



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 12:31 AM EDT

PDB ID : 5SFS  
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN COMPLEX WITH n2c(C)c1nc(nn1c(c2)C)CCc3nc(nn3C)N4CC[C@@H](C4)C, micromolar IC<sub>50</sub>=0.012855  
Authors : Joseph, C.; Flohr, A.; Benz, J.; Schlatter, D.; Rudolph, M.G.  
Deposited on : 2022-01-21  
Resolution : 2.24 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

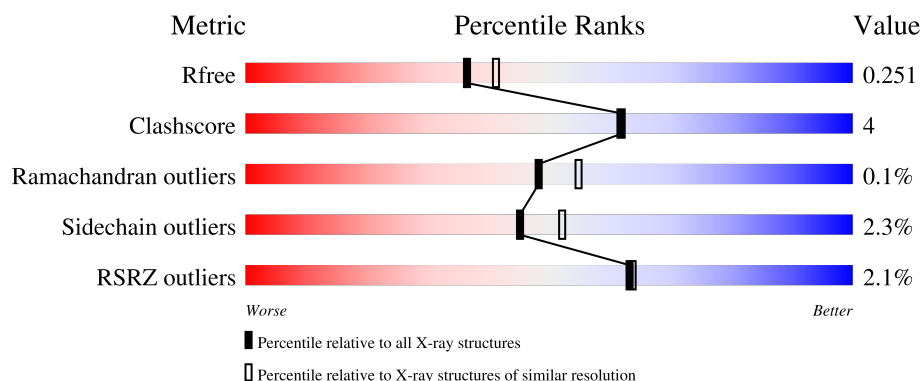
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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	3139 (2.26-2.22)
Clashscore	180529	3381 (2.26-2.22)
Ramachandran outliers	177936	3334 (2.26-2.22)
Sidechain outliers	177891	3335 (2.26-2.22)
RSRZ outliers	164620	3138 (2.26-2.22)

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>0%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	343	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>8%</div> </div> </div>
1	C	343	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	343	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10606 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	312	Total	C	N	O	S	0	0	0
			2537	1622	431	460	24			
1	B	317	Total	C	N	O	S	0	1	0
			2566	1639	436	467	24			
1	C	314	Total	C	N	O	S	0	0	0
			2546	1627	433	462	24			
1	D	313	Total	C	N	O	S	0	0	0
			2533	1620	432	457	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

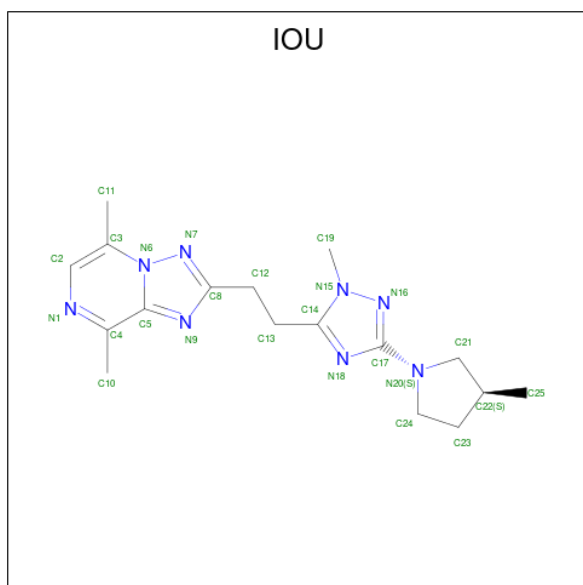
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 (4S)-5,8-dimethyl-2-(2-{1-methyl-3-[(3S)-3-methylpyrrolidin-1-yl]-1H-1,2,4-triazol-5-yl}ethyl)[1,2,4]triazolo[1,5-a]pyrazine (three-letter code: IOU) (formula: C<sub>17</sub>H<sub>24</sub>N<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			25	17	8		
4	B	1	Total	C	N	0	0
			25	17	8		
4	C	1	Total	C	N	0	0
			25	17	8		
4	D	1	Total	C	N	0	0
			25	17	8		

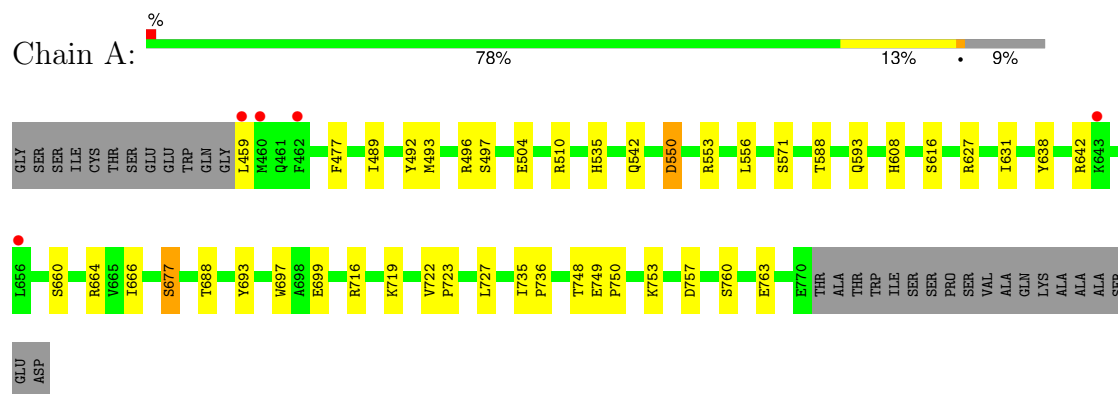
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total 79	O 79	0	0
5	B	99	Total 99	O 99	0	0
5	C	90	Total 90	O 90	0	0
5	D	48	Total 48	O 48	0	0

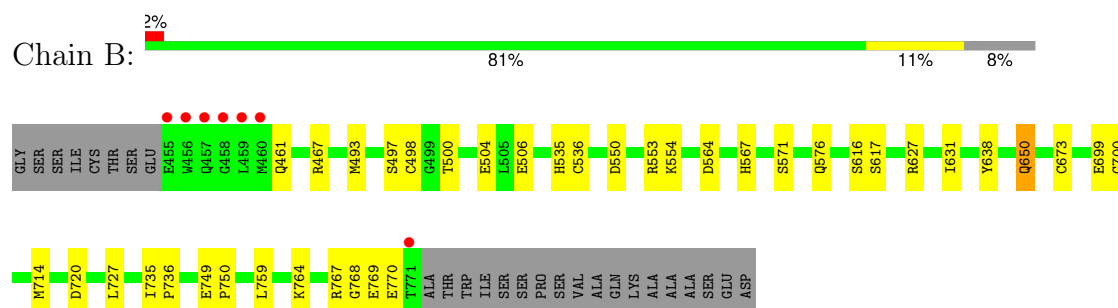
### 3 Residue-property plots [i](#)

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

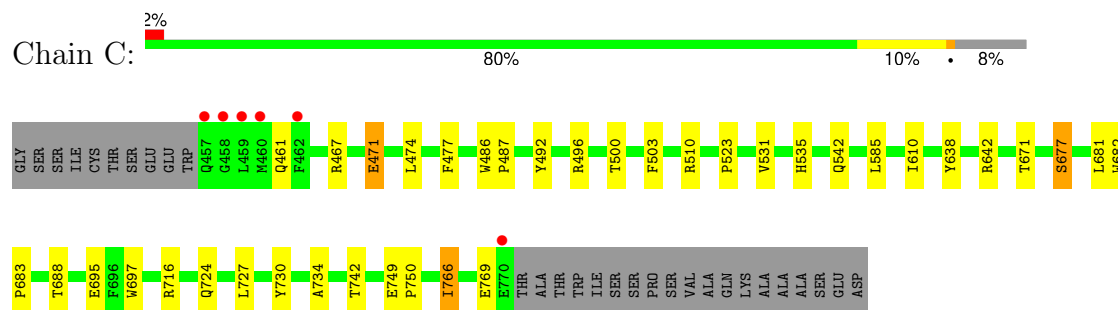
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



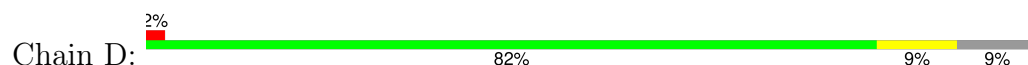
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

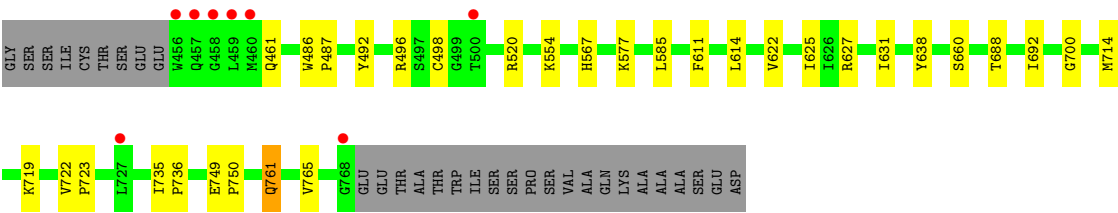


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- 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, $\alpha$ , $\beta$ , $\gamma$	135.57Å 135.57Å 235.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.61 – 2.24 43.61 – 2.24	Depositor EDS
% Data completeness (in resolution range)	95.0 (43.61-2.24) 95.0 (43.61-2.24)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.188 , 0.252 0.193 , 0.251	Depositor DCC
$R_{free}$ test set	3866 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: ZN, IOU, MG, CME

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	0.70	0/2588	0.81	0/3502
1	B	0.69	0/2620	0.82	0/3546
1	C	0.69	0/2597	0.83	1/3514 (0.0%)
1	D	0.71	0/2584	0.80	0/3497
All	All	0.70	0/10389	0.82	1/14059 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	510	ARG	NE-CZ-NH1	5.29	122.94	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	2537	0	2508	25	0
1	B	2566	0	2523	21	0
1	C	2546	0	2513	20	0
1	D	2533	0	2503	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	25	0	0	1	0
4	B	25	0	0	0	0
4	C	25	0	0	0	0
4	D	25	0	0	0	0
5	A	79	0	0	2	0
5	B	99	0	0	1	0
5	C	90	0	0	1	0
5	D	48	0	0	0	0
All	All	10606	0	10047	81	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 4.

All (81) 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	1.84	0.77
1:A:677:SER:HB3	5:A:951:HOH:O	1.85	0.75
1:D:761:GLN:HE21	1:D:761:GLN:HA	1.55	0.71
1:C:523:PRO:HD2	1:C:695:GLU:HG3	1.77	0.67
1:D:627:ARG:O	1:D:631:ILE:HG12	1.98	0.63
1:A:719:LYS:O	1:A:722:VAL:HG23	1.99	0.63
1:A:627:ARG:O	1:A:631:ILE:HG12	2.00	0.61
1:B:576:GLN:HG2	5:B:976:HOH:O	2.01	0.60
1:A:749:GLU:N	1:A:750:PRO:CD	2.65	0.59
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.88	0.55
1:B:749:GLU:N	1:B:750:PRO:CD	2.69	0.55
1:C:492:TYR:CZ	1:C:496:ARG:HD2	2.40	0.55
1:D:735:ILE:HB	1:D:736:PRO:HD3	1.88	0.54
1:A:493:MET:SD	1:A:535:HIS:HA	2.48	0.54
1:B:727:LEU:HD12	1:B:759:LEU:HD11	1.90	0.54
1:B:650:GLN:HE21	1:B:650:GLN:HA	1.71	0.54
1:B:727:LEU:HD12	1:B:759:LEU:CD1	2.38	0.53
1:B:700:GLY:HA3	1:B:714:MET:O	2.09	0.52
1:A:497:SER:O	1:A:553:ARG:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:TRP:HB3	1:C:531:VAL:HG21	1.91	0.52
1:C:724:GLN:HA	1:C:766:ILE:HD11	1.92	0.51
1:C:471:GLU:HA	1:C:474:LEU:HD12	1.92	0.51
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.47	0.50
1:A:497:SER:HA	1:A:542:GLN:NE2	2.27	0.50
1:B:571:SER:OG	1:B:699:GLU:OE2	2.30	0.49
1:C:638:TYR:CD1	1:C:671:THR:HG21	2.46	0.49
1:B:767:ARG:O	1:B:769:GLU:N	2.46	0.48
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.94	0.48
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.48	0.48
1:D:486:TRP:N	1:D:487:PRO:CD	2.78	0.47
1:B:550:ASP:N	1:B:550:ASP:OD1	2.48	0.47
1:B:650:GLN:HE21	1:B:650:GLN:CA	2.28	0.47
1:B:627:ARG:O	1:B:631:ILE:HG12	2.15	0.47
1:A:727:LEU:HD21	1:A:763:GLU:HG3	1.96	0.46
1:C:749:GLU:HB3	1:C:750:PRO:HD3	1.97	0.46
1:B:504:GLU:OE1	1:B:506:GLU:HB2	2.14	0.46
1:C:727:LEU:HD13	1:C:766:ILE:CD1	2.45	0.46
1:C:730:TYR:HA	1:C:734:ALA:HB3	1.98	0.46
1:D:700:GLY:HA3	1:D:714:MET:O	2.16	0.45
1:A:693:TYR:OH	4:A:803:IOU:N18	2.49	0.45
1:B:650:GLN:HA	1:B:650:GLN:NE2	2.31	0.45
1:C:467:ARG:O	1:C:471:GLU:HB2	2.16	0.45
1:B:764:LYS:HB3	1:B:770:GLU:HB3	1.99	0.45
1:D:498:CYS:SG	1:D:554:LYS:HG3	2.57	0.45
1:C:503:PHE:CE1	1:C:610:ILE:HD12	2.52	0.44
1:A:489:ILE:O	1:A:493:MET:HG3	2.17	0.44
1:D:622:VAL:HA	1:D:625:ILE:HD12	2.00	0.44
1:D:719:LYS:O	1:D:722:VAL:HG23	2.18	0.44
1:D:611:PHE:HB3	1:D:614:LEU:HD12	1.99	0.44
1:A:638:TYR:OH	1:A:642:ARG:HD3	2.18	0.44
1:B:536:CYS:SG	1:B:673:CYS:HA	2.58	0.44
1:C:542:GLN:NE2	1:C:542:GLN:HA	2.33	0.43
1:A:556:LEU:HD21	1:A:666:ILE:HG23	1.99	0.43
1:B:467:ARG:HG2	1:B:467:ARG:O	2.17	0.43
1:A:510:ARG:HG2	1:A:608:HIS:CE1	2.53	0.43
1:A:571:SER:OG	1:A:699:GLU:OE2	2.21	0.43
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.54	0.43
1:C:677:SER:HB3	1:C:688:THR:HG21	1.99	0.43
1:A:748:THR:C	1:A:750:PRO:HD2	2.39	0.43
1:B:493:MET:SD	1:B:535:HIS:HA	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:TYR:OH	1:C:642:ARG:HD3	2.19	0.43
1:B:564:ASP:O	1:B:567:HIS:HB2	2.19	0.42
1:D:722:VAL:N	1:D:723:PRO:CD	2.82	0.42
1:D:749:GLU:N	1:D:750:PRO:CD	2.82	0.42
1:D:761:GLN:O	1:D:765:VAL:HG23	2.18	0.42
1:A:550:ASP:OD1	1:A:550:ASP:N	2.52	0.42
1:C:697:TRP:HB3	1:C:716:ARG:HB3	2.02	0.42
1:A:588:THR:O	1:A:593:GLN:NE2	2.45	0.42
1:B:735:ILE:HB	1:B:736:PRO:HD3	2.02	0.42
1:D:520:ARG:HD2	1:D:567:HIS:O	2.20	0.42
1:A:677:SER:HB2	1:A:688:THR:HG21	2.03	0.41
1:A:697:TRP:HB3	1:A:716:ARG:HB3	2.02	0.41
1:C:461:GLN:HE21	1:C:500:THR:HG21	1.84	0.41
1:B:498:CYS:SG	1:B:554:LYS:HG3	2.61	0.41
1:D:688:THR:O	1:D:692:ILE:HG13	2.20	0.41
1:C:477:PHE:HB3	1:C:535:HIS:CE1	2.56	0.41
1:A:660:SER:O	1:A:664:ARG:HG3	2.21	0.41
1:A:753:LYS:HG3	5:A:963:HOH:O	2.20	0.41
1:C:682:TRP:N	1:C:683:PRO:CD	2.83	0.41
1:C:742:THR:HG22	5:C:943:HOH:O	2.21	0.41
1:C:486:TRP:N	1:C:487:PRO:CD	2.84	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	309/343 (90%)	299 (97%)	10 (3%)	0	100	100
1	B	315/343 (92%)	303 (96%)	11 (4%)	1 (0%)	37	39
1	C	311/343 (91%)	297 (96%)	14 (4%)	0	100	100
1	D	310/343 (90%)	297 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1245/1372 (91%)	1196 (96%)	48 (4%)	1 (0%)	48 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	768	GLY

### 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	281/305 (92%)	274 (98%)	7 (2%)	42 49
1	B	282/305 (92%)	274 (97%)	8 (3%)	38 44
1	C	281/305 (92%)	275 (98%)	6 (2%)	48 55
1	D	279/305 (92%)	273 (98%)	6 (2%)	47 54
All	All	1123/1220 (92%)	1096 (98%)	27 (2%)	45 50

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	LEU
1	A	504	GLU
1	A	550	ASP
1	A	616	SER
1	A	677	SER
1	A	757	ASP
1	A	760	SER
1	B	461	GLN
1	B	500	THR
1	B	616	SER
1	B	617	SER
1	B	638	TYR
1	B	650	GLN
1	B	720[A]	ASP

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Mol	Chain	Res	Type
1	B	720[B]	ASP
1	C	471	GLU
1	C	585	LEU
1	C	677	SER
1	C	681	LEU
1	C	766	ILE
1	C	769	GLU
1	D	461	GLN
1	D	577	LYS
1	D	585	LEU
1	D	638	TYR
1	D	660	SER
1	D	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	542	GLN
1	A	545	HIS
1	A	604	GLN
1	A	609	ASN
1	A	644	GLN
1	A	726	GLN
1	A	743	GLN
1	B	542	GLN
1	B	604	GLN
1	B	650	GLN
1	B	724	GLN
1	B	726	GLN
1	C	461	GLN
1	C	542	GLN
1	C	604	GLN
1	C	726	GLN
1	C	743	GLN
1	D	604	GLN
1	D	726	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	0.47	0	6,9,11	0.77	0
1	CME	C	509	1	8,9,10	0.48	0	6,9,11	0.39	0
1	CME	B	509	1	8,9,10	0.31	0	6,9,11	0.69	0
1	CME	D	509	1	8,9,10	0.45	0	6,9,11	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	A	509	1	-	2/5/8/10	-
1	CME	C	509	1	-	3/5/8/10	-
1	CME	B	509	1	-	2/5/8/10	-
1	CME	D	509	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	509	CME	SD-CE-CZ-OH
1	B	509	CME	SD-CE-CZ-OH

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Mol	Chain	Res	Type	Atoms
1	C	509	CME	SD-CE-CZ-OH
1	D	509	CME	SD-CE-CZ-OH
1	C	509	CME	CE-SD-SG-CB
1	B	509	CME	CZ-CE-SD-SG
1	A	509	CME	CE-SD-SG-CB
1	C	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	IOU	C	803	-	18,28,28	1.68	6 (33%)	16,41,41	2.66	6 (37%)
4	IOU	B	803	-	18,28,28	1.73	5 (27%)	16,41,41	2.93	5 (31%)
4	IOU	A	803	-	18,28,28	1.95	6 (33%)	16,41,41	3.03	8 (50%)
4	IOU	D	803	-	18,28,28	1.24	1 (5%)	16,41,41	3.80	8 (50%)

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	IOU	C	803	-	-	0/5/18/18	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IOU	B	803	-	-	1/5/18/18	0/4/4/4
4	IOU	A	803	-	-	0/5/18/18	0/4/4/4
4	IOU	D	803	-	-	2/5/18/18	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	IOU	C4-C5	-4.47	1.37	1.44
4	B	803	IOU	C12-C8	-3.86	1.45	1.50
4	C	803	IOU	C4-C5	-3.74	1.39	1.44
4	A	803	IOU	C12-C8	-3.50	1.46	1.50
4	B	803	IOU	C2-C3	-3.48	1.33	1.39
4	D	803	IOU	C14-N18	-3.03	1.29	1.34
4	B	803	IOU	C23-C24	-3.00	1.47	1.52
4	A	803	IOU	C14-N18	-2.63	1.30	1.34
4	A	803	IOU	C23-C24	-2.62	1.47	1.52
4	B	803	IOU	C14-N18	-2.61	1.30	1.34
4	C	803	IOU	C12-C8	-2.58	1.47	1.50
4	B	803	IOU	C4-C5	-2.42	1.41	1.44
4	C	803	IOU	C10-C4	-2.41	1.48	1.50
4	A	803	IOU	C2-C3	-2.23	1.35	1.39
4	C	803	IOU	C24-N20	-2.20	1.43	1.46
4	C	803	IOU	C2-C3	-2.19	1.35	1.39
4	C	803	IOU	C14-N18	-2.12	1.30	1.34
4	A	803	IOU	C5-N9	2.03	1.35	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	803	IOU	C14-N18-C17	10.20	109.73	103.90
4	B	803	IOU	C14-N18-C17	7.65	108.28	103.90
4	C	803	IOU	C14-N18-C17	5.82	107.23	103.90
4	D	803	IOU	C21-N20-C17	-5.67	114.27	123.41
4	C	803	IOU	C21-N20-C17	-5.62	114.34	123.41
4	B	803	IOU	C22-C21-N20	-5.39	97.50	103.45
4	D	803	IOU	C13-C14-N18	-5.28	116.65	124.22
4	A	803	IOU	C13-C14-N18	-5.23	116.72	124.22
4	A	803	IOU	C21-N20-C17	-4.97	115.40	123.41
4	A	803	IOU	C14-N18-C17	4.95	106.73	103.90
4	D	803	IOU	C24-N20-C17	-4.53	115.81	123.49
4	A	803	IOU	C22-C21-N20	-4.22	98.80	103.45
4	B	803	IOU	C24-C23-C22	-3.86	95.72	104.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	803	IOU	C10-C4-C5	-3.61	116.22	121.61
4	B	803	IOU	C12-C8-N9	3.45	132.19	122.54
4	C	803	IOU	C13-C12-C8	3.32	118.11	112.48
4	A	803	IOU	C12-C8-N9	3.21	131.52	122.54
4	A	803	IOU	C11-C3-N6	3.09	121.47	118.12
4	A	803	IOU	C24-N20-C17	-2.99	118.42	123.49
4	C	803	IOU	C13-C14-N18	-2.96	119.97	124.22
4	D	803	IOU	C10-C4-N1	2.95	123.15	117.64
4	C	803	IOU	C19-N15-C14	-2.90	125.92	128.87
4	D	803	IOU	C13-C12-C8	2.80	117.23	112.48
4	A	803	IOU	C10-C4-C5	-2.74	117.52	121.61
4	B	803	IOU	C11-C3-N6	2.67	121.00	118.12
4	C	803	IOU	C10-C4-C5	-2.65	117.66	121.61
4	D	803	IOU	C12-C8-N9	2.40	129.25	122.54

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	803	IOU	C13-C12-C8-N7
4	B	803	IOU	C13-C12-C8-N7
4	D	803	IOU	C12-C13-C14-N18

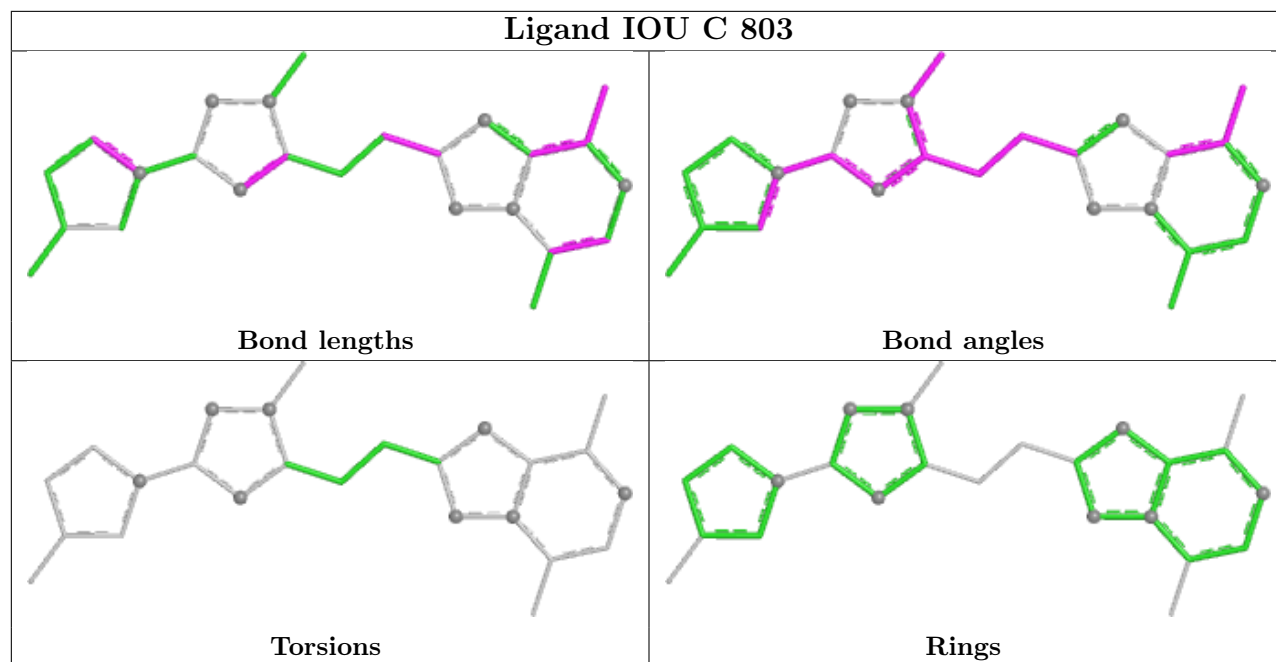
There are no ring outliers.

1 monomer is involved in 1 short contact:

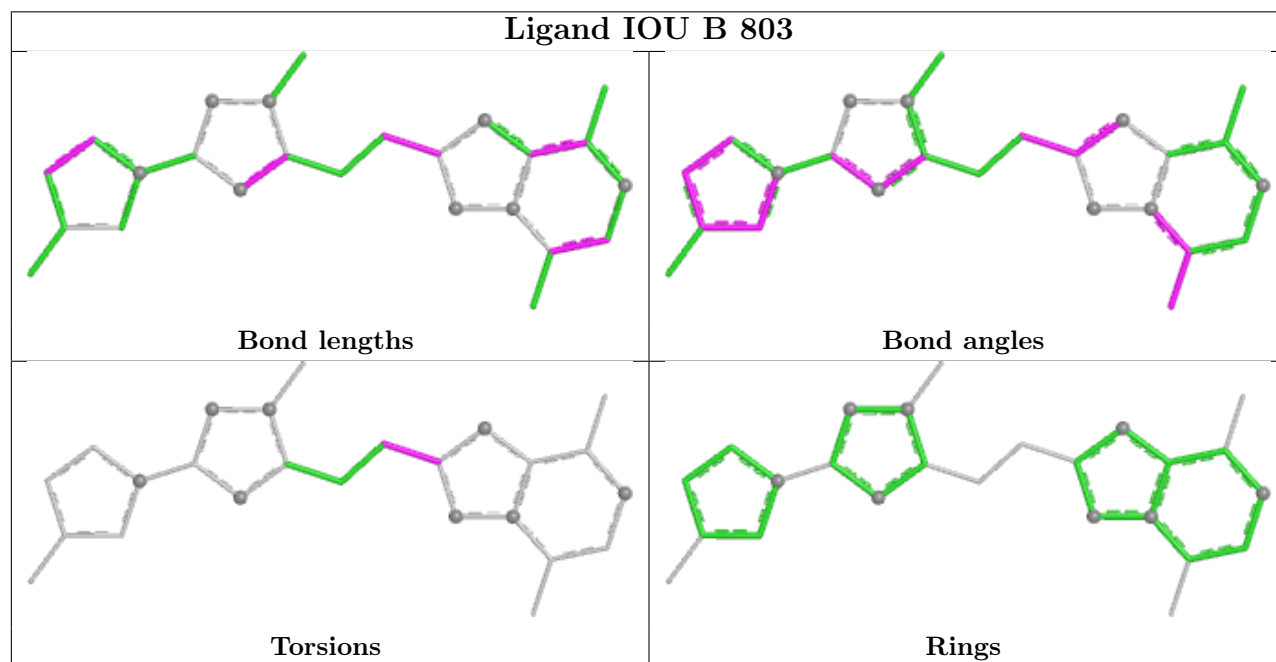
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	IOU	1	0

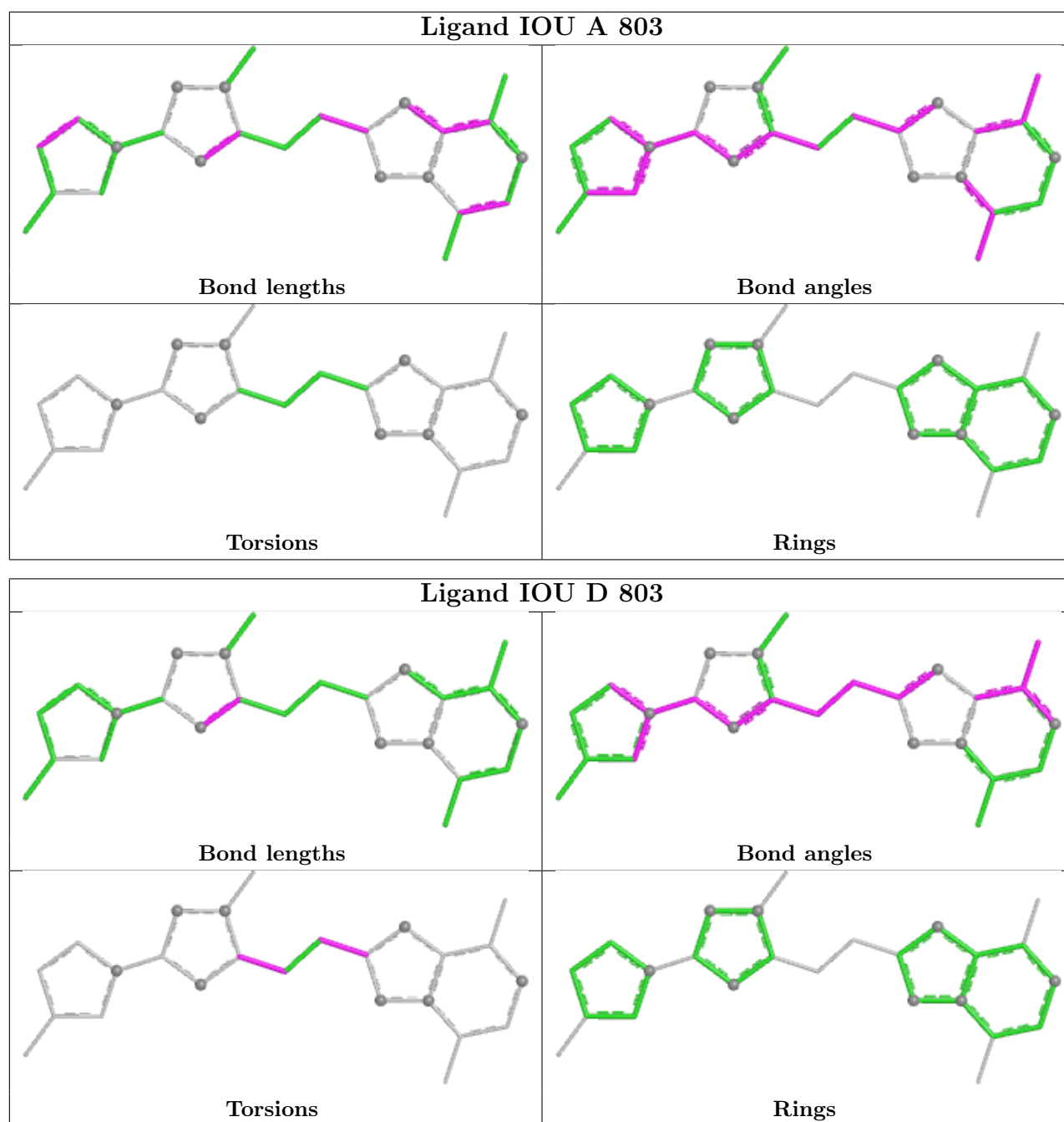
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand IOU C 803



## Ligand IOU B 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 ⓘ

### 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	311/343 (90%)	0.25	5 (1%) 70 71	35, 50, 81, 105	0
1	B	316/343 (92%)	0.20	7 (2%) 62 62	33, 48, 76, 140	1 (0%)
1	C	313/343 (91%)	0.12	6 (1%) 66 66	35, 49, 78, 119	0
1	D	312/343 (90%)	0.45	8 (2%) 57 58	42, 58, 82, 119	0
All	All	1252/1372 (91%)	0.26	26 (2%) 63 64	33, 52, 81, 140	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	456	TRP	8.2
1	A	459	LEU	6.4
1	B	456	TRP	6.2
1	B	771	THR	5.9
1	D	457	GLN	5.7
1	C	457	GLN	5.3
1	B	457	GLN	5.1
1	B	455	GLU	4.8
1	B	459	LEU	4.7
1	D	768	GLY	4.4
1	D	459	LEU	4.4
1	C	458	GLY	4.2
1	D	458	GLY	3.8
1	B	458	GLY	3.6
1	C	459	LEU	3.4
1	A	460	MET	3.0
1	D	460	MET	2.7
1	A	656	LEU	2.7
1	A	643	LYS	2.4
1	C	460	MET	2.4
1	B	460	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	727	LEU	2.2
1	C	770	GLU	2.2
1	D	500	THR	2.2
1	A	462	PHE	2.2
1	C	462	PHE	2.1

## 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(Å <sup>2</sup> )	Q<0.9
1	CME	B	509	10/11	0.77	0.19	41,62,110,116	0
1	CME	D	509	10/11	0.80	0.17	62,78,108,112	0
1	CME	A	509	10/11	0.83	0.17	55,67,110,110	0
1	CME	C	509	10/11	0.86	0.14	50,62,94,96	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(Å <sup>2</sup> )	Q<0.9
4	IOU	C	803	25/25	0.93	0.09	44,49,57,60	0
4	IOU	A	803	25/25	0.94	0.09	36,42,51,52	0
4	IOU	D	803	25/25	0.94	0.09	44,52,60,64	0
4	IOU	B	803	25/25	0.95	0.08	37,46,52,54	0
3	MG	A	802	1/1	0.99	0.03	44,44,44,44	0
3	MG	D	802	1/1	0.99	0.02	50,50,50,50	0
3	MG	C	802	1/1	1.00	0.01	37,37,37,37	0
2	ZN	B	801	1/1	1.00	0.01	41,41,41,41	0
2	ZN	C	801	1/1	1.00	0.02	44,44,44,44	0

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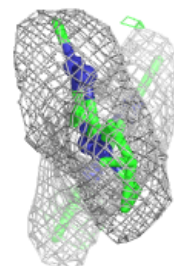
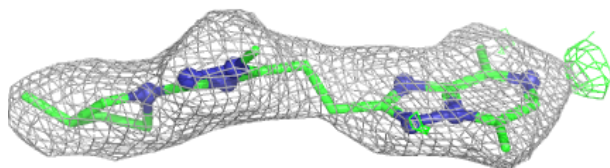
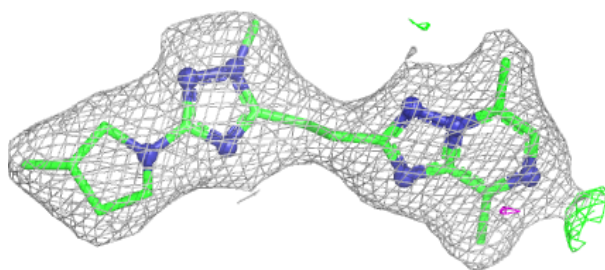
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	D	801	1/1	1.00	0.02	50,50,50,50	0
2	ZN	A	801	1/1	1.00	0.01	44,44,44,44	0
3	MG	B	802	1/1	1.00	0.02	36,36,36,36	0

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.

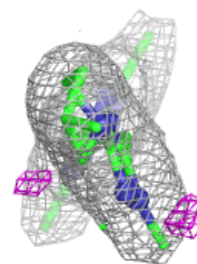
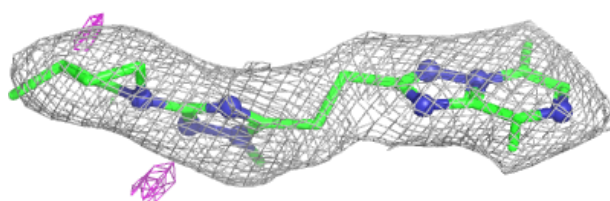
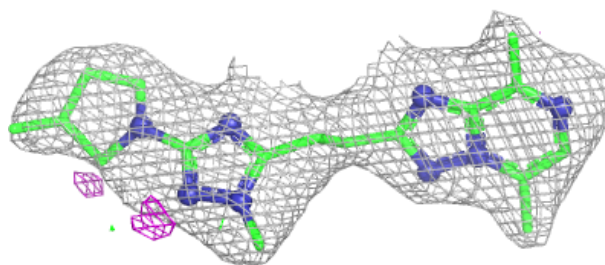
**Electron density around IOU C 803:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

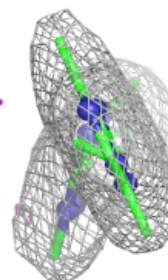
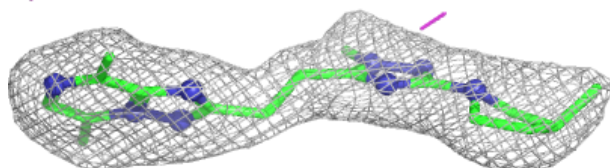
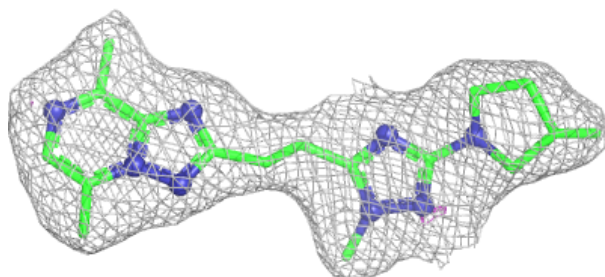


**Electron density around IOU A 803:**

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

**Electron density around IOU D 803:**

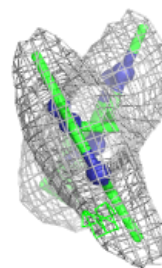
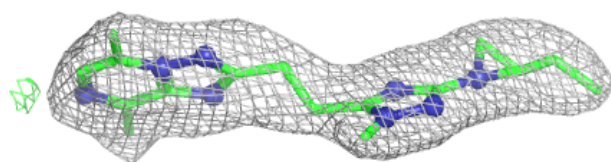
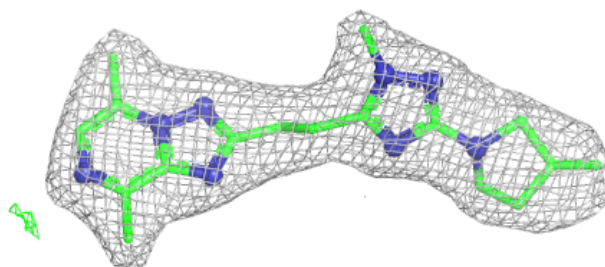
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around IOU 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.