wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2023 – 11:36 PM EDT

PDB ID	:	1Q6S
Title	:	THE STRUCTURE OF PHOSPHOTYROSINE PHOSPHATASE 1B IN COMPLEX WITH COMPOUND 9
Authors	:	Scapin, G.; Patel, S.B.; Becker, J.W.; Wang, Q.; Desponts, C.; Waddleton, D.; Skorey, K.; Cromlish, W.; Bayly, C.; Therien, M.; Gauthier, J.Y.; Li, C.S.; Lau, C.K.; Ramachandran, C.; Kennedy, B.P.; Asante-Appiah, E.
Deposited on	:	2003-08-13
Resolution	:	2.20 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

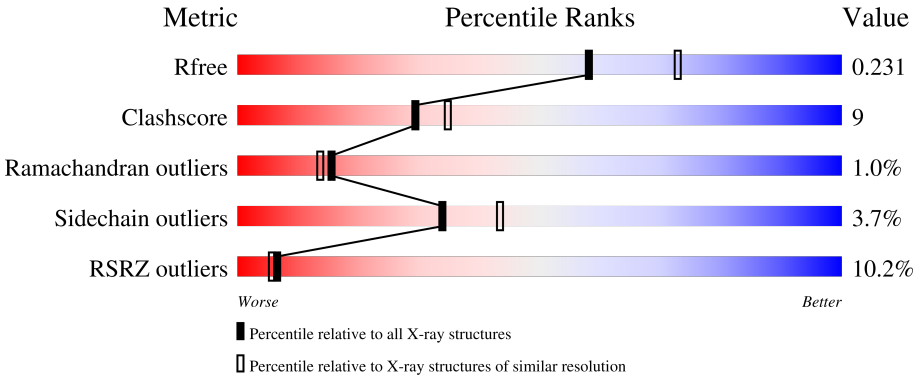
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	8% 77% 14% • 7%
1	B	310	11% 71% 20% • 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5211 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 Protein-tyrosine phosphatase, non-receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2349	1490	404	439	16			
1	B	289	Total	C	N	O	S	0	0	0
			2349	1490	404	439	16			

There are 24 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
B	989	MET	-	cloning artifact	UNP P18031
B	990	ASP	-	cloning artifact	UNP P18031
B	991	TYR	-	cloning artifact	UNP P18031
B	992	LYS	-	cloning artifact	UNP P18031
B	993	ASP	-	cloning artifact	UNP P18031
B	994	ASP	-	cloning artifact	UNP P18031
B	995	ASP	-	cloning artifact	UNP P18031
B	996	ASP	-	cloning artifact	UNP P18031
B	997	LYS	-	cloning artifact	UNP P18031
B	998	LEU	-	cloning artifact	UNP P18031
B	999	GLU	-	cloning artifact	UNP P18031
B	1000	PHE	-	cloning artifact	UNP P18031

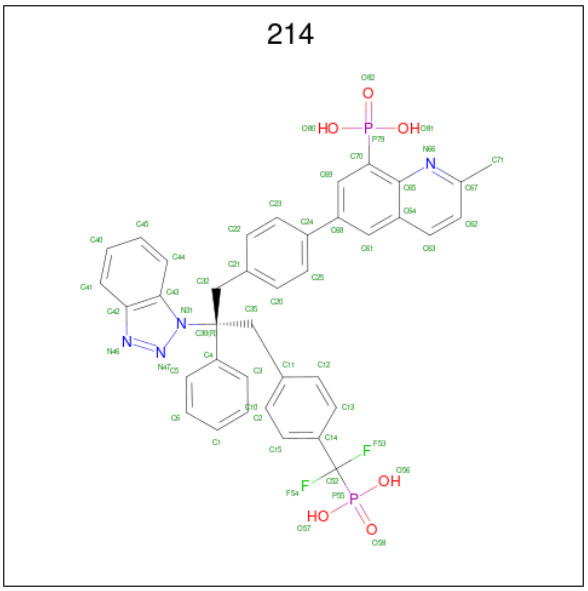
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

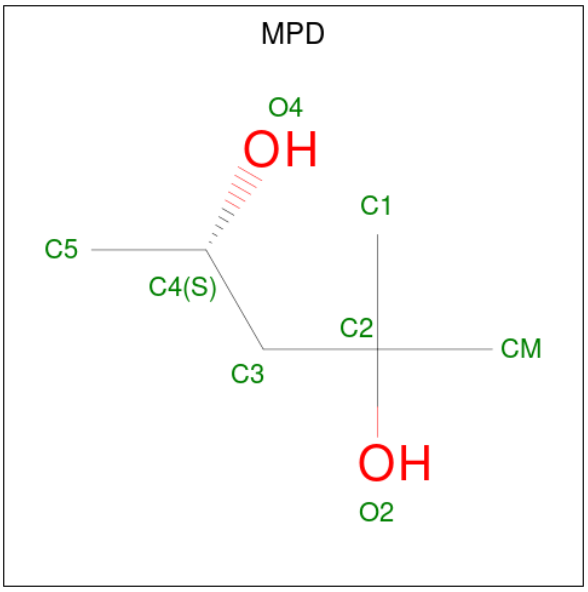
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is 6-[4-((2R)-2-(1H-1,2,3-BENZOTRIAZOL-1-YL)-3-{4-[DIFLUORO(PHOSPHONO)METHYL]PHENYL}-2-PHENYLPROPYL)PHENYL]-2-METHYLQUINOLIN-8-YL PHOSPHONIC ACID (three-letter code: 214) (formula: $C_{38}H_{32}F_2N_4O_6P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O P 52 38 2 4 6 2	0	0
4	B	1	Total C F N O P 52 38 2 4 6 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0

- Molecule 6 is water.

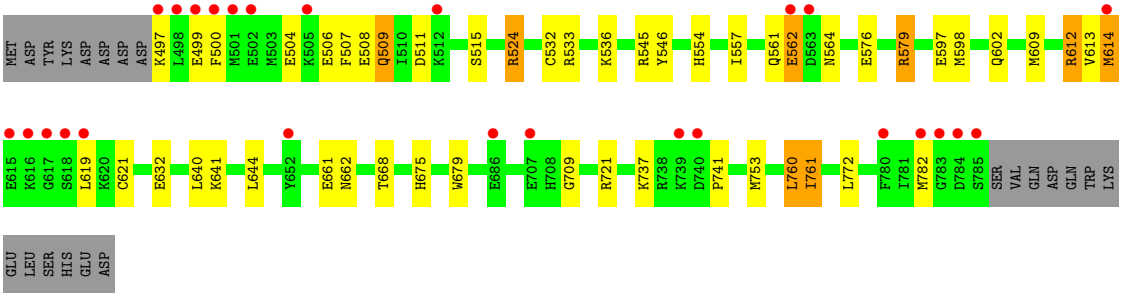
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	192	Total O 192 192	0	0
6	B	204	Total O 204 204	0	0

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.

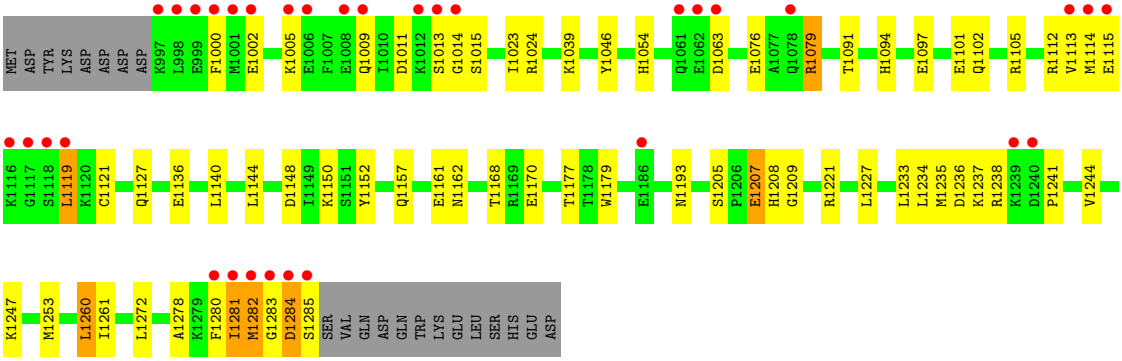
• Molecule 1: Protein-tyrosine phosphatase, non-receptor type 1

Chain A:



• Molecule 1: Protein-tyrosine phosphatase, non-receptor type 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.86Å 87.76Å 138.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.86 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.20) 95.5 (19.86-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 1.99Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.196 , 0.233 0.196 , 0.231	Depositor DCC
R_{free} test set	5034 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5211	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 214, CL, MPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.44	0/2402	0.64	1/3237 (0.0%)
1	B	0.45	0/2402	0.66	0/3237
All	All	0.44	0/4804	0.65	1/6474 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	524	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2349	0	2306	34	0
1	B	2349	0	2306	55	0
2	A	1	0	0	1	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	52	0	28	2	0
4	B	52	0	28	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	12	1	0
6	A	192	0	0	5	0
6	B	204	0	0	8	0
All	All	5211	0	4680	90	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 9.

The worst 5 of 90 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:1023:ILE:HD11	1:B:1247:LYS:HG3	1.50	0.93
1:B:1205:SER:OG	1:B:1207:GLU:HG2	1.84	0.78
1:B:1015:SER:HA	6:B:3277:HOH:O	1.86	0.75
1:B:1023:ILE:CD1	1:B:1247:LYS:HG3	2.16	0.75
1:B:1119:LEU:HD11	4:B:1301:214:H13	1.69	0.73

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	287/310 (93%)	275 (96%)	11 (4%)	1 (0%)	41 46
1	B	287/310 (93%)	267 (93%)	15 (5%)	5 (2%)	9 6
All	All	574/620 (93%)	542 (94%)	26 (4%)	6 (1%)	15 14

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1063	ASP

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Mol	Chain	Res	Type
1	B	1119	LEU
1	A	761	ILE
1	B	1261	ILE
1	B	1281	ILE

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	259/283 (92%)	250 (96%)	9 (4%)	36	46
1	B	259/283 (92%)	249 (96%)	10 (4%)	32	41
All	All	518/566 (92%)	499 (96%)	19 (4%)	34	43

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1144	LEU
1	B	1272	LEU
1	B	1282	MET
1	B	1260	LEU
1	A	782	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1094	HIS
1	B	1193	ASN
1	A	657	GLN
1	B	1054	HIS
1	B	1061	GLN

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 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	214	A	801	-	51,58,58	2.17	20 (39%)	61,89,89	1.77	13 (21%)
5	MPD	A	6000	-	7,7,7	2.07	2 (28%)	9,10,10	1.30	1 (11%)
4	214	B	1301	-	51,58,58	2.07	19 (37%)	61,89,89	1.71	11 (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
4	214	A	801	-	-	6/32/47/47	0/7/7/7
5	MPD	A	6000	-	-	1/5/5/5	-
4	214	B	1301	-	-	7/32/47/47	0/7/7/7

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1301	214	P55-O57	-5.51	1.44	1.54
4	A	801	214	C69-C70	5.04	1.42	1.37
4	A	801	214	C30-C4	4.90	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	214	P55-O57	-4.86	1.45	1.54
4	B	1301	214	C30-C4	4.86	1.58	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1301	214	C44-C43-N31	7.45	138.81	131.93
4	A	801	214	C44-C43-N31	7.05	138.44	131.93
4	A	801	214	C43-C42-N46	-4.37	103.13	108.58
4	B	1301	214	C43-C42-N46	-4.08	103.49	108.58
4	B	1301	214	C64-C65-N66	-3.57	117.90	122.64

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	214	C65-C70-P79-O81
4	A	801	214	C69-C70-P79-O81
4	B	1301	214	C65-C70-P79-O80
4	B	1301	214	C65-C70-P79-O81
4	B	1301	214	C69-C70-P79-O80

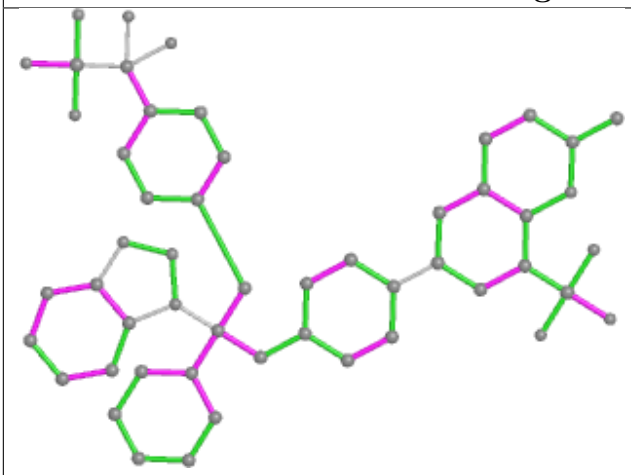
There are no ring outliers.

3 monomers are involved in 6 short contacts:

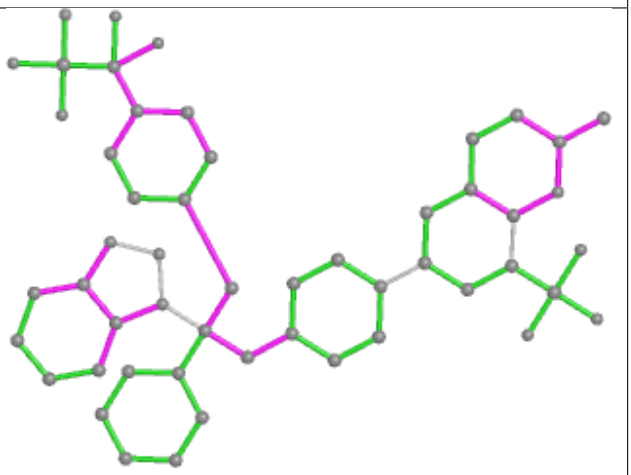
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	214	2	0
5	A	6000	MPD	1	0
4	B	1301	214	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

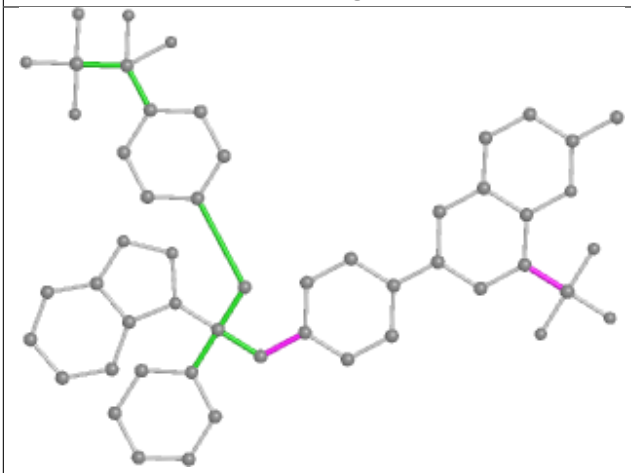
Ligand 214 A 801



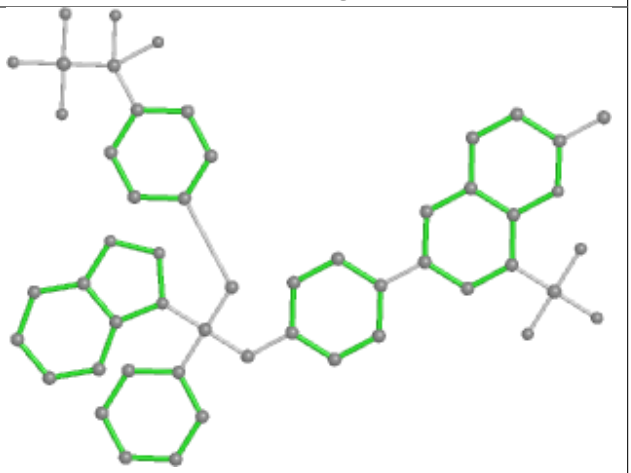
Bond lengths



Bond angles

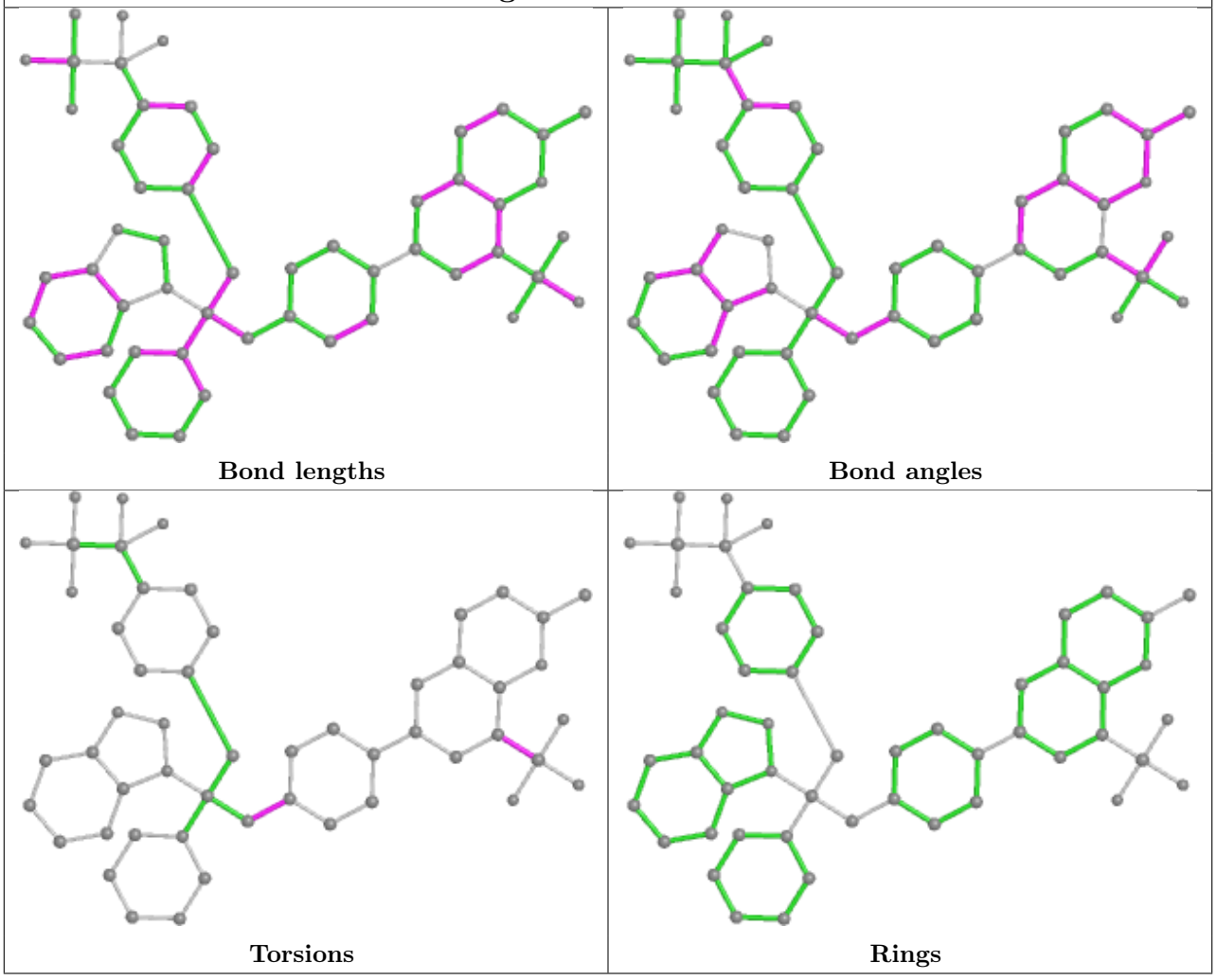


Torsions



Rings

Ligand 214 B 1301



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	289/310 (93%)	0.33	26 (8%)	9	8	13, 23, 52, 60	0
1	B	289/310 (93%)	0.41	33 (11%)	5	4	10, 23, 56, 63	0
All	All	578/620 (93%)	0.37	59 (10%)	6	6	10, 23, 54, 63	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	784	ASP	9.8
1	B	1116	LYS	9.3
1	A	785	SER	8.5
1	B	1115	GLU	8.2
1	B	1000	PHE	8.0

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

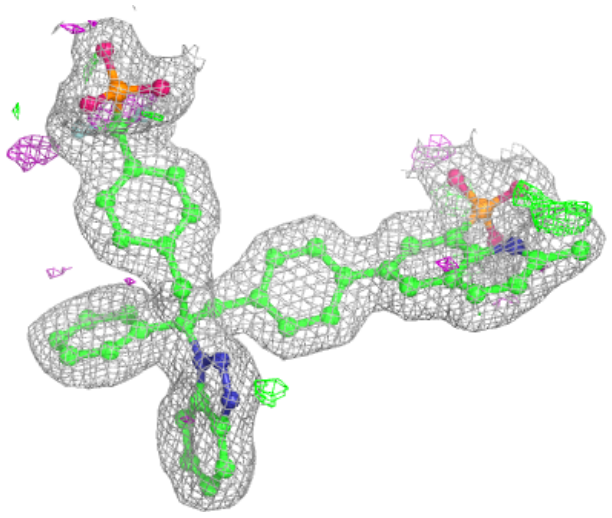
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

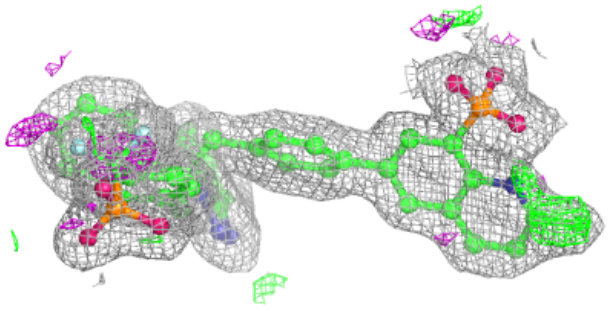
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MPD	A	6000	8/8	0.88	0.20	24,26,28,28	0
3	MG	A	4000	1/1	0.95	0.05	25,25,25,25	1
3	MG	B	5000	1/1	0.95	0.12	23,23,23,23	1
2	CL	B	2013	1/1	0.95	0.10	38,38,38,38	0
4	214	A	801	52/52	0.96	0.11	12,15,18,19	0
2	CL	A	2011	1/1	0.96	0.06	35,35,35,35	0
4	214	B	1301	52/52	0.97	0.10	10,13,17,18	0
2	CL	B	2012	1/1	0.99	0.07	32,32,32,32	0

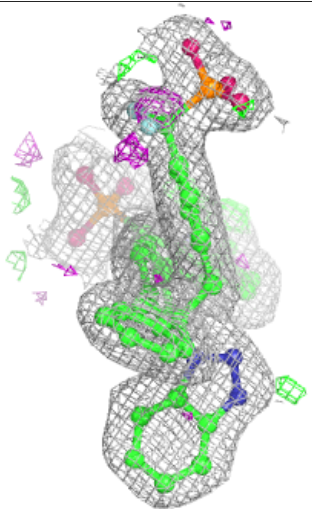
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 214 A 801:

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

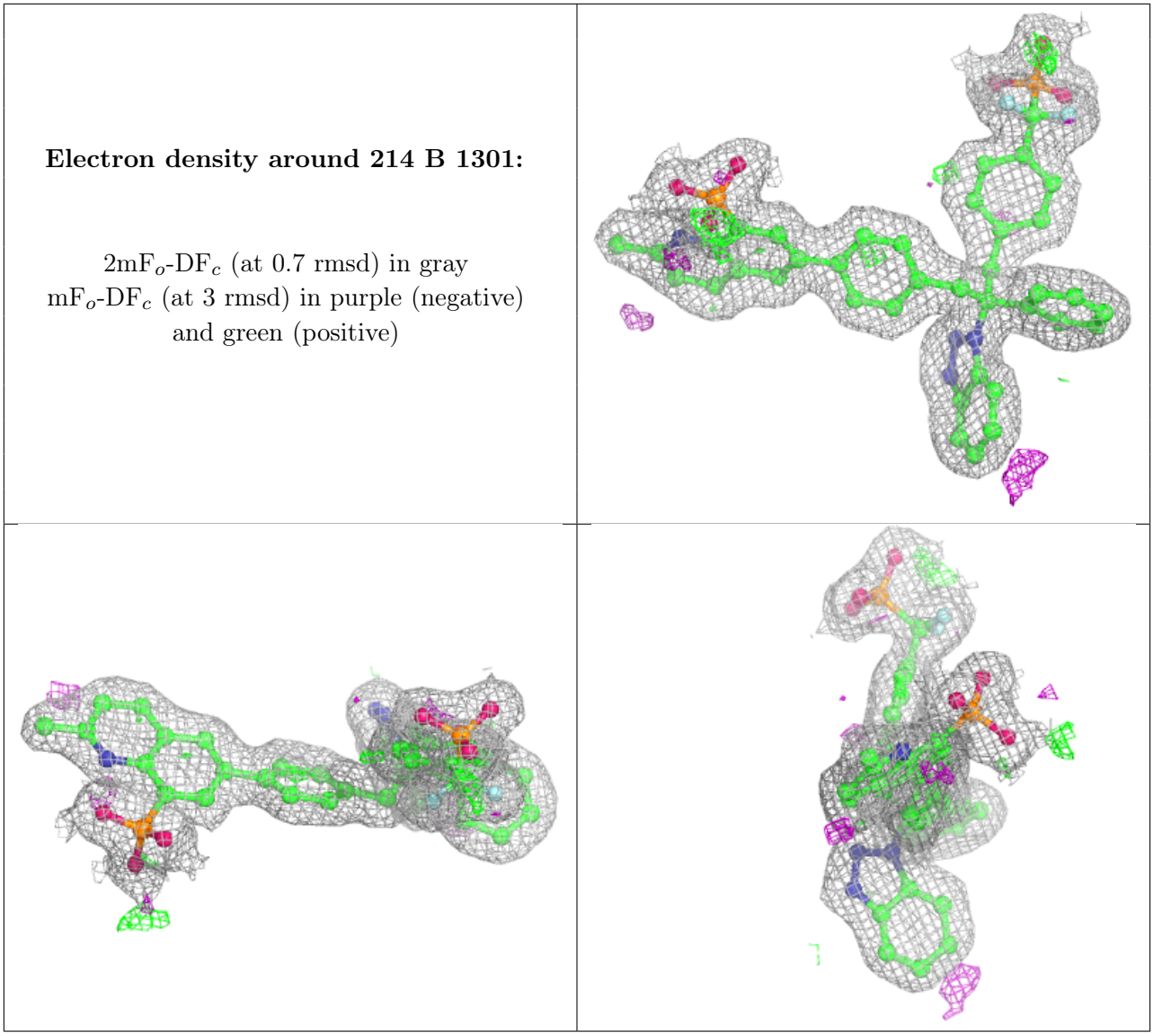






Electron density around 214 B 1301:

$2mF_o$-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.