



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 12:14 PM EDT

PDB ID : 2FJM  
Title : The structure of phosphotyrosine phosphatase 1B in complex with compound 2  
Authors : Asante-Appiah, E.; Patel, S.; Despons, C.; Taylor, J.M.; Lau, C.; Dufresne, C.; Therien, M.; Friesen, R.; Becker, J.W.; Leblanc, Y.; Scapin, G.  
Deposited on : 2006-01-03  
Resolution : 2.10 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 : 2.23.2  
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) : 2.23.2

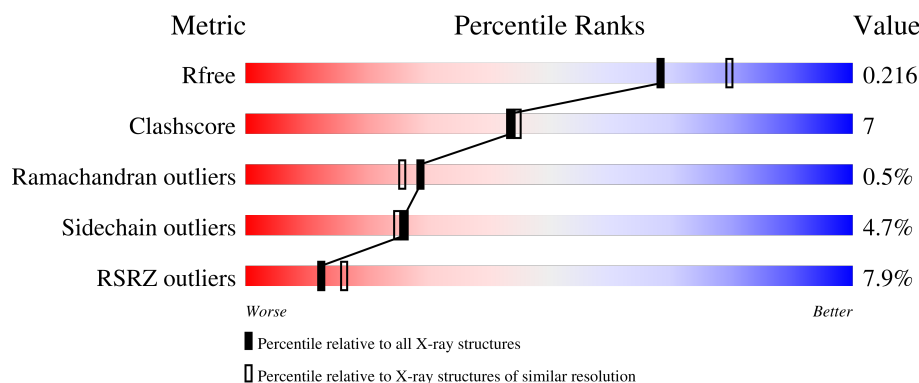
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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 of 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	310	<div> <div>10%</div> <div>78%</div> <div>14%</div> <div>8%</div> </div>
1	B	310	<div> <div>5%</div> <div>77%</div> <div>13%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	799	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5126 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 Tyrosine-protein phosphatase, non-receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	8	0
			2367	1506	404	442	15			
1	B	285	Total	C	N	O	S	0	9	0
			2371	1506	407	443	15			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	489	MET	-	cloning artifact	UNP P18031
A	490	ASP	-	cloning artifact	UNP P18031
A	491	TYR	-	cloning artifact	UNP P18031
A	492	LYS	-	cloning artifact	UNP P18031
A	493	ASP	-	cloning artifact	UNP P18031
A	494	ASP	-	cloning artifact	UNP P18031
A	495	ASP	-	cloning artifact	UNP P18031
A	496	ASP	-	cloning artifact	UNP P18031
A	497	LYS	-	cloning artifact	UNP P18031
A	498	LEU	-	cloning artifact	UNP P18031
A	499	GLU	-	cloning artifact	UNP P18031
A	500	PHE	-	cloning artifact	UNP P18031
A	619	VAL	LEU	engineered mutation	UNP P18031
B	489	MET	-	cloning artifact	UNP P18031
B	490	ASP	-	cloning artifact	UNP P18031
B	491	TYR	-	cloning artifact	UNP P18031
B	492	LYS	-	cloning artifact	UNP P18031
B	493	ASP	-	cloning artifact	UNP P18031
B	494	ASP	-	cloning artifact	UNP P18031
B	495	ASP	-	cloning artifact	UNP P18031
B	496	ASP	-	cloning artifact	UNP P18031
B	497	LYS	-	cloning artifact	UNP P18031
B	498	LEU	-	cloning artifact	UNP P18031
B	499	GLU	-	cloning artifact	UNP P18031
B	500	PHE	-	cloning artifact	UNP P18031

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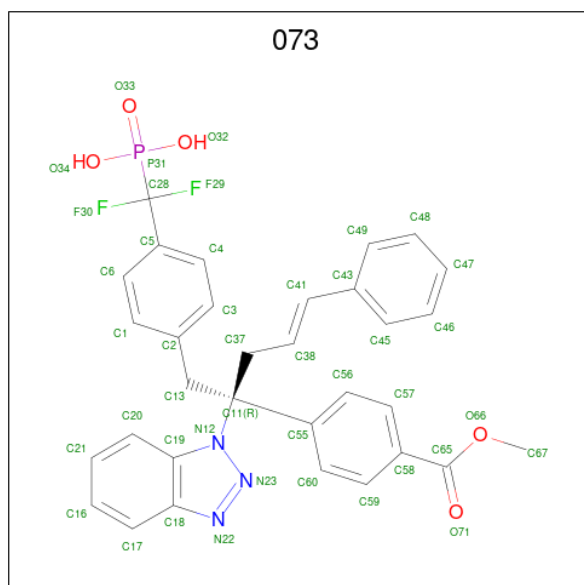
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Chain	Residue	Modelled	Actual	Comment	Reference
B	619	VAL	LEU	engineered mutation	UNP P18031

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0

- Molecule 3 is (4-{(2S,4E)-2-(1H-1,2,3-BENZOTRIAZOL-1-YL)-2-[4-(METHOXYCARBONYL)PHENYL]-5-PHENYLPENT-4-ENYL}PHENYL)(DIFLUORO)METHYLPHOSPHONIC ACID (three-letter code: 073) (formula: C<sub>32</sub>H<sub>28</sub>F<sub>2</sub>N<sub>3</sub>O<sub>5</sub>P).



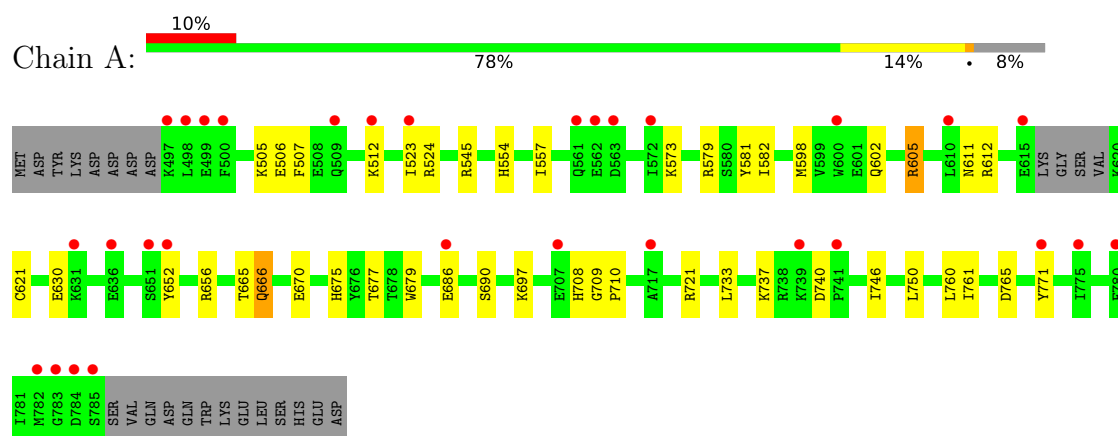
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total 145	O 145	0	0
5	B	154	Total 154	O 154	0	0

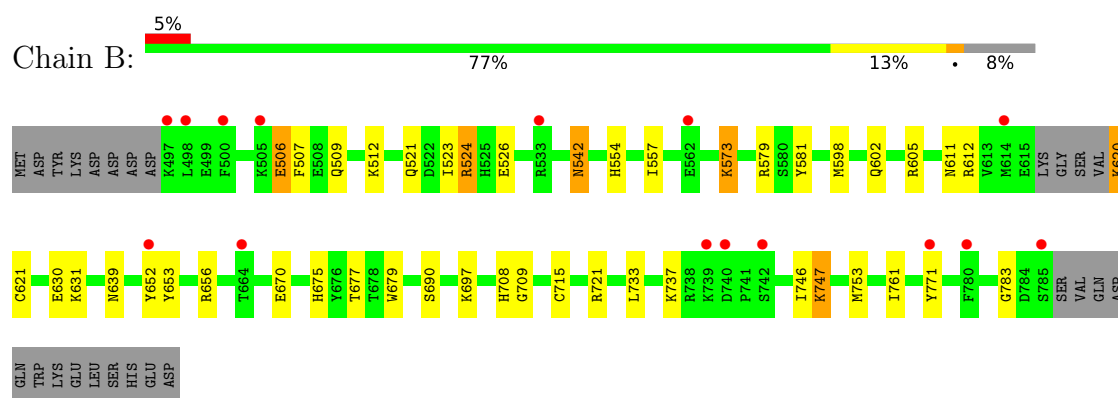
### 3 Residue-property plots [i](#)

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: Tyrosine-protein phosphatase, non-receptor type 1



- Molecule 1: Tyrosine-protein phosphatase, non-receptor type 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.43Å 86.62Å 139.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 14.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (15.00-2.10) 95.7 (14.99-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005, CNX	Depositor
R, $R_{free}$	0.192 , 0.217 0.189 , 0.216	Depositor DCC
$R_{free}$ test set	3007 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.470 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5126	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: MG, CL, 073

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	0.56	2/2453 (0.1%)	0.57	0/3304
1	B	0.54	2/2461 (0.1%)	0.58	0/3316
All	All	0.55	4/4914 (0.1%)	0.57	0/6620

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	630	GLU	CD-OE1	10.60	1.37	1.25
1	B	630	GLU	CD-OE1	9.21	1.35	1.25
1	A	630	GLU	CD-OE2	8.54	1.35	1.25
1	B	630	GLU	CD-OE2	6.72	1.33	1.25

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	2367	0	2307	36	0
1	B	2371	0	2305	39	0
2	A	1	0	0	2	0
2	B	1	0	0	1	0
3	A	43	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	43	0	26	0	0
4	B	1	0	0	0	0
5	A	145	0	0	4	0
5	B	154	0	0	3	0
All	All	5126	0	4664	64	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 (64) 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:A:524[B]:ARG:NH2	1:B:524[B]:ARG:NH1	1.74	1.36
1:A:524[B]:ARG:NH2	1:B:524[B]:ARG:CZ	2.01	1.23
1:A:524[B]:ARG:CZ	1:B:524[B]:ARG:NH2	2.29	0.95
1:A:524[A]:ARG:CZ	1:B:524[A]:ARG:NH2	2.39	0.86
1:A:524[B]:ARG:NH2	1:B:524[B]:ARG:HH12	1.73	0.83
1:A:524[B]:ARG:CZ	1:B:524[B]:ARG:HH22	1.95	0.78
1:A:524[B]:ARG:NH1	1:B:524[B]:ARG:HH22	1.81	0.78
1:A:524[B]:ARG:HD2	2:A:799:CL:CL	2.23	0.76
1:A:524[B]:ARG:NH2	1:B:524[B]:ARG:NH2	2.35	0.73
1:A:524[A]:ARG:NH2	1:B:524[A]:ARG:NH2	2.44	0.65
1:A:524[A]:ARG:NE	1:B:524[A]:ARG:NH2	2.48	0.62
1:B:611:ASN:O	1:B:675:HIS:HE1	1.84	0.60
1:B:521:GLN:OE1	1:B:524[B]:ARG:NH1	2.35	0.59
1:B:524[A]:ARG:HD2	2:B:799:CL:CL	2.41	0.58
1:A:524[B]:ARG:CD	2:A:799:CL:CL	2.89	0.57
1:A:611:ASN:O	1:A:675:HIS:HE1	1.88	0.57
1:A:605:ARG:NH2	1:A:670:GLU:OE1	2.33	0.56
1:B:523:ILE:HG12	1:B:747:LYS:HG2	1.89	0.55
1:A:746:ILE:HD12	1:A:771[B]:TYR:CD2	2.41	0.55
1:A:554:HIS:HD2	5:A:855:HOH:O	1.89	0.54
1:B:554:HIS:HD2	5:B:850:HOH:O	1.91	0.53
1:A:605:ARG:HG2	1:A:708:HIS:CD2	2.44	0.53
1:A:656:ARG:NH1	5:A:919:HOH:O	2.43	0.51
1:B:605:ARG:NH2	1:B:670:GLU:OE1	2.42	0.51
1:B:605:ARG:HD3	1:B:708:HIS:NE2	2.25	0.51
1:B:652[B]:TYR:CD2	1:B:653:TYR:HD2	2.29	0.50
1:A:557:ILE:HG21	1:A:598:MET:HG3	1.94	0.50
1:B:506:GLU:HA	1:B:509:GLN:HG2	1.94	0.49
1:B:656:ARG:NH1	5:B:925:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ILE:HG21	1:B:598:MET:HG3	1.96	0.48
1:A:573[B]:LYS:HE2	5:A:899:HOH:O	2.14	0.48
1:A:524[A]:ARG:NH2	5:A:886:HOH:O	2.39	0.47
1:B:579:ARG:CZ	1:B:733:LEU:HD11	2.45	0.47
1:A:507:PHE:HD1	1:A:771[B]:TYR:CD1	2.33	0.46
1:A:523:ILE:HG21	1:A:750:LEU:HD23	1.98	0.46
1:B:746:ILE:HD12	1:B:771[B]:TYR:CD1	2.51	0.46
1:B:620:LYS:HB2	1:B:621:CYS:H	1.52	0.45
1:B:679:TRP:CE2	1:B:721:ARG:HG2	2.50	0.45
1:A:656:ARG:HH12	1:A:675:HIS:HD2	1.64	0.45
1:B:579:ARG:HG2	1:B:581:TYR:CZ	2.52	0.45
1:A:679:TRP:CE2	1:A:721:ARG:HG2	2.52	0.45
1:B:656:ARG:HH12	1:B:675:HIS:CD2	2.35	0.45
1:B:679:TRP:NE1	1:B:721:ARG:HG2	2.31	0.45
1:B:507:PHE:HD1	1:B:771[B]:TYR:CD2	2.35	0.44
1:A:679:TRP:NE1	1:A:721:ARG:HG2	2.32	0.44
1:A:665:THR:O	1:A:666:GLN:HB2	2.17	0.44
1:B:656:ARG:HH12	1:B:675:HIS:HD2	1.66	0.43
1:B:605:ARG:NH1	1:B:670:GLU:OE1	2.51	0.43
1:A:545:ARG:NH2	1:A:621:CYS:HA	2.34	0.43
1:A:602:GLN:O	1:A:709:GLY:HA3	2.19	0.43
1:B:620:LYS:HA	5:B:864:HOH:O	2.18	0.43
1:A:579:ARG:HG2	1:A:581:TYR:CZ	2.53	0.43
1:B:602:GLN:O	1:B:709:GLY:HA3	2.19	0.43
1:B:612:ARG:HD3	1:B:677:THR:O	2.19	0.42
1:A:652[B]:TYR:CD2	1:A:690:SER:HB2	2.54	0.42
1:A:656:ARG:HH12	1:A:675:HIS:CD2	2.37	0.42
1:B:652[B]:TYR:CD2	1:B:690:SER:HB2	2.55	0.42
1:A:579:ARG:CZ	1:A:733:LEU:HD11	2.51	0.41
1:B:753:MET:HE2	1:B:753:MET:HB3	1.92	0.41
1:A:582:ILE:HG13	1:A:710:PRO:HB2	2.02	0.41
1:A:612:ARG:HD3	1:A:677:THR:O	2.20	0.41
1:B:542:ASN:N	1:B:542:ASN:HD22	2.18	0.41
1:A:524[B]:ARG:CZ	1:B:524[B]:ARG:CZ	2.69	0.40

There are no symmetry-related clashes.

## 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	289/310 (93%)	278 (96%)	10 (4%)	1 (0%)	41	41
1	B	290/310 (94%)	281 (97%)	7 (2%)	2 (1%)	22	18
All	All	579/620 (93%)	559 (96%)	17 (3%)	3 (0%)	29	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	761	ILE
1	B	761	ILE
1	B	783	GLY

### 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	263/283 (93%)	251 (95%)	12 (5%)	27	26
1	B	264/283 (93%)	249 (94%)	15 (6%)	20	18
All	All	527/566 (93%)	500 (95%)	27 (5%)	26	22

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	505	LYS
1	A	506	GLU
1	A	512	LYS

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Mol	Chain	Res	Type
1	A	605	ARG
1	A	666	GLN
1	A	686[A]	GLU
1	A	686[B]	GLU
1	A	697	LYS
1	A	737	LYS
1	A	740	ASP
1	A	760	LEU
1	A	765	ASP
1	B	506	GLU
1	B	512	LYS
1	B	524[A]	ARG
1	B	524[B]	ARG
1	B	526	GLU
1	B	542	ASN
1	B	573[A]	LYS
1	B	573[B]	LYS
1	B	620	LYS
1	B	631	LYS
1	B	639	ASN
1	B	697	LYS
1	B	715	CYS
1	B	737	LYS
1	B	747	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	554	HIS
1	A	639	ASN
1	A	657	GLN
1	A	675	HIS
1	A	708	HIS
1	B	542	ASN
1	B	554	HIS
1	B	639	ASN
1	B	675	HIS

### 5.3.3 RNA ⓘ

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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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$
3	073	A	800	-	41,47,47	1.49	6 (14%)	53,69,69	1.38	7 (13%)
3	073	B	801	-	41,47,47	1.41	5 (12%)	53,69,69	1.63	10 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	073	A	800	-	-	0/34/45/45	0/5/5/5
3	073	B	801	-	-	2/34/45/45	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	073	O66-C65	5.96	1.46	1.33
3	B	801	073	O66-C65	5.67	1.45	1.33
3	A	800	073	N22-N23	3.03	1.39	1.34
3	A	800	073	N23-N12	2.87	1.40	1.34
3	B	801	073	N22-N23	2.85	1.39	1.34
3	A	800	073	P31-O34	-2.70	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	073	N23-N12	2.61	1.39	1.34
3	A	800	073	P31-O32	-2.28	1.50	1.54
3	B	801	073	P31-O34	-2.15	1.50	1.54
3	A	800	073	C37-C38	2.06	1.53	1.50
3	B	801	073	P31-O32	-2.01	1.51	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	073	O66-C65-C58	5.09	120.06	112.34
3	A	800	073	O66-C65-C58	4.89	119.76	112.34
3	B	801	073	F30-C28-C5	-4.75	104.38	110.49
3	B	801	073	C20-C19-N12	4.21	135.81	131.93
3	A	800	073	C20-C19-N12	4.09	135.71	131.93
3	A	800	073	C67-O66-C65	3.36	122.31	115.83
3	B	801	073	C67-O66-C65	3.16	121.93	115.83
3	B	801	073	O32-P31-O34	2.91	116.22	107.99
3	A	800	073	F30-C28-C5	-2.90	106.75	110.49
3	B	801	073	O66-C65-O71	-2.74	118.08	123.45
3	A	800	073	O66-C65-O71	-2.53	118.50	123.45
3	B	801	073	P31-C28-C5	2.52	116.51	108.95
3	B	801	073	C37-C11-C13	2.50	114.18	110.14
3	B	801	073	C37-C38-C41	-2.17	120.60	123.94
3	A	800	073	P31-C28-C5	2.10	115.26	108.95
3	A	800	073	O32-P31-O34	2.03	113.72	107.99
3	B	801	073	F29-C28-F30	2.00	109.26	106.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

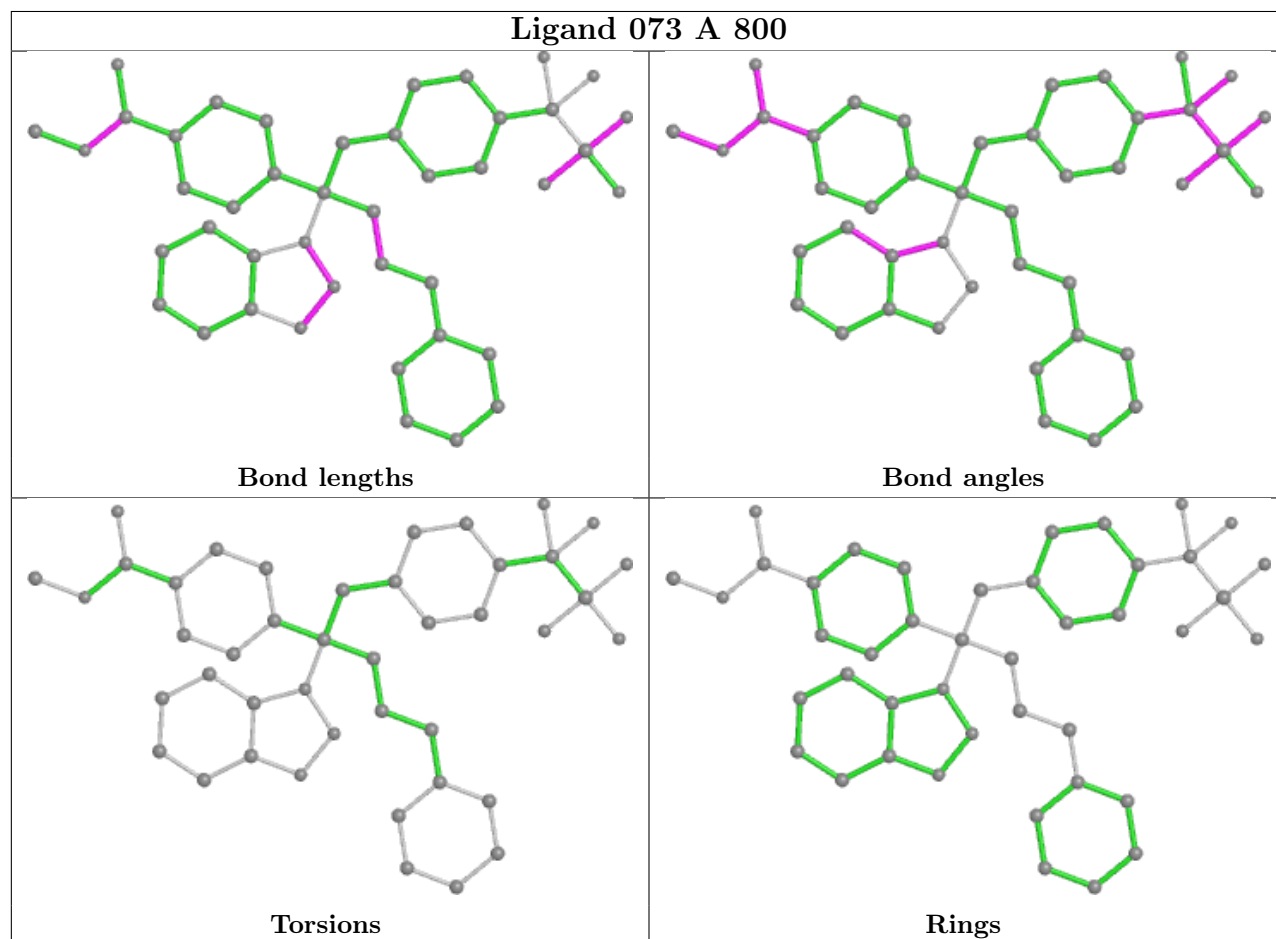
Mol	Chain	Res	Type	Atoms
3	B	801	073	C58-C65-O66-C67
3	B	801	073	O71-C65-O66-C67

There are no ring outliers.

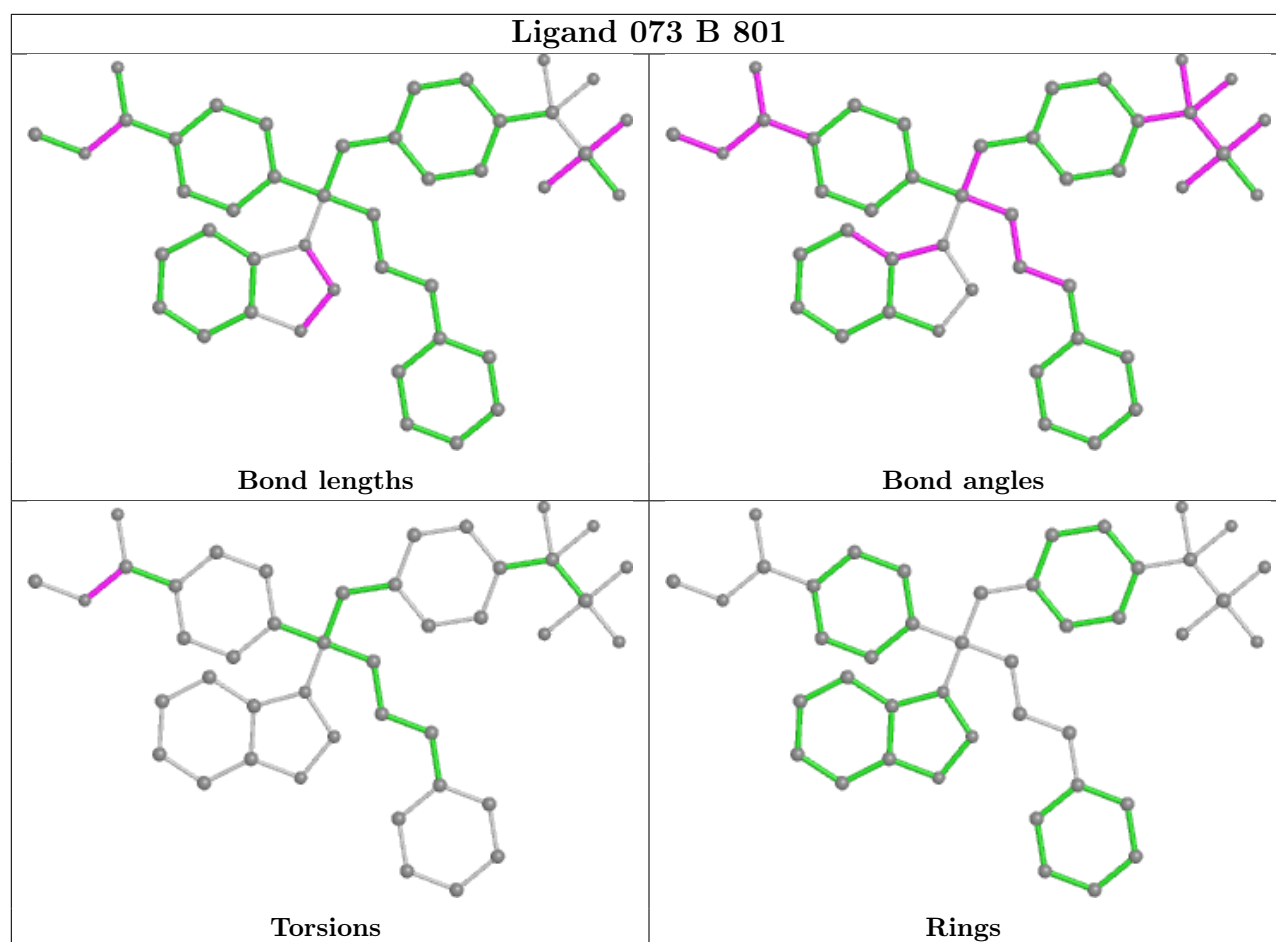
No monomer is involved in short contacts.

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

### 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	285/310 (91%)	0.79	30 (10%) <b>6</b> <b>8</b>	37, 44, 60, 79	0
1	B	285/310 (91%)	0.73	15 (5%) <b>26</b> <b>32</b>	37, 43, 60, 75	0
All	All	570/620 (91%)	0.76	45 (7%) <b>12</b> <b>16</b>	37, 43, 61, 79	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	785	SER	9.1
1	B	497	LYS	5.5
1	A	741	PRO	5.5
1	A	498	LEU	5.3
1	A	784	ASP	5.0
1	B	771[A]	TYR	4.6
1	A	500	PHE	4.4
1	B	500	PHE	4.3
1	B	498	LEU	4.3
1	B	739	LYS	4.2
1	B	505	LYS	4.1
1	A	785	SER	4.0
1	A	652[A]	TYR	3.7
1	A	783	GLY	3.7
1	B	652[A]	TYR	3.6
1	A	636	GLU	3.5
1	A	707[A]	GLU	3.4
1	A	771[A]	TYR	3.3
1	A	739	LYS	3.0
1	A	497	LYS	3.0
1	A	600	TRP	3.0
1	B	533[A]	ARG	2.9
1	B	740	ASP	2.9
1	A	717	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	614	MET	2.7
1	B	562	GLU	2.6
1	A	780	PHE	2.5
1	A	512	LYS	2.4
1	B	780	PHE	2.4
1	A	563	ASP	2.4
1	A	631	LYS	2.3
1	A	562	GLU	2.3
1	A	615	GLU	2.3
1	B	664	THR	2.3
1	A	782	MET	2.2
1	A	509	GLN	2.2
1	A	499	GLU	2.2
1	A	523	ILE	2.1
1	A	686[A]	GLU	2.1
1	A	561	GLN	2.1
1	A	651	SER	2.1
1	B	742	SER	2.0
1	A	775	ILE	2.0
1	A	610	LEU	2.0
1	A	572	ILE	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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	MG	B	800	1/1	0.86	0.09	59,59,59,59	0
3	073	B	801	43/43	0.92	0.13	26,30,38,44	0

*Continued on next page...*

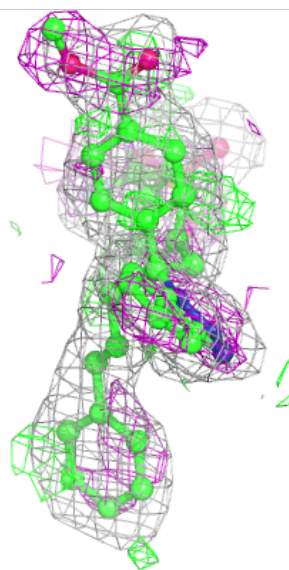
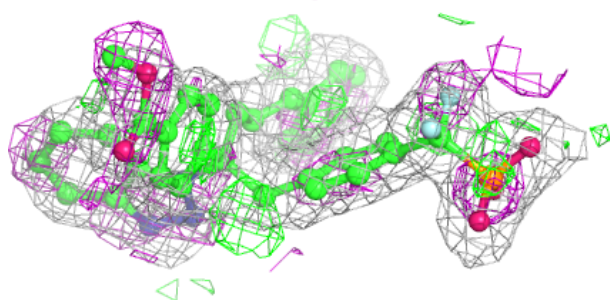
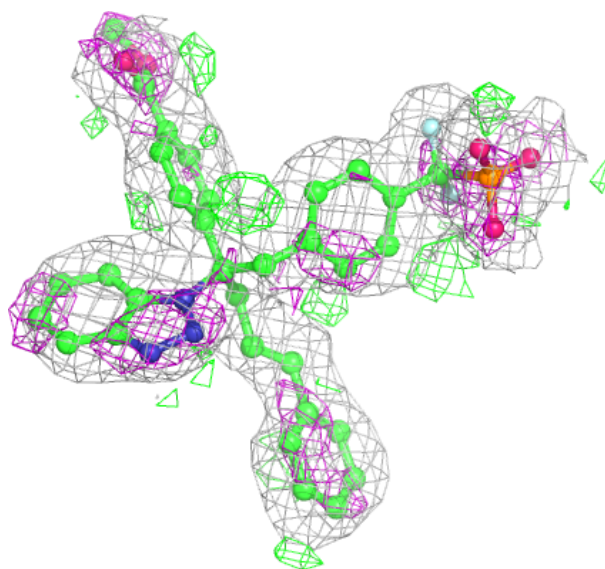
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	073	A	800	43/43	0.95	0.11	26,29,38,43	0
2	CL	A	799	1/1	0.97	0.07	29,29,29,29	0
2	CL	B	799	1/1	0.99	0.06	29,29,29,29	0

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.

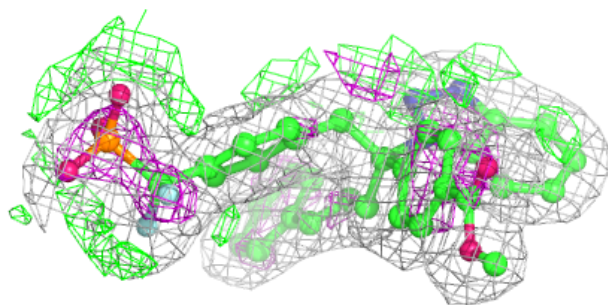
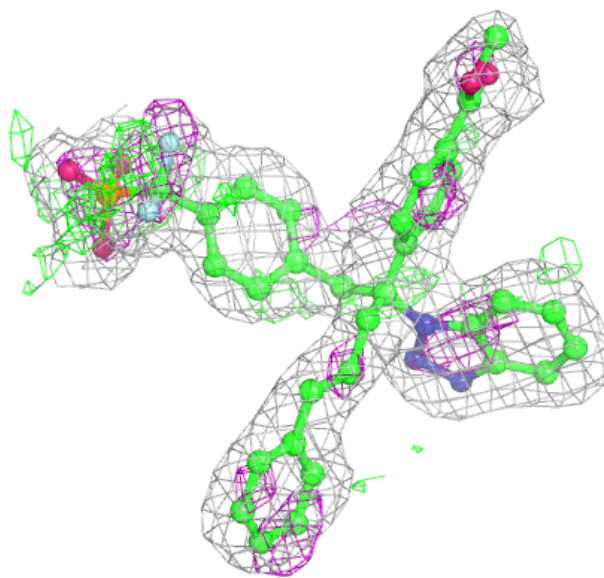
**Electron density around 073 B 801:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 073 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.