wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 07:29 am BST

PDB ID	:	3SUE
Title	:	Crystal structure of NS3/4A protease variant R155K in complex with MK-5172
Authors	:	Schiffer, C.A.; Romano, K.P.
Deposited on	:	2011-07-11
Resolution	:	2.20 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 (i)) were used in the production of this report:

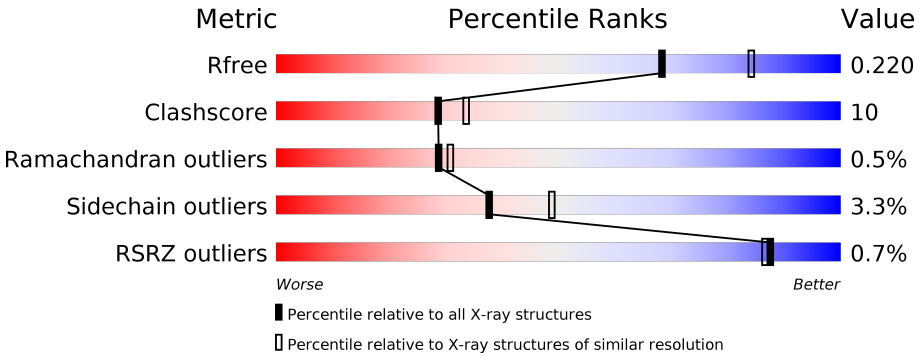
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	203	76% 16% • 6%
1	B	203	76% 17% 6%
1	C	203	75% 16% • 6%
1	D	203	% 68% 24% • 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SUE	A	1201	X	-	-	-
2	SUE	B	1201	X	-	-	-
2	SUE	C	1201	X	-	-	-
2	SUE	D	1201	X	-	-	-
3	ZN	C	1202	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5778 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
1	A	190	Total	C	N	O	S	0	0	0
			1360	844	243	267	6			
1	B	190	Total	C	N	O	S	0	0	0
			1351	841	241	263	6			
1	C	190	Total	C	N	O	S	0	0	0
			1359	845	242	266	6			
1	D	190	Total	C	N	O	S	0	0	0
			1337	834	239	258	6			

There are 112 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	1155	LYS	ARG	engineered mutation	UNP A8DG50
A	1159	SER	CYS	engineered mutation	UNP A8DG50
B	980	GLY	-	expression tag	UNP A8DG50
B	981	SER	-	expression tag	UNP A8DG50
B	982	HIS	-	expression tag	UNP A8DG50
B	983	MET	-	expression tag	UNP A8DG50
B	984	ALA	-	expression tag	UNP A8DG50
B	985	SER	-	expression tag	UNP A8DG50
B	986	MET	CYS	engineered mutation	UNP A8DG50
B	987	LYS	LEU	engineered mutation	UNP A8DG50
B	988	LYS	SER	engineered mutation	UNP A8DG50
B	989	LYS	THR	engineered mutation	UNP A8DG50
B	991	SER	CYS	SEE REMARK 999	UNP A8DG50
B	998	ILE	VAL	SEE REMARK 999	UNP A8DG50
B	999	ASN	ILE	SEE REMARK 999	UNP A8DG50
B	1001	SER	ALA	engineered mutation	UNP A8DG50
B	1002	GLY	PRO	engineered mutation	UNP A8DG50
B	1003	ASP	ILE	engineered mutation	UNP A8DG50
B	1013	GLU	LEU	engineered mutation	UNP A8DG50
B	1014	GLU	LEU	engineered mutation	UNP A8DG50
B	1017	GLN	ILE	engineered mutation	UNP A8DG50
B	1018	GLU	ILE	engineered mutation	UNP A8DG50
B	1021	GLN	LEU	engineered mutation	UNP A8DG50
B	1040	THR	ALA	engineered mutation	UNP A8DG50
B	1047	SER	CYS	engineered mutation	UNP A8DG50
B	1052	LEU	CYS	engineered mutation	UNP A8DG50
B	1072	THR	ILE	engineered mutation	UNP A8DG50
B	1086	GLN	PRO	engineered mutation	UNP A8DG50
B	1155	LYS	ARG	engineered mutation	UNP A8DG50
B	1159	SER	CYS	engineered mutation	UNP A8DG50
C	980	GLY	-	expression tag	UNP A8DG50
C	981	SER	-	expression tag	UNP A8DG50
C	982	HIS	-	expression tag	UNP A8DG50
C	983	MET	-	expression tag	UNP A8DG50
C	984	ALA	-	expression tag	UNP A8DG50
C	985	SER	-	expression tag	UNP A8DG50
C	986	MET	CYS	engineered mutation	UNP A8DG50

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Chain	Residue	Modelled	Actual	Comment	Reference
C	987	LYS	LEU	engineered mutation	UNP A8DG50
C	988	LYS	SER	engineered mutation	UNP A8DG50
C	989	LYS	THR	engineered mutation	UNP A8DG50
C	991	SER	CYS	SEE REMARK 999	UNP A8DG50
C	998	ILE	VAL	SEE REMARK 999	UNP A8DG50
C	999	ASN	ILE	SEE REMARK 999	UNP A8DG50
C	1001	SER	ALA	engineered mutation	UNP A8DG50
C	1002	GLY	PRO	engineered mutation	UNP A8DG50
C	1003	ASP	ILE	engineered mutation	UNP A8DG50
C	1013	GLU	LEU	engineered mutation	UNP A8DG50
C	1014	GLU	LEU	engineered mutation	UNP A8DG50
C	1017	GLN	ILE	engineered mutation	UNP A8DG50
C	1018	GLU	ILE	engineered mutation	UNP A8DG50
C	1021	GLN	LEU	engineered mutation	UNP A8DG50
C	1040	THR	ALA	engineered mutation	UNP A8DG50
C	1047	SER	CYS	engineered mutation	UNP A8DG50
C	1052	LEU	CYS	engineered mutation	UNP A8DG50
C	1072	THR	ILE	engineered mutation	UNP A8DG50
C	1086	GLN	PRO	engineered mutation	UNP A8DG50
C	1155	LYS	ARG	engineered mutation	UNP A8DG50
C	1159	SER	CYS	engineered mutation	UNP A8DG50
D	980	GLY	-	expression tag	UNP A8DG50
D	981	SER	-	expression tag	UNP A8DG50
D	982	HIS	-	expression tag	UNP A8DG50
D	983	MET	-	expression tag	UNP A8DG50
D	984	ALA	-	expression tag	UNP A8DG50
D	985	SER	-	expression tag	UNP A8DG50
D	986	MET	CYS	engineered mutation	UNP A8DG50
D	987	LYS	LEU	engineered mutation	UNP A8DG50
D	988	LYS	SER	engineered mutation	UNP A8DG50
D	989	LYS	THR	engineered mutation	UNP A8DG50
D	991	SER	CYS	SEE REMARK 999	UNP A8DG50
D	998	ILE	VAL	SEE REMARK 999	UNP A8DG50
D	999	ASN	ILE	SEE REMARK 999	UNP A8DG50
D	1001	SER	ALA	engineered mutation	UNP A8DG50
D	1002	GLY	PRO	engineered mutation	UNP A8DG50
D	1003	ASP	ILE	engineered mutation	UNP A8DG50
D	1013	GLU	LEU	engineered mutation	UNP A8DG50
D	1014	GLU	LEU	engineered mutation	UNP A8DG50
D	1017	GLN	ILE	engineered mutation	UNP A8DG50
D	1018	GLU	ILE	engineered mutation	UNP A8DG50
D	1021	GLN	LEU	engineered mutation	UNP A8DG50

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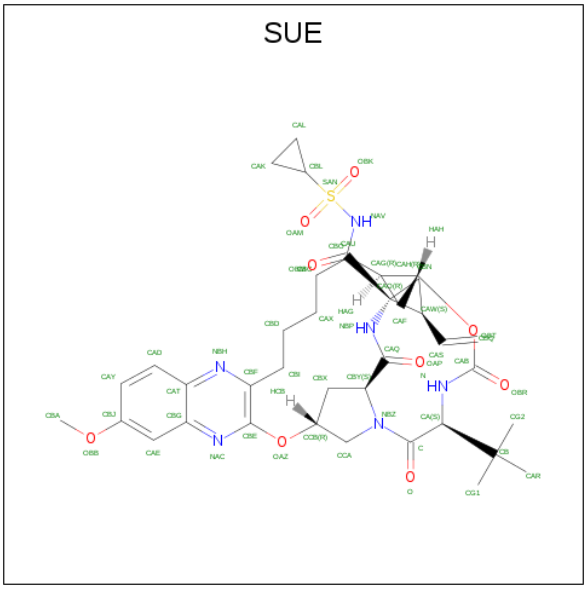
Chain	Residue	Modelled	Actual	Comment	Reference
D	1040	THR	ALA	engineered mutation	UNP A8DG50
D	1047	SER	CYS	engineered mutation	UNP A8DG50
D	1052	LEU	CYS	engineered mutation	UNP A8DG50
D	1072	THR	ILE	engineered mutation	UNP A8DG50
D	1086	GLN	PRO	engineered mutation	UNP A8DG50
D	1155	LYS	ARG	engineered mutation	UNP A8DG50
D	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]dioxadiazacyclononadecino[11,12-b]quinoxaline-8-carboxamide (three-letter code: SUE) (formula: $C_{38}H_{50}N_6O_9S$).



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is water.

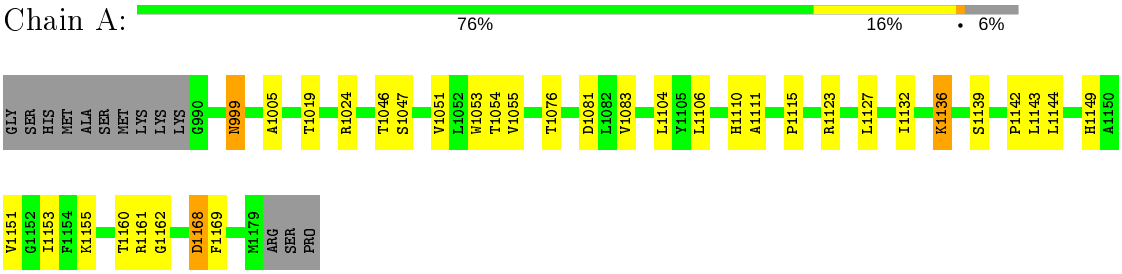
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	37	Total O 37 37	0	0
4	B	46	Total O 46 46	0	0
4	C	44	Total O 44 44	0	2
4	D	24	Total O 24 24	0	0

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.

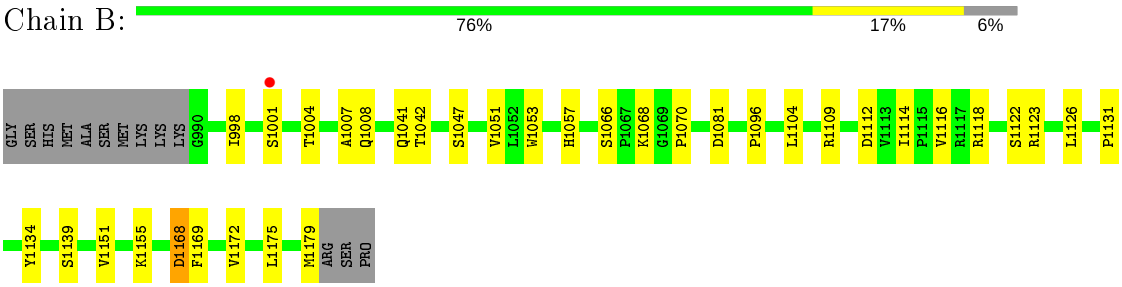
- Molecule 1: NS3 protease, NS4A protein

Chain A:



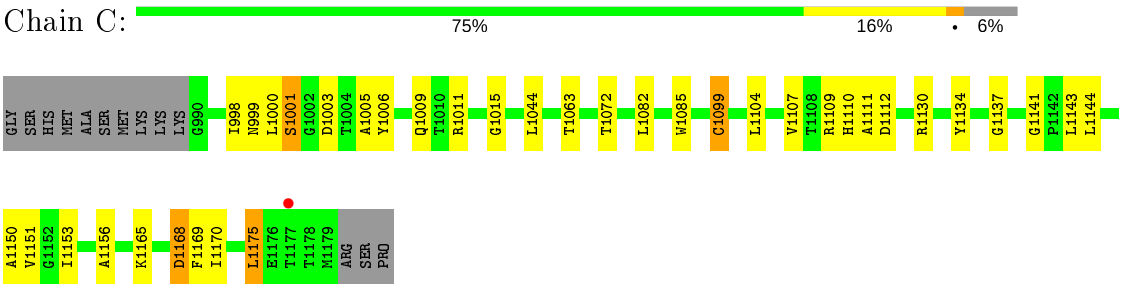
- Molecule 1: NS3 protease, NS4A protein

Chain B:



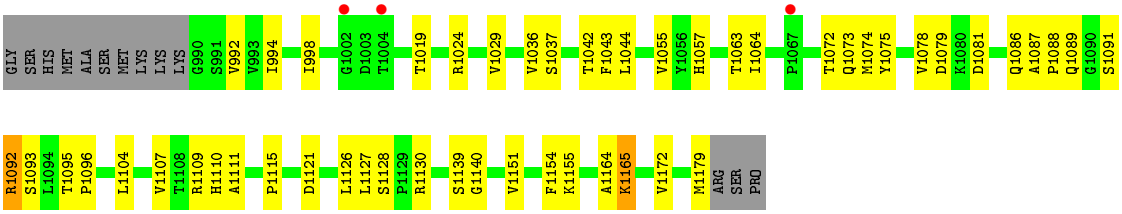
- Molecule 1: NS3 protease, NS4A protein

Chain C:



- Molecule 1: NS3 protease, NS4A protein

Chain D:


GLY SER HIS MET ALA SER MET LYS LYS LYS G990 S991 V992 V993 I994 I998 G1002 D1003 T1004 T1019 R1024 V1029 V1036 S1037 T1042 F1043 L1044 V1055 Y1056 H1057 T1063 I1064 P1067 T1072 Q1073 M1074 Y1075 V1078 D1079 K1080 D1081 Q1086 A1087 P1088 Q1089 G1090 S1091
R1092 S1093 L1094 T1095 P1096 L1104 V1107 T1108 R1109 H1110 A1111 P1115 D1121 L1126 L1127 S1128 P1129 R1130 S1139 G1140 V1151 F1154 K1155 A1164 K1165 V1172 M1179 ARG SER PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.34Å 103.32Å 73.50Å 90.00° 112.58° 90.00°	Depositor
Resolution (Å)	32.24 – 2.20 32.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (32.24-2.20) 91.3 (32.24-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.229 0.189 , 0.220	Depositor DCC
R_{free} test set	1812 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 15.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.542 for H, K, L 0.458 for -H, -K, H+L	Depositor
Outliers	0 of 36175 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5778	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: SUE, ZN

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	0/1384	0.62	0/1890
1	B	0.48	0/1375	0.64	0/1878
1	C	0.52	1/1383 (0.1%)	0.64	0/1888
1	D	0.47	0/1361	0.62	0/1860
All	All	0.48	1/5503 (0.0%)	0.63	0/7516

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1085	TRP	CD2-CE2	5.10	1.47	1.41

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	1360	0	1327	22	0
1	B	1351	0	1321	21	0
1	C	1359	0	1333	28	0
1	D	1337	0	1301	35	0
2	A	54	0	49	3	0
2	B	54	0	50	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	54	0	49	2	0
2	D	54	0	49	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	2	0
3	D	1	0	0	0	0
4	A	37	0	0	0	0
4	B	46	0	0	0	0
4	C	44	0	0	0	0
4	D	24	0	0	0	0
All	All	5778	0	5479	108	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 10.

The worst 5 of 108 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:B:1116:VAL:HG22	1:B:1126:LEU:HD23	1.63	0.81
1:C:1099:CYS:SG	3:C:1202:ZN:ZN	1.77	0.74
1:C:1099:CYS:HG	3:C:1202:ZN:ZN	1.01	0.72
1:D:1019:THR:HG23	1:D:1024:ARG:O	1.90	0.71
1:B:1112:ASP:HB3	1:B:1114:ILE:HD11	1.72	0.69

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	188/203 (93%)	185 (98%)	3 (2%)	0	100	100
1	B	188/203 (93%)	178 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	188/203 (93%)	181 (96%)	5 (3%)	2 (1%)	14 12
1	D	188/203 (93%)	181 (96%)	5 (3%)	2 (1%)	14 12
All	All	752/812 (93%)	725 (96%)	23 (3%)	4 (0%)	29 31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1001	SER
1	C	1003	ASP
1	D	1092	ARG
1	D	1088	PRO

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	144/165 (87%)	140 (97%)	4 (3%)	43 56
1	B	142/165 (86%)	138 (97%)	4 (3%)	43 56
1	C	144/165 (87%)	137 (95%)	7 (5%)	25 31
1	D	138/165 (84%)	134 (97%)	4 (3%)	42 54
All	All	568/660 (86%)	549 (97%)	19 (3%)	38 49

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1000	LEU
1	C	1099	CYS
1	D	1037	SER
1	B	1168	ASP
1	D	1064	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1086	GLN
1	A	1149	HIS
1	C	999	ASN
1	C	1149	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	C	1201	-	54,60,60	2.48	17 (31%)	73,92,92	2.75	21 (28%)
2	SUE	D	1201	-	54,60,60	3.07	18 (33%)	73,92,92	2.70	24 (32%)
2	SUE	A	1201	-	54,60,60	2.67	17 (31%)	73,92,92	2.81	17 (23%)
2	SUE	B	1201	-	54,60,60	2.83	18 (33%)	73,92,92	2.32	14 (19%)

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	SUE	C	1201	-	1/1/15/19	7/61/91/91	0/6/7/7
2	SUE	D	1201	-	1/1/15/19	13/61/91/91	0/6/7/7
2	SUE	A	1201	-	1/1/15/19	5/61/91/91	0/6/7/7
2	SUE	B	1201	-	1/1/15/19	3/61/91/91	0/6/7/7

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	SUE	SAN-NAV	-14.61	1.33	1.63
2	A	1201	SUE	CA-C	-11.29	1.37	1.53
2	C	1201	SUE	CA-C	-9.57	1.39	1.53
2	B	1201	SUE	CA-C	-9.16	1.40	1.53
2	D	1201	SUE	CA-C	-9.04	1.40	1.53

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	SUE	OBK-SAN-OAM	-18.80	105.14	119.24
2	D	1201	SUE	OBK-SAN-OAM	-15.19	107.84	119.24
2	C	1201	SUE	OBK-SAN-OAM	-14.00	108.74	119.24
2	B	1201	SUE	OBK-SAN-OAM	-13.43	109.16	119.24
2	C	1201	SUE	CBO-CAO-NBP	6.35	122.89	116.06

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	1201	SUE	NBZ
2	A	1201	SUE	NBZ
2	B	1201	SUE	NBZ
2	C	1201	SUE	NBZ

5 of 28 torsion outliers are listed below:

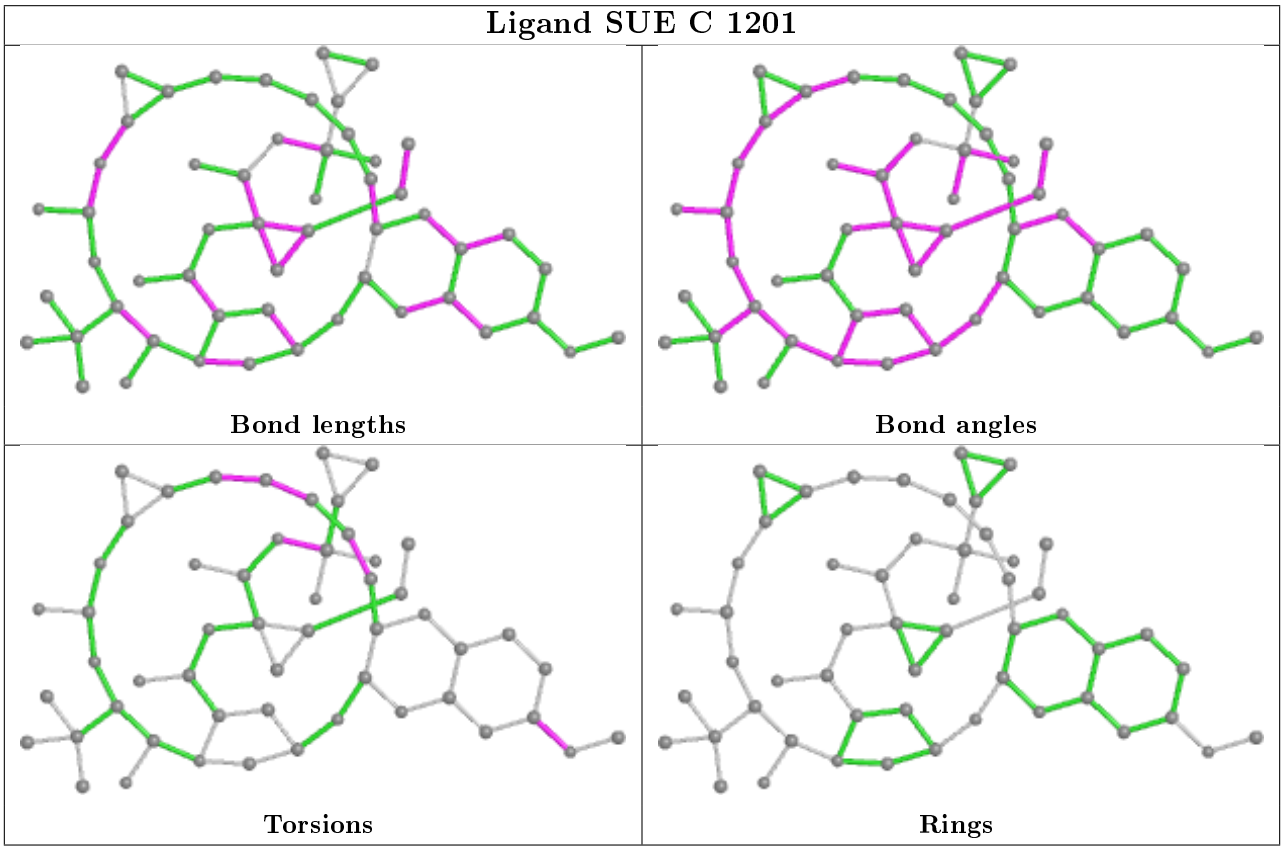
Mol	Chain	Res	Type	Atoms
2	D	1201	SUE	C-CA-CB-CAR
2	D	1201	SUE	C-CA-CB-CG1
2	D	1201	SUE	C-CA-CB-CG2
2	D	1201	SUE	N-CA-CB-CAR
2	D	1201	SUE	N-CA-CB-CG1

There are no ring outliers.

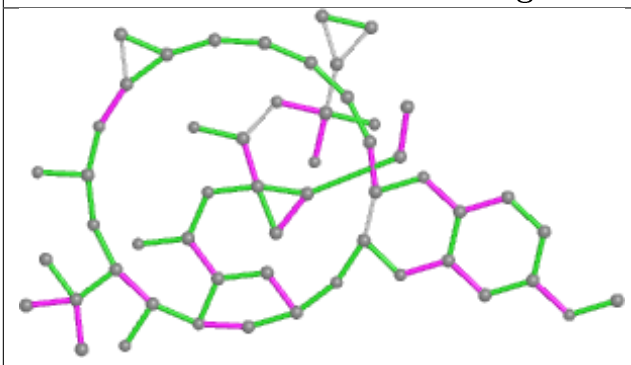
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1201	SUE	2	0
2	D	1201	SUE	4	0
2	A	1201	SUE	3	0
2	B	1201	SUE	5	0

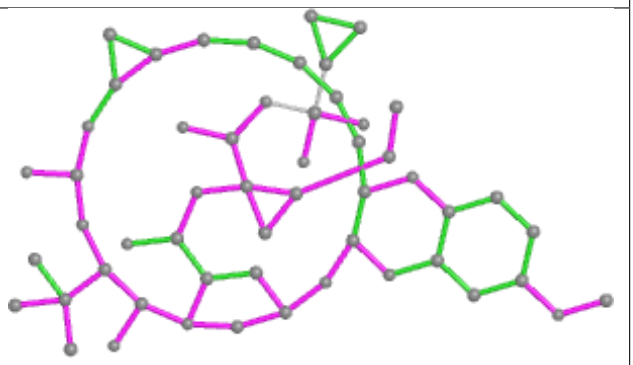
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



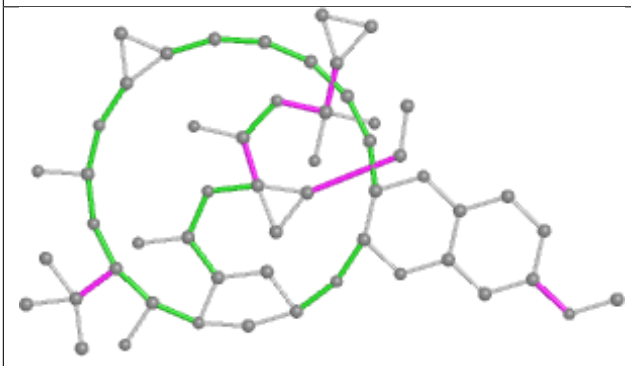
Ligand SUE D 1201



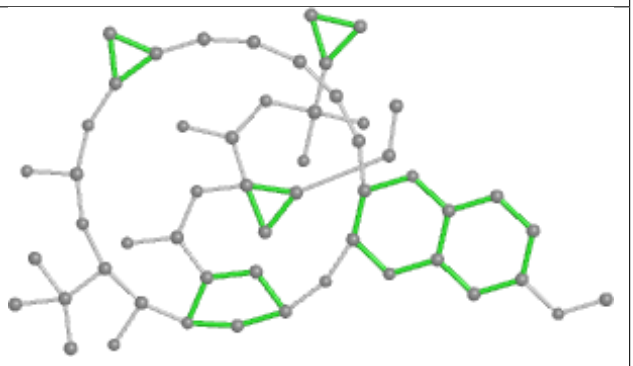
Bond lengths



Bond angles

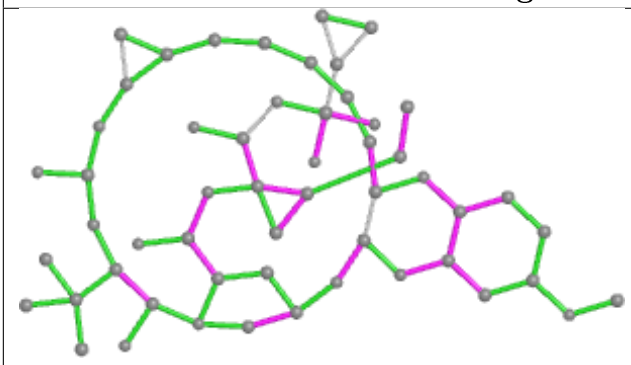


Torsions

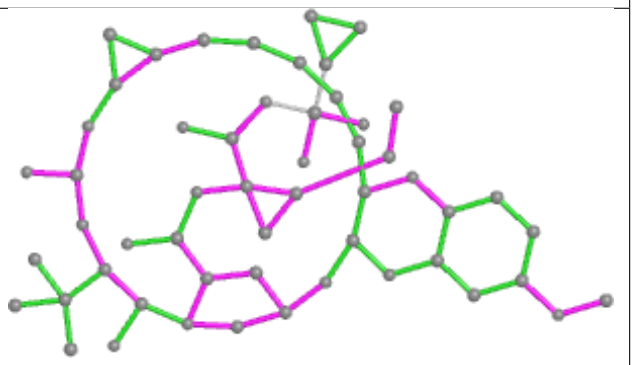


Rings

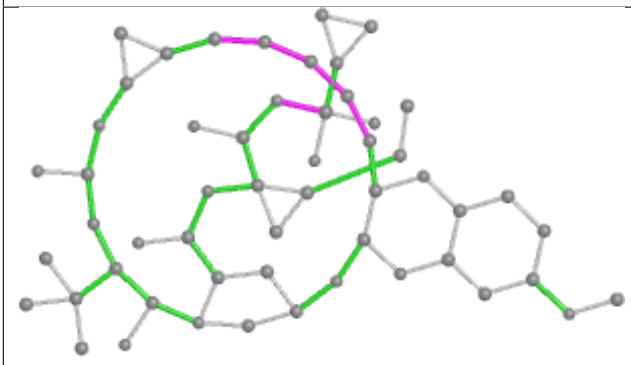
Ligand SUE A 1201



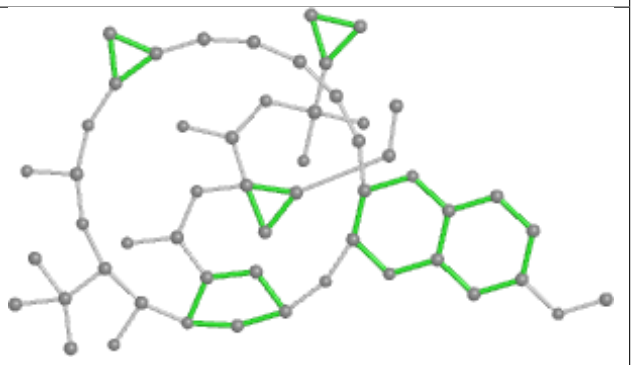
Bond lengths



Bond angles

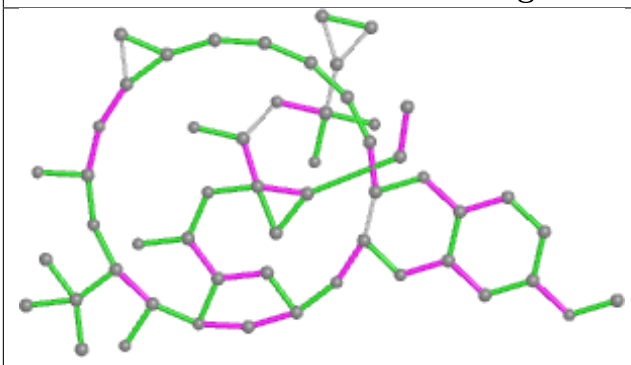


Torsions

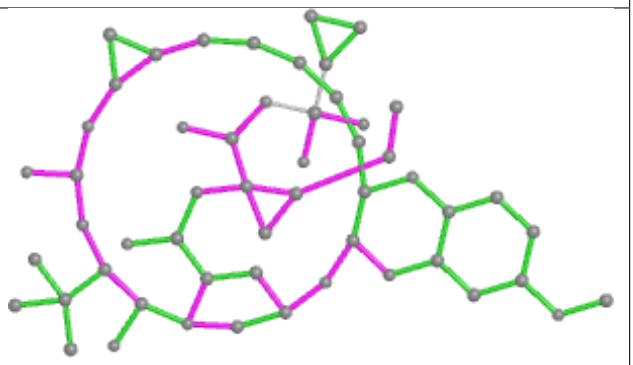


Rings

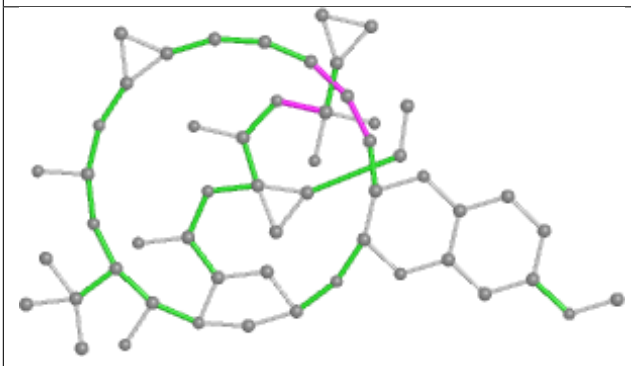
Ligand SUE B 1201



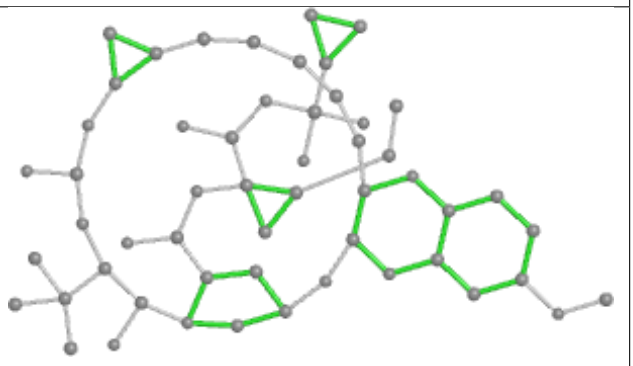
Bond lengths



Bond angles



Torsions



Rings

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	190/203 (93%)	-0.54	0 100 100	23, 38, 73, 130	0
1	B	190/203 (93%)	-0.60	1 (0%) 91 90	21, 35, 77, 95	0
1	C	190/203 (93%)	-0.54	1 (0%) 91 90	21, 34, 67, 115	0
1	D	190/203 (93%)	-0.46	3 (1%) 72 70	21, 39, 85, 138	0
All	All	760/812 (93%)	-0.53	5 (0%) 87 86	21, 37, 79, 138	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1177	THR	3.4
1	D	1004	THR	3.1
1	B	1001	SER	2.4
1	D	1002	GLY	2.2
1	D	1067	PRO	2.1

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,

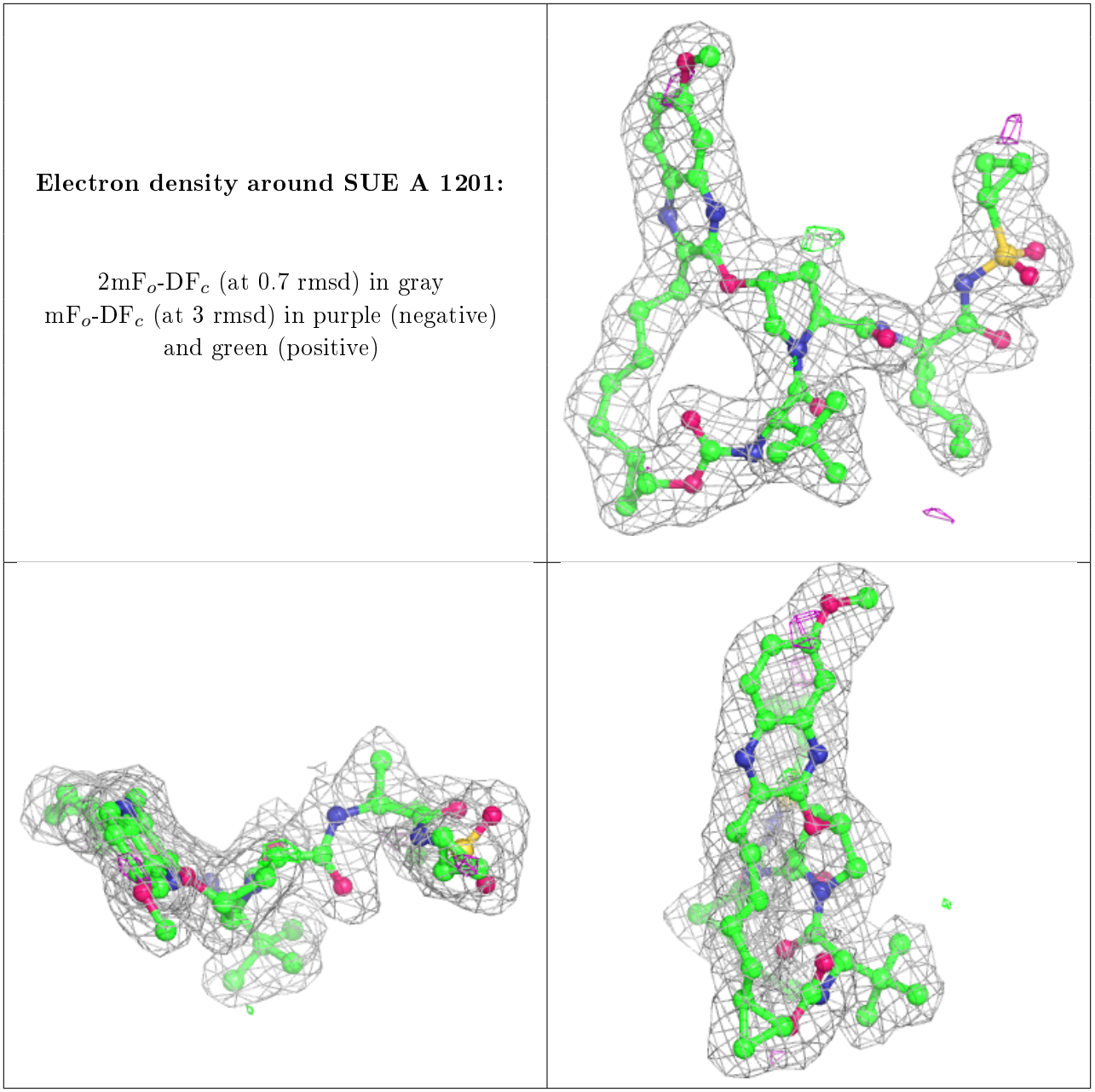
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SUE	A	1201	54/54	0.98	0.08	13,18,23,24	0
2	SUE	B	1201	54/54	0.98	0.07	15,18,24,26	0
2	SUE	C	1201	54/54	0.98	0.07	12,17,21,21	0
2	SUE	D	1201	54/54	0.99	0.06	10,15,18,19	0
3	ZN	A	1202	1/1	0.99	0.08	33,33,33,33	0
3	ZN	C	1202	1/1	0.99	0.03	25,25,25,25	0
3	ZN	B	1202	1/1	1.00	0.04	20,20,20,20	0
3	ZN	D	1202	1/1	1.00	0.04	24,24,24,24	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.

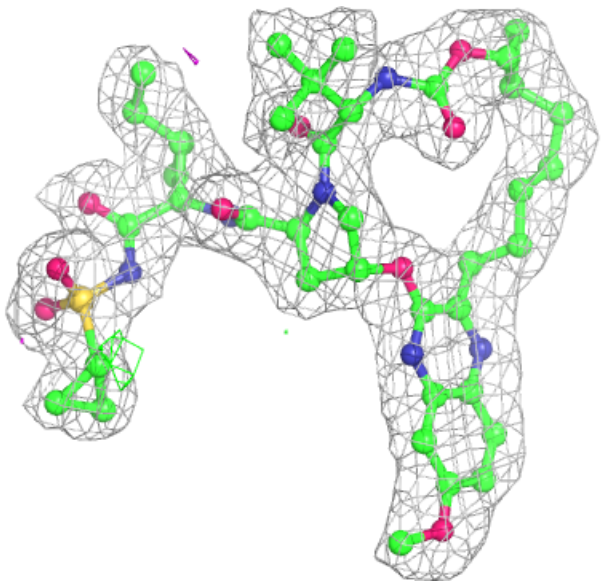
Electron density around SUE A 1201:

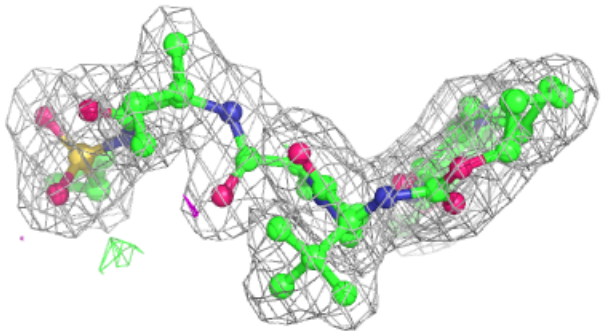
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

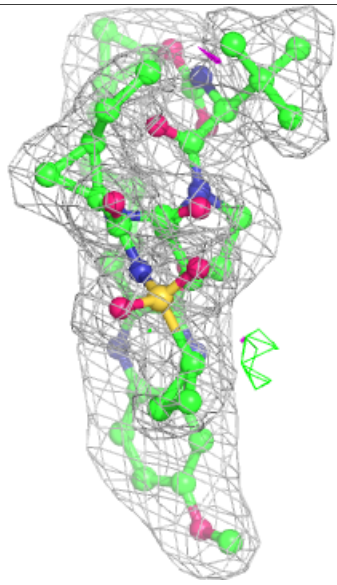


Electron density around SUE B 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

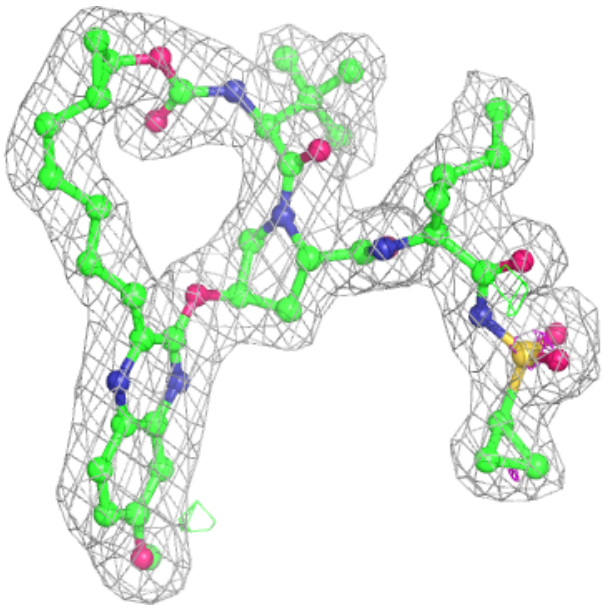


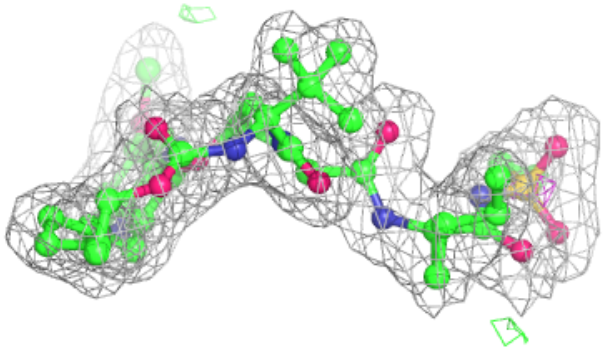


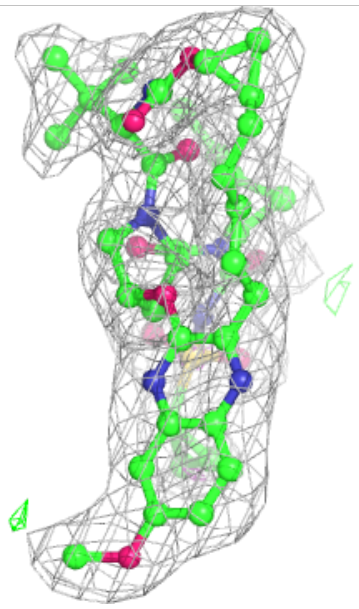


Electron density around SUE C 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

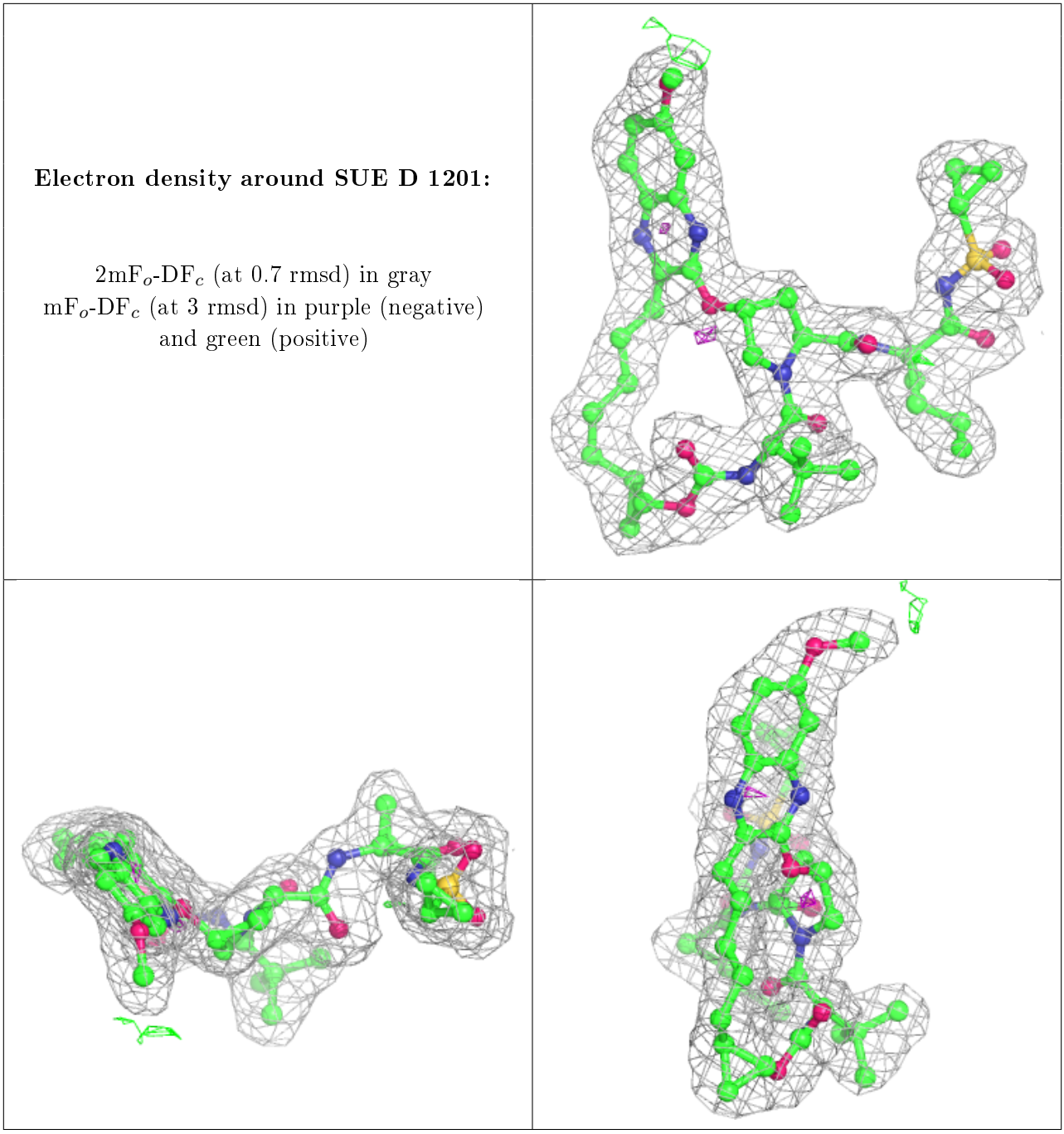






Electron density around SUE D 1201:

$2mF_o$-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.