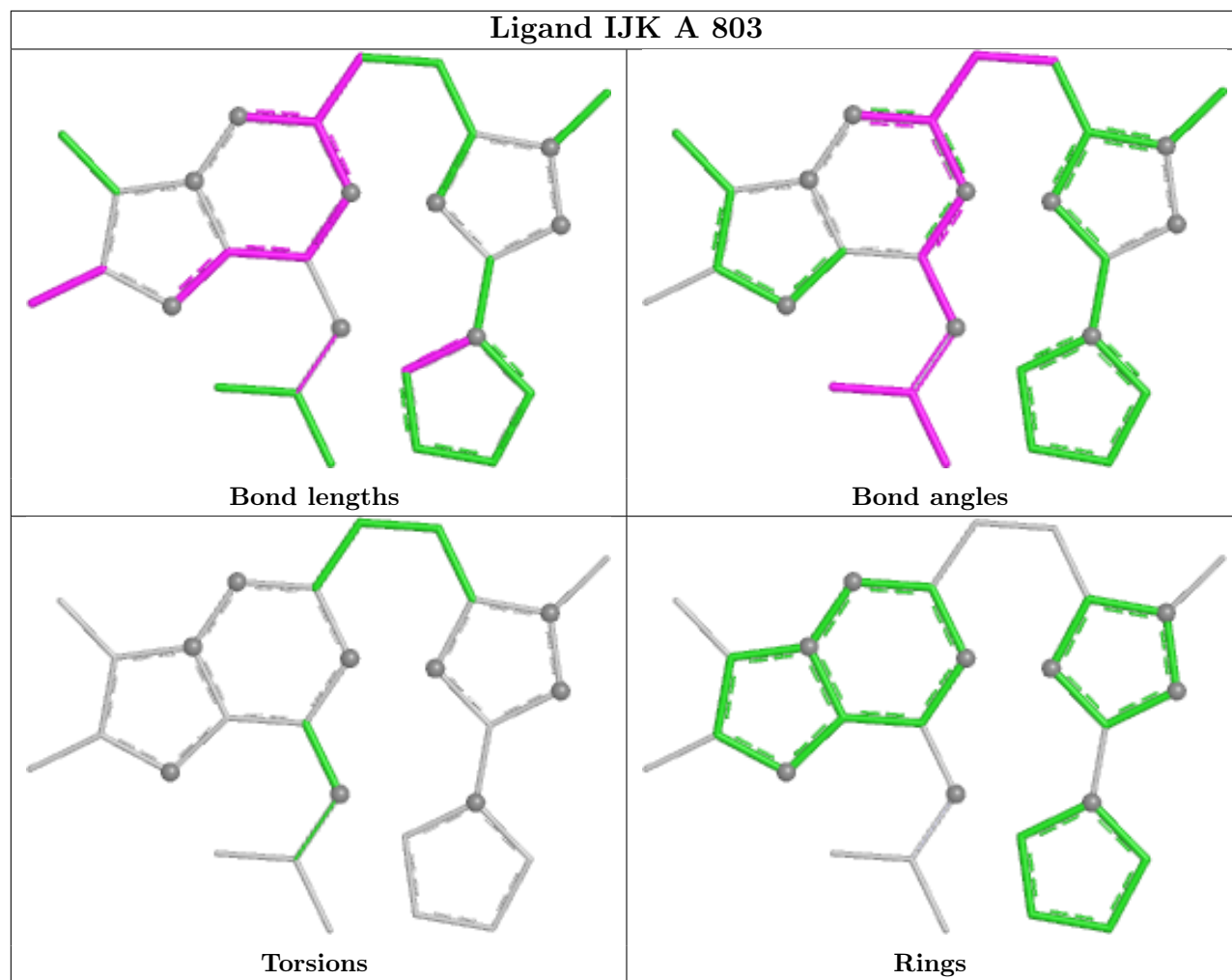
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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 IJK C 803







## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	312/343 (90%)	-0.27	2 (0%) 85 85	20, 35, 62, 92	1 (0%)
1	B	314/343 (91%)	-0.26	6 (1%) 66 65	23, 33, 59, 90	2 (0%)
1	C	312/343 (90%)	-0.31	2 (0%) 85 85	24, 36, 58, 102	0
1	D	310/343 (90%)	0.00	3 (0%) 79 79	28, 43, 67, 80	0
All	All	1248/1372 (90%)	-0.21	13 (1%) 79 79	20, 38, 63, 102	3 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	459	LEU	5.7
1	C	459	LEU	4.4
1	B	771	THR	4.2
1	D	768	GLY	4.2
1	D	459	LEU	4.1
1	B	457	GLN	3.6
1	A	458	GLY	3.5
1	B	458	GLY	3.3
1	C	458	GLY	3.2
1	D	458	GLY	3.0
1	A	459	LEU	2.9
1	B	460	MET	2.2
1	B	461	GLN	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
1	CME	D	509	10/11	0.86	0.16	40,53,105,105	0
1	CME	B	509	10/11	0.90	0.14	33,44,87,88	0
1	CME	C	509	10/11	0.91	0.12	36,43,81,82	0
1	CME	A	509	10/11	0.91	0.12	35,46,79,79	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

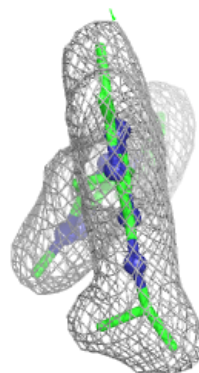
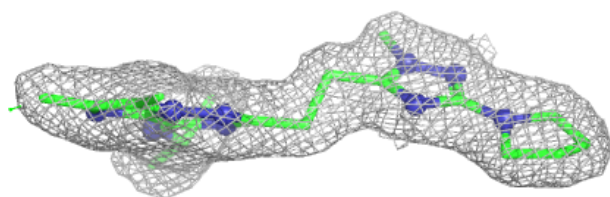
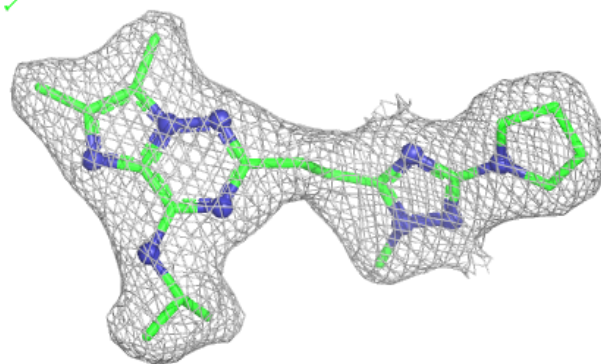
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	IJK	D	803	28/28	0.96	0.07	31,38,42,43	0
4	IJK	B	803	28/28	0.97	0.05	25,29,32,35	0
4	IJK	C	803	28/28	0.97	0.06	24,32,42,45	0
4	IJK	A	803	28/28	0.97	0.06	23,30,34,38	0
3	MG	B	802	1/1	0.99	0.02	24,24,24,24	0
3	MG	C	802	1/1	0.99	0.01	25,25,25,25	0
3	MG	A	802	1/1	0.99	0.03	26,26,26,26	0
3	MG	D	802	1/1	1.00	0.03	37,37,37,37	0
2	ZN	D	801	1/1	1.00	0.02	37,37,37,37	0
2	ZN	A	801	1/1	1.00	0.01	31,31,31,31	0
2	ZN	B	801	1/1	1.00	0.02	30,30,30,30	0
2	ZN	C	801	1/1	1.00	0.02	30,30,30,30	0

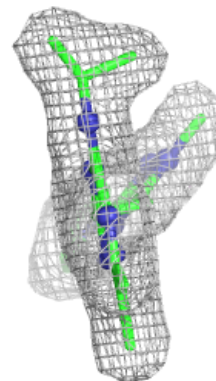
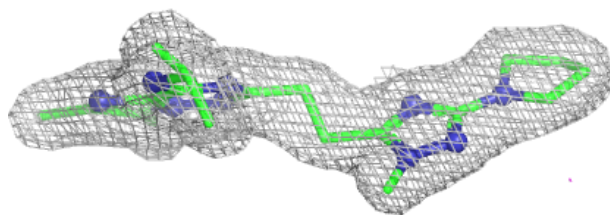
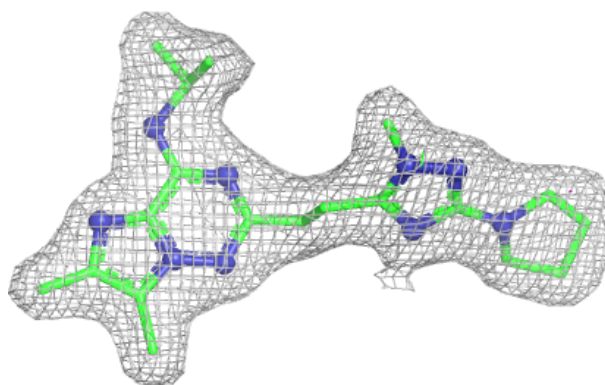
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around IJK D 803:**

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

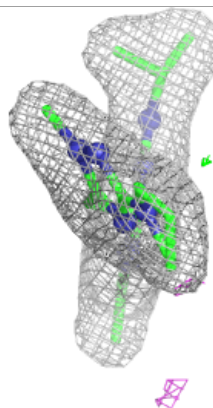
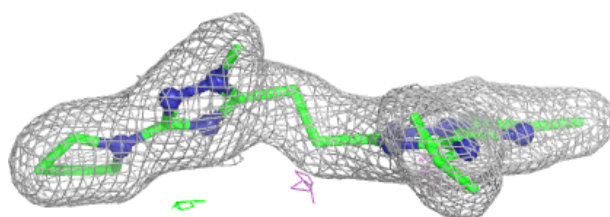
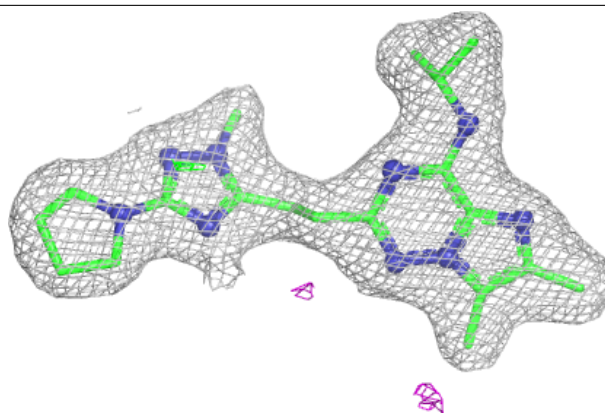
**Electron density around IJK B 803:**

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

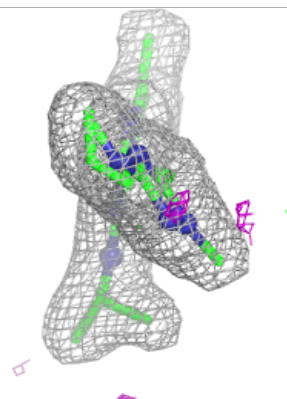
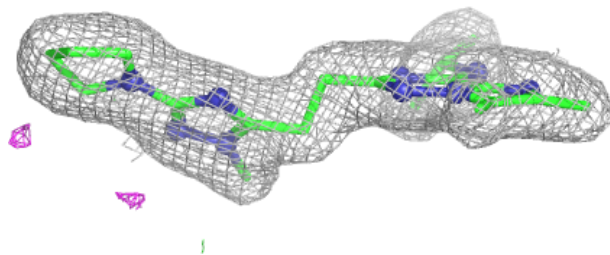
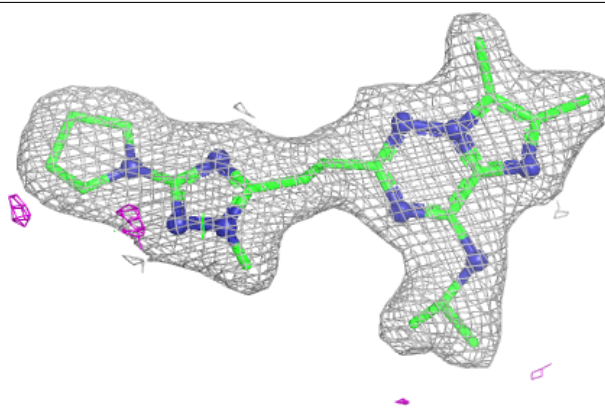


**Electron density around IJK C 803:**

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

**Electron density around IJK A 803:**

$2mF_o-DF_c$  (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.