



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 09:15 AM EDT

PDB ID : 6XOI
Title : Structure of SUMO1-ML00752641 adduct bound to SAE
Authors : Sintchak, M.; Lane, W.; Bump, N.
Deposited on : 2020-07-07
Resolution : 2.00 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 ⓘ 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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

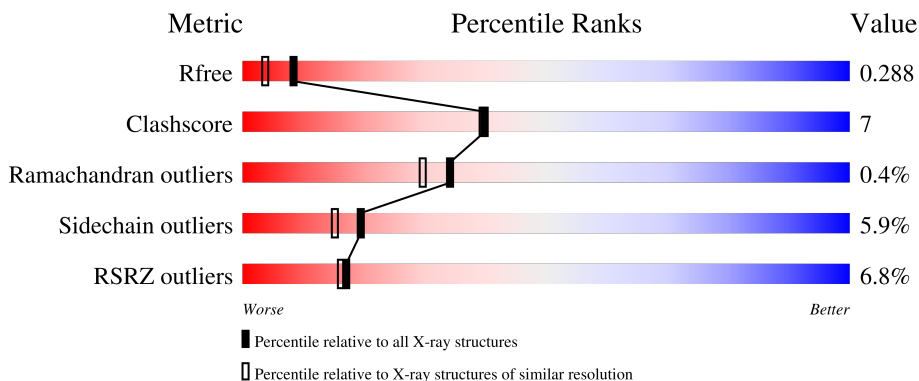
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	346	
2	B	640	
3	C	101	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6165 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 SUMO-activating enzyme subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	311	2394	1519	407	456	12	0	0	0

- Molecule 2 is a protein called SUMO-activating enzyme subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	403	3115	2011	524	561	19	0	0	0

- Molecule 3 is a protein called Small ubiquitin-related modifier 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	41	330	215	55	60	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

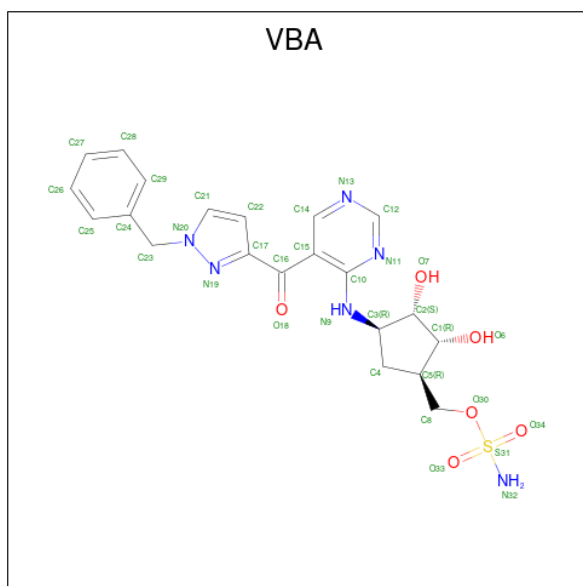


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0

- Molecule 6 is [(1R,2R,3S,4R)-4-{[5-(1-benzyl-1H-pyrazole-3-carbonyl)pyrimidin-4-yl]amino}-2,3-dihydroxycyclopentyl]methyl sulfamate (three-letter code: VBA) (formula: C₂₁H₂₄N₆O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O S 34 21 6 6 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	168	Total O 168 168	0	0
7	B	106	Total O 106 106	0	0
7	C	12	Total O 12 12	0	0

ASP
VAL
SER
GLN
GLU
GLU
GLU
ARG
SER
ARG
LYS
ARG
LYS
LEU
ASP
GLU
LYS
GLU
ASN
LEU
SER
ALA
LYS
ARG
SER
ARG
ILE
GLU
GLN
LYS
GLU
GLU
LEU
ASP
VAL
ILE
ALA
LEU
ASP

● Molecule 3: Small ubiquitin-related modifier 1

Chain C: 

MET
SER
ASP
GLN
GLU
ALA
LYS
PRO
SER
THR
GLU
ASP
LEU
GLY
ASP
LYS
LYS
GLU
GLY
GLU
Y21
I22
K23
L24
K25
V26
L27
D30
S31
S32
E33
I34
H35
F36
K37
V38
LYS
MET
THR
THR
HIS
HIS
LEU
LEU
LYS
LYS
LEU
LEU
LYS
GLU
GLU
SER
TYR
CYS
GLN
ARG
GLN
GLY
VAL
PRO
MET
ASN
S61

L62
R63
F64
L65
F66
E67
G68
R69
I71
A72
ASP
ASN
HIS
THR
PRO
LYS
GLU
LEU
GLY
MET
GLU
GLU
GLU
ASP
V87
V90
E93
G97
HIS
SER
THR
VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.22Å 72.40Å 127.41Å 90.00° 93.29° 90.00°	Depositor
Resolution (Å)	19.38 – 2.00 19.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.38-2.00) 95.7 (19.91-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.239 , 0.287 0.239 , 0.288	Depositor DCC
R_{free} test set	6927 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtrriage
Anisotropy	0.099	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6165	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, VBA, SO4

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	0.46	0/2437	0.78	0/3296
2	B	0.36	0/3172	0.75	0/4298
3	C	0.40	0/333	0.71	0/442
All	All	0.41	0/5942	0.76	0/8036

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	2394	0	2347	28	0
2	B	3115	0	3145	42	0
3	C	330	0	331	15	0
4	A	5	0	0	0	0
5	B	1	0	0	0	0
6	C	34	0	0	1	0
7	A	168	0	0	10	0
7	B	106	0	0	14	0
7	C	12	0	0	3	0
All	All	6165	0	5823	85	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.

The worst 5 of 85 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:152:LYS:HE3	7:A:622:HOH:O	1.21	1.26
2:B:382:ASN:HB2	7:B:876:HOH:O	1.50	1.09
2:B:256:THR:HB	7:B:825:HOH:O	1.54	1.05
2:B:305:LEU:HG	7:B:849:HOH:O	1.78	0.83
7:A:652:HOH:O	2:B:421:GLN:CG	2.27	0.81

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	307/346 (89%)	297 (97%)	8 (3%)	2 (1%)	22	16
2	B	387/640 (60%)	374 (97%)	12 (3%)	1 (0%)	41	37
3	C	35/101 (35%)	32 (91%)	3 (9%)	0	100	100
All	All	729/1087 (67%)	703 (96%)	23 (3%)	3 (0%)	34	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	SER
2	B	59	ARG
1	A	322	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	256/296 (86%)	244 (95%)	12 (5%)	26	22
2	B	338/552 (61%)	316 (94%)	22 (6%)	17	12
3	C	35/91 (38%)	32 (91%)	3 (9%)	10	6
All	All	629/939 (67%)	592 (94%)	37 (6%)	19	15

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	ARG
3	C	23	LYS
2	B	371	LYS
2	B	442	TYR
2	B	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	123	ASN
2	B	162	HIS
3	C	94	GLN
3	C	35	HIS
1	A	325	HIS

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 3 ligands modelled in this entry, 1 is 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
4	SO4	A	401	-	4,4,4	0.35	0	6,6,6	0.12	0
6	VBA	C	201	3	36,37,37	2.23	6 (16%)	46,53,53	2.06	17 (36%)

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
6	VBA	C	201	3	-	1/18/38/38	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	201	VBA	S31-N32	9.18	1.68	1.58
6	C	201	VBA	O30-S31	4.83	1.64	1.57
6	C	201	VBA	O33-S31	4.07	1.45	1.42
6	C	201	VBA	C10-N9	3.59	1.40	1.35
6	C	201	VBA	O34-S31	3.21	1.45	1.42

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	201	VBA	O34-S31-N32	6.14	118.42	109.14
6	C	201	VBA	C21-N20-N19	5.05	115.40	111.45
6	C	201	VBA	C4-C3-C2	-4.13	96.63	103.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	201	VBA	C14-C15-C10	3.96	118.43	114.55
6	C	201	VBA	C2-C3-N9	-2.67	106.98	112.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

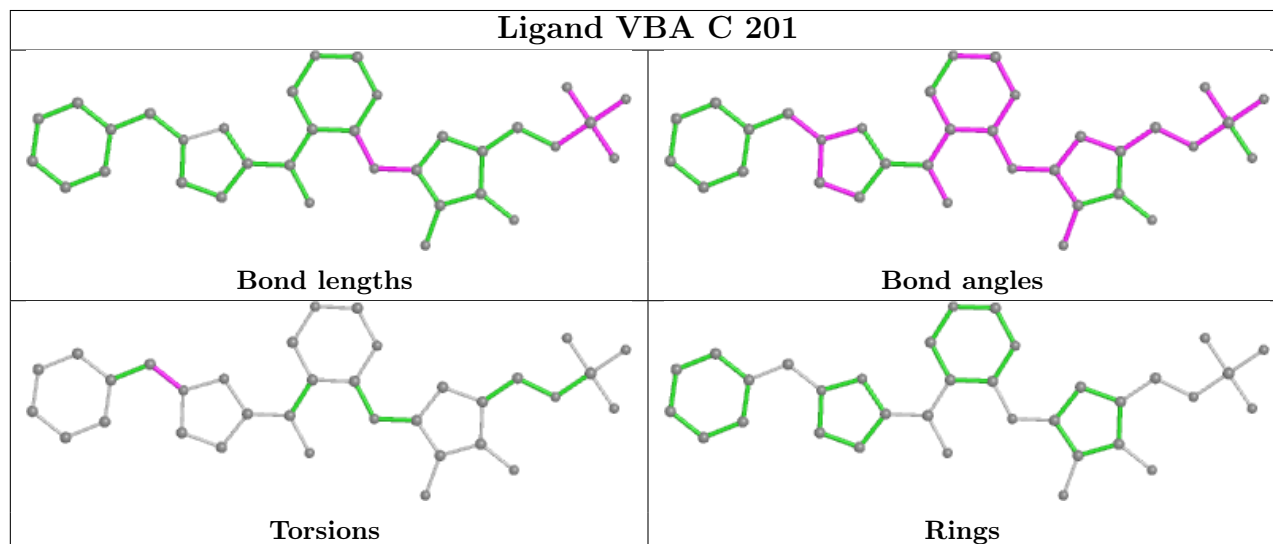
Mol	Chain	Res	Type	Atoms
6	C	201	VBA	C24-C23-N20-C21

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	201	VBA	1	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 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, 95th 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	311/346 (89%)	-0.14	4 (1%) 77 76	16, 30, 57, 78	0
2	B	403/640 (62%)	0.36	33 (8%) 11 11	16, 44, 75, 95	0
3	C	41/101 (40%)	1.54	14 (34%) 0 0	25, 67, 101, 108	0
All	All	755/1087 (69%)	0.22	51 (6%) 17 16	16, 37, 75, 108	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	34	ILE	6.7
3	C	61	SER	5.9
3	C	72	ALA	5.9
3	C	38	VAL	5.7
1	A	205	THR	5.5

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](#)

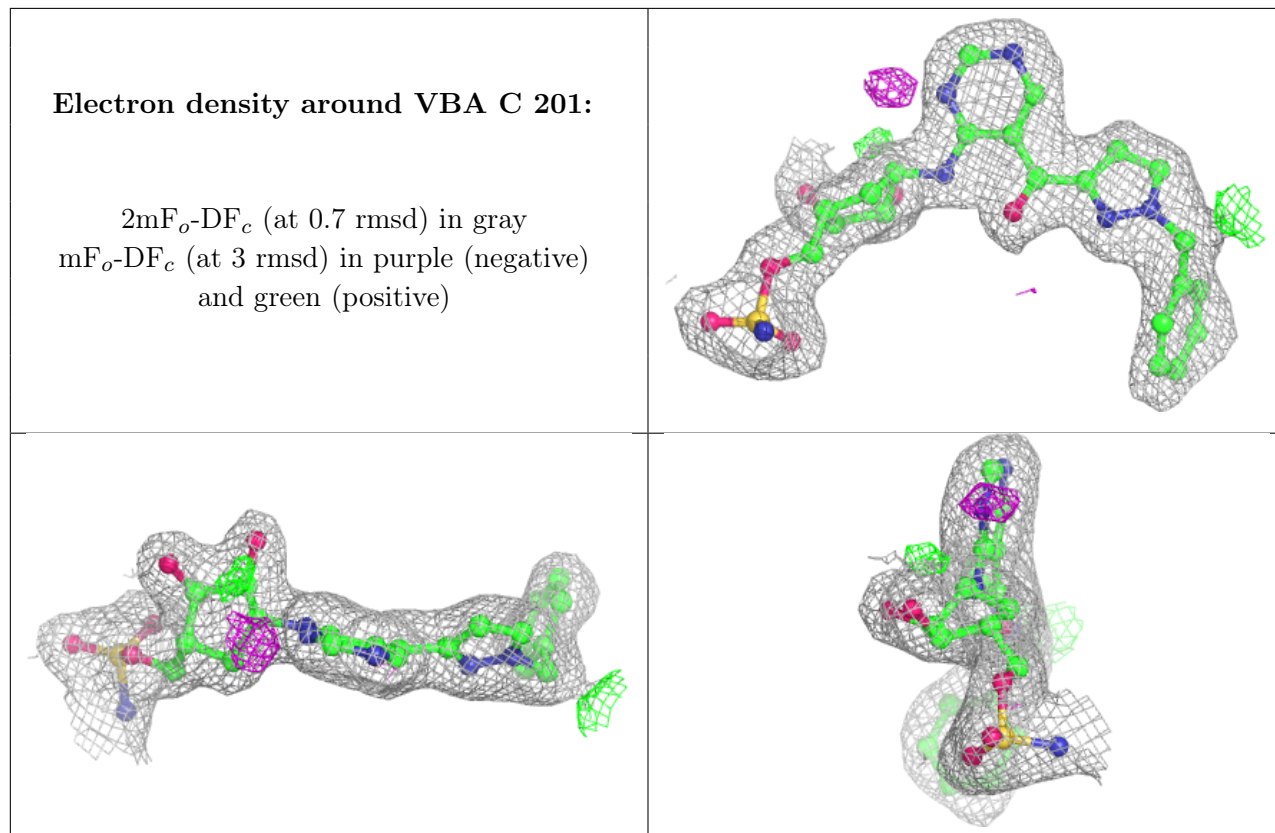
There are no monosaccharides in this entry.

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, 95th 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(\AA^2)	Q<0.9
6	VBA	C	201	34/34	0.94	0.11	20,28,54,57	0
5	ZN	B	700	1/1	0.97	0.05	41,41,41,41	0
4	SO4	A	401	5/5	0.98	0.09	39,47,48,52	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.



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

There are no such residues in this entry.