WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2020 – 05:52 AM BST

PDB ID	:	4TYD
Title	:	Structure-based design of a novel series of azetidine inhibitors of the hepatitis C virus NS3/4A serine protease
Authors	:	Parsy, C.
Deposited on	:	2014-07-08
Resolution	:	2.84 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

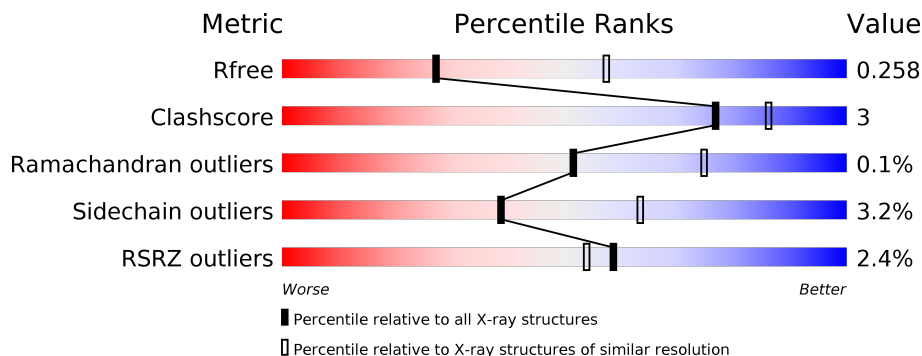|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		3.2%
RSRZ outliers		2.4%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	89% ... 6% •
1	B	203	% ... 89% ... 7% •
1	C	203	% ... 88% ... 8% •
1	D	203	2% ... 85% ... 10% •
1	E	203	% ... 85% ... 8% ... 6%
1	F	203	3% ... 87% ... 9% •

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Mol	Chain	Length	Quality of chain
1	G	203	% 84% 9% 6%
1	H	203	2% 89% 6% 5%
1	J	203	% 89% 7% ·
1	K	203	4% 91% · · ·
1	L	203	4% 84% 8% 8%
1	M	203	4% 85% 10% · ·

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	ZN	F	301	-	-	X	-
2	ZN	L	301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17686 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total 1425	C 887	N 260	O 268	S 10	0	0	0
1	B	196	Total 1439	C 895	N 265	O 269	S 10	0	0	0
1	C	196	Total 1439	C 896	N 263	O 270	S 10	0	0	0
1	D	195	Total 1434	C 893	N 262	O 269	S 10	0	0	0
1	E	190	Total 1393	C 869	N 253	O 262	S 9	0	0	0
1	F	195	Total 1430	C 890	N 261	O 269	S 10	0	0	0
1	G	190	Total 1393	C 869	N 253	O 262	S 9	0	0	0
1	H	193	Total 1418	C 882	N 259	O 267	S 10	0	0	0
1	J	196	Total 1439	C 895	N 265	O 269	S 10	0	0	0
1	K	194	Total 1424	C 887	N 260	O 267	S 10	0	0	0
1	L	187	Total 1374	C 857	N 250	O 258	S 9	0	0	0
1	M	195	Total 1430	C 890	N 261	O 269	S 10	0	0	0

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q0ZNA6
A	26	ARG	LYS	variant	UNP Q0ZNA6
A	181	ALA	-	expression tag	UNP Q0ZNA6
A	182	SER	-	expression tag	UNP Q0ZNA6
A	216	LYS	-	expression tag	UNP Q0ZNA6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	-	expression tag	UNP Q0ZNA6
A	218	LYS	-	expression tag	UNP Q0ZNA6
A	219	LYS	-	expression tag	UNP Q0ZNA6
A	220	LYS	-	expression tag	UNP Q0ZNA6
A	221	GLY	-	expression tag	UNP Q0ZNA6
A	222	SER	-	expression tag	UNP Q0ZNA6
A	223	VAL	-	expression tag	UNP Q0ZNA6
A	224	VAL	-	expression tag	UNP Q0ZNA6
A	225	ILE	-	expression tag	UNP Q0ZNA6
A	226	VAL	-	expression tag	UNP Q0ZNA6
A	227	GLY	-	expression tag	UNP Q0ZNA6
A	228	ARG	-	expression tag	UNP Q0ZNA6
A	229	ILE	-	expression tag	UNP Q0ZNA6
A	230	ILE	-	expression tag	UNP Q0ZNA6
A	231	LEU	-	expression tag	UNP Q0ZNA6
A	232	SER	-	expression tag	UNP Q0ZNA6
A	233	GLY	-	expression tag	UNP Q0ZNA6
A	234	ARG	-	expression tag	UNP Q0ZNA6
A	235	LYS	-	expression tag	UNP Q0ZNA6
B	0	MET	-	initiating methionine	UNP Q0ZNA6
B	26	ARG	LYS	variant	UNP Q0ZNA6
B	181	ALA	-	expression tag	UNP Q0ZNA6
B	215	SER	-	expression tag	UNP Q0ZNA6
B	216	LYS	-	expression tag	UNP Q0ZNA6
B	217	LYS	-	expression tag	UNP Q0ZNA6
B	218	LYS	-	expression tag	UNP Q0ZNA6
B	219	LYS	-	expression tag	UNP Q0ZNA6
B	220	LYS	-	expression tag	UNP Q0ZNA6
B	221	GLY	-	expression tag	UNP Q0ZNA6
B	222	SER	-	expression tag	UNP Q0ZNA6
B	223	VAL	-	expression tag	UNP Q0ZNA6
B	224	VAL	-	expression tag	UNP Q0ZNA6
B	225	ILE	-	expression tag	UNP Q0ZNA6
B	226	VAL	-	expression tag	UNP Q0ZNA6
B	227	GLY	-	expression tag	UNP Q0ZNA6
B	228	ARG	-	expression tag	UNP Q0ZNA6
B	229	ILE	-	expression tag	UNP Q0ZNA6
B	230	ILE	-	expression tag	UNP Q0ZNA6
B	231	LEU	-	expression tag	UNP Q0ZNA6
B	232	SER	-	expression tag	UNP Q0ZNA6
B	233	GLY	-	expression tag	UNP Q0ZNA6
B	234	ARG	-	expression tag	UNP Q0ZNA6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	235	LYS	-	expression tag	UNP Q0ZNA6
C	0	MET	-	initiating methionine	UNP Q0ZNA6
C	26	ARG	LYS	variant	UNP Q0ZNA6
C	181	ALA	-	expression tag	UNP Q0ZNA6
C	182	SER	-	expression tag	UNP Q0ZNA6
C	183	LYS	-	expression tag	UNP Q0ZNA6
C	217	LYS	-	expression tag	UNP Q0ZNA6
C	218	LYS	-	expression tag	UNP Q0ZNA6
C	219	LYS	-	expression tag	UNP Q0ZNA6
C	220	LYS	-	expression tag	UNP Q0ZNA6
C	221	GLY	-	expression tag	UNP Q0ZNA6
C	222	SER	-	expression tag	UNP Q0ZNA6
C	223	VAL	-	expression tag	UNP Q0ZNA6
C	224	VAL	-	expression tag	UNP Q0ZNA6
C	225	ILE	-	expression tag	UNP Q0ZNA6
C	226	VAL	-	expression tag	UNP Q0ZNA6
C	227	GLY	-	expression tag	UNP Q0ZNA6
C	228	ARG	-	expression tag	UNP Q0ZNA6
C	229	ILE	-	expression tag	UNP Q0ZNA6
C	230	ILE	-	expression tag	UNP Q0ZNA6
C	231	LEU	-	expression tag	UNP Q0ZNA6
C	232	SER	-	expression tag	UNP Q0ZNA6
C	233	GLY	-	expression tag	UNP Q0ZNA6
C	234	ARG	-	expression tag	UNP Q0ZNA6
C	235	LYS	-	expression tag	UNP Q0ZNA6
D	0	MET	-	initiating methionine	UNP Q0ZNA6
D	26	ARG	LYS	variant	UNP Q0ZNA6
D	181	ALA	-	expression tag	UNP Q0ZNA6
D	182	SER	-	expression tag	UNP Q0ZNA6
D	183	LYS	-	expression tag	UNP Q0ZNA6
D	217	LYS	-	expression tag	UNP Q0ZNA6
D	218	LYS	-	expression tag	UNP Q0ZNA6
D	219	LYS	-	expression tag	UNP Q0ZNA6
D	220	LYS	-	expression tag	UNP Q0ZNA6
D	221	GLY	-	expression tag	UNP Q0ZNA6
D	222	SER	-	expression tag	UNP Q0ZNA6
D	223	VAL	-	expression tag	UNP Q0ZNA6
D	224	VAL	-	expression tag	UNP Q0ZNA6
D	225	ILE	-	expression tag	UNP Q0ZNA6
D	226	VAL	-	expression tag	UNP Q0ZNA6
D	227	GLY	-	expression tag	UNP Q0ZNA6
D	228	ARG	-	expression tag	UNP Q0ZNA6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	229	ILE	-	expression tag	UNP Q0ZNA6
D	230	ILE	-	expression tag	UNP Q0ZNA6
D	231	LEU	-	expression tag	UNP Q0ZNA6
D	232	SER	-	expression tag	UNP Q0ZNA6
D	233	GLY	-	expression tag	UNP Q0ZNA6
D	234	ARG	-	expression tag	UNP Q0ZNA6
D	235	LYS	-	expression tag	UNP Q0ZNA6
E	0	MET	-	initiating methionine	UNP Q0ZNA6
E	26	ARG	LYS	variant	UNP Q0ZNA6
E	214	ALA	-	expression tag	UNP Q0ZNA6
E	215	SER	-	expression tag	UNP Q0ZNA6
E	216	LYS	-	expression tag	UNP Q0ZNA6
E	217	LYS	-	expression tag	UNP Q0ZNA6
E	218	LYS	-	expression tag	UNP Q0ZNA6
E	219	LYS	-	expression tag	UNP Q0ZNA6
E	220	LYS	-	expression tag	UNP Q0ZNA6
E	221	GLY	-	expression tag	UNP Q0ZNA6
E	222	SER	-	expression tag	UNP Q0ZNA6
E	223	VAL	-	expression tag	UNP Q0ZNA6
E	224	VAL	-	expression tag	UNP Q0ZNA6
E	225	ILE	-	expression tag	UNP Q0ZNA6
E	226	VAL	-	expression tag	UNP Q0ZNA6
E	227	GLY	-	expression tag	UNP Q0ZNA6
E	228	ARG	-	expression tag	UNP Q0ZNA6
E	229	ILE	-	expression tag	UNP Q0ZNA6
E	230	ILE	-	expression tag	UNP Q0ZNA6
E	231	LEU	-	expression tag	UNP Q0ZNA6
E	232	SER	-	expression tag	UNP Q0ZNA6
E	233	GLY	-	expression tag	UNP Q0ZNA6
E	234	ARG	-	expression tag	UNP Q0ZNA6
E	235	LYS	-	expression tag	UNP Q0ZNA6
F	0	MET	-	initiating methionine	UNP Q0ZNA6
F	26	ARG	LYS	variant	UNP Q0ZNA6
F	181	ALA	-	expression tag	UNP Q0ZNA6
F	182	SER	-	expression tag	UNP Q0ZNA6
F	216	LYS	-	expression tag	UNP Q0ZNA6
F	217	LYS	-	expression tag	UNP Q0ZNA6
F	218	LYS	-	expression tag	UNP Q0ZNA6
F	219	LYS	-	expression tag	UNP Q0ZNA6
F	220	LYS	-	expression tag	UNP Q0ZNA6
F	221	GLY	-	expression tag	UNP Q0ZNA6
F	222	SER	-	expression tag	UNP Q0ZNA6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	223	VAL	-	expression tag	UNP Q0ZNA6
F	224	VAL	-	expression tag	UNP Q0ZNA6
F	225	ILE	-	expression tag	UNP Q0ZNA6
F	226	VAL	-	expression tag	UNP Q0ZNA6
F	227	GLY	-	expression tag	UNP Q0ZNA6
F	228	ARG	-	expression tag	UNP Q0ZNA6
F	229	ILE	-	expression tag	UNP Q0ZNA6
F	230	ILE	-	expression tag	UNP Q0ZNA6
F	231	LEU	-	expression tag	UNP Q0ZNA6
F	232	SER	-	expression tag	UNP Q0ZNA6
F	233	GLY	-	expression tag	UNP Q0ZNA6
F	234	ARG	-	expression tag	UNP Q0ZNA6
F	235	LYS	-	expression tag	UNP Q0ZNA6
G	0	MET	-	initiating methionine	UNP Q0ZNA6
G	26	ARG	LYS	variant	UNP Q0ZNA6
G	214	ALA	-	expression tag	UNP Q0ZNA6
G	215	SER	-	expression tag	UNP Q0ZNA6
G	216	LYS	-	expression tag	UNP Q0ZNA6
G	217	LYS	-	expression tag	UNP Q0ZNA6
G	218	LYS	-	expression tag	UNP Q0ZNA6
G	219	LYS	-	expression tag	UNP Q0ZNA6
G	220	LYS	-	expression tag	UNP Q0ZNA6
G	221	GLY	-	expression tag	UNP Q0ZNA6
G	222	SER	-	expression tag	UNP Q0ZNA6
G	223	VAL	-	expression tag	UNP Q0ZNA6
G	224	VAL	-	expression tag	UNP Q0ZNA6
G	225	ILE	-	expression tag	UNP Q0ZNA6
G	226	VAL	-	expression tag	UNP Q0ZNA6
G	227	GLY	-	expression tag	UNP Q0ZNA6
G	228	ARG	-	expression tag	UNP Q0ZNA6
G	229	ILE	-	expression tag	UNP Q0ZNA6
G	230	ILE	-	expression tag	UNP Q0ZNA6
G	231	LEU	-	expression tag	UNP Q0ZNA6
G	232	SER	-	expression tag	UNP Q0ZNA6
G	233	GLY	-	expression tag	UNP Q0ZNA6
G	234	ARG	-	expression tag	UNP Q0ZNA6
G	235	LYS	-	expression tag	UNP Q0ZNA6
H	0	MET	-	initiating methionine	UNP Q0ZNA6
H	26	ARG	LYS	variant	UNP Q0ZNA6
H	181	ALA	-	expression tag	UNP Q0ZNA6
H	182	SER	-	expression tag	UNP Q0ZNA6
H	216	LYS	-	expression tag	UNP Q0ZNA6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	217	LYS	-	expression tag	UNP Q0ZNA6
H	218	LYS	-	expression tag	UNP Q0ZNA6
H	219	LYS	-	expression tag	UNP Q0ZNA6
H	220	LYS	-	expression tag	UNP Q0ZNA6
H	221	GLY	-	expression tag	UNP Q0ZNA6
H	222	SER	-	expression tag	UNP Q0ZNA6
H	223	VAL	-	expression tag	UNP Q0ZNA6
H	224	VAL	-	expression tag	UNP Q0ZNA6
H	225	ILE	-	expression tag	UNP Q0ZNA6
H	226	VAL	-	expression tag	UNP Q0ZNA6
H	227	GLY	-	expression tag	UNP Q0ZNA6
H	228	ARG	-	expression tag	UNP Q0ZNA6
H	229	ILE	-	expression tag	UNP Q0ZNA6
H	230	ILE	-	expression tag	UNP Q0ZNA6
H	231	LEU	-	expression tag	UNP Q0ZNA6
H	232	SER	-	expression tag	UNP Q0ZNA6
H	233	GLY	-	expression tag	UNP Q0ZNA6
H	234	ARG	-	expression tag	UNP Q0ZNA6
H	235	LYS	-	expression tag	UNP Q0ZNA6
J	0	MET	-	initiating methionine	UNP Q0ZNA6
J	26	ARG	LYS	variant	UNP Q0ZNA6
J	181	ALA	-	expression tag	UNP Q0ZNA6
J	215	SER	-	expression tag	UNP Q0ZNA6
J	216	LYS	-	expression tag	UNP Q0ZNA6
J	217	LYS	-	expression tag	UNP Q0ZNA6
J	218	LYS	-	expression tag	UNP Q0ZNA6
J	219	LYS	-	expression tag	UNP Q0ZNA6
J	220	LYS	-	expression tag	UNP Q0ZNA6
J	221	GLY	-	expression tag	UNP Q0ZNA6
J	222	SER	-	expression tag	UNP Q0ZNA6
J	223	VAL	-	expression tag	UNP Q0ZNA6
J	224	VAL	-	expression tag	UNP Q0ZNA6
J	225	ILE	-	expression tag	UNP Q0ZNA6
J	226	VAL	-	expression tag	UNP Q0ZNA6
J	227	GLY	-	expression tag	UNP Q0ZNA6
J	228	ARG	-	expression tag	UNP Q0ZNA6
J	229	ILE	-	expression tag	UNP Q0ZNA6
J	230	ILE	-	expression tag	UNP Q0ZNA6
J	231	LEU	-	expression tag	UNP Q0ZNA6
J	232	SER	-	expression tag	UNP Q0ZNA6
J	233	GLY	-	expression tag	UNP Q0ZNA6
J	234	ARG	-	expression tag	UNP Q0ZNA6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	235	LYS	-	expression tag	UNP Q0ZNA6
K	0	MET	-	initiating methionine	UNP Q0ZNA6
K	26	ARG	LYS	variant	UNP Q0ZNA6
K	181	ALA	-	expression tag	UNP Q0ZNA6
K	215	SER	-	expression tag	UNP Q0ZNA6
K	216	LYS	-	expression tag	UNP Q0ZNA6
K	217	LYS	-	expression tag	UNP Q0ZNA6
K	218	LYS	-	expression tag	UNP Q0ZNA6
K	219	LYS	-	expression tag	UNP Q0ZNA6
K	220	LYS	-	expression tag	UNP Q0ZNA6
K	221	GLY	-	expression tag	UNP Q0ZNA6
K	222	SER	-	expression tag	UNP Q0ZNA6
K	223	VAL	-	expression tag	UNP Q0ZNA6
K	224	VAL	-	expression tag	UNP Q0ZNA6
K	225	ILE	-	expression tag	UNP Q0ZNA6
K	226	VAL	-	expression tag	UNP Q0ZNA6
K	227	GLY	-	expression tag	UNP Q0ZNA6
K	228	ARG	-	expression tag	UNP Q0ZNA6
K	229	ILE	-	expression tag	UNP Q0ZNA6
K	230	ILE	-	expression tag	UNP Q0ZNA6
K	231	LEU	-	expression tag	UNP Q0ZNA6
K	232	SER	-	expression tag	UNP Q0ZNA6
K	233	GLY	-	expression tag	UNP Q0ZNA6
K	234	ARG	-	expression tag	UNP Q0ZNA6
K	235	LYS	-	expression tag	UNP Q0ZNA6
L	0	MET	-	initiating methionine	UNP Q0ZNA6
L	26	ARG	LYS	variant	UNP Q0ZNA6
L	214	ALA	-	expression tag	UNP Q0ZNA6
L	215	SER	-	expression tag	UNP Q0ZNA6
L	216	LYS	-	expression tag	UNP Q0ZNA6
L	217	LYS	-	expression tag	UNP Q0ZNA6
L	218	LYS	-	expression tag	UNP Q0ZNA6
L	219	LYS	-	expression tag	UNP Q0ZNA6
L	220	LYS	-	expression tag	UNP Q0ZNA6
L	221	GLY	-	expression tag	UNP Q0ZNA6
L	222	SER	-	expression tag	UNP Q0ZNA6
L	223	VAL	-	expression tag	UNP Q0ZNA6
L	224	VAL	-	expression tag	UNP Q0ZNA6
L	225	ILE	-	expression tag	UNP Q0ZNA6
L	226	VAL	-	expression tag	UNP Q0ZNA6
L	227	GLY	-	expression tag	UNP Q0ZNA6
L	228	ARG	-	expression tag	UNP Q0ZNA6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	229	ILE	-	expression tag	UNP Q0ZNA6
L	230	ILE	-	expression tag	UNP Q0ZNA6
L	231	LEU	-	expression tag	UNP Q0ZNA6
L	232	SER	-	expression tag	UNP Q0ZNA6
L	233	GLY	-	expression tag	UNP Q0ZNA6
L	234	ARG	-	expression tag	UNP Q0ZNA6
L	235	LYS	-	expression tag	UNP Q0ZNA6
M	0	MET	-	initiating methionine	UNP Q0ZNA6
M	26	ARG	LYS	variant	UNP Q0ZNA6
M	181	ALA	-	expression tag	UNP Q0ZNA6
M	182	SER	-	expression tag	UNP Q0ZNA6
M	216	LYS	-	expression tag	UNP Q0ZNA6
M	217	LYS	-	expression tag	UNP Q0ZNA6
M	218	LYS	-	expression tag	UNP Q0ZNA6
M	219	LYS	-	expression tag	UNP Q0ZNA6
M	220	LYS	-	expression tag	UNP Q0ZNA6
M	221	GLY	-	expression tag	UNP Q0ZNA6
M	222	SER	-	expression tag	UNP Q0ZNA6
M	223	VAL	-	expression tag	UNP Q0ZNA6
M	224	VAL	-	expression tag	UNP Q0ZNA6
M	225	ILE	-	expression tag	UNP Q0ZNA6
M	226	VAL	-	expression tag	UNP Q0ZNA6
M	227	GLY	-	expression tag	UNP Q0ZNA6
M	228	ARG	-	expression tag	UNP Q0ZNA6
M	229	ILE	-	expression tag	UNP Q0ZNA6
M	230	ILE	-	expression tag	UNP Q0ZNA6
M	231	LEU	-	expression tag	UNP Q0ZNA6
M	232	SER	-	expression tag	UNP Q0ZNA6
M	233	GLY	-	expression tag	UNP Q0ZNA6
M	234	ARG	-	expression tag	UNP Q0ZNA6
M	235	LYS	-	expression tag	UNP Q0ZNA6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Zn 1	0	0
2	J	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	K	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0
2	L	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0
2	M	1	Total 1	Zn 1	0	0

- Molecule 3 is (4R,6S,7Z,15S,17S)-17-[({7-methoxy-2-[4-(propan-2-yl)-1,3-thiazol-2-yl]quinolin-4-yl}oxy)methyl]-13-methyl-N-[(1-methylcyclopropyl)sulfonyl]-2,14-dioxo-1,3,13-triazatricyclo[13.2.0.0 4,6]heptadec-7-ene-4-carboxamide (three-letter code: 3EO) (formula: $C_{37}H_{46}N_6O_7S_2$).
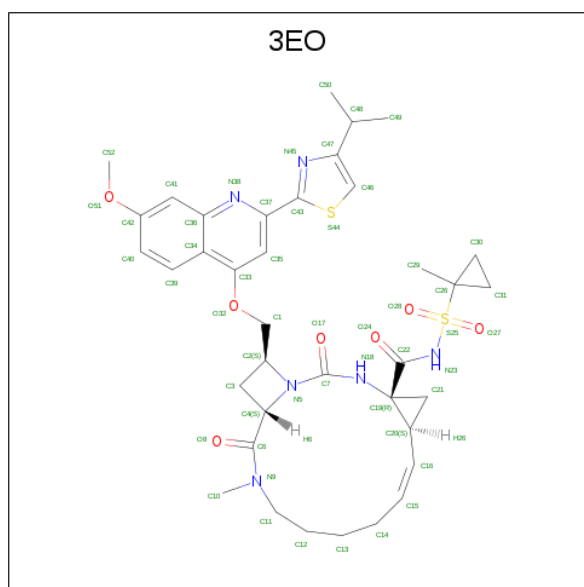
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 52	C 37	N 6	O 7	S 2	0	0
3	B	1	Total 52	C 37	N 6	O 7	S 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 52	C 37	N 6	O 7	S 2	0	0
3	D	1	Total 52	C 37	N 6	O 7	S 2	0	0
3	E	1	Total 52	C 37	N 6	O 7	S 2	0	0
3	F	1	Total 52	C 37	N 6	O 7	S 2	0	0
3	G	1	Total 52	C 37	N 6	O 7	S 2	0	0
3	H	1	Total 52	C 37	N 6	O 7	S 2	0	0
3	J	1	Total 52	C 37	N 6	O 7	S 2	0	0
3	K	1	Total 52	C 37	N 6	O 7	S 2	0	0
3	L	1	Total 52	C 37	N 6	O 7	S 2	0	0
3	M	1	Total 52	C 37	N 6	O 7	S 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total 2	Cl 2	0	0
4	H	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	C	2	Total 2	Cl 2	0	0
4	A	1	Total 1	Cl 1	0	0
4	F	3	Total 3	Cl 3	0	0
4	M	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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:

- Molecule 1: NS3 protease

Chain B:
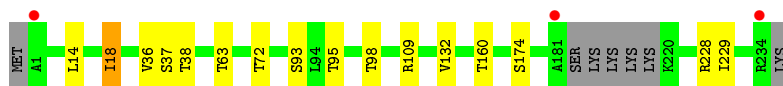
- Molecule 1: NS3 protease

Chain C:

- Molecule 1: NS3 protease

Chain D:

- Molecule 1: NS3 protease

Chain E:

- Molecule 1: NS3 protease
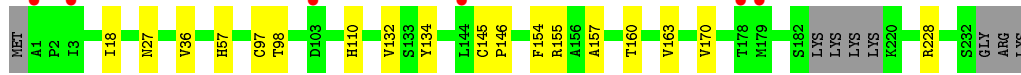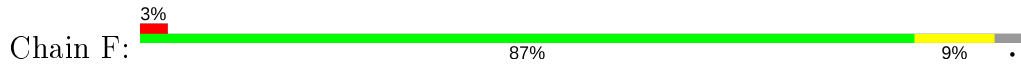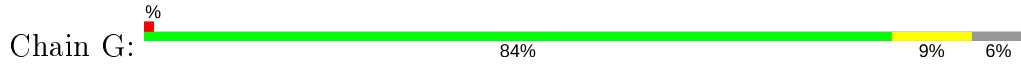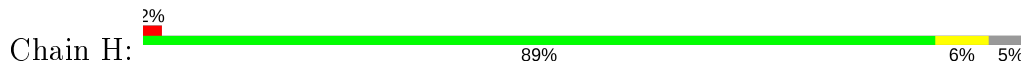
Chain F:

• Molecule 1: NS3 protease

Chain G:

• Molecule 1: NS3 protease

Chain H:

• Molecule 1: NS3 protease

Chain J:

• Molecule 1: NS3 protease

Chain K:

• Molecule 1: NS3 protease

Chain L:

• Molecule 1: NS3 protease

Chain M:
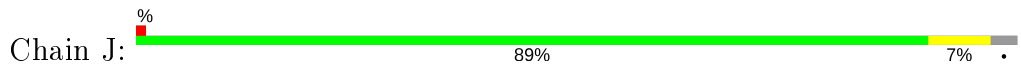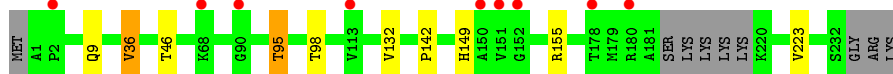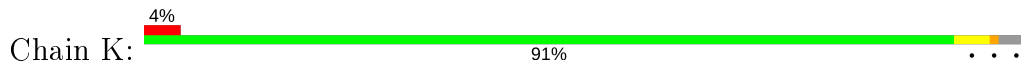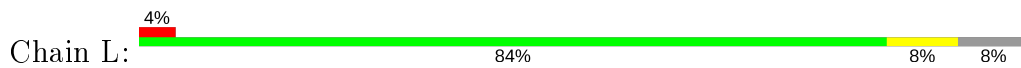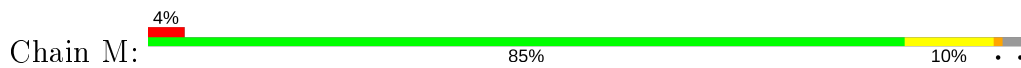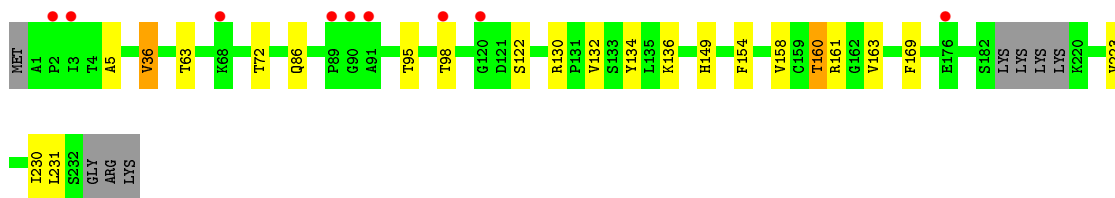
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	140.69Å 143.20Å 240.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.84 49.12 – 2.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-2.84) 99.7 (49.12-2.84)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.267 0.214 , 0.258	Depositor DCC
R_{free} test set	997 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.5	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.059 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17686	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3EO, ZN, CL

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	0.36	0/1450	0.56	0/1971
1	B	0.38	0/1464	0.57	0/1990
1	C	0.35	0/1464	0.57	0/1990
1	D	0.36	0/1459	0.54	0/1982
1	E	0.35	0/1418	0.56	0/1930
1	F	0.34	0/1455	0.55	0/1979
1	G	0.35	0/1418	0.57	0/1930
1	H	0.35	0/1442	0.54	0/1960
1	J	0.36	0/1464	0.55	0/1990
1	K	0.33	0/1449	0.53	0/1971
1	L	0.33	0/1398	0.53	0/1901
1	M	0.36	0/1455	0.56	0/1979
All	All	0.35	0/17336	0.55	0/23573

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1425	0	1448	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1439	0	1466	9	0
1	C	1439	0	1468	13	0
1	D	1434	0	1462	16	0
1	E	1393	0	1416	10	0
1	F	1430	0	1456	14	0
1	G	1393	0	1416	7	0
1	H	1418	0	1441	8	0
1	J	1439	0	1466	7	0
1	K	1424	0	1451	6	0
1	L	1374	0	1396	11	0
1	M	1430	0	1455	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	2	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	2	0
2	M	1	0	0	0	0
3	A	52	0	45	4	0
3	B	52	0	45	3	0
3	C	52	0	45	3	0
3	D	52	0	45	4	0
3	E	52	0	45	4	0
3	F	52	0	45	4	0
3	G	52	0	45	2	0
3	H	52	0	45	3	0
3	J	52	0	45	5	0
3	K	52	0	45	2	0
3	L	52	0	45	3	0
3	M	52	0	45	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	H	1	0	0	0	0
4	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	1	0	0	0	0
All	All	17686	0	17881	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 3.

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:L:97:CYS:SG	2:L:301:ZN:ZN	1.52	0.98
3:B:302:3EO:H32	1:E:132:VAL:HG11	1.62	0.80
1:F:97:CYS:SG	2:F:301:ZN:ZN	1.72	0.79
3:G:302:3EO:H32	1:M:132:VAL:HG11	1.68	0.76
1:B:132:VAL:HG11	3:C:302:3EO:H32	1.68	0.75

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	190/203 (94%)	182 (96%)	8 (4%)	0	100	100
1	B	192/203 (95%)	185 (96%)	7 (4%)	0	100	100
1	C	192/203 (95%)	187 (97%)	5 (3%)	0	100	100
1	D	191/203 (94%)	188 (98%)	3 (2%)	0	100	100
1	E	186/203 (92%)	179 (96%)	6 (3%)	1 (0%)	29	51
1	F	191/203 (94%)	185 (97%)	6 (3%)	0	100	100
1	G	186/203 (92%)	181 (97%)	4 (2%)	1 (0%)	29	51
1	H	189/203 (93%)	183 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	192/203 (95%)	188 (98%)	4 (2%)	0	100	100
1	K	190/203 (94%)	184 (97%)	6 (3%)	0	100	100
1	L	183/203 (90%)	176 (96%)	7 (4%)	0	100	100
1	M	191/203 (94%)	183 (96%)	8 (4%)	0	100	100
All	All	2273/2436 (93%)	2201 (97%)	70 (3%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	2	PRO
1	E	132	VAL

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	158/165 (96%)	152 (96%)	6 (4%)	33	59
1	B	158/165 (96%)	150 (95%)	8 (5%)	24	45
1	C	159/165 (96%)	154 (97%)	5 (3%)	40	64
1	D	159/165 (96%)	152 (96%)	7 (4%)	28	53
1	E	154/165 (93%)	149 (97%)	5 (3%)	39	63
1	F	158/165 (96%)	155 (98%)	3 (2%)	57	77
1	G	154/165 (93%)	148 (96%)	6 (4%)	32	58
1	H	157/165 (95%)	155 (99%)	2 (1%)	69	84
1	J	158/165 (96%)	152 (96%)	6 (4%)	33	59
1	K	157/165 (95%)	154 (98%)	3 (2%)	57	77
1	L	152/165 (92%)	148 (97%)	4 (3%)	46	70
1	M	158/165 (96%)	152 (96%)	6 (4%)	33	59
All	All	1882/1980 (95%)	1821 (97%)	61 (3%)	39	63

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	98	THR
1	G	93	SER
1	M	86	GLN
1	E	130	ARG
1	E	177	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	8	GLN
1	G	34	GLN
1	M	27	ASN
1	F	27	ASN
1	F	34	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 23 are monoatomic - leaving 12 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	3EO	G	302	-	51,58,58	2.29	11 (21%)	62,89,89	2.53	21 (33%)
3	3EO	A	302	-	51,58,58	2.31	11 (21%)	62,89,89	2.28	17 (27%)
3	3EO	C	302	-	51,58,58	2.25	11 (21%)	62,89,89	2.51	21 (33%)
3	3EO	B	302	-	51,58,58	2.28	12 (23%)	62,89,89	2.47	20 (32%)
3	3EO	M	302	-	51,58,58	2.24	13 (25%)	62,89,89	2.41	22 (35%)
3	3EO	K	302	-	51,58,58	2.30	12 (23%)	62,89,89	2.52	21 (33%)
3	3EO	J	302	-	51,58,58	2.24	11 (21%)	62,89,89	2.45	22 (35%)
3	3EO	D	302	-	51,58,58	2.30	11 (21%)	62,89,89	2.43	21 (33%)
3	3EO	F	302	-	51,58,58	2.26	11 (21%)	62,89,89	2.27	21 (33%)
3	3EO	L	302	-	51,58,58	2.33	12 (23%)	62,89,89	2.39	21 (33%)
3	3EO	H	302	-	51,58,58	2.28	12 (23%)	62,89,89	2.51	20 (32%)
3	3EO	E	302	-	51,58,58	2.25	12 (23%)	62,89,89	2.38	19 (30%)

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	3EO	G	302	-	-	9/44/85/85	0/6/7/7
3	3EO	A	302	-	-	4/44/85/85	0/6/7/7
3	3EO	C	302	-	-	8/44/85/85	0/6/7/7
3	3EO	B	302	-	-	8/44/85/85	0/6/7/7
3	3EO	M	302	-	-	7/44/85/85	0/6/7/7
3	3EO	K	302	-	-	14/44/85/85	0/6/7/7
3	3EO	J	302	-	-	7/44/85/85	0/6/7/7
3	3EO	D	302	-	-	3/44/85/85	0/6/7/7
3	3EO	F	302	-	-	6/44/85/85	0/6/7/7
3	3EO	L	302	-	-	8/44/85/85	0/6/7/7
3	3EO	H	302	-	-	9/44/85/85	0/6/7/7
3	3EO	E	302	-	-	8/44/85/85	0/6/7/7

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	3EO	C43-S44	-10.37	1.59	1.73
3	L	302	3EO	C43-S44	-10.25	1.59	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	3EO	C43-S44	-10.10	1.59	1.73
3	G	302	3EO	C43-S44	-10.09	1.59	1.73
3	K	302	3EO	C43-S44	-9.95	1.59	1.73

The worst 5 of 246 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	3EO	C3-C4-N5	7.32	95.05	88.20
3	H	302	3EO	C3-C4-N5	7.19	94.92	88.20
3	F	302	3EO	C3-C4-N5	7.13	94.87	88.20
3	C	302	3EO	C31-C26-C30	7.00	63.20	59.54
3	D	302	3EO	C3-C4-N5	6.99	94.74	88.20

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	3EO	C12-C11-N9-C6
3	B	302	3EO	C12-C11-N9-C10
3	B	302	3EO	N38-C37-C43-N45
3	B	302	3EO	C22-N23-S25-C26
3	F	302	3EO	C3-C4-C6-N9

There are no ring outliers.

12 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	302	3EO	2	0
3	A	302	3EO	4	0
3	C	302	3EO	3	0
3	B	302	3EO	3	0
3	M	302	3EO	4	0
3	K	302	3EO	2	0
3	J	302	3EO	5	0
3	D	302	3EO	4	0
3	F	302	3EO	4	0
3	L	302	3EO	3	0
3	H	302	3EO	3	0
3	E	302	3EO	4	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 3EO G 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO C 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO M 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO K 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO J 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO D 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO F 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO L 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO H 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3EO E 302

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 (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	194/203 (95%)	-0.09	0	100	100	48, 64, 91, 123	0
1	B	196/203 (96%)	-0.14	3 (1%)	73	70	43, 60, 85, 117	0
1	C	196/203 (96%)	0.02	2 (1%)	82	79	47, 62, 92, 113	0
1	D	195/203 (96%)	-0.01	4 (2%)	63	58	47, 64, 92, 124	0
1	E	190/203 (93%)	-0.02	3 (1%)	72	68	42, 63, 97, 122	0
1	F	195/203 (96%)	0.15	6 (3%)	49	42	45, 67, 104, 130	0
1	G	190/203 (93%)	0.01	2 (1%)	80	78	40, 64, 91, 126	0
1	H	193/203 (95%)	-0.09	5 (2%)	56	51	48, 74, 111, 135	0
1	J	196/203 (96%)	-0.03	3 (1%)	73	70	50, 72, 97, 120	0
1	K	194/203 (95%)	0.38	9 (4%)	32	25	55, 84, 114, 142	0
1	L	187/203 (92%)	0.43	9 (4%)	30	23	54, 87, 113, 130	0
1	M	195/203 (96%)	0.21	9 (4%)	32	25	46, 70, 105, 129	0
All	All	2321/2436 (95%)	0.07	55 (2%)	59	54	40, 69, 107, 142	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	174	SER	5.2
1	M	90	GLY	4.9
1	G	1	ALA	4.6
1	L	230	ILE	4.5
1	B	1	ALA	4.2

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(Å^2)	Q<0.9
4	CL	F	303	1/1	0.82	0.14	69,69,69,69	0
4	CL	F	304	1/1	0.86	0.08	62,62,62,62	0
4	CL	B	303	1/1	0.87	0.14	68,68,68,68	0
4	CL	C	304	1/1	0.89	0.17	64,64,64,64	0
2	ZN	H	301	1/1	0.89	0.15	120,120,120,120	0
4	CL	E	304	1/1	0.89	0.09	59,59,59,59	0
2	ZN	K	301	1/1	0.91	0.09	123,123,123,123	0
4	CL	M	303	1/1	0.92	0.17	54,54,54,54	0
4	CL	F	305	1/1	0.93	0.10	55,55,55,55	0
4	CL	A	303	1/1	0.93	0.17	55,55,55,55	0
4	CL	H	303	1/1	0.93	0.09	59,59,59,59	0
2	ZN	L	301	1/1	0.94	0.10	120,120,120,120	0
3	3EO	K	302	52/52	0.94	0.19	59,64,72,73	0
2	ZN	D	301	1/1	0.94	0.17	94,94,94,94	0
3	3EO	J	302	52/52	0.95	0.20	55,59,64,65	0
3	3EO	M	302	52/52	0.95	0.18	45,56,70,71	0
3	3EO	L	302	52/52	0.95	0.21	63,66,74,74	0
2	ZN	J	301	1/1	0.96	0.14	92,92,92,92	0
4	CL	C	303	1/1	0.96	0.11	55,55,55,55	0
4	CL	E	303	1/1	0.96	0.17	46,46,46,46	0
2	ZN	F	301	1/1	0.96	0.10	96,96,96,96	0
3	3EO	F	302	52/52	0.97	0.17	49,53,58,59	0
3	3EO	B	302	52/52	0.97	0.19	41,51,55,56	0
3	3EO	H	302	52/52	0.97	0.17	51,55,58,59	0
2	ZN	G	301	1/1	0.97	0.09	85,85,85,85	0
2	ZN	C	301	1/1	0.97	0.11	86,86,86,86	0
3	3EO	C	302	52/52	0.97	0.17	48,56,60,61	0
3	3EO	A	302	52/52	0.97	0.18	43,49,51,53	0
3	3EO	D	302	52/52	0.97	0.18	46,53,60,61	0
3	3EO	E	302	52/52	0.97	0.18	45,51,56,57	0
2	ZN	A	301	1/1	0.98	0.11	80,80,80,80	0
3	3EO	G	302	52/52	0.98	0.20	47,51,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	ZN	B	301	1/1	0.99	0.18	77,77,77,77	0
2	ZN	M	301	1/1	0.99	0.10	77,77,77,77	0
2	ZN	E	301	1/1	0.99	0.11	53,53,53,53	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.
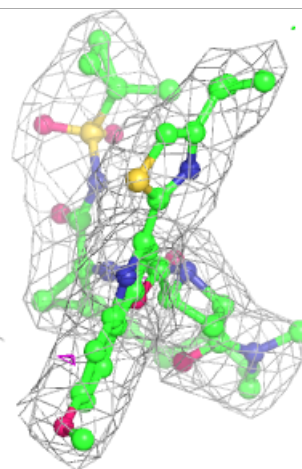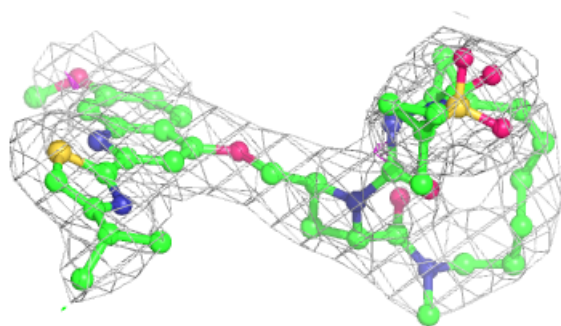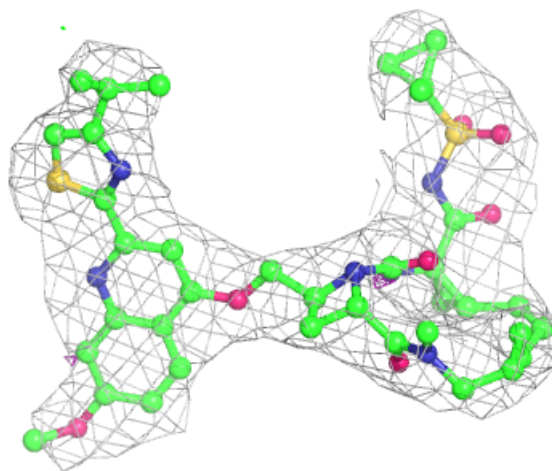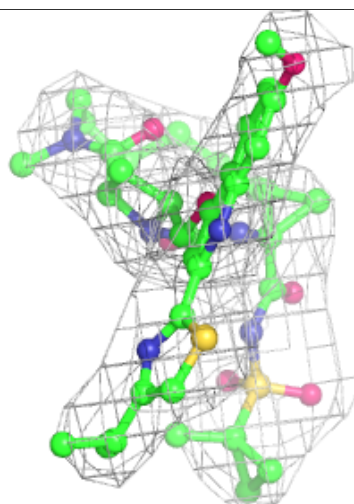
Electron density around 3EO K 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
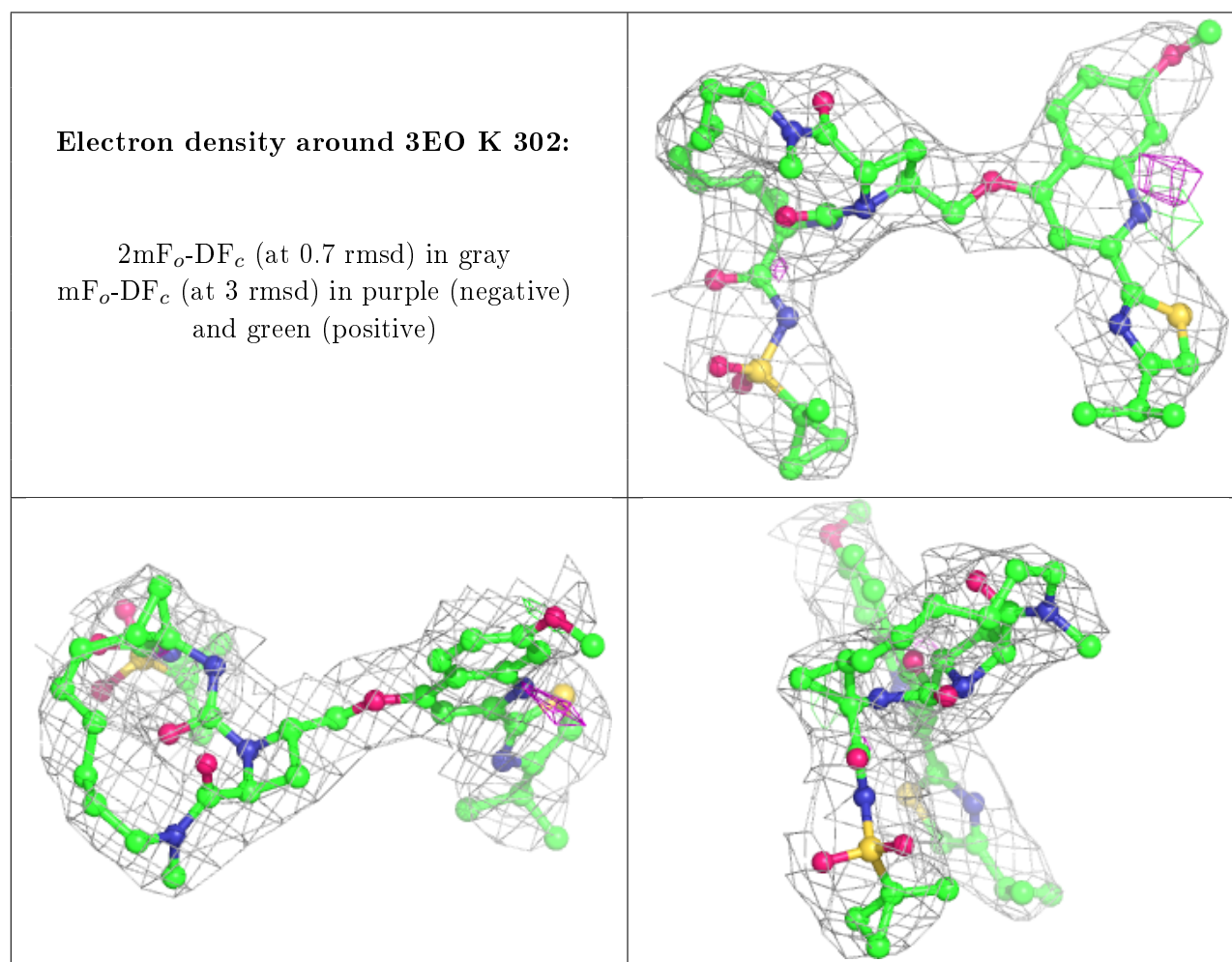
Electron density around 3EO J 302:

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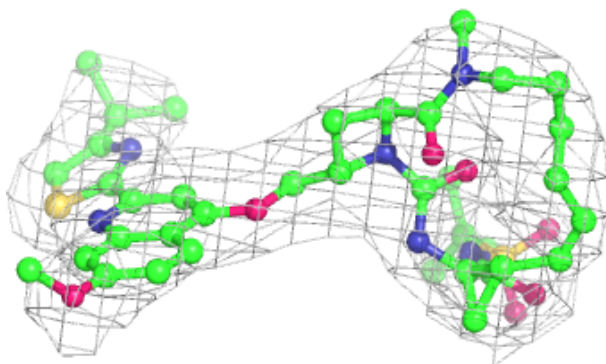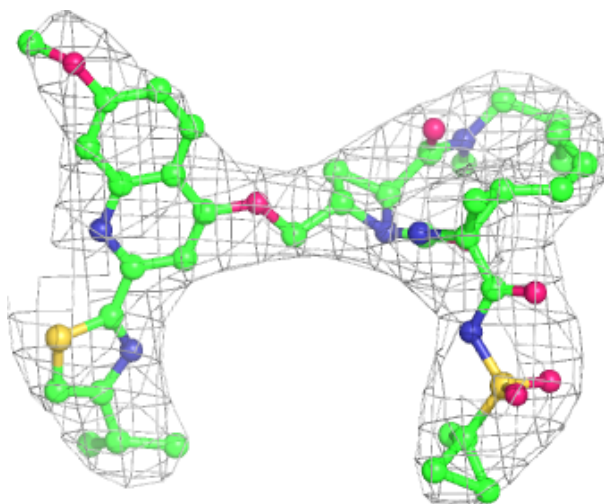and green (positive)

Electron density around 3EO M 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
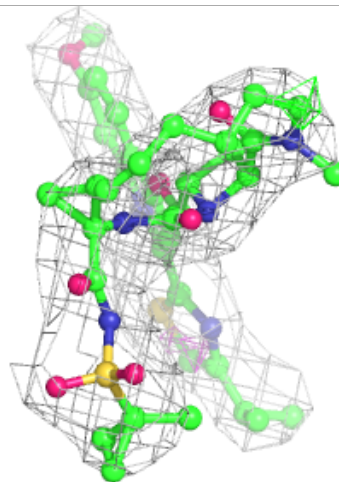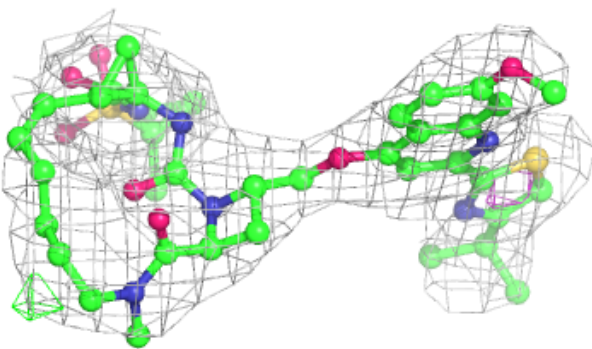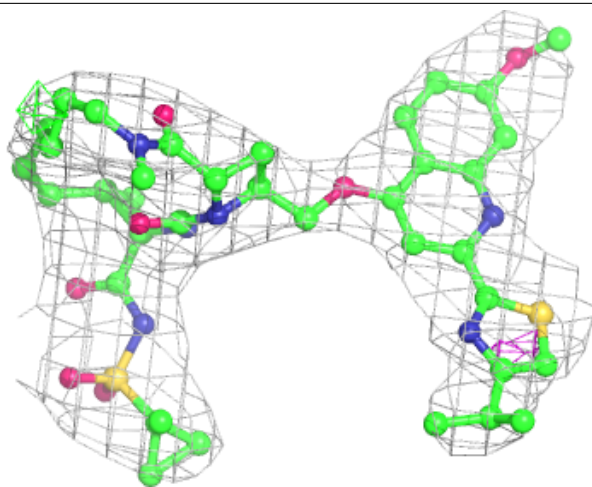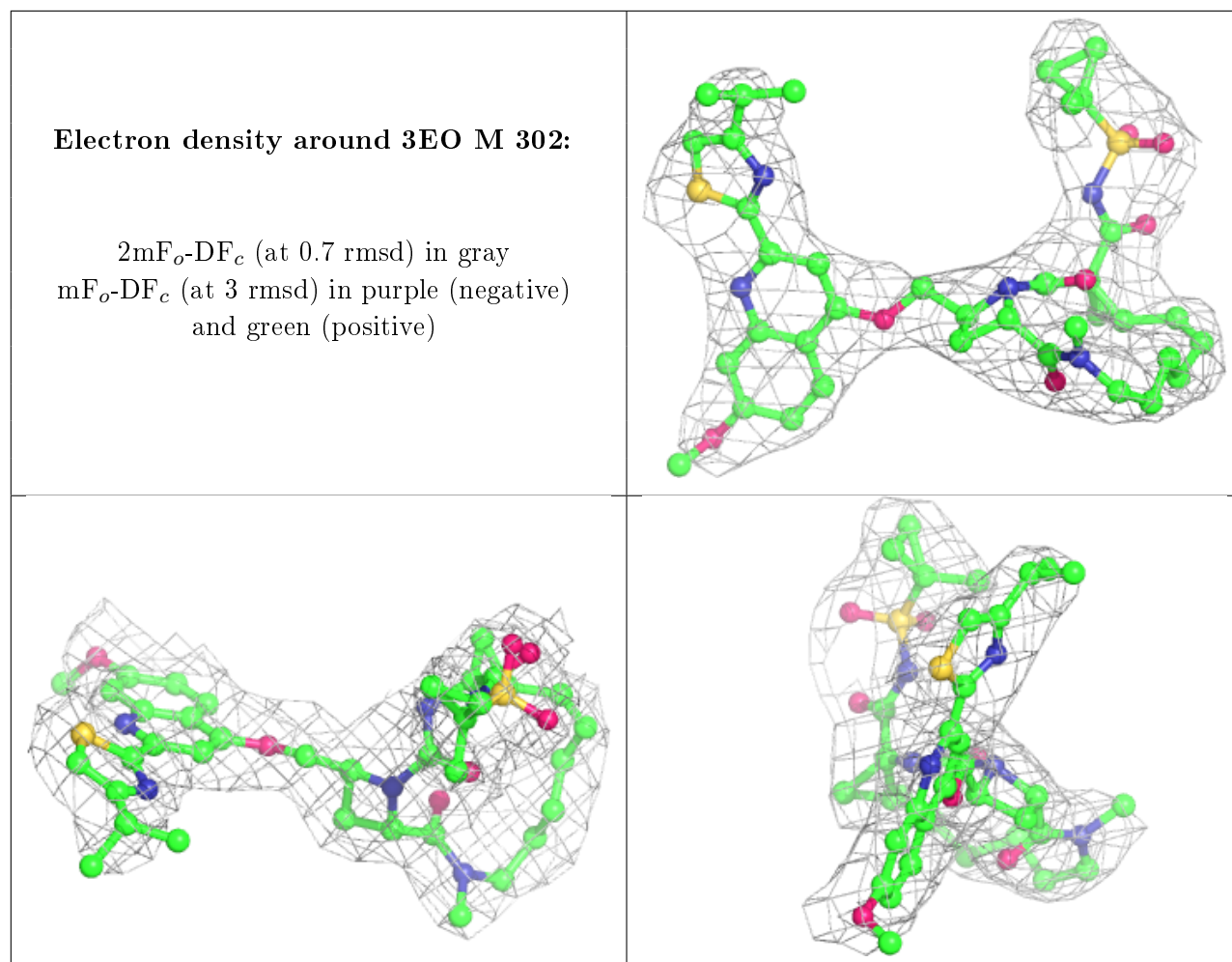
Electron density around 3EO L 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
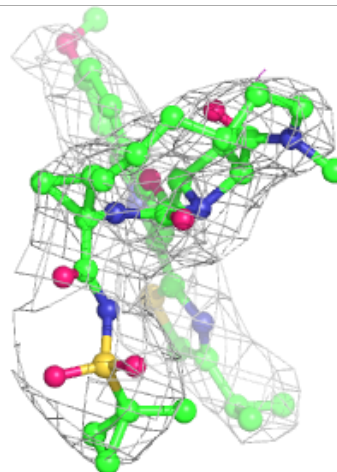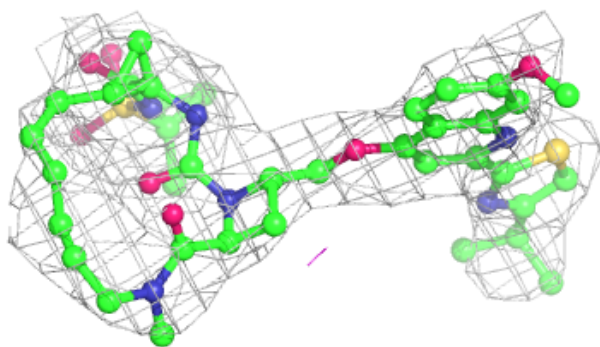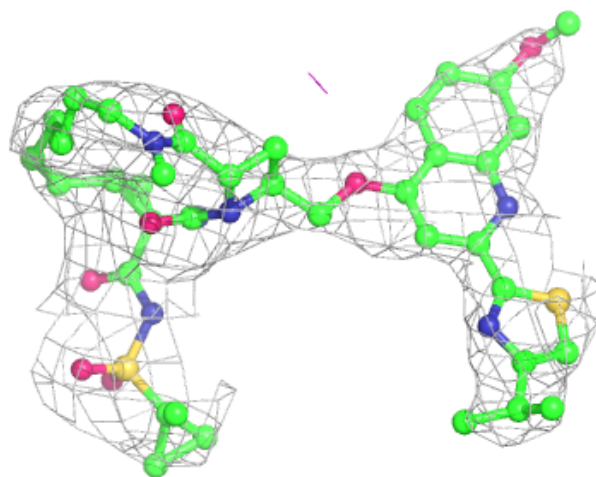
Electron density around 3EO F 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
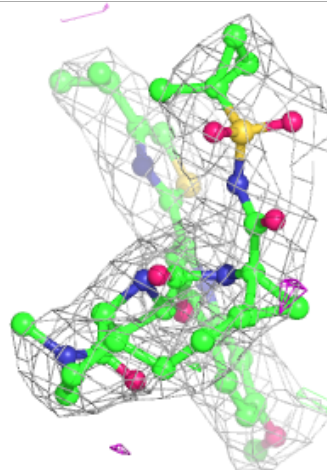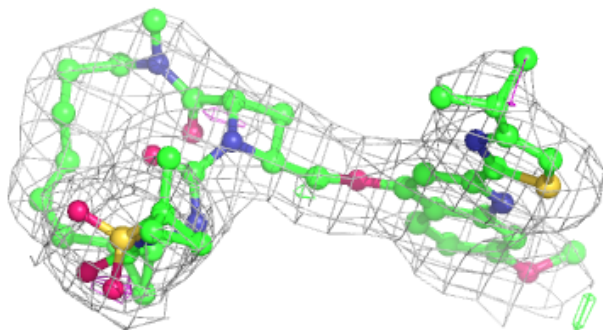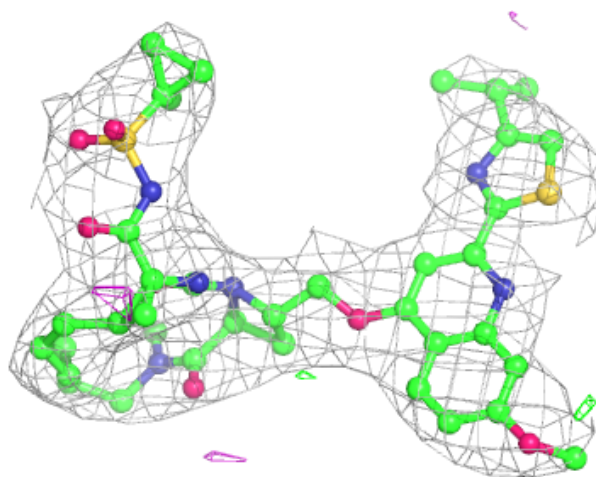
Electron density around 3EO B 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
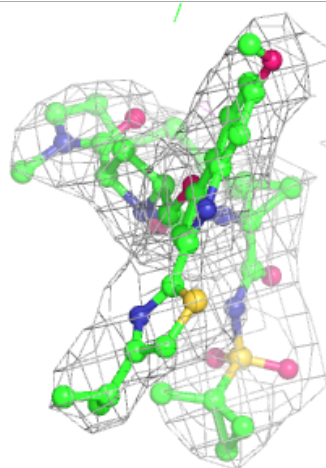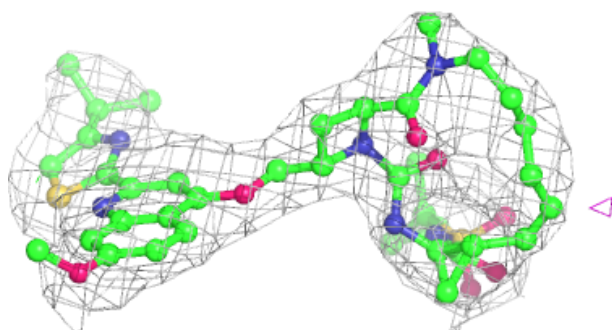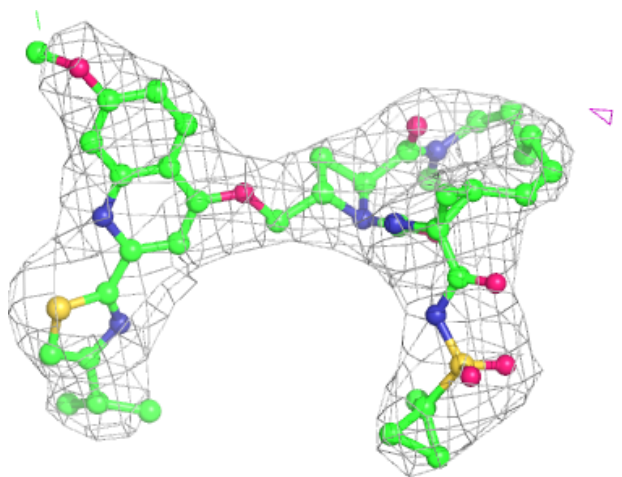
Electron density around 3EO H 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
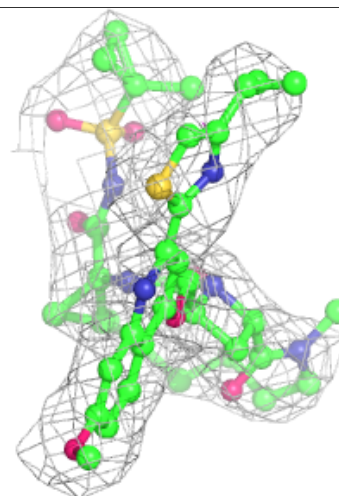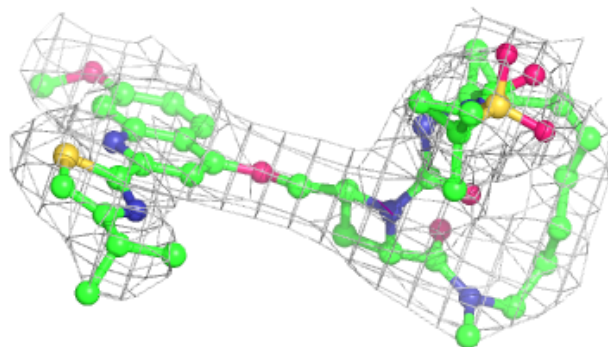mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
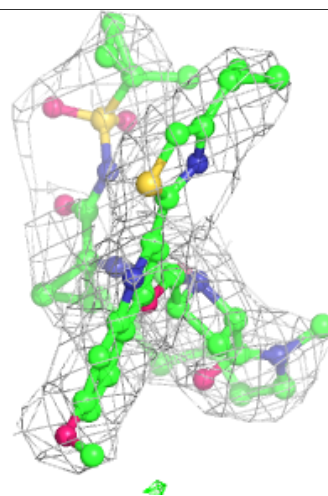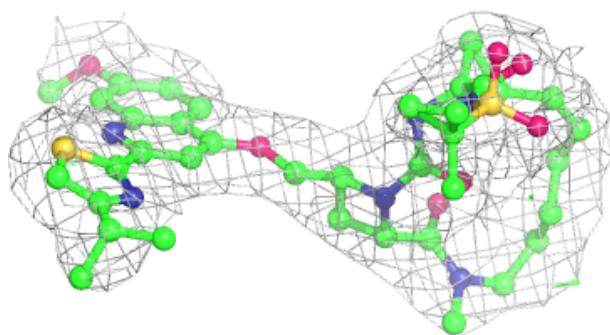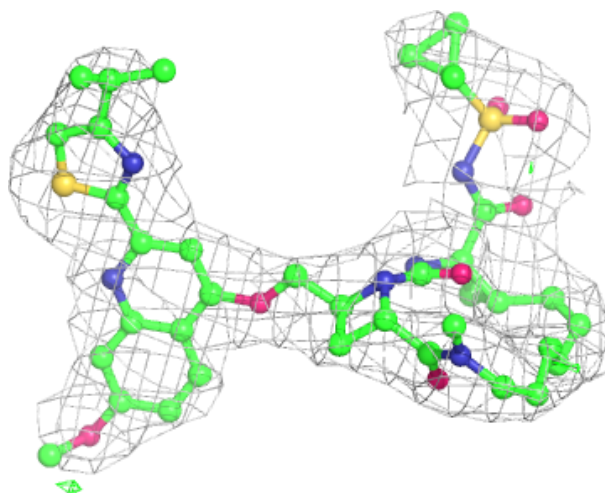
Electron density around 3EO C 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
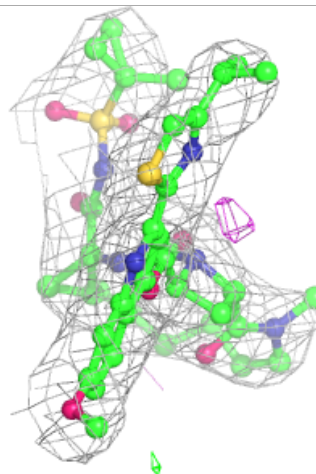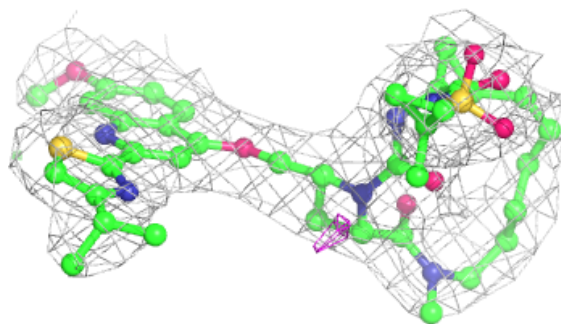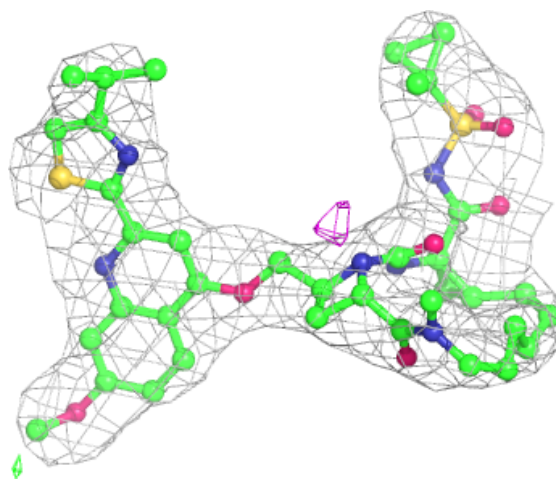
Electron density around 3EO A 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
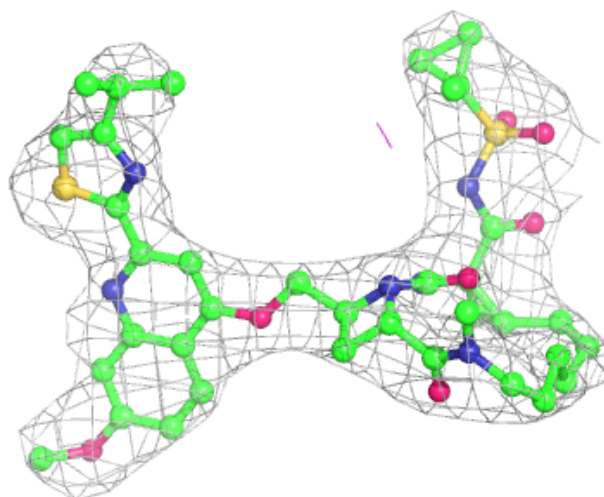and green (positive)
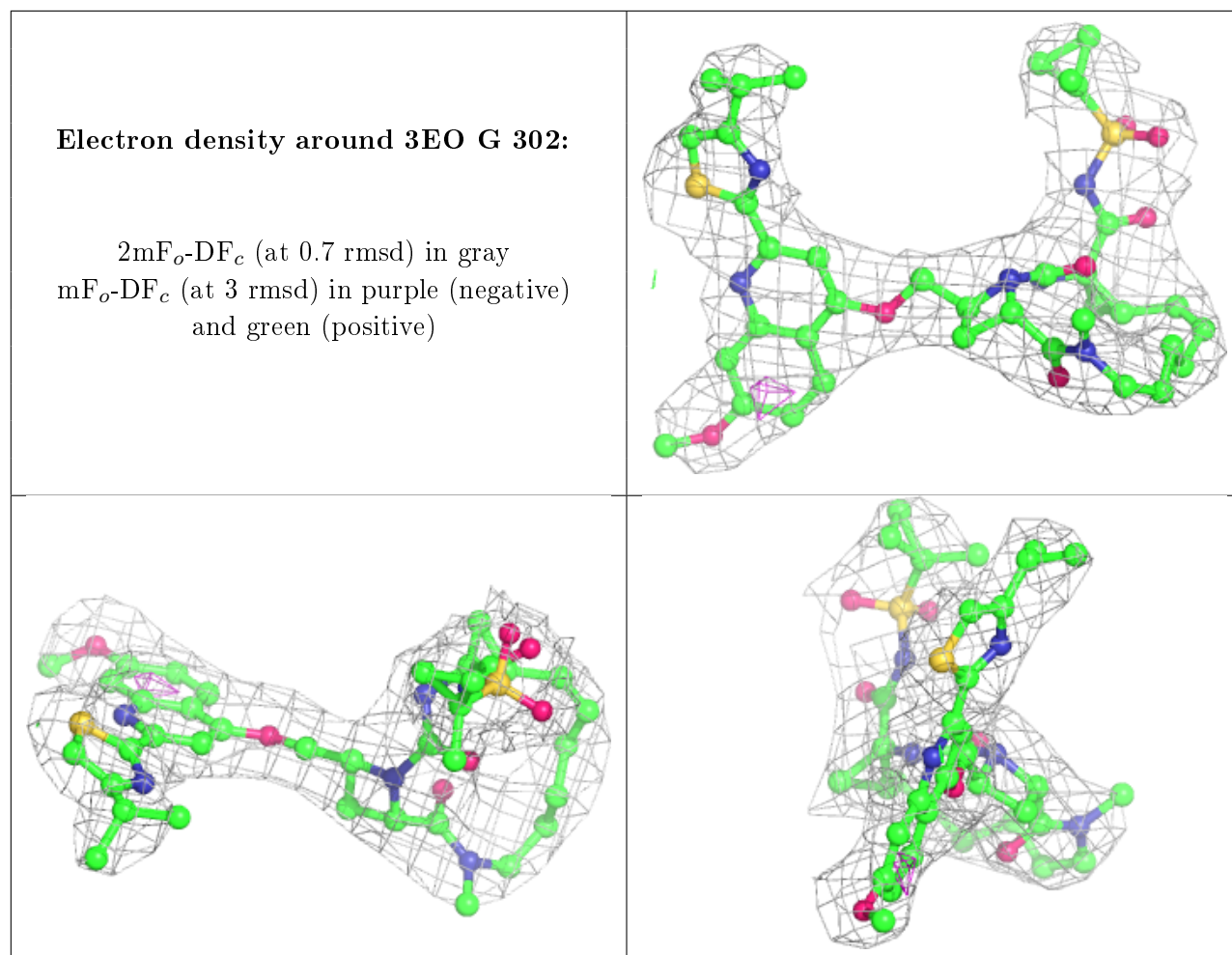
Electron density around 3EO D 302:

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

Electron density around 3EO E 302:

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

Electron density around 3EO G 302:

$2mF_o$-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.