



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:23 AM UTC

PDB ID : 6XOI / pdb_00006xoi
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

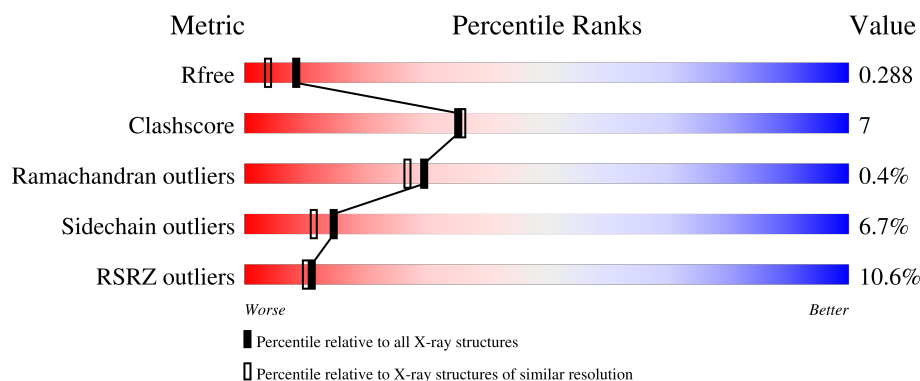
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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% 76% 12% 10%
2	B	640	9% 52% 9% 37%
3	C	101	19% 27% 12% 59%

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
1	A	311	Total	C	N	O	S	0	0	0
			2394	1519	407	456	12			

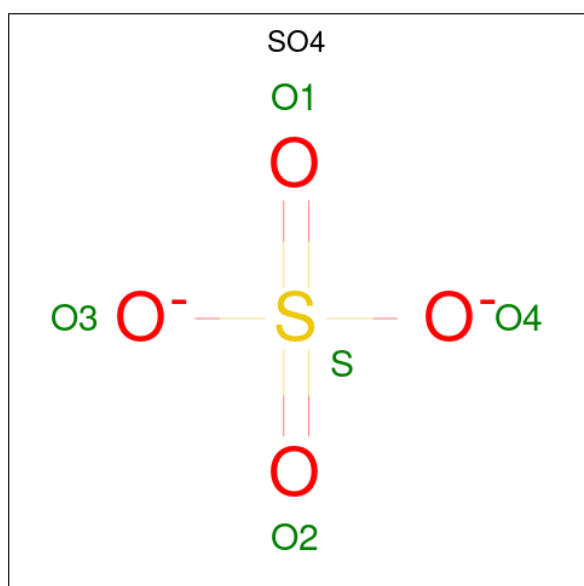
- Molecule 2 is a protein called SUMO-activating enzyme subunit 2.

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

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

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

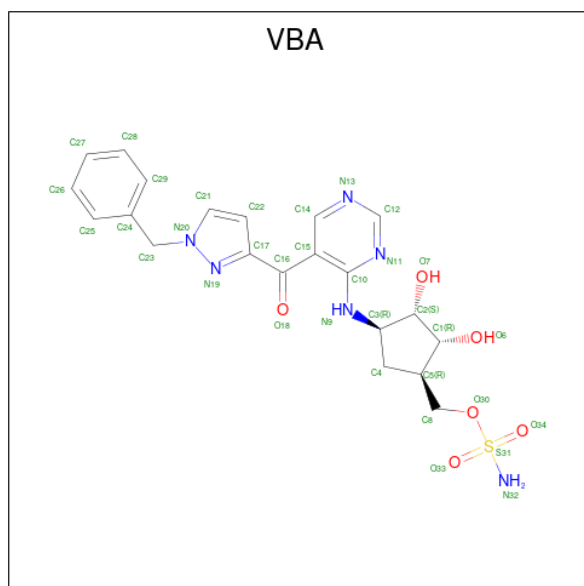


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

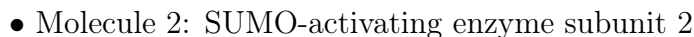
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 (CCD ID: VBA) (formula: C₂₁H₂₄N₆O₆S) (labeled as "Ligand of Interest" by depositor).



- Molecule 1: SUMO-activating enzyme subunit 1



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 19.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.38-2.00) 95.6 (19.38-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.01Å)	Xtriage
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	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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	0.62	1/2437 (0.0%)	1.11	3/3296 (0.1%)
2	B	0.55	0/3172	1.09	1/4298 (0.0%)
3	C	0.52	0/333	0.96	0/442
All	All	0.58	1/5942 (0.0%)	1.09	4/8036 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	HIS	CE1-NE2	5.45	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	GLU	CB-CA-C	5.80	119.32	109.80
1	A	177	GLU	CB-CG-CD	5.78	122.43	112.60
2	B	86	LYS	CB-CA-C	5.51	119.93	110.01
1	A	104	PRO	CB-CA-C	-5.30	104.32	111.85

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	2394	0	2347	29	0
2	B	3115	0	3145	43	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	87	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 (87) 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
1:A:69:GLU:OE1	1:A:91:ARG:NH2	2.13	0.80
2:B:33:LEU:HD13	2:B:80:VAL:HG21	1.62	0.80
2:B:277:LYS:HG2	7:B:892:HOH:O	1.82	0.79
2:B:308:LYS:HE2	7:B:882:HOH:O	1.88	0.73
1:A:105:MET:HE3	1:A:105:MET:HA	1.72	0.72
3:C:23:LYS:NZ	3:C:35:HIS:HD2	1.89	0.70
3:C:23:LYS:HZ1	3:C:35:HIS:CD2	2.13	0.65
3:C:23:LYS:NZ	3:C:35:HIS:CD2	2.64	0.65
2:B:185:CYS:SG	2:B:368:MET:HE1	2.37	0.63
1:A:253:LYS:HE2	7:A:617:HOH:O	2.01	0.61
1:A:325:HIS:HD2	7:A:648:HOH:O	1.84	0.60
2:B:157:GLU:OE1	2:B:162:HIS:CD2	2.55	0.60
2:B:327:GLU:HA	2:B:330:ARG:HH11	1.65	0.60
3:C:25:LYS:HG3	3:C:87:VAL:HG22	1.82	0.60
2:B:33:LEU:HD13	2:B:80:VAL:CG2	2.33	0.57
1:A:277:LEU:HD12	1:A:284:PRO:HA	1.85	0.57
1:A:312:GLN:HG2	7:B:901:HOH:O	2.04	0.57
2:B:401:GLU:HG2	7:B:801:HOH:O	2.05	0.57
3:C:93:GLU:HB2	7:C:309:HOH:O	2.07	0.54
2:B:152:LYS:HG3	2:B:410:ILE:HD13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:OD1	1:A:225:SER:HB2	2.08	0.54
2:B:407:SER:HB3	2:B:409:LYS:HD2	1.90	0.53
2:B:44:ILE:O	2:B:89:ILE:HA	2.08	0.53
1:A:230:LYS:HD3	7:A:592:HOH:O	2.09	0.53
1:A:174:PHE:HE1	1:A:211:VAL:HG23	1.72	0.52
3:C:27:ILE:HD12	3:C:87:VAL:HG11	1.91	0.52
1:A:91:ARG:HD3	7:A:513:HOH:O	2.09	0.51
1:A:175:VAL:HG21	1:A:206:MET:CB	2.41	0.51
2:B:185:CYS:SG	2:B:368:MET:CE	2.98	0.51
1:A:175:VAL:CG2	1:A:206:MET:CB	2.89	0.51
1:A:325:HIS:HE1	7:A:644:HOH:O	1.93	0.50
2:B:418:LEU:HD13	2:B:429:LEU:HD21	1.94	0.50
1:A:11:ILE:HG22	1:A:35:ARG:HD3	1.94	0.50
3:C:23:LYS:HZ1	3:C:35:HIS:HD2	1.50	0.50
2:B:157:GLU:OE1	2:B:162:HIS:HD2	1.95	0.49
2:B:438:ASN:OD1	2:B:438:ASN:C	2.55	0.49
2:B:277:LYS:CG	7:B:892:HOH:O	2.51	0.49
2:B:543:GLU:HG3	7:B:895:HOH:O	2.13	0.49
1:A:152:LYS:CE	7:A:622:HOH:O	2.08	0.48
2:B:80:VAL:HA	2:B:83:PHE:CE2	2.49	0.48
2:B:395:ALA:HA	2:B:398:ILE:HD12	1.96	0.48
2:B:16:ALA:O	2:B:42:SER:OG	2.32	0.48
2:B:176:ARG:CB	7:B:891:HOH:O	2.62	0.48
3:C:93:GLU:HG3	7:C:309:HOH:O	2.13	0.47
3:C:34:ILE:HB	7:C:307:HOH:O	2.14	0.47
2:B:152:LYS:HB3	2:B:155:VAL:HB	1.96	0.47
2:B:11:LEU:HG	2:B:407:SER:OG	2.14	0.47
2:B:157:GLU:OE2	2:B:435:ASP:CB	2.63	0.47
2:B:122:ARG:HG2	2:B:138:GLU:OE1	2.15	0.47
1:A:159:PHE:CG	1:A:246:LEU:HD13	2.50	0.47
1:A:241:PHE:HB3	1:A:277:LEU:HD21	1.97	0.47
1:A:163:GLY:HA3	1:A:306:VAL:HG21	1.96	0.46
2:B:119:ARG:HD3	2:B:159:TYR:OH	2.15	0.46
2:B:289:SER:HB2	7:B:865:HOH:O	2.15	0.46
2:B:305:LEU:CG	7:B:849:HOH:O	2.48	0.46
2:B:194:ASN:O	2:B:198:GLY:N	2.46	0.46
6:C:201:VBA:O18	6:C:201:VBA:N9	2.48	0.45
7:A:618:HOH:O	2:B:82:GLN:HG3	2.16	0.45
3:C:62:LEU:HD22	3:C:90:VAL:CG1	2.47	0.45
2:B:256:THR:CB	7:B:825:HOH:O	2.34	0.44
3:C:64:PHE:CD2	3:C:90:VAL:HG22	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:GLN:O	2:B:78:GLU:HG3	2.17	0.44
2:B:76:ALA:O	2:B:80:VAL:HG23	2.18	0.44
1:A:326:ASN:HA	1:A:327:ASN:HA	1.78	0.43
1:A:277:LEU:CD1	1:A:284:PRO:HA	2.47	0.43
1:A:162:HIS:HE1	7:A:636:HOH:O	2.02	0.43
1:A:51:ILE:HD11	1:A:310:LEU:HD23	2.01	0.42
3:C:23:LYS:HZ3	3:C:35:HIS:HD2	1.66	0.42
3:C:30:ASP:O	3:C:31:SER:HB2	2.18	0.42
1:A:296:PHE:O	1:A:297:SER:HB2	2.19	0.42
2:B:34:LYS:O	2:B:38:LEU:HG	2.18	0.42
2:B:262:ASP:O	2:B:266:LEU:HB2	2.19	0.42
2:B:157:GLU:OE2	2:B:435:ASP:HB2	2.20	0.42
1:A:275:ASP:O	1:A:279:SER:HB2	2.18	0.42
1:A:299:MET:HE2	1:A:299:MET:HB3	1.93	0.42
2:B:382:ASN:CB	7:B:876:HOH:O	2.33	0.41
3:C:23:LYS:HZ3	3:C:35:HIS:CD2	2.37	0.41
2:B:435:ASP:OD2	3:C:70:ARG:NH1	2.50	0.41
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.89	0.41
1:A:11:ILE:HG22	1:A:35:ARG:CD	2.51	0.41
2:B:371:LYS:HD3	2:B:379:MET:HE1	2.03	0.40
1:A:66:LEU:HD21	1:A:113:GLU:O	2.20	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	307/346 (89%)	297 (97%)	8 (3%)	2 (1%)	18	14
2	B	387/640 (60%)	374 (97%)	12 (3%)	1 (0%)	36	35
3	C	35/101 (35%)	32 (91%)	3 (9%)	0	100	100
All	All	729/1087 (67%)	703 (96%)	23 (3%)	3 (0%)	30	27

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 ⓘ

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%)	241 (94%)	15 (6%)	18	14
2	B	338/552 (61%)	314 (93%)	24 (7%)	13	10
3	C	35/91 (38%)	32 (91%)	3 (9%)	10	6
All	All	629/939 (67%)	587 (93%)	42 (7%)	15	11

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	40	LEU
1	A	84	THR
1	A	86	SER
1	A	110	VAL
1	A	131	LEU
1	A	152	LYS
1	A	159	PHE
1	A	177	GLU
1	A	225	SER
1	A	230	LYS
1	A	279	SER
1	A	280	LEU
1	A	334	MET
1	A	335	LYS
2	B	11	LEU
2	B	15	VAL
2	B	32	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	33	LEU
2	B	46	LEU
2	B	65	LYS
2	B	86	LYS
2	B	138	GLU
2	B	152	LYS
2	B	158	CYS
2	B	263	ILE
2	B	270	ASP
2	B	275	LYS
2	B	290	GLN
2	B	308	LYS
2	B	311	GLN
2	B	328	THR
2	B	330	ARG
2	B	362	ARG
2	B	371	LYS
2	B	407	SER
2	B	414	ARG
2	B	442	TYR
2	B	465	GLN
3	C	21	TYR
3	C	23	LYS
3	C	34	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	149	ASN
1	A	162	HIS
1	A	325	HIS
2	B	43	HIS
2	B	93	HIS
2	B	123	ASN
2	B	162	HIS
2	B	288	GLN
3	C	29	GLN
3	C	35	HIS
3	C	94	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 oligosaccharides 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	0.33	0	6,6,6	0.11	0
6	VBA	C	201	3	37,37,37	2.06	7 (18%)	49,53,53	1.96	16 (32%)

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	-	3/22/38/38	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	201	VBA	S31-N32	8.53	1.68	1.58
6	C	201	VBA	O30-S31	4.89	1.64	1.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	201	VBA	C10-N9	3.48	1.40	1.35
6	C	201	VBA	O33-S31	3.13	1.45	1.42
6	C	201	VBA	O34-S31	2.48	1.45	1.42
6	C	201	VBA	C3-N9	2.19	1.49	1.45
6	C	201	VBA	C15-C10	-2.02	1.40	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	201	VBA	O34-S31-N32	6.43	118.42	109.13
6	C	201	VBA	C4-C3-C2	-4.13	96.63	103.17
6	C	201	VBA	C14-C15-C10	3.74	118.43	114.67
6	C	201	VBA	C22-C21-N20	-3.51	104.14	107.30
6	C	201	VBA	C21-N20-N19	3.50	115.40	112.03
6	C	201	VBA	O18-C16-C17	2.70	121.94	117.68
6	C	201	VBA	C2-C3-N9	-2.62	106.98	112.24
6	C	201	VBA	C4-C5-C8	-2.55	107.73	112.78
6	C	201	VBA	C4-C3-N9	-2.45	107.20	112.51
6	C	201	VBA	C15-C10-N11	-2.38	118.88	121.88
6	C	201	VBA	O7-C2-C3	-2.37	106.58	112.92
6	C	201	VBA	C22-C17-C16	2.33	129.97	124.45
6	C	201	VBA	O30-S31-N32	-2.29	98.17	105.54
6	C	201	VBA	N9-C10-N11	2.21	121.13	118.00
6	C	201	VBA	C23-N20-C21	-2.16	124.47	127.79
6	C	201	VBA	C8-O30-S31	2.13	120.01	117.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	201	VBA	C15-C16-C17-N19
6	C	201	VBA	O18-C16-C17-N19
6	C	201	VBA	C15-C16-C17-C22

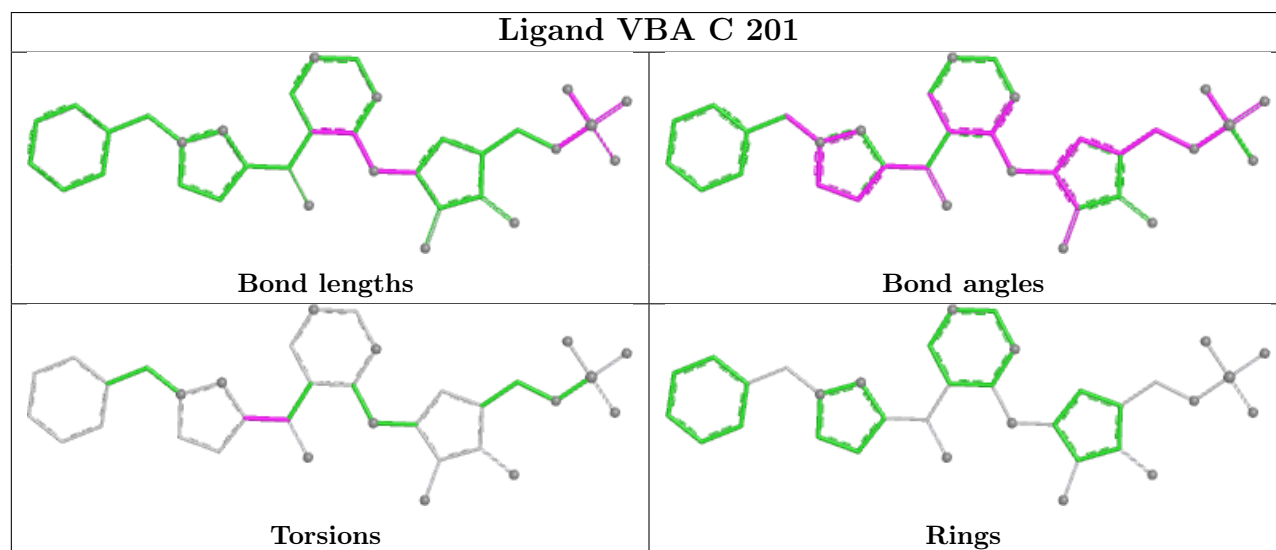
There are no ring outliers.

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

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, 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%)	0.01	6 (1%) 66 66	16, 30, 57, 78	0
2	B	403/640 (62%)	0.73	55 (13%) 7 6	16, 44, 75, 95	0
3	C	41/101 (40%)	2.07	19 (46%) 0 1	25, 67, 101, 108	0
All	All	755/1087 (69%)	0.51	80 (10%) 11 10	16, 37, 75, 108	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	38	VAL	7.0
1	A	9	GLY	6.2
3	C	34	ILE	5.5
2	B	547	VAL	4.7
3	C	62	LEU	4.4
3	C	68	GLY	4.3
3	C	22	ILE	4.2
2	B	462	LEU	4.2
3	C	35	HIS	4.1
2	B	342	LEU	4.0
2	B	544	PHE	3.9
2	B	265	TYR	3.9
2	B	266	LEU	3.9
3	C	23	LYS	3.9
2	B	273	TRP	3.8
2	B	522	PHE	3.7
3	C	26	VAL	3.5
2	B	408	GLY	3.5
2	B	17	GLY	3.4
2	B	542	VAL	3.4
3	C	72	ALA	3.4
3	C	21	TYR	3.3
3	C	33	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	305	LEU	3.2
2	B	533	LEU	3.1
1	A	225	SER	3.1
3	C	32	SER	3.0
2	B	280	VAL	3.0
2	B	532	ILE	3.0
1	A	205	THR	3.0
2	B	531	ASN	2.9
2	B	162	HIS	2.9
2	B	268	THR	2.8
1	A	226	SER	2.8
2	B	198	GLY	2.8
3	C	24	LEU	2.8
3	C	27	ILE	2.8
2	B	341	GLU	2.7
2	B	476	VAL	2.7
2	B	267	LEU	2.7
2	B	467	LYS	2.7
1	A	10	GLY	2.7
2	B	269	MET	2.6
3	C	61	SER	2.6
3	C	37	LYS	2.6
2	B	42	SER	2.6
3	C	36	PHE	2.5
2	B	195	GLN	2.5
2	B	252	VAL	2.5
3	C	28	GLY	2.5
2	B	270	ASP	2.4
2	B	477	ALA	2.4
2	B	470	LYS	2.4
2	B	290	GLN	2.4
2	B	469	VAL	2.4
2	B	251	PRO	2.4
3	C	66	PHE	2.4
2	B	175	ILE	2.3
2	B	173	CYS	2.3
2	B	254	LEU	2.3
2	B	464	LEU	2.3
2	B	282	LEU	2.2
2	B	284	TRP	2.2
2	B	331	VAL	2.2
2	B	445	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	328	THR	2.2
2	B	478	PRO	2.2
2	B	350	SER	2.2
2	B	451	THR	2.2
2	B	197	PHE	2.1
2	B	365	ILE	2.1
2	B	171	PRO	2.1
2	B	468	ILE	2.1
1	A	175	VAL	2.1
2	B	16	ALA	2.1
2	B	174	THR	2.1
2	B	407	SER	2.1
2	B	193	PHE	2.1
2	B	272	LEU	2.0
2	B	184	HIS	2.0

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](#)

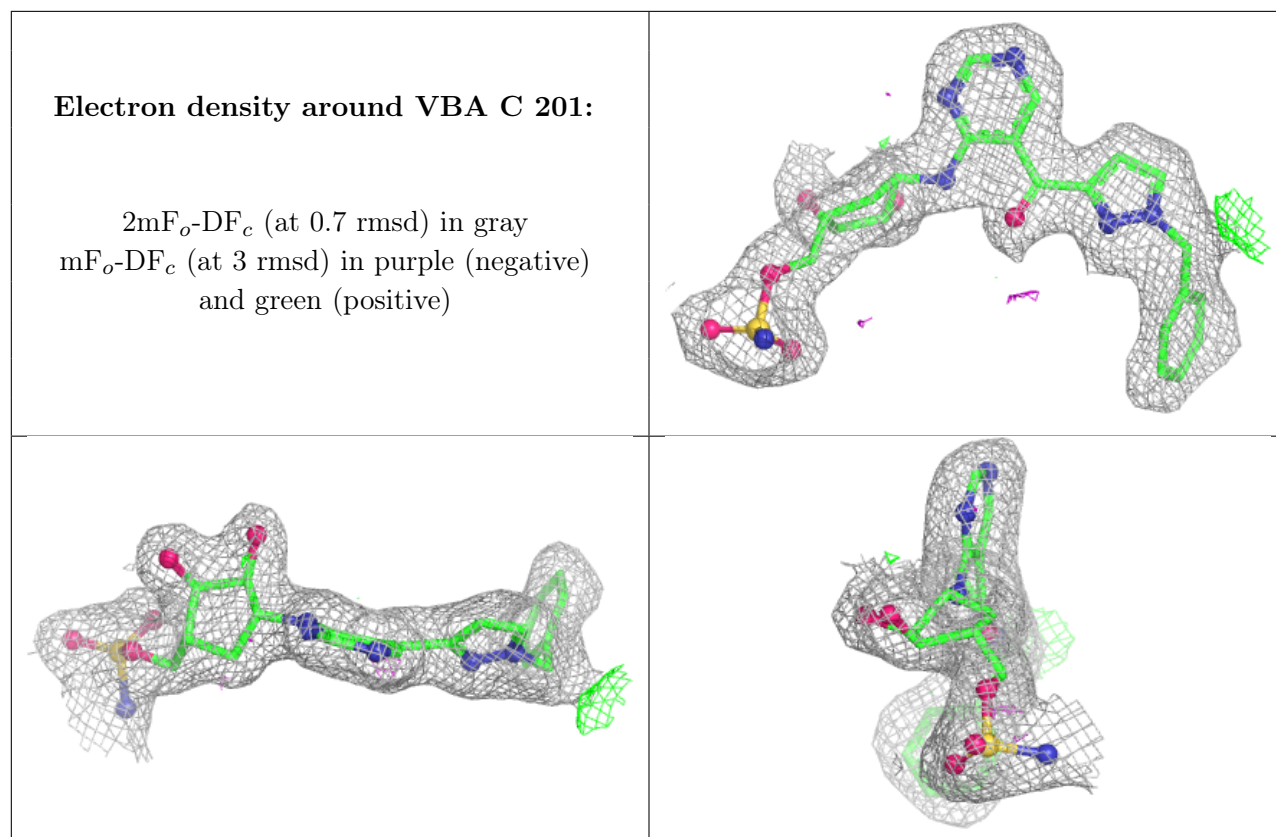
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
4	SO4	A	401	5/5	0.95	0.08	39,47,48,52	0
5	ZN	B	700	1/1	0.97	0.04	41,41,41,41	0
6	VBA	C	201	34/34	0.97	0.07	20,28,54,57	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.