wwPDB X-ray Structure Validation Summary Report (i)

May 24, 2020 – 01:52 am BST

PDB ID	:	6GNN
Title	:	Exoenzyme T from Pseudomonas aeruginosa in complex with human 14-3-3 protein beta, tetrameric crystal form bound to STO1101
Authors	:	Karlberg, T.; Pinto, A.F.; Hornyak, P.; Thorsell, A.G.; Nareoja, K.; Schuler, H.
Deposited on	:	2018-05-31
Resolution	:	3.79 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 following versions of software and data (see references (1)) were used in the production of this report:

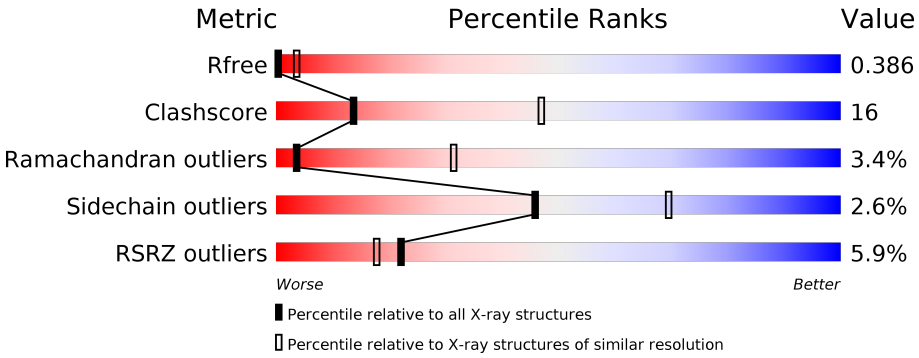
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

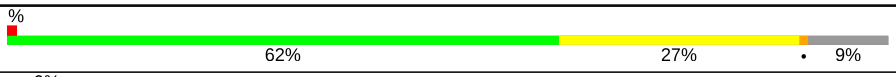
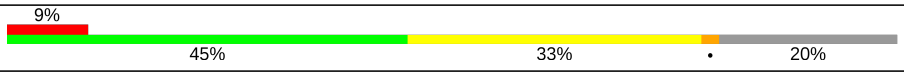
The reported resolution of this entry is 3.79 Å.

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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 >=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	248	
2	C	246	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3322 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 14-3-3 protein beta/alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1811	1137	303	362	9			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	GLU	-	expression tag	UNP P31946
A	241	ASN	-	expression tag	UNP P31946
A	242	LEU	-	expression tag	UNP P31946
A	243	TYR	-	expression tag	UNP P31946
A	244	PHE	-	expression tag	UNP P31946
A	245	GLN	-	expression tag	UNP P31946
A	246	SER	-	expression tag	UNP P31946
A	247	LEU	-	expression tag	UNP P31946
A	248	GLU	-	expression tag	UNP P31946

- Molecule 2 is a protein called Exoenzyme T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	198	Total	C	N	O	S	0	0	0
			1493	915	265	310	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	209	MET	-	initiating methionine	UNP Q9I788
C	210	GLY	-	expression tag	UNP Q9I788
C	211	SER	-	expression tag	UNP Q9I788
C	212	SER	-	expression tag	UNP Q9I788
C	213	HIS	-	expression tag	UNP Q9I788
C	214	HIS	-	expression tag	UNP Q9I788
C	215	HIS	-	expression tag	UNP Q9I788

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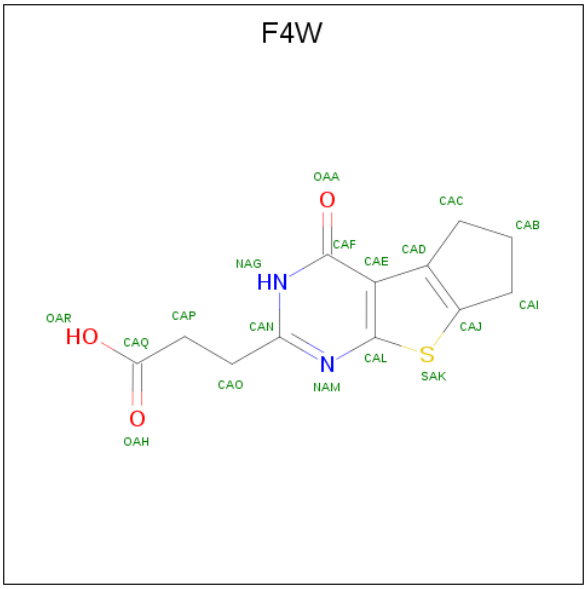
Chain	Residue	Modelled	Actual	Comment	Reference
C	216	HIS	-	expression tag	UNP Q9I788
C	217	HIS	-	expression tag	UNP Q9I788
C	218	HIS	-	expression tag	UNP Q9I788
C	219	SER	-	expression tag	UNP Q9I788
C	220	GLN	-	expression tag	UNP Q9I788
C	221	ASP	-	expression tag	UNP Q9I788
C	222	PRO	-	expression tag	UNP Q9I788
C	223	ASN	-	expression tag	UNP Q9I788
C	224	SER	-	expression tag	UNP Q9I788
C	225	GLU	-	expression tag	UNP Q9I788
C	226	ASN	-	expression tag	UNP Q9I788
C	227	LEU	-	expression tag	UNP Q9I788
C	228	TYR	-	expression tag	UNP Q9I788
C	229	PHE	-	expression tag	UNP Q9I788
C	230	GLN	-	expression tag	UNP Q9I788
C	231	GLY	-	expression tag	UNP Q9I788
C	349	SER	GLY	conflict	UNP Q9I788

- Molecule 3 is 3-(12-oxidanylidene-7-thia-9,11-diazatricyclo[6.4.0.0^{2,6}]dodeca-1(8),2(6),9-trien-10-yl)propanoic acid (three-letter code: F4W) (formula: $C_{12}H_{12}N_2O_3S$).



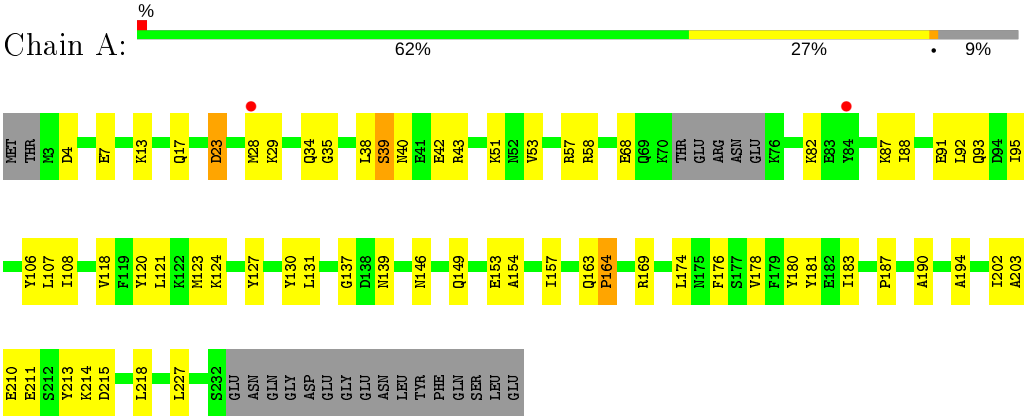
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			18	12	2	3	1		

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.

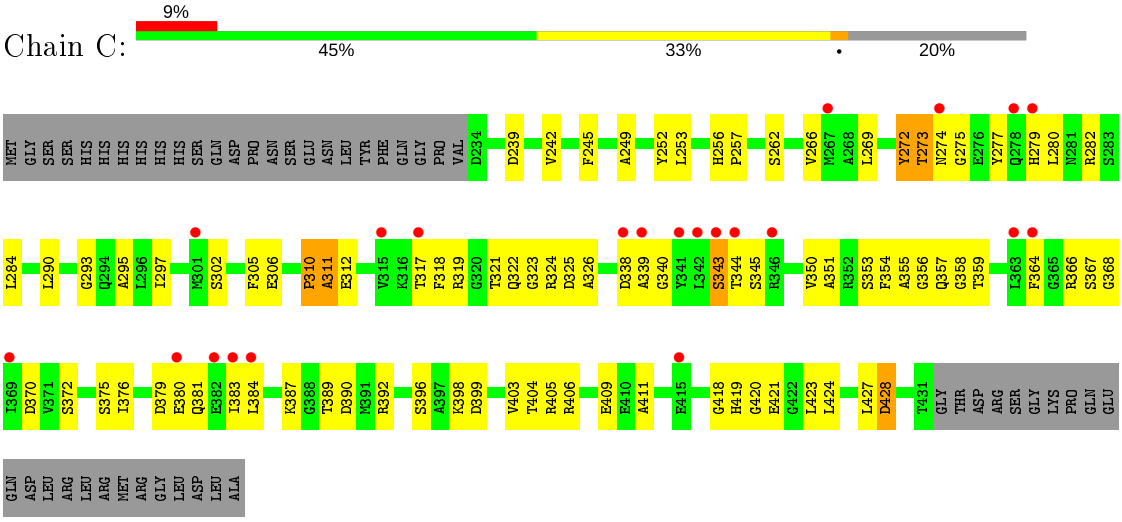
- Molecule 1: 14-3-3 protein beta/alpha

Chain A:



- Molecule 2: Exoenzyme T

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	115.38Å 60.30Å 81.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.44 – 3.79 53.44 – 3.79	Depositor EDS
% Data completeness (in resolution range)	98.5 (53.44-3.79) 98.9 (53.44-3.79)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.285 , 0.385 0.286 , 0.386	Depositor DCC
R_{free} test set	314 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å^2)	122.6	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 84.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3322	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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: F4W

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	0.25	0/1837	0.38	0/2471
2	C	0.28	0/1513	0.48	0/2037
All	All	0.26	0/3350	0.43	0/4508

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

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	1811	0	1796	48	0
2	C	1493	0	1428	64	0
3	C	18	0	0	3	0
All	All	3322	0	3224	104	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 16.

The worst 5 of 104 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:29:LYS:HG3	1:A:102:LEU:HD11	1.59	0.84
2:C:321:THR:OG1	2:C:359:THR:OG1	1.99	0.79
1:A:4:ASP:HB3	1:A:7:GLU:HG2	1.65	0.78
2:C:392:ARG:NH1	2:C:409:GLU:OE1	2.22	0.73
2:C:269:LEU:O	2:C:273:THR:OG1	2.11	0.68

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	221/248 (89%)	204 (92%)	14 (6%)	3 (1%)	11 46
2	C	196/246 (80%)	151 (77%)	34 (17%)	11 (6%)	2 21
All	All	417/494 (84%)	355 (85%)	48 (12%)	14 (3%)	3 31

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	273	THR
2	C	310	PRO
2	C	257	PRO
2	C	272	TYR
2	C	370	ASP

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	199/220 (90%)	193 (97%)	6 (3%)	41 66
2	C	152/194 (78%)	149 (98%)	3 (2%)	55 75
All	All	351/414 (85%)	342 (97%)	9 (3%)	46 69

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
2	C	343	SER
2	C	252	TYR
1	A	39	SER
1	A	176	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	$\#\|Z\| > 2$
3	F4W	C	501	-	13,20,20	3.10	6 (46%)	12,29,29	4.00	9 (75%)

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	F4W	C	501	-	-	1/3/11/11	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	F4W	OAA-CAF	6.27	1.40	1.24
3	C	501	F4W	CAB-CAI	4.41	1.66	1.53
3	C	501	F4W	CAB-CAC	4.35	1.66	1.53
3	C	501	F4W	CAC-CAD	-3.85	1.46	1.51
3	C	501	F4W	CAE-CAL	-3.67	1.36	1.42

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	F4W	CAI-CAJ-CAD	8.29	117.05	111.09
3	C	501	F4W	CAN-NAM-CAL	7.48	121.85	115.56
3	C	501	F4W	CAC-CAD-CAJ	3.98	115.66	110.96
3	C	501	F4W	CAE-CAF-NAG	-3.84	120.68	124.09
3	C	501	F4W	NAM-CAN-NAG	-3.69	121.18	126.06

There are no chirality outliers.

All (1) torsion outliers are listed below:

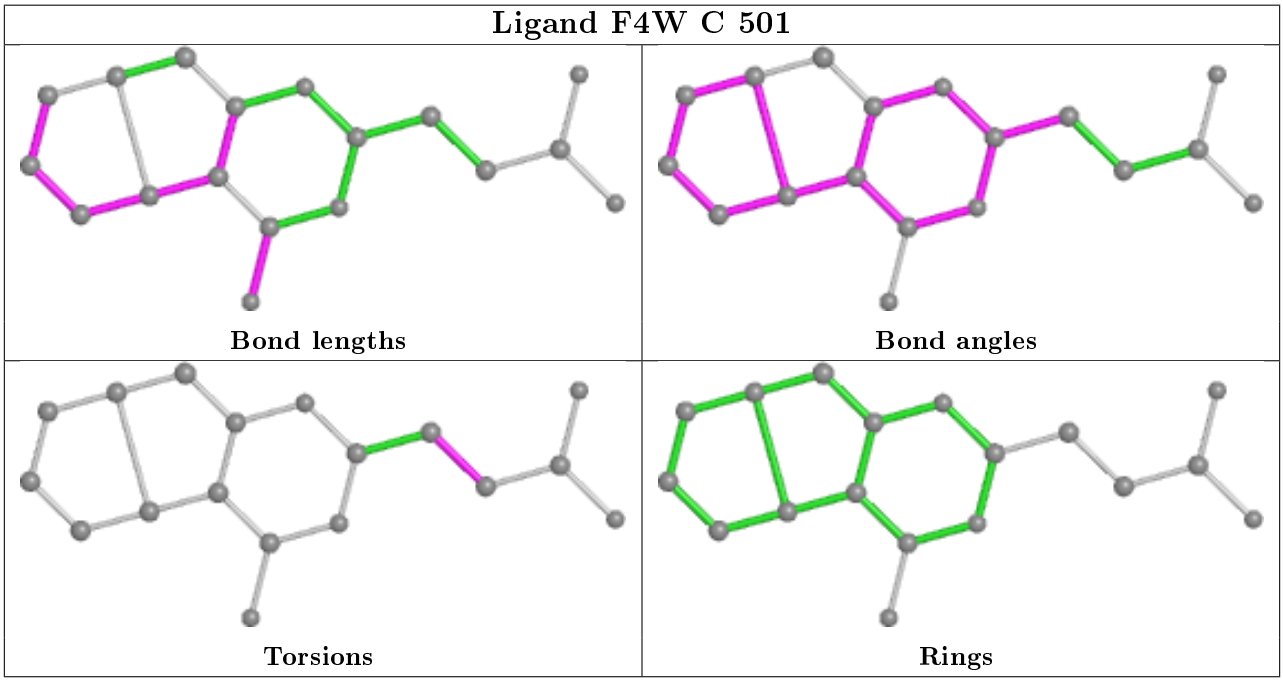
Mol	Chain	Res	Type	Atoms
3	C	501	F4W	CAN-CAO-CAP-CAQ

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	F4W	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.



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	225/248 (90%)	0.16	3 (1%) 77 70	98, 126, 157, 167	0
2	C	198/246 (80%)	0.55	22 (11%) 5 5	90, 121, 147, 174	0
All	All	423/494 (85%)	0.34	25 (5%) 22 18	90, 125, 154, 174	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	382	GLU	5.5
2	C	384	LEU	3.9
2	C	369	ILE	3.8
2	C	383	ILE	3.5
2	C	342	LEU	3.2

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 carbohydrates in this entry.

6.4 Ligands

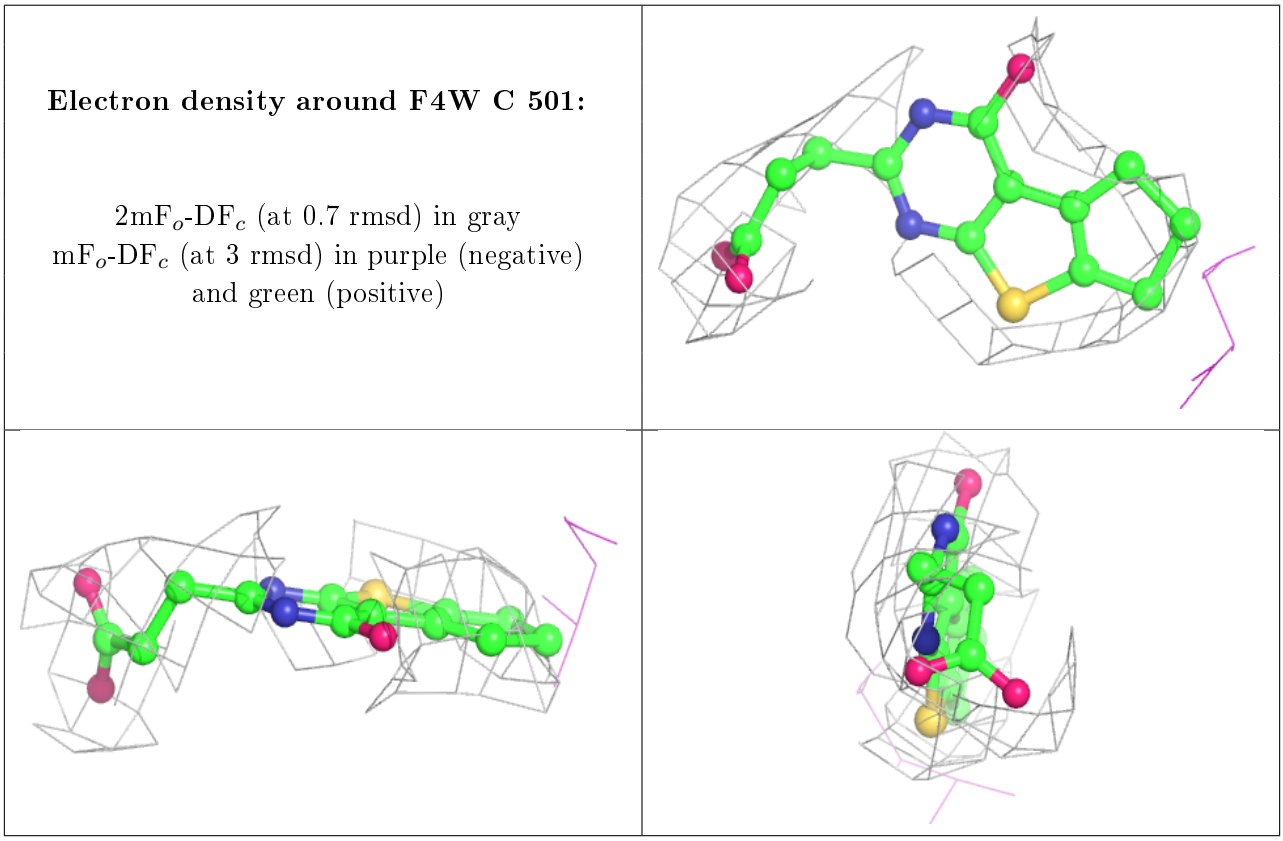
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	F4W	C	501	18/18	0.89	0.34	106,113,122,135	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 F4W C 501:

$2mF_o$-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

There are no such residues in this entry.