



wwPDB X-ray Structure Validation Summary Report

Sep 19, 2014 – 07:13 AM EDT

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 wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

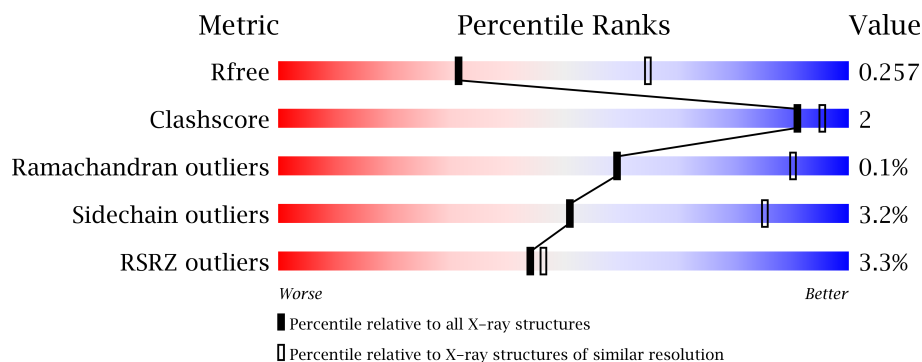
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

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}	66092	2270 (2.88-2.80)
Clashscore	79885	2848 (2.88-2.80)
Ramachandran outliers	78287	2786 (2.88-2.80)
Sidechain outliers	78261	2789 (2.88-2.80)
RSRZ outliers	66119	2274 (2.88-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	203	
1	B	203	
1	C	203	
1	D	203	
1	E	203	
1	F	203	
1	G	203	
1	H	203	
1	J	203	
1	K	203	
1	L	203	
1	M	203	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17686 atoms, of which 0 are hydrogen and 0 are deuterium.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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).

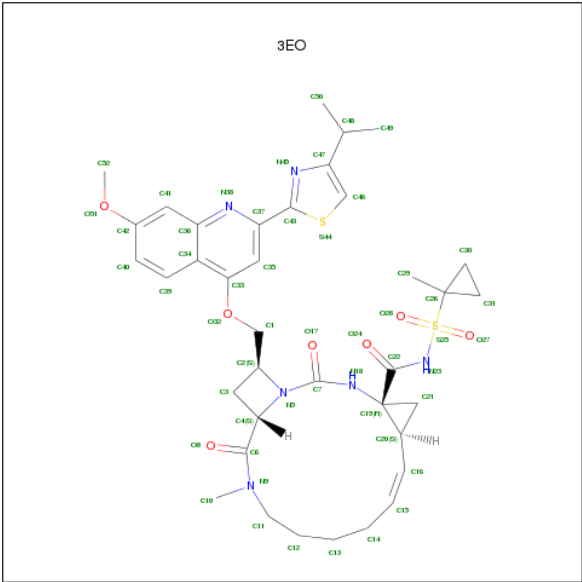
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

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		
3	B	1	Total	C	N	O	S	0	0
			52	37	6	7	2		

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 5 is water.

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

- Molecule 1: NS3 protease

Chain G:



- Molecule 1: NS3 protease

Chain H:



- Molecule 1: NS3 protease

Chain J:



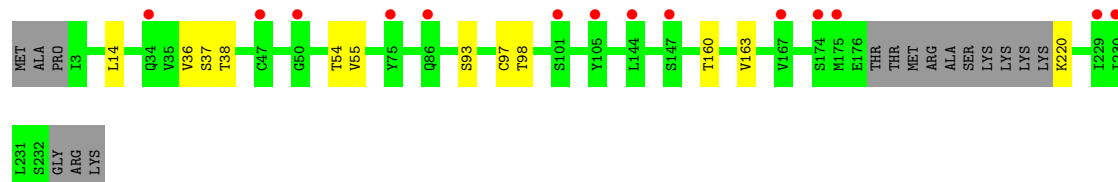
- Molecule 1: NS3 protease

Chain K:



- Molecule 1: NS3 protease

Chain L:



- Molecule 1: NS3 protease

Chain M:



4 Data and refinement statistics

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}	13.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.267 0.215 , 0.257	Depositor DCC
R_{free} test set	997 reflections (1.77%)	DCC
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 , 34.7	EDS
Estimated twinning fraction	0.059 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 57364 reflections	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.

5 Model quality

5.1 Standard geometry

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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1425	0	1448	4	0
1	B	1439	0	1466	7	0
1	C	1439	0	1468	8	0
1	D	1434	0	1462	12	0
1	E	1393	0	1416	7	0
1	F	1430	0	1456	8	0
1	G	1393	0	1416	5	0
1	H	1418	0	1441	5	0
1	J	1439	0	1466	5	0
1	K	1424	0	1451	5	0
1	L	1374	0	1396	6	0
1	M	1430	0	1455	8	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	0	0	0
3	B	52	0	0	0	0
3	C	52	0	0	0	0
3	D	52	0	0	0	0
3	E	52	0	0	0	0
3	F	52	0	0	0	0
3	G	52	0	0	0	0
3	H	52	0	0	0	0
3	J	52	0	0	1	0
3	K	52	0	0	1	0
3	L	52	0	0	0	0
3	M	52	0	0	0	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	1	0	0	0	0
All	All	17686	0	17341	69	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

The worst 5 of 69 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:97:CYS:SG	2:L:301:ZN:ZN	1.52	0.98
1:F:97:CYS:SG	2:F:301:ZN:ZN	1.72	0.79
1:L:97:CYS:HG	2:L:301:ZN:ZN	0.42	0.74
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

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%)	38	75
1	F	191/203 (94%)	185 (97%)	6 (3%)	0	100	100
1	G	186/203 (92%)	181 (97%)	4 (2%)	1 (0%)	38	75
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	59	90

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/165 (96%)	152 (96%)	6 (4%)	44	80
1	B	158/165 (96%)	150 (95%)	8 (5%)	33	68
1	C	159/165 (96%)	154 (97%)	5 (3%)	52	86
1	D	159/165 (96%)	152 (96%)	7 (4%)	39	75
1	E	154/165 (93%)	149 (97%)	5 (3%)	51	85
1	F	158/165 (96%)	155 (98%)	3 (2%)	69	94
1	G	154/165 (93%)	148 (96%)	6 (4%)	43	80
1	H	157/165 (95%)	155 (99%)	2 (1%)	80	97
1	J	158/165 (96%)	152 (96%)	6 (4%)	44	80
1	K	157/165 (95%)	154 (98%)	3 (2%)	69	94
1	L	152/165 (92%)	148 (97%)	4 (3%)	59	89
1	M	158/165 (96%)	152 (96%)	6 (4%)	44	80
All	All	1882/1980 (95%)	1821 (97%)	61 (3%)	51	85

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

Mol	Chain	Res	Type
1	E	98	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	27	ASN
1	G	149	HIS
1	M	27	ASN
1	G	34	GLN
1	H	27	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	302	-	58,58,58	2.16	12 (20%)	86,89,89	3.05	34 (39%)
3	3EO	B	302	-	58,58,58	2.11	12 (20%)	86,89,89	3.05	34 (39%)
3	3EO	C	302	-	58,58,58	2.10	13 (22%)	86,89,89	3.00	36 (41%)
3	3EO	D	302	-	58,58,58	2.13	11 (18%)	86,89,89	3.12	35 (40%)
3	3EO	E	302	-	58,58,58	2.09	12 (20%)	86,89,89	3.01	33 (38%)
3	3EO	F	302	-	58,58,58	2.10	11 (18%)	86,89,89	2.87	33 (38%)
3	3EO	G	302	-	58,58,58	2.14	12 (20%)	86,89,89	3.16	39 (45%)
3	3EO	H	302	-	58,58,58	2.11	12 (20%)	86,89,89	3.17	37 (43%)
3	3EO	J	302	-	58,58,58	2.06	11 (18%)	86,89,89	3.03	36 (41%)
3	3EO	K	302	-	58,58,58	2.13	11 (18%)	86,89,89	3.12	36 (41%)
3	3EO	L	302	-	58,58,58	2.16	11 (18%)	86,89,89	3.00	35 (40%)
3	3EO	M	302	-	58,58,58	2.08	13 (22%)	86,89,89	3.09	38 (44%)

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	A	302	-	-	0/46/85/85	0/4/7/7
3	3EO	B	302	-	-	0/46/85/85	0/4/7/7
3	3EO	C	302	-	-	0/46/85/85	0/4/7/7
3	3EO	D	302	-	-	0/46/85/85	0/4/7/7
3	3EO	E	302	-	-	0/46/85/85	0/4/7/7
3	3EO	F	302	-	-	0/46/85/85	0/4/7/7
3	3EO	G	302	-	-	0/46/85/85	0/4/7/7
3	3EO	H	302	-	-	0/46/85/85	0/4/7/7
3	3EO	J	302	-	-	0/46/85/85	0/4/7/7
3	3EO	K	302	-	-	0/46/85/85	0/4/7/7
3	3EO	L	302	-	-	0/46/85/85	0/4/7/7
3	3EO	M	302	-	-	0/46/85/85	0/4/7/7

The worst 5 of 141 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

The worst 5 of 426 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	3EO	N18-C7-N5	15.72	126.94	116.83
3	H	302	3EO	N18-C7-N5	15.13	126.55	116.83
3	D	302	3EO	N18-C7-N5	14.98	126.46	116.83
3	M	302	3EO	N18-C7-N5	14.87	126.39	116.83
3	G	302	3EO	N18-C7-N5	14.73	126.30	116.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.01	0 100 100	48, 64, 91, 123	0
1	B	196/203 (96%)	-0.06	4 (2%) 62 65	43, 60, 85, 117	0
1	C	196/203 (96%)	0.11	3 (1%) 70 72	47, 62, 92, 113	0
1	D	195/203 (96%)	0.03	5 (2%) 53 56	47, 64, 92, 124	0
1	E	190/203 (93%)	0.05	5 (2%) 53 56	42, 63, 97, 122	0
1	F	195/203 (96%)	0.24	9 (4%) 31 33	45, 67, 104, 130	0
1	G	190/203 (93%)	0.05	3 (1%) 68 70	40, 64, 91, 126	0
1	H	193/203 (95%)	-0.05	6 (3%) 47 49	48, 74, 111, 135	0
1	J	196/203 (96%)	0.05	7 (3%) 41 42	50, 72, 97, 120	0
1	K	194/203 (95%)	0.51	11 (5%) 23 23	55, 84, 114, 142	0
1	L	187/203 (92%)	0.53	14 (7%) 14 13	54, 87, 113, 130	0
1	M	195/203 (96%)	0.24	9 (4%) 31 33	46, 70, 105, 129	0
All	All	2321/2436 (95%)	0.14	76 (3%) 44 46	40, 69, 107, 142	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1	ALA	6.1
1	M	90	GLY	5.1
1	M	2	PRO	4.9
1	B	1	ALA	4.7
1	L	144	LEU	4.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	D	301	1/1	0.18	1.97	94,94,94,94	0
2	ZN	B	301	1/1	0.20	1.02	77,77,77,77	0
4	CL	M	303	1/1	0.20	1.01	54,54,54,54	0
3	3EO	G	302	52/52	0.20	0.98	47,51,55,55	0
3	3EO	B	302	52/52	0.19	0.72	41,51,55,56	0
3	3EO	A	302	52/52	0.18	0.64	43,49,51,53	0
3	3EO	E	302	52/52	0.18	0.56	45,51,56,57	0
2	ZN	H	301	1/1	0.15	0.41	120,120,120,120	0
3	3EO	L	302	52/52	0.20	0.37	63,66,74,74	0
2	ZN	J	301	1/1	0.15	0.31	92,92,92,92	0
3	3EO	H	302	52/52	0.18	0.28	51,55,58,59	0
4	CL	E	303	1/1	0.17	0.21	46,46,46,46	0
3	3EO	J	302	52/52	0.19	0.21	55,59,64,65	0
3	3EO	D	302	52/52	0.18	0.16	46,53,60,61	0
3	3EO	M	302	52/52	0.17	0.12	45,56,70,71	0
3	3EO	K	302	52/52	0.19	0.09	59,64,72,73	0
3	3EO	F	302	52/52	0.17	-0.17	49,53,58,59	0
3	3EO	C	302	52/52	0.17	-0.24	48,56,60,61	0
4	CL	C	304	1/1	0.16	-0.29	64,64,64,64	0
2	ZN	A	301	1/1	0.11	-0.57	80,80,80,80	0
4	CL	B	303	1/1	0.16	-0.66	68,68,68,68	0
4	CL	A	303	1/1	0.16	-0.77	55,55,55,55	0
2	ZN	M	301	1/1	0.11	-0.80	77,77,77,77	0
2	ZN	E	301	1/1	0.12	-0.80	53,53,53,53	0
2	ZN	G	301	1/1	0.09	-1.23	85,85,85,85	0
2	ZN	C	301	1/1	0.10	-1.24	86,86,86,86	0
4	CL	F	303	1/1	0.12	-1.34	69,69,69,69	0
2	ZN	L	301	1/1	0.10	-1.82	120,120,120,120	0
2	ZN	F	301	1/1	0.10	-1.90	96,96,96,96	0
4	CL	E	304	1/1	0.09	-2.57	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CL	C	303	1/1	0.11	-2.72	55,55,55,55	0
2	ZN	K	301	1/1	0.07	-3.06	123,123,123,123	0
4	CL	F	304	1/1	0.07	-3.20	62,62,62,62	0
4	CL	F	305	1/1	0.11	-3.32	55,55,55,55	0
4	CL	H	303	1/1	0.08	-4.93	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.