



Full wwPDB X-ray Structure Validation 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)

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 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	:	2.13.1
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

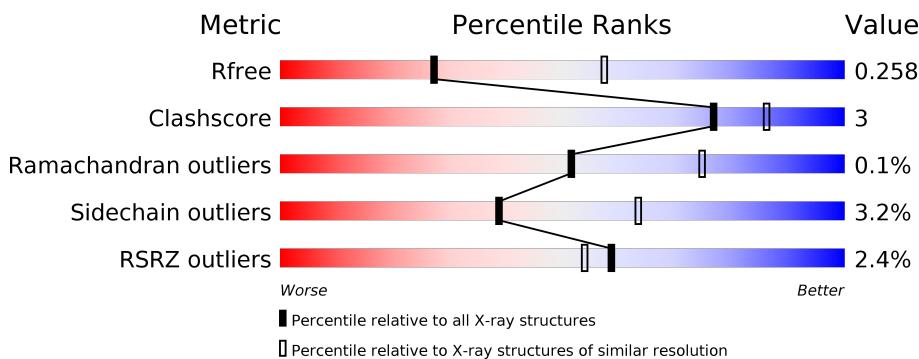
1 Overall quality at a glance

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	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.



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

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).

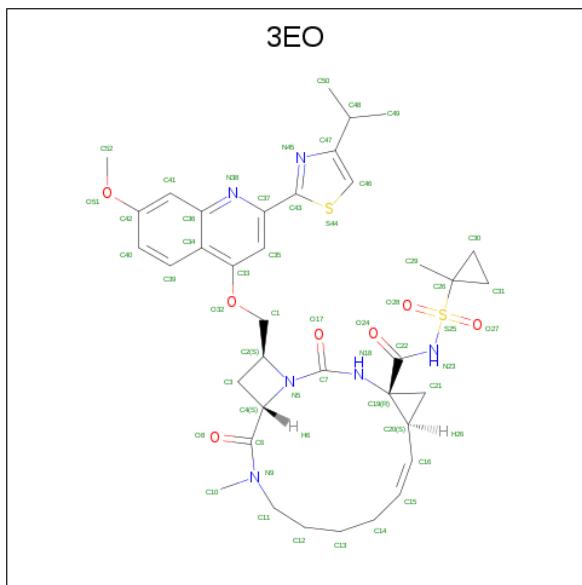
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0

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

- 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: C₃₇H₄₆N₆O₇S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			52	37	6	7	2		

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			52	37	6	7	2		

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

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

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

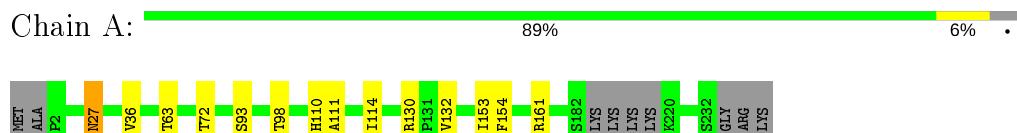
- Molecule 5 is water.

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

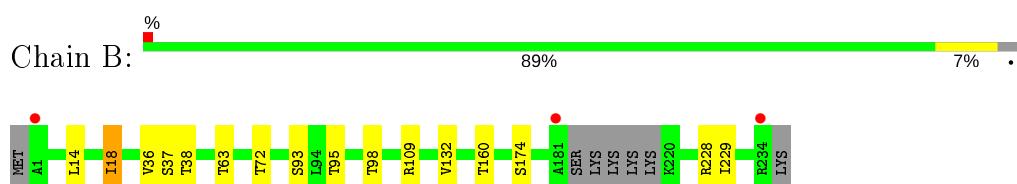
3 Residue-property plots

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.

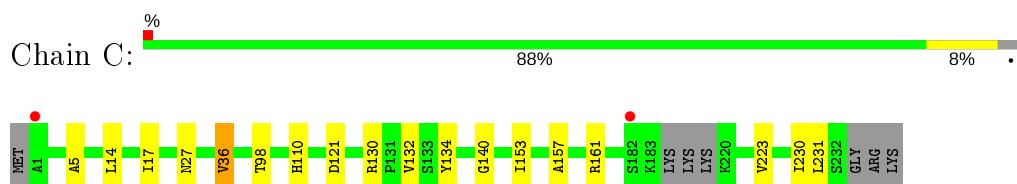
- Molecule 1: NS3 protease



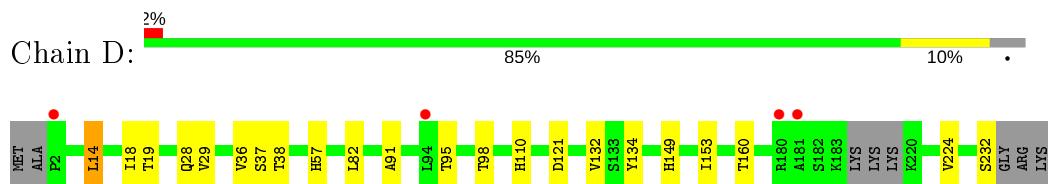
- Molecule 1: NS3 protease



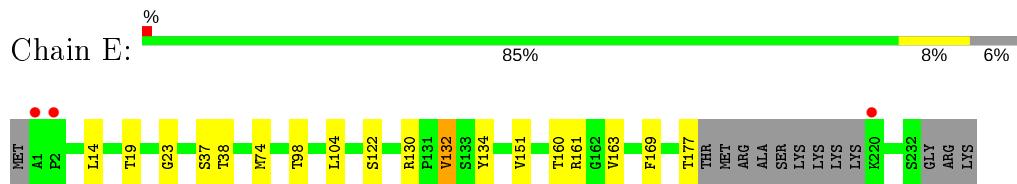
- Molecule 1: NS3 protease



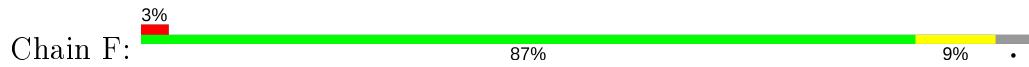
- Molecule 1: NS3 protease



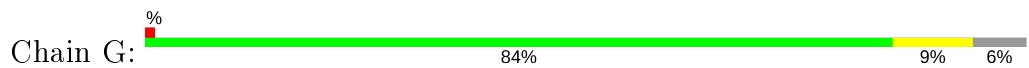
- Molecule 1: NS3 protease



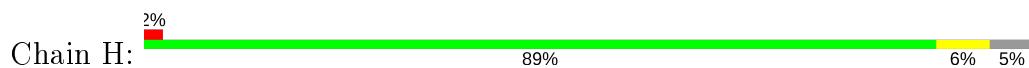
- Molecule 1: NS3 protease



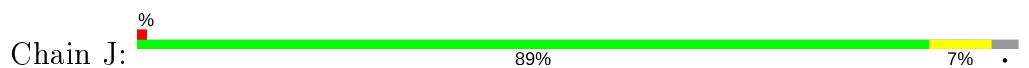
- Molecule 1: NS3 protease



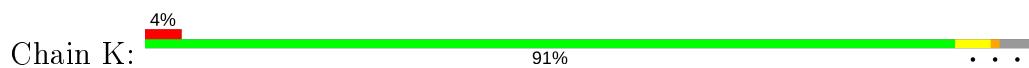
- Molecule 1: NS3 protease



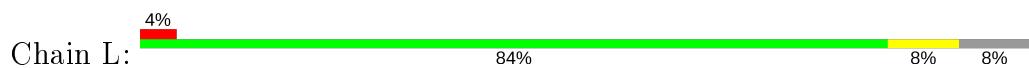
- Molecule 1: NS3 protease



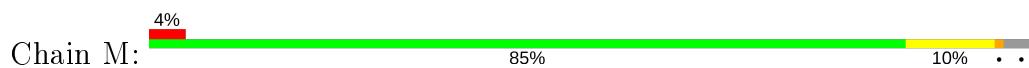
- Molecule 1: NS3 protease

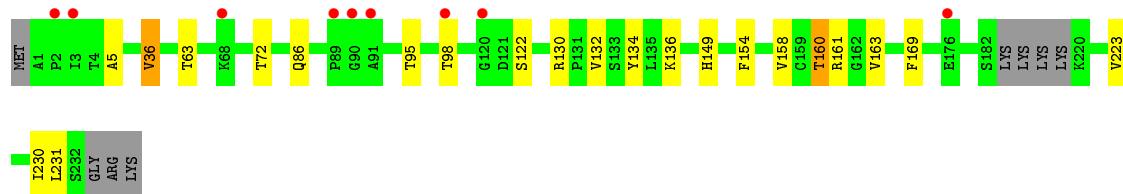


- Molecule 1: NS3 protease



- Molecule 1: NS3 protease





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	140.69 Å 143.20 Å 240.55 Å 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
$\langle I/\sigma(I) \rangle^{\text{1}}$	2.14 (at 2.86 Å)	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	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	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.*

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: 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.

All (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
1:L:97:CYS:HG	2:L:301:ZN:ZN	0.42	0.74
3:J:302:3EO:H32	1:L:132:VAL:HG11	1.72	0.70
1:G:132:VAL:HG11	3:H:302:3EO:H32	1.75	0.69
1:H:132:VAL:HG11	3:M:302:3EO:H32	1.76	0.68
1:C:132:VAL:HG11	3:E:302:3EO:H32	1.76	0.67
1:J:132:VAL:HG11	3:K:302:3EO:H32	1.78	0.66
3:J:302:3EO:H32	1:L:132:VAL:CG1	2.26	0.65
3:D:302:3EO:H32	1:F:132:VAL:HG11	1.78	0.64
3:D:302:3EO:H43	1:F:134:TYR:HA	1.80	0.63
3:G:302:3EO:H43	1:M:134:TYR:HA	1.80	0.63
1:C:134:TYR:HA	3:E:302:3EO:H43	1.81	0.62
3:B:302:3EO:H32	1:E:132:VAL:CG1	2.29	0.62
1:A:132:VAL:HG11	3:F:302:3EO:H32	1.82	0.61
1:K:132:VAL:HG11	3:L:302:3EO:H32	1.81	0.61
3:D:302:3EO:H42	1:F:110:HIS:CD2	2.37	0.59
1:E:160:THR:O	1:E:163:VAL:HG12	2.03	0.59
1:H:73:GLN:NE2	1:H:76:THR:OG1	2.35	0.59
1:L:37:SER:OG	1:L:38:THR:O	2.19	0.58
1:B:37:SER:OG	1:B:38:THR:O	2.20	0.57
1:D:37:SER:OG	1:D:38:THR:O	2.22	0.57
1:G:134:TYR:HA	3:H:302:3EO:H43	1.87	0.56
3:A:302:3EO:H43	1:D:134:TYR:HA	1.89	0.55
3:A:302:3EO:H42	1:D:110:HIS:CD2	2.42	0.54
1:D:95:THR:HG23	1:D:149:HIS:CD2	2.45	0.52
1:H:136:LYS:HA	3:H:302:3EO:H12	1.92	0.52
1:D:29:VAL:HG11	1:D:91:ALA:HB2	1.92	0.51
1:B:18:ILE:CD1	1:D:18:ILE:HD13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:VAL:CG1	3:E:302:3EO:H32	2.41	0.51
1:B:109:ARG:HA	1:B:229:ILE:HD11	1.92	0.50
1:F:154:PHE:CE2	3:F:302:3EO:H13	2.47	0.50
1:J:37:SER:OG	1:J:38:THR:O	2.28	0.50
1:E:37:SER:OG	1:E:38:THR:O	2.27	0.50
1:C:36:VAL:HG13	1:C:223:VAL:HG13	1.93	0.49
1:C:110:HIS:CD2	3:E:302:3EO:H42	2.48	0.48
1:G:109:ARG:HA	1:G:229:ILE:HD11	1.95	0.48
1:K:36:VAL:HG13	1:K:223:VAL:CG1	2.44	0.48
1:J:157:ALA:HB3	3:J:302:3EO:H27	1.94	0.48
1:B:18:ILE:HG12	1:D:18:ILE:HD13	1.95	0.48
1:B:18:ILE:HD11	1:D:18:ILE:HD13	1.96	0.48
1:C:27:ASN:HD22	1:F:27:ASN:HD22	1.60	0.48
1:A:27:ASN:HD22	1:A:27:ASN:N	2.12	0.47
1:K:155:ARG:HG2	3:K:302:3EO:C39	2.45	0.47
1:D:82:LEU:CD1	1:D:153:ILE:HD11	2.44	0.47
1:H:5:ALA:HB2	1:H:231:LEU:HD23	1.96	0.47
3:A:302:3EO:H32	1:D:132:VAL:HG11	1.97	0.46
1:J:76:THR:HG23	1:J:83:VAL:HG12	1.97	0.46
1:B:63:THR:HG22	1:B:72:THR:HA	1.98	0.46
1:G:46:THR:HG21	1:G:142:PRO:HB3	1.96	0.46
3:J:302:3EO:H43	1:L:134:TYR:HA	1.98	0.46
1:G:36:VAL:HG13	1:G:223:VAL:HG13	1.97	0.46
1:K:46:THR:HG21	1:K:142:PRO:HB3	1.96	0.46
1:L:154:PHE:CE2	3:L:302:3EO:H13	2.51	0.46
3:B:302:3EO:H43	1:E:134:TYR:HA	1.97	0.45
1:B:132:VAL:CG1	3:C:302:3EO:H32	2.42	0.45
1:B:14:LEU:HG	1:C:17:ILE:HG21	1.98	0.45
1:F:97:CYS:HG	2:F:301:ZN:ZN	1.24	0.45
1:D:57:HIS:HB2	3:D:302:3EO:H40	1.99	0.45
1:A:114:ILE:HG23	1:A:130:ARG:NH1	2.32	0.44
1:C:157:ALA:HB3	3:C:302:3EO:H28	1.99	0.44
1:E:104:LEU:HD22	1:E:151:VAL:HG21	2.00	0.44
1:A:154:PHE:CE2	3:A:302:3EO:H13	2.53	0.44
1:M:36:VAL:HG13	1:M:223:VAL:CG1	2.48	0.44
1:L:157:ALA:HB3	3:L:302:3EO:H27	2.00	0.44
1:G:82:LEU:CD1	1:G:153:ILE:HD11	2.47	0.44
1:J:157:ALA:HB3	3:J:302:3EO:C14	2.48	0.44
1:M:122:SER:HB2	1:M:169:PHE:O	2.17	0.44
1:C:27:ASN:HD22	1:F:27:ASN:ND2	2.16	0.44
1:F:157:ALA:HB3	3:F:302:3EO:H27	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:THR:HG22	1:H:72:THR:HA	1.99	0.43
1:D:14:LEU:HD11	1:E:14:LEU:HD11	2.00	0.43
1:D:14:LEU:O	1:D:18:ILE:HD12	2.18	0.43
1:G:1:ALA:O	1:G:3:ILE:N	2.52	0.43
1:M:5:ALA:HB2	1:M:231:LEU:HD23	2.01	0.43
1:C:5:ALA:HB2	1:C:231:LEU:HD23	2.01	0.43
1:F:160:THR:O	1:F:163:VAL:HG12	2.18	0.43
1:C:140:GLY:HA2	1:C:153:ILE:HD12	2.01	0.42
1:L:160:THR:O	1:L:163:VAL:HG12	2.19	0.42
1:M:63:THR:HG22	1:M:72:THR:HA	2.01	0.42
1:K:95:THR:HG23	1:K:149:HIS:CD2	2.54	0.42
1:D:82:LEU:HD12	1:D:153:ILE:HD11	2.02	0.42
1:F:155:ARG:HD3	1:F:170:VAL:HG23	2.02	0.42
1:J:230:ILE:HD12	1:J:230:ILE:N	2.34	0.42
1:L:54:THR:OG1	1:L:55:VAL:N	2.52	0.42
1:M:136:LYS:HA	3:M:302:3EO:H12	2.01	0.42
1:D:19:THR:HG21	1:D:224:VAL:HG13	2.01	0.42
1:H:160:THR:O	1:H:163:VAL:HG12	2.20	0.41
1:C:230:ILE:N	1:C:230:ILE:HD12	2.36	0.41
1:F:57:HIS:CE1	3:F:302:3EO:H1	2.56	0.41
1:A:110:HIS:O	1:A:111:ALA:HB3	2.21	0.41
1:H:132:VAL:CG1	3:M:302:3EO:H32	2.48	0.41
1:M:95:THR:HG23	1:M:149:HIS:CD2	2.55	0.41
1:A:63:THR:HG22	1:A:72:THR:HA	2.02	0.41
1:K:9:GLN:OE1	1:L:220:LYS:N	2.54	0.41
1:M:154:PHE:CE2	3:M:302:3EO:H13	2.56	0.41
1:D:14:LEU:HD11	1:E:14:LEU:CD1	2.51	0.41
1:J:29:VAL:HG11	1:J:91:ALA:HB2	2.02	0.41
1:H:161:ARG:HG2	1:M:158:VAL:HG13	2.02	0.41
1:F:145:CYS:HB2	1:F:146:PRO:HD2	2.03	0.40
1:E:19:THR:O	1:E:23:GLY:N	2.52	0.40
1:M:230:ILE:HD12	1:M:230:ILE:N	2.36	0.40
1:C:14:LEU:HB3	1:F:18:ILE:HD11	2.02	0.40
1:E:122:SER:HB2	1:E:169:PHE:O	2.21	0.40
1:M:160:THR:O	1:M:163:VAL:HG12	2.21	0.40

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	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
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

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	36	VAL
1	A	93	SER
1	A	98	THR
1	A	153	ILE
1	A	161	ARG
1	B	18	ILE
1	B	36	VAL
1	B	93	SER
1	B	95	THR
1	B	98	THR
1	B	160	THR
1	B	174	SER
1	B	228	ARG
1	C	36	VAL
1	C	98	THR
1	C	121	ASP
1	C	130	ARG
1	C	161	ARG
1	D	14	LEU
1	D	28	GLN
1	D	36	VAL

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Mol	Chain	Res	Type
1	D	98	THR
1	D	121	ASP
1	D	160	THR
1	D	232	SER
1	E	74	MET
1	E	98	THR
1	E	130	ARG
1	E	161	ARG
1	E	177	THR
1	F	36	VAL
1	F	98	THR
1	F	228	ARG
1	G	93	SER
1	G	98	THR
1	G	151	VAL
1	G	160	THR
1	G	161	ARG
1	G	176	GLU
1	H	130	ARG
1	H	232	SER
1	J	36	VAL
1	J	98	THR
1	J	130	ARG
1	J	160	THR
1	J	228	ARG
1	J	234	ARG
1	K	36	VAL
1	K	95	THR
1	K	98	THR
1	L	14	LEU
1	L	36	VAL
1	L	93	SER
1	L	98	THR
1	M	36	VAL
1	M	86	GLN
1	M	98	THR
1	M	130	ARG
1	M	160	THR
1	M	161	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	34	GLN
1	B	27	ASN
1	B	34	GLN
1	C	27	ASN
1	C	34	GLN
1	C	110	HIS
1	C	149	HIS
1	D	27	ASN
1	D	34	GLN
1	D	73	GLN
1	D	110	HIS
1	D	149	HIS
1	E	27	ASN
1	E	34	GLN
1	F	8	GLN
1	F	27	ASN
1	F	34	GLN
1	F	110	HIS
1	G	34	GLN
1	G	149	HIS
1	H	27	ASN
1	H	34	GLN
1	H	73	GLN
1	J	27	ASN
1	J	34	GLN
1	J	149	HIS
1	K	9	GLN
1	K	34	GLN
1	K	149	HIS
1	L	27	ASN
1	L	34	GLN
1	M	27	ASN
1	M	34	GLN
1	M	149	HIS

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 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

All (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
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
3	H	302	3EO	C43-S44	-9.88	1.60	1.73
3	B	302	3EO	C43-S44	-9.87	1.60	1.73
3	F	302	3EO	C43-S44	-9.76	1.60	1.73
3	C	302	3EO	C43-S44	-9.74	1.60	1.73
3	E	302	3EO	C43-S44	-9.51	1.60	1.73
3	M	302	3EO	C43-S44	-9.33	1.60	1.73
3	J	302	3EO	C43-S44	-9.26	1.60	1.73
3	F	302	3EO	C46-S44	-7.29	1.59	1.70
3	G	302	3EO	C46-S44	-7.22	1.59	1.70
3	H	302	3EO	C46-S44	-7.22	1.59	1.70
3	A	302	3EO	C46-S44	-7.16	1.59	1.70
3	B	302	3EO	C46-S44	-7.14	1.59	1.70
3	C	302	3EO	C46-S44	-7.13	1.59	1.70
3	E	302	3EO	C46-S44	-7.06	1.59	1.70
3	L	302	3EO	C46-S44	-7.04	1.59	1.70
3	K	302	3EO	C46-S44	-6.97	1.59	1.70
3	M	302	3EO	C46-S44	-6.96	1.59	1.70
3	J	302	3EO	C46-S44	-6.95	1.59	1.70
3	D	302	3EO	C46-S44	-6.73	1.60	1.70
3	K	302	3EO	C21-C19	5.16	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	3EO	C21-C19	4.90	1.56	1.51
3	G	302	3EO	C21-C19	4.77	1.56	1.51
3	J	302	3EO	C21-C19	4.63	1.55	1.51
3	M	302	3EO	C21-C19	4.59	1.55	1.51
3	H	302	3EO	C21-C19	4.57	1.55	1.51
3	L	302	3EO	C21-C19	4.55	1.55	1.51
3	E	302	3EO	C21-C19	4.53	1.55	1.51
3	D	302	3EO	C21-C19	4.50	1.55	1.51
3	A	302	3EO	C21-C19	4.28	1.55	1.51
3	C	302	3EO	C21-C19	4.21	1.55	1.51
3	F	302	3EO	C21-C19	4.07	1.55	1.51
3	D	302	3EO	C20-C16	4.00	1.54	1.49
3	L	302	3EO	C20-C16	3.95	1.54	1.49
3	F	302	3EO	C20-C16	3.91	1.54	1.49
3	J	302	3EO	C37-N38	3.88	1.39	1.33
3	A	302	3EO	C37-N38	3.87	1.39	1.33
3	C	302	3EO	C20-C16	3.84	1.54	1.49
3	E	302	3EO	C37-N38	3.75	1.38	1.33
3	F	302	3EO	C37-N38	3.74	1.38	1.33
3	G	302	3EO	C20-C16	3.74	1.54	1.49
3	J	302	3EO	C20-C16	3.72	1.54	1.49
3	H	302	3EO	C37-N38	3.69	1.38	1.33
3	B	302	3EO	C20-C16	3.68	1.54	1.49
3	E	302	3EO	C20-C16	3.66	1.53	1.49
3	K	302	3EO	C37-N38	3.63	1.38	1.33
3	K	302	3EO	C20-C16	3.58	1.53	1.49
3	M	302	3EO	C37-N38	3.58	1.38	1.33
3	C	302	3EO	C37-N38	3.52	1.38	1.33
3	D	302	3EO	C37-N38	3.46	1.38	1.33
3	L	302	3EO	C37-N38	3.44	1.38	1.33
3	A	302	3EO	C20-C16	3.44	1.53	1.49
3	M	302	3EO	C20-C16	3.30	1.53	1.49
3	B	302	3EO	C37-N38	3.29	1.38	1.33
3	A	302	3EO	C6-N9	3.26	1.40	1.35
3	H	302	3EO	C20-C16	3.25	1.53	1.49
3	C	302	3EO	C31-C30	3.22	1.58	1.50
3	L	302	3EO	C6-N9	3.20	1.40	1.35
3	J	302	3EO	C31-C30	3.20	1.58	1.50
3	G	302	3EO	C37-N38	3.20	1.37	1.33
3	F	302	3EO	C31-C30	3.19	1.58	1.50
3	K	302	3EO	C6-N9	3.19	1.40	1.35
3	E	302	3EO	C31-C30	3.17	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	302	3EO	C31-C30	3.13	1.57	1.50
3	D	302	3EO	C31-C30	3.09	1.57	1.50
3	M	302	3EO	C6-N9	3.08	1.40	1.35
3	B	302	3EO	C31-C30	3.08	1.57	1.50
3	H	302	3EO	C31-C30	3.08	1.57	1.50
3	K	302	3EO	C31-C30	3.08	1.57	1.50
3	E	302	3EO	C6-N9	3.04	1.40	1.35
3	A	302	3EO	C31-C30	3.04	1.57	1.50
3	H	302	3EO	C6-N9	3.02	1.40	1.35
3	J	302	3EO	S25-N23	3.02	1.64	1.60
3	G	302	3EO	C31-C30	3.01	1.57	1.50
3	M	302	3EO	C31-C30	3.01	1.57	1.50
3	M	302	3EO	C43-N45	2.89	1.35	1.31
3	D	302	3EO	C3-C4	-2.89	1.51	1.55
3	J	302	3EO	C6-N9	2.88	1.40	1.35
3	L	302	3EO	S25-N23	2.83	1.64	1.60
3	C	302	3EO	C6-N9	2.80	1.40	1.35
3	M	302	3EO	C3-C4	-2.74	1.51	1.55
3	H	302	3EO	S25-N23	2.70	1.64	1.60
3	F	302	3EO	C3-C4	-2.66	1.51	1.55
3	G	302	3EO	C6-N9	2.66	1.39	1.35
3	A	302	3EO	C3-C4	-2.65	1.51	1.55
3	B	302	3EO	S25-N23	2.62	1.64	1.60
3	H	302	3EO	C3-C4	-2.62	1.52	1.55
3	J	302	3EO	C3-C4	-2.60	1.52	1.55
3	B	302	3EO	C43-N45	2.60	1.35	1.31
3	E	302	3EO	C3-C4	-2.60	1.52	1.55
3	L	302	3EO	C3-C4	-2.59	1.52	1.55
3	D	302	3EO	C43-N45	2.59	1.35	1.31
3	K	302	3EO	C43-N45	2.57	1.35	1.31
3	K	302	3EO	C3-C4	-2.56	1.52	1.55
3	M	302	3EO	S25-N23	2.54	1.64	1.60
3	C	302	3EO	C19-C20	-2.52	1.49	1.54
3	L	302	3EO	C43-N45	2.52	1.35	1.31
3	F	302	3EO	C6-N9	2.51	1.39	1.35
3	C	302	3EO	C3-C4	-2.51	1.52	1.55
3	B	302	3EO	C6-N9	2.50	1.39	1.35
3	F	302	3EO	C43-N45	2.48	1.35	1.31
3	A	302	3EO	C43-N45	2.47	1.35	1.31
3	K	302	3EO	C19-C20	-2.47	1.49	1.54
3	D	302	3EO	S25-N23	2.46	1.64	1.60
3	B	302	3EO	C3-C4	-2.46	1.52	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	3EO	C43-N45	2.44	1.35	1.31
3	G	302	3EO	S25-N23	2.44	1.63	1.60
3	E	302	3EO	S25-N23	2.44	1.63	1.60
3	J	302	3EO	C43-N45	2.43	1.35	1.31
3	G	302	3EO	C19-C20	-2.42	1.49	1.54
3	G	302	3EO	C3-C4	-2.40	1.52	1.55
3	M	302	3EO	C19-C20	-2.37	1.50	1.54
3	D	302	3EO	C6-N9	2.37	1.39	1.35
3	C	302	3EO	S25-N23	2.36	1.63	1.60
3	J	302	3EO	C19-C20	-2.34	1.50	1.54
3	D	302	3EO	C19-C20	-2.33	1.50	1.54
3	K	302	3EO	S25-N23	2.33	1.63	1.60
3	F	302	3EO	C19-C20	-2.32	1.50	1.54
3	C	302	3EO	C43-N45	2.31	1.34	1.31
3	E	302	3EO	C19-C20	-2.30	1.50	1.54
3	B	302	3EO	C19-C20	-2.30	1.50	1.54
3	F	302	3EO	S25-N23	2.27	1.63	1.60
3	H	302	3EO	C43-N45	2.24	1.34	1.31
3	H	302	3EO	C19-N18	2.20	1.49	1.45
3	L	302	3EO	C26-S25	-2.20	1.79	1.81
3	A	302	3EO	C19-C20	-2.18	1.50	1.54
3	E	302	3EO	C41-C36	-2.16	1.38	1.41
3	H	302	3EO	C19-C20	-2.13	1.50	1.54
3	M	302	3EO	C19-N18	2.10	1.49	1.45
3	E	302	3EO	C43-N45	2.09	1.34	1.31
3	A	302	3EO	C19-N18	2.04	1.49	1.45
3	M	302	3EO	C26-S25	-2.03	1.80	1.81
3	L	302	3EO	C19-C20	-2.03	1.50	1.54
3	B	302	3EO	C41-C36	-2.02	1.38	1.41
3	K	302	3EO	C19-N18	2.02	1.49	1.45

All (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
3	J	302	3EO	C31-C26-C30	6.94	63.17	59.54
3	B	302	3EO	C3-C4-N5	6.90	94.66	88.20
3	M	302	3EO	C3-C4-N5	6.84	94.60	88.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	3EO	C3-C4-N5	6.80	94.56	88.20
3	L	302	3EO	C3-C4-N5	6.72	94.49	88.20
3	G	302	3EO	C3-C4-N5	6.72	94.49	88.20
3	L	302	3EO	C31-C26-C30	6.66	63.03	59.54
3	A	302	3EO	C3-C4-N5	6.65	94.43	88.20
3	F	302	3EO	C31-C26-C30	6.62	63.00	59.54
3	A	302	3EO	C31-C26-C30	6.61	63.00	59.54
3	B	302	3EO	C31-C26-C30	6.60	62.99	59.54
3	M	302	3EO	C31-C26-C30	6.59	62.99	59.54
3	D	302	3EO	C31-C26-C30	6.58	62.98	59.54
3	E	302	3EO	C31-C26-C30	6.54	62.96	59.54
3	H	302	3EO	C31-C26-C30	6.53	62.96	59.54
3	K	302	3EO	C31-C26-C30	6.49	62.94	59.54
3	J	302	3EO	C3-C4-N5	6.32	94.11	88.20
3	K	302	3EO	C3-C4-N5	6.30	94.10	88.20
3	G	302	3EO	C31-C26-C30	6.28	62.82	59.54
3	L	302	3EO	O27-S25-O28	-6.03	108.34	120.57
3	E	302	3EO	O27-S25-O28	-6.01	108.37	120.57
3	B	302	3EO	O27-S25-O28	-5.97	108.46	120.57
3	C	302	3EO	O27-S25-O28	-5.95	108.49	120.57
3	J	302	3EO	O27-S25-O28	-5.84	108.72	120.57
3	H	302	3EO	O27-S25-O28	-5.79	108.82	120.57
3	G	302	3EO	O27-S25-O28	-5.74	108.92	120.57
3	D	302	3EO	O27-S25-O28	-5.55	109.30	120.57
3	K	302	3EO	O27-S25-O28	-5.45	109.52	120.57
3	G	302	3EO	C22-N23-S25	-5.44	115.29	124.08
3	C	302	3EO	C22-N23-S25	-5.29	115.54	124.08
3	A	302	3EO	O27-S25-O28	-5.16	110.09	120.57
3	D	302	3EO	C22-N23-S25	-5.16	115.75	124.08
3	M	302	3EO	O27-S25-O28	-5.07	110.27	120.57
3	K	302	3EO	O28-S25-C26	4.99	111.61	107.60
3	C	302	3EO	C46-C47-C48	-4.95	121.63	129.25
3	K	302	3EO	C21-C20-C19	4.89	62.04	59.09
3	M	302	3EO	C22-N23-S25	-4.88	116.20	124.08
3	A	302	3EO	C22-N23-S25	-4.81	116.31	124.08
3	K	302	3EO	C46-C47-C48	-4.81	121.86	129.25
3	B	302	3EO	C46-C47-C48	-4.79	121.88	129.25
3	L	302	3EO	C46-C47-C48	-4.74	121.97	129.25
3	G	302	3EO	C21-C20-C19	4.72	61.94	59.09
3	J	302	3EO	C46-C47-C48	-4.66	122.08	129.25
3	F	302	3EO	C46-C47-C48	-4.66	122.08	129.25
3	G	302	3EO	C46-C47-C48	-4.65	122.10	129.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	3EO	C21-C20-C19	4.60	61.87	59.09
3	H	302	3EO	C46-C47-C48	-4.60	122.18	129.25
3	B	302	3EO	C22-N23-S25	-4.54	116.74	124.08
3	C	302	3EO	C37-N38-C36	4.52	121.42	118.06
3	M	302	3EO	C46-C47-C48	-4.51	122.31	129.25
3	J	302	3EO	C21-C20-C19	4.51	61.81	59.09
3	F	302	3EO	O27-S25-O28	-4.49	111.45	120.57
3	A	302	3EO	C46-C47-C48	-4.48	122.36	129.25
3	M	302	3EO	C21-C20-C19	4.44	61.77	59.09
3	K	302	3EO	C37-N38-C36	4.38	121.32	118.06
3	A	302	3EO	O17-C7-N5	-4.38	114.65	121.72
3	H	302	3EO	O27-S25-C26	4.37	111.11	107.60
3	E	302	3EO	C21-C20-C19	4.33	61.71	59.09
3	D	302	3EO	C21-C20-C19	4.29	61.68	59.09
3	E	302	3EO	C22-N23-S25	-4.27	117.18	124.08
3	D	302	3EO	C46-C47-C48	-4.27	122.69	129.25
3	C	302	3EO	C21-C20-C19	4.26	61.66	59.09
3	G	302	3EO	O28-S25-C26	4.26	111.02	107.60
3	H	302	3EO	C21-C20-C19	4.24	61.65	59.09
3	D	302	3EO	O17-C7-N5	-4.24	114.87	121.72
3	A	302	3EO	C21-C20-C19	4.20	61.63	59.09
3	H	302	3EO	C37-N38-C36	4.18	121.17	118.06
3	J	302	3EO	C37-N38-C36	4.17	121.16	118.06
3	K	302	3EO	C19-C21-C20	-4.15	57.71	61.56
3	H	302	3EO	C22-N23-S25	-4.15	117.38	124.08
3	L	302	3EO	C21-C20-C19	4.14	61.59	59.09
3	K	302	3EO	O27-S25-C26	4.13	110.92	107.60
3	G	302	3EO	O17-C7-N5	-4.12	115.06	121.72
3	G	302	3EO	C37-N38-C36	4.11	121.11	118.06
3	G	302	3EO	C19-C22-N23	4.09	122.78	115.70
3	J	302	3EO	O27-S25-C26	4.08	110.87	107.60
3	E	302	3EO	C46-C47-C48	-4.07	122.99	129.25
3	B	302	3EO	O27-S25-C26	3.99	110.80	107.60
3	M	302	3EO	O27-S25-C26	3.99	110.80	107.60
3	C	302	3EO	C19-C21-C20	-3.94	57.91	61.56
3	G	302	3EO	C19-C21-C20	-3.92	57.92	61.56
3	B	302	3EO	C19-C21-C20	-3.92	57.92	61.56
3	H	302	3EO	C19-C22-N23	3.92	122.48	115.70
3	M	302	3EO	C37-N38-C36	3.92	120.97	118.06
3	C	302	3EO	O27-S25-C26	3.91	110.74	107.60
3	M	302	3EO	C19-C21-C20	-3.91	57.94	61.56
3	B	302	3EO	C10-N9-C11	-3.88	108.00	115.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	3EO	C37-N38-C36	3.88	120.94	118.06
3	D	302	3EO	C19-C21-C20	-3.87	57.97	61.56
3	H	302	3EO	O17-C7-N5	-3.87	115.47	121.72
3	L	302	3EO	C37-N38-C36	3.87	120.94	118.06
3	F	302	3EO	C21-C20-C19	3.86	61.42	59.09
3	J	302	3EO	C19-C21-C20	-3.85	57.99	61.56
3	L	302	3EO	C19-N18-C7	-3.85	115.15	123.89
3	J	302	3EO	O17-C7-N5	-3.83	115.53	121.72
3	E	302	3EO	C19-C21-C20	-3.83	58.01	61.56
3	F	302	3EO	C19-C21-C20	-3.81	58.03	61.56
3	F	302	3EO	C22-N23-S25	-3.77	117.98	124.08
3	H	302	3EO	C19-C21-C20	-3.69	58.14	61.56
3	M	302	3EO	C19-C22-N23	3.66	122.03	115.70
3	B	302	3EO	C19-C22-N23	3.66	122.03	115.70
3	L	302	3EO	C19-C21-C20	-3.61	58.21	61.56
3	E	302	3EO	C37-N38-C36	3.60	120.74	118.06
3	H	302	3EO	O28-S25-C26	3.59	110.48	107.60
3	A	302	3EO	C19-C21-C20	-3.57	58.25	61.56
3	M	302	3EO	C19-N18-C7	-3.57	115.78	123.89
3	D	302	3EO	C19-N18-C7	-3.56	115.81	123.89
3	K	302	3EO	C21-C20-C16	3.55	129.00	120.03
3	G	302	3EO	C19-N18-C7	-3.54	115.84	123.89
3	J	302	3EO	C19-C22-N23	3.53	121.81	115.70
3	F	302	3EO	O27-S25-C26	3.53	110.43	107.60
3	L	302	3EO	C19-C22-N23	3.53	121.80	115.70
3	M	302	3EO	C10-N9-C11	-3.51	108.76	115.89
3	J	302	3EO	C19-N18-C7	-3.50	115.95	123.89
3	F	302	3EO	C19-N18-C7	-3.49	115.97	123.89
3	C	302	3EO	C19-C22-N23	3.48	121.72	115.70
3	B	302	3EO	O17-C7-N5	-3.45	116.14	121.72
3	H	302	3EO	C19-N18-C7	-3.45	116.06	123.89
3	J	302	3EO	C22-N23-S25	-3.45	118.51	124.08
3	K	302	3EO	O17-C7-N5	-3.43	116.18	121.72
3	C	302	3EO	O17-C7-N5	-3.43	116.18	121.72
3	F	302	3EO	C52-O51-C42	3.43	124.95	117.51
3	D	302	3EO	O28-S25-C26	3.43	110.35	107.60
3	K	302	3EO	C22-N23-S25	-3.42	118.55	124.08
3	K	302	3EO	C19-N18-C7	-3.41	116.15	123.89
3	D	302	3EO	C19-C22-N23	3.40	121.58	115.70
3	L	302	3EO	C10-N9-C11	-3.36	109.06	115.89
3	A	302	3EO	C52-O51-C42	3.36	124.80	117.51
3	E	302	3EO	O17-C7-N5	-3.36	116.30	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	3EO	C10-N9-C11	-3.35	109.10	115.89
3	E	302	3EO	C19-N18-C7	-3.34	116.30	123.89
3	F	302	3EO	C37-N38-C36	3.30	120.51	118.06
3	L	302	3EO	O17-C7-N5	-3.29	116.41	121.72
3	L	302	3EO	C22-N23-S25	-3.27	118.80	124.08
3	C	302	3EO	C34-C36-N38	-3.26	119.35	122.81
3	E	302	3EO	C52-O51-C42	3.24	124.53	117.51
3	H	302	3EO	C10-N9-C11	-3.21	109.37	115.89
3	D	302	3EO	C37-N38-C36	3.20	120.44	118.06
3	J	302	3EO	C10-N9-C11	-3.19	109.41	115.89
3	B	302	3EO	C19-N18-C7	-3.17	116.70	123.89
3	D	302	3EO	C52-O51-C42	3.17	124.38	117.51
3	H	302	3EO	C1-O32-C33	3.16	128.60	118.25
3	E	302	3EO	C19-C22-N23	3.14	121.13	115.70
3	J	302	3EO	O28-S25-C26	3.12	110.10	107.60
3	E	302	3EO	C1-O32-C33	3.08	128.33	118.25
3	A	302	3EO	O27-S25-C26	3.07	110.06	107.60
3	K	302	3EO	C21-C19-N18	3.07	121.92	117.80
3	J	302	3EO	C34-C36-N38	-3.02	119.61	122.81
3	C	302	3EO	C10-N9-C11	-3.02	109.76	115.89
3	K	302	3EO	C35-C37-N38	-3.01	119.49	122.23
3	K	302	3EO	C1-O32-C33	2.99	128.03	118.25
3	J	302	3EO	C1-O32-C33	2.97	127.98	118.25
3	M	302	3EO	C35-C37-N38	-2.95	119.54	122.23
3	M	302	3EO	O17-C7-N5	-2.94	116.97	121.72
3	C	302	3EO	C52-O51-C42	2.93	123.86	117.51
3	F	302	3EO	C1-O32-C33	2.90	127.72	118.25
3	J	302	3EO	C21-C20-C16	2.86	127.26	120.03
3	D	302	3EO	C34-C36-N38	-2.86	119.78	122.81
3	F	302	3EO	O17-C7-N5	-2.85	117.11	121.72
3	H	302	3EO	C34-C36-N38	-2.85	119.79	122.81
3	B	302	3EO	C34-C36-N38	-2.85	119.79	122.81
3	M	302	3EO	C1-O32-C33	2.83	127.50	118.25
3	K	302	3EO	C34-C36-N38	-2.82	119.82	122.81
3	G	302	3EO	C10-N9-C11	-2.82	110.17	115.89
3	A	302	3EO	C4-C6-N9	2.81	125.20	119.40
3	E	302	3EO	C35-C37-N38	-2.80	119.67	122.23
3	K	302	3EO	C10-N9-C11	-2.80	110.21	115.89
3	L	302	3EO	C34-C36-N38	-2.78	119.86	122.81
3	F	302	3EO	C4-C6-N9	2.77	125.13	119.40
3	L	302	3EO	C1-O32-C33	2.73	127.19	118.25
3	C	302	3EO	C1-O32-C33	2.73	127.19	118.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	302	3EO	C35-C37-N38	-2.73	119.74	122.23
3	B	302	3EO	C52-O51-C42	2.71	123.40	117.51
3	A	302	3EO	C19-C22-N23	2.71	120.38	115.70
3	G	302	3EO	C35-C37-N38	-2.70	119.76	122.23
3	F	302	3EO	C35-C37-N38	-2.66	119.80	122.23
3	G	302	3EO	C52-O51-C42	2.66	123.29	117.51
3	J	302	3EO	C35-C37-N38	-2.65	119.81	122.23
3	L	302	3EO	O27-S25-C26	2.64	109.72	107.60
3	A	302	3EO	C1-O32-C33	2.63	126.85	118.25
3	B	302	3EO	C1-O32-C33	2.62	126.81	118.25
3	G	302	3EO	C1-O32-C33	2.61	126.78	118.25
3	H	302	3EO	C52-O51-C42	2.60	123.15	117.51
3	D	302	3EO	C1-O32-C33	2.57	126.67	118.25
3	K	302	3EO	C52-O51-C42	2.57	123.09	117.51
3	L	302	3EO	C48-C47-N45	2.56	124.46	120.30
3	C	302	3EO	C12-C13-C14	-2.54	102.74	113.79
3	D	302	3EO	C4-C6-N9	2.54	124.64	119.40
3	G	302	3EO	C34-C36-N38	-2.53	120.13	122.81
3	D	302	3EO	C43-C37-N38	2.49	119.92	117.28
3	C	302	3EO	C48-C47-N45	2.49	124.35	120.30
3	C	302	3EO	C19-N18-C7	-2.48	118.26	123.89
3	A	302	3EO	C19-N18-C7	-2.44	118.36	123.89
3	M	302	3EO	C34-C36-N38	-2.43	120.23	122.81
3	F	302	3EO	C48-C47-N45	2.40	124.20	120.30
3	M	302	3EO	C52-O51-C42	2.39	122.70	117.51
3	F	302	3EO	C21-C20-C16	2.39	126.06	120.03
3	F	302	3EO	C34-C36-N38	-2.39	120.28	122.81
3	J	302	3EO	C52-O51-C42	2.37	122.65	117.51
3	E	302	3EO	O27-S25-C26	2.35	109.49	107.60
3	B	302	3EO	C21-C20-C16	2.35	125.97	120.03
3	B	302	3EO	C12-C13-C14	-2.35	103.56	113.79
3	L	302	3EO	C35-C37-N38	-2.32	120.11	122.23
3	L	302	3EO	C52-O51-C42	2.31	122.53	117.51
3	A	302	3EO	C34-C36-N38	-2.31	120.37	122.81
3	D	302	3EO	O27-S25-C26	2.30	109.44	107.60
3	G	302	3EO	C12-C13-C14	-2.29	103.81	113.79
3	H	302	3EO	C21-C20-C16	2.29	125.82	120.03
3	M	302	3EO	O17-C7-N18	-2.29	116.64	121.05
3	C	302	3EO	C21-C20-C16	2.28	125.80	120.03
3	F	302	3EO	C19-C22-N23	2.28	119.63	115.70
3	B	302	3EO	C35-C37-N38	-2.27	120.16	122.23
3	H	302	3EO	C48-C47-N45	2.27	123.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	302	3EO	C19-C22-N23	2.23	119.56	115.70
3	M	302	3EO	C12-C13-C14	-2.23	104.07	113.79
3	E	302	3EO	C34-C36-N38	-2.21	120.47	122.81
3	L	302	3EO	C37-C43-N45	2.20	130.12	124.47
3	J	302	3EO	C48-C47-N45	2.19	123.87	120.30
3	G	302	3EO	C21-C20-C16	2.19	125.57	120.03
3	M	302	3EO	C48-C47-N45	2.19	123.86	120.30
3	D	302	3EO	C21-C20-C16	2.16	125.48	120.03
3	D	302	3EO	C35-C37-N38	-2.15	120.27	122.23
3	E	302	3EO	C12-C13-C14	-2.14	104.45	113.79
3	M	302	3EO	O51-C42-C41	-2.14	118.61	124.43
3	L	302	3EO	C21-C20-C16	2.13	125.42	120.03
3	M	302	3EO	C21-C20-C16	2.11	125.36	120.03
3	F	302	3EO	O51-C42-C41	-2.10	118.70	124.43
3	D	302	3EO	C21-C19-N18	2.09	120.60	117.80
3	C	302	3EO	C35-C37-N38	-2.09	120.33	122.23
3	A	302	3EO	C37-N38-C36	2.09	119.61	118.06
3	C	302	3EO	C41-C36-C34	2.08	122.05	119.65
3	G	302	3EO	C21-C19-N18	2.08	120.59	117.80
3	J	302	3EO	C4-C6-N9	2.06	123.66	119.40
3	F	302	3EO	O8-C6-C4	-2.05	115.94	120.22
3	A	302	3EO	C10-N9-C11	-2.03	111.76	115.89
3	K	302	3EO	C48-C47-N45	2.02	123.58	120.30
3	B	302	3EO	C12-C11-N9	2.02	119.57	112.55
3	E	302	3EO	C21-C20-C16	2.01	125.12	120.03
3	L	302	3EO	O51-C42-C41	-2.01	118.95	124.43
3	J	302	3EO	C12-C13-C14	-2.01	105.05	113.79
3	G	302	3EO	C4-C6-N9	2.00	123.53	119.40

There are no chirality outliers.

All (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
3	F	302	3EO	C22-N23-S25-C26
3	H	302	3EO	C12-C11-N9-C6
3	H	302	3EO	C12-C11-N9-C10
3	H	302	3EO	C20-C19-N18-C7

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Mol	Chain	Res	Type	Atoms
3	H	302	3EO	C22-N23-S25-C26
3	G	302	3EO	C12-C11-N9-C6
3	G	302	3EO	C12-C11-N9-C10
3	G	302	3EO	C22-N23-S25-C26
3	A	302	3EO	N38-C37-C43-N45
3	A	302	3EO	C22-N23-S25-C26
3	M	302	3EO	C12-C11-N9-C6
3	M	302	3EO	C12-C11-N9-C10
3	M	302	3EO	C22-N23-S25-C26
3	L	302	3EO	C12-C11-N9-C6
3	L	302	3EO	C12-C11-N9-C10
3	L	302	3EO	C22-N23-S25-C26
3	K	302	3EO	C3-C4-C6-N9
3	K	302	3EO	N38-C37-C43-N45
3	K	302	3EO	C22-N23-S25-C26
3	J	302	3EO	C12-C11-N9-C6
3	J	302	3EO	C12-C11-N9-C10
3	J	302	3EO	C22-N23-S25-C26
3	D	302	3EO	C22-N23-S25-C26
3	C	302	3EO	C12-C11-N9-C6
3	C	302	3EO	C22-N23-S25-C26
3	E	302	3EO	C3-C4-C6-N9
3	E	302	3EO	C12-C11-N9-C6
3	E	302	3EO	C12-C11-N9-C10
3	E	302	3EO	C22-N23-S25-C26
3	M	302	3EO	C41-C42-O51-C52
3	M	302	3EO	C40-C42-O51-C52
3	K	302	3EO	C40-C42-O51-C52
3	L	302	3EO	C40-C42-O51-C52
3	L	302	3EO	C41-C42-O51-C52
3	H	302	3EO	C40-C42-O51-C52
3	K	302	3EO	C41-C42-O51-C52
3	J	302	3EO	C40-C42-O51-C52
3	D	302	3EO	C40-C42-O51-C52
3	C	302	3EO	C40-C42-O51-C52
3	B	302	3EO	C40-C42-O51-C52
3	B	302	3EO	C41-C42-O51-C52
3	H	302	3EO	C41-C42-O51-C52
3	J	302	3EO	C41-C42-O51-C52
3	D	302	3EO	C41-C42-O51-C52
3	C	302	3EO	C41-C42-O51-C52
3	F	302	3EO	C40-C42-O51-C52

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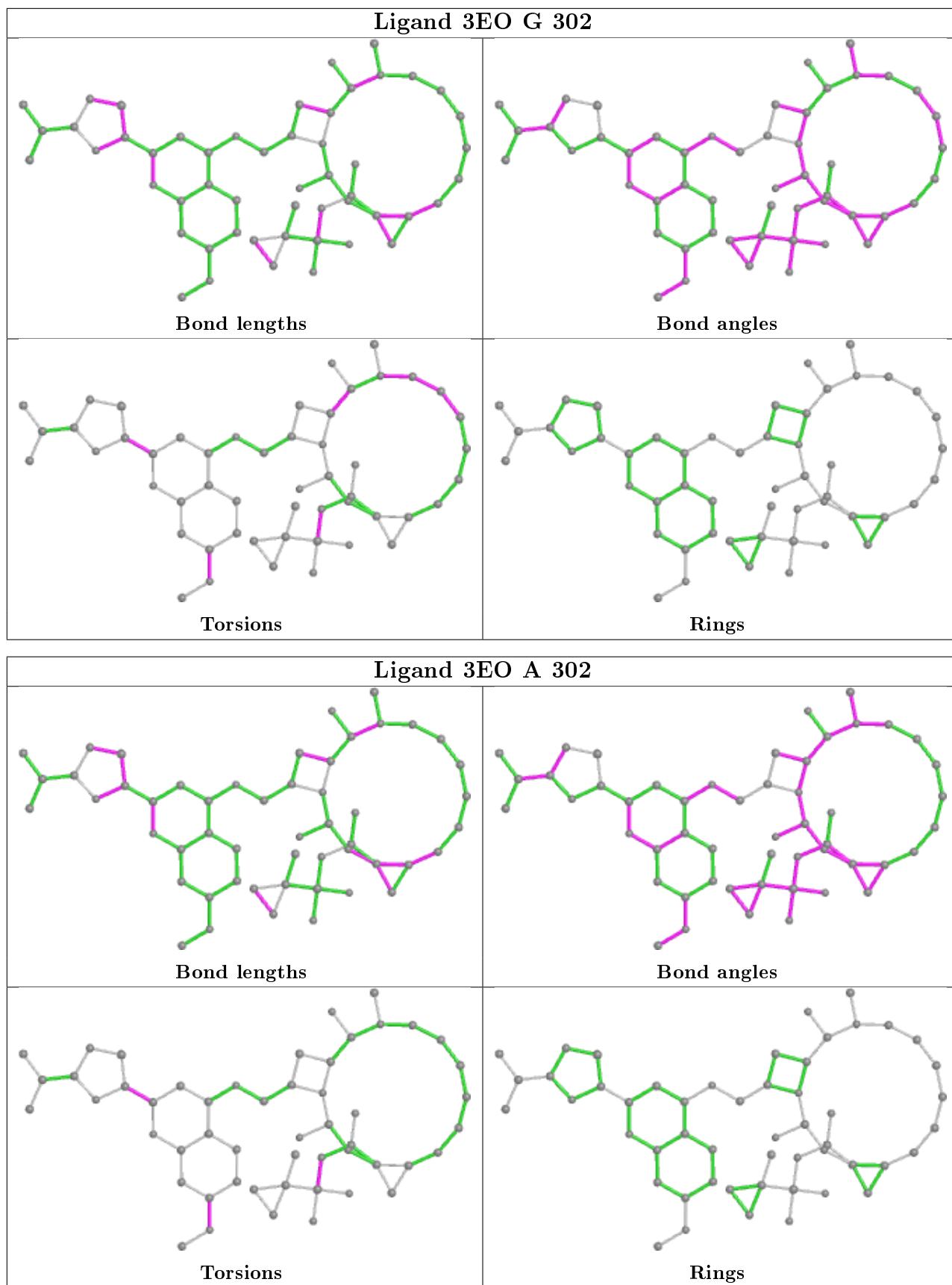
Mol	Chain	Res	Type	Atoms
3	F	302	3EO	C41-C42-O51-C52
3	G	302	3EO	C40-C42-O51-C52
3	G	302	3EO	C41-C42-O51-C52
3	K	302	3EO	C22-N23-S25-O27
3	A	302	3EO	C40-C42-O51-C52
3	A	302	3EO	C41-C42-O51-C52
3	E	302	3EO	C40-C42-O51-C52
3	E	302	3EO	C41-C42-O51-C52
3	M	302	3EO	C22-N23-S25-O28
3	K	302	3EO	N9-C11-C12-C13
3	C	302	3EO	N9-C11-C12-C13
3	C	302	3EO	C12-C11-N9-C10
3	K	302	3EO	C11-C12-C13-C14
3	G	302	3EO	N9-C11-C12-C13
3	K	302	3EO	C21-C19-C22-N23
3	K	302	3EO	C21-C19-C22-O24
3	G	302	3EO	C11-C12-C13-C14
3	B	302	3EO	C11-C12-C13-C14
3	B	302	3EO	N5-C4-C6-O8
3	F	302	3EO	N5-C4-C6-O8
3	H	302	3EO	N5-C4-C6-O8
3	G	302	3EO	N5-C4-C6-O8
3	L	302	3EO	N5-C4-C6-O8
3	K	302	3EO	N5-C4-C6-O8
3	J	302	3EO	N5-C4-C6-O8
3	C	302	3EO	N5-C4-C6-O8
3	E	302	3EO	N5-C4-C6-O8
3	C	302	3EO	C11-C12-C13-C14
3	L	302	3EO	C11-C12-C13-C14
3	H	302	3EO	C21-C19-N18-C7
3	J	302	3EO	C11-C12-C13-C14
3	H	302	3EO	C11-C12-C13-C14
3	K	302	3EO	C12-C13-C14-C15
3	L	302	3EO	C22-N23-S25-O28
3	F	302	3EO	O32-C1-C2-N5
3	G	302	3EO	N38-C37-C43-N45
3	K	302	3EO	C12-C11-N9-C10
3	E	302	3EO	C11-C12-C13-C14
3	K	302	3EO	C15-C16-C20-C19
3	M	302	3EO	C11-C12-C13-C14

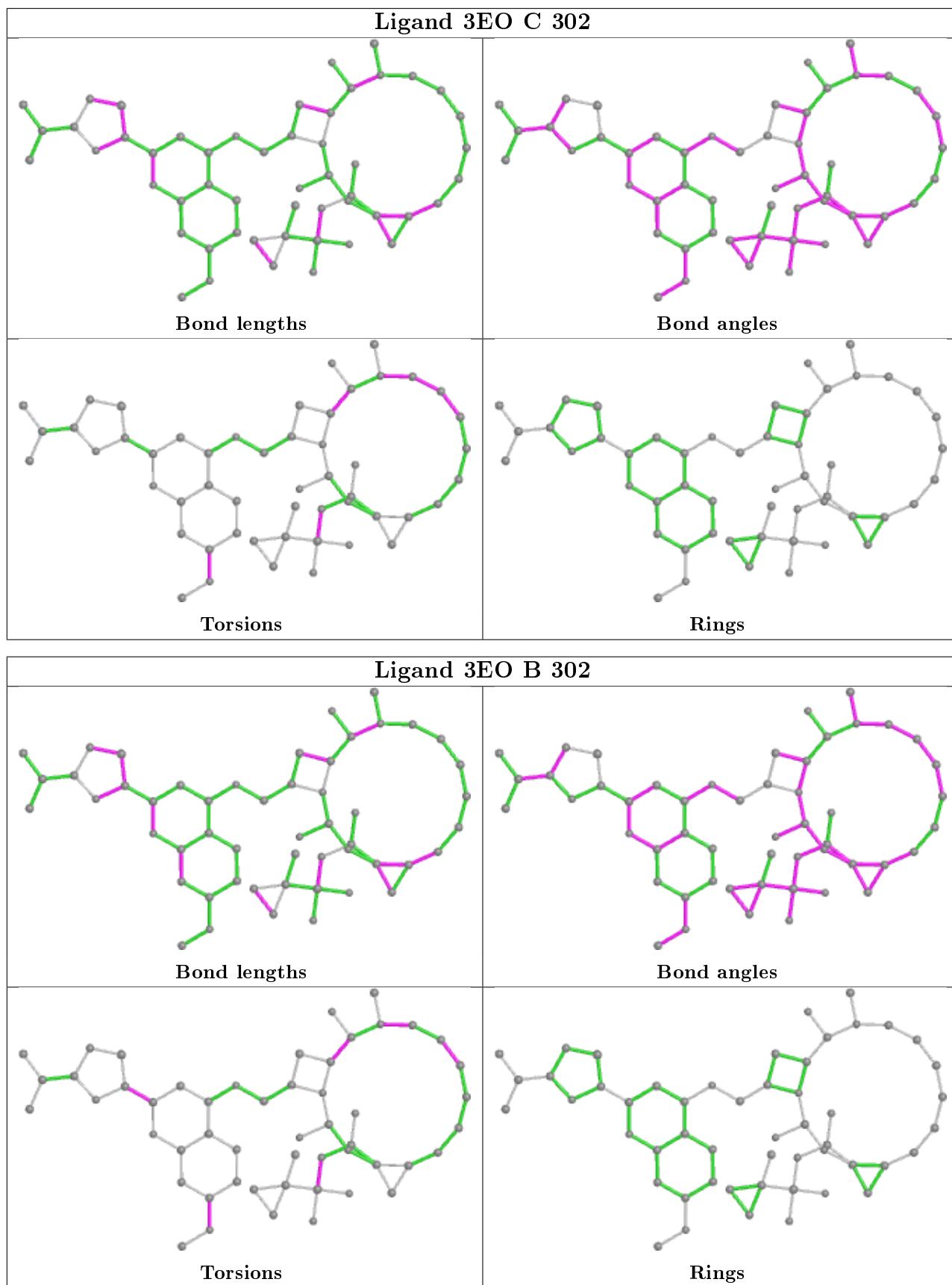
There are no ring outliers.

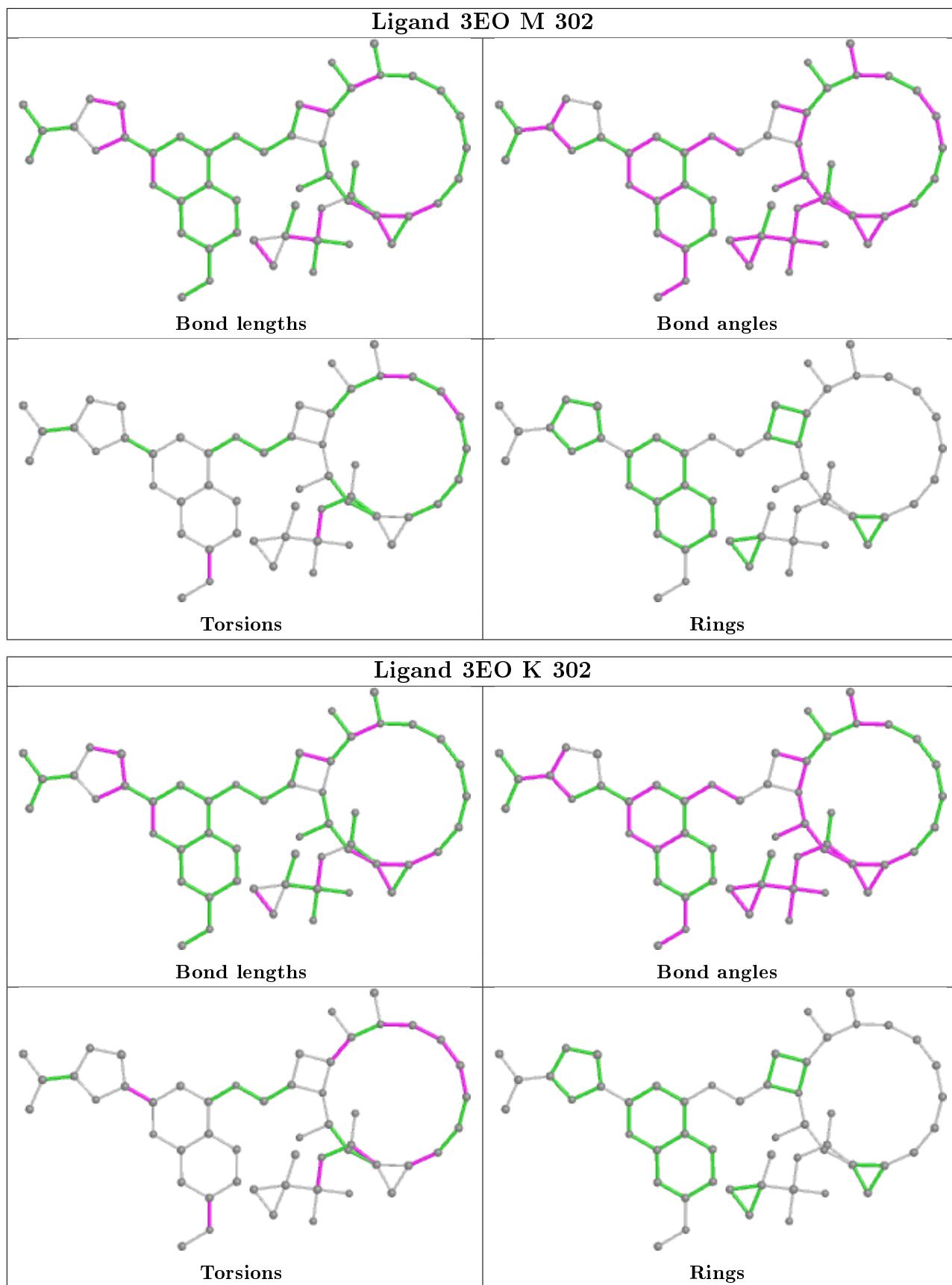
12 monomers are involved in 41 short contacts:

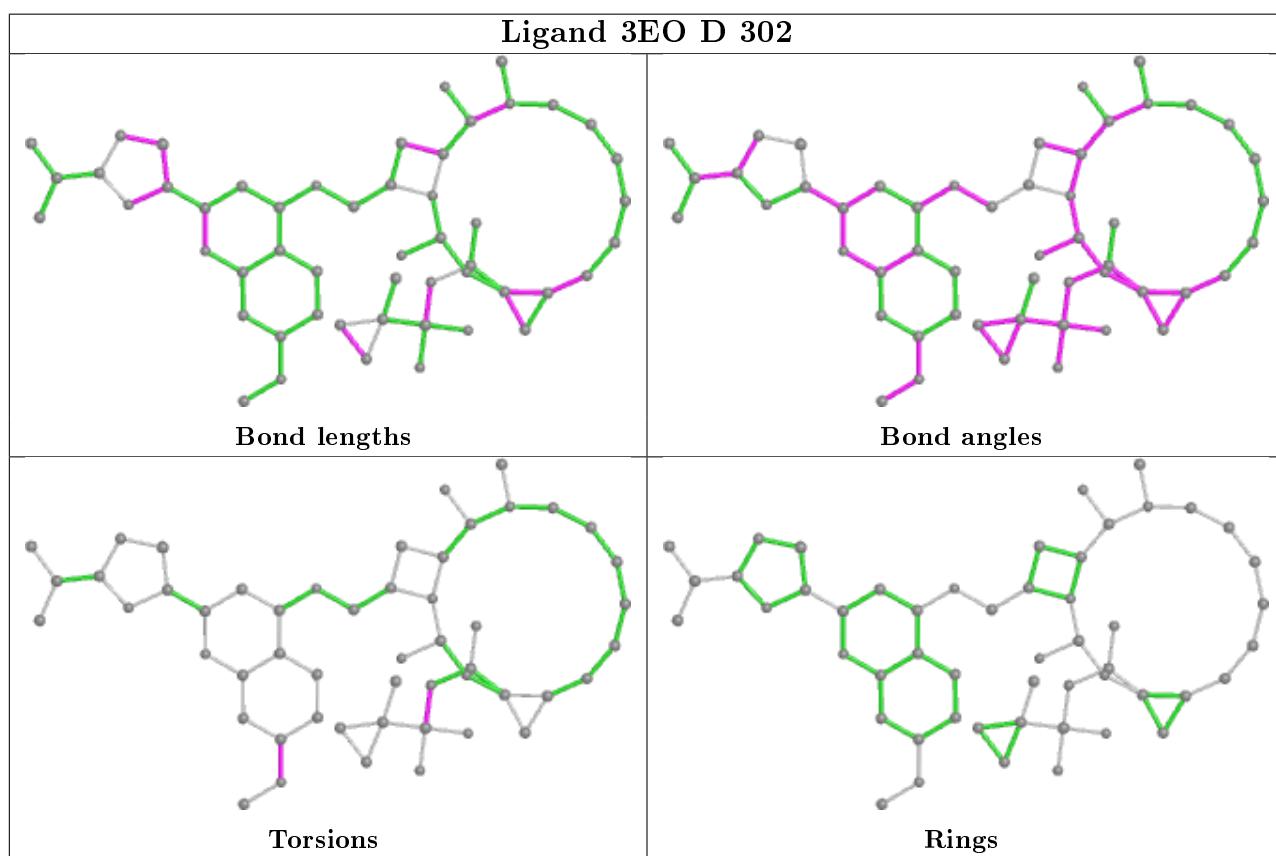
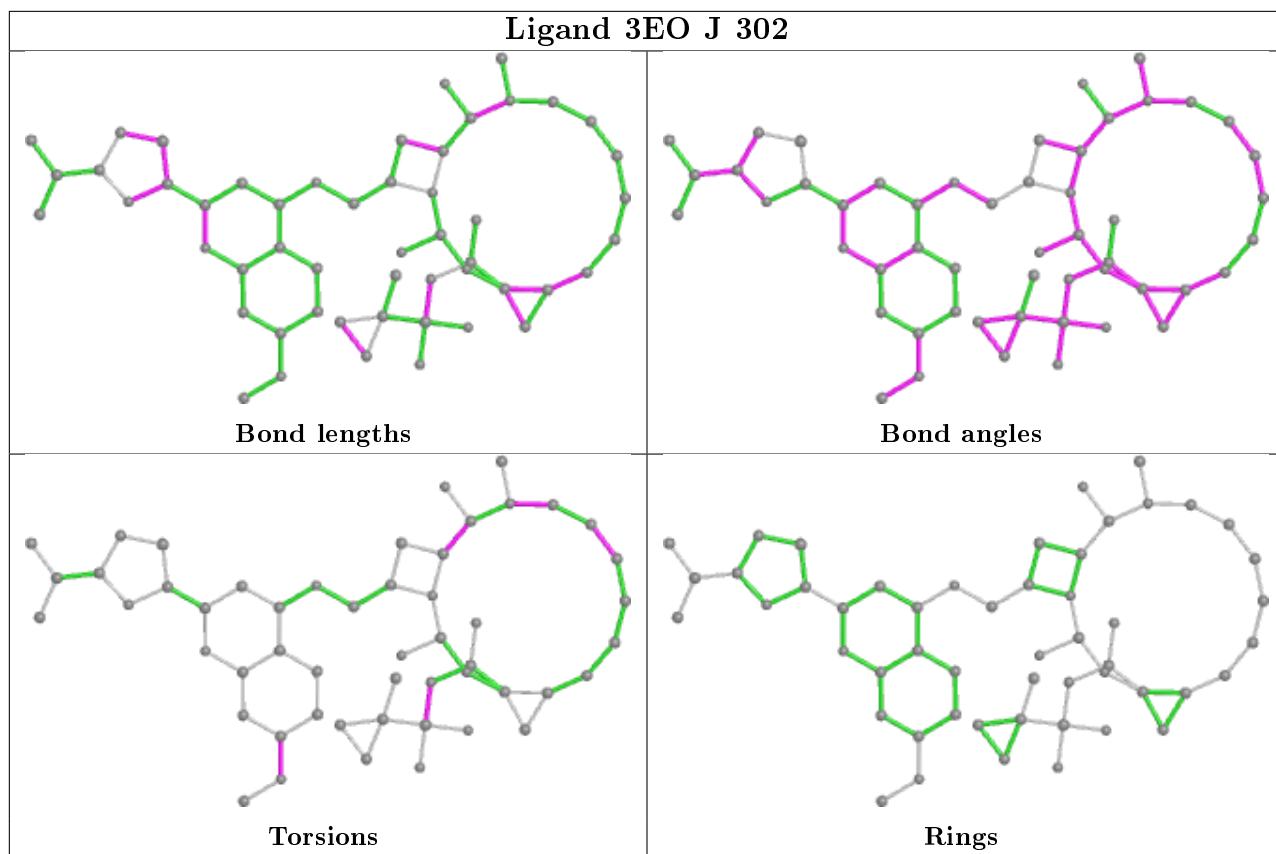
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	302	3EO	2	0
3	A	302	3EO	4	0
3	C	302	3EO	3	0
3	B	302	3EO	3	0
3	M	302	3EO	4	0
3	K	302	3EO	2	0
3	J	302	3EO	5	0
3	D	302	3EO	4	0
3	F	302	3EO	4	0
3	L	302	3EO	3	0
3	H	302	3EO	3	0
3	E	302	3EO	4	0

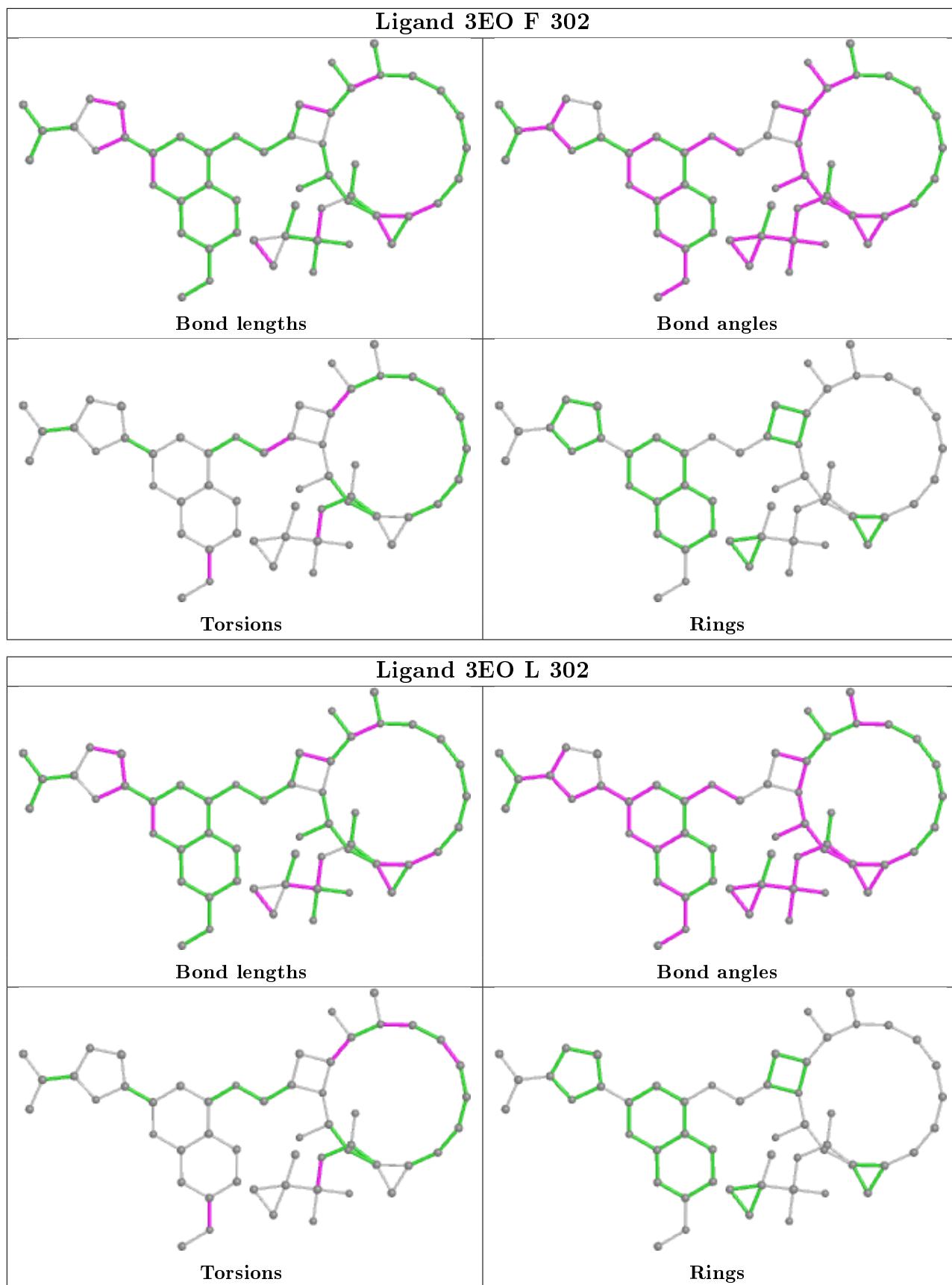
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

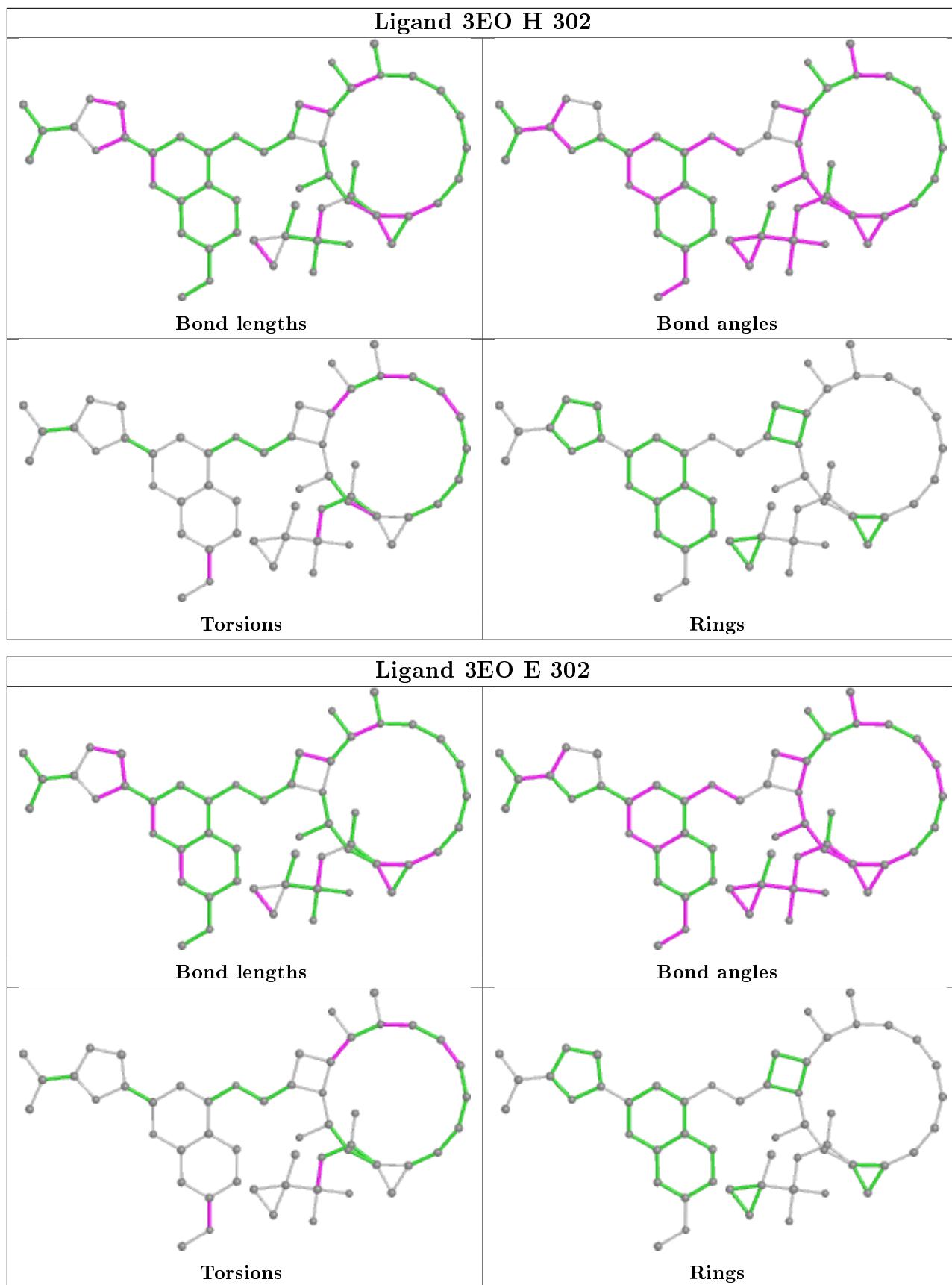












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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

All (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
1	J	181	ALA	4.1
1	F	178	THR	4.1
1	M	2	PRO	4.1
1	L	144	LEU	3.8
1	K	151	VAL	3.8
1	C	182	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	98	THR	3.4
1	D	181	ALA	3.4
1	L	75	TYR	3.3
1	F	3	ILE	3.2
1	K	152	GLY	3.2
1	L	50	GLY	3.2
1	L	175	MET	3.1
1	F	179	MET	3.1
1	F	144	LEU	2.8
1	H	182	SER	2.8
1	L	229	ILE	2.7
1	H	8	GLN	2.7
1	B	181	ALA	2.7
1	C	1	ALA	2.7
1	M	3	ILE	2.7
1	M	89	PRO	2.6
1	D	2	PRO	2.6
1	K	113	VAL	2.5
1	F	1	ALA	2.5
1	H	3	ILE	2.5
1	E	220	LYS	2.5
1	K	68	LYS	2.4
1	D	94	LEU	2.4
1	B	234	ARG	2.4
1	E	1	ALA	2.4
1	M	120	GLY	2.4
1	K	150	ALA	2.4
1	M	91	ALA	2.4
1	K	180	ARG	2.4
1	G	2	PRO	2.3
1	K	178	THR	2.3
1	D	180	ARG	2.3
1	L	86	GLN	2.3
1	H	6	TYR	2.3
1	K	90	GLY	2.2
1	L	47	CYS	2.2
1	M	176	GLU	2.2
1	E	2	PRO	2.2
1	J	75	TYR	2.2
1	M	68	LYS	2.2
1	J	180	ARG	2.1
1	K	2	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	174	SER	2.0
1	F	103	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

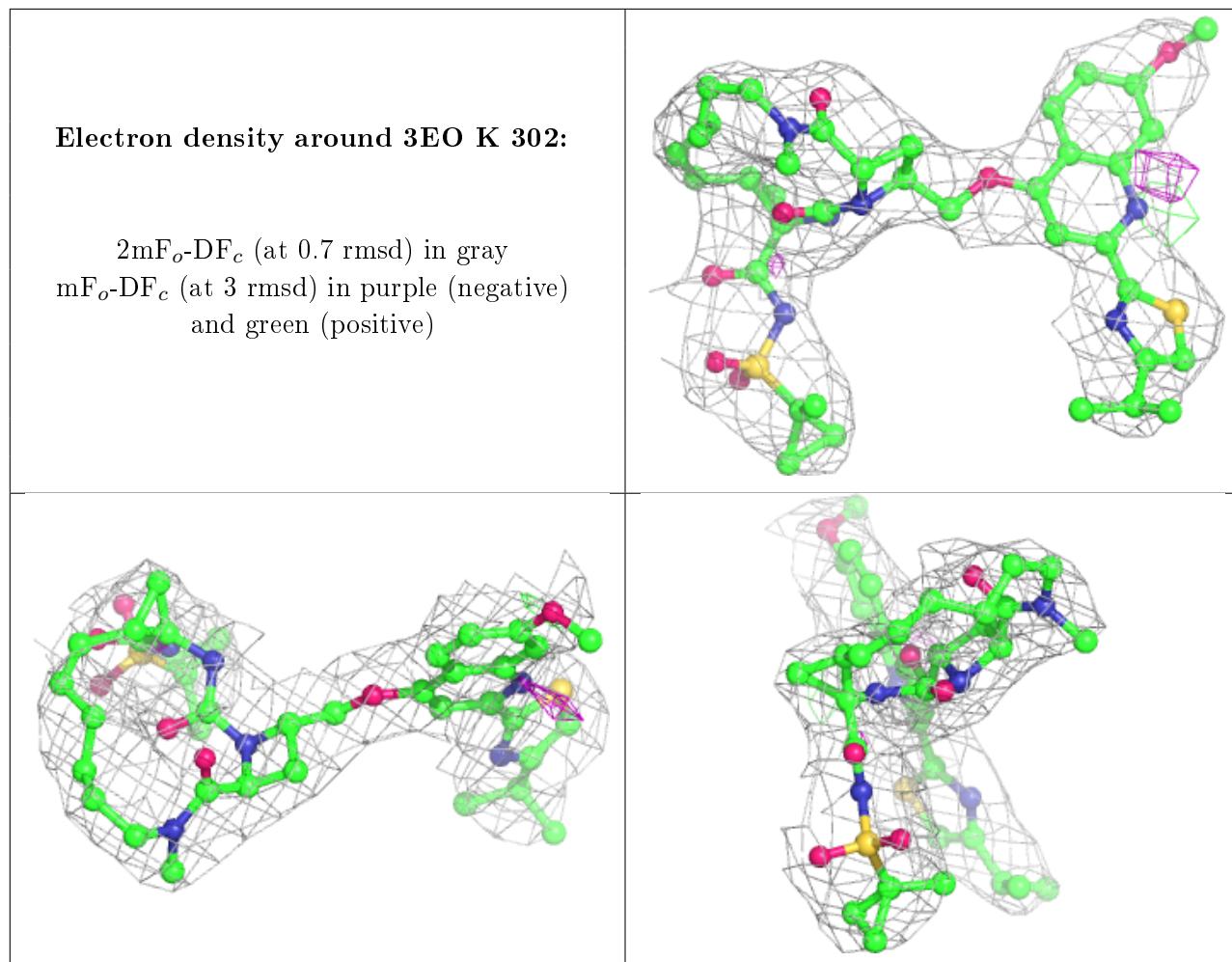
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	F	303	1/1	0.82	0.14	69,69,69,69	0
4	CL	F	304	1/1	0.86	0.08	62,62,62,62	0
4	CL	B	303	1/1	0.87	0.14	68,68,68,68	0
4	CL	C	304	1/1	0.89	0.17	64,64,64,64	0
2	ZN	H	301	1/1	0.89	0.15	120,120,120,120	0
4	CL	E	304	1/1	0.89	0.09	59,59,59,59	0
2	ZN	K	301	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

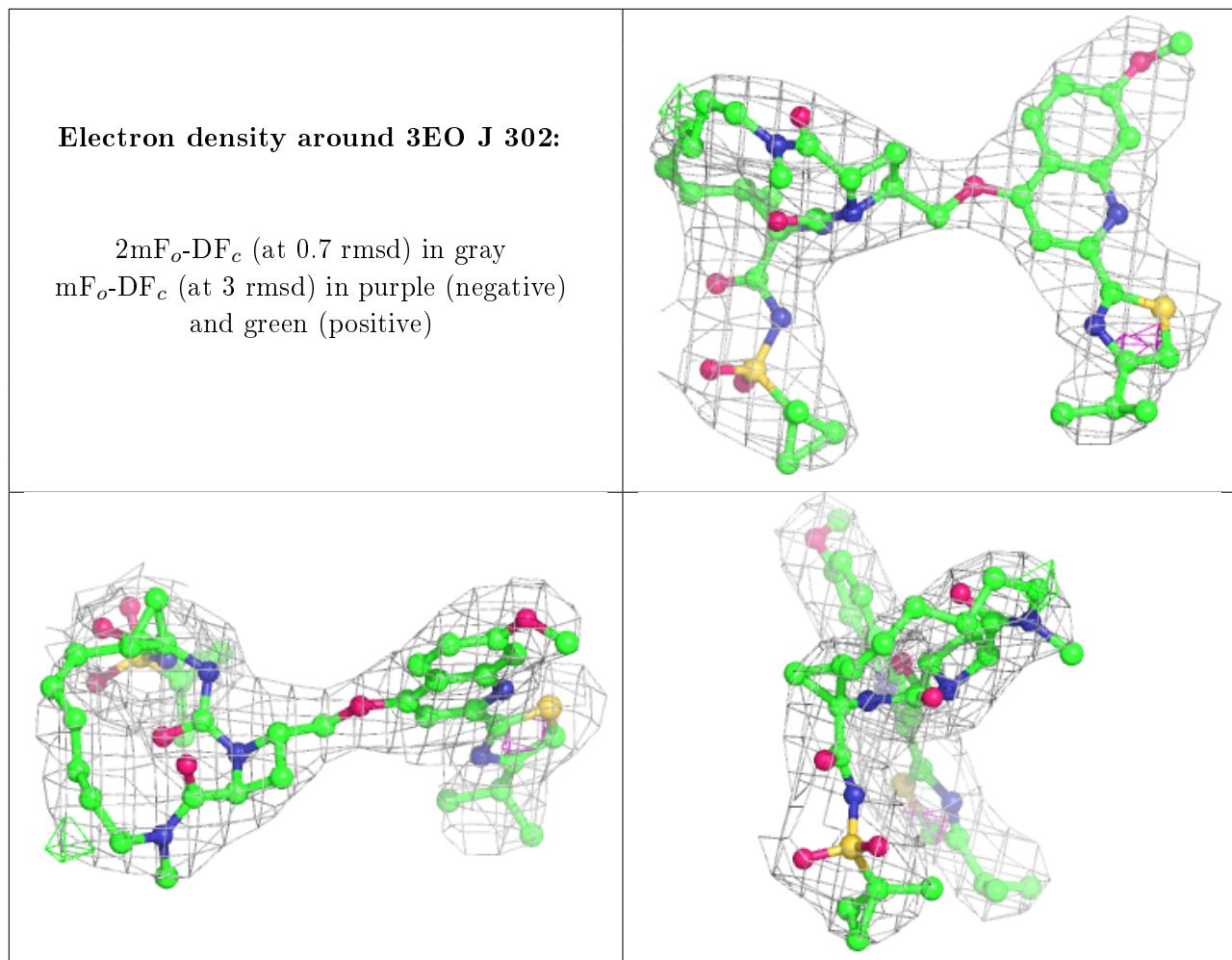
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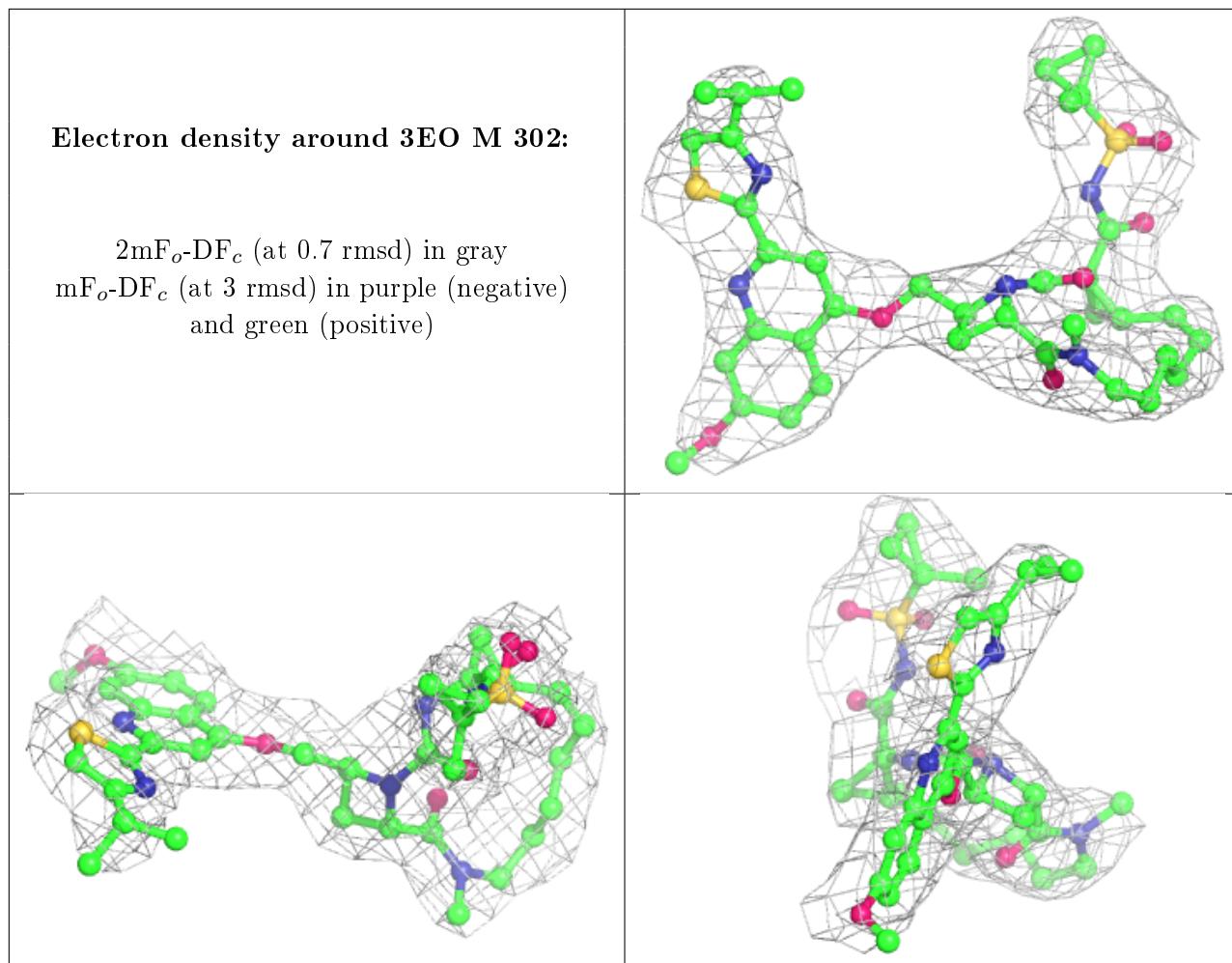
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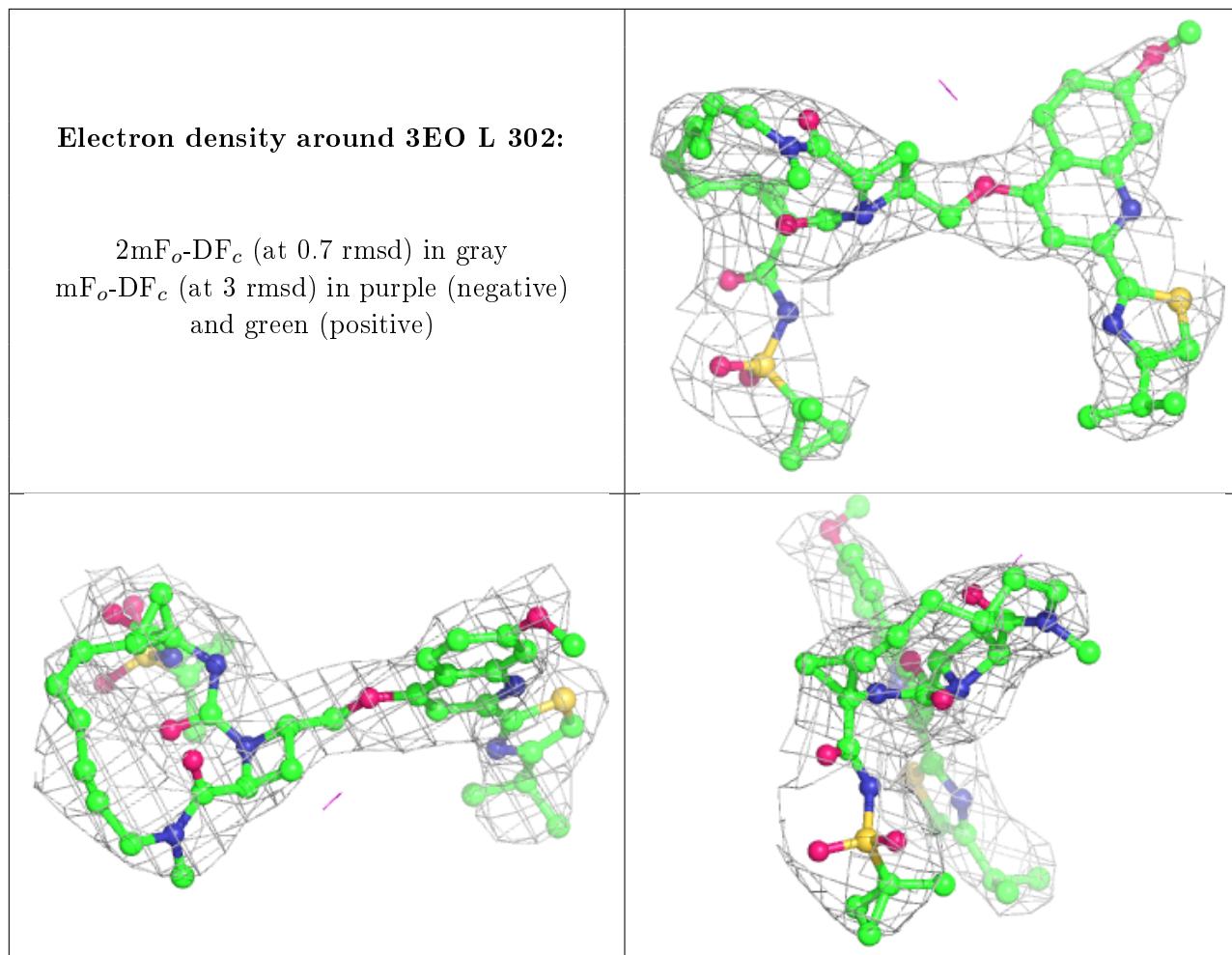
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	3EO	F	302	52/52	0.97	0.17	49,53,58,59	0
3	3EO	B	302	52/52	0.97	0.19	41,51,55,56	0
3	3EO	H	302	52/52	0.97	0.17	51,55,58,59	0
2	ZN	G	301	1/1	0.97	0.09	85,85,85,85	0
2	ZN	C	301	1/1	0.97	0.11	86,86,86,86	0
3	3EO	C	302	52/52	0.97	0.17	48,56,60,61	0
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
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

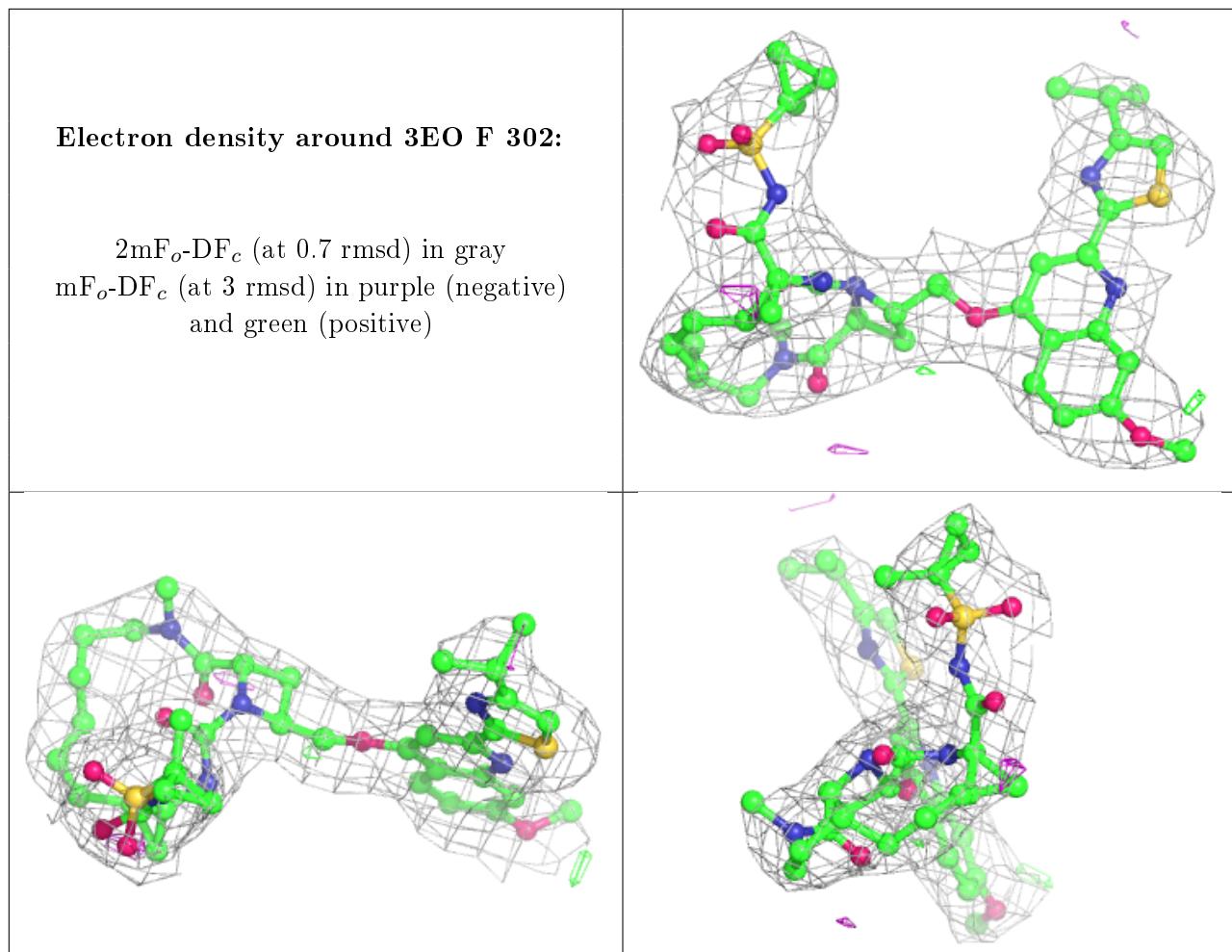
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

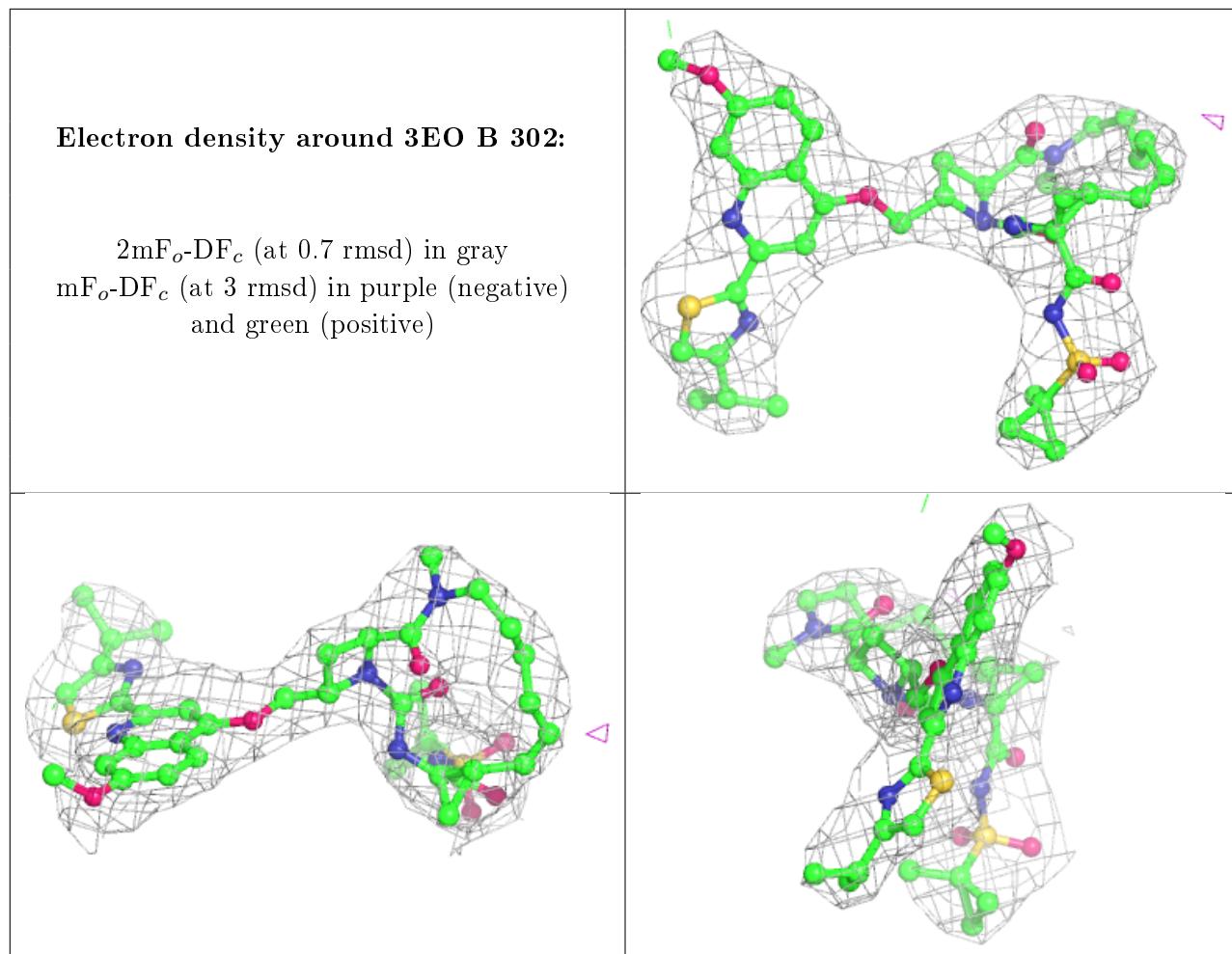


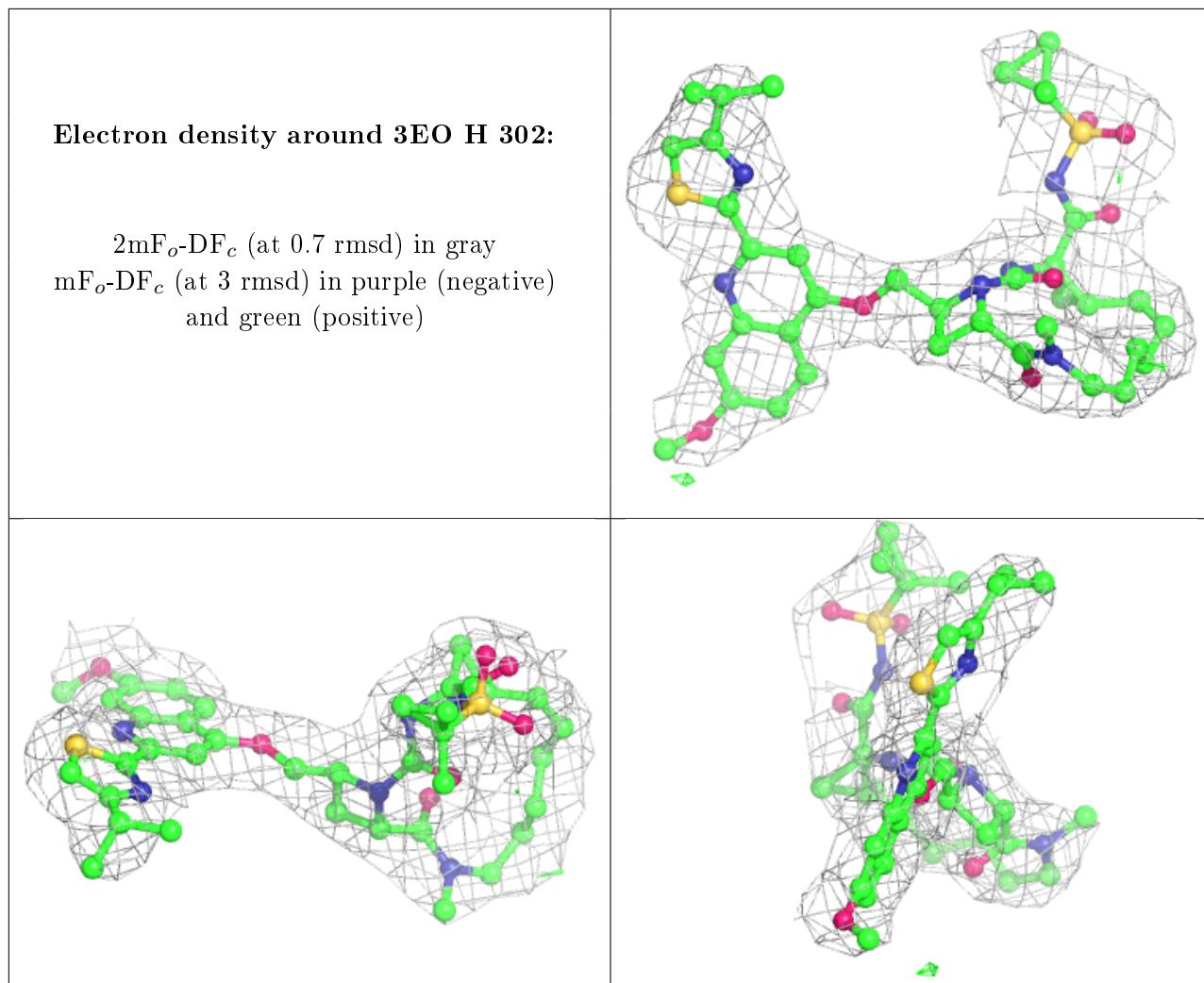


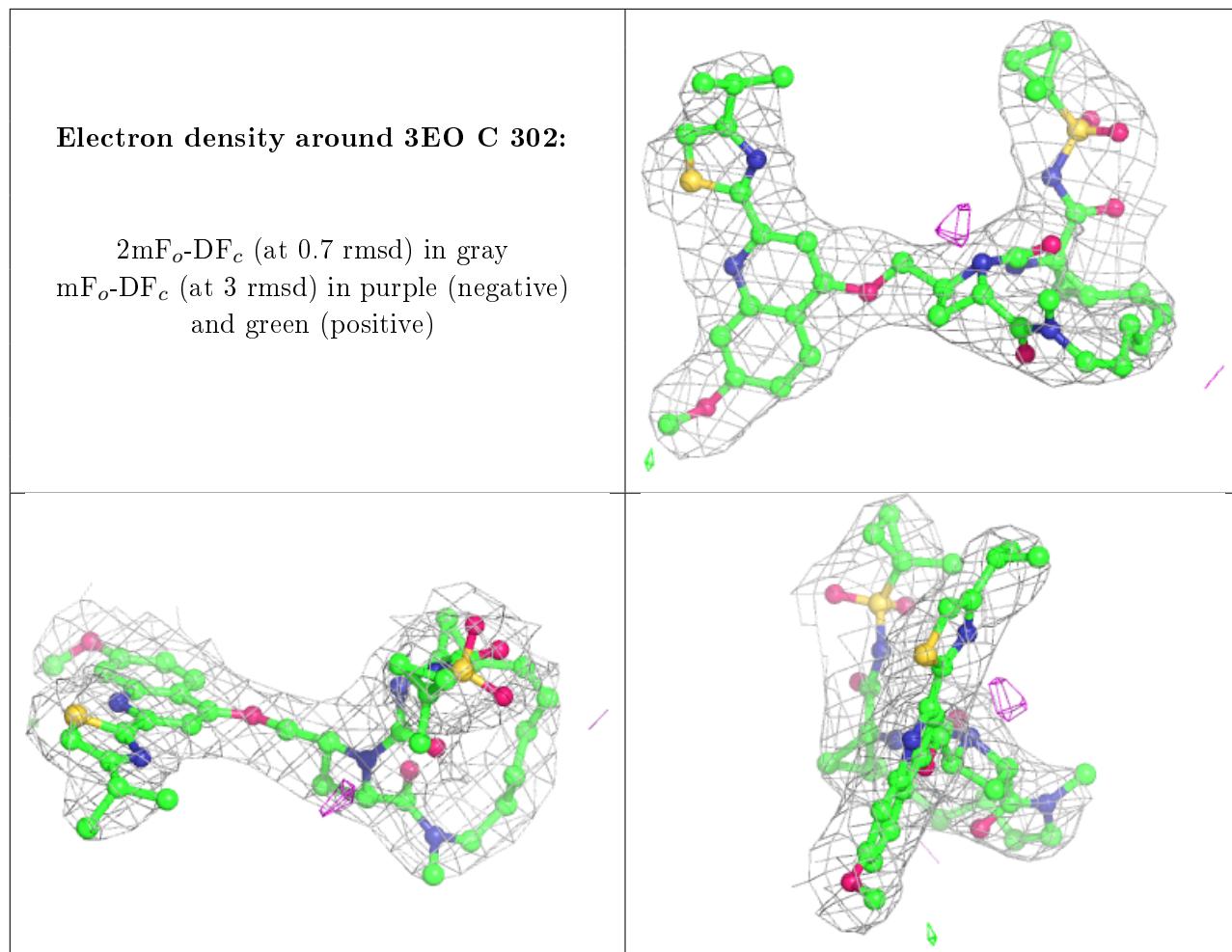


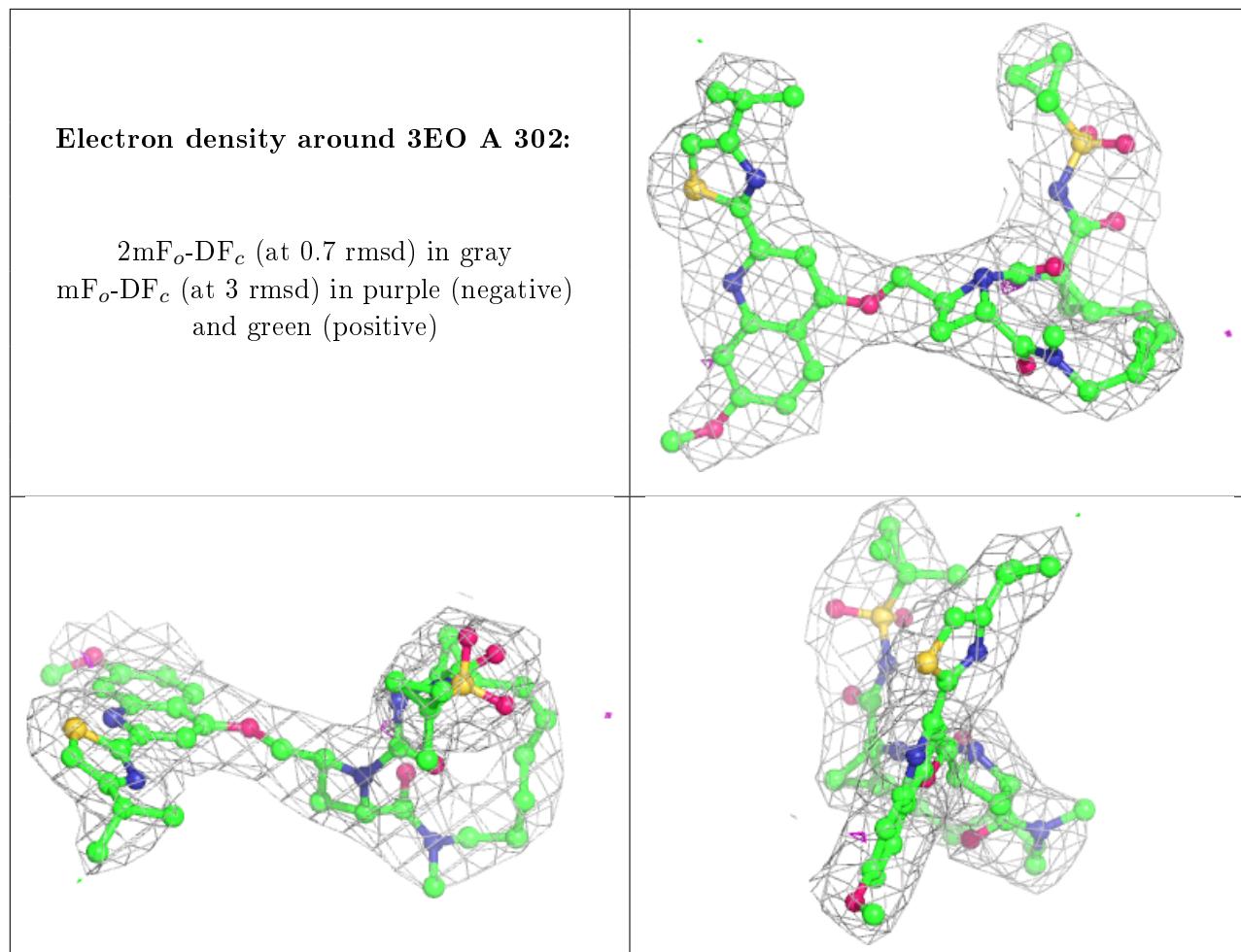


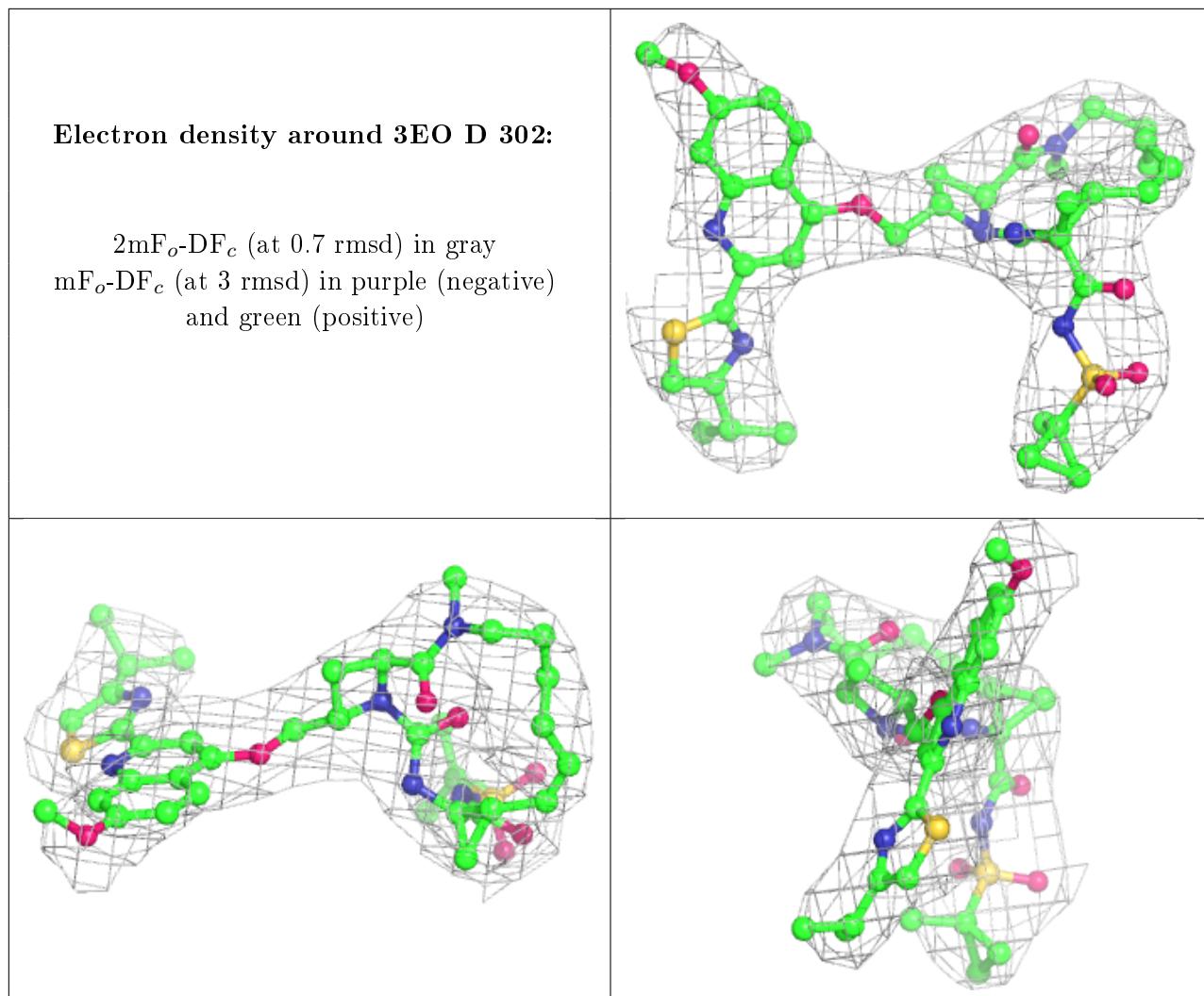


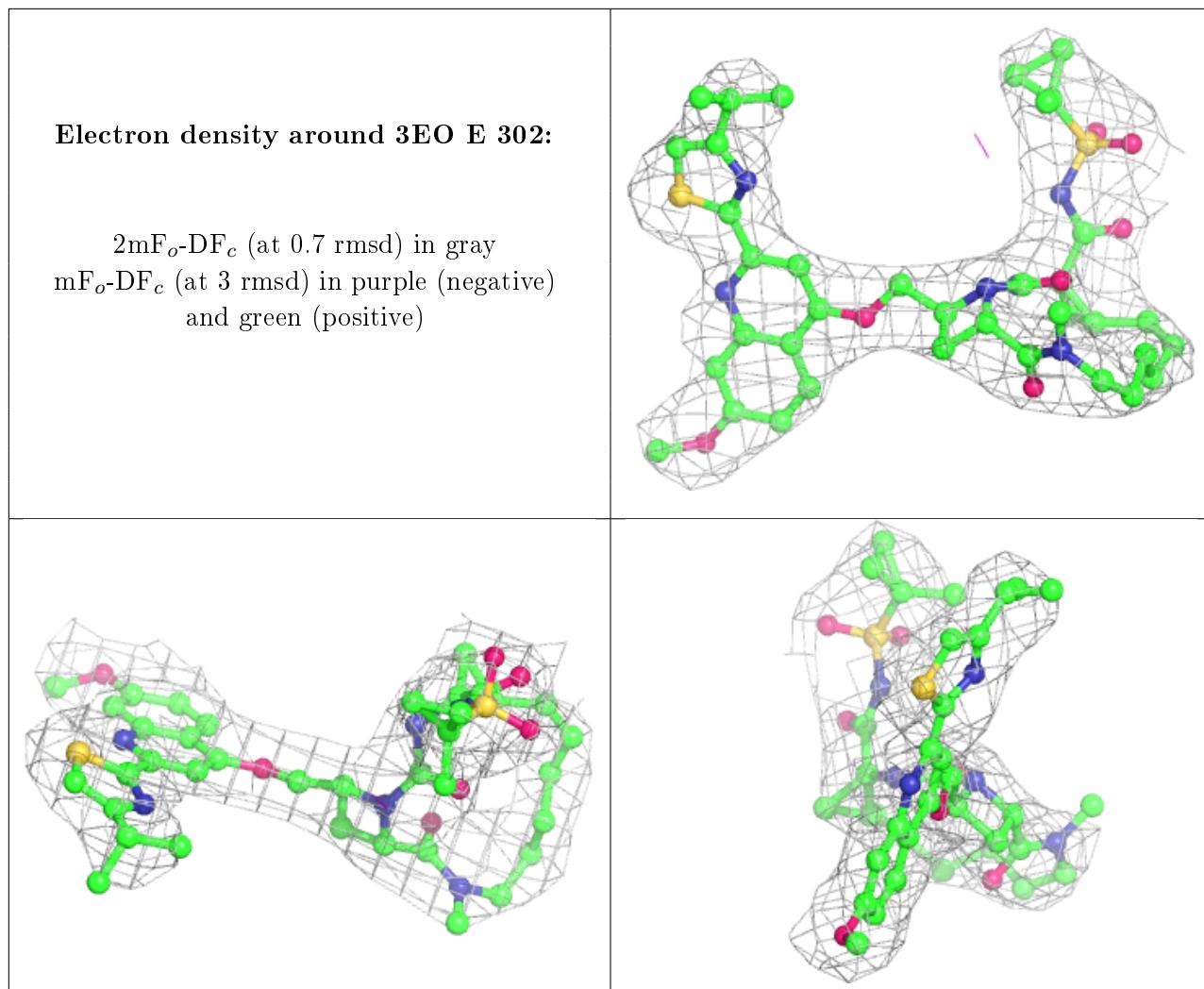


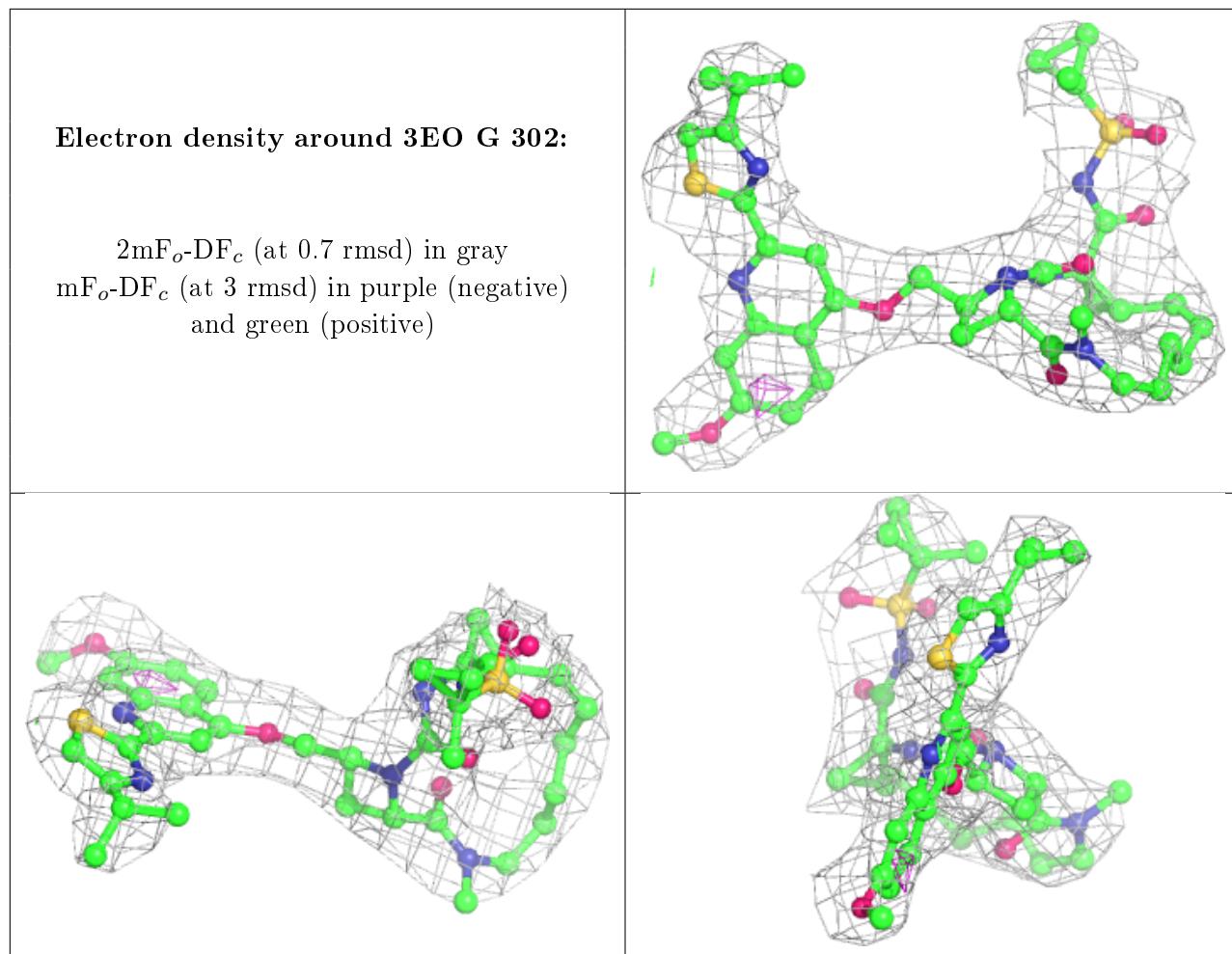












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.