



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2022 – 07:14 PM EDT

PDB ID : 5SIF  
Title : Crystal Structure of human phosphodiesterase 10 in complex with 3-[2-(2,5-difluorophenyl)pyrazol-3-yl]-1-(3-methylsulfonylphenyl)pyridazin-4-one  
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Deposited on : 2022-02-01  
Resolution : 2.20 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 : 2.31.2  
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) : 2.31.2

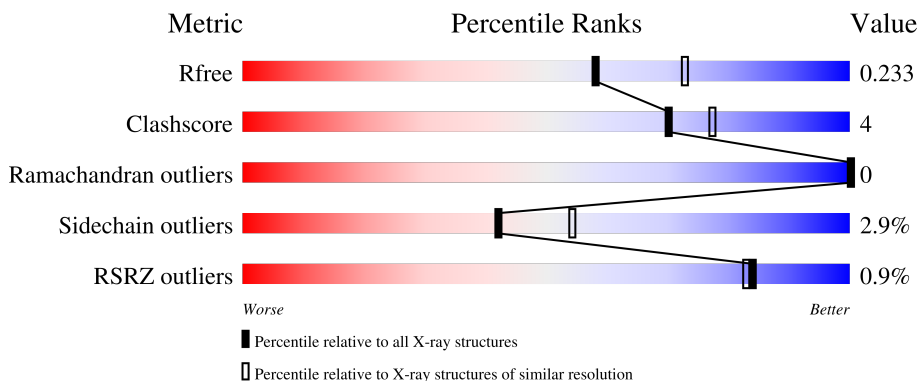
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	 82% 8% 9%
1	B	343	 81% 10% 8%
1	C	343	 83% 8% 9%
1	D	343	 80% 10% 9%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10856 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
			Total	C	N	O	S			
1	A	313	Total 2541	C 1624	N 432	O 461	S 24	0	0	0
1	B	315	Total 2559	C 1635	N 437	O 463	S 24	0	1	0
1	C	313	Total 2541	C 1624	N 432	O 461	S 24	0	0	0
1	D	311	Total 2523	C 1614	N 430	O 455	S 24	0	0	0

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 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

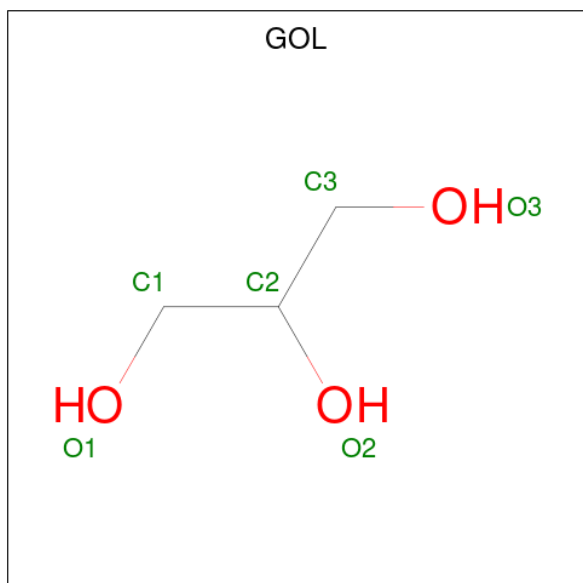
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

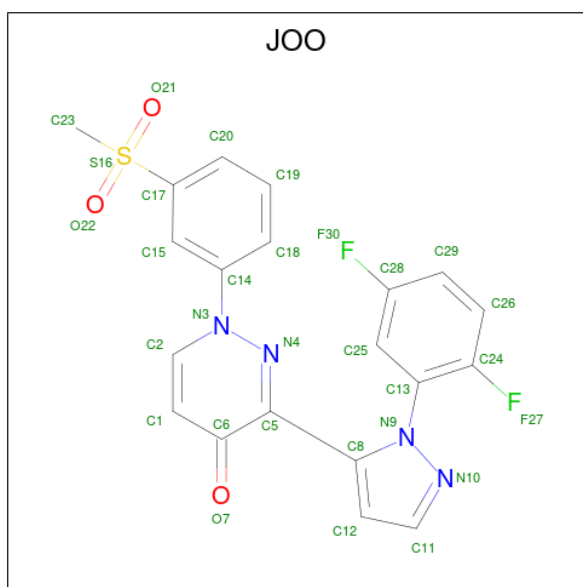
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is 3-[1-(2,5-difluorophenyl)-1H-pyrazol-5-yl]-1-[3-(methanesulfonyl)phenyl]pyridazin-4(1H)-one (three-letter code: JOO) (formula: C<sub>20</sub>H<sub>14</sub>F<sub>2</sub>N<sub>4</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
6	A	1	Total 30	C 20	F 2	N 4	O 3	S 1	0	0
6	B	1	Total 30	C 20	F 2	N 4	O 3	S 1	0	0
6	C	1	Total 30	C 20	F 2	N 4	O 3	S 1	0	0
6	D	1	Total 30	C 20	F 2	N 4	O 3	S 1	0	0

- Molecule 7 is PRASEODYMIUM ION (three-letter code: PR) (formula: Pr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	5	Total 5	Pr 5	0	0
7	C	3	Total 3	Pr 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	142	Total 142	O 142	0	0
8	B	152	Total 152	O 152	0	0
8	C	146	Total 146	O 146	0	0

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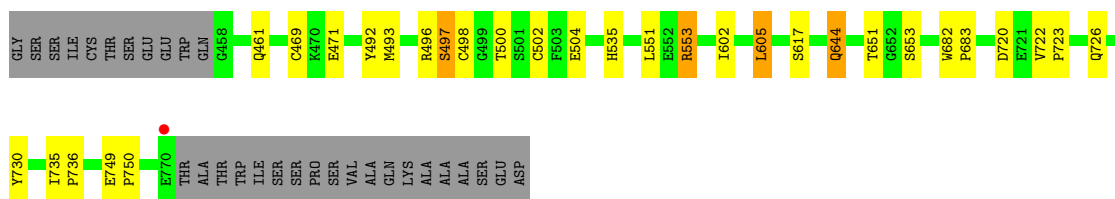
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	D	109	Total 109	O 109	0	0

### 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.

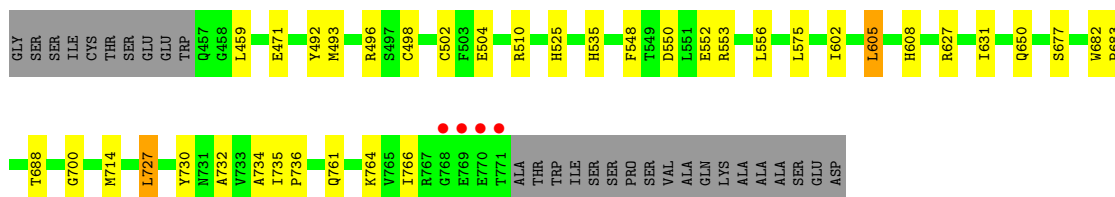
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain A: 




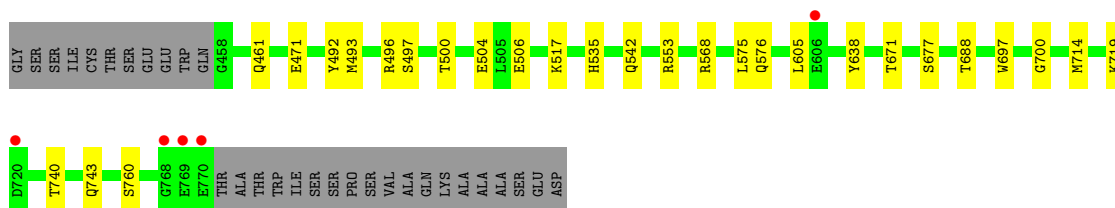
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain B: 




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

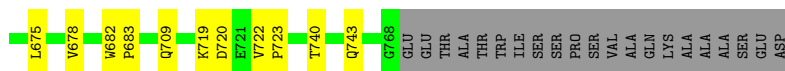
Chain C: 



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

Chain D: 







## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.13Å 135.13Å 235.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.45 – 2.20 41.47 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.3 (41.45-2.20) 88.3 (41.47-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.182 , 0.231 0.189 , 0.233	Depositor DCC
$R_{free}$ test set	3834 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10856	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: JOO, PR, CME, MG, GOL, ZN, CL

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	0.65	0/2592	0.75	0/3507
1	B	0.65	0/2613	0.75	0/3535
1	C	0.66	0/2592	0.75	0/3507
1	D	0.66	0/2574	0.73	0/3483
All	All	0.66	0/10371	0.75	0/14032

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	2541	0	2513	20	0
1	B	2559	0	2528	19	0
1	C	2541	0	2511	14	0
1	D	2523	0	2501	18	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
5	A	6	0	8	0	0
6	A	30	0	0	0	0
6	B	30	0	0	1	0
6	C	30	0	0	0	0
6	D	30	0	0	0	0
7	B	5	0	0	0	0
7	C	3	0	0	0	0
8	A	142	0	0	3	1
8	B	152	0	0	1	0
8	C	146	0	0	3	1
8	D	109	0	0	3	1
All	All	10856	0	10061	71	2

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 (71) 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:D:620:GLU:OE1	8:D:901:HOH:O	2.03	0.75
1:A:469:CYS:SG	8:A:1027:HOH:O	2.47	0.71
1:C:493:MET:O	1:C:497:SER:HB2	1.89	0.71
1:A:493:MET:O	1:A:497:SER:HB2	1.94	0.67
1:A:498:CYS:HG	1:A:502:CYS:HG	1.43	0.64
1:D:469:CYS:SG	8:D:1008:HOH:O	2.55	0.64
1:B:727:LEU:HD12	1:B:766:ILE:CD1	2.30	0.62
1:C:553:ARG:NH1	8:C:902:HOH:O	2.33	0.61
1:D:644:GLN:HE21	1:D:644:GLN:HA	1.65	0.60
1:D:719:LYS:O	1:D:722:VAL:HG23	2.02	0.60
1:D:493:MET:O	1:D:497:SER:HB2	2.02	0.59
1:C:492:TYR:CZ	1:C:496:ARG:HD2	2.37	0.59
1:A:461:GLN:HE22	1:A:500:THR:HG21	1.68	0.57
1:C:740:THR:HA	1:C:743:GLN:HE21	1.69	0.57
1:C:461:GLN:NE2	1:C:500:THR:HG21	2.19	0.56
1:B:548:PHE:O	1:B:553:ARG:NH2	2.39	0.54
1:D:740:THR:HA	1:D:743:GLN:HE21	1.72	0.54
1:A:602:ILE:HA	1:A:605:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:ARG:NH1	8:C:906:HOH:O	2.41	0.53
1:C:638:TYR:CD1	1:C:671:THR:HG21	2.46	0.51
1:B:510:ARG:HG2	1:B:608:HIS:CE1	2.47	0.49
1:D:602:ILE:O	1:D:605:LEU:HB2	2.12	0.49
1:D:675:LEU:O	1:D:678:VAL:HG22	2.13	0.49
1:B:677:SER:HB2	1:B:688:THR:HG21	1.94	0.49
1:B:727:LEU:HD12	1:B:766:ILE:HD12	1.95	0.48
1:A:469:CYS:SG	8:A:1022:HOH:O	2.61	0.47
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.95	0.47
1:B:735:ILE:HB	1:B:736:PRO:HD3	1.96	0.47
1:A:461:GLN:NE2	1:A:461:GLN:HA	2.29	0.47
1:B:682:TRP:HB3	1:B:683:PRO:HD3	1.96	0.47
1:D:720:ASP:OD1	1:D:720:ASP:N	2.47	0.47
1:A:749:GLU:N	1:A:750:PRO:CD	2.78	0.46
1:B:730:TYR:HA	1:B:734:ALA:HB3	1.97	0.46
1:D:575:LEU:HD11	1:D:591:MET:SD	2.56	0.46
1:A:461:GLN:NE2	1:A:500:THR:HG21	2.30	0.45
1:B:700:GLY:HA3	1:B:714:MET:O	2.17	0.45
1:C:697:TRP:CZ2	1:C:719:LYS:HG3	2.52	0.45
1:B:498:CYS:O	1:B:502:CYS:SG	2.75	0.44
1:B:550:ASP:OD1	1:B:553:ARG:NH1	2.51	0.44
1:C:677:SER:HB2	1:C:688:THR:HG21	1.99	0.44
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.88	0.44
1:C:542:GLN:NE2	1:C:542:GLN:HA	2.33	0.44
1:C:506:GLU:OE2	8:C:901:HOH:O	2.20	0.44
1:D:462:PHE:CE1	1:D:491:VAL:HG11	2.53	0.44
1:D:550:ASP:OD1	1:D:553:ARG:NH2	2.46	0.44
1:A:461:GLN:HE22	1:A:500:THR:CG2	2.30	0.43
1:A:553:ARG:NH1	8:A:904:HOH:O	2.35	0.43
1:C:493:MET:SD	1:C:535:HIS:HA	2.59	0.43
1:D:722:VAL:HB	1:D:723:PRO:HD3	1.99	0.43
1:C:740:THR:HA	1:C:743:GLN:NE2	2.33	0.42
1:B:602:ILE:O	1:B:605:LEU:HB2	2.19	0.42
1:D:682:TRP:N	1:D:683:PRO:CD	2.82	0.42
1:A:735:ILE:HB	1:A:736:PRO:HD3	2.02	0.42
1:A:493:MET:SD	1:A:535:HIS:HA	2.60	0.42
1:A:726:GLN:O	1:A:730:TYR:HD1	2.02	0.42
1:B:493:MET:SD	1:B:535:HIS:HA	2.60	0.42
1:A:651:THR:OG1	1:A:653:SER:OG	2.34	0.42
1:B:492:TYR:CZ	1:B:496:ARG:HD2	2.55	0.41
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:TRP:N	1:A:683:PRO:CD	2.84	0.41
1:B:761:GLN:HE22	1:B:764:LYS:HE3	1.85	0.41
1:D:538:TYR:O	1:D:542:GLN:HG2	2.21	0.41
1:D:682:TRP:HB3	1:D:683:PRO:HD3	2.03	0.41
1:B:525:HIS:HE1	6:B:808:JOO:F30	1.94	0.41
1:D:565:LEU:O	1:D:595:HIS:ND1	2.48	0.41
1:D:598:GLN:NE2	8:D:905:HOH:O	2.41	0.41
1:B:732:ALA:HB2	8:B:923:HOH:O	2.21	0.40
1:C:700:GLY:HA3	1:C:714:MET:O	2.22	0.40
1:B:552:GLU:O	1:B:556:LEU:HG	2.21	0.40
1:B:627:ARG:O	1:B:631:ILE:HG12	2.21	0.40
1:A:644:GLN:HE21	1:A:644:GLN:HA	1.86	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:1046:HOH:O	8:C:1046:HOH:O[2_655]	1.90	0.30
8:A:975:HOH:O	8:D:928:HOH:O[7_554]	2.17	0.03

## 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	310/343 (90%)	298 (96%)	12 (4%)	0	100	100
1	B	313/343 (91%)	305 (97%)	8 (3%)	0	100	100
1	C	310/343 (90%)	301 (97%)	9 (3%)	0	100	100
1	D	308/343 (90%)	296 (96%)	12 (4%)	0	100	100
All	All	1241/1372 (90%)	1200 (97%)	41 (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	281/305 (92%)	273 (97%)	8 (3%)	43	56
1	B	282/305 (92%)	275 (98%)	7 (2%)	47	60
1	C	281/305 (92%)	274 (98%)	7 (2%)	47	60
1	D	279/305 (92%)	269 (96%)	10 (4%)	35	45
All	All	1123/1220 (92%)	1091 (97%)	32 (3%)	42	56

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	GLU
1	A	497	SER
1	A	504	GLU
1	A	553	ARG
1	A	605	LEU
1	A	617	SER
1	A	644	GLN
1	A	720	ASP
1	B	459	LEU
1	B	471	GLU
1	B	504	GLU
1	B	575	LEU
1	B	605	LEU
1	B	650	GLN
1	B	727	LEU
1	C	471	GLU
1	C	504	GLU
1	C	517	LYS
1	C	575	LEU
1	C	576	GLN
1	C	605	LEU
1	C	760	SER
1	D	459	LEU
1	D	498	CYS

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Mol	Chain	Res	Type
1	D	504	GLU
1	D	557	LEU
1	D	573	SER
1	D	588	THR
1	D	605	LEU
1	D	621	GLN
1	D	644	GLN
1	D	709	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	495	HIS
1	A	542	GLN
1	A	604	GLN
1	A	644	GLN
1	A	724	GLN
1	A	743	GLN
1	B	484	ASN
1	B	576	GLN
1	B	604	GLN
1	B	731	ASN
1	B	743	GLN
1	B	761	GLN
1	C	461	GLN
1	C	542	GLN
1	C	576	GLN
1	C	604	GLN
1	C	743	GLN
1	D	461	GLN
1	D	542	GLN
1	D	604	GLN
1	D	644	GLN
1	D	650	GLN
1	D	709	GLN
1	D	743	GLN
1	D	761	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](#)

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	D	509	1	8,9,10	0.44	0	5,9,11	0.90	0
1	CME	A	509	1	8,9,10	0.59	0	5,9,11	0.55	0
1	CME	C	509	1	8,9,10	0.41	0	5,9,11	0.43	0
1	CME	B	509	1	8,9,10	0.30	0	5,9,11	0.44	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	D	509	1	-	2/5/8/10	-
1	CME	A	509	1	-	2/5/8/10	-
1	CME	C	509	1	-	2/5/8/10	-
1	CME	B	509	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) 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	CE-SD-SG-CB
1	D	509	CME	CE-SD-SG-CB
1	A	509	CME	CZ-CE-SD-SG
1	C	509	CME	CZ-CE-SD-SG
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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 17 are monoatomic - leaving 5 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
6	JOO	A	805	-	30,33,33	1.56	5 (16%)	37,49,49	2.42	13 (35%)
5	GOL	A	804	-	5,5,5	0.13	0	5,5,5	0.39	0
6	JOO	D	803	-	30,33,33	1.35	3 (10%)	37,49,49	2.47	10 (27%)
6	JOO	B	808	-	30,33,33	1.27	4 (13%)	37,49,49	2.37	10 (27%)
6	JOO	C	806	-	30,33,33	1.30	2 (6%)	37,49,49	2.80	17 (45%)

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
6	JOO	A	805	-	-	3/14/18/18	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	804	-	-	3/4/4/4	-
6	JOO	D	803	-	-	3/14/18/18	0/4/4/4
6	JOO	B	808	-	-	4/14/18/18	0/4/4/4
6	JOO	C	806	-	-	3/14/18/18	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	805	JOO	N3-N4	-5.49	1.28	1.38
6	D	803	JOO	N3-N4	-4.70	1.29	1.38
6	C	806	JOO	N3-N4	-4.66	1.29	1.38
6	B	808	JOO	N3-N4	-4.60	1.29	1.38
6	A	805	JOO	C8-C5	-3.13	1.46	1.49
6	A	805	JOO	C17-S16	2.78	1.80	1.77
6	D	803	JOO	C8-C5	-2.65	1.46	1.49
6	B	808	JOO	C8-C5	-2.56	1.46	1.49
6	C	806	JOO	C23-S16	2.29	1.84	1.75
6	A	805	JOO	C23-S16	2.28	1.84	1.75
6	D	803	JOO	C23-S16	2.13	1.83	1.75
6	B	808	JOO	C23-S16	2.11	1.83	1.75
6	B	808	JOO	C17-S16	2.10	1.79	1.77
6	A	805	JOO	C12-C8	-2.10	1.36	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	806	JOO	C11-N10-N9	7.76	109.34	103.70
6	A	805	JOO	C11-N10-N9	6.96	108.76	103.70
6	D	803	JOO	C11-N10-N9	6.79	108.64	103.70
6	B	808	JOO	C24-C13-N9	6.47	123.81	117.86
6	B	808	JOO	O21-S16-C17	-6.32	103.09	108.25
6	D	803	JOO	C24-C13-N9	6.25	123.62	117.86
6	A	805	JOO	F27-C24-C13	-6.24	116.22	121.04
6	B	808	JOO	C11-N10-N9	6.16	108.18	103.70
6	C	806	JOO	F27-C24-C13	-5.78	116.57	121.04
6	D	803	JOO	O22-S16-C17	-5.74	103.56	108.25
6	A	805	JOO	C2-C1-C6	-5.68	117.34	121.31
6	C	806	JOO	O21-S16-C17	-5.43	103.82	108.25
6	C	806	JOO	O21-S16-C23	5.02	115.72	108.49
6	C	806	JOO	C26-C24-C13	4.97	124.25	120.19
6	D	803	JOO	C26-C24-C13	4.80	124.11	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	803	JOO	C2-C1-C6	-4.58	118.11	121.31
6	A	805	JOO	C1-C2-N3	4.44	122.36	117.70
6	C	806	JOO	C5-N4-N3	3.85	123.91	118.76
6	B	808	JOO	C2-C1-C6	-3.76	118.69	121.31
6	A	805	JOO	C23-S16-C17	-3.74	100.17	104.58
6	C	806	JOO	C23-S16-C17	-3.63	100.29	104.58
6	C	806	JOO	C2-C1-C6	-3.61	118.79	121.31
6	B	808	JOO	C15-C17-S16	3.38	121.75	119.06
6	D	803	JOO	C14-N3-C2	3.30	123.42	118.50
6	B	808	JOO	C5-N4-N3	3.23	123.08	118.76
6	C	806	JOO	C1-C2-N3	3.04	120.89	117.70
6	B	808	JOO	O21-S16-C23	3.03	112.85	108.49
6	D	803	JOO	O21-S16-C23	2.95	112.74	108.49
6	D	803	JOO	C5-N4-N3	2.81	122.52	118.76
6	C	806	JOO	C14-N3-C2	2.70	122.52	118.50
6	C	806	JOO	C25-C13-C24	-2.67	116.85	119.65
6	C	806	JOO	O7-C6-C5	2.60	123.56	121.13
6	A	805	JOO	C1-C6-C5	-2.52	115.59	117.84
6	C	806	JOO	C24-C13-N9	2.52	120.18	117.86
6	A	805	JOO	O21-S16-C23	2.52	112.11	108.49
6	A	805	JOO	O22-S16-C23	2.44	112.00	108.49
6	C	806	JOO	C29-C28-C25	-2.41	120.16	123.29
6	A	805	JOO	C20-C17-S16	2.39	121.80	119.58
6	A	805	JOO	C26-C24-C13	2.34	122.10	120.19
6	A	805	JOO	C14-C15-C17	2.23	120.70	118.97
6	B	808	JOO	C1-C2-N3	2.23	120.04	117.70
6	B	808	JOO	C19-C20-C17	2.22	121.26	118.95
6	D	803	JOO	C1-C2-N3	2.14	119.94	117.70
6	A	805	JOO	C14-N3-N4	2.14	116.37	113.80
6	C	806	JOO	C1-C6-C5	-2.13	115.94	117.84
6	A	805	JOO	C19-C20-C17	2.10	121.14	118.95
6	C	806	JOO	C26-C29-C28	2.09	120.52	118.36
6	B	808	JOO	C14-N3-N4	2.08	116.30	113.80
6	C	806	JOO	C13-C25-C28	2.06	120.48	117.47
6	D	803	JOO	C29-C26-C24	-2.04	116.58	119.05

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	804	GOL	C1-C2-C3-O3
6	B	808	JOO	C25-C13-N9-N10

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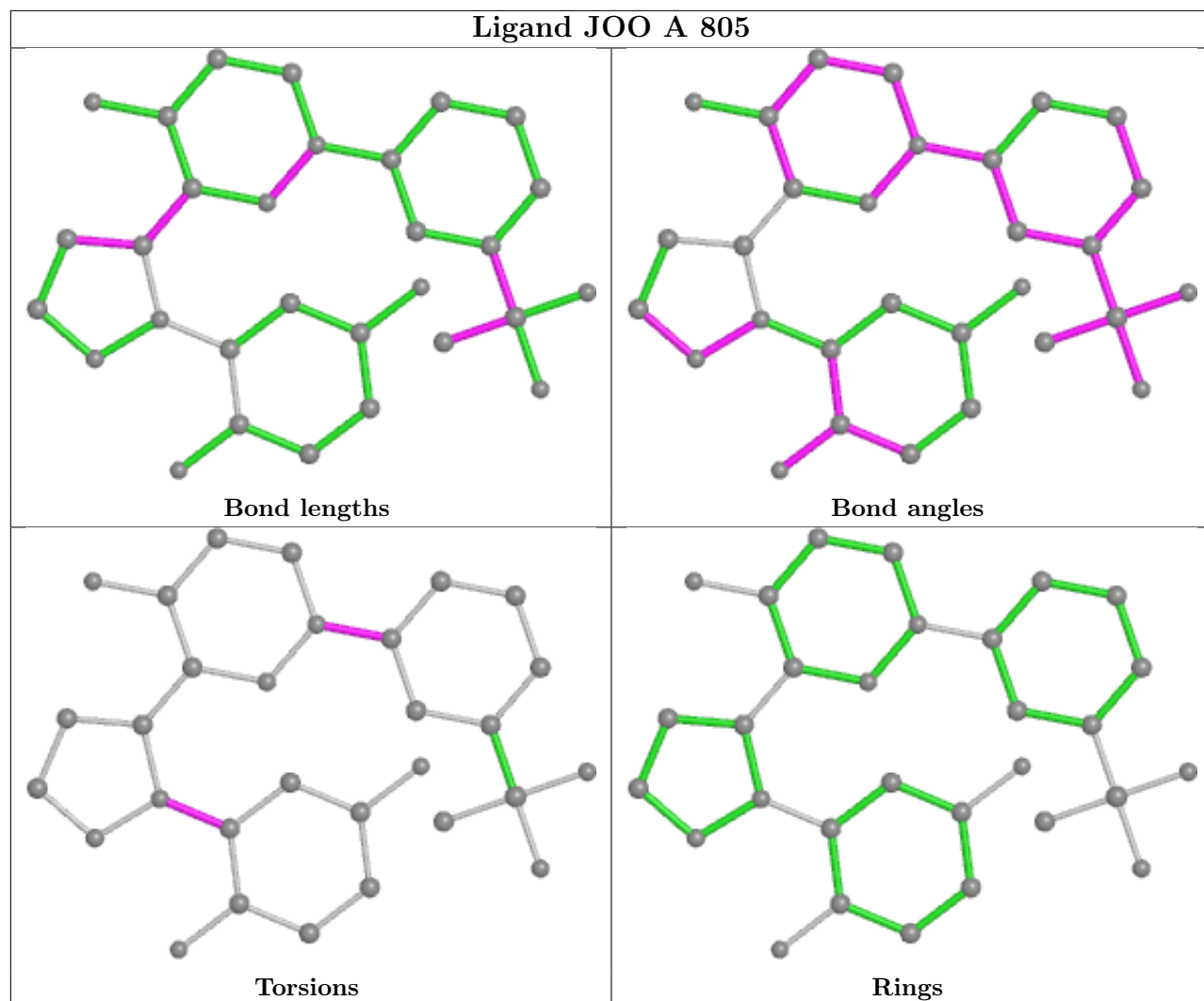
Mol	Chain	Res	Type	Atoms
5	A	804	GOL	O1-C1-C2-C3
5	A	804	GOL	O2-C2-C3-O3
6	A	805	JOO	C15-C14-N3-N4
6	A	805	JOO	C18-C14-N3-N4
6	B	808	JOO	C15-C14-N3-N4
6	D	803	JOO	C15-C14-N3-N4
6	A	805	JOO	C25-C13-N9-N10
6	B	808	JOO	C18-C14-N3-C2
6	C	806	JOO	C15-C14-N3-N4
6	D	803	JOO	C18-C14-N3-N4
6	D	803	JOO	C25-C13-N9-N10
6	C	806	JOO	C18-C14-N3-C2
6	B	808	JOO	C18-C14-N3-N4
6	C	806	JOO	C18-C14-N3-N4

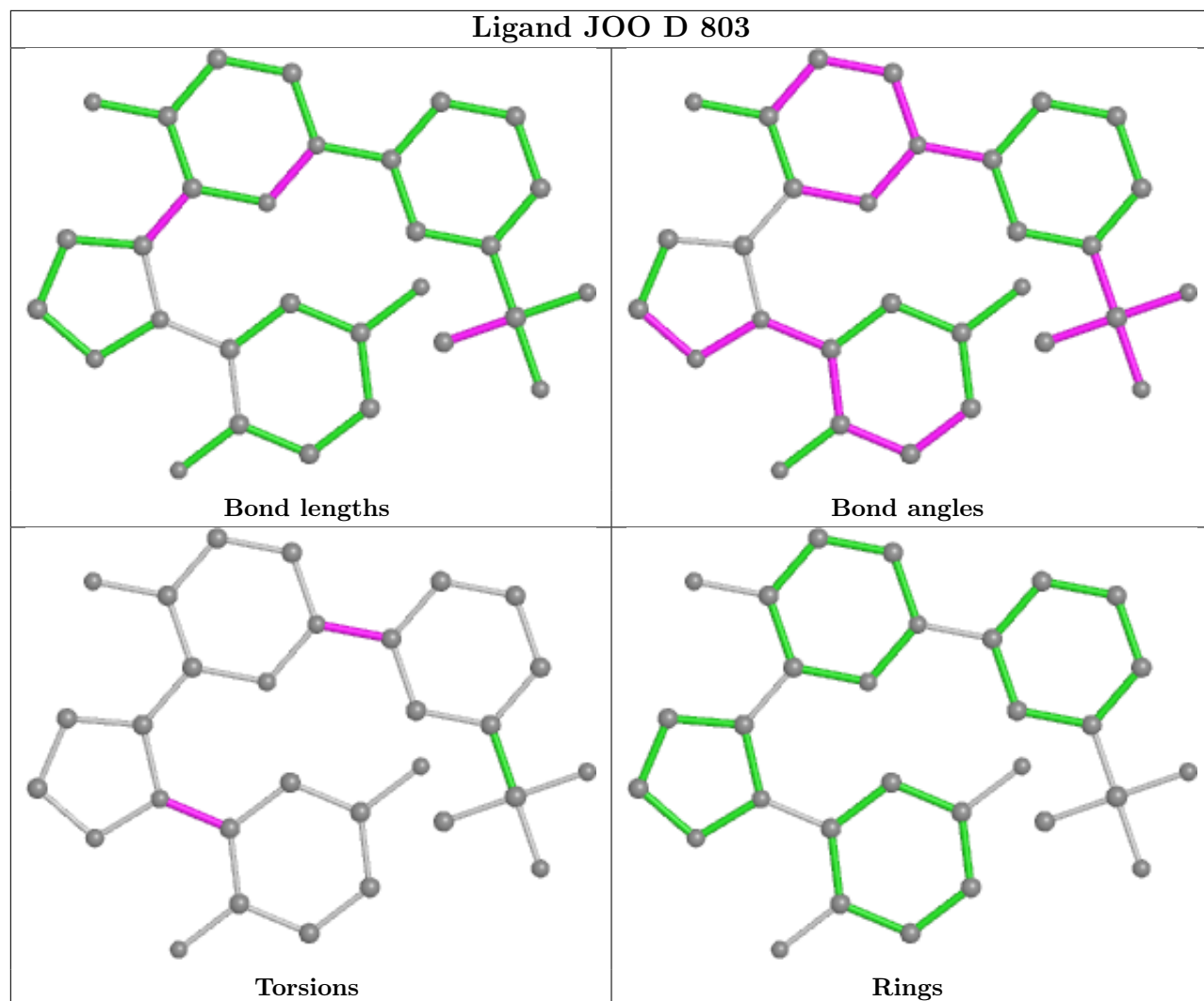
There are no ring outliers.

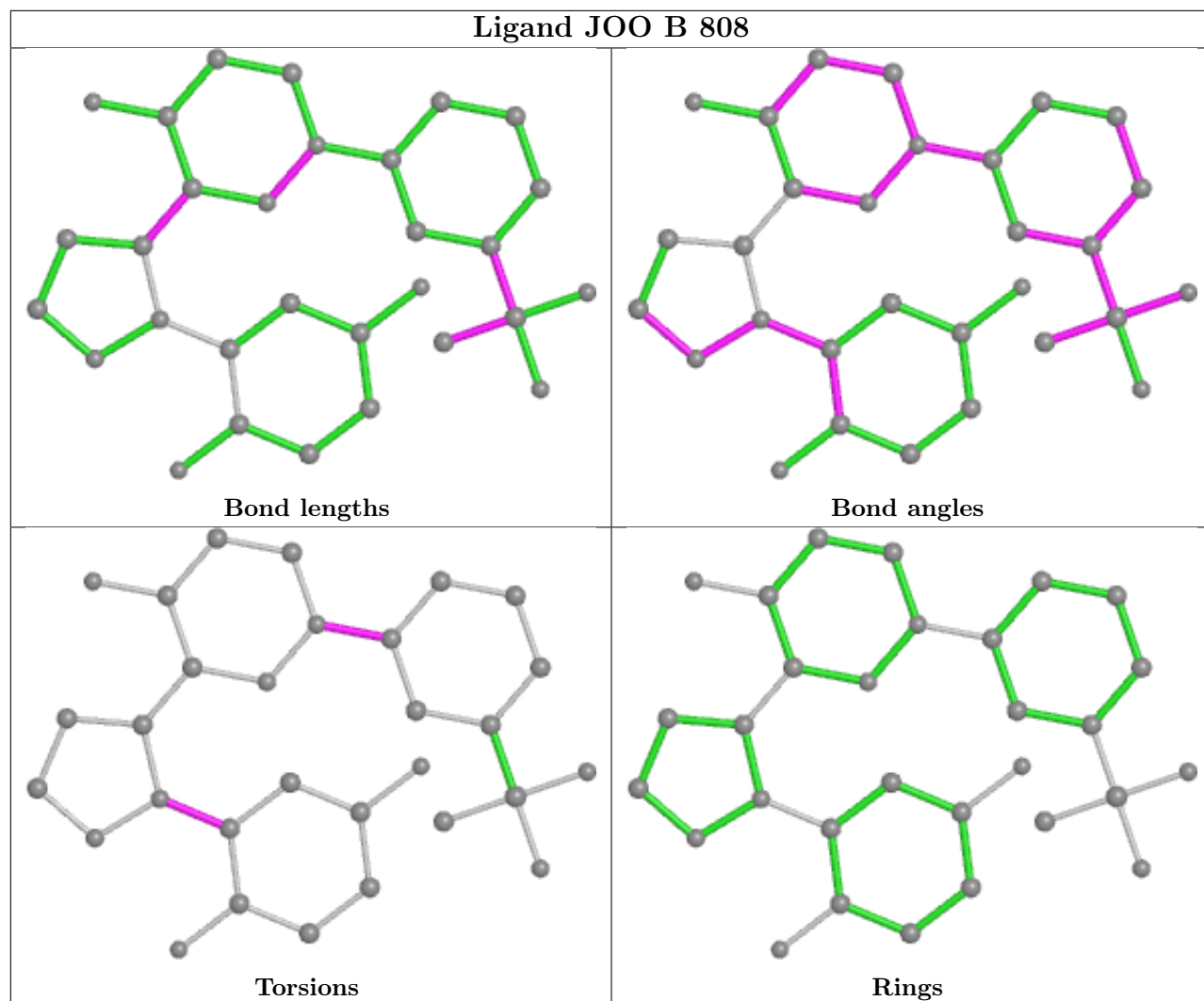
1 monomer is involved in 1 short contact:

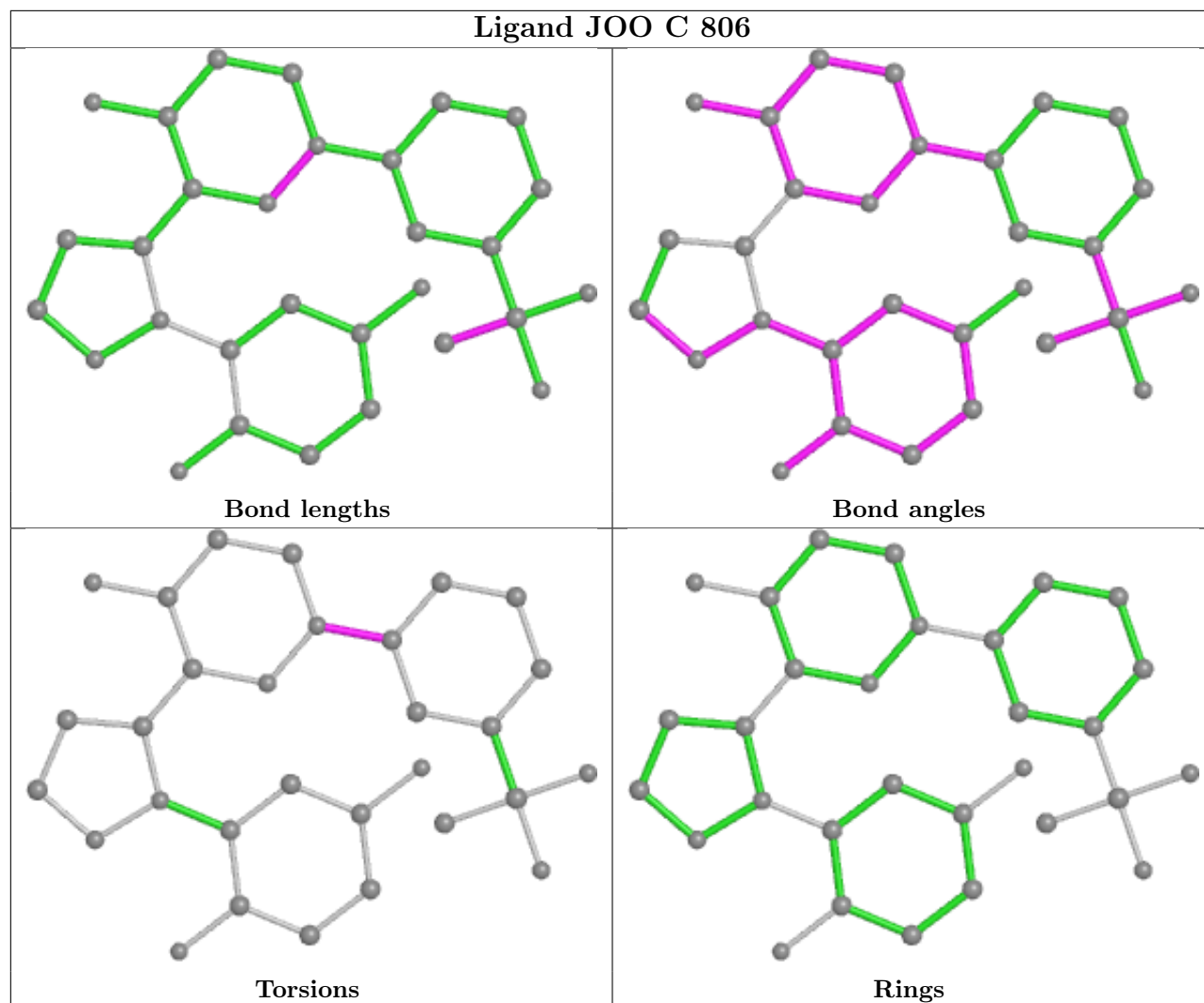
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	808	JOO	1	0

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 [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%)	-0.45	1 (0%) 94 93	24, 36, 60, 81	0
1	B	314/343 (91%)	-0.42	4 (1%) 77 75	24, 35, 61, 93	0
1	C	312/343 (90%)	-0.49	5 (1%) 72 70	25, 37, 59, 89	0
1	D	310/343 (90%)	-0.50	1 (0%) 94 93	29, 42, 65, 87	0
All	All	1248/1372 (90%)	-0.47	11 (0%) 84 83	24, 38, 61, 93	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	769	GLU	3.3
1	C	768	GLY	3.1
1	A	770	GLU	2.9
1	B	768	GLY	2.8
1	C	770	GLU	2.8
1	B	771	THR	2.7
1	C	720	ASP	2.6
1	B	770	GLU	2.6
1	B	769	GLU	2.4
1	C	606	GLU	2.2
1	D	460	MET	2.0

### 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	D	509	10/11	0.92	0.11	42,52,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CME	C	509	10/11	0.93	0.11	41,51,77,77	0
1	CME	A	509	10/11	0.94	0.14	40,48,76,77	0
1	CME	B	509	10/11	0.94	0.16	39,47,81,84	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

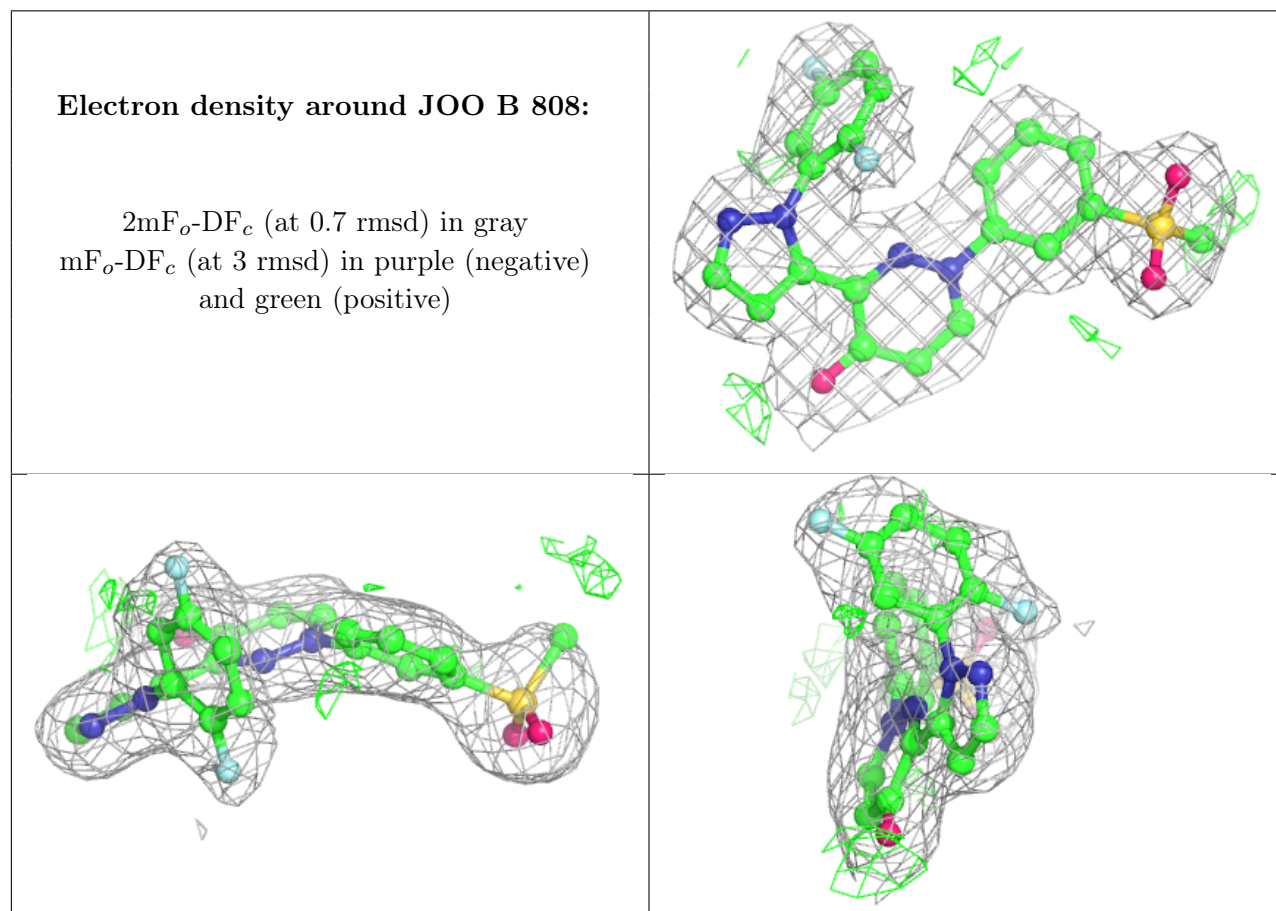
### 6.4 Ligands [i](#)

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
7	PR	B	806	1/1	0.81	0.04	114,114,114,114	0
7	PR	B	804	1/1	0.82	0.22	164,164,164,164	0
5	GOL	A	804	6/6	0.84	0.16	63,66,67,70	0
7	PR	C	804	1/1	0.89	0.37	157,157,157,157	0
7	PR	C	805	1/1	0.91	0.28	155,155,155,155	0
6	JOO	B	808	30/30	0.93	0.11	32,39,57,63	0
6	JOO	C	806	30/30	0.93	0.12	31,41,60,66	0
6	JOO	A	805	30/30	0.93	0.12	33,43,61,68	0
6	JOO	D	803	30/30	0.94	0.10	35,43,66,72	0
7	PR	B	807	1/1	0.94	0.17	125,125,125,125	0
7	PR	B	805	1/1	0.95	0.14	125,125,125,125	0
7	PR	C	803	1/1	0.95	0.09	129,129,129,129	0
3	MG	B	802	1/1	0.96	0.09	23,23,23,23	0
3	MG	D	802	1/1	0.96	0.04	32,32,32,32	0
3	MG	C	802	1/1	0.97	0.07	24,24,24,24	0
4	CL	A	803	1/1	0.97	0.06	57,57,57,57	0
7	PR	B	803	1/1	0.99	0.03	87,87,87,87	0
3	MG	A	802	1/1	0.99	0.07	22,22,22,22	0
2	ZN	C	801	1/1	1.00	0.08	31,31,31,31	0
2	ZN	D	801	1/1	1.00	0.08	35,35,35,35	0
2	ZN	A	801	1/1	1.00	0.10	29,29,29,29	0
2	ZN	B	801	1/1	1.00	0.08	29,29,29,29	0

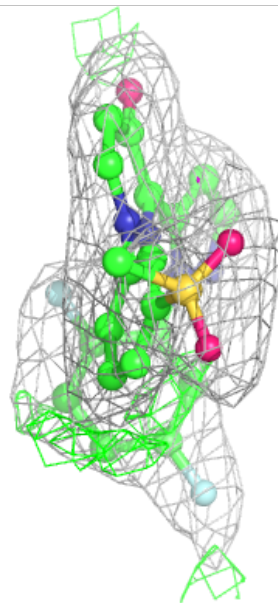
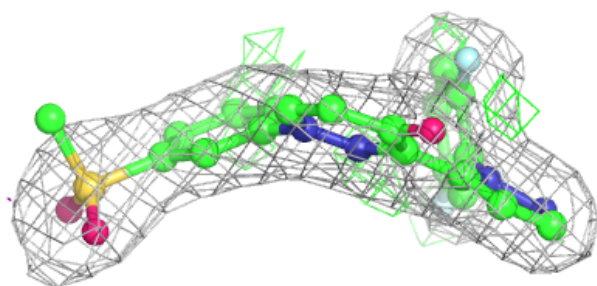
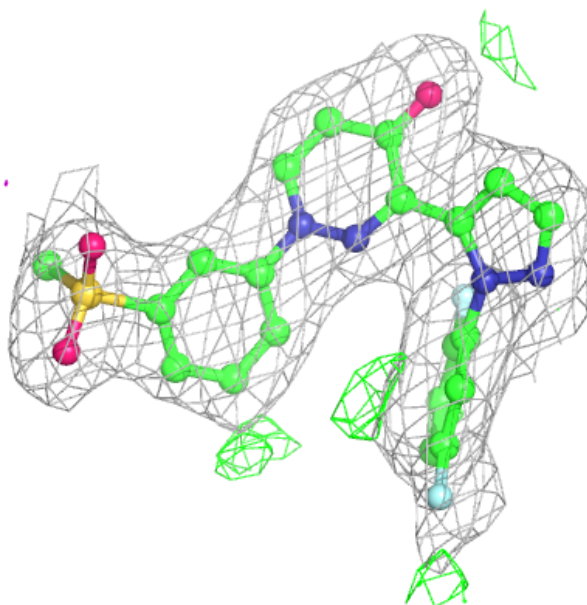
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



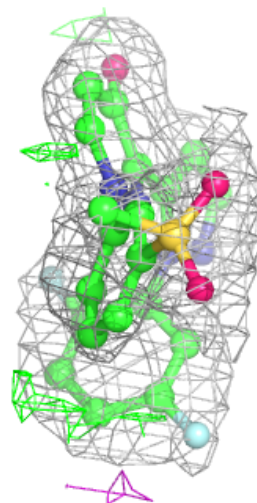
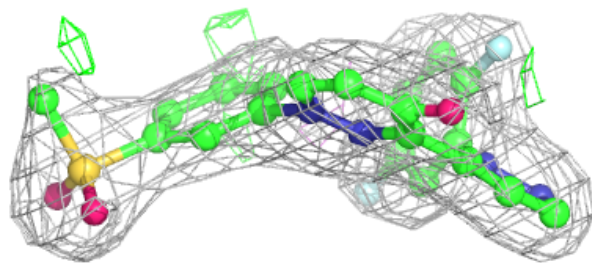
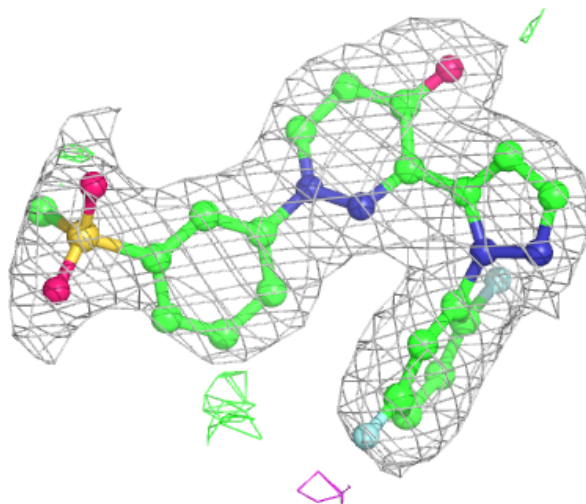
**Electron density around JOO C 806:**

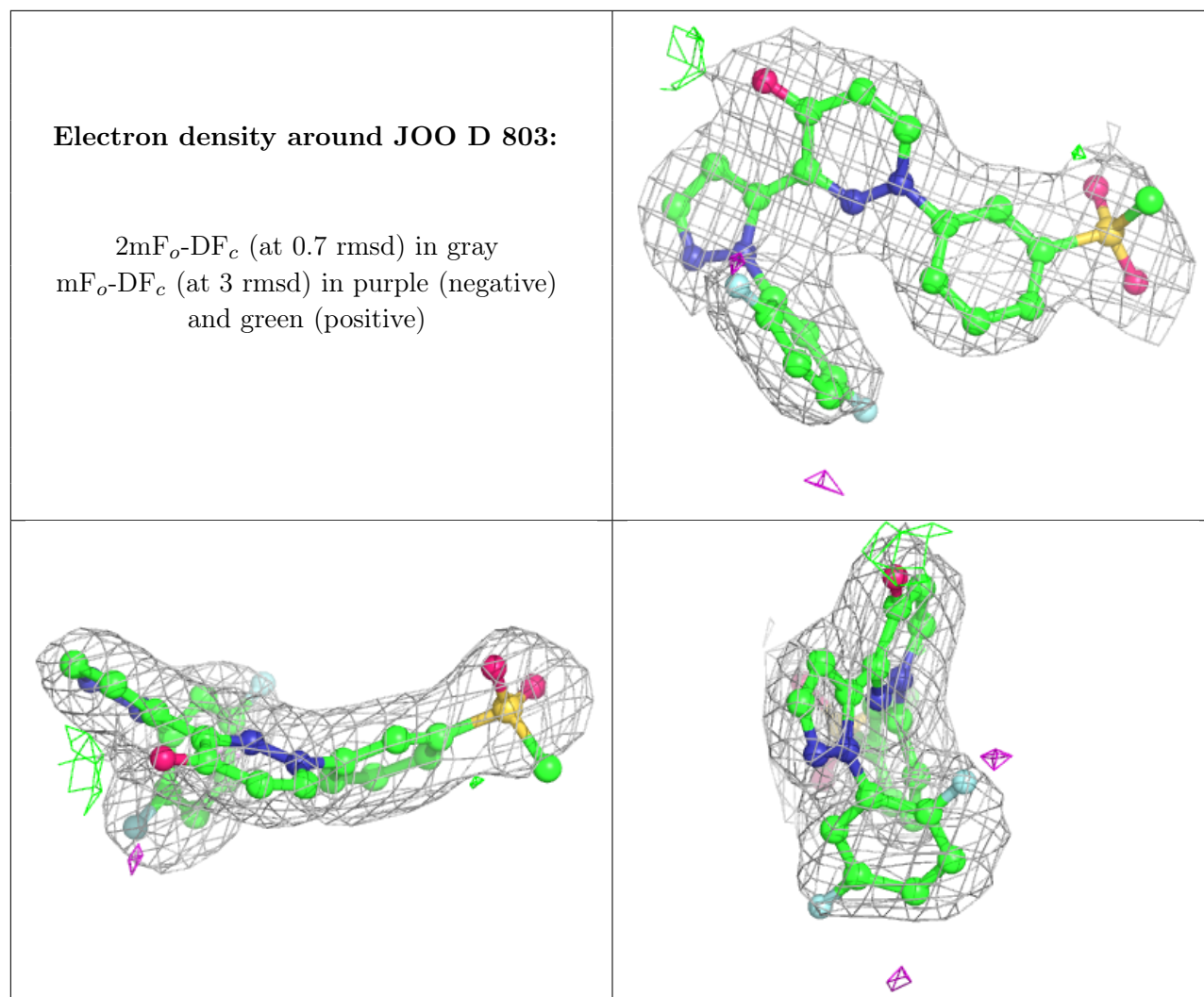
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around JOO A 805:**

$2mF_o-DF_c$  (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.