



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2020 – 08:10 PM BST

PDB ID : 6XUG  
Title : Human Ecto-5'-nucleotidase (CD73) in complex with A2410 (compound 53 in publication) in the closed form in crystal form IV  
Authors : Strater, N.  
Deposited on : 2020-01-19  
Resolution : 2.09 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.14.5  
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) : 2.14.5

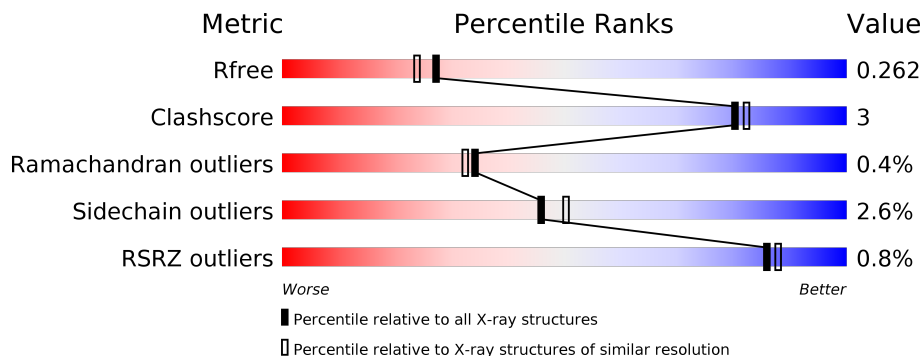
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	538	 % 87% 8% . .
1	B	538	 % 86% 9% . .

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8997 atoms, of which 32 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 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	515	4039	2577	683	761	18	0	7	0
1	B	514	4003	2547	680	758	18	0	1	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ASP	ASN	conflict	UNP P21589
A	311	ASP	ASN	conflict	UNP P21589
A	333	ASP	ASN	conflict	UNP P21589
A	403	ASP	ASN	conflict	UNP P21589
A	550	GLY	-	expression tag	UNP P21589
A	551	GLY	-	expression tag	UNP P21589
A	552	GLY	-	expression tag	UNP P21589
A	553	GLY	-	expression tag	UNP P21589
A	554	ALA	-	expression tag	UNP P21589
A	555	GLY	-	expression tag	UNP P21589
A	556	GLY	-	expression tag	UNP P21589
A	557	GLY	-	expression tag	UNP P21589
A	558	GLY	-	expression tag	UNP P21589
A	559	HIS	-	expression tag	UNP P21589
A	560	HIS	-	expression tag	UNP P21589
A	561	HIS	-	expression tag	UNP P21589
A	562	HIS	-	expression tag	UNP P21589
A	563	HIS	-	expression tag	UNP P21589
A	564	HIS	-	expression tag	UNP P21589
B	53	ASP	ASN	conflict	UNP P21589
B	311	ASP	ASN	conflict	UNP P21589
B	333	ASP	ASN	conflict	UNP P21589
B	403	ASP	ASN	conflict	UNP P21589
B	550	GLY	-	expression tag	UNP P21589
B	551	GLY	-	expression tag	UNP P21589

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Chain	Residue	Modelled	Actual	Comment	Reference
B	552	GLY	-	expression tag	UNP P21589
B	553	GLY	-	expression tag	UNP P21589
B	554	ALA	-	expression tag	UNP P21589
B	555	GLY	-	expression tag	UNP P21589
B	556	GLY	-	expression tag	UNP P21589
B	557	GLY	-	expression tag	UNP P21589
B	558	GLY	-	expression tag	UNP P21589
B	559	HIS	-	expression tag	UNP P21589
B	560	HIS	-	expression tag	UNP P21589
B	561	HIS	-	expression tag	UNP P21589
B	562	HIS	-	expression tag	UNP P21589
B	563	HIS	-	expression tag	UNP P21589
B	564	HIS	-	expression tag	UNP P21589

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

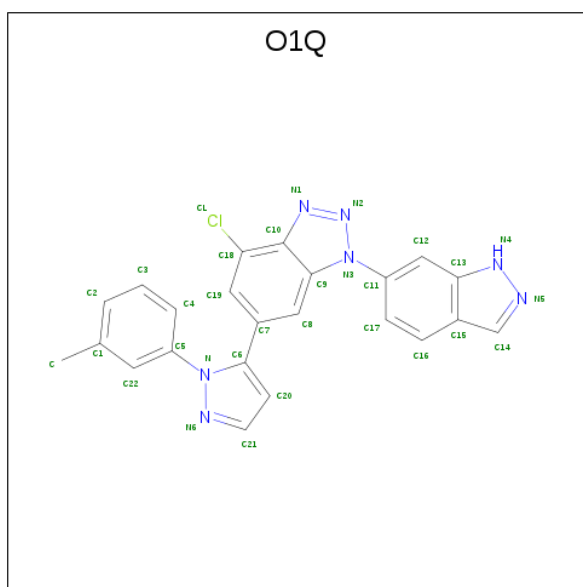
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 4-chloranyl-1-(1 {H}-indazol-6-yl)-6-[2-(3-methylphenyl)pyrazol-3-yl]benzotriazole (three-letter code: O1Q) (formula: C<sub>23</sub>H<sub>16</sub>ClN<sub>7</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	H	N	16	0
			47	23	1	16	7		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	H	N		
5	B	1	47	23	1	16	7	16	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	439	Total	O	0	0
			439	439		
6	B	406	Total	O	0	0
			406	406		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.75Å 230.01Å 54.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.67 – 2.09 86.82 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (72.67-2.09) 99.6 (86.82-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.08Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.188 , 0.237 0.207 , 0.262	Depositor DCC
$R_{free}$ test set	3452 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtrriage
Anisotropy	0.769	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 63.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0833e-03. 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: PO4, CA, ZN, O1Q

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	0.52	0/4142	0.72	0/5608
1	B	0.51	0/4086	0.71	0/5531
All	All	0.51	0/8228	0.71	0/11139

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	4039	0	4057	20	0
1	B	4003	0	4004	24	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	31	16	0	0	0
5	B	31	16	0	0	0
6	A	439	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	406	0	0	3	0
All	All	8965	32	8061	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 44 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:HIS:HA	6:B:753:HOH:O	1.80	0.82
1:A:243:HIS:HA	6:A:792:HOH:O	1.80	0.80
1:B:296:GLU:HG2	6:B:985:HOH:O	2.00	0.60
1:B:273:ARG:HD2	6:B:790:HOH:O	2.03	0.58
1:B:175:GLY:HA2	1:B:218:LEU:O	2.05	0.56

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	518/538 (96%)	494 (95%)	22 (4%)	2 (0%)	34	32
1	B	511/538 (95%)	489 (96%)	20 (4%)	2 (0%)	34	32
All	All	1029/1076 (96%)	983 (96%)	42 (4%)	4 (0%)	34	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	SER
1	B	335	SER
1	A	88	GLN

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Mol	Chain	Res	Type
1	B	88	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	450/457 (98%)	439 (98%)	11 (2%)	49	53
1	B	443/457 (97%)	431 (97%)	12 (3%)	44	48
All	All	893/914 (98%)	870 (97%)	23 (3%)	46	50

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	LYS
1	B	228	LEU
1	B	520	SER
1	B	170	VAL
1	B	365	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN
1	A	499	ASN
1	B	499	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	O1Q	A	605	-	32,36,36	0.86	1 (3%)	38,53,53	1.03	3 (7%)
5	O1Q	B	605	-	32,36,36	0.87	2 (6%)	38,53,53	1.02	3 (7%)
4	PO4	B	604	2	4,4,4	2.39	2 (50%)	6,6,6	1.40	1 (16%)
4	PO4	A	604	2	4,4,4	1.77	1 (25%)	6,6,6	1.12	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
5	O1Q	A	605	-	-	7/12/12/12	0/6/6/6
5	O1Q	B	605	-	-	7/12/12/12	0/6/6/6

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	PO4	P-O1	3.87	1.59	1.50
5	B	605	O1Q	C18-C10	-2.12	1.39	1.42
4	B	604	PO4	P-O2	2.06	1.60	1.54
4	A	604	PO4	P-O2	2.04	1.60	1.54
5	A	605	O1Q	C18-C10	-2.03	1.40	1.42

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	O1Q	C7-C8-C9	-3.61	118.01	121.87
5	B	605	O1Q	C7-C8-C9	-3.40	118.24	121.87
5	A	605	O1Q	C8-C9-C10	3.28	123.66	120.55
5	B	605	O1Q	C8-C9-C10	3.06	123.45	120.55
4	B	604	PO4	O3-P-O1	-2.92	100.20	110.89

There are no chirality outliers.

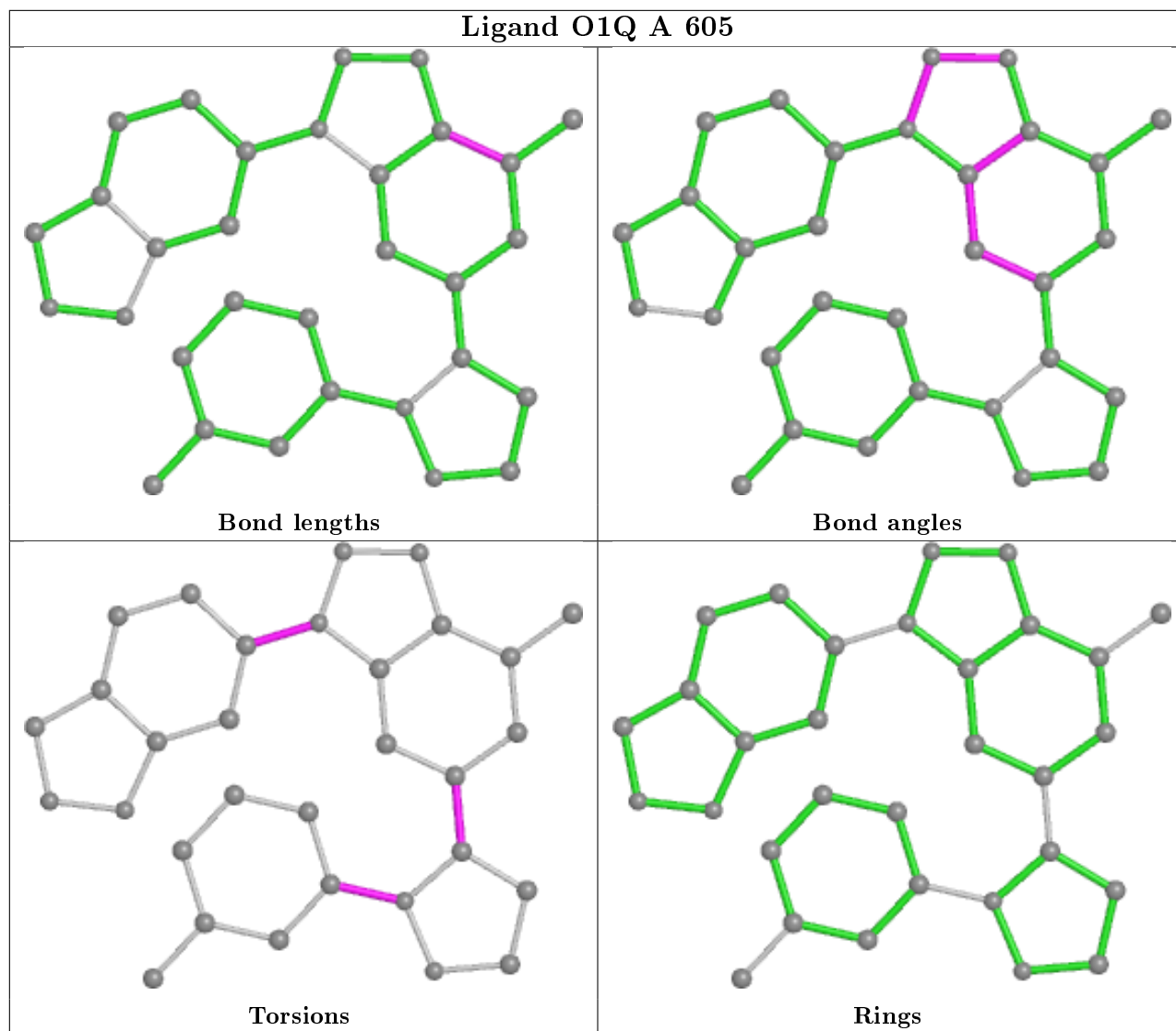
5 of 14 torsion outliers are listed below:

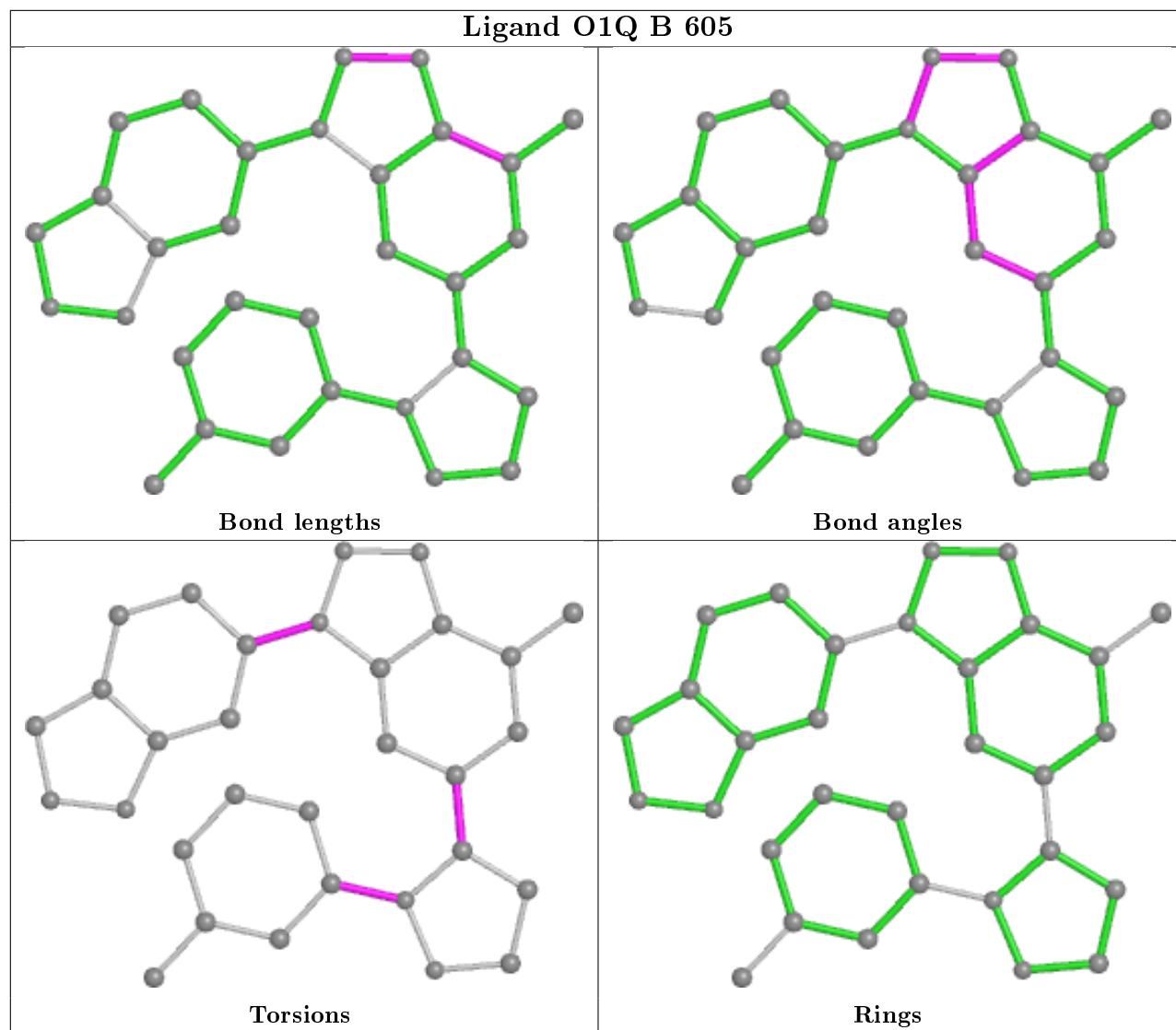
Mol	Chain	Res	Type	Atoms
5	A	605	O1Q	N-C6-C7-C8
5	A	605	O1Q	C20-C6-C7-C19
5	B	605	O1Q	C20-C6-C7-C8
5	A	605	O1Q	C20-C6-C7-C8
5	A	605	O1Q	N-C6-C7-C19

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	515/538 (95%)	-0.46	5 (0%) 82 85	19, 36, 61, 107	1 (0%)
1	B	514/538 (95%)	-0.41	3 (0%) 89 91	22, 39, 69, 108	0
All	All	1029/1076 (95%)	-0.43	8 (0%) 86 88	19, 37, 64, 108	1 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	SER	4.6
1	A	408	TRP	4.1
1	A	336	THR	3.3
1	B	335	SER	3.3
1	A	334	TYR	3.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

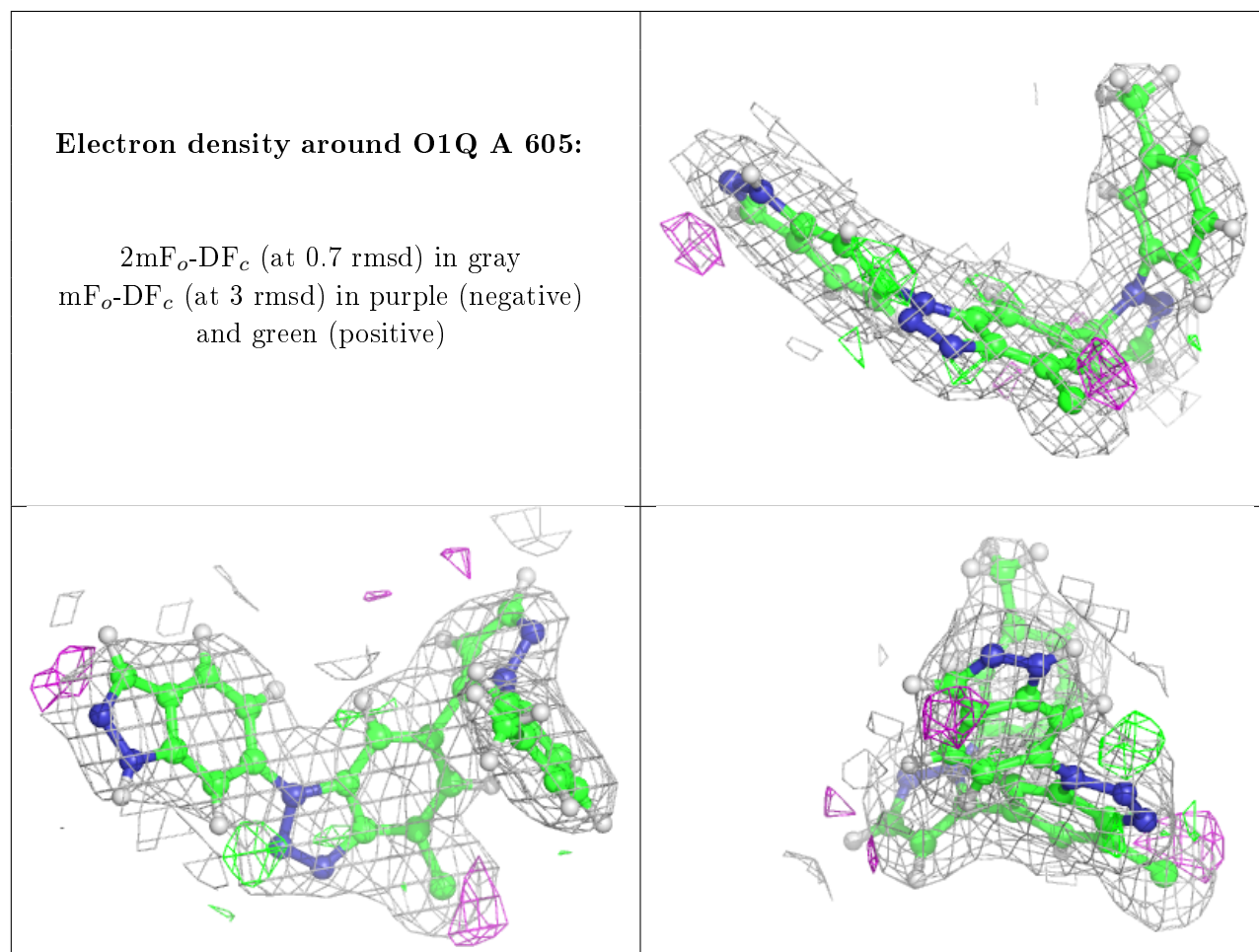
### 6.4 Ligands [i](#)

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



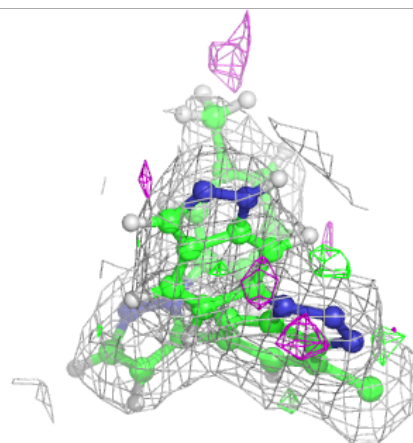
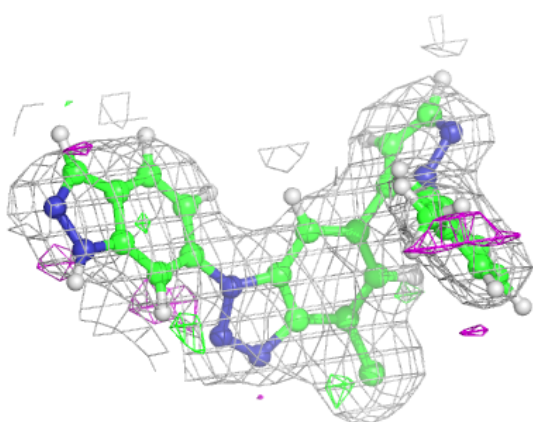
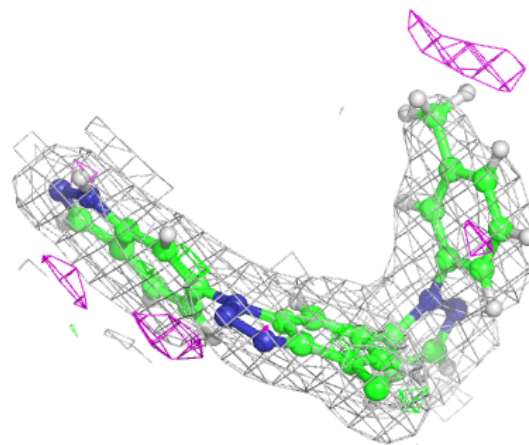
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	O1Q	A	605	31/31	0.93	0.09	12,19,25,28	16
5	O1Q	B	605	31/31	0.94	0.09	8,20,25,26	16
3	CA	B	603	1/1	0.97	0.08	59,59,59,59	0
4	PO4	B	604	5/5	0.98	0.11	29,30,33,34	0
3	CA	A	603	1/1	0.99	0.03	50,50,50,50	0
2	ZN	A	601	1/1	0.99	0.06	40,40,40,40	0
4	PO4	A	604	5/5	0.99	0.11	31,31,32,34	0
2	ZN	B	601	1/1	0.99	0.04	45,45,45,45	0
2	ZN	B	602	1/1	1.00	0.08	29,29,29,29	0
2	ZN	A	602	1/1	1.00	0.08	28,28,28,28	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 O1Q B 605:**

$2mF_o-DF_c$  (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.