



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 24, 2024 – 06:11 PM EST

PDB ID : 8W3D
Title : TAS-120 covalent structure with FGFR2 molecular brake mutant
Authors : Hoffman, I.D.; Nelson, K.J.; Bensen, D.C.; Bailey, J.B.
Deposited on : 2024-02-22
Resolution : 2.04 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

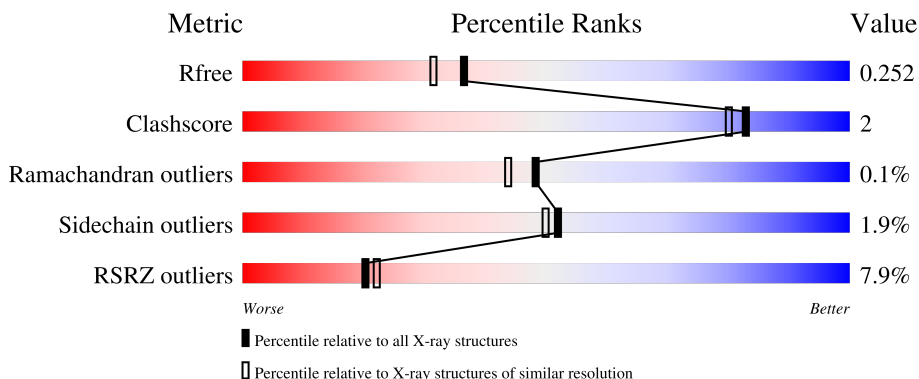
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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 ≥ 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	324	 8% 86% 6% 8%
1	B	324	 7% 83% 5% 12%
1	C	324	 5% 89% 5% 7%
1	D	324	 8% 83% 8% 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10120 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 Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	2393	1526	404	440	23	0	1	0
1	B	286	2292	1464	389	417	22	0	2	0
1	C	300	2416	1540	407	446	23	0	4	0
1	D	296	2379	1518	401	438	22	0	3	0

There are 60 discrepancies between the modelled and reference sequences:

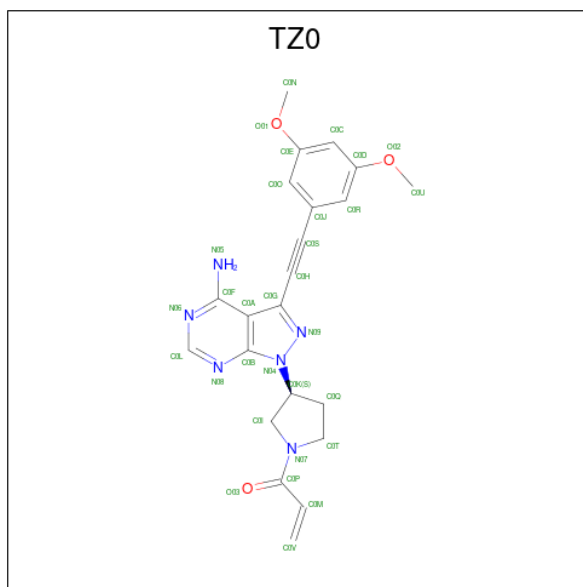
Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	initiating methionine	UNP P21802
A	446	GLY	-	expression tag	UNP P21802
A	447	SER	-	expression tag	UNP P21802
A	448	SER	-	expression tag	UNP P21802
A	449	HIS	-	expression tag	UNP P21802
A	450	HIS	-	expression tag	UNP P21802
A	451	HIS	-	expression tag	UNP P21802
A	452	HIS	-	expression tag	UNP P21802
A	453	HIS	-	expression tag	UNP P21802
A	454	HIS	-	expression tag	UNP P21802
A	455	SER	-	expression tag	UNP P21802
A	456	GLN	-	expression tag	UNP P21802
A	457	ASP	-	expression tag	UNP P21802
A	549	LYS	ASN	engineered mutation	UNP P21802
A	650	VAL	ASP	engineered mutation	UNP P21802
B	445	MET	-	initiating methionine	UNP P21802
B	446	GLY	-	expression tag	UNP P21802
B	447	SER	-	expression tag	UNP P21802
B	448	SER	-	expression tag	UNP P21802
B	449	HIS	-	expression tag	UNP P21802
B	450	HIS	-	expression tag	UNP P21802

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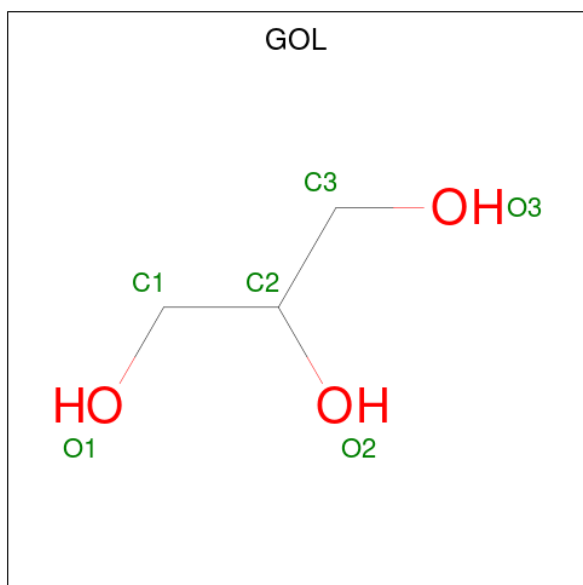
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	expression tag	UNP P21802
B	452	HIS	-	expression tag	UNP P21802
B	453	HIS	-	expression tag	UNP P21802
B	454	HIS	-	expression tag	UNP P21802
B	455	SER	-	expression tag	UNP P21802
B	456	GLN	-	expression tag	UNP P21802
B	457	ASP	-	expression tag	UNP P21802
B	549	LYS	ASN	engineered mutation	UNP P21802
B	650	VAL	ASP	engineered mutation	UNP P21802
C	445	MET	-	initiating methionine	UNP P21802
C	446	GLY	-	expression tag	UNP P21802
C	447	SER	-	expression tag	UNP P21802
C	448	SER	-	expression tag	UNP P21802
C	449	HIS	-	expression tag	UNP P21802
C	450	HIS	-	expression tag	UNP P21802
C	451	HIS	-	expression tag	UNP P21802
C	452	HIS	-	expression tag	UNP P21802
C	453	HIS	-	expression tag	UNP P21802
C	454	HIS	-	expression tag	UNP P21802
C	455	SER	-	expression tag	UNP P21802
C	456	GLN	-	expression tag	UNP P21802
C	457	ASP	-	expression tag	UNP P21802
C	549	LYS	ASN	engineered mutation	UNP P21802
C	650	VAL	ASP	engineered mutation	UNP P21802
D	445	MET	-	initiating methionine	UNP P21802
D	446	GLY	-	expression tag	UNP P21802
D	447	SER	-	expression tag	UNP P21802
D	448	SER	-	expression tag	UNP P21802
D	449	HIS	-	expression tag	UNP P21802
D	450	HIS	-	expression tag	UNP P21802
D	451	HIS	-	expression tag	UNP P21802
D	452	HIS	-	expression tag	UNP P21802
D	453	HIS	-	expression tag	UNP P21802
D	454	HIS	-	expression tag	UNP P21802
D	455	SER	-	expression tag	UNP P21802
D	456	GLN	-	expression tag	UNP P21802
D	457	ASP	-	expression tag	UNP P21802
D	549	LYS	ASN	engineered mutation	UNP P21802
D	650	VAL	ASP	engineered mutation	UNP P21802

- Molecule 2 is 1-[(3S)-3-{4-amino-3-[(3,5-dimethoxyphenyl)ethynyl]-1H-pyrazolo[3,4-d]pyrimidin-1-yl}pyrrolidin-1-yl]prop-2-en-1-one (three-letter code: TZ0) (formula: C₂₂H₂₂N₆O₃) (labeled as "Ligand of Interest" by depositor).



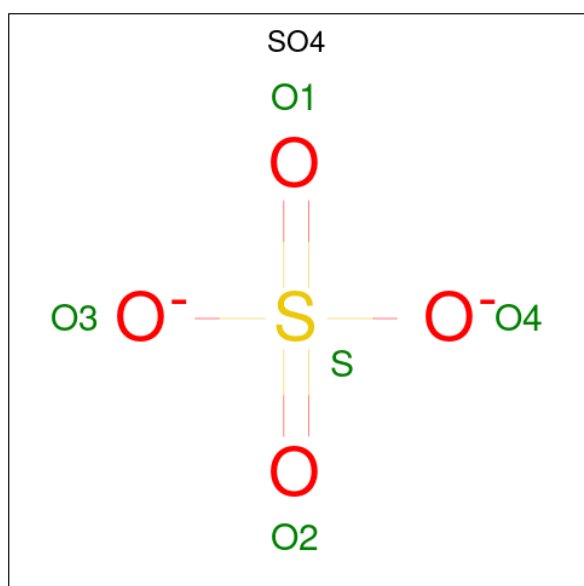
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			31	22	6	3		
2	B	1	Total	C	N	O	0	0
			31	22	6	3		
2	C	1	Total	C	N	O	0	0
			31	22	6	3		
2	D	1	Total	C	N	O	0	0
			31	22	6	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		

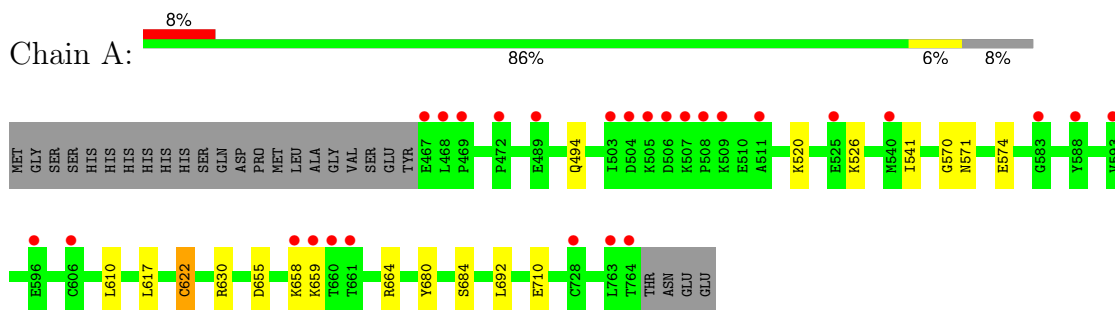
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	100	Total	O	0	0
			100	100		
5	B	104	Total	O	0	0
			104	104		
5	C	109	Total	O	0	0
			109	109		
5	D	134	Total	O	0	0
			134	134		

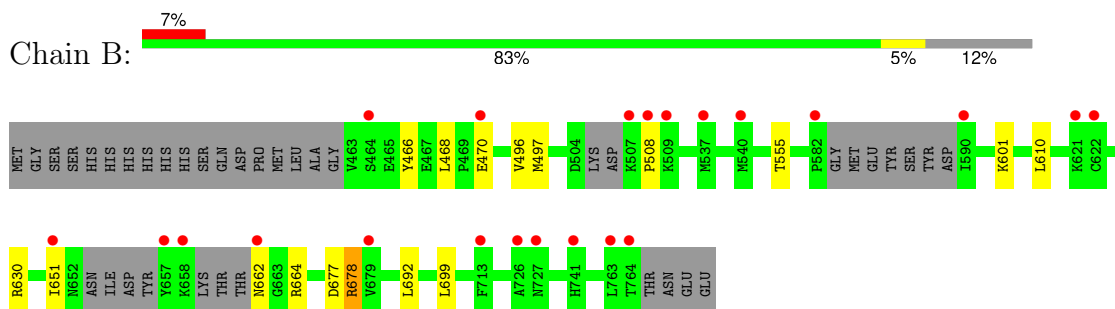
3 Residue-property plots [i](#)

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.

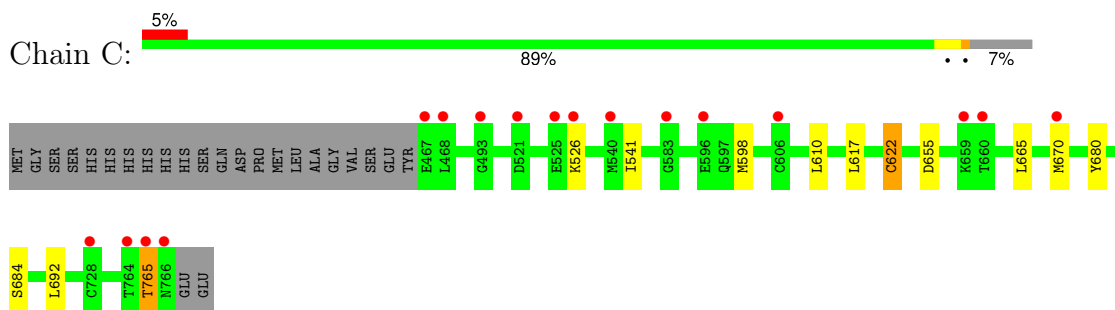
- Molecule 1: Fibroblast growth factor receptor 2



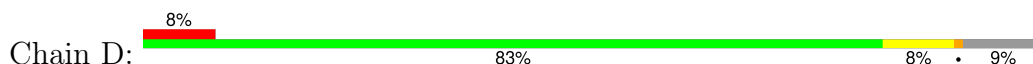
- Molecule 1: Fibroblast growth factor receptor 2

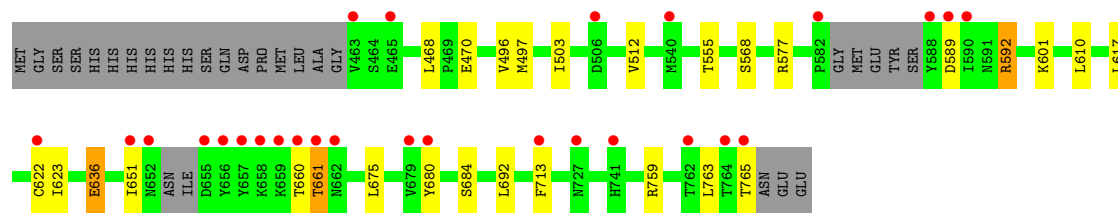


- Molecule 1: Fibroblast growth factor receptor 2



- Molecule 1: Fibroblast growth factor receptor 2





4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.13Å 129.87Å 132.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.04 33.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.00-2.04) 99.7 (33.00-2.04)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.219 , 0.250 0.226 , 0.252	Depositor DCC
R_{free} test set	2002 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtrriage
Anisotropy	0.215	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10120	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0097e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, TZ0, GOL

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	0.27	0/2448	0.53	0/3307
1	B	0.28	0/2341	0.52	0/3157
1	C	0.28	0/2474	0.55	0/3342
1	D	0.28	0/2432	0.54	0/3284
All	All	0.28	0/9695	0.53	0/13090

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	2393	0	2408	10	0
1	B	2292	0	2314	8	0
1	C	2416	0	2431	12	0
1	D	2379	0	2393	17	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	C	31	0	0	0	0
2	D	31	0	0	0	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	16	0	0
3	D	6	0	8	0	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	15	0	0	0	0
5	A	100	0	0	0	0
5	B	104	0	0	0	0
5	C	109	0	0	0	0
5	D	134	0	0	0	0
All	All	10120	0	9578	44	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 2.

All (44) 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:589:ASP:HB2	1:D:592:ARG:HD2	1.73	0.68
1:D:503:ILE:HG22	1:D:512:VAL:CG2	2.24	0.67
1:D:759:ARG:O	1:D:763:LEU:HD23	1.94	0.67
1:B:468:LEU:HD23	1:B:555:THR:HB	1.80	0.64
1:C:665:LEU:HB3	1:C:670[A]:MET:CE	2.28	0.63
1:C:665:LEU:HB3	1:C:670[B]:MET:CE	2.28	0.62
1:D:468:LEU:HD23	1:D:555:THR:HB	1.80	0.62
1:C:598:MET:CE	1:C:598:MET:HA	2.29	0.62
1:C:665:LEU:HB3	1:C:670[A]:MET:SD	2.41	0.61
1:C:665:LEU:HB3	1:C:670[B]:MET:SD	2.43	0.58
1:B:508:PRO:HB2	1:C:765:THR:HG23	1.86	0.58
1:D:568:SER:OG	1:D:636:GLU:HG2	2.06	0.55
1:D:589:ASP:HB2	1:D:592:ARG:CD	2.36	0.55
1:C:541:ILE:HD13	1:C:617:LEU:HD21	1.90	0.54
1:D:660:THR:O	1:D:661:THR:HB	2.07	0.54
1:D:617:LEU:HG	1:D:622[B]:CYS:SG	2.48	0.54
1:A:541:ILE:HD13	1:A:617:LEU:HD21	1.91	0.53
1:C:598:MET:HA	1:C:598:MET:HE2	1.94	0.50
1:B:662:ASN:HD22	1:B:678:ARG:HA	1.77	0.49
1:A:658:LYS:O	1:A:659:LYS:HG2	2.12	0.49
1:D:503:ILE:HG22	1:D:512:VAL:HG21	1.94	0.49
1:B:610:LEU:HD13	1:B:692:LEU:HD21	1.96	0.47
1:B:699:LEU:HD12	1:B:699:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:LEU:HD13	1:A:692:LEU:HD21	1.96	0.46
1:A:570:GLY:HA3	1:A:574:GLU:OE2	2.15	0.46
1:C:610:LEU:HD13	1:C:692:LEU:HD21	1.96	0.46
1:A:571:ASN:O	1:A:574:GLU:HG2	2.16	0.46
1:A:526:LYS:HG2	1:B:664:ARG:CZ	2.46	0.46
1:D:610:LEU:HD13	1:D:692:LEU:HD21	1.97	0.46
1:D:577:ARG:O	1:D:592:ARG:NH1	2.48	0.46
1:D:496:VAL:HG12	1:D:497:MET:O	2.16	0.45
1:A:617:LEU:HD22	1:A:622:CYS:SG	2.57	0.45
1:B:496:VAL:HG12	1:B:497:MET:O	2.17	0.44
1:C:665:LEU:HB3	1:C:670[A]:MET:HE3	2.00	0.44
1:D:503:ILE:HG22	1:D:512:VAL:HG22	2.00	0.44
1:A:710:GLU:HB3	1:B:466:TYR:CD2	2.53	0.44
1:C:617:LEU:HD22	1:C:622[A]:CYS:SG	2.60	0.42
1:C:680:TYR:CE1	1:C:684:SER:HB2	2.55	0.41
1:D:675:LEU:HD21	1:D:713:PHE:CD1	2.56	0.41
1:A:680:TYR:CE1	1:A:684:SER:HB2	2.55	0.41
1:D:503:ILE:CG2	1:D:512:VAL:CG2	2.97	0.40
1:D:680:TYR:CE1	1:D:684:SER:HB2	2.57	0.40
1:A:494:GLN:HE21	1:A:520:LYS:HG2	1.87	0.40
1:D:622[B]:CYS:SG	1:D:623:ILE:N	2.91	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	297/324 (92%)	292 (98%)	5 (2%)	0	100	100
1	B	277/324 (86%)	273 (99%)	4 (1%)	0	100	100
1	C	300/324 (93%)	297 (99%)	3 (1%)	0	100	100
1	D	291/324 (90%)	285 (98%)	5 (2%)	1 (0%)	37	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1165/1296 (90%)	1147 (98%)	17 (2%)	1 (0%)	48 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	661	THR

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	263/285 (92%)	259 (98%)	4 (2%)	60 60
1	B	252/285 (88%)	246 (98%)	6 (2%)	44 40
1	C	266/285 (93%)	262 (98%)	4 (2%)	60 60
1	D	262/285 (92%)	256 (98%)	6 (2%)	45 41
All	All	1043/1140 (92%)	1023 (98%)	20 (2%)	52 50

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	622	CYS
1	A	630	ARG
1	A	655	ASP
1	A	664	ARG
1	B	470	GLU
1	B	601	LYS
1	B	630	ARG
1	B	651	ILE
1	B	677	ASP
1	B	678	ARG
1	C	526	LYS
1	C	622[A]	CYS
1	C	655	ASP
1	C	765	THR

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Mol	Chain	Res	Type
1	D	470	GLU
1	D	592	ARG
1	D	601	LYS
1	D	636	GLU
1	D	651	ILE
1	D	765	THR

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

Mol	Chain	Res	Type
1	A	494	GLN
1	A	597	GLN
1	B	727	ASN
1	C	597	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	802	-	5,5,5	0.10	0	5,5,5	0.28	0
2	TZ0	A	801	1	32,34,34	1.87	6 (18%)	34,48,48	2.18	9 (26%)
3	GOL	D	802	-	5,5,5	0.09	0	5,5,5	0.27	0
4	SO4	A	804	-	4,4,4	0.34	0	6,6,6	0.07	0
3	GOL	A	802	-	5,5,5	0.10	0	5,5,5	0.26	0
3	GOL	B	803	-	5,5,5	0.12	0	5,5,5	0.36	0
4	SO4	A	803	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	A	805	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	D	804	-	4,4,4	0.34	0	6,6,6	0.06	0
2	TZ0	D	801	1	32,34,34	1.96	7 (21%)	34,48,48	2.10	7 (20%)
4	SO4	B	804	-	4,4,4	0.33	0	6,6,6	0.07	0
2	TZ0	B	801	1	32,34,34	1.90	7 (21%)	34,48,48	2.05	7 (20%)
4	SO4	D	803	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	C	802	-	4,4,4	0.34	0	6,6,6	0.08	0
4	SO4	B	805	-	4,4,4	0.33	0	6,6,6	0.07	0
2	TZ0	C	801	1	32,34,34	1.93	6 (18%)	34,48,48	2.13	8 (23%)
4	SO4	D	805	-	4,4,4	0.34	0	6,6,6	0.07	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
3	GOL	B	802	-	-	4/4/4/4	-
2	TZ0	A	801	1	-	0/12/28/28	0/4/4/4
3	GOL	D	802	-	-	2/4/4/4	-
3	GOL	A	802	-	-	1/4/4/4	-
3	GOL	B	803	-	-	2/4/4/4	-
2	TZ0	D	801	1	-	1/12/28/28	0/4/4/4
2	TZ0	B	801	1	-	1/12/28/28	0/4/4/4
2	TZ0	C	801	1	-	2/12/28/28	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	TZ0	C0L-N08	5.20	1.40	1.32
2	D	801	TZ0	C0G-C0A	-5.20	1.33	1.41
2	C	801	TZ0	C0L-N08	5.17	1.40	1.32
2	D	801	TZ0	C0V-C0M	4.96	1.54	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	TZ0	C0V-C0M	4.95	1.54	1.30
2	D	801	TZ0	C0L-N08	4.94	1.39	1.32
2	B	801	TZ0	C0G-C0A	-4.90	1.34	1.41
2	C	801	TZ0	C0V-C0M	4.89	1.53	1.30
2	A	801	TZ0	C0V-C0M	4.85	1.53	1.30
2	B	801	TZ0	C0L-N08	4.69	1.39	1.32
2	C	801	TZ0	C0G-C0A	-4.43	1.34	1.41
2	A	801	TZ0	C0G-C0A	-4.21	1.35	1.41
2	D	801	TZ0	C0L-N06	3.52	1.40	1.33
2	A	801	TZ0	C0L-N06	3.47	1.40	1.33
2	C	801	TZ0	C0L-N06	3.47	1.40	1.33
2	B	801	TZ0	C0L-N06	3.42	1.40	1.33
2	C	801	TZ0	C0A-C0B	-3.14	1.34	1.43
2	A	801	TZ0	C0A-C0B	-3.10	1.34	1.43
2	B	801	TZ0	N09-N04	-3.09	1.33	1.37
2	D	801	TZ0	N09-N04	-2.98	1.33	1.37
2	B	801	TZ0	C0A-C0B	-2.95	1.35	1.43
2	D	801	TZ0	C0A-C0B	-2.92	1.35	1.43
2	C	801	TZ0	N09-N04	-2.84	1.34	1.37
2	A	801	TZ0	N09-N04	-2.48	1.34	1.37
2	D	801	TZ0	C0M-C0P	2.41	1.55	1.49
2	B	801	TZ0	C0M-C0P	2.08	1.55	1.49

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	TZ0	N08-C0L-N06	-7.53	118.45	128.67
2	D	801	TZ0	N08-C0L-N06	-7.33	118.72	128.67
2	C	801	TZ0	N08-C0L-N06	-7.33	118.73	128.67
2	B	801	TZ0	N08-C0L-N06	-7.23	118.86	128.67
2	A	801	TZ0	C0V-C0M-C0P	-4.95	111.21	121.27
2	C	801	TZ0	C0V-C0M-C0P	-4.92	111.29	121.27
2	D	801	TZ0	C0V-C0M-C0P	-4.60	111.92	121.27
2	B	801	TZ0	C0V-C0M-C0P	-4.57	112.00	121.27
2	D	801	TZ0	C0G-N09-N04	4.18	107.31	104.32
2	C	801	TZ0	C0K-N04-N09	3.91	126.79	119.35
2	D	801	TZ0	C0K-N04-N09	3.64	126.28	119.35
2	B	801	TZ0	C0K-N04-N09	3.63	126.27	119.35
2	B	801	TZ0	C0G-N09-N04	3.45	106.79	104.32
2	A	801	TZ0	C0K-N04-N09	3.45	125.92	119.35
2	D	801	TZ0	C0T-N07-C0I	-3.42	108.39	112.38
2	A	801	TZ0	C0Q-C0T-N07	3.34	107.23	102.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	TZ0	C0G-N09-N04	3.27	106.66	104.32
2	B	801	TZ0	C0T-N07-C0I	-3.18	108.67	112.38
2	C	801	TZ0	C0T-N07-C0I	-3.15	108.69	112.38
2	A	801	TZ0	C0G-N09-N04	2.85	106.36	104.32
2	A	801	TZ0	C0Q-C0K-N04	-2.85	108.25	112.11
2	B	801	TZ0	C0Q-C0T-N07	2.58	106.25	102.93
2	C	801	TZ0	C0A-C0F-N05	-2.52	118.23	122.70
2	A	801	TZ0	C0A-C0F-N05	-2.49	118.28	122.70
2	C	801	TZ0	C0Q-C0K-C0I	2.39	106.24	102.22
2	A	801	TZ0	C0T-N07-C0I	-2.36	109.62	112.38
2	C	801	TZ0	C0Q-C0T-N07	2.26	105.83	102.93
2	D	801	TZ0	C0Q-C0T-N07	2.23	105.80	102.93
2	D	801	TZ0	C0Q-C0K-C0I	2.23	105.97	102.22
2	A	801	TZ0	C0Q-C0K-C0I	2.19	105.92	102.22
2	B	801	TZ0	C0Q-C0K-C0I	2.03	105.65	102.22

There are no chirality outliers.

All (13) torsion outliers are listed below:

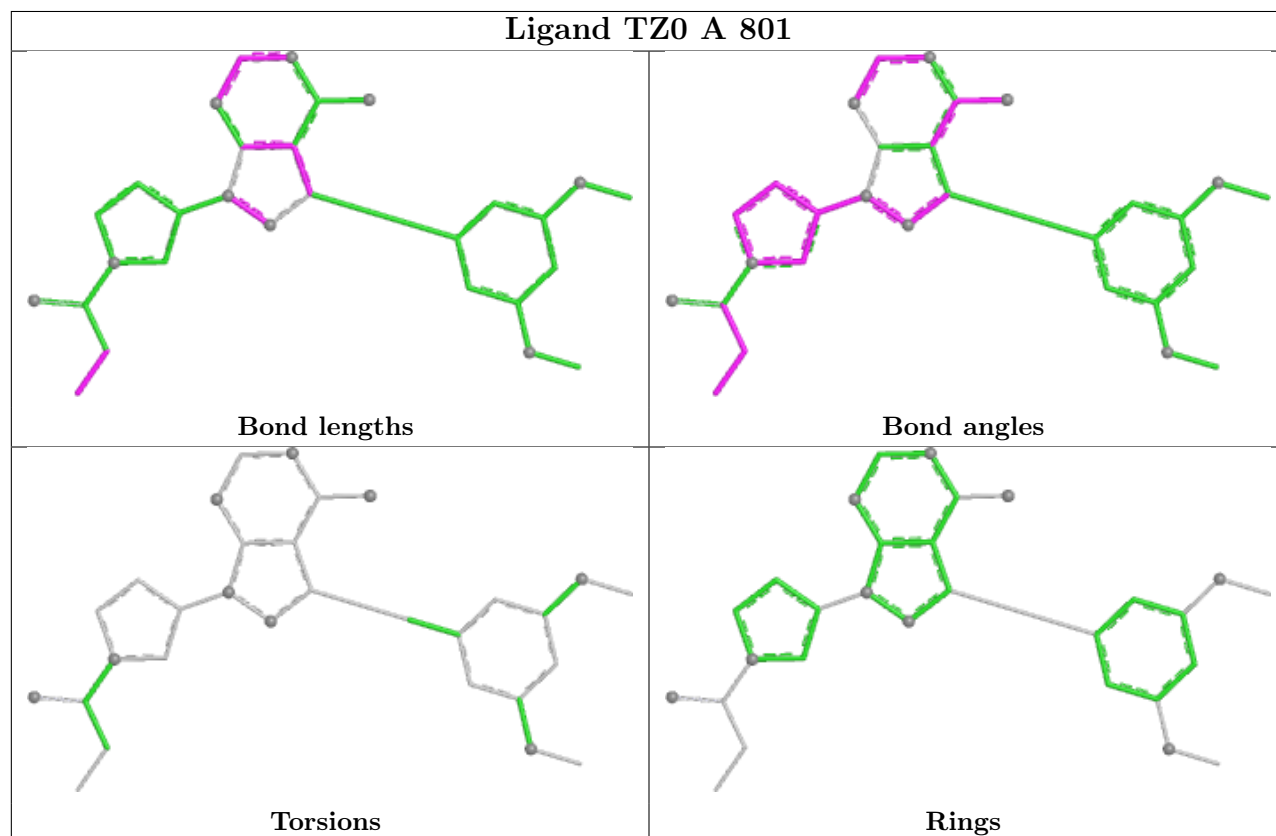
Mol	Chain	Res	Type	Atoms
3	B	802	GOL	O1-C1-C2-O2
3	B	802	GOL	O1-C1-C2-C3
3	B	802	GOL	C1-C2-C3-O3
3	B	802	GOL	O2-C2-C3-O3
3	D	802	GOL	O1-C1-C2-C3
3	D	802	GOL	O1-C1-C2-O2
2	C	801	TZ0	C0R-C0D-O02-C0U
2	C	801	TZ0	C0C-C0D-O02-C0U
3	B	803	GOL	C1-C2-C3-O3
3	A	802	GOL	O2-C2-C3-O3
3	B	803	GOL	O2-C2-C3-O3
2	B	801	TZ0	C0V-C0M-C0P-N07
2	D	801	TZ0	C0C-C0E-O01-C0N

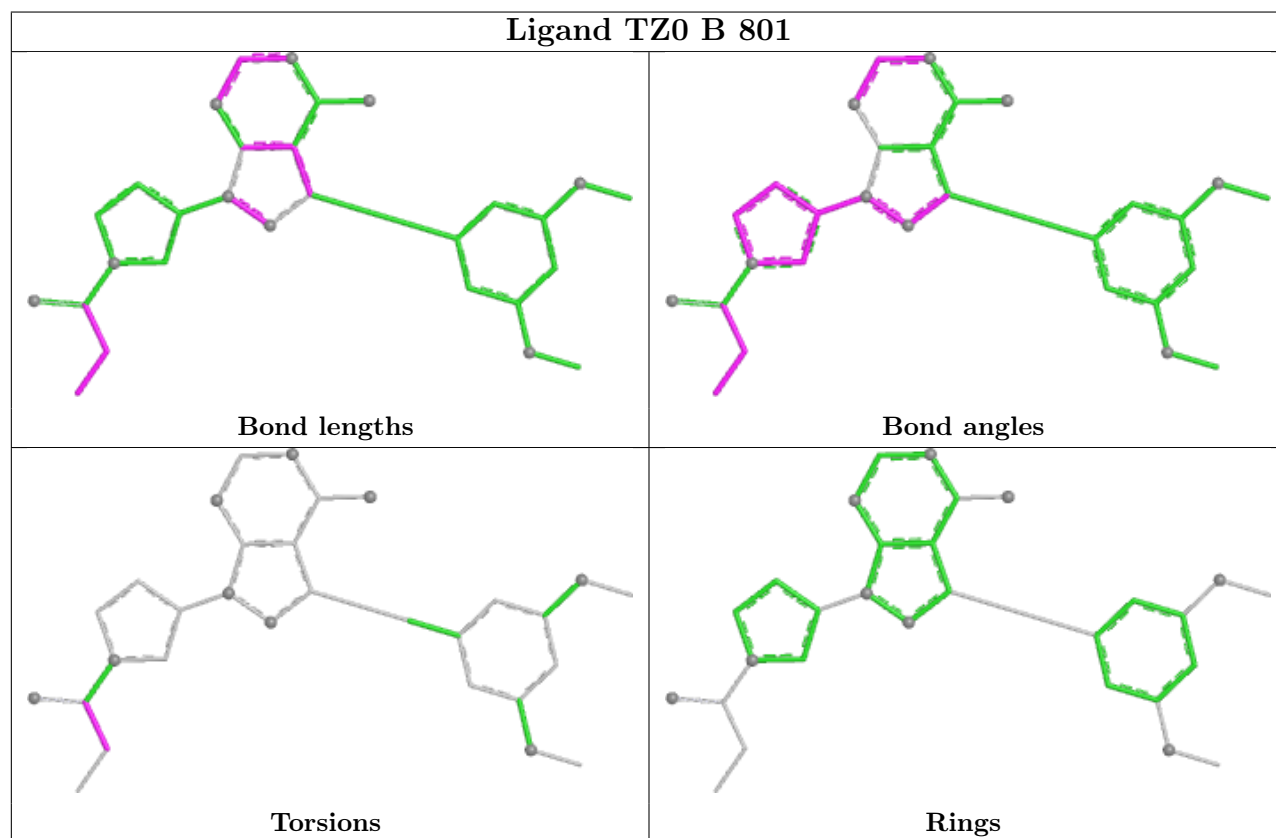
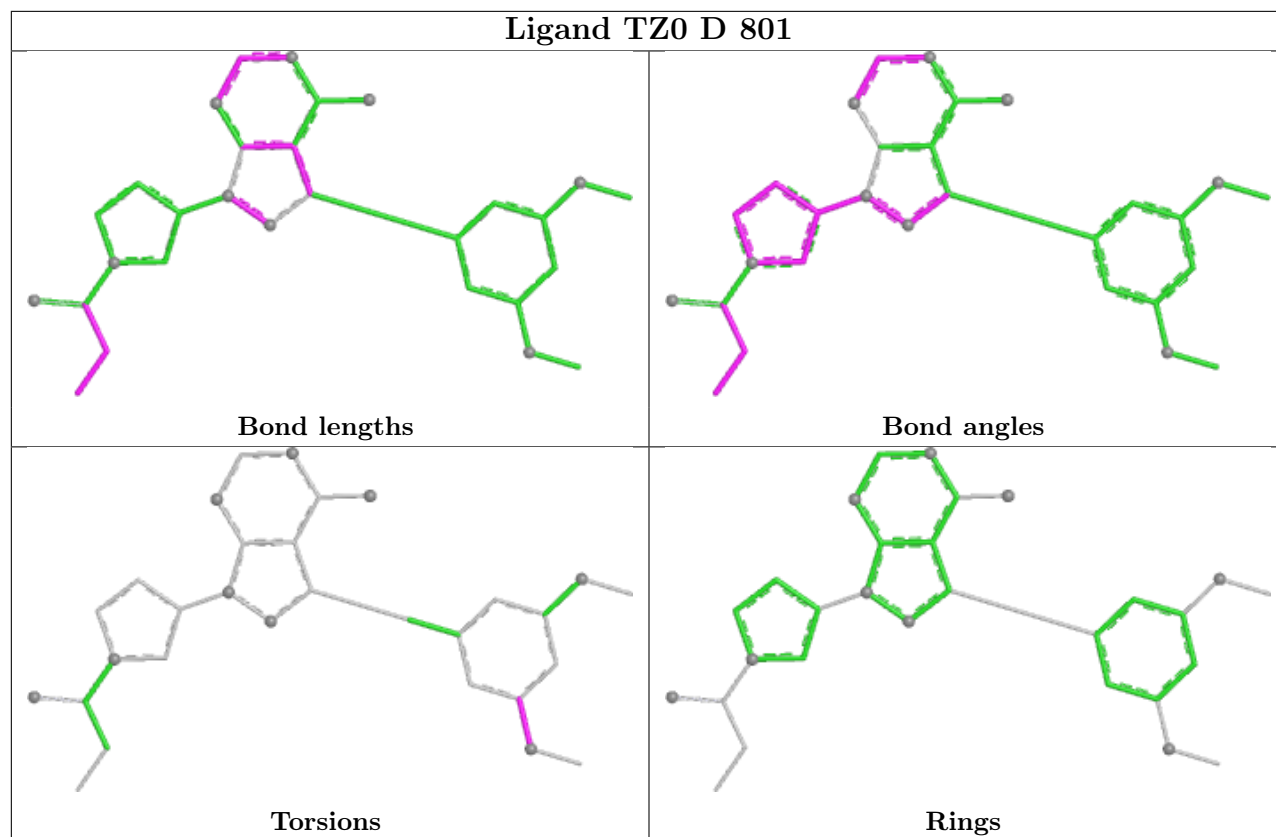
There are no ring outliers.

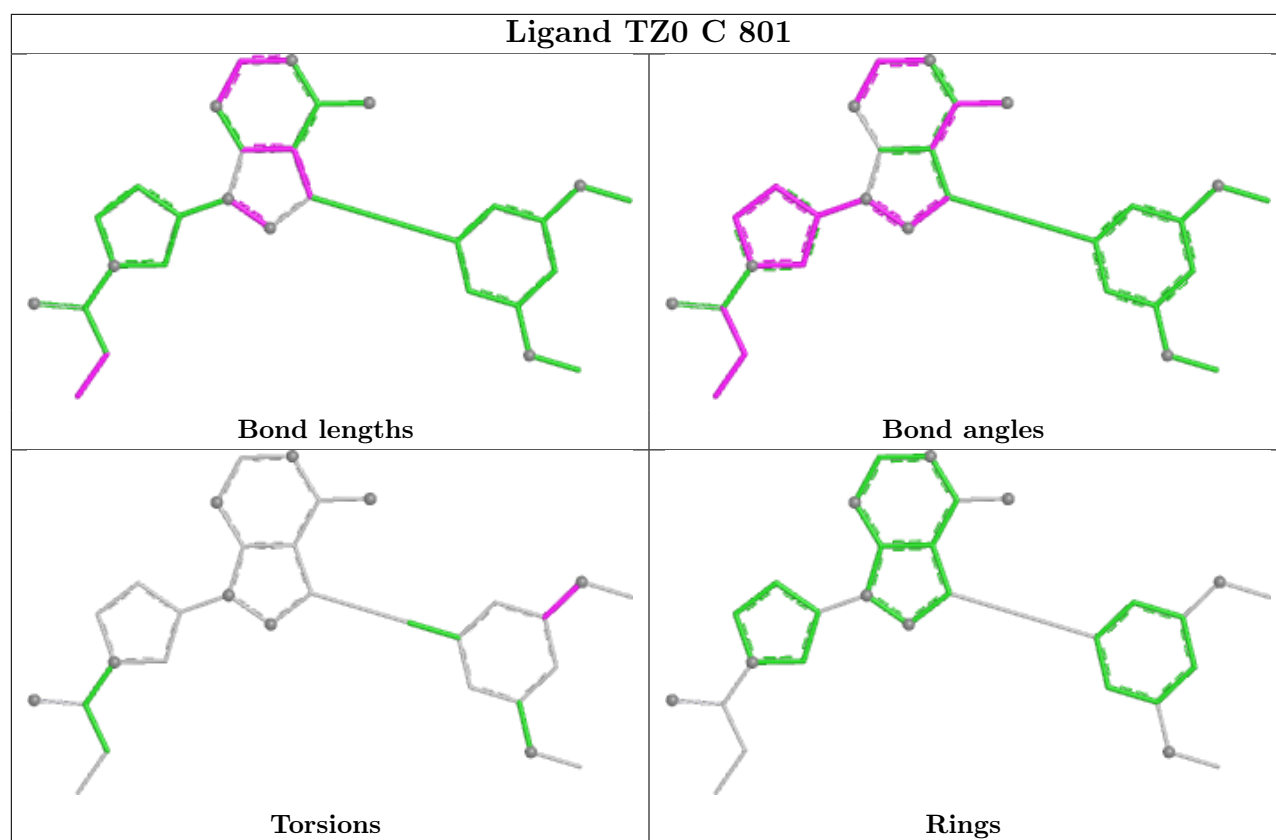
No monomer is involved in short contacts.

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.







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, 95th 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 ²)	Q<0.9
1	A	298/324 (91%)	0.61	27 (9%) 16 18	21, 39, 74, 117	1 (0%)
1	B	286/324 (88%)	0.62	22 (7%) 21 23	22, 38, 70, 93	1 (0%)
1	C	300/324 (92%)	0.42	17 (5%) 30 32	19, 37, 63, 91	2 (0%)
1	D	296/324 (91%)	0.62	27 (9%) 16 18	22, 37, 70, 101	1 (0%)
All	All	1180/1296 (91%)	0.57	93 (7%) 20 22	19, 37, 70, 117	5 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	661	THR	5.9
1	D	657	TYR	5.6
1	A	468	LEU	5.0
1	B	657	TYR	4.9
1	B	590	ILE	4.4
1	D	765	THR	4.3
1	D	588	TYR	4.3
1	B	662	ASN	4.3
1	A	508	PRO	4.2
1	B	622[A]	CYS	4.0
1	A	764	THR	4.0
1	B	540	MET	3.9
1	D	656	TYR	3.9
1	D	658	LYS	3.9
1	D	660	THR	3.8
1	D	590	ILE	3.8
1	A	660	THR	3.7
1	A	659	LYS	3.7
1	C	606[A]	CYS	3.6
1	A	506	ASP	3.5
1	D	463	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	662	ASN	3.5
1	C	468	LEU	3.5
1	B	764	THR	3.3
1	A	728	CYS	3.3
1	A	472	PRO	3.2
1	D	589	ASP	3.2
1	A	505	LYS	3.2
1	D	764	THR	3.1
1	A	583	GLY	3.1
1	D	659	LYS	3.1
1	C	660	THR	3.0
1	A	469	PRO	3.0
1	A	593	VAL	3.0
1	A	507	LYS	3.0
1	C	766	ASN	3.0
1	B	508	PRO	2.9
1	A	540	MET	2.8
1	A	509	LYS	2.8
1	B	727	ASN	2.8
1	A	504	ASP	2.7
1	D	582	PRO	2.7
1	A	489	GLU	2.7
1	C	765	THR	2.7
1	B	470	GLU	2.7
1	C	764	THR	2.6
1	D	713	PHE	2.6
1	B	507	LYS	2.6
1	C	540	MET	2.6
1	A	606[A]	CYS	2.6
1	A	467	GLU	2.6
1	B	713	PHE	2.5
1	C	728	CYS	2.5
1	D	727	ASN	2.5
1	C	467	GLU	2.4
1	D	680	TYR	2.4
1	D	741	HIS	2.4
1	D	465	GLU	2.4
1	B	537	MET	2.4
1	A	511	ALA	2.3
1	A	661	THR	2.3
1	B	582	PRO	2.3
1	B	763	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	525	GLU	2.2
1	D	655	ASP	2.2
1	D	679	VAL	2.2
1	B	726	ALA	2.2
1	A	658	LYS	2.2
1	B	658	LYS	2.2
1	C	670[A]	MET	2.2
1	C	525	GLU	2.2
1	B	679	VAL	2.2
1	C	596	GLU	2.2
1	A	763	LEU	2.2
1	A	588	TYR	2.2
1	D	762	THR	2.2
1	B	509	LYS	2.2
1	C	526	LYS	2.2
1	D	540	MET	2.2
1	C	659	LYS	2.1
1	A	596	GLU	2.1
1	A	503	ILE	2.1
1	B	651	ILE	2.1
1	C	521	ASP	2.1
1	C	493	GLY	2.1
1	D	622[A]	CYS	2.1
1	B	621	LYS	2.1
1	B	464	SER	2.1
1	D	651	ILE	2.1
1	D	506	ASP	2.1
1	B	741	HIS	2.1
1	C	583	GLY	2.0
1	D	652	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

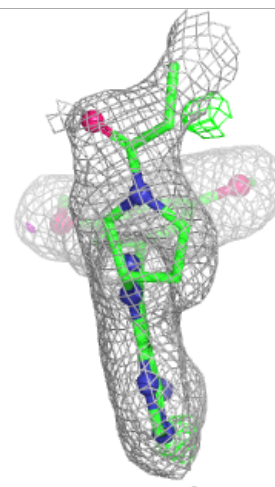
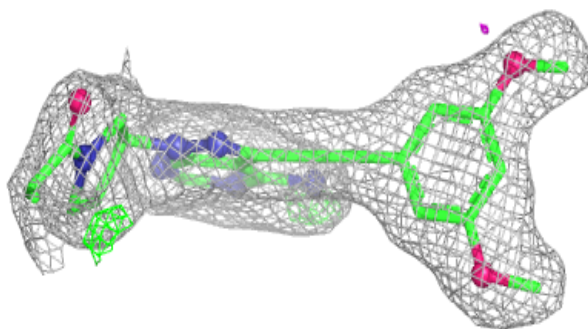
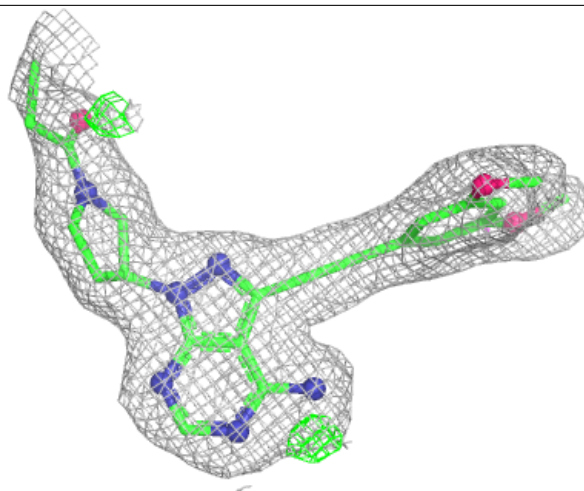
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	805	5/5	0.58	0.16	99,101,105,105	0
4	SO4	D	805	5/5	0.63	0.19	111,113,117,119	0
4	SO4	B	805	5/5	0.69	0.14	90,93,98,98	0
4	SO4	D	803	5/5	0.70	0.14	79,82,89,93	0
3	GOL	B	803	6/6	0.75	0.15	49,54,55,60	0
4	SO4	A	803	5/5	0.78	0.12	68,71,75,82	0
4	SO4	D	804	5/5	0.82	0.17	73,75,77,82	5
4	SO4	A	804	5/5	0.83	0.13	64,70,77,81	0
4	SO4	B	804	5/5	0.83	0.10	79,80,84,87	0
4	SO4	C	802	5/5	0.84	0.11	64,66,71,71	0
3	GOL	B	802	6/6	0.85	0.12	43,53,59,59	0
3	GOL	A	802	6/6	0.86	0.15	52,58,62,65	0
3	GOL	D	802	6/6	0.90	0.10	44,48,49,56	0
2	TZ0	A	801	31/31	0.94	0.08	25,29,44,48	0
2	TZ0	C	801	31/31	0.95	0.07	23,25,40,43	0
2	TZ0	D	801	31/31	0.95	0.07	20,25,35,36	0
2	TZ0	B	801	31/31	0.95	0.07	22,27,36,38	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.

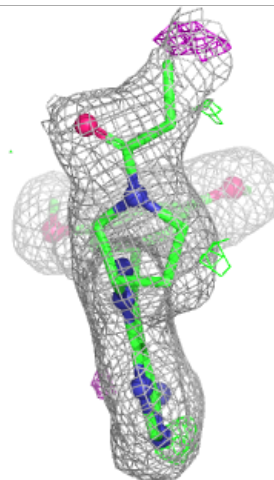
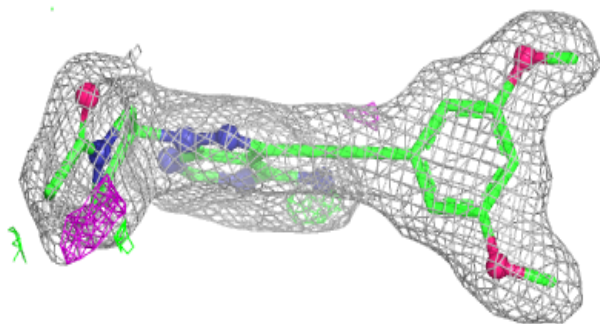
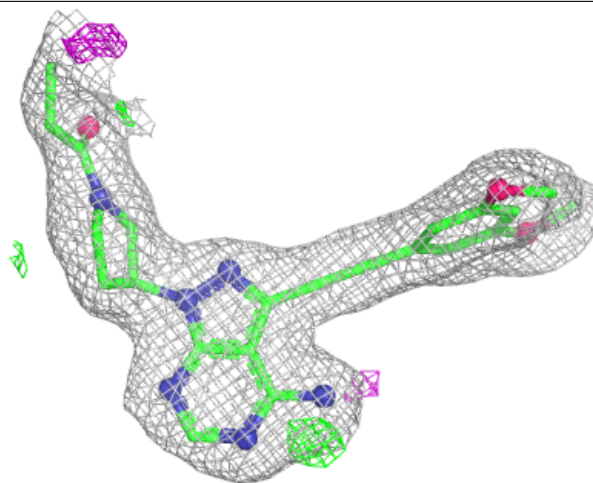
Electron density around TZ0 A 801:

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



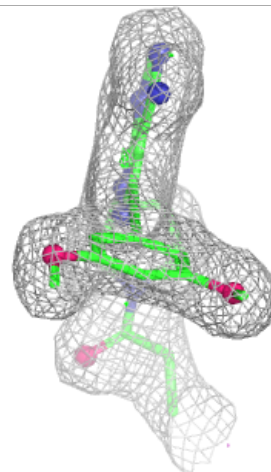
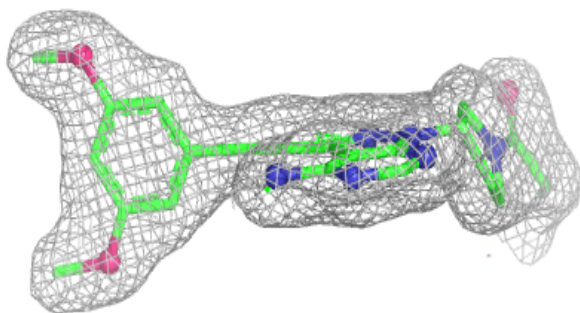
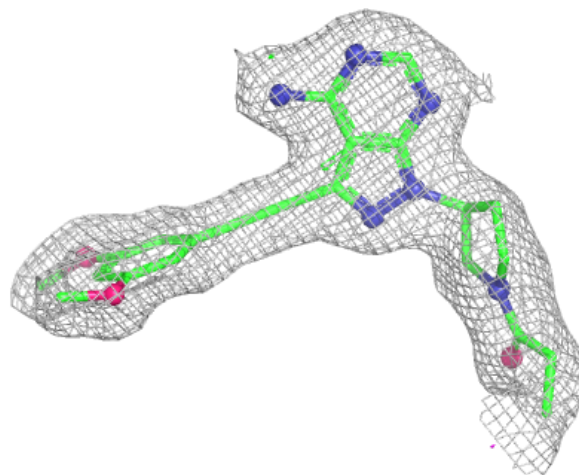
Electron density around TZ0 C 801:

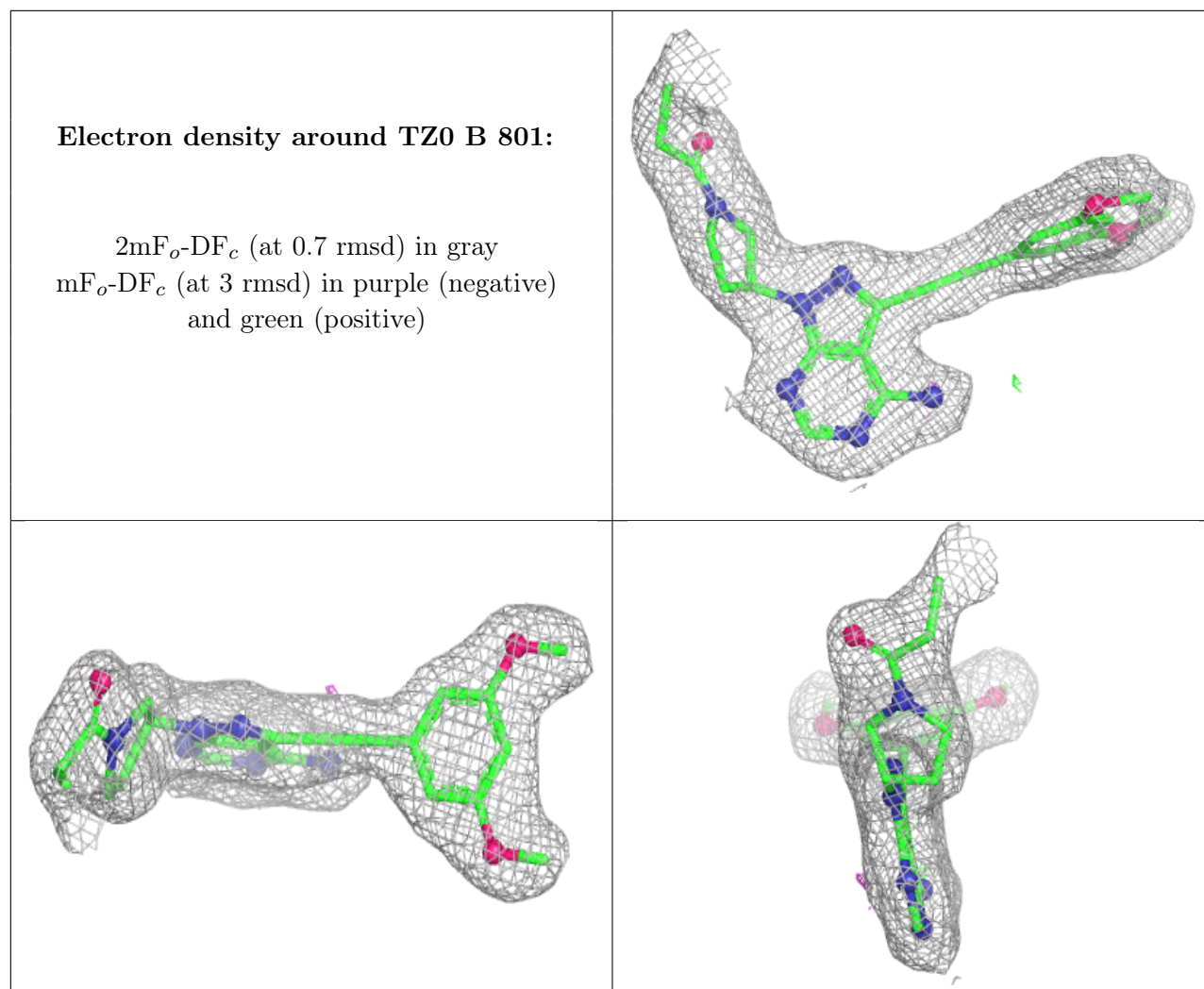
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TZ0 D 801:

$2mF_o-DF_c$ (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.