



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:38 AM UTC

PDB ID : 6C2M / pdb_00006c2m
Title : Crystal structure of HCV NS3/4A protease variant Y56H in complex with MK-5172
Authors : Matthew, A.N.; Schiffer, C.A.
Deposited on : 2018-01-08
Resolution : 1.86 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

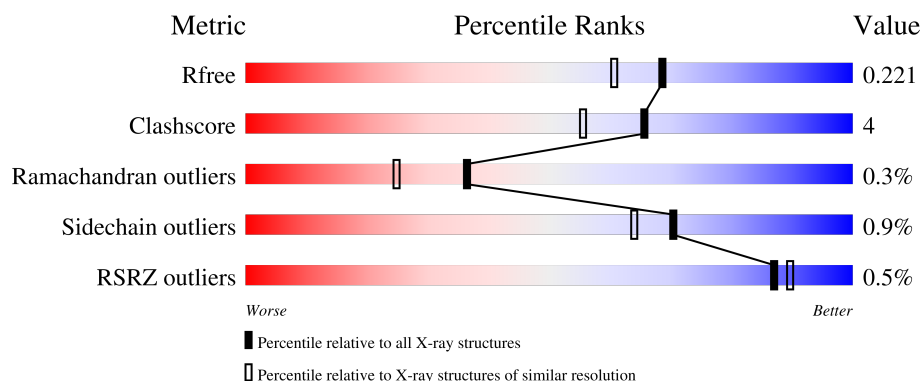
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	197	91% 5% . .
1	B	197	94% . .
1	C	197	% 88% 8% . .
1	D	197	2% 83% 13% . .

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
3	SUE	A	1202	X	-	-	-
3	SUE	B	1202	X	-	-	-
3	SUE	C	1203	X	-	-	-
3	SUE	D	1202	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11237 atoms, of which 5409 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	191	Total	C	H	N	O	S	0	1	0
			2669	840	1312	243	268	6			
1	B	191	Total	C	H	N	O	S	0	1	0
			2640	836	1295	238	265	6			
1	C	191	Total	C	H	N	O	S	0	1	0
			2649	838	1302	242	261	6			
1	D	191	Total	C	H	N	O	S	0	1	0
			2645	837	1300	242	260	6			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	expression tag	UNP C1KIK8
A	984	ALA	-	expression tag	UNP C1KIK8
A	985	SER	-	expression tag	UNP C1KIK8
A	986	MET	-	expression tag	UNP C1KIK8
A	987	LYS	-	expression tag	UNP C1KIK8
A	988	LYS	-	expression tag	UNP C1KIK8
A	989	LYS	-	expression tag	UNP C1KIK8
A	990	GLY	-	expression tag	UNP C1KIK8
A	991	SER	-	expression tag	UNP C1KIK8
A	992	VAL	-	expression tag	UNP C1KIK8
A	993	VAL	-	expression tag	UNP C1KIK8
A	994	ILE	-	expression tag	UNP C1KIK8
A	995	VAL	-	expression tag	UNP C1KIK8
A	996	GLY	-	expression tag	UNP C1KIK8
A	997	ARG	-	expression tag	UNP C1KIK8
A	998	ILE	-	expression tag	UNP C1KIK8
A	999	ASN	-	expression tag	UNP C1KIK8
A	1000	LEU	-	expression tag	UNP C1KIK8
A	1001	SER	-	expression tag	UNP C1KIK8
A	1002	GLY	-	expression tag	UNP C1KIK8
A	1003	ASP	-	expression tag	UNP C1KIK8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1013	GLU	LEU	engineered mutation	UNP C1KIK8
A	1014	GLU	LEU	engineered mutation	UNP C1KIK8
A	1017	GLN	ILE	engineered mutation	UNP C1KIK8
A	1018	GLU	ILE	engineered mutation	UNP C1KIK8
A	1021	GLN	LEU	engineered mutation	UNP C1KIK8
A	1040	THR	ALA	engineered mutation	UNP C1KIK8
A	1047	SER	CYS	engineered mutation	UNP C1KIK8
A	1052	LEU	CYS	engineered mutation	UNP C1KIK8
A	1056	HIS	TYR	engineered mutation	UNP C1KIK8
A	1072	THR	ILE	engineered mutation	UNP C1KIK8
A	1086	GLN	PRO	engineered mutation	UNP C1KIK8
A	1159	SER	CYS	engineered mutation	UNP C1KIK8
B	983	MET	-	expression tag	UNP C1KIK8
B	984	ALA	-	expression tag	UNP C1KIK8
B	985	SER	-	expression tag	UNP C1KIK8
B	986	MET	-	expression tag	UNP C1KIK8
B	987	LYS	-	expression tag	UNP C1KIK8
B	988	LYS	-	expression tag	UNP C1KIK8
B	989	LYS	-	expression tag	UNP C1KIK8
B	990	GLY	-	expression tag	UNP C1KIK8
B	991	SER	-	expression tag	UNP C1KIK8
B	992	VAL	-	expression tag	UNP C1KIK8
B	993	VAL	-	expression tag	UNP C1KIK8
B	994	ILE	-	expression tag	UNP C1KIK8
B	995	VAL	-	expression tag	UNP C1KIK8
B	996	GLY	-	expression tag	UNP C1KIK8
B	997	ARG	-	expression tag	UNP C1KIK8
B	998	ILE	-	expression tag	UNP C1KIK8
B	999	ASN	-	expression tag	UNP C1KIK8
B	1000	LEU	-	expression tag	UNP C1KIK8
B	1001	SER	-	expression tag	UNP C1KIK8
B	1002	GLY	-	expression tag	UNP C1KIK8
B	1003	ASP	-	expression tag	UNP C1KIK8
B	1013	GLU	LEU	engineered mutation	UNP C1KIK8
B	1014	GLU	LEU	engineered mutation	UNP C1KIK8
B	1017	GLN	ILE	engineered mutation	UNP C1KIK8
B	1018	GLU	ILE	engineered mutation	UNP C1KIK8
B	1021	GLN	LEU	engineered mutation	UNP C1KIK8
B	1040	THR	ALA	engineered mutation	UNP C1KIK8
B	1047	SER	CYS	engineered mutation	UNP C1KIK8
B	1052	LEU	CYS	engineered mutation	UNP C1KIK8
B	1056	HIS	TYR	engineered mutation	UNP C1KIK8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1072	THR	ILE	engineered mutation	UNP C1KIK8
B	1086	GLN	PRO	engineered mutation	UNP C1KIK8
B	1159	SER	CYS	engineered mutation	UNP C1KIK8
C	983	MET	-	expression tag	UNP C1KIK8
C	984	ALA	-	expression tag	UNP C1KIK8
C	985	SER	-	expression tag	UNP C1KIK8
C	986	MET	-	expression tag	UNP C1KIK8
C	987	LYS	-	expression tag	UNP C1KIK8
C	988	LYS	-	expression tag	UNP C1KIK8
C	989	LYS	-	expression tag	UNP C1KIK8
C	990	GLY	-	expression tag	UNP C1KIK8
C	991	SER	-	expression tag	UNP C1KIK8
C	992	VAL	-	expression tag	UNP C1KIK8
C	993	VAL	-	expression tag	UNP C1KIK8
C	994	ILE	-	expression tag	UNP C1KIK8
C	995	VAL	-	expression tag	UNP C1KIK8
C	996	GLY	-	expression tag	UNP C1KIK8
C	997	ARG	-	expression tag	UNP C1KIK8
C	998	ILE	-	expression tag	UNP C1KIK8
C	999	ASN	-	expression tag	UNP C1KIK8
C	1000	LEU	-	expression tag	UNP C1KIK8
C	1001	SER	-	expression tag	UNP C1KIK8
C	1002	GLY	-	expression tag	UNP C1KIK8
C	1003	ASP	-	expression tag	UNP C1KIK8
C	1013	GLU	LEU	engineered mutation	UNP C1KIK8
C	1014	GLU	LEU	engineered mutation	UNP C1KIK8
C	1017	GLN	ILE	engineered mutation	UNP C1KIK8
C	1018	GLU	ILE	engineered mutation	UNP C1KIK8
C	1021	GLN	LEU	engineered mutation	UNP C1KIK8
C	1040	THR	ALA	engineered mutation	UNP C1KIK8
C	1047	SER	CYS	engineered mutation	UNP C1KIK8
C	1052	LEU	CYS	engineered mutation	UNP C1KIK8
C	1056	HIS	TYR	engineered mutation	UNP C1KIK8
C	1072	THR	ILE	engineered mutation	UNP C1KIK8
C	1086	GLN	PRO	engineered mutation	UNP C1KIK8
C	1159	SER	CYS	engineered mutation	UNP C1KIK8
D	983	MET	-	expression tag	UNP C1KIK8
D	984	ALA	-	expression tag	UNP C1KIK8
D	985	SER	-	expression tag	UNP C1KIK8
D	986	MET	-	expression tag	UNP C1KIK8
D	987	LYS	-	expression tag	UNP C1KIK8
D	988	LYS	-	expression tag	UNP C1KIK8

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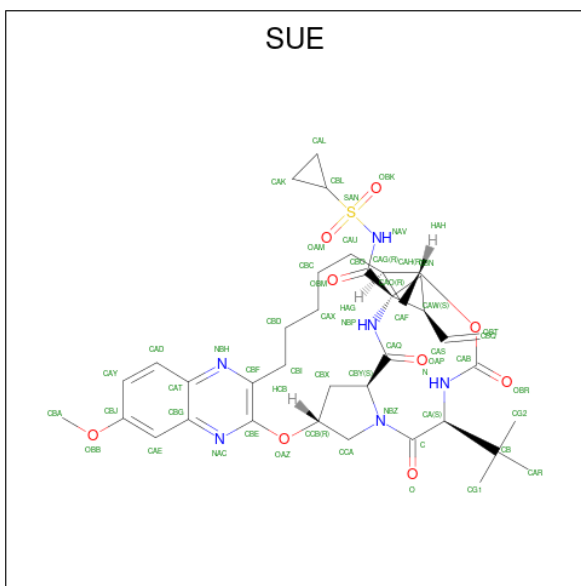
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Chain	Residue	Modelled	Actual	Comment	Reference
D	989	LYS	-	expression tag	UNP C1KIK8
D	990	GLY	-	expression tag	UNP C1KIK8
D	991	SER	-	expression tag	UNP C1KIK8
D	992	VAL	-	expression tag	UNP C1KIK8
D	993	VAL	-	expression tag	UNP C1KIK8
D	994	ILE	-	expression tag	UNP C1KIK8
D	995	VAL	-	expression tag	UNP C1KIK8
D	996	GLY	-	expression tag	UNP C1KIK8
D	997	ARG	-	expression tag	UNP C1KIK8
D	998	ILE	-	expression tag	UNP C1KIK8
D	999	ASN	-	expression tag	UNP C1KIK8
D	1000	LEU	-	expression tag	UNP C1KIK8
D	1001	SER	-	expression tag	UNP C1KIK8
D	1002	GLY	-	expression tag	UNP C1KIK8
D	1003	ASP	-	expression tag	UNP C1KIK8
D	1013	GLU	LEU	engineered mutation	UNP C1KIK8
D	1014	GLU	LEU	engineered mutation	UNP C1KIK8
D	1017	GLN	ILE	engineered mutation	UNP C1KIK8
D	1018	GLU	ILE	engineered mutation	UNP C1KIK8
D	1021	GLN	LEU	engineered mutation	UNP C1KIK8
D	1040	THR	ALA	engineered mutation	UNP C1KIK8
D	1047	SER	CYS	engineered mutation	UNP C1KIK8
D	1052	LEU	CYS	engineered mutation	UNP C1KIK8
D	1056	HIS	TYR	engineered mutation	UNP C1KIK8
D	1072	THR	ILE	engineered mutation	UNP C1KIK8
D	1086	GLN	PRO	engineered mutation	UNP C1KIK8
D	1159	SER	CYS	engineered mutation	UNP C1KIK8

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

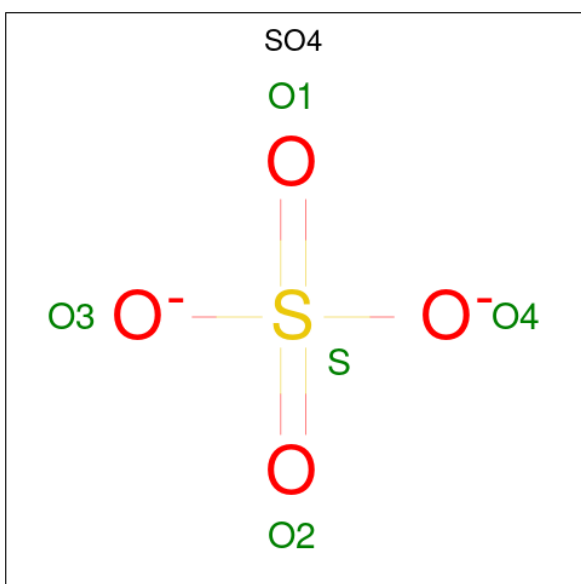
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is (1aR,5S,8S,10R,22aR)-5-tert-butyl-N-{(1R,2S)-1-[(cyclopropylsulfonyl)carbamoyl]-2-ethenylcyclopropyl}-14-methoxy-3,6-di oxo-1,1a,3,4,5,6,9,10,18,19,20,21,22,22a-tetradecahydro-8H-7,10-methanocyclopropano[18,19][1,10,3,6]dioxadiazacyclononadec ino[11,12-b]

quinoxaline-8-carboxamide (CCD ID: SUE) (formula: $\text{C}_{38}\text{H}_{50}\text{N}_6\text{O}_9\text{S}$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 104	C 38	H 50	N 6	O 9	S 1	0	0
3	B	1	Total 104	C 38	H 50	N 6	O 9	S 1	0	0
3	C	1	Total 104	C 38	H 50	N 6	O 9	S 1	0	0
3	D	1	Total 104	C 38	H 50	N 6	O 9	S 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		
5	B	63	Total	O	0	0
			63	63		
5	C	45	Total	O	0	0
			45	45		
5	D	36	Total	O	0	0
			36	36		

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

Chain A:  91% 5% ..



- Molecule 1: NS3 protease

Chain B:  94% ..



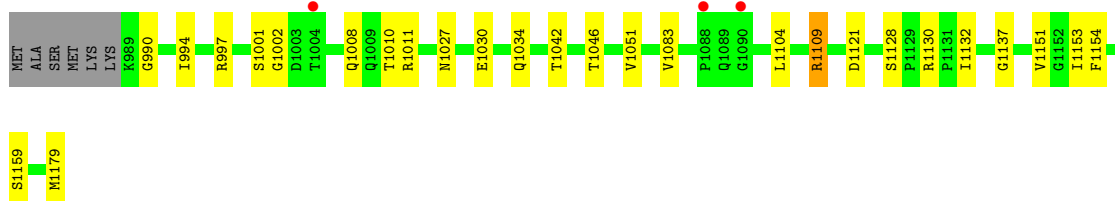
- Molecule 1: NS3 protease

Chain C:  88% 8% ..



- Molecule 1: NS3 protease

Chain D:  83% 13% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.63Å 103.33Å 73.96Å 90.00° 112.01° 90.00°	Depositor
Resolution (Å)	35.73 – 1.86 35.73 – 1.86	Depositor EDS
% Data completeness (in resolution range)	95.8 (35.73-1.86) 93.0 (35.73-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.85Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.180 , 0.224 (Not available) , 0.221	Depositor DCC
R_{free} test set	1983 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.247 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11237	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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: SUE, SO4, 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	0.24	0/1384	0.46	1/1891 (0.1%)
1	B	0.23	0/1372	0.42	0/1877
1	C	0.25	0/1374	0.42	0/1878
1	D	0.23	0/1372	0.42	0/1876
All	All	0.23	0/5502	0.43	1/7522 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1151	VAL	N-CA-C	-5.92	107.05	112.96

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	1357	1312	1312	7	0
1	B	1345	1295	1295	4	0
1	C	1347	1302	1303	11	0
1	D	1345	1300	1298	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	54	50	47	2	0
3	B	54	50	48	1	0
3	C	54	50	48	1	0
3	D	54	50	49	1	0
4	C	5	0	0	0	0
5	A	65	0	0	1	2
5	B	63	0	0	1	2
5	C	45	0	0	1	1
5	D	36	0	0	4	1
All	All	5828	5409	5400	42	3

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 4.

All (42) 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)
3:A:1202:SUE:OBK	5:A:1301:HOH:O	1.98	0.79
1:D:1001:SER:O	5:D:1301:HOH:O	2.01	0.79
1:D:997:ARG:NH2	1:D:1008:GLN:OE1	2.34	0.61
1:B:1078:VAL:HG23	3:B:1202:SUE:HAY	1.83	0.59
1:D:1132:ILE:HD11	1:D:1159:SER:HB3	1.86	0.58
1:A:1135:LEU:C	3:A:1202:SUE:HBQA	2.34	0.53
1:B:1179:MET:O	5:B:1301:HOH:O	2.19	0.52
1:D:1109:ARG:HG3	1:D:1137:GLY:O	2.12	0.49
1:A:999:ASN:HB3	1:A:1001:SER:HB2	1.92	0.49
1:D:994:ILE:O	1:D:1011:ARG:HD3	2.13	0.48
1:C:1173:GLU:O	1:C:1177:THR:N	2.40	0.48
1:C:1174:SER:HA	1:C:1177:THR:HB	1.96	0.48
1:A:1047[B]:SER:HB3	1:A:1093:SER:HG	1.77	0.48
1:D:1132:ILE:HD11	1:D:1159:SER:CB	2.45	0.47
1:D:1121:ASP:OD1	1:D:1121:ASP:N	2.48	0.46
1:D:1010:THR:OG1	5:D:1302:HOH:O	2.21	0.45
1:D:1042:THR:HG21	1:D:1109:ARG:NH2	2.33	0.43
1:A:1114:ILE:HD11	1:A:1134:TYR:HE2	1.83	0.43
1:C:1176:GLU:HA	1:C:1179:MET:SD	2.58	0.43
1:D:1027:ASN:O	5:D:1303:HOH:O	2.21	0.43
1:C:1104:LEU:HD22	1:C:1151:VAL:HG21	2.01	0.43
1:D:1128:SER:HB2	1:D:1130:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:ASN:O	1:A:1005:ALA:HA	2.19	0.42
1:D:1154:PHE:CE2	3:D:1202:SUE:HBN	2.53	0.42
1:D:1109:ARG:HD2	1:D:1137:GLY:O	2.20	0.42
1:C:1121:ASP:OD1	1:C:1121:ASP:N	2.52	0.42
1:C:1175:LEU:O	1:C:1179:MET:SD	2.77	0.42
1:D:1030:GLU:O	1:D:1034:GLN:NE2	2.39	0.42
1:B:1159:SER:HA	1:B:1163:VAL:O	2.19	0.41
1:D:1002:GLY:HA2	5:D:1301:HOH:O	2.20	0.41
1:D:1042:THR:HG21	1:D:1109:ARG:HH21	1.85	0.41
1:C:1154:PHE:CE2	3:C:1203:SUE:HBN	2.55	0.41
1:C:1011:ARG:NH2	5:C:1301:HOH:O	2.27	0.41
1:C:1101:SER:O	1:C:1118:ARG:NH2	2.51	0.41
1:C:1075:TYR:CD1	1:C:1075:TYR:C	2.98	0.40
1:D:1046:THR:HB	1:D:1153:ILE:CD1	2.51	0.40
1:A:1001:SER:HA	1:B:1068:LYS:HZ2	1.86	0.40
1:A:1132:ILE:HD11	1:A:1159:SER:CB	2.52	0.40
1:C:1006:TYR:HA	1:C:1111:ALA:CB	2.52	0.40
1:D:997:ARG:HD3	1:D:1030:GLU:C	2.47	0.40
1:D:1051:VAL:HG21	1:D:1179:MET:HE3	2.04	0.40
1:D:1104:LEU:HD22	1:D:1151:VAL:HG21	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1348:HOH:O	5:B:1315:HOH:O[2_545]	1.97	0.23
5:C:1338:HOH:O	5:D:1309:HOH:O[2_645]	2.07	0.13
5:A:1340:HOH:O	5:B:1338:HOH:O[2_645]	2.19	0.01

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	190/197 (96%)	179 (94%)	10 (5%)	1 (0%)	24	13
1	B	190/197 (96%)	185 (97%)	5 (3%)	0	100	100
1	C	190/197 (96%)	186 (98%)	4 (2%)	0	100	100
1	D	190/197 (96%)	179 (94%)	10 (5%)	1 (0%)	24	13
All	All	760/788 (96%)	729 (96%)	29 (4%)	2 (0%)	36	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1001	SER
1	D	990	GLY

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	143/160 (89%)	143 (100%)	0	100	100
1	B	140/160 (88%)	139 (99%)	1 (1%)	76	70
1	C	139/160 (87%)	137 (99%)	2 (1%)	59	49
1	D	138/160 (86%)	136 (99%)	2 (1%)	59	49
All	All	560/640 (88%)	555 (99%)	5 (1%)	70	64

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1133	SER
1	C	1074	MET
1	C	1177	THR
1	D	1083	VAL
1	D	1109	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1028	GLN
1	D	999	ASN

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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
3	SUE	C	1203	-	55,60,60	4.05	22 (40%)	74,92,92	2.39	15 (20%)
3	SUE	A	1202	-	55,60,60	3.91	20 (36%)	74,92,92	2.25	14 (18%)
4	SO4	C	1201	-	4,4,4	0.25	0	6,6,6	0.19	0
3	SUE	D	1202	-	55,60,60	4.06	21 (38%)	74,92,92	2.32	16 (21%)
3	SUE	B	1202	-	55,60,60	3.95	21 (38%)	74,92,92	2.31	17 (22%)

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	SUE	D	1202	-	1/1/19/19	3/61/91/91	0/6/7/7
3	SUE	A	1202	-	1/1/19/19	6/61/91/91	0/6/7/7
3	SUE	C	1203	-	1/1/19/19	9/61/91/91	0/6/7/7
3	SUE	B	1202	-	1/1/19/19	6/61/91/91	0/6/7/7

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	SUE	CBF-NBH	11.51	1.46	1.32
3	C	1203	SUE	CBF-NBH	11.39	1.46	1.32
3	B	1202	SUE	CBF-NBH	11.11	1.45	1.32
3	A	1202	SUE	CBF-NBH	10.81	1.45	1.32
3	C	1203	SUE	CAE-CBJ	10.15	1.54	1.37
3	D	1202	SUE	CAE-CBJ	9.92	1.54	1.37
3	B	1202	SUE	CAE-CBJ	9.77	1.53	1.37
3	A	1202	SUE	CAE-CBJ	9.66	1.53	1.37
3	A	1202	SUE	CAY-CBJ	9.19	1.55	1.38
3	C	1203	SUE	CAY-CBJ	9.17	1.55	1.38
3	D	1202	SUE	CAY-CBJ	9.13	1.55	1.38
3	B	1202	SUE	CAY-CBJ	9.03	1.55	1.38
3	D	1202	SUE	CAE-CBG	8.51	1.54	1.41
3	C	1203	SUE	CAD-CAT	8.34	1.55	1.41
3	C	1203	SUE	CAE-CBG	8.34	1.54	1.41
3	A	1202	SUE	CAD-CAY	8.31	1.54	1.36
3	C	1203	SUE	CAD-CAY	8.31	1.54	1.36
3	B	1202	SUE	CAD-CAY	8.26	1.54	1.36
3	A	1202	SUE	CAE-CBG	8.25	1.54	1.41
3	B	1202	SUE	CAE-CBG	8.13	1.54	1.41
3	D	1202	SUE	CAD-CAY	8.11	1.54	1.36
3	D	1202	SUE	CAD-CAT	8.05	1.55	1.41
3	B	1202	SUE	CAD-CAT	7.91	1.55	1.41
3	A	1202	SUE	CAD-CAT	7.87	1.55	1.41
3	C	1203	SUE	CBG-NAC	7.55	1.49	1.37
3	D	1202	SUE	CAT-NBH	7.50	1.49	1.37
3	C	1203	SUE	CAT-NBH	7.41	1.49	1.37
3	D	1202	SUE	CBG-NAC	7.12	1.48	1.37
3	B	1202	SUE	CAT-NBH	6.95	1.48	1.37
3	B	1202	SUE	CBG-NAC	6.93	1.48	1.37
3	A	1202	SUE	CAT-NBH	6.83	1.48	1.37
3	D	1202	SUE	CBE-NAC	6.75	1.45	1.30
3	C	1203	SUE	CBE-NAC	6.63	1.45	1.30
3	C	1203	SUE	CAQ-NBP	6.56	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1202	SUE	C-NBZ	6.55	1.49	1.34
3	A	1202	SUE	CBE-NAC	6.54	1.45	1.30
3	A	1202	SUE	CBG-NAC	6.53	1.47	1.37
3	B	1202	SUE	CAQ-NBP	6.41	1.47	1.34
3	B	1202	SUE	CBE-NAC	6.40	1.44	1.30
3	A	1202	SUE	C-NBZ	6.37	1.49	1.34
3	D	1202	SUE	CAQ-NBP	6.37	1.47	1.34
3	D	1202	SUE	C-NBZ	6.29	1.48	1.34
3	C	1203	SUE	C-NBZ	6.24	1.48	1.34
3	A	1202	SUE	CAQ-NBP	5.90	1.46	1.34
3	D	1202	SUE	CAB-N	5.13	1.47	1.34
3	B	1202	SUE	CAB-N	4.91	1.46	1.34
3	A	1202	SUE	CAB-N	4.89	1.46	1.34
3	D	1202	SUE	CBG-CAT	4.63	1.51	1.42
3	C	1203	SUE	CBG-CAT	4.63	1.51	1.42
3	C	1203	SUE	CAB-N	4.51	1.45	1.34
3	D	1202	SUE	OBT-CAB	4.19	1.42	1.35
3	B	1202	SUE	CBG-CAT	4.19	1.50	1.42
3	A	1202	SUE	CBG-CAT	3.97	1.50	1.42
3	A	1202	SUE	OBT-CAB	3.73	1.41	1.35
3	B	1202	SUE	OBT-CAB	3.58	1.41	1.35
3	A	1202	SUE	OAM-SAN	3.48	1.47	1.43
3	C	1203	SUE	OBT-CAB	3.42	1.41	1.35
3	C	1203	SUE	OAZ-CBE	3.26	1.43	1.36
3	A	1202	SUE	OAZ-CBE	3.14	1.43	1.36
3	D	1202	SUE	OAM-SAN	3.13	1.47	1.43
3	D	1202	SUE	OBK-SAN	3.10	1.47	1.43
3	B	1202	SUE	OAM-SAN	3.02	1.47	1.43
3	B	1202	SUE	OBK-SAN	2.98	1.47	1.43
3	D	1202	SUE	OAZ-CBE	2.96	1.42	1.36
3	C	1203	SUE	OBT-CAH	-2.94	1.41	1.46
3	C	1203	SUE	OAM-SAN	2.81	1.46	1.43
3	A	1202	SUE	OBK-SAN	2.74	1.46	1.43
3	D	1202	SUE	OBT-CAH	-2.66	1.41	1.46
3	A	1202	SUE	OBT-CAH	-2.66	1.41	1.46
3	B	1202	SUE	OBT-CAH	-2.60	1.41	1.46
3	B	1202	SUE	OAZ-CBE	2.57	1.42	1.36
3	D	1202	SUE	OBM-CBO	-2.56	1.18	1.22
3	A	1202	SUE	CAG-CAH	2.56	1.53	1.49
3	C	1203	SUE	OBM-CBO	-2.52	1.18	1.22
3	D	1202	SUE	CAG-CAH	2.47	1.53	1.49
3	B	1202	SUE	CAG-CAH	2.34	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	SUE	OBM-CBO	-2.31	1.18	1.22
3	C	1203	SUE	CBN-CAO	2.29	1.53	1.51
3	D	1202	SUE	OAP-CAQ	-2.25	1.19	1.23
3	C	1203	SUE	CAG-CAH	2.24	1.52	1.49
3	B	1202	SUE	OBM-CBO	-2.24	1.19	1.22
3	C	1203	SUE	OBK-SAN	2.18	1.46	1.43
3	B	1202	SUE	CBN-CAO	2.13	1.53	1.51
3	C	1203	SUE	O-C	-2.01	1.18	1.22

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1203	SUE	OBK-SAN-OAM	-12.33	100.87	118.88
3	D	1202	SUE	OBK-SAN-OAM	-11.12	102.64	118.88
3	B	1202	SUE	OBK-SAN-OAM	-11.10	102.68	118.88
3	A	1202	SUE	OBK-SAN-OAM	-10.96	102.88	118.88
3	D	1202	SUE	CAU-CAG-CAH	8.35	140.12	122.56
3	C	1203	SUE	CAU-CAG-CAH	7.61	138.56	122.56
3	B	1202	SUE	CAU-CAG-CAH	7.07	137.42	122.56
3	A	1202	SUE	CAU-CAG-CAH	7.00	137.28	122.56
3	C	1203	SUE	OAM-SAN-CBL	6.67	116.87	107.98
3	B	1202	SUE	OBT-CAB-N	6.02	117.94	110.26
3	A	1202	SUE	CBO-CAO-NBP	5.92	122.42	116.10
3	A	1202	SUE	CAW-CAO-NBP	-5.91	106.23	117.25
3	D	1202	SUE	CBO-CAO-NBP	5.71	122.19	116.10
3	B	1202	SUE	CBO-CAO-NBP	5.70	122.19	116.10
3	D	1202	SUE	OBT-CAB-N	5.39	117.14	110.26
3	C	1203	SUE	CBO-CAO-NBP	5.32	121.78	116.10
3	C	1203	SUE	CAW-CAO-NBP	-4.26	109.31	117.25
3	C	1203	SUE	OBT-CAB-N	4.22	115.64	110.26
3	B	1202	SUE	CAW-CAO-NBP	-4.11	109.57	117.25
3	A	1202	SUE	OBT-CAB-N	4.00	115.36	110.26
3	D	1202	SUE	CBX-CCB-CCA	-3.86	100.47	103.69
3	D	1202	SUE	CB-CA-C	-3.64	108.38	113.23
3	A	1202	SUE	CBX-CCB-CCA	-3.43	100.83	103.69
3	B	1202	SUE	CBX-CBY-CAQ	3.38	117.84	111.36
3	B	1202	SUE	CAH-OBT-CAB	-3.25	112.61	117.09
3	D	1202	SUE	OBK-SAN-CBL	3.16	112.20	107.98
3	D	1202	SUE	CAW-CAO-NBP	-3.11	111.45	117.25
3	C	1203	SUE	CBX-CCB-CCA	-3.09	101.11	103.69
3	B	1202	SUE	CBX-CCB-CCA	-3.00	101.19	103.69
3	D	1202	SUE	CCA-NBZ-CBY	-2.92	107.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	SUE	CBD-CBI-CBF	-2.90	105.89	112.85
3	A	1202	SUE	CBC-CAU-CAG	-2.89	105.19	115.11
3	D	1202	SUE	OBR-CAB-N	-2.87	120.15	124.86
3	C	1203	SUE	CCA-NBZ-CBY	-2.77	108.17	111.83
3	B	1202	SUE	OBR-CAB-N	-2.74	120.36	124.86
3	B	1202	SUE	CAQ-CBY-NBZ	-2.74	105.03	112.50
3	B	1202	SUE	CBC-CAU-CAG	-2.73	105.75	115.11
3	A	1202	SUE	CBX-CBY-CAQ	2.72	116.57	111.36
3	B	1202	SUE	CCA-NBZ-CBY	-2.70	108.25	111.83
3	D	1202	SUE	CAQ-CBY-NBZ	-2.60	105.41	112.50
3	C	1203	SUE	OBR-CAB-N	-2.59	120.62	124.86
3	A	1202	SUE	CAQ-CBY-NBZ	-2.52	105.63	112.50
3	C	1203	SUE	CBX-CBY-CAQ	2.51	116.16	111.36
3	B	1202	SUE	CAO-CBO-NAV	2.45	119.82	115.68
3	A	1202	SUE	CCB-CCA-NBZ	-2.45	99.64	102.66
3	C	1203	SUE	CAQ-CBY-NBZ	-2.45	105.83	112.50
3	C	1203	SUE	CAW-CAS-CBQ	-2.40	117.97	125.39
3	D	1202	SUE	CAW-CAS-CBQ	-2.38	118.02	125.39
3	A	1202	SUE	CCA-NBZ-CBY	-2.36	108.71	111.83
3	C	1203	SUE	CBX-CBY-NBZ	2.27	105.88	103.17
3	B	1202	SUE	CAW-CAS-CBQ	-2.26	118.40	125.39
3	C	1203	SUE	CB-CA-C	-2.26	110.22	113.23
3	A	1202	SUE	OBR-CAB-N	-2.25	121.17	124.86
3	C	1203	SUE	CBD-CBI-CBF	-2.23	107.49	112.85
3	A	1202	SUE	CBD-CBI-CBF	-2.19	107.58	112.85
3	D	1202	SUE	CAO-CBO-NAV	2.16	119.34	115.68
3	D	1202	SUE	CAE-CBG-CAT	2.14	121.88	119.50
3	A	1202	SUE	OBK-SAN-CBL	2.12	110.80	107.98
3	B	1202	SUE	CAE-CBG-CAT	2.10	121.84	119.50
3	D	1202	SUE	CAX-CBD-CBI	-2.08	105.04	113.74
3	B	1202	SUE	CBX-CBY-NBZ	2.05	105.61	103.17
3	D	1202	SUE	CBI-CBF-CBE	-2.05	117.33	122.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1202	SUE	NBZ
3	B	1202	SUE	NBZ
3	C	1203	SUE	NBZ
3	D	1202	SUE	NBZ

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	SUE	CAH-CAG-CAU-CBC
3	A	1202	SUE	CBQ-CAS-CAW-CBN
3	B	1202	SUE	CAX-CBD-CBI-CBF
3	C	1203	SUE	CBO-NAV-SAN-OAM
3	C	1203	SUE	CBO-NAV-SAN-CBL
3	D	1202	SUE	CAF-CAH-OBT-CAB
3	C	1203	SUE	CAX-CBD-CBI-CBF
3	B	1202	SUE	CAG-CAU-CBC-CAX
3	C	1203	SUE	CBD-CAX-CBC-CAU
3	B	1202	SUE	CBD-CAX-CBC-CAU
3	C	1203	SUE	CBC-CAX-CBD-CBI
3	B	1202	SUE	NBH-CBF-CBI-CBD
3	C	1203	SUE	CAH-CAG-CAU-CBC
3	B	1202	SUE	CBE-CBF-CBI-CBD
3	C	1203	SUE	CAF-CAG-CAU-CBC
3	A	1202	SUE	CBO-NAV-SAN-CBL
3	B	1202	SUE	CBO-NAV-SAN-CBL
3	D	1202	SUE	CBO-NAV-SAN-CBL
3	D	1202	SUE	NBP-CAQ-CBY-NBZ
3	A	1202	SUE	CBD-CAX-CBC-CAU
3	C	1203	SUE	NBP-CAQ-CBY-NBZ
3	A	1202	SUE	CBQ-CAS-CAW-CAO
3	C	1203	SUE	CAG-CAU-CBC-CAX
3	A	1202	SUE	CBC-CAX-CBD-CBI

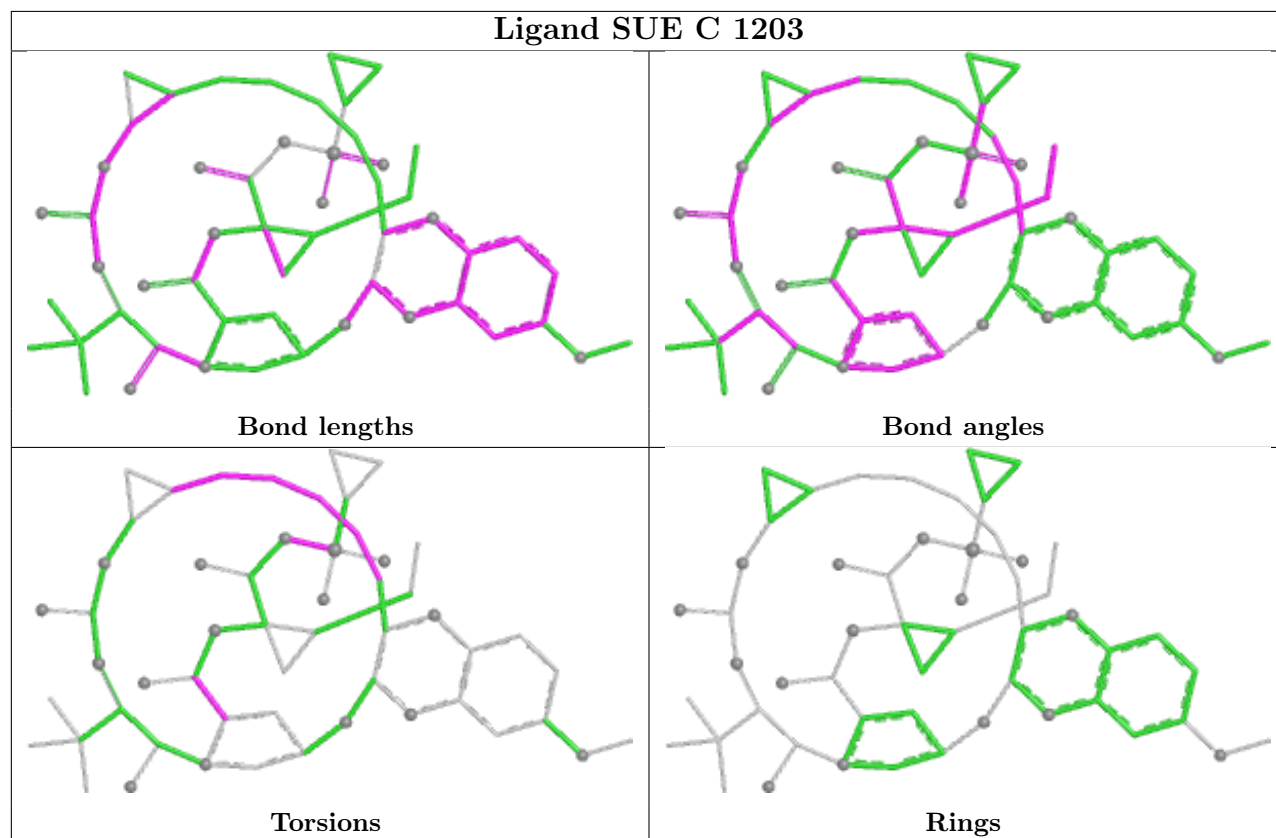
There are no ring outliers.

4 monomers are involved in 5 short contacts:

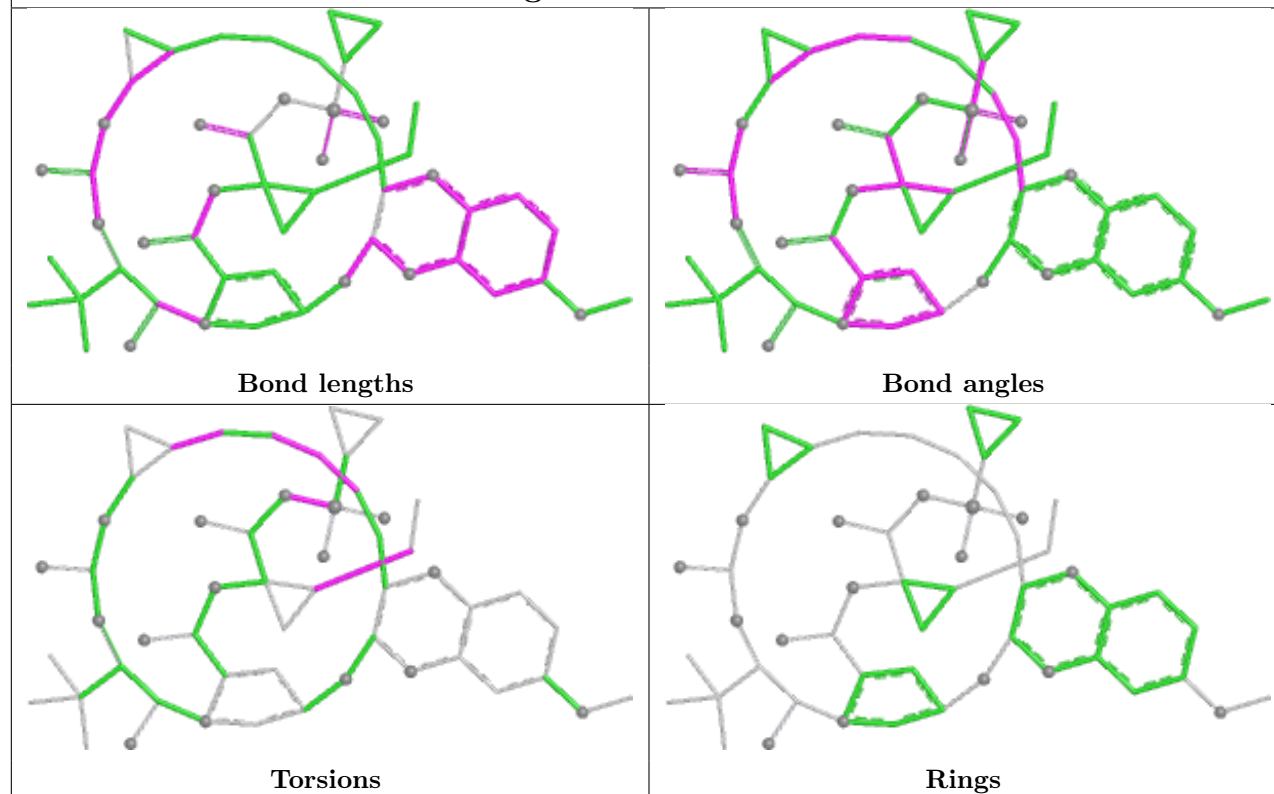
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1203	SUE	1	0
3	A	1202	SUE	2	0
3	D	1202	SUE	1	0
3	B	1202	SUE	1	0

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

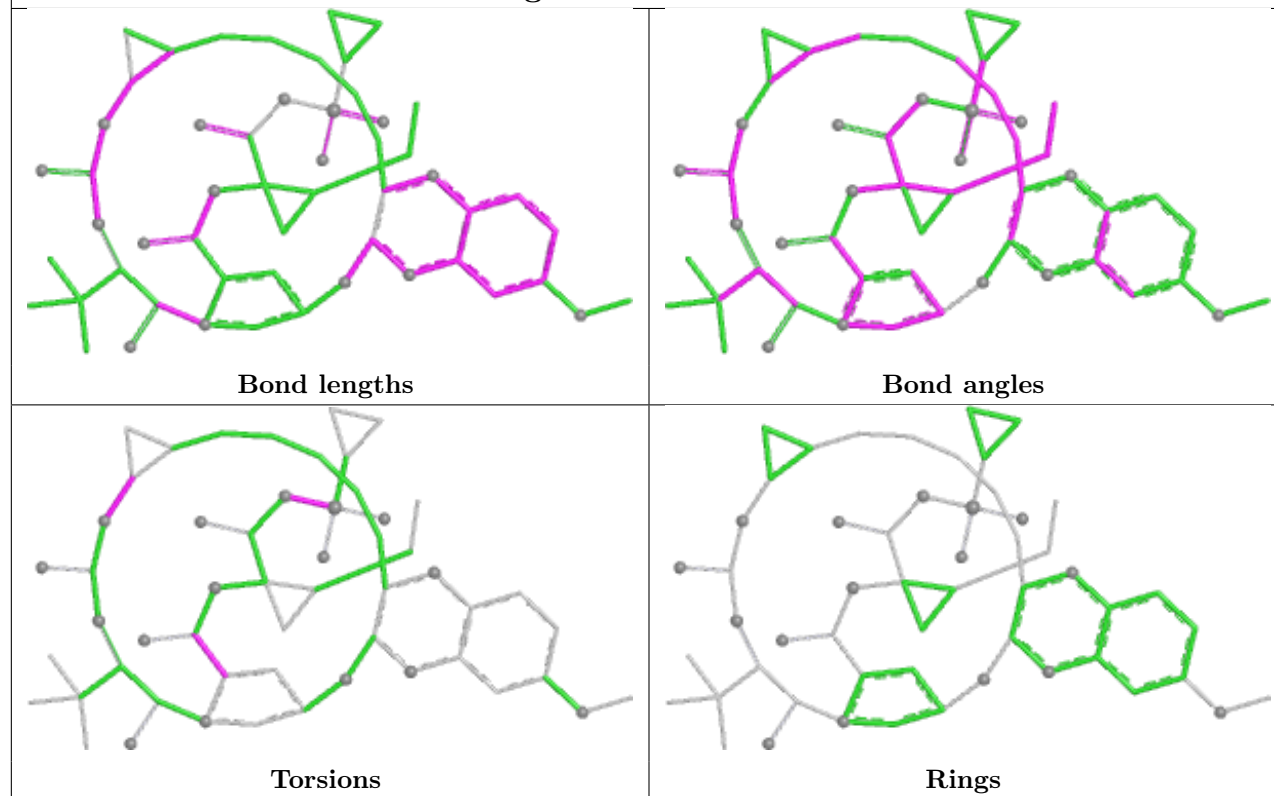
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

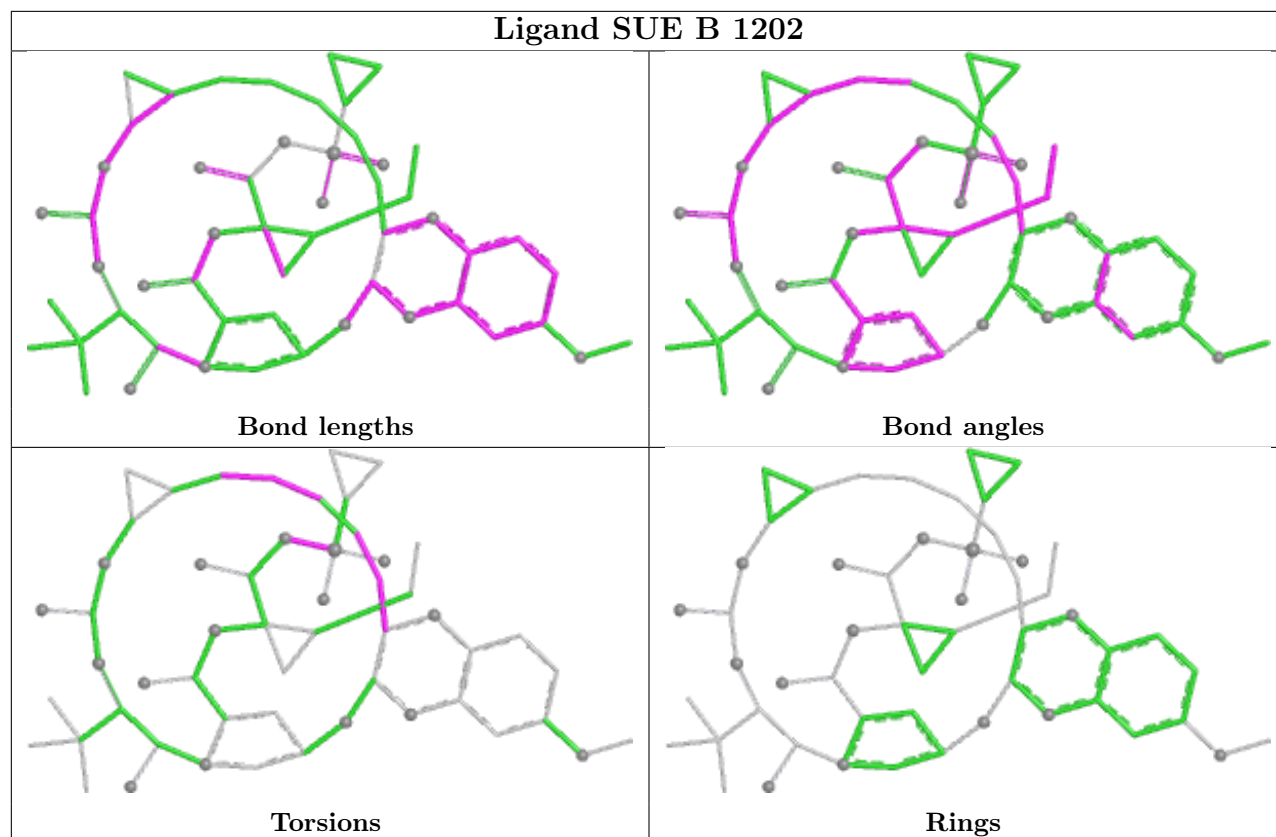


Ligand SUE A 1202



Ligand SUE D 1202





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	191/197 (96%)	-0.97	0	100 100	10, 27, 54, 80	1 (0%)
1	B	191/197 (96%)	-0.98	0	100 100	9, 28, 50, 87	1 (0%)
1	C	191/197 (96%)	-0.89	1 (0%)	87 90	13, 28, 52, 92	1 (0%)
1	D	191/197 (96%)	-0.69	3 (1%)	70 74	15, 33, 73, 86	1 (0%)
All	All	764/788 (96%)	-0.88	4 (0%)	87 90	9, 29, 60, 92	4 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1177	THR	2.5
1	D	1090	GLY	2.4
1	D	1004	THR	2.3
1	D	1088	PRO	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](#)

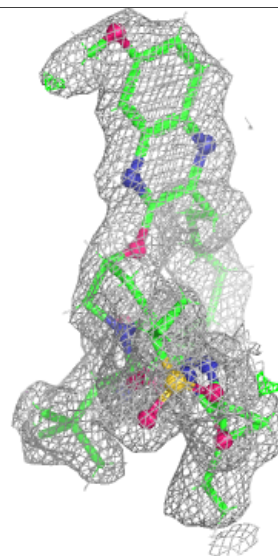
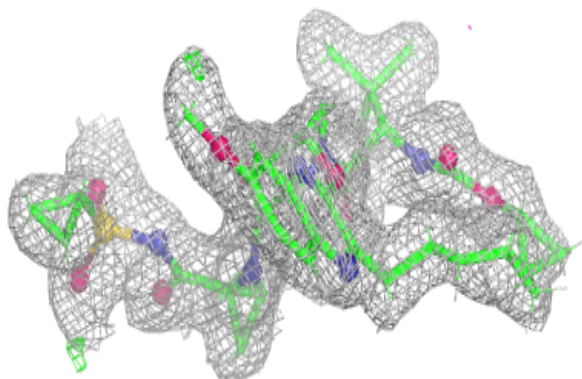
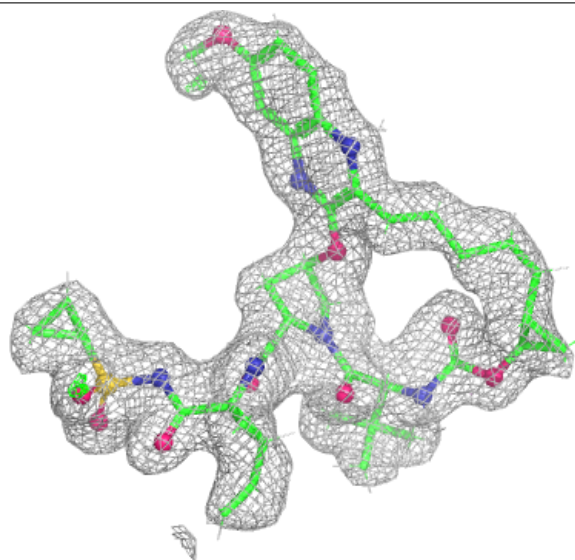
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
3	SUE	A	1202	54/54	0.99	0.04	16,29,43,55	0
3	SUE	B	1202	54/54	0.99	0.04	17,27,39,41	0
3	SUE	C	1203	54/54	0.99	0.04	14,22,36,45	0
3	SUE	D	1202	54/54	0.99	0.04	11,25,40,54	0
2	ZN	A	1201	1/1	1.00	0.02	24,24,24,24	0
2	ZN	B	1201	1/1	1.00	0.01	26,26,26,26	0
2	ZN	C	1202	1/1	1.00	0.02	24,24,24,24	0
2	ZN	D	1201	1/1	1.00	0.02	27,27,27,27	0
4	SO4	C	1201	5/5	1.00	0.03	23,36,41,43	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.

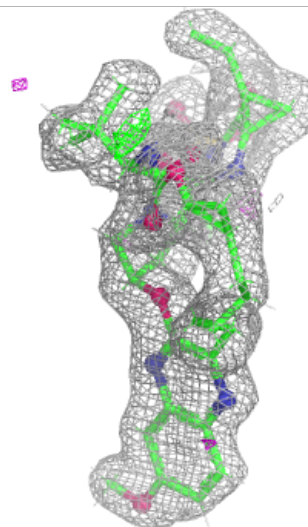
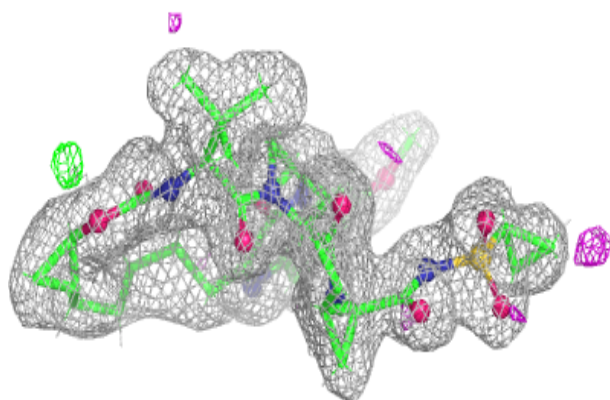
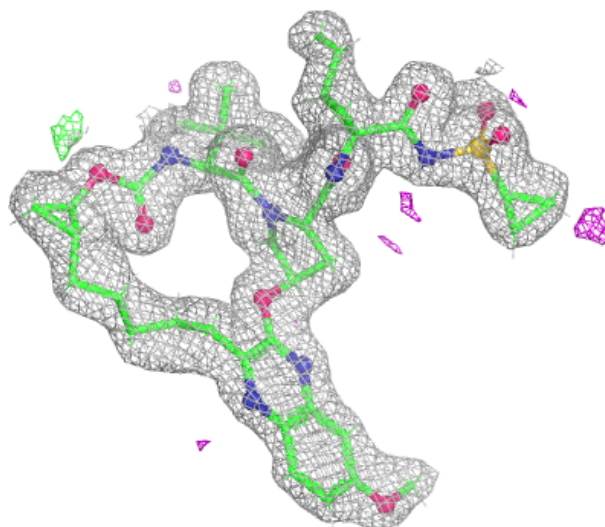
Electron density around SUE A 1202:

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



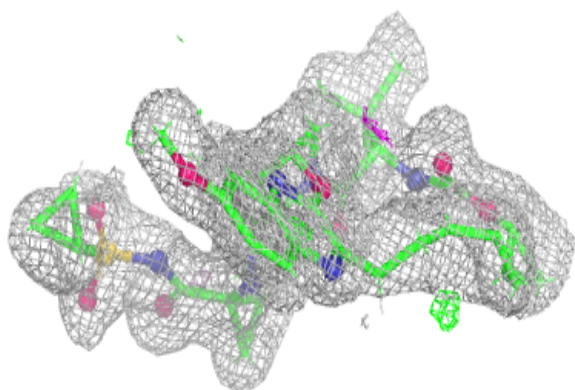
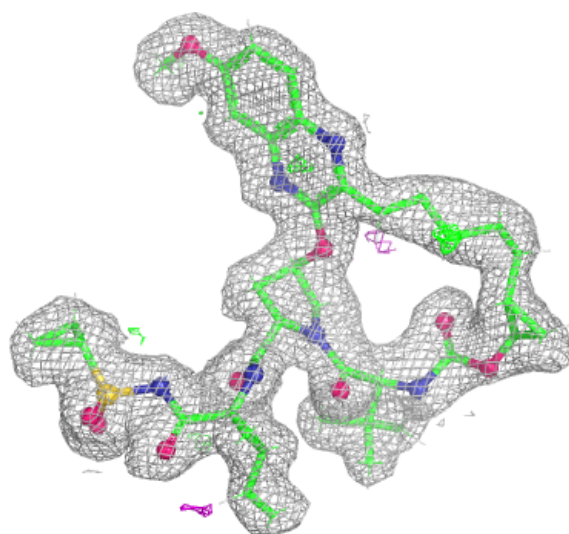
Electron density around SUE B 1202:

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



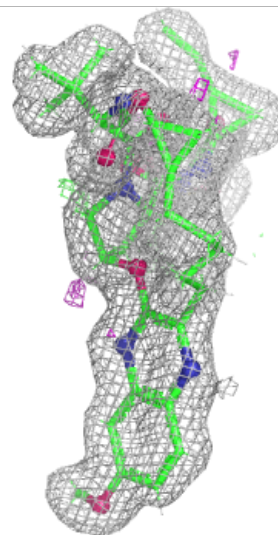
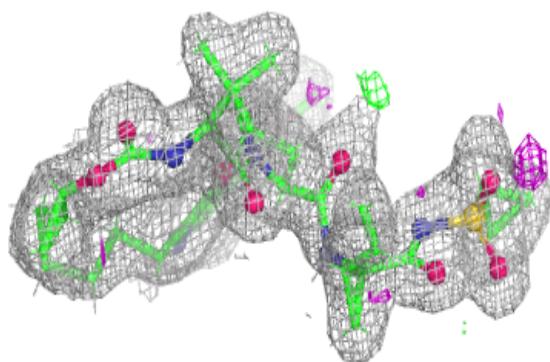
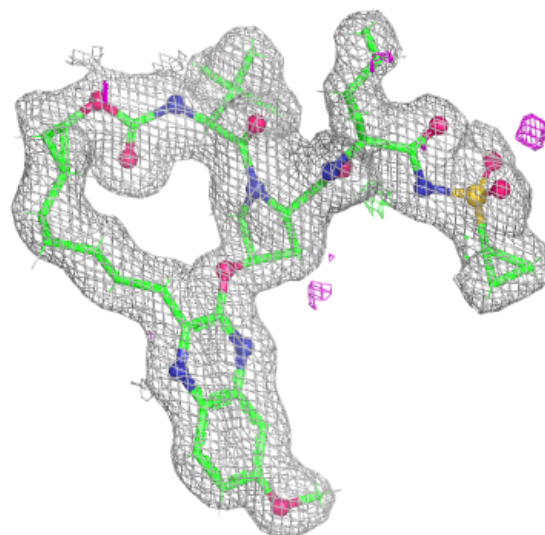
Electron density around SUE C 1203:

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



Electron density around SUE D 1202:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.