Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 08:30 AM EDT

PDB ID	:	6UQD
Title	:	Co-complex of S. pyogenes 10782 streptopain bound with a SuFEx-based optimized small molecule inhibitor
Authors	:	Wolan, D.W.; Woehl, J.L.; Kitamura, S.
Deposited on	:	2019-10-18
Resolution	:	2.02 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.02 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4319 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.

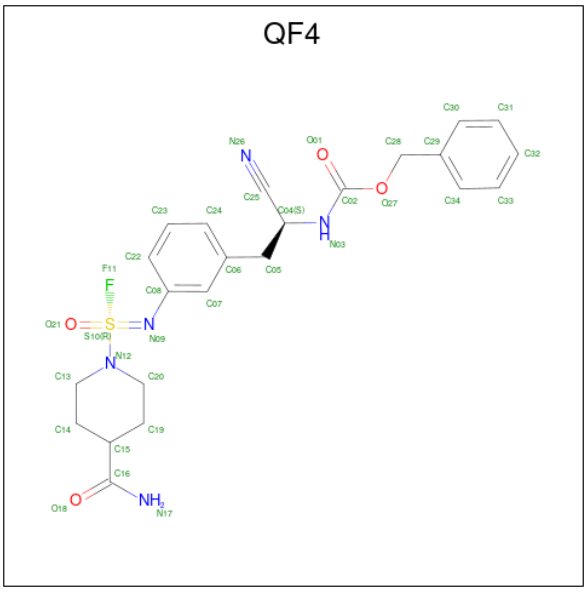
- Molecule 1 is a protein called Streptopain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	1	0
			1907	1203	334	365	5			
1	B	254	Total	C	N	O	S	0	3	0
			1959	1236	342	376	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP P0C0J0
A	154	ASN	ASP	conflict	UNP P0C0J0
A	399	LEU	-	expression tag	UNP P0C0J0
A	400	GLU	-	expression tag	UNP P0C0J0
A	401	HIS	-	expression tag	UNP P0C0J0
A	402	HIS	-	expression tag	UNP P0C0J0
A	403	HIS	-	expression tag	UNP P0C0J0
A	404	HIS	-	expression tag	UNP P0C0J0
A	405	HIS	-	expression tag	UNP P0C0J0
A	406	HIS	-	expression tag	UNP P0C0J0
B	27	MET	-	initiating methionine	UNP P0C0J0
B	154	ASN	ASP	conflict	UNP P0C0J0
B	399	LEU	-	expression tag	UNP P0C0J0
B	400	GLU	-	expression tag	UNP P0C0J0
B	401	HIS	-	expression tag	UNP P0C0J0
B	402	HIS	-	expression tag	UNP P0C0J0
B	403	HIS	-	expression tag	UNP P0C0J0
B	404	HIS	-	expression tag	UNP P0C0J0
B	405	HIS	-	expression tag	UNP P0C0J0
B	406	HIS	-	expression tag	UNP P0C0J0

- Molecule 2 is benzyl [(1S)-2-(3-{[(4-carbamoylpiperidin-1-yl)(fluoro)oxo-lambda 6 -sulfanylidene]amino}phenyl)-1-cyanoethyl]carbamate (three-letter code: QF4) (formula: $C_{23}H_{26}FN_5O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			34	23	1	5	4	1		
2	B	1	Total	C	F	N	O	S	0	0
			34	23	1	5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	196	Total	O	0	0
			196	196		
3	B	189	Total	O	0	0
			189	189		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.62Å 115.52Å 50.27Å 90.00° 112.58° 90.00°	Depositor
Resolution (Å)	43.07 – 2.02	Depositor
% Data completeness (in resolution range)	93.0 (43.07-2.02)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.215 , 0.257	Depositor
Wilson B-factor (Å^2)	10.5	Xtriage
Anisotropy	0.058	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4319	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.57% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

2 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	QF4	B	501	-	31,36,36	4.40	12 (38%)	37,49,49	4.69	7 (18%)
2	QF4	A	501	-	31,36,36	2.70	12 (38%)	37,49,49	1.92	7 (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
2	QF4	B	501	-	-	10/21/40/40	0/3/3/3
2	QF4	A	501	-	-	11/21/40/40	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	QF4	O21-S10	21.15	1.61	1.40
2	A	501	QF4	O21-S10	6.75	1.47	1.40
2	A	501	QF4	C13-N12	5.71	1.53	1.47
2	A	501	QF4	C16-N17	5.09	1.45	1.32
2	B	501	QF4	C16-N17	5.05	1.45	1.32
2	A	501	QF4	C20-N12	4.99	1.53	1.47
2	B	501	QF4	C02-N03	4.83	1.46	1.34
2	A	501	QF4	C02-N03	4.79	1.46	1.34
2	B	501	QF4	C13-N12	4.77	1.52	1.47
2	A	501	QF4	F11-S10	4.44	1.61	1.53
2	B	501	QF4	C20-N12	4.27	1.52	1.47
2	B	501	QF4	C04-C25	3.40	1.52	1.48
2	B	501	QF4	F11-S10	-3.14	1.47	1.53
2	A	501	QF4	C19-C15	-3.10	1.45	1.53
2	A	501	QF4	C14-C15	-2.99	1.45	1.53
2	A	501	QF4	C04-C25	2.95	1.52	1.48
2	A	501	QF4	O27-C02	2.86	1.40	1.35
2	B	501	QF4	O27-C02	2.81	1.40	1.35
2	B	501	QF4	C19-C15	-2.70	1.46	1.53
2	B	501	QF4	C14-C15	-2.58	1.46	1.53
2	A	501	QF4	O18-C16	-2.56	1.18	1.23
2	B	501	QF4	O18-C16	-2.52	1.19	1.23
2	B	501	QF4	O27-C28	-2.50	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	QF4	O27-C28	-2.39	1.40	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	QF4	F11-S10-N09	-26.74	93.83	112.21
2	A	501	QF4	F11-S10-N09	7.55	117.39	112.21
2	B	501	QF4	C20-N12-C13	-5.88	105.66	112.17
2	A	501	QF4	O27-C02-N03	4.84	120.33	110.50
2	B	501	QF4	O27-C02-N03	4.55	119.76	110.50
2	A	501	QF4	C14-C13-N12	4.36	115.37	109.43
2	A	501	QF4	O01-C02-N03	-3.04	119.86	124.85
2	B	501	QF4	O01-C02-N03	-2.61	120.58	124.85
2	B	501	QF4	C15-C16-N17	2.44	120.46	116.54
2	B	501	QF4	O27-C02-O01	-2.39	119.66	124.25
2	A	501	QF4	C19-C20-N12	2.38	112.67	109.43
2	A	501	QF4	O27-C02-O01	-2.32	119.80	124.25
2	A	501	QF4	C15-C16-N17	2.26	120.18	116.54
2	B	501	QF4	C19-C15-C14	2.23	114.68	109.97

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	QF4	C13-N12-S10-O21
2	A	501	QF4	C20-N12-S10-O21
2	A	501	QF4	C14-C15-C16-N17
2	A	501	QF4	C14-C15-C16-O18
2	A	501	QF4	C25-C04-C05-C06
2	A	501	QF4	C07-C08-N09-S10
2	B	501	QF4	C13-N12-S10-O21
2	B	501	QF4	C20-N12-S10-O21
2	B	501	QF4	C14-C15-C16-N17
2	B	501	QF4	C14-C15-C16-O18
2	B	501	QF4	N03-C02-O27-C28
2	B	501	QF4	O01-C02-O27-C28
2	A	501	QF4	N03-C02-O27-C28
2	A	501	QF4	O01-C02-O27-C28
2	B	501	QF4	O27-C02-N03-C04
2	B	501	QF4	O01-C02-N03-C04
2	B	501	QF4	N03-C04-C05-C06
2	A	501	QF4	N03-C04-C05-C06

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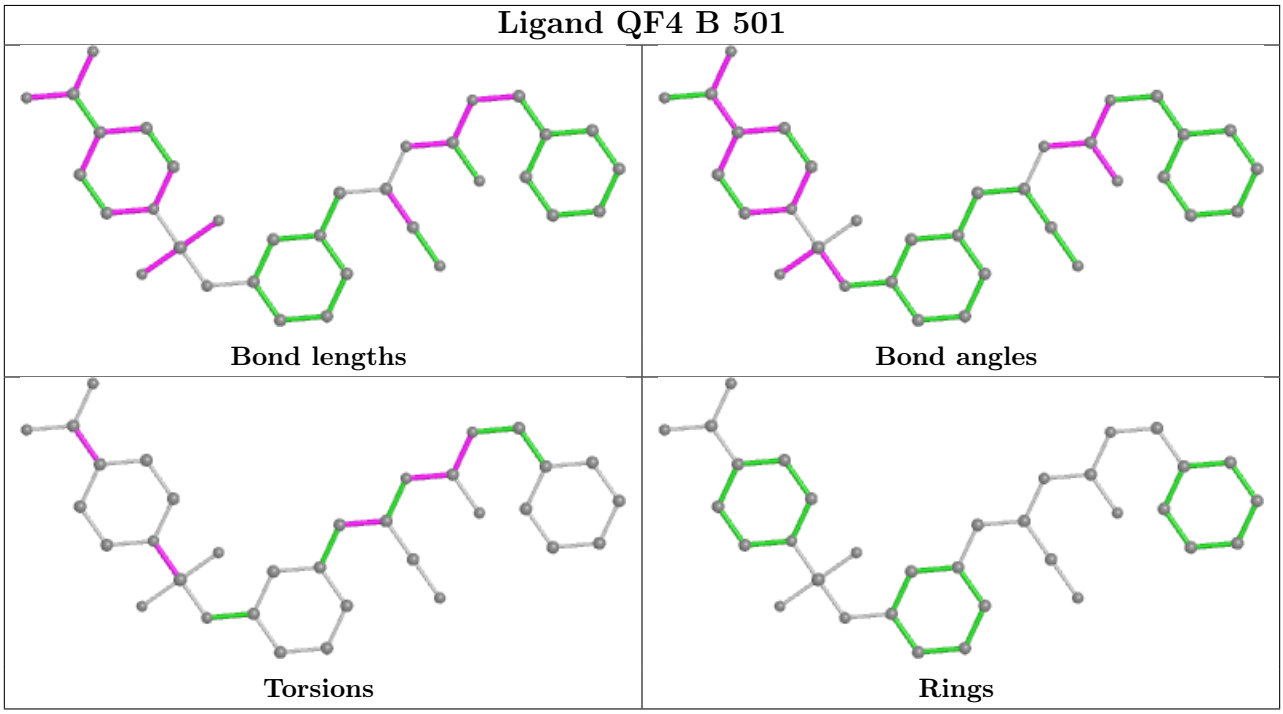
Mol	Chain	Res	Type	Atoms
2	B	501	QF4	C25-C04-C05-C06
2	A	501	QF4	C22-C08-N09-S10
2	A	501	QF4	O27-C02-N03-C04

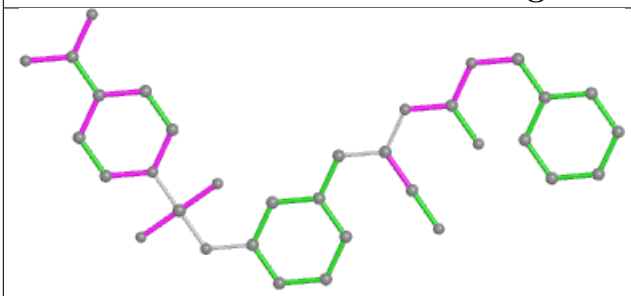
There are no ring outliers.

No monomer is involved in short contacts.

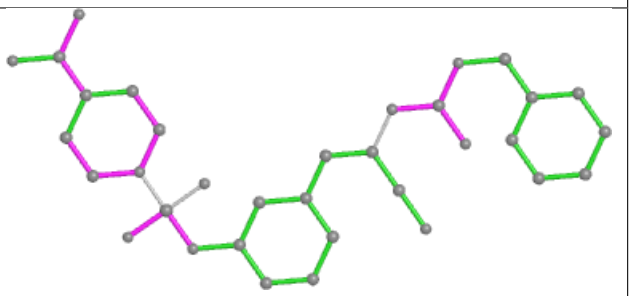
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



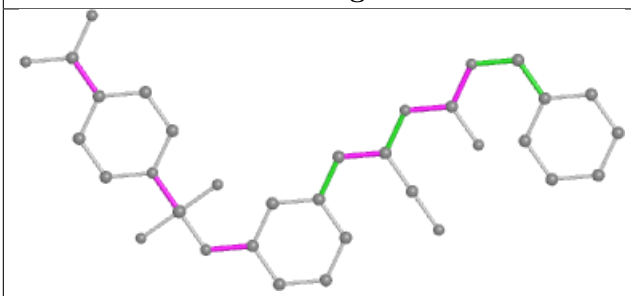
Ligand QF4 A 501



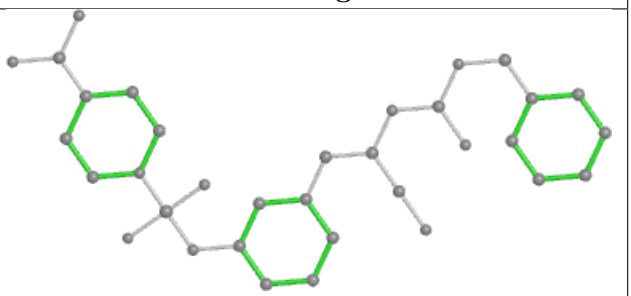
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.