



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 01:08 PM EST

PDB ID : 3SUG
Title : Crystal structure of NS3/4A protease variant A156T in complex with MK-5172
Authors : Schiffer, C.A.; Romano, K.P.
Deposited on : 2011-07-11
Resolution : 1.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

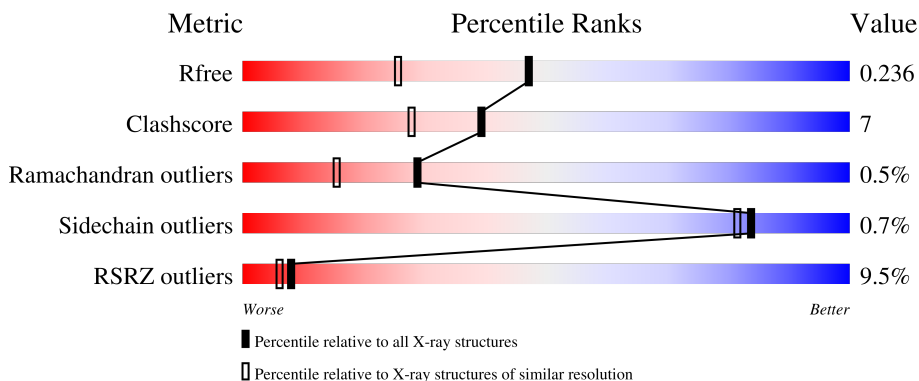
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	203	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SUE	A	1201	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1605 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 NS3 protease, NS4A protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1447	896	261	282	8	0	1	0

There are 29 discrepancies between the modelled and reference sequences:

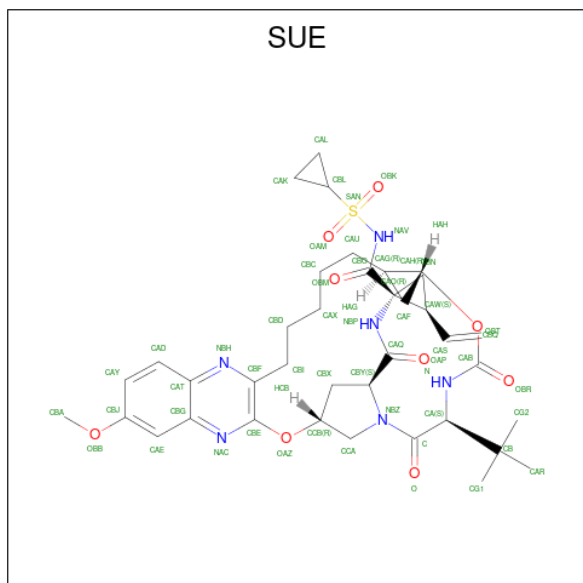
Chain	Residue	Modelled	Actual	Comment	Reference
A	980	GLY	-	expression tag	UNP A8DG50
A	981	SER	-	expression tag	UNP A8DG50
A	982	HIS	-	expression tag	UNP A8DG50
A	983	MET	-	expression tag	UNP A8DG50
A	984	ALA	-	expression tag	UNP A8DG50
A	985	SER	-	expression tag	UNP A8DG50
A	986	MET	CYS	engineered mutation	UNP A8DG50
A	987	LYS	LEU	engineered mutation	UNP A8DG50
A	988	LYS	SER	engineered mutation	UNP A8DG50
A	989	LYS	THR	engineered mutation	UNP A8DG50
A	991	SER	CYS	SEE REMARK 999	UNP A8DG50
A	998	ILE	VAL	SEE REMARK 999	UNP A8DG50
A	999	ASN	ILE	SEE REMARK 999	UNP A8DG50
A	1001	SER	ALA	engineered mutation	UNP A8DG50
A	1002	GLY	PRO	engineered mutation	UNP A8DG50
A	1003	ASP	ILE	engineered mutation	UNP A8DG50
A	1013	GLU	LEU	engineered mutation	UNP A8DG50
A	1014	GLU	LEU	engineered mutation	UNP A8DG50
A	1017	GLN	ILE	engineered mutation	UNP A8DG50
A	1018	GLU	ILE	engineered mutation	UNP A8DG50
A	1021	GLN	LEU	engineered mutation	UNP A8DG50
A	1040	THR	ALA	engineered mutation	UNP A8DG50
A	1047	SER	CYS	engineered mutation	UNP A8DG50
A	1052	LEU	CYS	engineered mutation	UNP A8DG50
A	1072	THR	ILE	engineered mutation	UNP A8DG50
A	1086	GLN	PRO	engineered mutation	UNP A8DG50
A	1139	ALA	SER	engineered mutation	UNP A8DG50

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1156	THR	ALA	engineered mutation	UNP A8DG50
A	1159	SER	CYS	engineered mutation	UNP A8DG50

- Molecule 2 is (1aR,5S,8S,10R,22aR)-5-tert-butyl-N-{(1R,2S)-1-[(cyclopropylsulfonyl)carbamoyl]-2-ethenylcyclopropyl}-14-methoxy-3,6-dioxo-1,1a,3,4,5,6,9,10,18,19,20,21,22,22a-tetradecahydro-8H-7,10-methanocyclopropa[18,19][1,10,3,6]dioxadiazacyclonadecino[11,12-b]quinoxaline-8-carboxamide (three-letter code: SUE) (formula: C₃₈H₅₀N₆O₉S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	54	38	6	9	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0

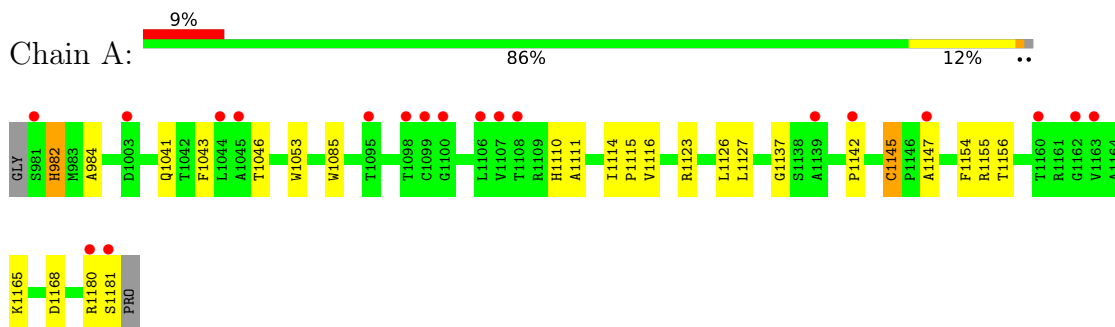
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	97	Total O 98 98	0	1

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: NS3 protease, NS4A protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.88Å 58.25Å 62.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.68 – 1.80 23.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.9 (23.68-1.80) 90.0 (23.68-1.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 1.80Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.234 0.201 , 0.236	Depositor DCC
R_{free} test set	859 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtrriage
Anisotropy	0.607	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1605	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% 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, SO4, SUE

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	0.50	2/1475 (0.1%)	0.70	1/2009 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1053	TRP	CD2-CE2	5.56	1.48	1.41
1	A	1085	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1145	CYS	CA-CB-SG	5.86	124.54	114.00

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	1447	0	1420	21	0
2	A	54	0	49	9	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	98	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1605	0	1469	22	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 (22) 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:1155:ARG:HG2	1:A:1156:THR:HG23	1.44	0.99
1:A:982:HIS:CE1	1:A:984:ALA:HB3	2.16	0.79
1:A:1156:THR:HG21	2:A:1201:SUE:HBIA	1.64	0.79
1:A:1115:PRO:HB2	1:A:1127:LEU:HD22	1.66	0.77
1:A:982:HIS:HE1	1:A:984:ALA:HB3	1.60	0.64
1:A:1155:ARG:HH21	2:A:1201:SUE:HBI	1.68	0.56
1:A:1123:ARG:NE	1:A:1168:ASP:OD1	2.42	0.53
1:A:1155:ARG:HH22	2:A:1201:SUE:HAX	1.74	0.51
1:A:1155:ARG:NH2	2:A:1201:SUE:HBI	2.26	0.51
1:A:1041:GLN:OE1	2:A:1201:SUE:HAK	2.13	0.49
1:A:1156:THR:HG22	2:A:1201:SUE:HBV	1.95	0.49
1:A:1116:VAL:HG22	1:A:1126:LEU:HD23	1.96	0.48
1:A:1156:THR:HA	2:A:1201:SUE:HBNA	1.96	0.47
1:A:1180:ARG:O	1:A:1181:SER:CB	2.64	0.46
1:A:1154:PHE:CE2	2:A:1201:SUE:HBN	2.52	0.45
1:A:1115:PRO:CB	1:A:1127:LEU:HD22	2.43	0.45
1:A:1110:HIS:O	1:A:1111:ALA:HB3	2.18	0.44
1:A:1043:PHE:HA	1:A:1137:GLY:O	2.18	0.44
1:A:1145:CYS:SG	1:A:1147:ALA:HB3	2.58	0.43
1:A:1114:ILE:HG21	1:A:1126:LEU:HD22	2.02	0.42
2:A:1201:SUE:O	2:A:1201:SUE:CAQ	2.68	0.41
1:A:1046:THR:HG21	1:A:1142:PRO:HB3	2.03	0.41

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	200/203 (98%)	197 (98%)	2 (1%)	1 (0%)	29 15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	982	HIS

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	154/165 (93%)	153 (99%)	1 (1%)	86 84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1165	LYS

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

Mol	Chain	Res	Type
1	A	982	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
2	SUE	A	1201	-	54,60,60	2.74	15 (27%)	73,92,92	2.06	15 (20%)
3	SO4	A	1202	-	4,4,4	0.38	0	6,6,6	0.47	0

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SUE	A	1201	-	1/1/15/19	4/61/91/91	0/6/7/7

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	SUE	OBK-SAN	9.90	1.54	1.43
2	A	1201	SUE	CA-C	-8.34	1.41	1.53
2	A	1201	SUE	OAM-SAN	8.27	1.52	1.43
2	A	1201	SUE	CBQ-CAS	4.83	1.54	1.29
2	A	1201	SUE	CBI-CBF	-4.80	1.38	1.51
2	A	1201	SUE	SAN-NAV	-4.75	1.53	1.63
2	A	1201	SUE	CBY-CAQ	-4.61	1.42	1.52
2	A	1201	SUE	CAG-CAH	3.20	1.54	1.49
2	A	1201	SUE	CBY-NBZ	2.80	1.52	1.47
2	A	1201	SUE	CAB-N	2.54	1.41	1.34
2	A	1201	SUE	CA-N	2.48	1.49	1.45
2	A	1201	SUE	CAO-NBP	2.17	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	SUE	CBN-CAO	-2.12	1.48	1.51
2	A	1201	SUE	CBF-NBH	2.01	1.34	1.32
2	A	1201	SUE	CBE-NAC	2.01	1.35	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	SUE	OBK-SAN-OAM	-10.45	111.40	119.24
2	A	1201	SUE	OBT-CAB-N	5.15	117.00	110.32
2	A	1201	SUE	CA-C-NBZ	4.16	123.52	118.52
2	A	1201	SUE	CBO-CAO-NBP	3.84	120.19	116.06
2	A	1201	SUE	OBR-CAB-N	-3.53	119.07	124.85
2	A	1201	SUE	CCA-NBZ-CBY	-3.21	107.07	111.70
2	A	1201	SUE	CAU-CAG-CAH	-3.04	115.44	122.75
2	A	1201	SUE	CBD-CBI-CBF	-3.02	105.54	112.79
2	A	1201	SUE	CBX-CBY-NBZ	3.00	107.06	103.10
2	A	1201	SUE	CAX-CBD-CBI	-2.82	102.80	113.76
2	A	1201	SUE	OAZ-CBE-NAC	2.66	123.50	118.91
2	A	1201	SUE	CBF-NBH-CAT	2.54	120.81	117.67
2	A	1201	SUE	CBN-CAO-NBP	-2.50	114.43	117.80
2	A	1201	SUE	C-CA-N	2.14	109.67	107.34
2	A	1201	SUE	O-C-NBZ	-2.11	117.62	121.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1201	SUE	NBZ

All (4) torsion outliers are listed below:

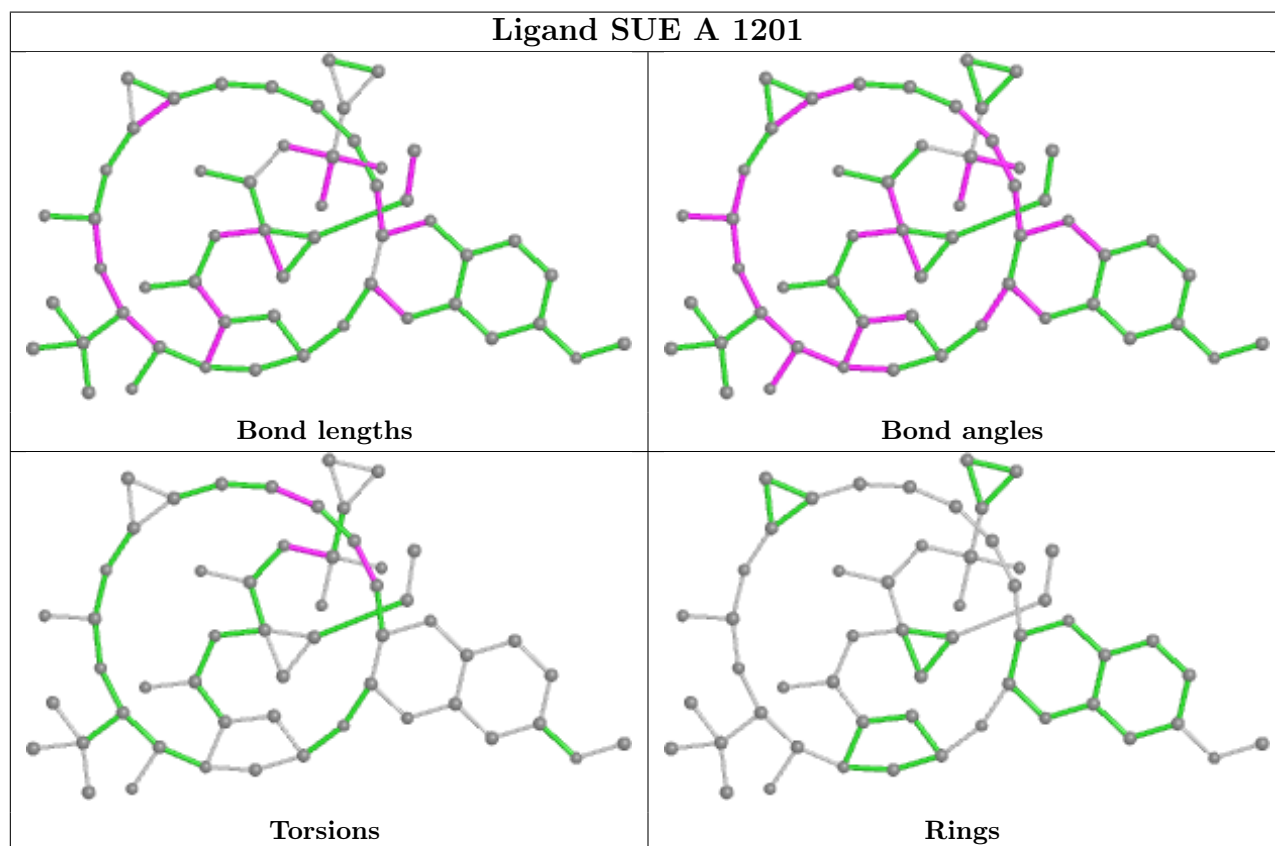
Mol	Chain	Res	Type	Atoms
2	A	1201	SUE	CBO-NAV-SAN-OBK
2	A	1201	SUE	CBO-NAV-SAN-CBL
2	A	1201	SUE	CAX-CBD-CBI-CBF
2	A	1201	SUE	CBD-CAX-CBC-CAU

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	SUE	9	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	201/203 (99%)	0.39	19 (9%) 8 6	27, 39, 61, 80	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1181	SER	6.0
1	A	1160	THR	3.7
1	A	1180	ARG	3.7
1	A	1098	THR	3.3
1	A	1107	VAL	3.2
1	A	1162	GLY	2.9
1	A	1147	ALA	2.9
1	A	1142	PRO	2.9
1	A	1099	CYS	2.7
1	A	1106	LEU	2.6
1	A	1100	GLY	2.6
1	A	1003	ASP	2.5
1	A	981	SER	2.4
1	A	1139	ALA	2.4
1	A	1108	THR	2.4
1	A	1045	ALA	2.3
1	A	1044	LEU	2.3
1	A	1095	THR	2.1
1	A	1163	VAL	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](#)

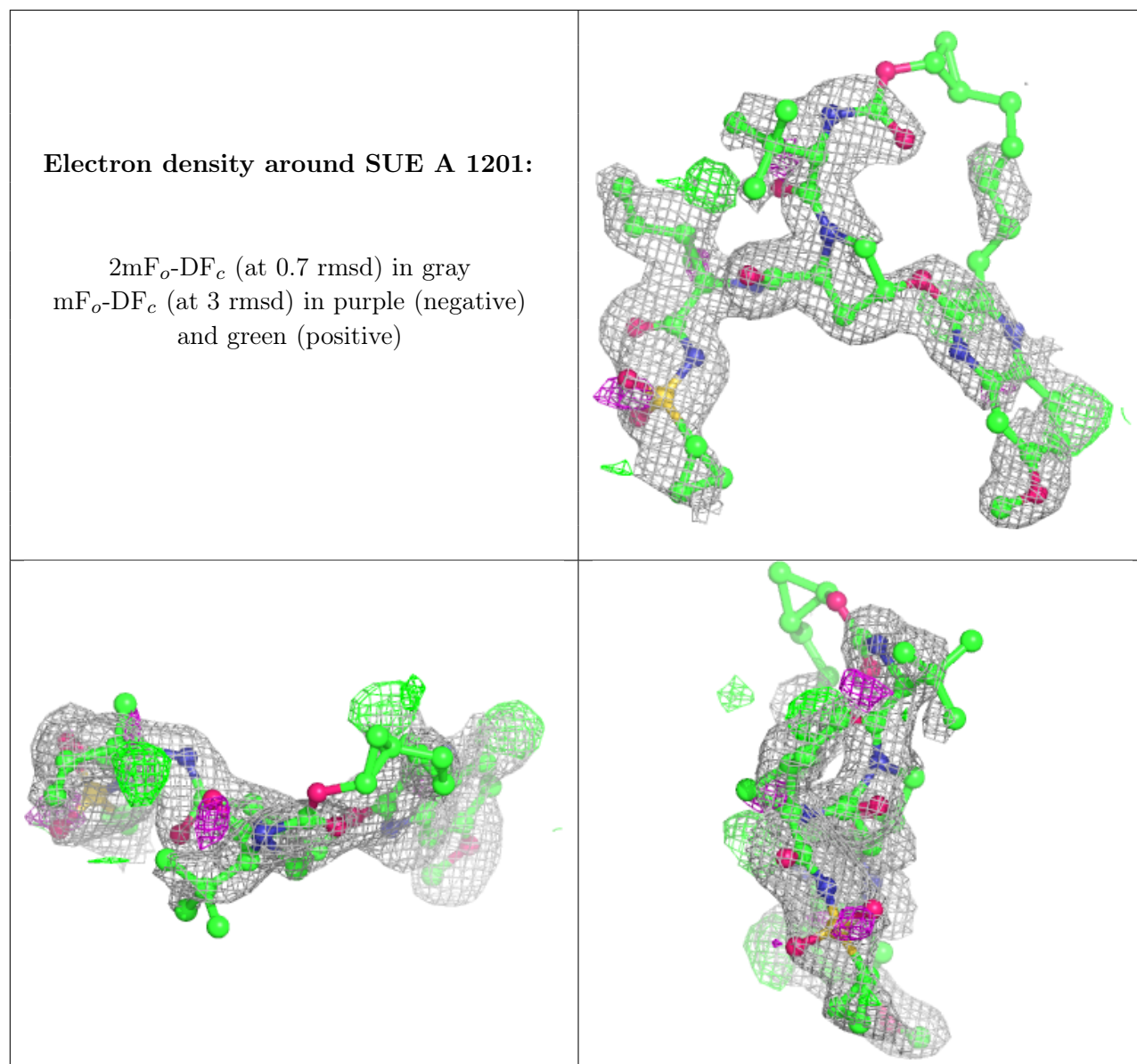
There are no monosaccharides in this entry.

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
2	SUE	A	1201	54/54	0.77	0.30	40,60,78,81	54
4	ZN	A	1203	1/1	0.92	0.09	51,51,51,51	0
3	SO4	A	1202	5/5	0.98	0.13	41,44,47,49	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.