



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 AM UTC

PDB ID : 8W3B / pdb_00008w3b
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 : 2.23 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

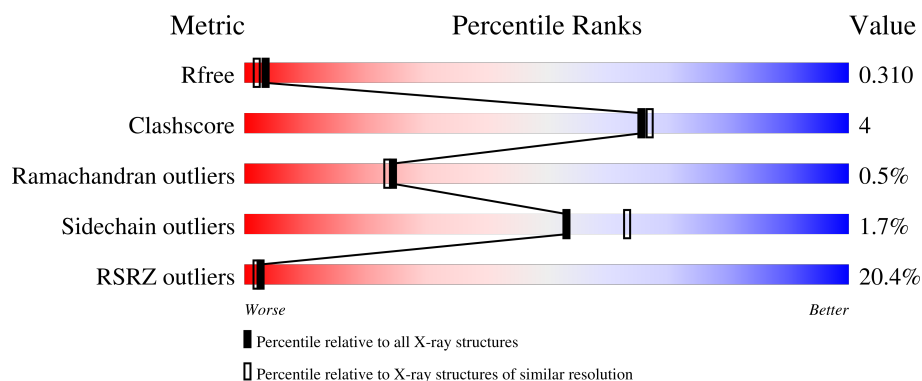
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (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 ≥ 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	17% 76% 10% 14%
1	B	324	16% 78% 8% 14%
1	C	324	16% 79% 10% 9%
1	D	324	22% 79% 6% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9349 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
1	A	279	Total	C	N	O	S	0	0	0
			2237	1427	379	410	21			
1	B	278	Total	C	N	O	S	0	0	0
			2220	1417	379	403	21			
1	C	294	Total	C	N	O	S	0	1	0
			2363	1508	399	433	23			
1	D	280	Total	C	N	O	S	0	0	0
			2241	1431	381	408	21			

There are 60 discrepancies between the modelled and reference sequences:

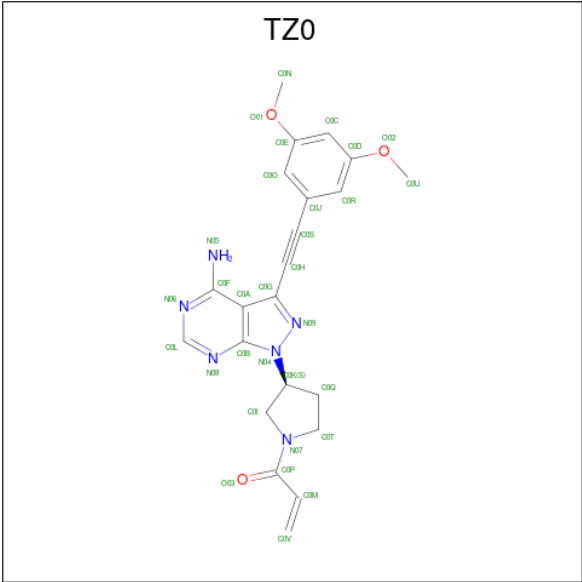
Chain	Residue	Modelled	Actual	Comment	Reference
A	445	MET	-	initiating methionine	UNP P21802
A	446	GLY	-	expression tag	UNP P21802
A	447	SER	-	expression tag	UNP P21802
A	448	SER	-	expression tag	UNP P21802
A	449	HIS	-	expression tag	UNP P21802
A	450	HIS	-	expression tag	UNP P21802
A	451	HIS	-	expression 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	HIS	ASN	variant	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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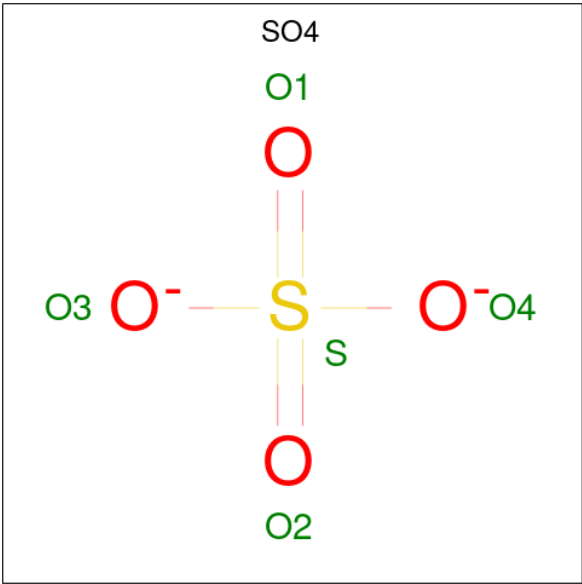
Chain	Residue	Modelled	Actual	Comment	Reference
B	451	HIS	-	expression tag	UNP P21802
B	452	HIS	-	expression tag	UNP P21802
B	453	HIS	-	expression tag	UNP P21802
B	454	HIS	-	expression tag	UNP P21802
B	455	SER	-	expression tag	UNP P21802
B	456	GLN	-	expression tag	UNP P21802
B	457	ASP	-	expression tag	UNP P21802
B	549	HIS	ASN	variant	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	HIS	ASN	variant	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	HIS	ASN	variant	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 (CCD ID: TZ0) (formula: C₂₂H₂₂N₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

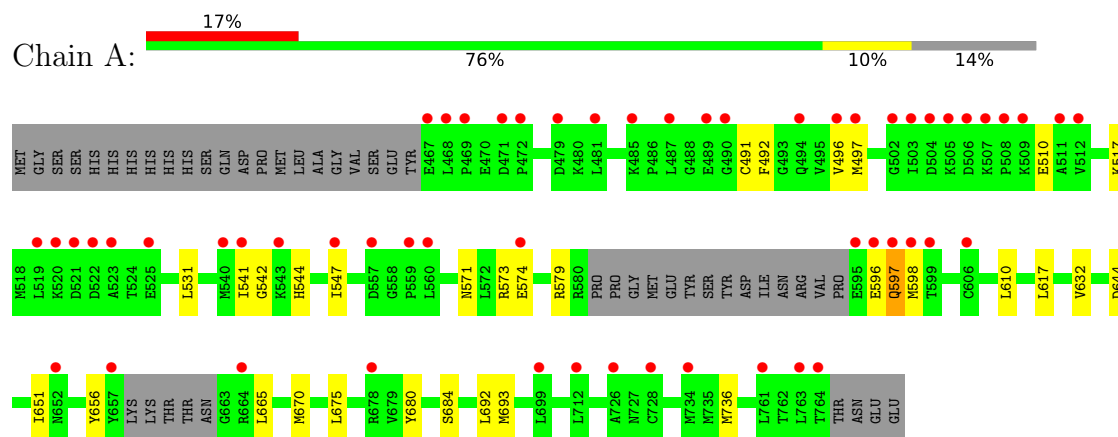
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	39	Total O 39 39	0	0
4	B	35	Total O 35 35	0	0
4	C	35	Total O 35 35	0	0
4	D	40	Total O 40 40	0	0

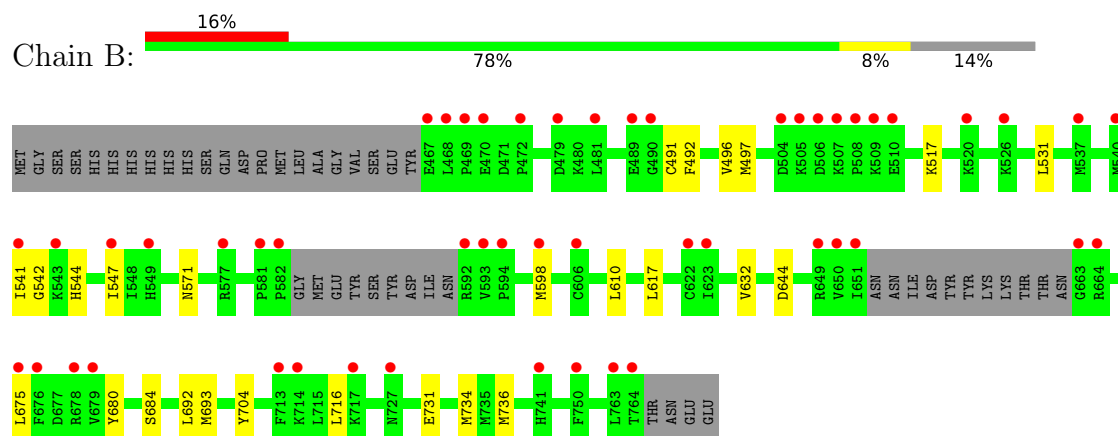
3 Residue-property plots [i](#)

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.

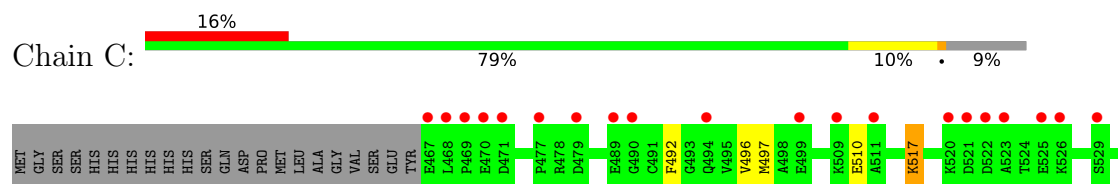
• Molecule 1: Fibroblast growth factor receptor 2

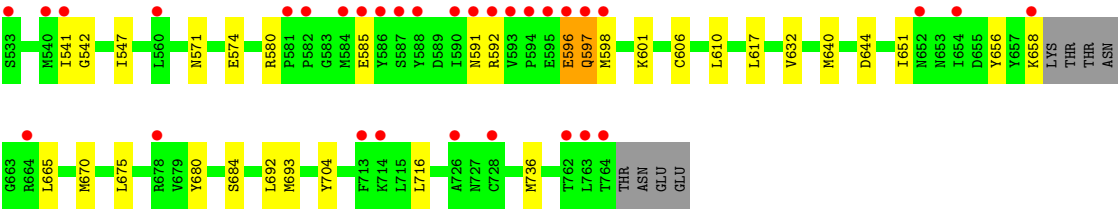


• Molecule 1: Fibroblast growth factor receptor 2

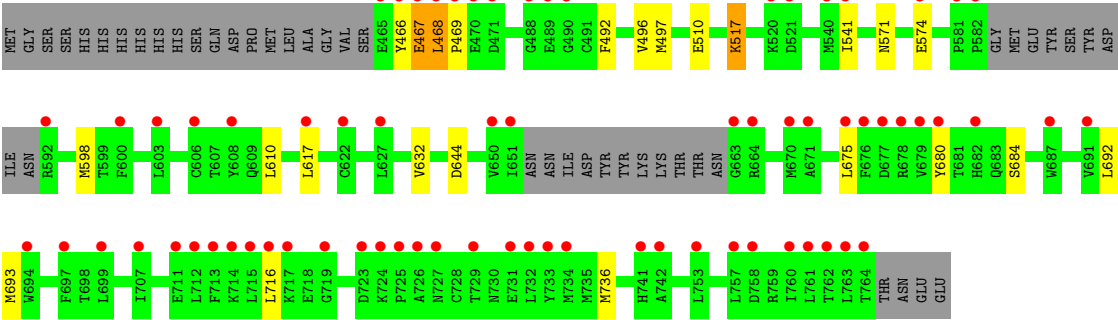
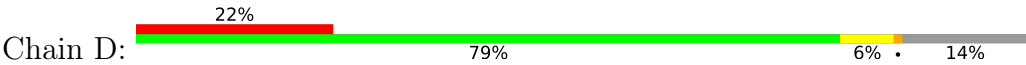


• Molecule 1: Fibroblast growth factor receptor 2





● Molecule 1: Fibroblast growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.31Å 131.40Å 134.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.23 50.01 – 2.23	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.01-2.23) 98.2 (50.01-2.23)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.291 , 0.312 0.289 , 0.310	Depositor DCC
R_{free} test set	3459 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9349	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.40 % 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 2.3746e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: TZ0, SO4

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	0.44	0/2283	0.94	0/3080
1	B	0.44	0/2267	0.93	1/3060 (0.0%)
1	C	0.44	0/2418	0.93	1/3266 (0.0%)
1	D	0.44	0/2289	0.93	0/3090
All	All	0.44	0/9257	0.93	2/12496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	704	TYR	CB-CA-C	5.58	115.85	111.00
1	B	704	TYR	CB-CA-C	5.07	115.41	111.00

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	2237	0	2244	21	0
1	B	2220	0	2242	16	0
1	C	2363	0	2368	17	0
1	D	2241	0	2257	15	0
2	A	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	0	1	0
2	C	31	0	0	0	0
2	D	31	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	39	0	0	0	0
4	B	35	0	0	0	0
4	C	35	0	0	0	0
4	D	40	0	0	0	0
All	All	9349	0	9111	69	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 (69) 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:492:PHE:O	1:D:517:LYS:HE2	1.73	0.89
1:C:492:PHE:O	1:C:517:LYS:HE2	1.73	0.86
1:A:492:PHE:O	1:A:517:LYS:HE3	1.78	0.84
1:B:492:PHE:O	1:B:517:LYS:HE3	1.78	0.84
1:D:466:TYR:OH	1:D:468:LEU:HD12	1.79	0.83
1:C:606[B]:CYS:SG	1:C:640:MET:HE3	2.36	0.65
1:C:596:GLU:O	1:C:597:GLN:O	2.21	0.58
1:A:573:ARG:HH11	1:A:573:ARG:HG2	1.69	0.58
1:C:693:MET:HB3	1:C:736:MET:HE2	1.86	0.57
1:A:693:MET:HB3	1:A:736:MET:HE2	1.87	0.57
1:B:731:GLU:HA	1:B:734:MET:CE	2.35	0.57
1:A:596:GLU:O	1:A:597:GLN:O	2.22	0.56
1:A:598:MET:HA	1:A:598:MET:HE2	1.85	0.56
1:D:466:TYR:HH	1:D:468:LEU:HD12	1.71	0.56
1:D:693:MET:HB3	1:D:736:MET:HE2	1.88	0.55
1:A:517:LYS:HD3	1:A:531:LEU:HD13	1.87	0.55
1:D:598:MET:HA	1:D:598:MET:HE2	1.89	0.54
1:C:598:MET:HA	1:C:598:MET:HE2	1.88	0.54
1:B:693:MET:HB3	1:B:736:MET:HE2	1.90	0.54
1:A:579:ARG:HD3	1:A:598:MET:HE3	1.88	0.54
1:B:598:MET:HA	1:B:598:MET:HE2	1.89	0.53
1:A:517:LYS:HD3	1:A:531:LEU:CD1	2.39	0.52
1:B:544:HIS:HB3	1:B:547:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:LYS:HD3	1:B:531:LEU:CD1	2.40	0.52
1:C:610:LEU:HD13	1:C:692:LEU:HD21	1.89	0.52
1:A:544:HIS:HB3	1:A:547:ILE:HG12	1.91	0.52
1:A:610:LEU:HD13	1:A:692:LEU:HD21	1.90	0.52
1:D:610:LEU:HD13	1:D:692:LEU:HD21	1.90	0.52
1:C:547:ILE:HD11	1:C:617:LEU:HG	1.91	0.52
1:B:517:LYS:HD3	1:B:531:LEU:HD13	1.91	0.52
1:B:610:LEU:HD13	1:B:692:LEU:HD21	1.91	0.52
1:C:680:TYR:CE1	1:C:684:SER:HB2	2.47	0.50
1:A:680:TYR:CE1	1:A:684:SER:HB2	2.47	0.49
1:D:468:LEU:HD23	1:D:469:PRO:HD2	1.94	0.49
1:B:731:GLU:HA	1:B:734:MET:HE2	1.93	0.49
1:B:680:TYR:CE1	1:B:684:SER:HB2	2.47	0.49
1:D:680:TYR:CE1	1:D:684:SER:HB2	2.47	0.48
1:D:541:ILE:HG21	1:D:617:LEU:HD21	1.97	0.47
1:D:466:TYR:C	1:D:467:GLU:HG2	2.38	0.47
1:C:651:ILE:HG22	1:C:656:TYR:HD1	1.79	0.47
1:A:541:ILE:HD13	1:A:547:ILE:HD12	1.96	0.46
1:B:541:ILE:HD13	1:B:547:ILE:HD12	1.96	0.46
1:B:491:CYS:HB2	2:B:801:TZ0:C0P	2.45	0.46
1:C:571:ASN:OD1	1:C:574:GLU:HG2	2.15	0.46
1:A:651:ILE:HG22	1:A:656:TYR:HD1	1.80	0.46
1:A:571:ASN:OD1	1:A:574:GLU:HG2	2.15	0.46
1:D:571:ASN:OD1	1:D:574:GLU:HG2	2.16	0.46
1:D:617:LEU:HA	1:D:617:LEU:HD23	1.83	0.45
1:A:573:ARG:HG2	1:A:573:ARG:NH1	2.30	0.44
1:B:496:VAL:HG12	1:B:497:MET:O	2.18	0.43
1:D:541:ILE:HG21	1:D:617:LEU:CD2	2.49	0.43
1:A:496:VAL:HG12	1:A:497:MET:O	2.18	0.43
1:D:496:VAL:HG12	1:D:497:MET:O	2.18	0.43
1:D:571:ASN:HA	1:D:632:VAL:O	2.19	0.43
1:B:571:ASN:HA	1:B:632:VAL:O	2.18	0.43
1:C:591:ASN:O	1:C:592:ARG:HB2	2.18	0.43
1:C:571:ASN:HA	1:C:632:VAL:O	2.18	0.43
1:C:496:VAL:HG12	1:C:497:MET:O	2.18	0.42
1:C:541:ILE:HD12	1:C:542:GLY:O	2.19	0.42
1:A:541:ILE:HD12	1:A:542:GLY:O	2.20	0.42
1:A:571:ASN:HA	1:A:632:VAL:O	2.19	0.42
1:C:617:LEU:HD23	1:C:617:LEU:HA	1.83	0.42
1:C:580:ARG:NH1	1:C:585:GLU:O	2.53	0.42
1:A:617:LEU:HD23	1:A:617:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:ILE:HD12	1:B:542:GLY:O	2.20	0.42
1:A:491:CYS:HB2	2:A:801:TZ0:C0P	2.50	0.41
1:C:665:LEU:HD12	1:C:670:MET:HE3	2.02	0.41
1:B:617:LEU:HD23	1:B:617:LEU:HA	1.83	0.41
1:A:665:LEU:HD12	1:A:670:MET:HE3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/324 (84%)	268 (98%)	3 (1%)	2 (1%)	18	16
1	B	272/324 (84%)	267 (98%)	4 (2%)	1 (0%)	30	30
1	C	291/324 (90%)	284 (98%)	5 (2%)	2 (1%)	18	16
1	D	274/324 (85%)	269 (98%)	4 (2%)	1 (0%)	30	30
All	All	1110/1296 (86%)	1088 (98%)	16 (1%)	6 (0%)	24	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	597	GLN
1	C	597	GLN
1	A	644	ASP
1	B	644	ASP
1	C	644	ASP
1	D	644	ASP

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	244/285 (86%)	242 (99%)	2 (1%)	73	80
1	B	243/285 (85%)	241 (99%)	2 (1%)	73	80
1	C	259/285 (91%)	252 (97%)	7 (3%)	39	47
1	D	245/285 (86%)	239 (98%)	6 (2%)	43	51
All	All	991/1140 (87%)	974 (98%)	17 (2%)	53	63

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	510	GLU
1	A	675	LEU
1	B	675	LEU
1	B	716	LEU
1	C	510	GLU
1	C	517	LYS
1	C	596	GLU
1	C	601	LYS
1	C	658	LYS
1	C	675	LEU
1	C	716	LEU
1	D	467	GLU
1	D	468	LEU
1	D	510	GLU
1	D	517	LYS
1	D	675	LEU
1	D	716	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	GLN
1	D	597	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	TZ0	C	801	1	32,34,34	2.16	8 (25%)	44,48,48	2.71	16 (36%)
3	SO4	B	802	-	4,4,4	0.34	0	6,6,6	0.08	0
2	TZ0	D	801	1	32,34,34	2.09	7 (21%)	44,48,48	2.67	16 (36%)
2	TZ0	B	801	1	32,34,34	2.05	6 (18%)	44,48,48	2.67	15 (34%)
2	TZ0	A	801	1	32,34,34	2.07	6 (18%)	44,48,48	2.65	13 (29%)
3	SO4	A	802	-	4,4,4	0.34	0	6,6,6	0.09	0
3	SO4	C	802	-	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
2	TZ0	C	801	1	-	6/17/28/28	0/4/4/4
2	TZ0	D	801	1	-	11/17/28/28	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TZ0	B	801	1	-	8/17/28/28	0/4/4/4
2	TZ0	A	801	1	-	6/17/28/28	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	TZ0	C0A-C0F	-6.68	1.35	1.42
2	C	801	TZ0	C0A-C0F	-6.60	1.35	1.42
2	B	801	TZ0	C0A-C0F	-6.60	1.35	1.42
2	A	801	TZ0	C0A-C0F	-6.42	1.35	1.42
2	A	801	TZ0	C0V-C0M	4.96	1.54	1.30
2	D	801	TZ0	C0V-C0M	4.91	1.54	1.30
2	C	801	TZ0	C0V-C0M	4.86	1.53	1.30
2	B	801	TZ0	C0V-C0M	4.85	1.53	1.30
2	C	801	TZ0	C0A-C0B	-4.71	1.34	1.40
2	D	801	TZ0	C0A-C0B	-4.66	1.34	1.40
2	B	801	TZ0	C0A-C0B	-4.55	1.34	1.40
2	A	801	TZ0	C0A-C0B	-4.35	1.35	1.40
2	A	801	TZ0	C0L-N08	3.86	1.40	1.33
2	C	801	TZ0	C0L-N08	3.80	1.40	1.33
2	A	801	TZ0	C0L-N06	3.70	1.40	1.33
2	D	801	TZ0	C0L-N08	3.69	1.40	1.33
2	B	801	TZ0	C0L-N08	3.65	1.40	1.33
2	B	801	TZ0	C0L-N06	3.61	1.40	1.33
2	C	801	TZ0	C0L-N06	3.60	1.40	1.33
2	D	801	TZ0	C0L-N06	3.34	1.39	1.33
2	C	801	TZ0	C0H-C0S	-2.96	1.15	1.20
2	D	801	TZ0	N04-N09	-2.49	1.33	1.38
2	D	801	TZ0	C0K-N04	2.29	1.50	1.46
2	A	801	TZ0	N04-N09	-2.28	1.34	1.38
2	B	801	TZ0	N04-N09	-2.27	1.34	1.38
2	C	801	TZ0	N04-N09	-2.20	1.34	1.38
2	C	801	TZ0	C0K-N04	2.17	1.50	1.46

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	TZ0	N08-C0L-N06	-7.12	117.81	128.58
2	B	801	TZ0	N08-C0L-N06	-7.07	117.88	128.58
2	C	801	TZ0	N08-C0L-N06	-6.83	118.24	128.58
2	A	801	TZ0	N08-C0L-N06	-6.69	118.45	128.58
2	C	801	TZ0	C0F-C0A-C0B	6.28	120.44	115.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	TZ0	C0F-C0A-C0B	6.15	120.35	115.74
2	B	801	TZ0	C0F-C0A-C0B	6.07	120.29	115.74
2	B	801	TZ0	C0A-C0B-N08	-5.97	120.63	126.97
2	A	801	TZ0	C0A-C0B-N08	-5.90	120.70	126.97
2	C	801	TZ0	C0A-C0B-N08	-5.86	120.75	126.97
2	D	801	TZ0	C0F-C0A-C0B	5.86	120.13	115.74
2	D	801	TZ0	C0A-C0B-N08	-5.70	120.92	126.97
2	D	801	TZ0	C0V-C0M-C0P	-5.60	109.91	121.27
2	A	801	TZ0	C0V-C0M-C0P	-5.46	110.19	121.27
2	B	801	TZ0	C0V-C0M-C0P	-5.42	110.27	121.27
2	C	801	TZ0	C0V-C0M-C0P	-5.35	110.42	121.27
2	C	801	TZ0	C0F-C0A-C0G	-5.23	133.70	139.12
2	A	801	TZ0	C0F-C0A-C0G	-4.96	133.98	139.12
2	B	801	TZ0	C0F-C0A-C0G	-4.89	134.05	139.12
2	D	801	TZ0	C0F-C0A-C0G	-4.86	134.09	139.12
2	C	801	TZ0	C0B-N04-N09	-4.72	107.88	110.90
2	B	801	TZ0	C0B-N04-N09	-4.66	107.92	110.90
2	A	801	TZ0	C0B-N04-N09	-4.60	107.95	110.90
2	D	801	TZ0	C0B-N04-N09	-4.55	107.99	110.90
2	C	801	TZ0	C0A-C0F-N05	-4.20	117.85	123.40
2	D	801	TZ0	C0A-C0F-N05	-4.10	117.99	123.40
2	D	801	TZ0	C0T-N07-C0I	-4.07	107.62	112.38
2	A	801	TZ0	C0A-C0F-N05	-3.98	118.14	123.40
2	B	801	TZ0	C0A-C0F-N05	-3.92	118.23	123.40
2	A	801	TZ0	C0A-C0F-N06	3.73	121.98	118.64
2	C	801	TZ0	C0A-C0F-N06	3.55	121.83	118.64
2	B	801	TZ0	C0A-C0F-N06	3.54	121.82	118.64
2	B	801	TZ0	C0L-N08-C0B	3.42	120.19	111.83
2	D	801	TZ0	C0G-N09-N04	3.41	107.06	103.81
2	A	801	TZ0	C0G-N09-N04	3.40	107.05	103.81
2	A	801	TZ0	N08-C0B-N04	3.39	130.46	126.05
2	D	801	TZ0	C0A-C0F-N06	3.37	121.67	118.64
2	B	801	TZ0	N08-C0B-N04	3.36	130.43	126.05
2	C	801	TZ0	C0G-N09-N04	3.33	106.99	103.81
2	C	801	TZ0	N08-C0B-N04	3.33	130.38	126.05
2	D	801	TZ0	C0L-N08-C0B	3.32	119.94	111.83
2	C	801	TZ0	C0L-N08-C0B	3.31	119.90	111.83
2	A	801	TZ0	C0L-N08-C0B	3.28	119.85	111.83
2	D	801	TZ0	N08-C0B-N04	3.27	130.31	126.05
2	B	801	TZ0	C0G-N09-N04	3.17	106.83	103.81
2	A	801	TZ0	C0T-N07-C0I	-2.96	108.93	112.38
2	C	801	TZ0	C0Q-C0T-N07	2.92	106.69	102.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	TZ0	C0Q-C0T-N07	2.79	106.53	102.93
2	B	801	TZ0	C0A-C0B-N04	2.75	108.94	107.19
2	C	801	TZ0	C0A-C0B-N04	2.63	108.86	107.19
2	A	801	TZ0	C0A-C0B-N04	2.58	108.83	107.19
2	D	801	TZ0	C0A-C0B-N04	2.48	108.77	107.19
2	C	801	TZ0	C0Q-C0K-C0I	2.47	106.39	102.22
2	C	801	TZ0	C0K-N04-N09	2.47	125.68	119.89
2	B	801	TZ0	C0T-N07-C0I	-2.42	109.55	112.38
2	B	801	TZ0	C0K-N04-N09	2.30	125.28	119.89
2	C	801	TZ0	C0T-N07-C0I	-2.22	109.79	112.38
2	D	801	TZ0	C0A-C0G-C0H	2.15	128.77	123.49
2	D	801	TZ0	C0K-N04-N09	2.12	124.86	119.89
2	D	801	TZ0	C0Q-C0K-C0I	2.10	105.75	102.22

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	TZ0	C0G-C0H-C0S-C0J
2	B	801	TZ0	C0G-C0H-C0S-C0J
2	B	801	TZ0	C0I-C0K-N04-N09
2	B	801	TZ0	C0Q-C0K-N04-C0B
2	C	801	TZ0	C0I-C0K-N04-N09
2	C	801	TZ0	C0Q-C0K-N04-C0B
2	D	801	TZ0	C0G-C0H-C0S-C0J
2	D	801	TZ0	C0I-C0K-N04-N09
2	D	801	TZ0	C0Q-C0K-N04-C0B
2	D	801	TZ0	C0O-C0E-O01-C0N
2	D	801	TZ0	C0C-C0E-O01-C0N
2	D	801	TZ0	C0V-C0M-C0P-O03
2	B	801	TZ0	C0V-C0M-C0P-N07
2	A	801	TZ0	C0I-C0K-N04-N09
2	D	801	TZ0	C0Q-C0K-N04-N09
2	C	801	TZ0	C0G-C0H-C0S-C0J
2	B	801	TZ0	C0C-C0D-O02-C0U
2	B	801	TZ0	C0R-C0D-O02-C0U
2	B	801	TZ0	C0V-C0M-C0P-O03
2	A	801	TZ0	C0V-C0M-C0P-N07
2	D	801	TZ0	C0V-C0M-C0P-N07
2	A	801	TZ0	C0Q-C0K-N04-C0B
2	D	801	TZ0	C0I-C0K-N04-C0B
2	A	801	TZ0	C0Q-C0K-N04-N09

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Mol	Chain	Res	Type	Atoms
2	C	801	TZ0	C0Q-C0K-N04-N09
2	C	801	TZ0	C0V-C0M-C0P-N07
2	D	801	TZ0	C0C-C0D-O02-C0U
2	D	801	TZ0	C0R-C0D-O02-C0U
2	B	801	TZ0	C0Q-C0K-N04-N09
2	A	801	TZ0	C0V-C0M-C0P-O03
2	C	801	TZ0	C0V-C0M-C0P-O03

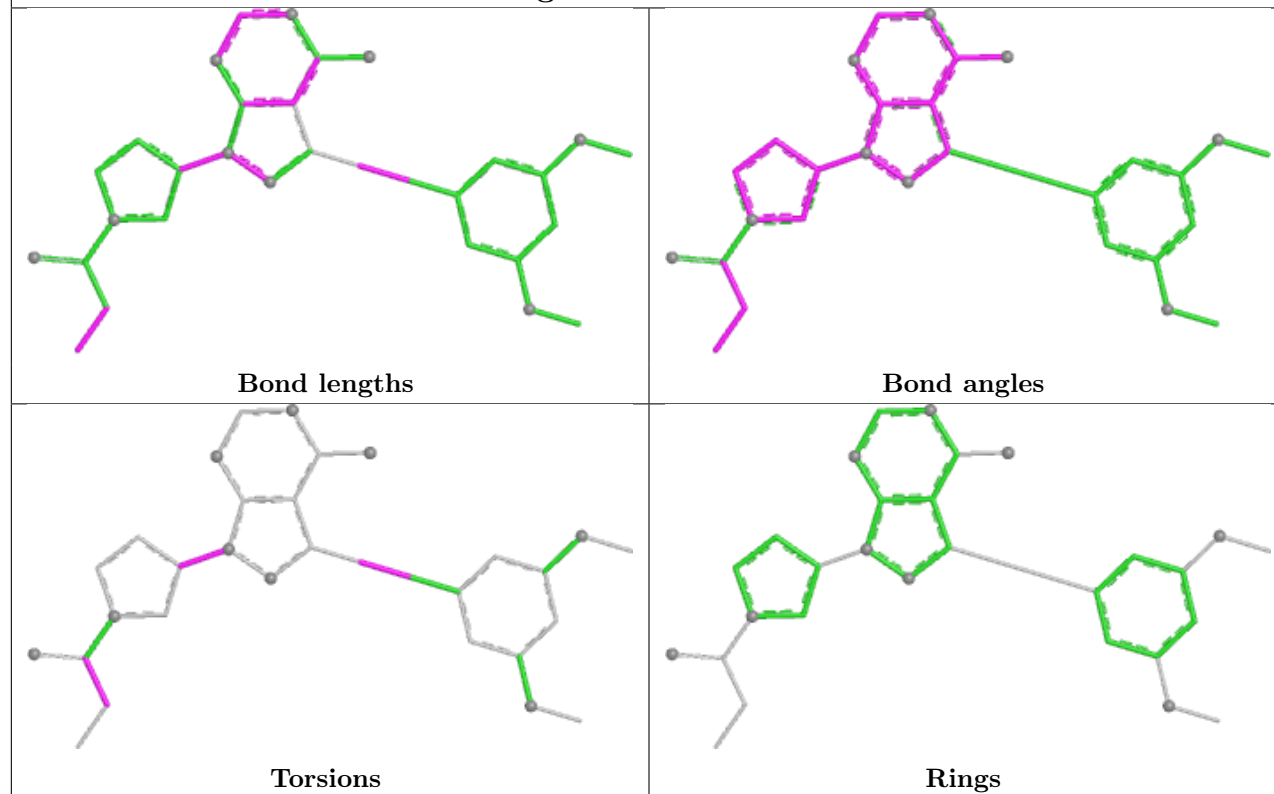
There are no ring outliers.

2 monomers are involved in 2 short contacts:

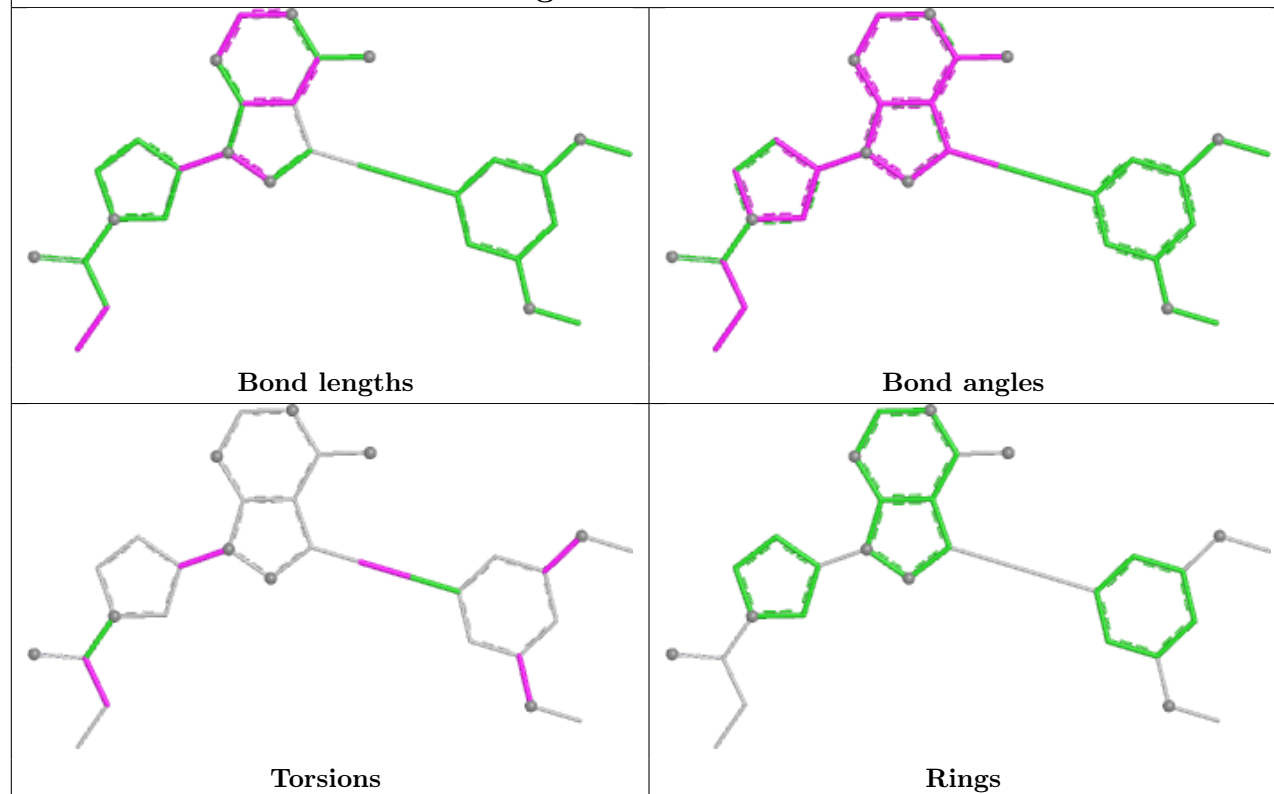
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	TZ0	1	0
2	A	801	TZ0	1	0

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.

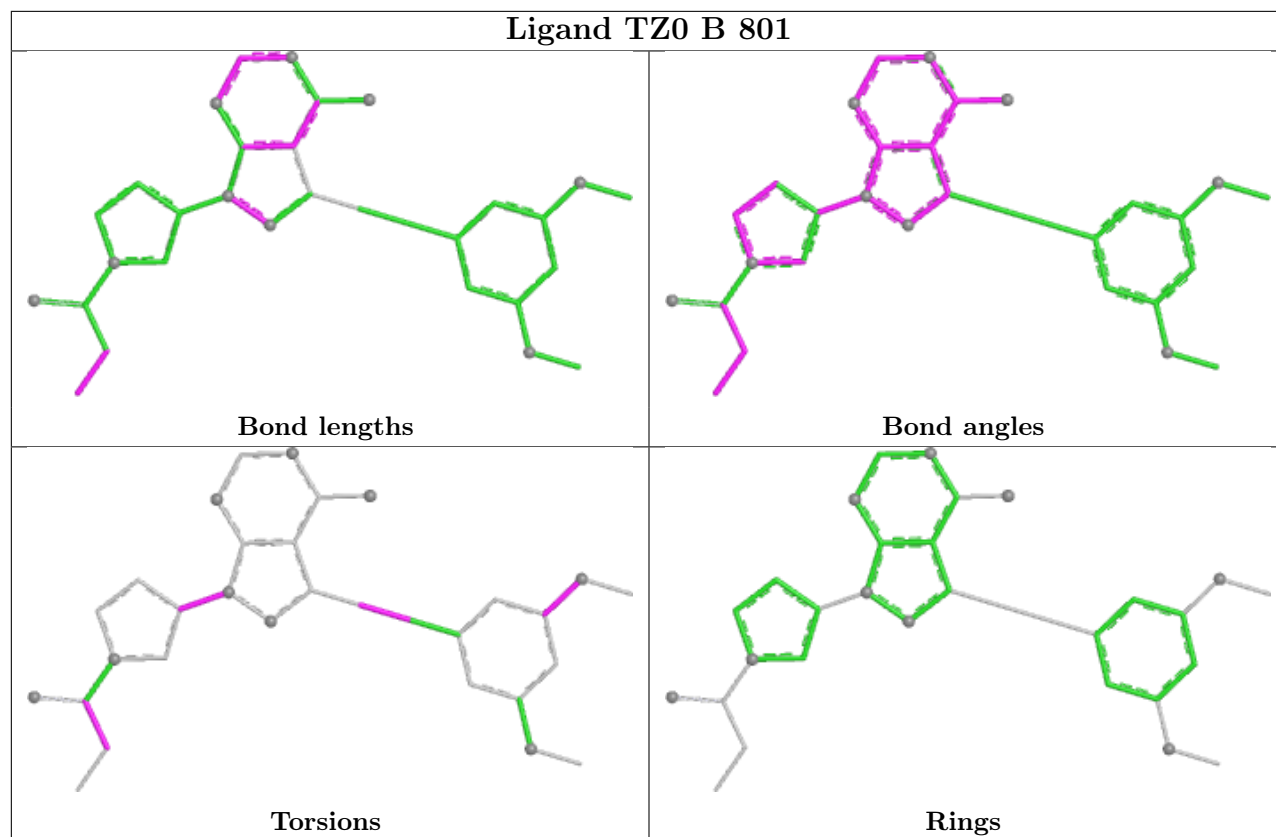
Ligand TZ0 C 801



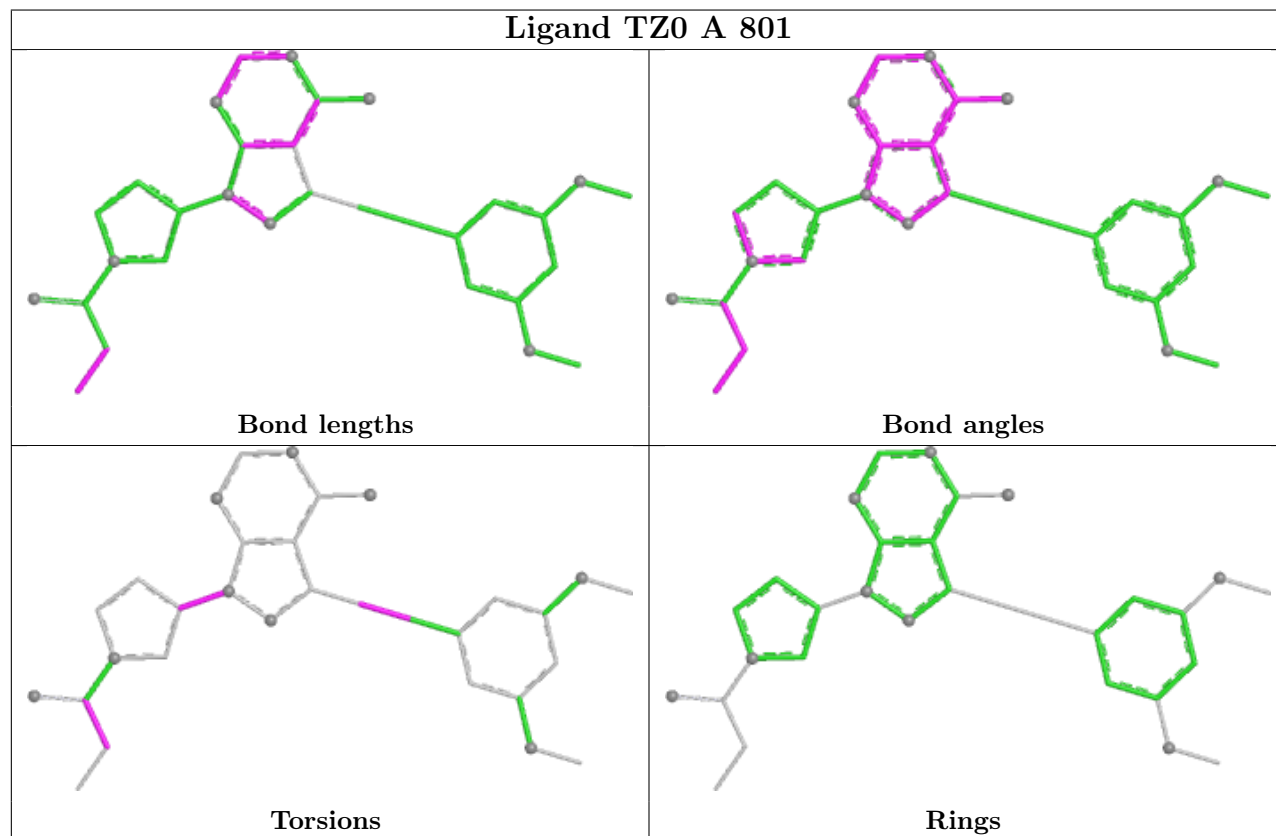
Ligand TZ0 D 801



Ligand TZ0 B 801



Ligand TZ0 A 801



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, 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	279/324 (86%)	1.33	56 (20%) 3 2	26, 45, 74, 99	0
1	B	278/324 (85%)	1.31	51 (18%) 3 2	24, 42, 68, 82	0
1	C	294/324 (90%)	1.23	52 (17%) 4 3	21, 41, 71, 84	1 (0%)
1	D	280/324 (86%)	1.46	72 (25%) 1 1	25, 44, 69, 88	0
All	All	1131/1296 (87%)	1.33	231 (20%) 3 2	21, 43, 71, 99	1 (0%)

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	470	GLU	5.1
1	A	764	THR	5.0
1	C	581	PRO	4.9
1	D	764	THR	4.9
1	A	728	CYS	4.8
1	A	509	LYS	4.7
1	C	764	THR	4.6
1	A	508	PRO	4.6
1	B	468	LEU	4.6
1	A	763	LEU	4.5
1	B	540	MET	4.5
1	A	595	GLU	4.4
1	D	582	PRO	4.3
1	C	590	ILE	4.3
1	D	650	VAL	4.3
1	D	726	ALA	4.2
1	A	734	MET	4.2
1	C	586	TYR	4.1
1	B	467	GLU	4.1
1	D	663	GLY	4.1
1	B	508	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	764	THR	4.1
1	B	651	ILE	4.1
1	D	622	CYS	4.0
1	C	592	ARG	4.0
1	D	600	PHE	3.9
1	C	582	PRO	3.9
1	A	520	LYS	3.9
1	B	592	ARG	3.9
1	B	581	PRO	3.9
1	D	606	CYS	3.8
1	B	622	CYS	3.8
1	B	509	LYS	3.8
1	B	506	ASP	3.8
1	A	505	LYS	3.7
1	C	467	GLU	3.7
1	D	466	TYR	3.7
1	C	594	PRO	3.7
1	D	467	GLU	3.7
1	D	468	LEU	3.7
1	C	658	LYS	3.7
1	C	588	TYR	3.6
1	D	713	PHE	3.6
1	D	760	ILE	3.6
1	A	467	GLU	3.6
1	D	734	MET	3.5
1	C	470	GLU	3.5
1	D	742	ALA	3.5
1	A	574	GLU	3.4
1	A	596	GLU	3.4
1	C	763	LEU	3.4
1	C	593	VAL	3.3
1	D	469	PRO	3.3
1	D	540	MET	3.3
1	B	582	PRO	3.3
1	D	727	ASN	3.2
1	B	750	PHE	3.2
1	B	650	VAL	3.2
1	A	598	MET	3.2
1	A	468	LEU	3.2
1	D	763	LEU	3.1
1	D	716	LEU	3.1
1	D	731	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	623	ILE	3.1
1	A	489	GLU	3.1
1	C	596	GLU	3.1
1	A	472	PRO	3.1
1	C	541	ILE	3.0
1	B	663	GLY	3.0
1	D	490	GLY	3.0
1	B	763	LEU	3.0
1	D	541	ILE	3.0
1	C	490	GLY	3.0
1	B	469	PRO	3.0
1	D	675	LEU	2.9
1	A	606	CYS	2.9
1	D	679	VAL	2.9
1	D	714	LYS	2.9
1	C	597	GLN	2.9
1	B	537	MET	2.9
1	D	680	TYR	2.9
1	D	723	ASP	2.9
1	B	717	LYS	2.9
1	C	728	CYS	2.9
1	B	727	ASN	2.9
1	D	757	LEU	2.9
1	C	540	MET	2.9
1	A	652	ASN	2.9
1	C	521	ASP	2.9
1	C	520	LYS	2.8
1	C	591	ASN	2.8
1	B	490	GLY	2.8
1	D	488	GLY	2.8
1	D	732	LEU	2.8
1	B	713	PHE	2.8
1	B	547	ILE	2.8
1	A	494	GLN	2.8
1	A	507	LYS	2.8
1	B	664	ARG	2.8
1	D	724	LYS	2.8
1	D	592	ARG	2.8
1	A	503	ILE	2.7
1	D	762	THR	2.7
1	A	469	PRO	2.7
1	B	606	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	472	PRO	2.7
1	B	549	HIS	2.7
1	A	521	ASP	2.7
1	D	651	ILE	2.7
1	C	678	ARG	2.7
1	B	507	LYS	2.6
1	D	676	PHE	2.6
1	A	506	ASP	2.6
1	A	522	ASP	2.6
1	B	594	PRO	2.6
1	C	489	GLU	2.6
1	D	677	ASP	2.6
1	C	713	PHE	2.6
1	D	697	PHE	2.6
1	A	599	THR	2.6
1	D	729	THR	2.6
1	C	587	SER	2.6
1	D	717	LYS	2.6
1	C	469	PRO	2.6
1	B	481	LEU	2.5
1	D	694	TRP	2.5
1	B	520	LYS	2.5
1	D	682	HIS	2.5
1	B	675	LEU	2.5
1	C	468	LEU	2.5
1	C	584	MET	2.5
1	C	598	MET	2.5
1	D	671	ALA	2.5
1	A	502	GLY	2.5
1	C	529	SER	2.5
1	D	715	LEU	2.5
1	C	479	ASP	2.5
1	A	678	ARG	2.5
1	D	664	ARG	2.5
1	D	699	LEU	2.5
1	B	598	MET	2.5
1	C	522	ASP	2.5
1	D	581	PRO	2.5
1	A	512	VAL	2.4
1	A	487	LEU	2.4
1	D	670	MET	2.4
1	A	479	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	496	VAL	2.4
1	B	541	ILE	2.4
1	D	627	LEU	2.4
1	C	664	ARG	2.4
1	D	711	GLU	2.4
1	B	505	LYS	2.4
1	C	509	LYS	2.4
1	A	664	ARG	2.4
1	A	504	ASP	2.4
1	A	497	MET	2.4
1	A	541	ILE	2.4
1	A	519	LEU	2.4
1	D	761	LEU	2.4
1	A	543	LYS	2.3
1	A	540	MET	2.3
1	B	741	HIS	2.3
1	A	511	ALA	2.3
1	A	523	ALA	2.3
1	B	593	VAL	2.3
1	D	741	HIS	2.3
1	B	479	ASP	2.3
1	C	526	LYS	2.3
1	A	726	ALA	2.3
1	D	465	GLU	2.3
1	B	676	PHE	2.3
1	A	712	LEU	2.3
1	B	543	LYS	2.3
1	D	712	LEU	2.3
1	C	523	ALA	2.3
1	C	533	SER	2.3
1	D	470	GLU	2.3
1	A	761	LEU	2.2
1	D	753	LEU	2.2
1	D	521	ASP	2.2
1	A	490	GLY	2.2
1	A	657	TYR	2.2
1	C	585	GLU	2.2
1	C	595	GLU	2.2
1	C	762	THR	2.2
1	A	560	LEU	2.2
1	A	481	LEU	2.2
1	D	603	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	557	ASP	2.2
1	B	504	ASP	2.2
1	B	649	ARG	2.2
1	D	489	GLU	2.2
1	A	547	ILE	2.2
1	C	652	ASN	2.2
1	A	525	GLU	2.2
1	C	560	LEU	2.1
1	B	510	GLU	2.1
1	B	526	LYS	2.1
1	A	559	PRO	2.1
1	D	719	GLY	2.1
1	B	489	GLU	2.1
1	C	714	LYS	2.1
1	A	699	LEU	2.1
1	C	525	GLU	2.1
1	C	471	ASP	2.1
1	A	597	GLN	2.1
1	D	678	ARG	2.1
1	A	485	LYS	2.1
1	C	499	GLU	2.1
1	C	477	PRO	2.1
1	D	608	TYR	2.1
1	D	733	TYR	2.1
1	B	679	VAL	2.1
1	D	687	TRP	2.1
1	B	714	LYS	2.0
1	C	511	ALA	2.0
1	C	726	ALA	2.0
1	D	574	GLU	2.0
1	C	494	GLN	2.0
1	A	471	ASP	2.0
1	D	471	ASP	2.0
1	D	617	LEU	2.0
1	D	707	ILE	2.0
1	B	577	ARG	2.0
1	D	691	VAL	2.0
1	D	758	ASP	2.0
1	B	678	ARG	2.0
1	C	654	ILE	2.0
1	D	725	PRO	2.0
1	D	520	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

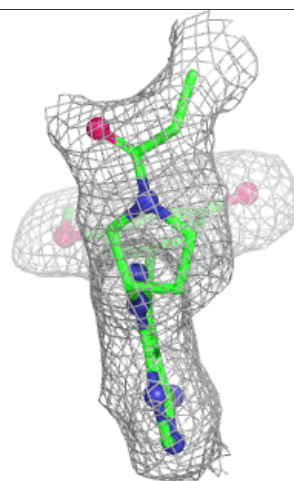
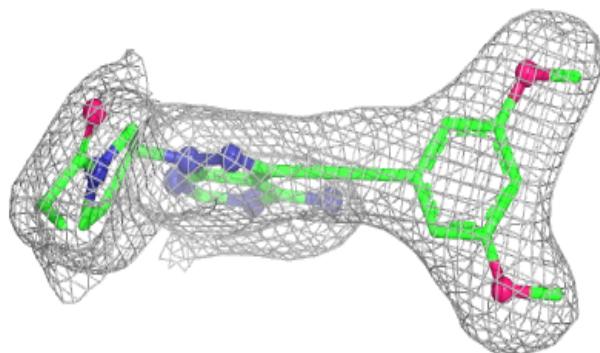
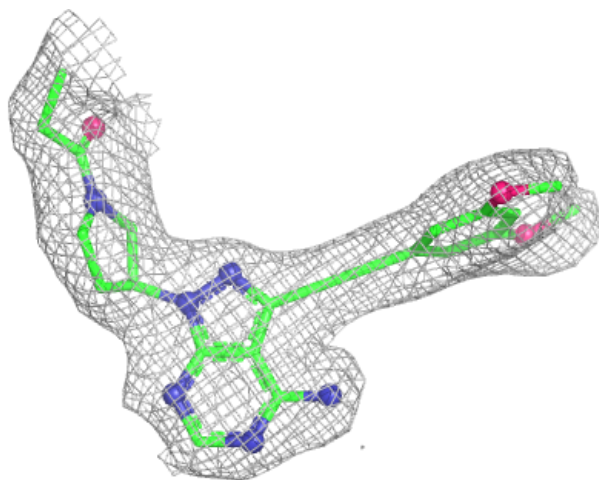
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	802	5/5	0.53	0.26	106,108,112,115	0
3	SO4	A	802	5/5	0.76	0.15	79,82,85,85	0
3	SO4	C	802	5/5	0.81	0.14	72,77,79,79	0
2	TZ0	C	801	31/31	0.91	0.09	26,29,33,37	0
2	TZ0	A	801	31/31	0.92	0.09	26,31,35,38	0
2	TZ0	D	801	31/31	0.94	0.08	23,25,29,31	0
2	TZ0	B	801	31/31	0.94	0.08	23,27,28,31	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.

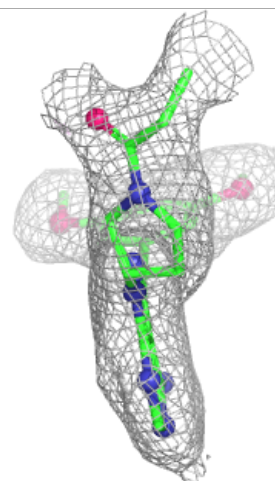
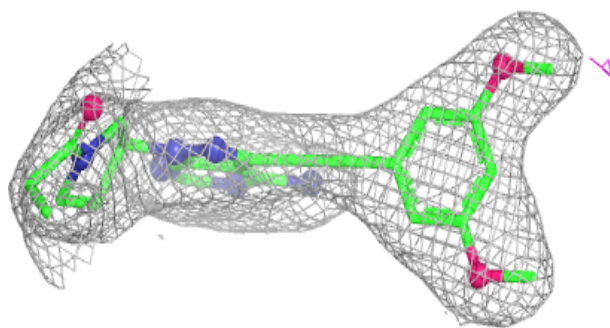
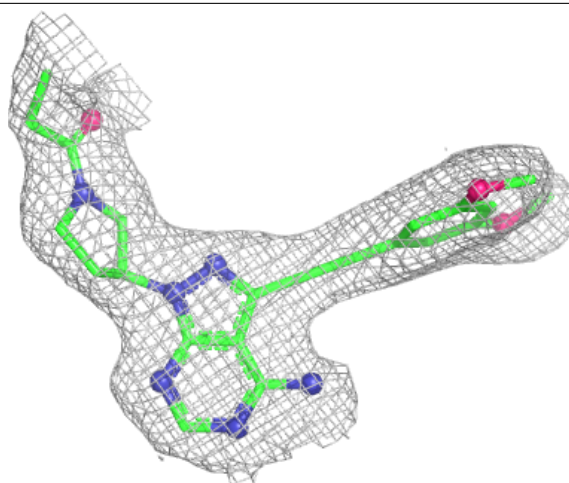
Electron density around TZ0 C 801:

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



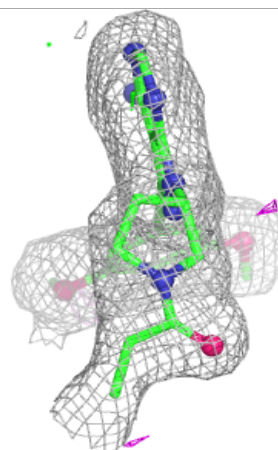
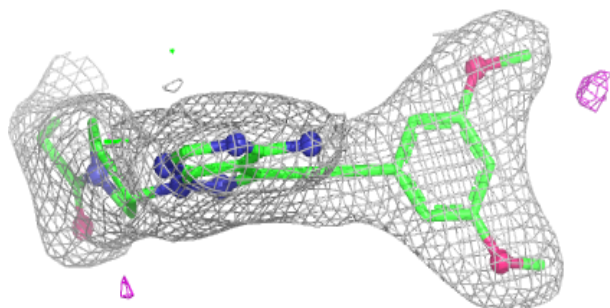
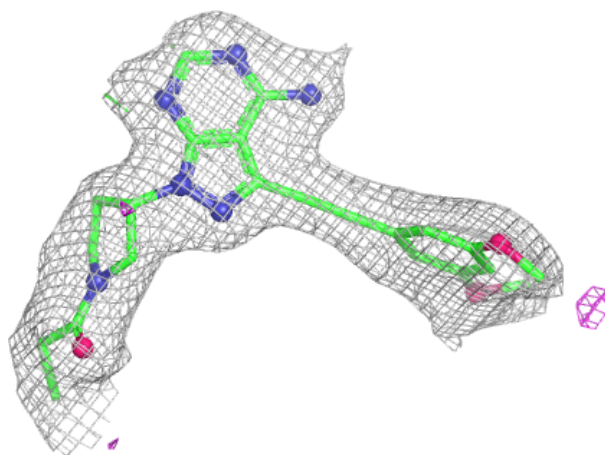
Electron density around TZ0 A 801:

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



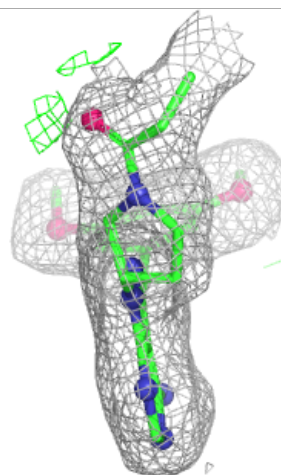
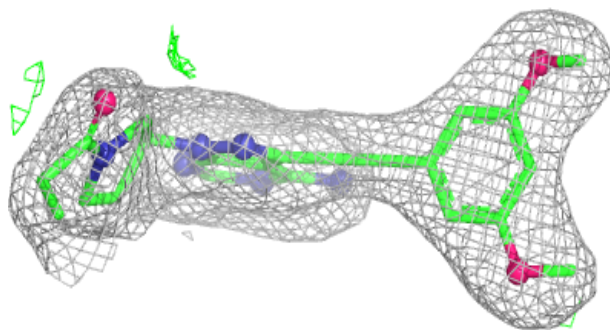
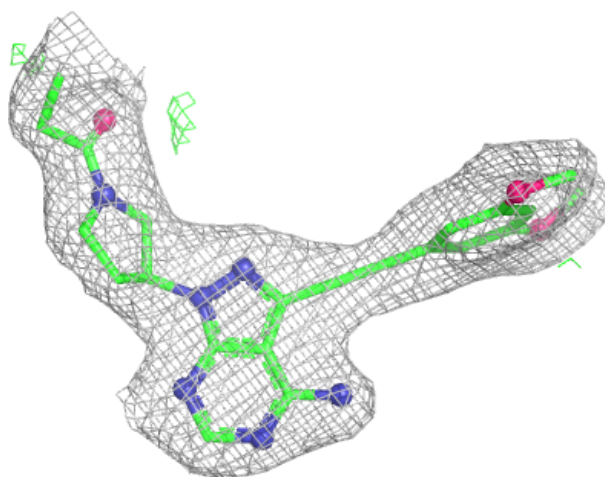
Electron density around TZ0 D 801:

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



Electron density around TZ0 B 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.