



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:46 am BST

PDB ID : 6P68  
Title : Crystal structure of FGFR1-Y563C (FGFR4 surrogate) covalently bound to compound 22.  
Authors : Larsen, N.A.  
Deposited on : 2019-06-03  
Resolution : 2.90 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.

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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	:	2.11
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)	:	2.11

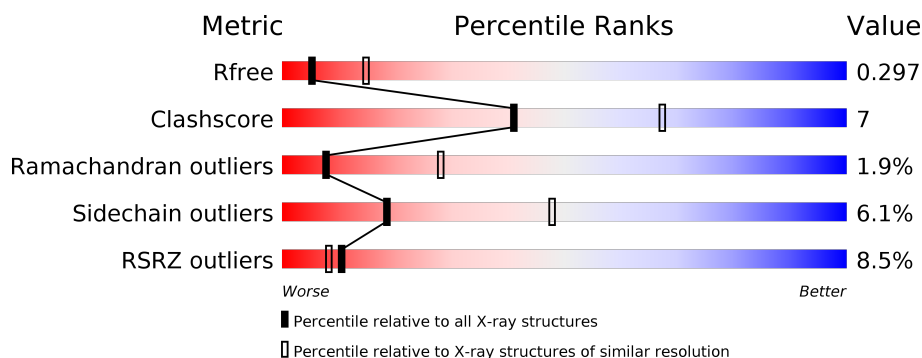
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	309	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	B	309	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 7%</div> </div> </div>
1	C	309	<div> <div>14%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6913 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.

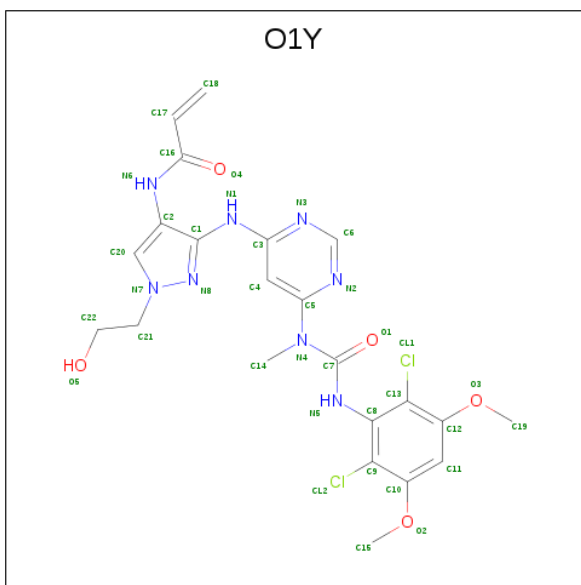
- Molecule 1 is a protein called Fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2268	1442	385	423	18			
1	B	286	Total	C	N	O	S	0	0	0
			2261	1437	384	422	18			
1	C	286	Total	C	N	O	S	0	0	0
			2259	1437	384	420	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	GLY	-	expression tag	UNP P11362
A	488	ALA	CYS	engineered mutation	UNP P11362
A	563	CYS	TYR	engineered mutation	UNP P11362
A	584	SER	CYS	conflict	UNP P11362
B	457	GLY	-	expression tag	UNP P11362
B	488	ALA	CYS	engineered mutation	UNP P11362
B	563	CYS	TYR	engineered mutation	UNP P11362
B	584	SER	CYS	conflict	UNP P11362
C	457	GLY	-	expression tag	UNP P11362
C	488	ALA	CYS	engineered mutation	UNP P11362
C	563	CYS	TYR	engineered mutation	UNP P11362
C	584	SER	CYS	conflict	UNP P11362

- Molecule 2 is N-{3-[(6-{[(2,6-dichloro-3,5-dimethoxyphenyl)carbamoyl](methyl)amino}pyrimidin-4-yl)amino]-1-(2-hydroxyethyl)-1H-pyrazol-4-yl}prop-2-enamide (three-letter code: O1Y) (formula: C<sub>22</sub>H<sub>24</sub>Cl<sub>2</sub>N<sub>8</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			37	22	2	8	5		
2	B	1	Total	C	Cl	N	O	0	0
			37	22	2	8	5		
2	C	1	Total	C	Cl	N	O	0	0
			37	22	2	8	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

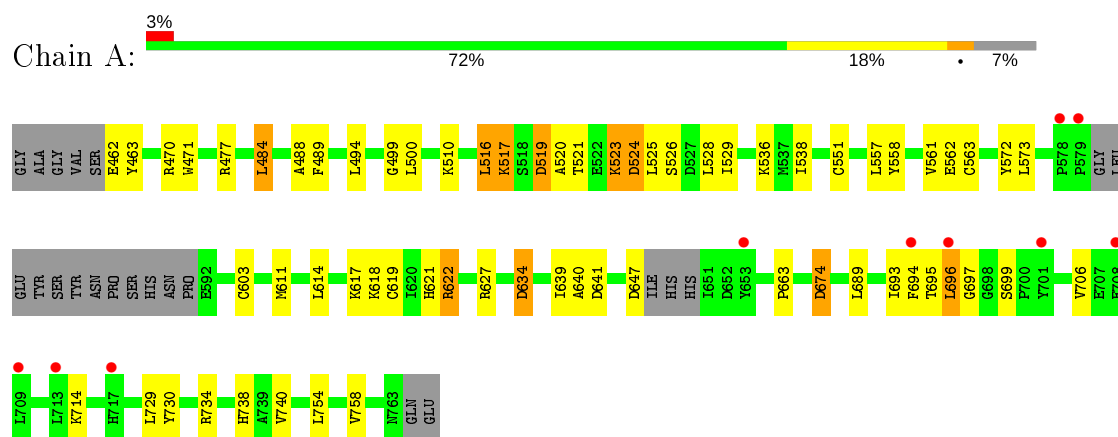
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		
4	C	1	Total	O	0	0
			1	1		

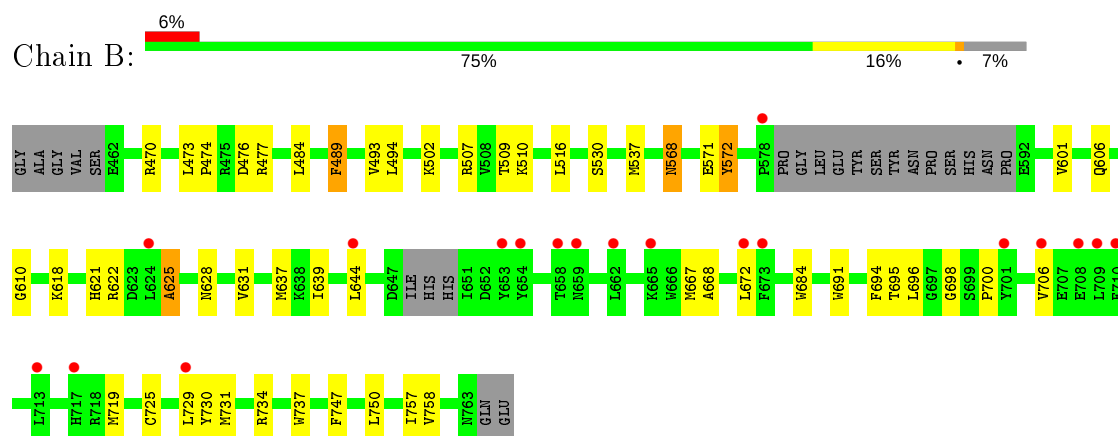
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

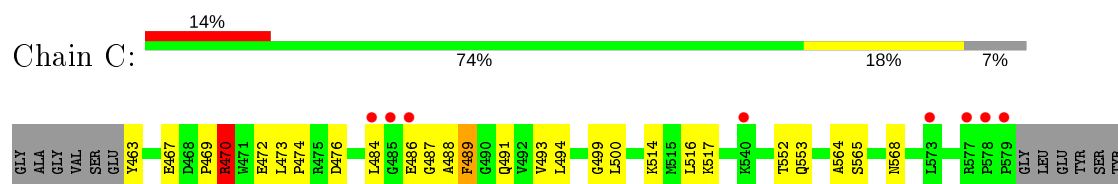
- Molecule 1: Fibroblast growth factor receptor 1

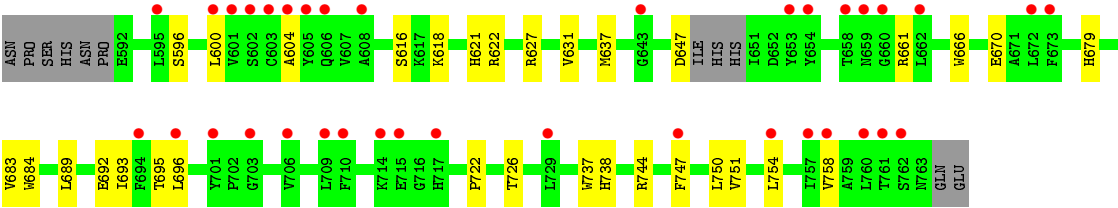


- Molecule 1: Fibroblast growth factor receptor 1



- Molecule 1: Fibroblast growth factor receptor 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.50 Å   79.27 Å   96.72 Å 90.00°   110.53°   90.00°	Depositor
Resolution (Å)	48.28 – 2.90 48.28 – 2.95	Depositor EDS
% Data completeness (in resolution range)	94.0 (48.28-2.90) 96.1 (48.28-2.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 2.96 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.226   ,   0.303 0.215   ,   0.297	Depositor DCC
$R_{free}$ test set	1395 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6913	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: SO4, O1Y

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	0.57	0/2313	0.80	0/3126
1	B	0.48	0/2305	0.67	0/3114
1	C	0.48	0/2304	0.72	0/3114
All	All	0.51	0/6922	0.73	0/9354

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	2268	0	2267	37	0
1	B	2261	0	2260	31	0
1	C	2259	0	2261	25	0
2	A	37	0	0	4	0
2	B	37	0	0	2	0
2	C	37	0	0	5	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
All	All	6913	0	6788	97	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 7.

All (97) 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:C:565:SER:HA	2:C:801:O1Y:C17	2.08	0.82
2:A:801:O1Y:N2	2:A:801:O1Y:N5	2.34	0.71
1:A:689:LEU:HD23	1:A:689:LEU:O	1.92	0.69
2:C:801:O1Y:N2	2:C:801:O1Y:N5	2.39	0.66
1:A:754:LEU:O	1:A:758:VAL:HG23	1.95	0.66
1:A:484:LEU:HD21	1:A:494:LEU:HD21	1.77	0.65
1:A:738:HIS:HD2	1:A:740:VAL:H	1.44	0.65
2:B:801:O1Y:N2	2:B:801:O1Y:N5	2.46	0.62
1:B:484:LEU:HD12	1:B:484:LEU:O	2.00	0.62
1:C:514:LYS:HE2	2:C:801:O1Y:C19	2.29	0.62
1:B:473:LEU:HD12	1:B:474:PRO:HD2	1.83	0.60
1:A:640:ALA:HB1	2:A:801:O1Y:CL2	2.38	0.59
1:A:484:LEU:HD21	1:A:494:LEU:CD2	2.32	0.59
1:A:471:TRP:CD1	1:A:536:LYS:HE2	2.39	0.57
1:B:484:LEU:HD23	1:B:494:LEU:HG	1.87	0.56
1:C:670:GLU:OE2	1:C:744:ARG:NH1	2.37	0.56
1:C:473:LEU:HD12	1:C:474:PRO:HD2	1.86	0.56
1:A:611:MET:SD	1:A:639:ILE:HD13	2.46	0.55
1:A:477:ARG:NE	1:A:477:ARG:HA	2.21	0.55
1:A:516:LEU:HD21	1:A:525:LEU:HA	1.89	0.55
1:A:523:LYS:O	1:A:526:SER:N	2.41	0.54
1:A:689:LEU:O	1:A:693:ILE:HG13	2.08	0.54
1:C:484:LEU:HD21	1:C:494:LEU:HD21	1.89	0.53
1:B:631:VAL:HG13	1:B:637:MET:CE	2.39	0.53
1:A:621:HIS:O	1:A:622:ARG:HB2	2.09	0.52
1:B:568:ASN:OD1	1:B:568:ASN:C	2.47	0.52
1:B:695:THR:O	1:B:696:LEU:C	2.49	0.51
1:C:695:THR:HG22	1:C:722:PRO:HB3	1.92	0.51
1:B:572:TYR:CE2	1:B:631:VAL:HG11	2.45	0.51
1:B:621:HIS:O	1:B:622:ARG:HB2	2.10	0.51
1:B:668:ALA:HB2	1:B:684:TRP:CB	2.41	0.51
1:B:719:MET:O	1:B:730:TYR:OH	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:HIS:O	1:C:683:VAL:HG23	2.10	0.51
1:A:603:CYS:SG	1:A:693:ILE:HD13	2.51	0.51
2:B:801:O1Y:C20	2:B:801:O1Y:O4	2.57	0.50
1:A:617:LYS:O	1:A:618:LYS:HB2	2.09	0.50
1:C:564:ALA:O	2:C:801:O1Y:N6	2.46	0.49
1:C:684:TRP:CE3	1:C:737:TRP:HA	2.48	0.48
1:B:476:ASP:OD1	1:B:476:ASP:N	2.43	0.48
1:B:610:GLY:HA3	1:B:639:ILE:HD12	1.95	0.48
1:A:614:LEU:HB3	1:A:619:CYS:HB3	1.95	0.47
1:A:674:ASP:N	1:A:674:ASP:OD1	2.48	0.47
1:A:517:LYS:O	1:A:520:ALA:HB2	2.15	0.47
1:B:668:ALA:HB2	1:B:684:TRP:HB3	1.95	0.47
1:A:499:GLY:O	1:A:500:LEU:HB2	2.15	0.46
1:A:463:TYR:CD2	1:A:525:LEU:HD22	2.51	0.46
1:A:561:VAL:HG23	1:A:562:GLU:N	2.30	0.46
1:A:523:LYS:O	1:A:524:ASP:C	2.53	0.46
1:C:472:GLU:OE1	1:C:552:THR:OG1	2.34	0.46
1:B:484:LEU:CD1	1:B:484:LEU:O	2.63	0.46
1:A:634:ASP:N	1:A:634:ASP:OD1	2.49	0.45
1:B:601:VAL:HG12	1:B:758:VAL:HG22	1.98	0.45
1:B:695:THR:OG1	1:B:698:GLY:N	2.45	0.45
1:B:747:PHE:HA	1:B:750:LEU:HD12	1.98	0.45
1:A:528:LEU:HD23	1:A:557:LEU:HD23	1.99	0.45
1:B:601:VAL:HG12	1:B:758:VAL:CG2	2.47	0.45
1:A:730:TYR:O	1:A:734:ARG:HG2	2.16	0.45
1:A:477:ARG:NE	1:A:477:ARG:CA	2.80	0.44
1:C:499:GLY:O	1:C:500:LEU:HB2	2.16	0.44
2:A:801:O1Y:C20	2:A:801:O1Y:O4	2.63	0.44
1:B:572:TYR:CD2	1:B:631:VAL:HG11	2.53	0.44
1:C:484:LEU:HD22	2:C:801:O1Y:C21	2.47	0.44
1:A:695:THR:O	1:A:696:LEU:C	2.53	0.43
1:B:729:LEU:HD21	1:B:757:ILE:HD13	2.00	0.43
1:C:604:ALA:HB2	1:C:693:ILE:HD13	2.00	0.43
1:B:684:TRP:CZ3	1:B:737:TRP:O	2.71	0.43
1:C:683:VAL:HG13	1:C:750:LEU:HD11	1.99	0.43
1:A:519:ASP:OD1	1:A:519:ASP:N	2.52	0.43
1:A:694:PHE:CZ	1:A:729:LEU:HD13	2.53	0.43
1:C:486:GLU:HG2	1:C:491:GLN:HB3	2.01	0.43
1:C:661:ARG:HD3	1:C:666:TRP:HH2	1.83	0.43
1:C:754:LEU:O	1:C:758:VAL:HG23	2.19	0.42
1:B:625:ALA:O	1:B:628:ASN:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:TRP:CE3	1:B:737:TRP:HA	2.54	0.42
1:B:730:TYR:CZ	1:B:734:ARG:HD3	2.55	0.42
1:B:606:GLN:HB3	1:B:637:MET:HB2	2.01	0.42
1:B:667:MET:HE2	1:B:672:LEU:HA	2.00	0.42
1:B:473:LEU:HD11	1:B:477:ARG:CB	2.50	0.42
1:C:467:GLU:OE2	1:C:553:GLN:HG3	2.20	0.42
1:C:568:ASN:OD1	1:C:568:ASN:C	2.58	0.41
1:A:573:LEU:HD23	1:A:573:LEU:HA	1.90	0.41
1:C:631:VAL:HG13	1:C:637:MET:HE2	2.02	0.41
1:C:689:LEU:O	1:C:692:GLU:HB2	2.20	0.41
1:B:694:PHE:CZ	1:B:729:LEU:HD13	2.54	0.41
1:C:469:PRO:O	1:C:470:ARG:C	2.58	0.41
1:C:747:PHE:O	1:C:751:VAL:HG23	2.21	0.41
1:A:484:LEU:CD2	1:A:494:LEU:HD21	2.48	0.41
1:A:551:CYS:HB2	1:A:558:TYR:HB2	2.02	0.41
1:A:523:LYS:O	1:A:525:LEU:N	2.53	0.41
1:A:538:ILE:HG13	1:B:537:MET:HE1	2.01	0.41
1:C:476:ASP:OD1	1:C:476:ASP:C	2.59	0.41
1:A:462:GLU:HG3	1:A:463:TYR:N	2.36	0.40
1:B:691:TRP:CZ3	1:B:700:PRO:HA	2.56	0.40
1:A:641:ASP:H	2:A:801:O1Y:C15	2.35	0.40
1:A:695:THR:O	1:A:697:GLY:N	2.54	0.40
1:C:621:HIS:O	1:C:622:ARG:HB2	2.22	0.40
1:B:730:TYR:O	1:B:731:MET:C	2.60	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	281/309 (91%)	252 (90%)	24 (8%)	5 (2%)	<b>8</b> 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	280/309 (91%)	249 (89%)	26 (9%)	5 (2%)	8	29
1	C	280/309 (91%)	247 (88%)	27 (10%)	6 (2%)	7	26
All	All	841/927 (91%)	748 (89%)	77 (9%)	16 (2%)	8	28

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	489	PHE
1	B	571	GLU
1	B	572	TYR
1	C	489	PHE
1	A	488	ALA
1	A	524	ASP
1	A	696	LEU
1	C	488	ALA
1	C	600	LEU
1	C	696	LEU
1	C	487	GLY
1	A	622	ARG
1	B	625	ALA
1	C	470	ARG
1	A	706	VAL
1	B	706	VAL

### 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	247/269 (92%)	228 (92%)	19 (8%)	13	35
1	B	246/269 (91%)	233 (95%)	13 (5%)	22	54
1	C	246/269 (91%)	233 (95%)	13 (5%)	22	54
All	All	739/807 (92%)	694 (94%)	45 (6%)	18	48

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	470	ARG
1	A	484	LEU
1	A	489	PHE
1	A	510	LYS
1	A	516	LEU
1	A	517	LYS
1	A	519	ASP
1	A	521	THR
1	A	523	LYS
1	A	529	ILE
1	A	563	CYS
1	A	572	TYR
1	A	627	ARG
1	A	634	ASP
1	A	647	ASP
1	A	663	PRO
1	A	674	ASP
1	A	699	SER
1	A	714	LYS
1	B	470	ARG
1	B	489	PHE
1	B	493	VAL
1	B	502	LYS
1	B	507	ARG
1	B	509	THR
1	B	510	LYS
1	B	516	LEU
1	B	530	SER
1	B	568	ASN
1	B	618	LYS
1	B	644	LEU
1	B	725	CYS
1	C	463	TYR
1	C	470	ARG
1	C	489	PHE
1	C	493	VAL
1	C	516	LEU
1	C	517	LYS
1	C	596	SER
1	C	616	SER
1	C	618	LYS
1	C	627	ARG
1	C	647	ASP

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Mol	Chain	Res	Type
1	C	726	THR
1	C	738	HIS

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

Mol	Chain	Res	Type
1	A	738	HIS
1	B	738	HIS
1	B	763	ASN
1	C	679	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	O1Y	B	801	1	35,39,39	2.00	10 (28%)	38,54,54	3.77	13 (34%)
3	SO4	B	802	-	4,4,4	0.46	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	O1Y	A	801	1	35,39,39	2.84	10 (28%)	38,54,54	2.76	9 (23%)
3	SO4	A	802	-	4,4,4	0.38	0	6,6,6	0.27	0
2	O1Y	C	801	1	35,39,39	3.02	11 (31%)	38,54,54	3.13	10 (26%)

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	O1Y	B	801	1	-	7/25/29/29	0/3/3/3
2	O1Y	A	801	1	-	5/25/29/29	0/3/3/3
2	O1Y	C	801	1	-	5/25/29/29	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	O1Y	C9-CL2	-10.63	1.50	1.72
2	A	801	O1Y	C13-CL1	-8.26	1.55	1.72
2	C	801	O1Y	C13-CL1	-6.94	1.57	1.72
2	A	801	O1Y	C9-CL2	-6.55	1.58	1.72
2	A	801	O1Y	C8-N5	-6.25	1.31	1.43
2	C	801	O1Y	C20-C2	-6.02	1.31	1.38
2	A	801	O1Y	C20-C2	-5.91	1.32	1.38
2	B	801	O1Y	C9-CL2	-5.40	1.61	1.72
2	C	801	O1Y	C8-N5	-4.92	1.34	1.43
2	C	801	O1Y	C2-N6	-4.72	1.32	1.41
2	A	801	O1Y	C18-C17	4.57	1.52	1.30
2	A	801	O1Y	C2-N6	-4.44	1.33	1.41
2	C	801	O1Y	C18-C17	4.30	1.51	1.30
2	B	801	O1Y	C18-C17	4.18	1.51	1.30
2	B	801	O1Y	C20-C2	-4.13	1.33	1.38
2	B	801	O1Y	C8-N5	-3.97	1.35	1.43
2	A	801	O1Y	C3-N1	-3.74	1.32	1.38
2	B	801	O1Y	C17-C16	3.54	1.54	1.48
2	B	801	O1Y	C2-N6	-3.42	1.35	1.41
2	C	801	O1Y	C3-N1	-2.96	1.33	1.38
2	A	801	O1Y	C1-N1	-2.76	1.32	1.36
2	B	801	O1Y	C6-N2	2.75	1.39	1.33
2	C	801	O1Y	C20-N7	-2.71	1.32	1.35
2	A	801	O1Y	C17-C16	2.56	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	O1Y	C13-CL1	-2.36	1.67	1.72
2	C	801	O1Y	O3-C12	-2.35	1.33	1.37
2	C	801	O1Y	C6-N2	2.33	1.38	1.33
2	C	801	O1Y	C1-N1	-2.17	1.33	1.36
2	B	801	O1Y	C6-N3	2.11	1.37	1.33
2	B	801	O1Y	C20-N7	-2.09	1.33	1.35
2	A	801	O1Y	C20-N7	-2.02	1.33	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	O1Y	C18-C17-C16	-16.33	103.59	122.27
2	C	801	O1Y	C18-C17-C16	-13.11	107.28	122.27
2	A	801	O1Y	C6-N2-C5	9.41	123.16	114.94
2	A	801	O1Y	C18-C17-C16	-8.92	112.07	122.27
2	B	801	O1Y	C6-N2-C5	8.84	122.66	114.94
2	A	801	O1Y	N2-C6-N3	-6.88	117.84	128.60
2	C	801	O1Y	C15-O2-C10	-6.37	107.92	117.53
2	B	801	O1Y	C17-C16-N6	6.33	118.01	113.84
2	B	801	O1Y	N2-C6-N3	-6.15	118.97	128.60
2	C	801	O1Y	C6-N2-C5	6.12	120.29	114.94
2	B	801	O1Y	C21-N7-C20	-4.70	118.76	129.82
2	C	801	O1Y	N2-C6-N3	-4.68	121.28	128.60
2	C	801	O1Y	C19-O3-C12	-4.61	110.57	117.53
2	C	801	O1Y	N2-C5-N4	4.51	118.97	115.28
2	B	801	O1Y	C2-N6-C16	-3.24	119.68	127.15
2	B	801	O1Y	O4-C16-C17	-3.17	117.65	122.72
2	B	801	O1Y	C20-N7-N8	-3.08	109.04	111.45
2	C	801	O1Y	C2-N6-C16	-3.04	120.13	127.15
2	C	801	O1Y	C21-N7-C20	-3.01	122.74	129.82
2	B	801	O1Y	N2-C5-N4	2.92	117.67	115.28
2	A	801	O1Y	C4-C5-N2	-2.81	117.87	122.73
2	C	801	O1Y	C4-C5-N2	-2.80	117.88	122.73
2	A	801	O1Y	N2-C5-N4	2.77	117.55	115.28
2	B	801	O1Y	C4-C5-N2	-2.77	117.94	122.73
2	A	801	O1Y	C2-N6-C16	-2.76	120.78	127.15
2	C	801	O1Y	C4-C3-N3	-2.63	119.09	122.75
2	B	801	O1Y	C4-C3-N3	-2.49	119.28	122.75
2	B	801	O1Y	O1-C7-N5	-2.29	118.53	123.61
2	B	801	O1Y	C15-O2-C10	-2.26	114.12	117.53
2	A	801	O1Y	C21-N7-C20	-2.17	124.72	129.82
2	A	801	O1Y	C9-C8-C13	2.04	122.46	118.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	O1Y	C10-C9-CL2	2.03	123.59	119.84

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	O1Y	O4-C16-C17-C18
2	B	801	O1Y	N6-C16-C17-C18
2	B	801	O1Y	C22-C21-N7-C20
2	B	801	O1Y	C22-C21-N7-N8
2	A	801	O1Y	O4-C16-C17-C18
2	A	801	O1Y	N6-C16-C17-C18
2	A	801	O1Y	C22-C21-N7-C20
2	A	801	O1Y	C22-C21-N7-N8
2	C	801	O1Y	O4-C16-C17-C18
2	C	801	O1Y	N6-C16-C17-C18
2	B	801	O1Y	N3-C3-N1-C1
2	B	801	O1Y	C4-C3-N1-C1
2	C	801	O1Y	C4-C3-N1-C1
2	C	801	O1Y	N3-C3-N1-C1
2	B	801	O1Y	N7-C21-C22-O5
2	C	801	O1Y	N7-C21-C22-O5
2	A	801	O1Y	N7-C21-C22-O5

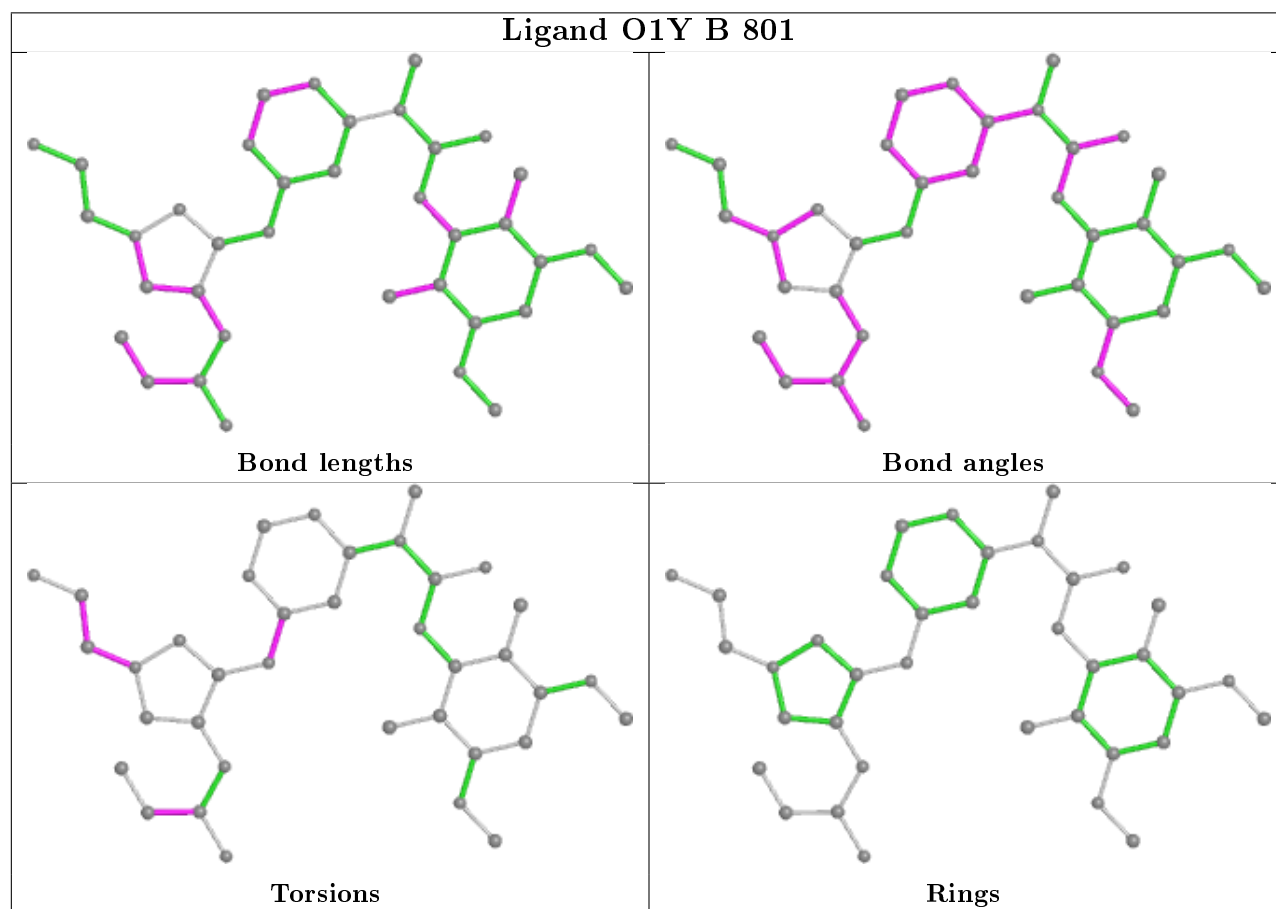
There are no ring outliers.

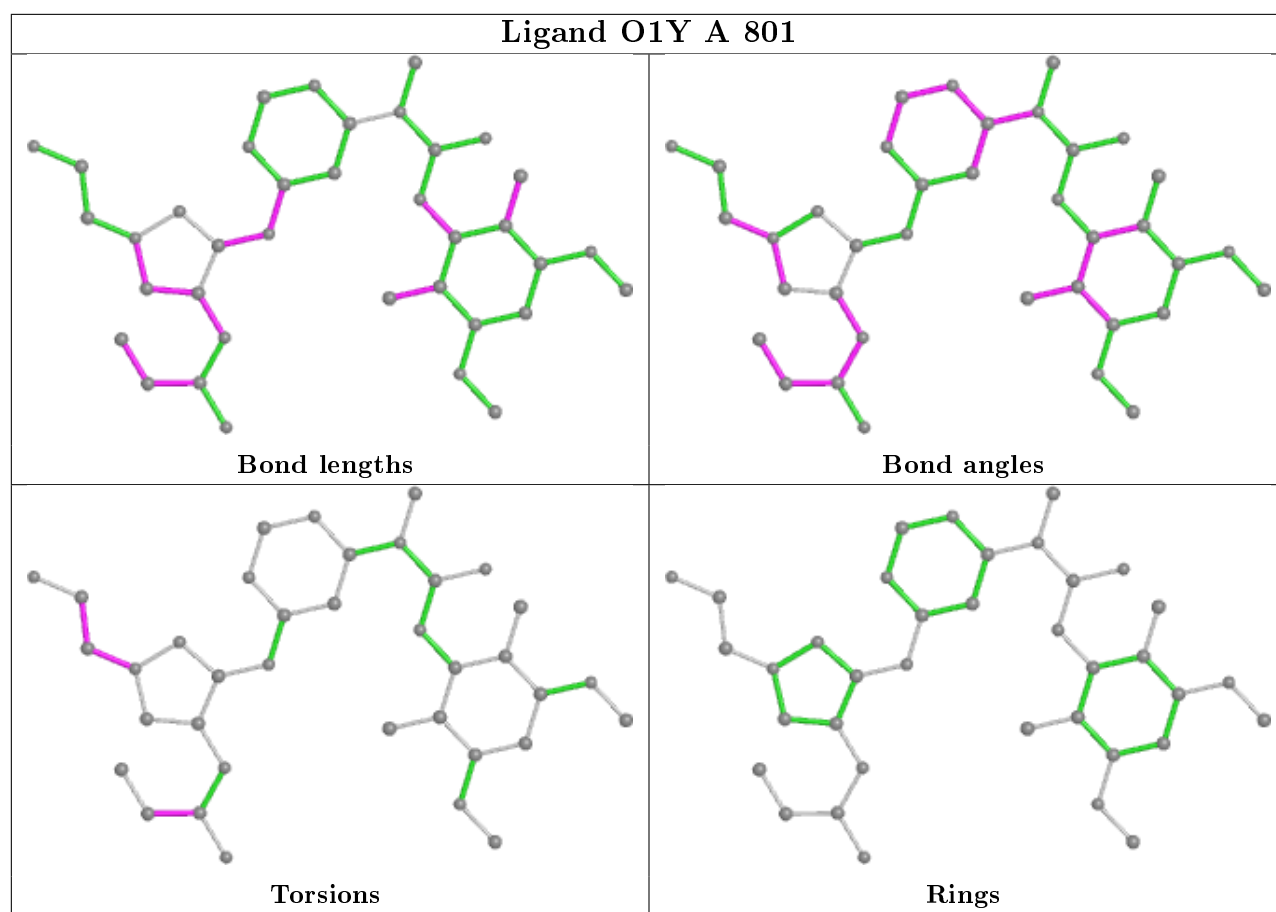
3 monomers are involved in 11 short contacts:

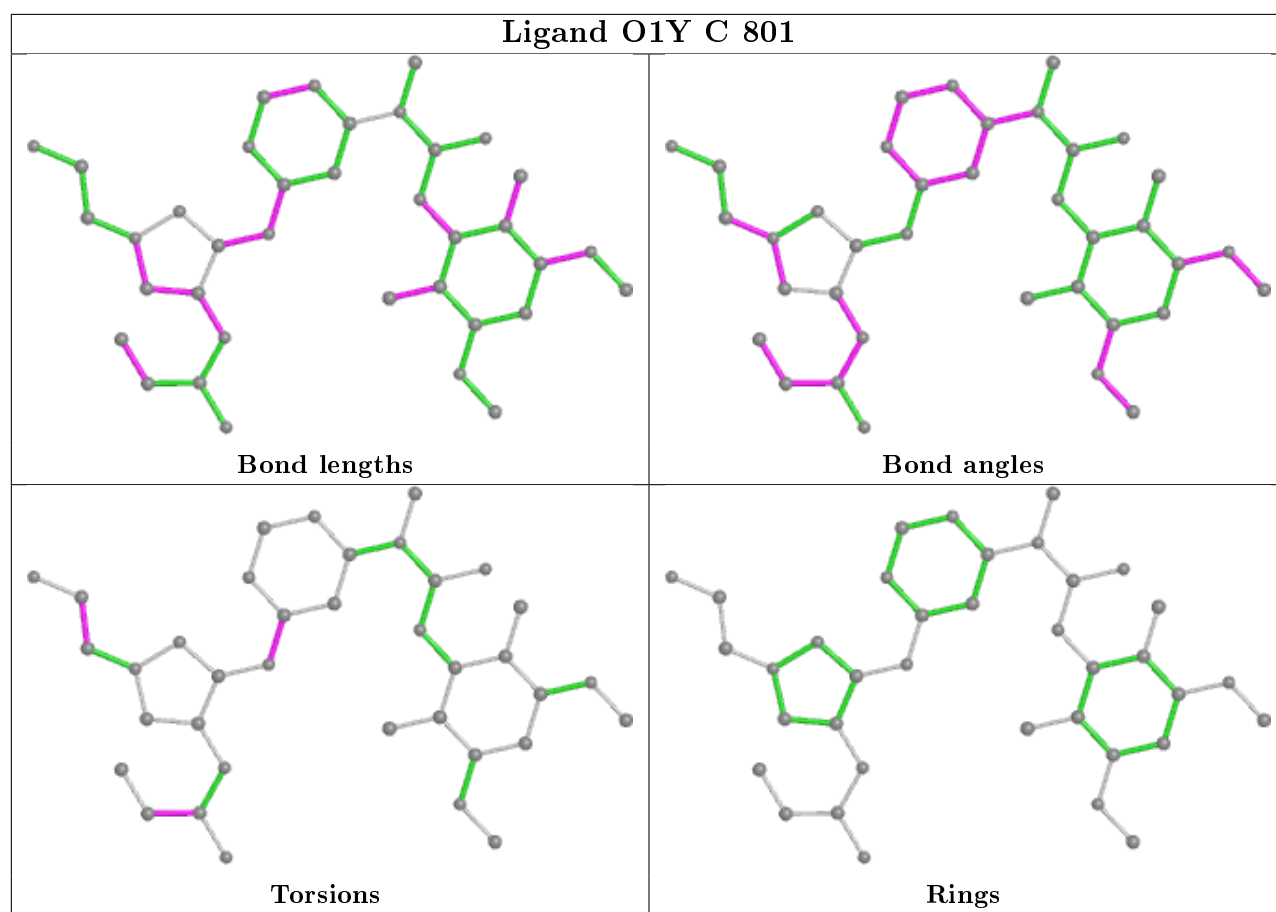
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	O1Y	2	0
2	A	801	O1Y	4	0
2	C	801	O1Y	5	0

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	287/309 (92%)	0.23	10 (3%) 44 38	58, 89, 153, 190	0
1	B	286/309 (92%)	0.37	19 (6%) 18 14	74, 106, 158, 198	0
1	C	286/309 (92%)	0.65	44 (15%) 2 1	70, 116, 181, 211	0
All	All	859/927 (92%)	0.42	73 (8%) 10 8	58, 104, 169, 211	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	579	PRO	8.1
1	C	603	CYS	7.2
1	C	578	PRO	6.9
1	C	653	TYR	6.2
1	B	662	LEU	6.2
1	C	485	GLY	5.7
1	C	710	PHE	5.6
1	C	654	TYR	5.0
1	C	577	ARG	4.6
1	B	717	HIS	4.6
1	C	605	TYR	4.3
1	B	673	PHE	4.2
1	B	654	TYR	4.2
1	C	604	ALA	4.1
1	A	578	PRO	3.7
1	A	709	LEU	3.6
1	C	486	GLU	3.6
1	C	643	GLY	3.6
1	C	729	LEU	3.5
1	B	672	LEU	3.5
1	A	701	TYR	3.5
1	C	601	VAL	3.4
1	B	709	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	659	ASN	3.3
1	C	694	PHE	3.3
1	C	761	THR	3.3
1	C	573	LEU	3.3
1	B	665	LYS	3.2
1	C	709	LEU	3.2
1	C	673	PHE	3.0
1	A	713	LEU	3.0
1	C	714	LYS	3.0
1	A	579	PRO	2.9
1	A	696	LEU	2.9
1	B	708	GLU	2.8
1	B	701	TYR	2.8
1	A	653	TYR	2.8
1	C	660	GLY	2.7
1	B	658	THR	2.7
1	C	701	TYR	2.6
1	C	715	GLU	2.6
1	C	608	ALA	2.5
1	C	659	ASN	2.5
1	C	703	GLY	2.5
1	A	694	PHE	2.5
1	C	696	LEU	2.5
1	A	717	HIS	2.5
1	C	600	LEU	2.5
1	C	762	SER	2.4
1	C	760	LEU	2.4
1	C	717	HIS	2.4
1	B	624	LEU	2.4
1	C	662	LEU	2.4
1	C	747	PHE	2.4
1	C	672	LEU	2.4
1	B	578	PRO	2.3
1	B	653	TYR	2.3
1	B	706	VAL	2.3
1	C	595	LEU	2.3
1	C	602	SER	2.2
1	B	729	LEU	2.2
1	C	540	LYS	2.2
1	C	754	LEU	2.2
1	C	758	VAL	2.2
1	C	658	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	713	LEU	2.2
1	C	757	ILE	2.1
1	B	644	LEU	2.1
1	C	606	GLN	2.1
1	A	708	GLU	2.1
1	C	484	LEU	2.0
1	C	706	VAL	2.0
1	B	710	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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, 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.

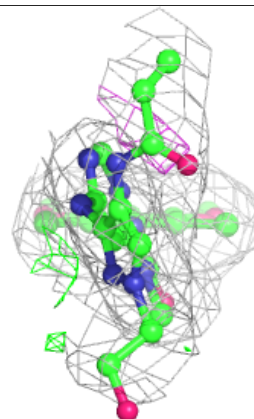
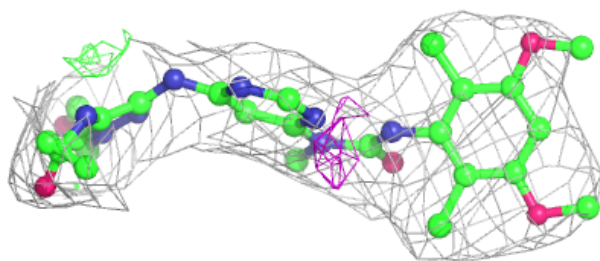
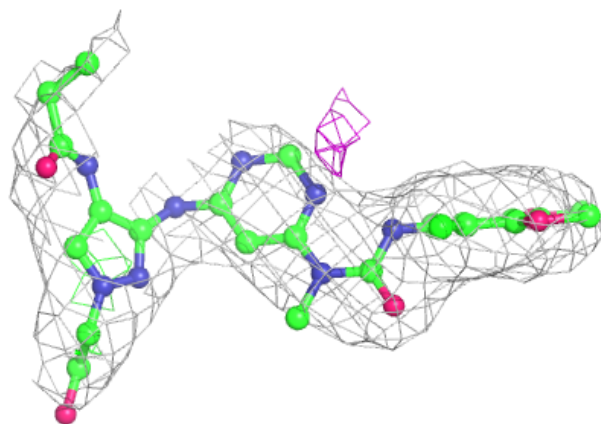
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	B	802	5/5	0.82	0.27	115,120,127,139	0
3	SO4	A	802	5/5	0.89	0.20	115,123,130,130	0
2	O1Y	C	801	37/37	0.92	0.18	87,112,141,144	0
2	O1Y	B	801	37/37	0.93	0.21	86,107,151,161	0
2	O1Y	A	801	37/37	0.93	0.19	71,89,137,155	0

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.

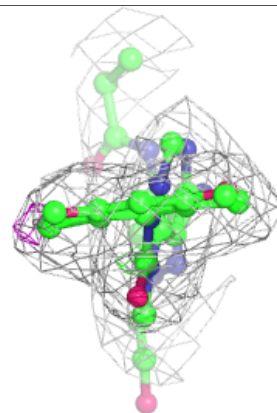
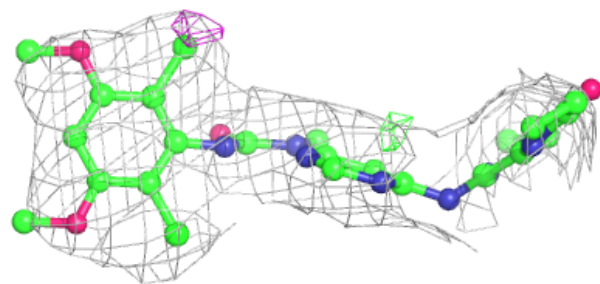
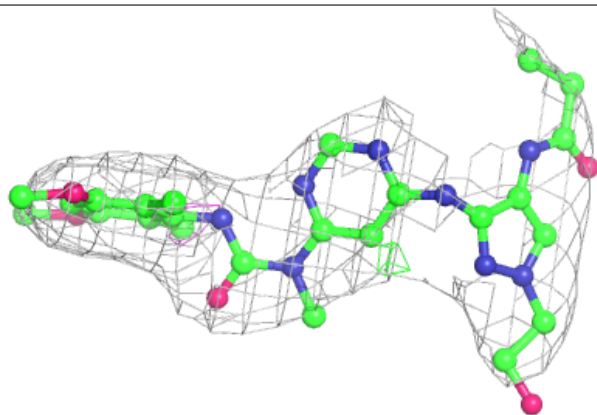


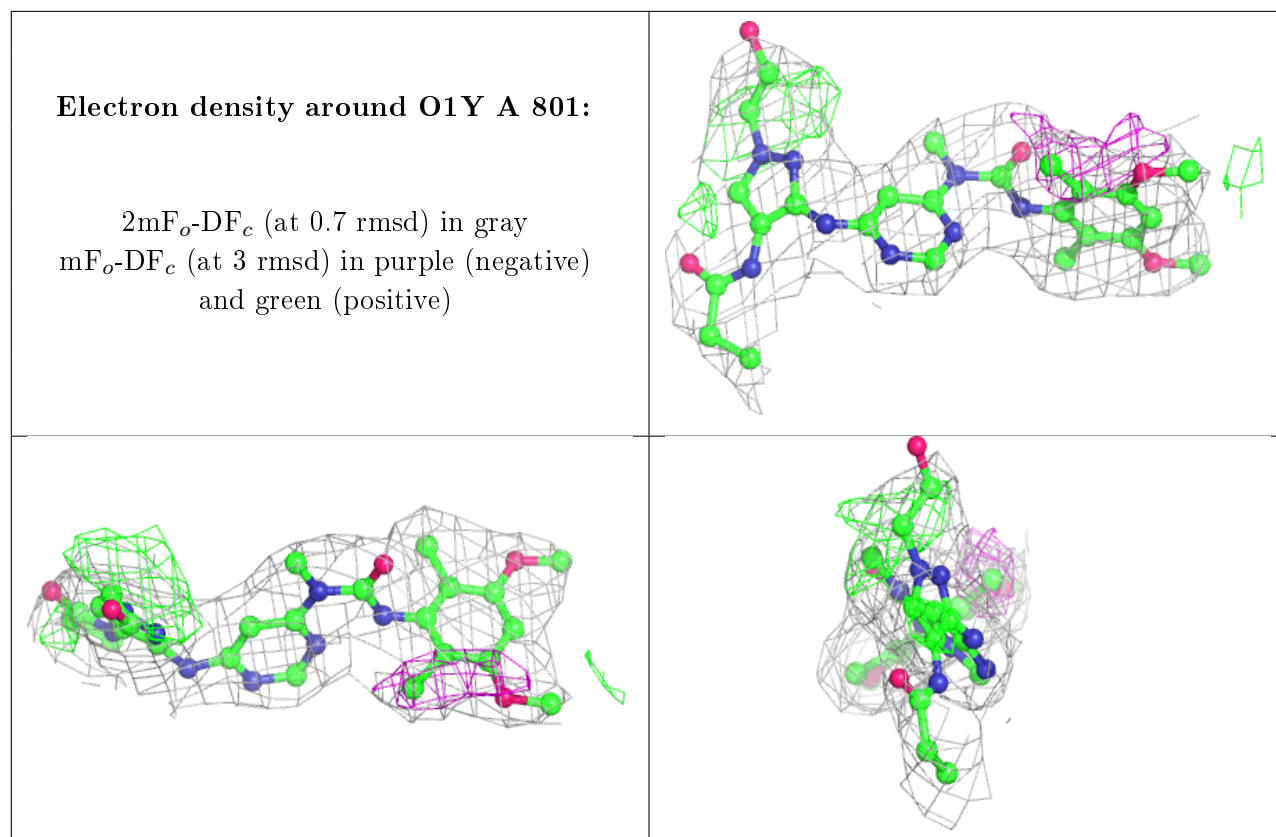
**Electron density around O1Y C 801:**

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

**Electron density around O1Y 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.