



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:08 pm BST

PDB ID : 6AGX  
Title : The cocrystal structure of FGFR2 bound with compound 14 harboring 5H-pyrrolo[2,3-b]pyrazine scaffold  
Authors : Xiong, B.  
Deposited on : 2018-08-15  
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

The 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

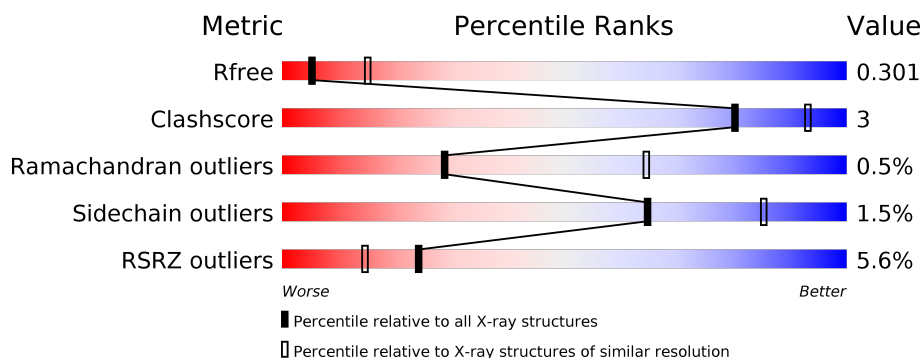
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	298	<div> <div>7%</div> <div>84%</div> <div>10%</div> <div>• •</div> </div>
1	B	298	<div> <div>5%</div> <div>92%</div> <div>8%</div> </div>
1	C	298	<div> <div>5%</div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
1	D	298	<div> <div>4%</div> <div>95%</div> <div>5%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9544 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.

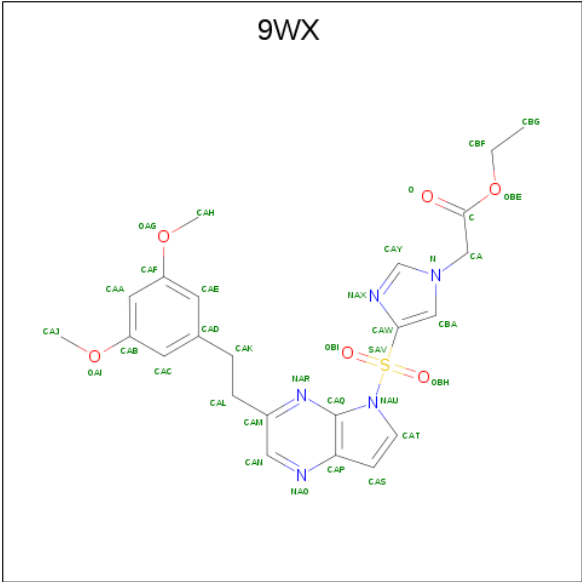
- Molecule 1 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	P	S	0	2	0
			2292	1457	389	422	1	23			
1	B	298	Total	C	N	O	P	S	0	2	0
			2414	1526	404	456	4	24			
1	C	284	Total	C	N	O	P	S	0	2	0
			2284	1451	388	421	1	23			
1	D	298	Total	C	N	O	P	S	0	2	0
			2414	1526	404	456	4	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	628	THR	ALA	engineered mutation	UNP P21802
B	628	THR	ALA	engineered mutation	UNP P21802
C	628	THR	ALA	engineered mutation	UNP P21802
D	628	THR	ALA	engineered mutation	UNP P21802

- Molecule 2 is ethyl [4-({3-[2-(3,5-dimethoxyphenyl)ethyl]-5H-pyrrolo[2,3-b]pyrazin-5-yl}sulfonyl)-1H-imidazol-1-yl]acetate (three-letter code: 9WX) (formula: C<sub>23</sub>H<sub>25</sub>N<sub>5</sub>O<sub>6</sub>S).

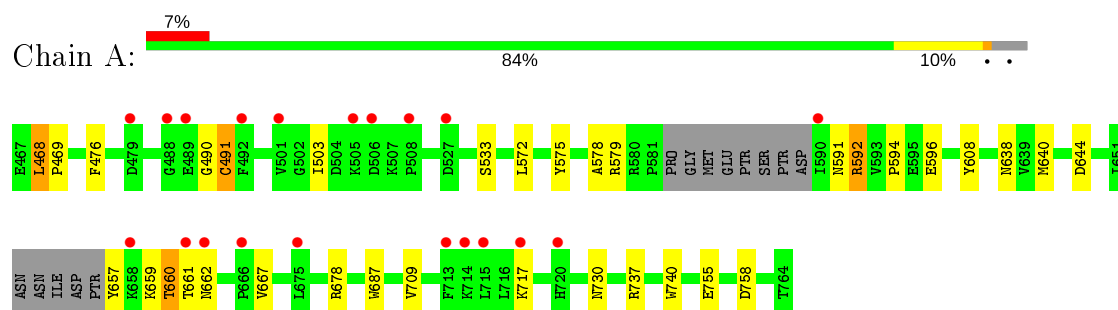


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	23	5	6	1		
2	B	1	Total	C	N	O	S	0	0
			35	23	5	6	1		
2	C	1	Total	C	N	O	S	0	0
			35	23	5	6	1		
2	D	1	Total	C	N	O	S	0	0
			35	23	5	6	1		

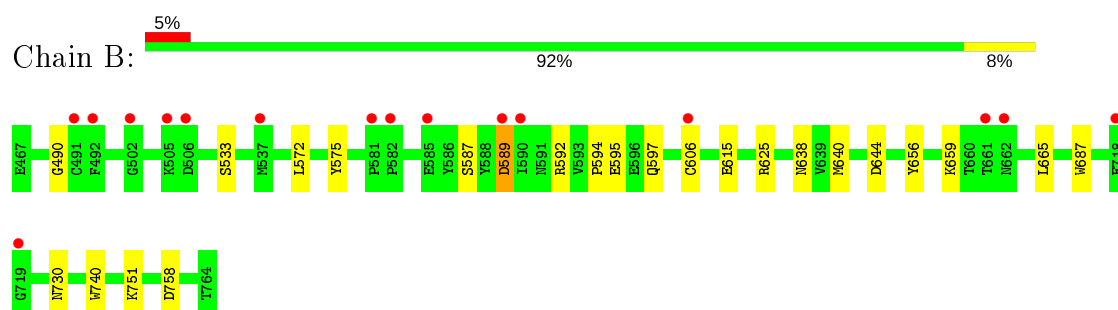
### 3 Residue-property plots [i](#)

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.

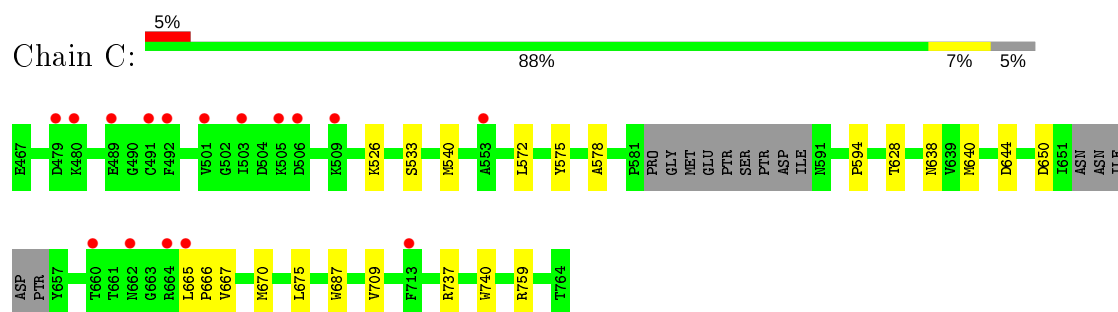
#### • Molecule 1: Fibroblast growth factor receptor 2



#### • 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 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.32Å 78.27Å 99.25Å 90.00° 96.47° 90.00°	Depositor
Resolution (Å)	45.22 – 2.95 45.22 – 2.95	Depositor EDS
% Data completeness (in resolution range)	90.7 (45.22-2.95) 90.7 (45.22-2.95)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.251 , 0.298 0.253 , 0.301	Depositor DCC
$R_{free}$ test set	1269 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 27.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	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 41.62 % 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 2.2997e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PTR, 9WX

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	0.34	0/2327	0.55	0/3139
1	B	0.34	0/2401	0.55	0/3238
1	C	0.35	0/2319	0.55	0/3128
1	D	0.33	0/2401	0.54	0/3238
All	All	0.34	0/9448	0.55	0/12743

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	737	ARG	Sidechain
1	D	737	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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	2292	0	2315	18	1
1	B	2414	0	2396	12	1
1	C	2284	0	2304	16	0
1	D	2414	0	2396	8	0
2	A	35	0	0	0	0
2	B	35	0	0	1	0
2	C	35	0	0	0	0
2	D	35	0	0	0	0
All	All	9544	0	9411	51	1

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 3.

All (51) 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:665:LEU:HB2	1:C:670:MET:CE	1.87	1.04
1:C:665:LEU:HB2	1:C:670:MET:HE1	1.45	0.98
1:A:579:ARG:HG2	1:A:596:GLU:O	1.93	0.68
1:B:572:LEU:HD13	1:B:640:MET:HE1	1.77	0.66
1:D:572:LEU:HD13	1:D:640:MET:HE1	1.76	0.66
1:A:490:GLY:O	1:A:491:CYS:HB2	1.95	0.65
1:C:572:LEU:HD13	1:C:640:MET:HE1	1.78	0.64
1:A:572:LEU:HD13	1:A:640:MET:HE1	1.81	0.62
1:A:476:PHE:CD1	1:A:503:ILE:HD12	2.35	0.61
1:C:665:LEU:HB2	1:C:670:MET:HE2	1.82	0.61
1:C:578:ALA:O	1:C:594:PRO:HD2	2.02	0.59
1:B:659:LYS:HZ2	1:B:665:LEU:HD11	1.67	0.58
1:A:608:TYR:OH	1:C:759:ARG:HG2	2.03	0.58
1:A:490:GLY:O	1:A:491:CYS:CB	2.51	0.57
1:C:575:TYR:OH	1:C:638:ASN:ND2	2.38	0.56
1:D:575:TYR:OH	1:D:638:ASN:ND2	2.38	0.56
1:A:578:ALA:O	1:A:594:PRO:HD2	2.06	0.55
1:D:743:VAL:HB	1:D:746:GLN:HG3	1.89	0.55
1:A:575:TYR:OH	1:A:638:ASN:ND2	2.39	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:TYR:OH	1:B:638:ASN:ND2	2.37	0.54
1:B:594:PRO:HD2	1:B:595:GLU:OE2	2.07	0.53
1:B:606[B]:CYS:SG	1:B:640:MET:SD	3.01	0.53
1:A:660:THR:C	1:A:662:ASN:H	2.14	0.51
1:B:490:GLY:HA3	2:B:800:9WX:CBF	2.41	0.51
1:A:667:VAL:HG11	1:A:709:VAL:HG13	1.93	0.50
1:B:625:ARG:HD2	1:B:659:LYS:NZ	2.27	0.50
1:B:687:TRP:CE3	1:B:740:TRP:HA	2.48	0.48
1:C:540:MET:HE1	1:C:650:ASP:OD2	2.14	0.48
1:C:667:VAL:HG11	1:C:709:VAL:HG13	1.96	0.48
1:A:591:ASN:O	1:A:592:ARG:HB2	2.14	0.47
1:C:670:MET:SD	1:C:675:LEU:HG	2.54	0.47
1:A:657:PTR:P	1:A:660:THR:HG22	2.55	0.47
1:D:687:TRP:CE3	1:D:740:TRP:HA	2.50	0.46
1:B:615:GLU:OE1	1:B:751:LYS:HA	2.16	0.46
1:A:687:TRP:CE3	1:A:740:TRP:HA	2.51	0.46
1:C:687:TRP:CE3	1:C:740:TRP:HA	2.52	0.45
1:C:572:LEU:HD13	1:C:640:MET:CE	2.45	0.45
1:D:572:LEU:HD13	1:D:640:MET:CE	2.45	0.45
1:A:572:LEU:HD13	1:A:640:MET:CE	2.45	0.45
1:A:661:THR:HG22	1:A:678:ARG:HD3	1.99	0.44
1:B:587:SER:OG	1:B:592:ARG:HD3	2.18	0.44
1:C:526:LYS:HD3	1:D:662:ASN:HB3	2.00	0.44
1:B:572:LEU:HD13	1:B:640:MET:CE	2.47	0.44
1:C:540:MET:CE	1:C:650:ASP:OD2	2.66	0.44
1:A:660:THR:O	1:A:661:THR:OG1	2.33	0.43
1:A:659:LYS:C	1:A:661:THR:H	2.22	0.42
1:A:468:LEU:HD23	1:A:469:PRO:HD2	2.00	0.42
1:C:709:VAL:HG21	1:D:523:ALA:HB3	2.02	0.41
1:D:656:PTR:CD1	1:D:656:PTR:N	2.84	0.41
1:C:665:LEU:HA	1:C:666:PRO:HD3	1.93	0.40
1:B:656:PTR:N	1:B:656:PTR:CD2	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:LYS:O	1:B:589:ASP:OD1[2_556]	1.97	0.23

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/298 (94%)	268 (95%)	10 (4%)	3 (1%)	14	46
1	B	294/298 (99%)	285 (97%)	8 (3%)	1 (0%)	41	73
1	C	280/298 (94%)	272 (97%)	7 (2%)	1 (0%)	34	69
1	D	294/298 (99%)	285 (97%)	8 (3%)	1 (0%)	41	73
All	All	1149/1192 (96%)	1110 (97%)	33 (3%)	6 (0%)	29	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	CYS
1	A	644	ASP
1	C	644	ASP
1	D	644	ASP
1	B	644	ASP
1	A	592	ARG

### 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	252/259 (97%)	246 (98%)	6 (2%)	49	77
1	B	261/259 (101%)	256 (98%)	5 (2%)	57	81
1	C	251/259 (97%)	248 (99%)	3 (1%)	71	88
1	D	261/259 (101%)	260 (100%)	1 (0%)	91	96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1025/1036 (99%)	1010 (98%)	15 (2%)	65 85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	LEU
1	A	533	SER
1	A	660	THR
1	A	730	ASN
1	A	755	GLU
1	A	758	ASP
1	B	533	SER
1	B	589	ASP
1	B	597	GLN
1	B	730	ASN
1	B	758	ASP
1	C	533	SER
1	C	628	THR
1	C	737	ARG
1	D	533	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	ASN
1	A	597	GLN
1	A	631	ASN
1	A	730	ASN
1	B	730	ASN
1	C	730	ASN
1	D	730	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PTR	D	656	1	15,16,17	0.77	0	19,22,24	1.03	2 (10%)
1	PTR	D	588	1	15,16,17	0.78	0	19,22,24	1.17	2 (10%)
1	PTR	C	657	1	15,16,17	0.63	0	19,22,24	1.26	1 (5%)
1	PTR	D	657	1	15,16,17	0.82	0	19,22,24	1.15	1 (5%)
1	PTR	A	657	1	15,16,17	0.71	0	19,22,24	1.20	2 (10%)
1	PTR	B	657	1	15,16,17	1.07	1 (6%)	19,22,24	0.93	0
1	PTR	B	588	1	15,16,17	0.85	1 (6%)	19,22,24	1.13	1 (5%)
1	PTR	B	586	1	15,16,17	0.82	0	19,22,24	1.09	1 (5%)
1	PTR	D	586	1	15,16,17	0.82	0	19,22,24	0.91	2 (10%)
1	PTR	B	656	1	15,16,17	0.88	1 (6%)	19,22,24	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	D	656	1	-	0/10/11/13	0/1/1/1
1	PTR	D	588	1	-	0/10/11/13	0/1/1/1
1	PTR	C	657	1	-	0/10/11/13	0/1/1/1
1	PTR	D	657	1	-	0/10/11/13	0/1/1/1
1	PTR	A	657	1	-	0/10/11/13	0/1/1/1
1	PTR	B	657	1	-	2/10/11/13	0/1/1/1
1	PTR	B	588	1	-	0/10/11/13	0/1/1/1
1	PTR	B	586	1	-	2/10/11/13	0/1/1/1
1	PTR	D	586	1	-	2/10/11/13	0/1/1/1
1	PTR	B	656	1	-	0/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	657	PTR	P-OH	3.59	1.64	1.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	656	PTR	P-OH	2.58	1.63	1.59
1	B	588	PTR	P-OH	2.24	1.62	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	586	PTR	CG-CB-CA	-3.14	107.75	114.10
1	C	657	PTR	OH-P-O1P	-2.88	98.46	109.31
1	B	588	PTR	CG-CB-CA	-2.76	108.52	114.10
1	A	657	PTR	OH-P-O1P	-2.51	99.86	109.31
1	D	656	PTR	CG-CB-CA	-2.31	109.42	114.10
1	D	657	PTR	P-OH-CZ	2.26	131.00	123.75
1	D	588	PTR	CB-CA-C	-2.24	107.27	111.47
1	A	657	PTR	O3P-P-O2P	2.23	116.17	107.64
1	D	586	PTR	CG-CB-CA	-2.15	109.76	114.10
1	D	586	PTR	O3P-P-O2P	2.09	115.63	107.64
1	D	656	PTR	O3P-P-O2P	2.08	115.58	107.64
1	D	588	PTR	OH-P-O1P	-2.00	101.75	109.31

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	586	PTR	O-C-CA-CB
1	D	586	PTR	O-C-CA-CB
1	B	586	PTR	C-CA-CB-CG
1	D	586	PTR	C-CA-CB-CG
1	B	657	PTR	CE1-CZ-OH-P
1	B	657	PTR	CE2-CZ-OH-P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	656	PTR	1	0
1	A	657	PTR	1	0
1	B	656	PTR	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	9WX	A	800	-	35,38,38	2.65	10 (28%)	35,54,54	2.09	10 (28%)
2	9WX	D	800	-	35,38,38	2.81	11 (31%)	35,54,54	1.96	8 (22%)
2	9WX	B	800	-	35,38,38	2.68	12 (34%)	35,54,54	1.73	8 (22%)
2	9WX	C	800	-	35,38,38	2.67	10 (28%)	35,54,54	1.79	8 (22%)

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	9WX	A	800	-	-	9/16/28/28	0/4/4/4
2	9WX	D	800	-	-	10/16/28/28	0/4/4/4
2	9WX	B	800	-	-	9/16/28/28	0/4/4/4
2	9WX	C	800	-	-	4/16/28/28	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	9WX	OBI-SAV	8.67	1.54	1.43
2	A	800	9WX	OBI-SAV	8.49	1.54	1.43
2	D	800	9WX	OBH-SAV	8.37	1.54	1.43
2	D	800	9WX	OBI-SAV	8.37	1.54	1.43
2	B	800	9WX	OBI-SAV	8.18	1.53	1.43
2	A	800	9WX	OBH-SAV	8.16	1.53	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	9WX	OBH-SAV	8.09	1.53	1.43
2	B	800	9WX	OBH-SAV	7.90	1.53	1.43
2	D	800	9WX	CAW-SAV	5.62	1.83	1.78
2	A	800	9WX	CAN-NAO	5.34	1.40	1.31
2	C	800	9WX	CAN-NAO	5.19	1.40	1.31
2	D	800	9WX	CAN-NAO	5.15	1.40	1.31
2	B	800	9WX	CAN-NAO	4.96	1.39	1.31
2	B	800	9WX	CAL-CAM	-4.92	1.40	1.51
2	A	800	9WX	CAL-CAM	-4.52	1.41	1.51
2	D	800	9WX	CAL-CAM	-4.27	1.41	1.51
2	C	800	9WX	CAL-CAM	-4.14	1.42	1.51
2	C	800	9WX	CAK-CAD	-3.61	1.41	1.51
2	C	800	9WX	CBA-N	-3.58	1.33	1.38
2	B	800	9WX	CAK-CAD	-3.58	1.41	1.51
2	D	800	9WX	CAK-CAD	-3.54	1.41	1.51
2	A	800	9WX	CAK-CAD	-3.35	1.42	1.51
2	B	800	9WX	CBA-N	-3.20	1.33	1.38
2	B	800	9WX	CBA-CAW	-2.99	1.32	1.37
2	C	800	9WX	CBA-CAW	-2.90	1.32	1.37
2	B	800	9WX	CAT-NAU	-2.77	1.33	1.38
2	D	800	9WX	CBA-N	-2.75	1.34	1.38
2	A	800	9WX	CBA-N	-2.74	1.34	1.38
2	D	800	9WX	CAT-NAU	-2.61	1.33	1.38
2	D	800	9WX	CAS-CAP	-2.44	1.32	1.42
2	A	800	9WX	CBA-CAW	-2.39	1.33	1.37
2	A	800	9WX	CAT-NAU	-2.38	1.34	1.38
2	C	800	9WX	CAT-NAU	-2.35	1.34	1.38
2	D	800	9WX	CBA-CAW	-2.34	1.33	1.37
2	D	800	9WX	CAP-CAQ	-2.33	1.34	1.40
2	C	800	9WX	CAS-CAP	-2.32	1.32	1.42
2	C	800	9WX	CAP-CAQ	-2.29	1.34	1.40
2	A	800	9WX	CAP-CAQ	-2.28	1.34	1.40
2	A	800	9WX	CAS-CAP	-2.28	1.33	1.42
2	B	800	9WX	CAP-CAQ	-2.24	1.35	1.40
2	B	800	9WX	CAS-CAP	-2.20	1.33	1.42
2	B	800	9WX	CA-N	2.18	1.51	1.47
2	B	800	9WX	CA-C	2.10	1.56	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	9WX	CAL-CAM-NAR	5.31	124.11	116.03

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	9WX	CA-N-CAY	-5.18	119.66	125.61
2	D	800	9WX	CA-N-CAY	-5.14	119.70	125.61
2	C	800	9WX	CAL-CAM-NAR	4.86	123.43	116.03
2	D	800	9WX	CAL-CAM-NAR	4.53	122.93	116.03
2	B	800	9WX	CAL-CAM-NAR	4.51	122.90	116.03
2	A	800	9WX	CA-N-CBA	4.50	132.33	126.25
2	D	800	9WX	CA-N-CBA	4.34	132.11	126.25
2	A	800	9WX	CAM-CAN-NAO	-4.14	119.07	123.13
2	C	800	9WX	CAM-CAN-NAO	-4.13	119.08	123.13
2	C	800	9WX	CAN-CAM-NAR	-3.99	118.24	120.85
2	D	800	9WX	CAM-CAN-NAO	-3.88	119.33	123.13
2	D	800	9WX	CAN-CAM-NAR	-3.87	118.32	120.85
2	A	800	9WX	CAN-CAM-NAR	-3.60	118.50	120.85
2	B	800	9WX	CAM-CAN-NAO	-3.54	119.66	123.13
2	B	800	9WX	CA-N-CAY	3.51	129.64	125.61
2	C	800	9WX	CAM-NAR-CAQ	3.42	122.11	117.71
2	B	800	9WX	CAN-CAM-NAR	-3.37	118.65	120.85
2	A	800	9WX	CAM-NAR-CAQ	3.26	121.89	117.71
2	B	800	9WX	CA-N-CBA	-3.02	122.18	126.25
2	D	800	9WX	CAM-NAR-CAQ	2.98	121.54	117.71
2	B	800	9WX	CAM-NAR-CAQ	2.83	121.35	117.71
2	B	800	9WX	OBI-SAV-OBH	-2.72	108.44	117.71
2	C	800	9WX	OBI-SAV-OBH	-2.71	108.48	117.71
2	D	800	9WX	OBI-SAV-OBH	-2.60	108.84	117.71
2	A	800	9WX	OBE-C-CA	2.56	115.97	109.29
2	D	800	9WX	OBE-C-CA	2.56	115.97	109.29
2	C	800	9WX	CBF-OBE-C	-2.55	109.31	116.73
2	A	800	9WX	OBI-SAV-OBH	-2.49	109.23	117.71
2	C	800	9WX	CAN-NAO-CAP	2.27	119.65	116.91
2	A	800	9WX	CAN-NAO-CAP	2.05	119.38	116.91
2	B	800	9WX	OBE-C-CA	2.03	114.60	109.29
2	A	800	9WX	CAJ-OAI-CAB	2.03	121.91	117.51
2	C	800	9WX	OBE-C-CA	2.01	114.53	109.29

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	9WX	C-CA-N-CBA
2	D	800	9WX	CA-C-OBE-CBF
2	D	800	9WX	OBE-C-CA-N
2	D	800	9WX	O-C-CA-N

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	800	9WX	C-CA-N-CBA
2	B	800	9WX	OBE-C-CA-N
2	C	800	9WX	CA-C-OBE-CBF
2	D	800	9WX	O-C-OBE-CBF
2	A	800	9WX	CA-C-OBE-CBF
2	B	800	9WX	CA-C-OBE-CBF
2	A	800	9WX	O-C-OBE-CBF
2	B	800	9WX	O-C-OBE-CBF
2	A	800	9WX	CAE-CAF-OAG-CAH
2	C	800	9WX	CAE-CAF-OAG-CAH
2	A	800	9WX	CAA-CAF-OAG-CAH
2	C	800	9WX	CAA-CAF-OAG-CAH
2	C	800	9WX	O-C-OBE-CBF
2	B	800	9WX	CAC-CAB-OAI-CAJ
2	B	800	9WX	CAA-CAB-OAI-CAJ
2	D	800	9WX	CAE-CAF-OAG-CAH
2	D	800	9WX	CAA-CAF-OAG-CAH
2	A	800	9WX	O-C-CA-N
2	A	800	9WX	C-CA-N-CAY
2	B	800	9WX	CAA-CAF-OAG-CAH
2	A	800	9WX	OBE-C-CA-N
2	B	800	9WX	CAE-CAF-OAG-CAH
2	A	800	9WX	CBG-CBF-OBE-C
2	D	800	9WX	CAK-CAL-CAM-CAN
2	D	800	9WX	CAK-CAL-CAM-NAR
2	D	800	9WX	C-CA-N-CAY
2	B	800	9WX	C-CA-N-CAY
2	B	800	9WX	CAK-CAL-CAM-NAR

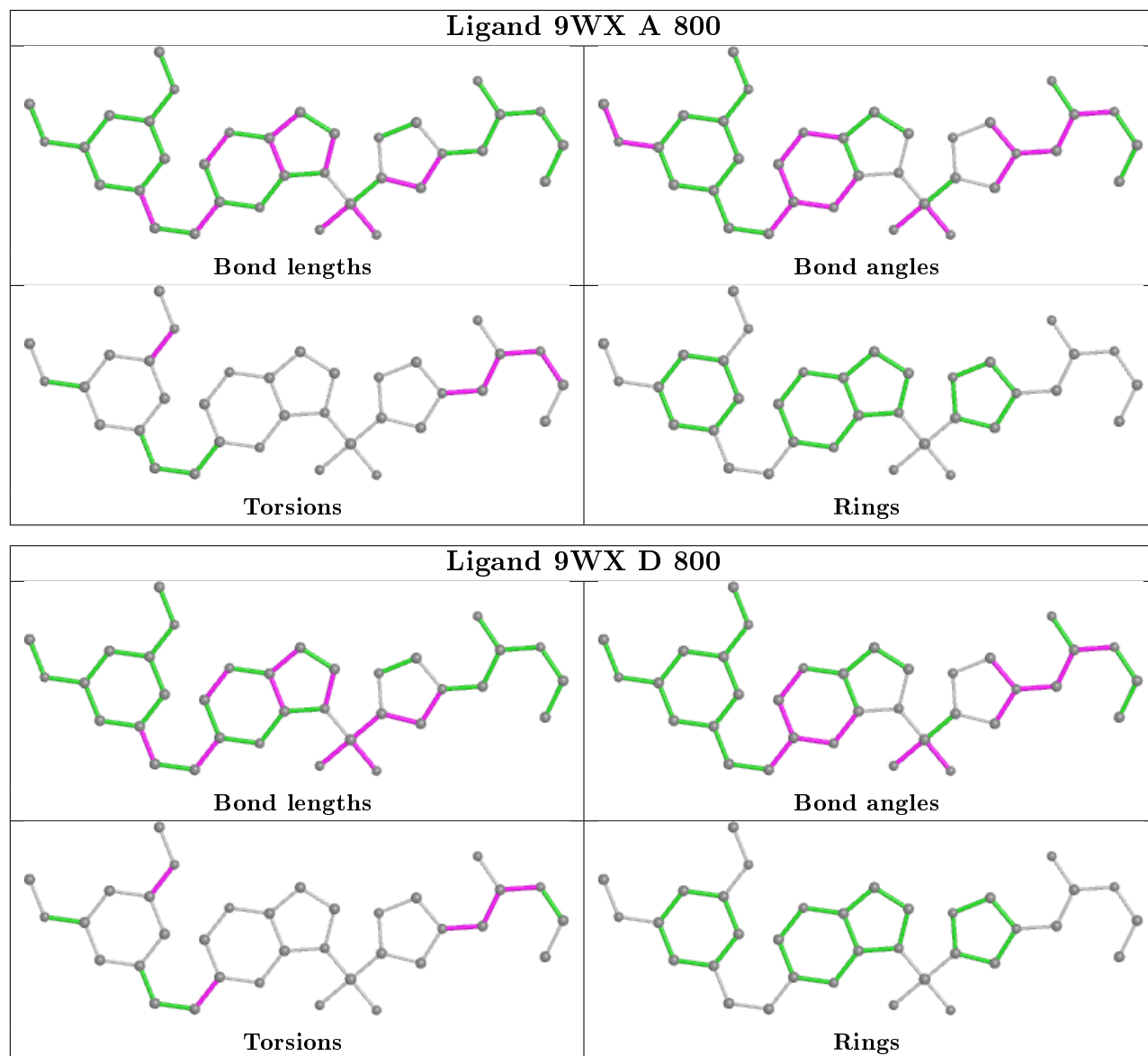
There are no ring outliers.

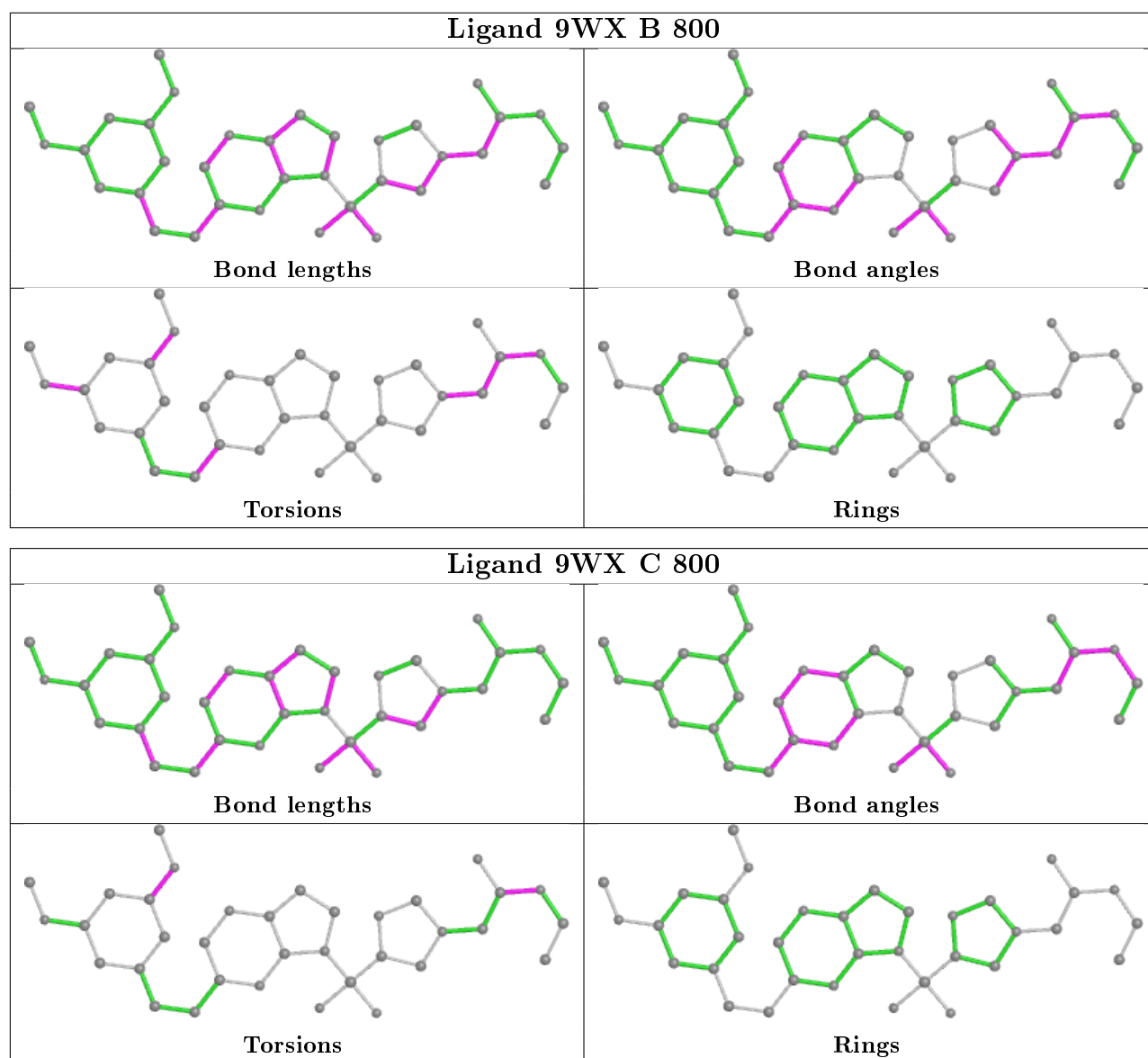
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	9WX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	284/298 (95%)	0.43	20 (7%) 16 9	36, 64, 106, 127	1 (0%)
1	B	294/298 (98%)	0.38	16 (5%) 25 16	34, 57, 100, 125	1 (0%)
1	C	283/298 (94%)	0.31	16 (5%) 23 14	33, 53, 97, 114	1 (0%)
1	D	294/298 (98%)	0.29	13 (4%) 34 21	29, 51, 91, 128	1 (0%)
All	All	1155/1192 (96%)	0.35	65 (5%) 24 15	29, 56, 102, 128	4 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	CYS	6.4
1	B	506	ASP	6.1
1	D	491	CYS	5.1
1	A	714	LYS	5.0
1	B	582	PRO	4.4
1	A	662	ASN	4.3
1	B	719	GLY	4.2
1	A	506	ASP	4.1
1	C	491	CYS	4.0
1	B	581	PRO	4.0
1	C	505	LYS	4.0
1	D	506	ASP	3.9
1	C	506	ASP	3.9
1	A	505	LYS	3.9
1	D	503	ILE	3.7
1	B	589	ASP	3.7
1	B	492	PHE	3.5
1	A	508	PRO	3.5
1	B	585	GLU	3.4
1	A	720	HIS	3.4
1	D	581	PRO	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	479	ASP	3.1
1	A	489	GLU	3.1
1	A	658	LYS	3.0
1	D	504	ASP	3.0
1	A	661	THR	2.9
1	A	666	PRO	2.9
1	C	660	THR	2.8
1	D	540	MET	2.7
1	D	510	GLU	2.7
1	B	502	GLY	2.7
1	B	590	ILE	2.6
1	A	492	PHE	2.6
1	C	503	ILE	2.6
1	A	501	VAL	2.6
1	C	492	PHE	2.6
1	B	718	GLU	2.5
1	B	662	ASN	2.5
1	C	489	GLU	2.5
1	A	713	PHE	2.5
1	C	509	LYS	2.5
1	A	527	ASP	2.4
1	D	508	PRO	2.4
1	C	501	VAL	2.4
1	D	655	ASP	2.4
1	A	488	GLY	2.3
1	A	715	LEU	2.3
1	C	664	ARG	2.3
1	A	717	LYS	2.3
1	D	557	ASP	2.3
1	D	505	LYS	2.2
1	A	675	LEU	2.2
1	A	590	ILE	2.2
1	C	480	LYS	2.1
1	B	606[A]	CYS	2.1
1	C	662	ASN	2.1
1	D	474	TRP	2.1
1	C	479	ASP	2.1
1	B	661	THR	2.1
1	B	537	MET	2.1
1	C	665	LEU	2.0
1	C	713	PHE	2.1
1	C	553	ALA	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	479	ASP	2.0
1	B	505	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PTR	B	588	16/17	0.68	0.34	106,116,146,148	0
1	PTR	D	588	16/17	0.81	0.18	72,77,96,98	0
1	PTR	B	586	16/17	0.81	0.27	93,99,117,117	0
1	PTR	D	586	16/17	0.87	0.29	60,70,73,75	0
1	PTR	B	656	16/17	0.87	0.20	69,84,100,108	0
1	PTR	A	657	16/17	0.88	0.20	70,72,85,87	0
1	PTR	D	656	16/17	0.91	0.20	47,53,67,68	0
1	PTR	C	657	16/17	0.92	0.18	49,51,57,61	0
1	PTR	B	657	16/17	0.93	0.14	52,57,67,69	0
1	PTR	D	657	16/17	0.94	0.17	45,48,56,57	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

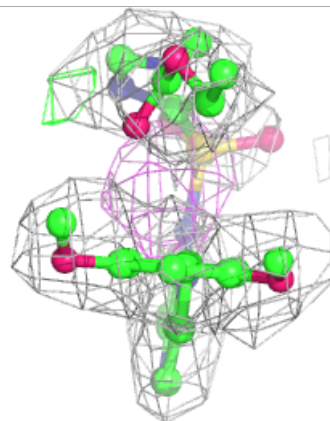
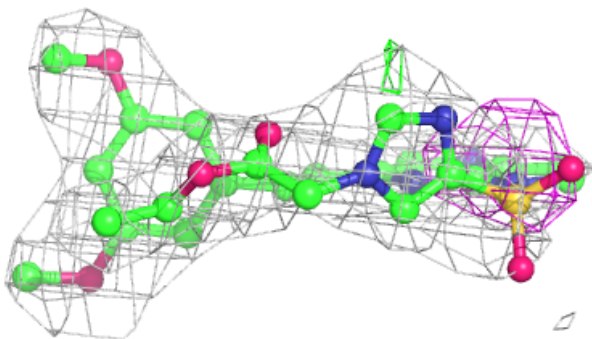
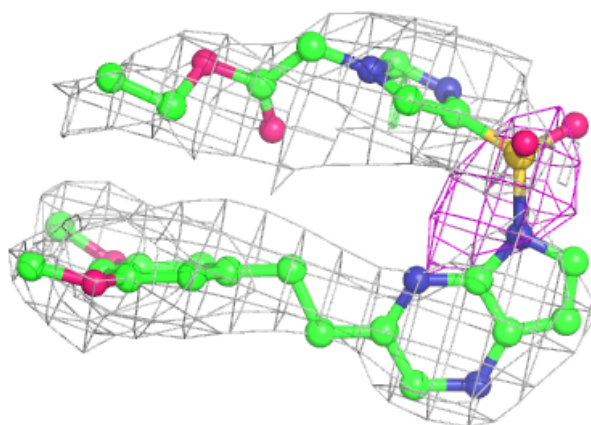
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	9WX	C	800	35/35	0.79	0.28	49,78,102,108	0
2	9WX	B	800	35/35	0.88	0.25	51,60,101,103	0
2	9WX	A	800	35/35	0.88	0.21	51,68,91,92	0
2	9WX	D	800	35/35	0.89	0.25	43,57,100,104	0

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.

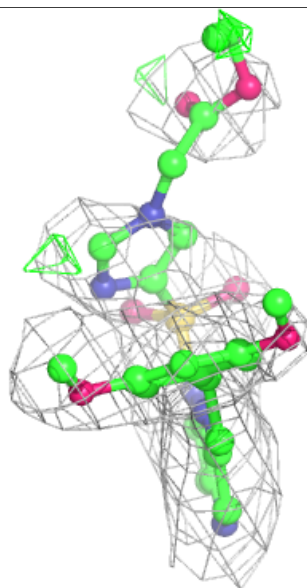
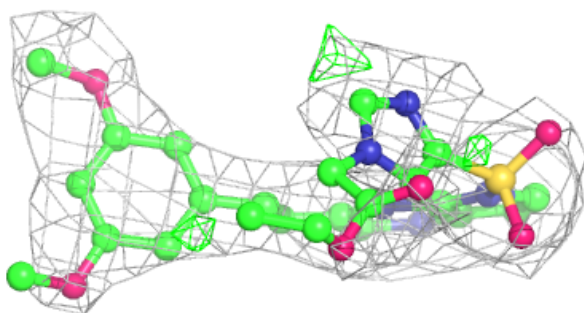
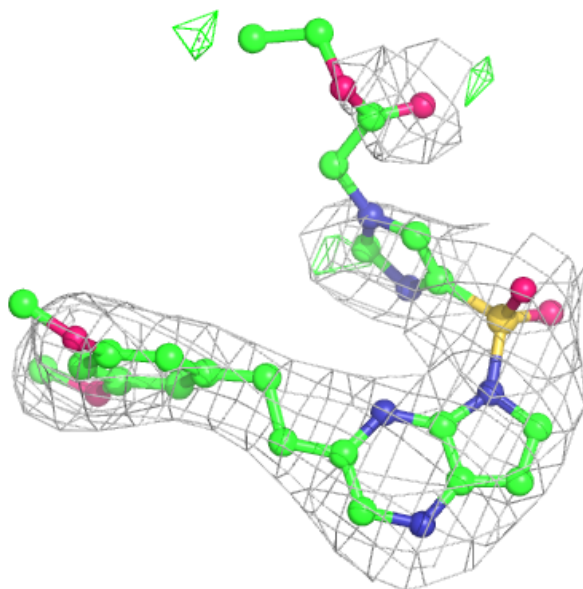
**Electron density around 9WX C 800:**

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



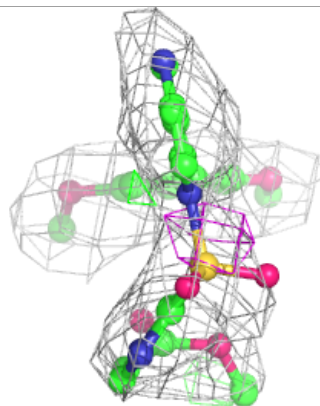
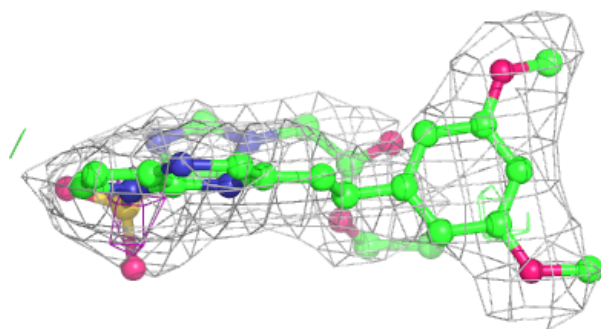
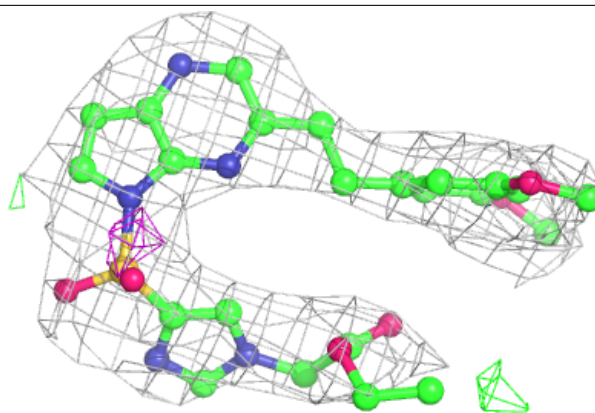
**Electron density around 9WX B 800:**

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



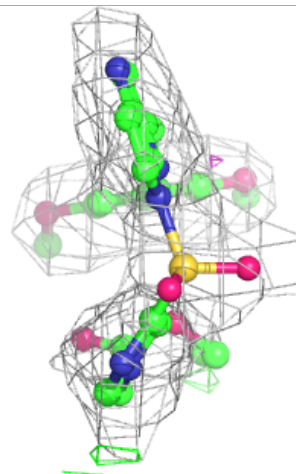
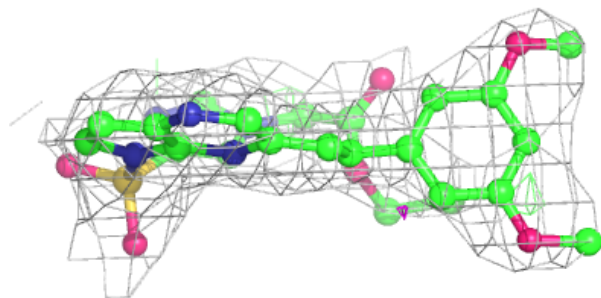
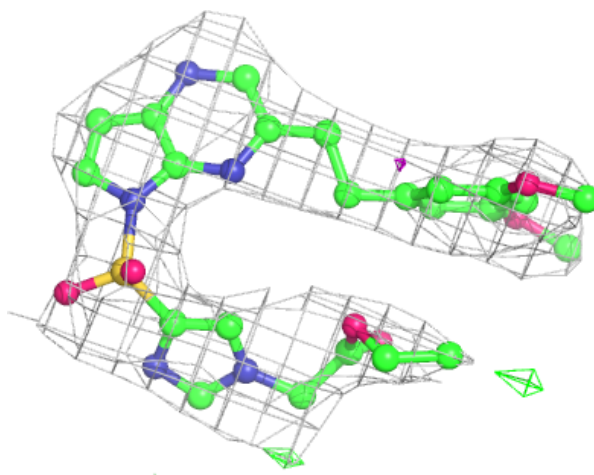
**Electron density around 9WX A 800:**

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



**Electron density around 9WX D 800:**

$2mF_o-DF_c$  (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.