Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:42 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

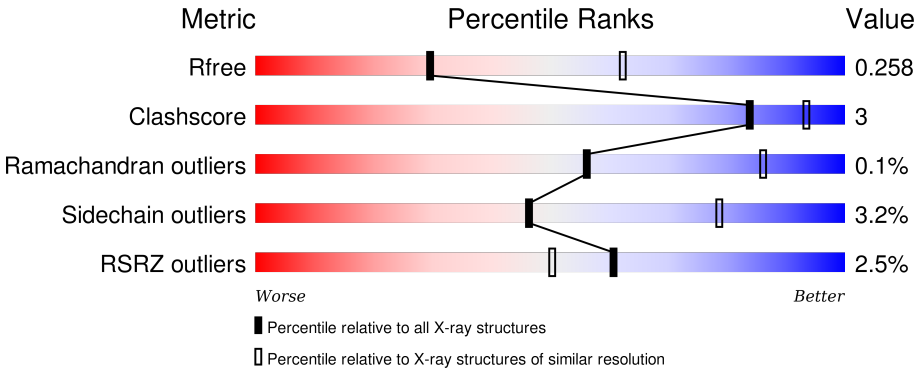
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 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}	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	203	89% 6% ·
1	B	203	% 89% 7% ·
1	C	203	% 88% 8% ·
1	D	203	2% 85% 10% ·
1	E	203	% 85% 8% 6%

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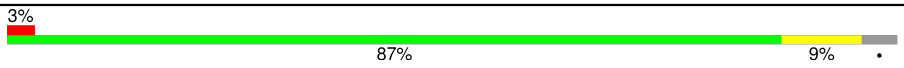
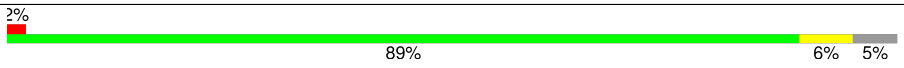
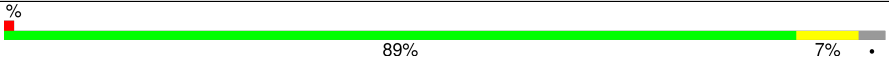
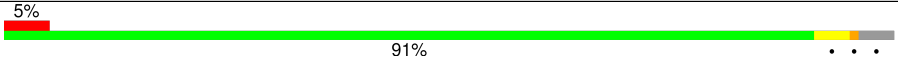
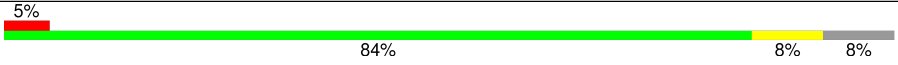
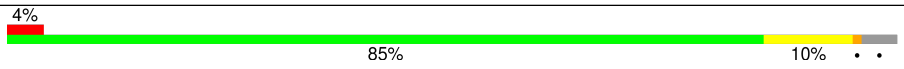
Mol	Chain	Length	Quality of chain
1	F	203	
1	G	203	
1	H	203	
1	J	203	
1	K	203	
1	L	203	
1	M	203	

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

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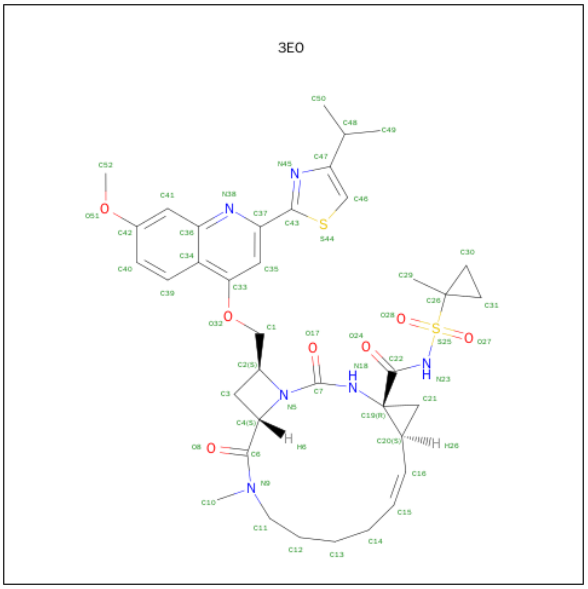
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	M	1	Total Zn 1 1	0	0

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



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

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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.

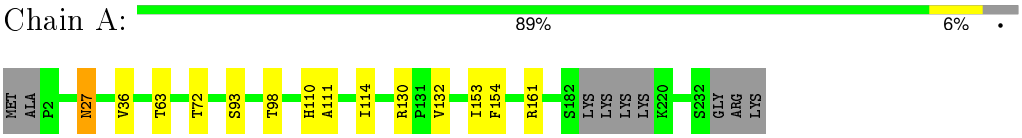
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

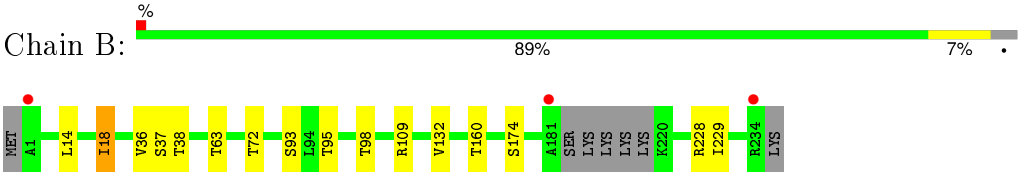
- Molecule 1: NS3 protease

Chain A:



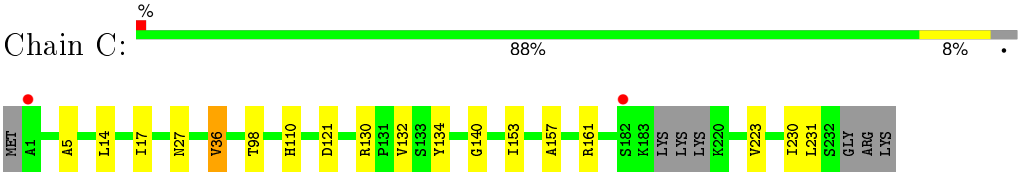
- Molecule 1: NS3 protease

Chain B:



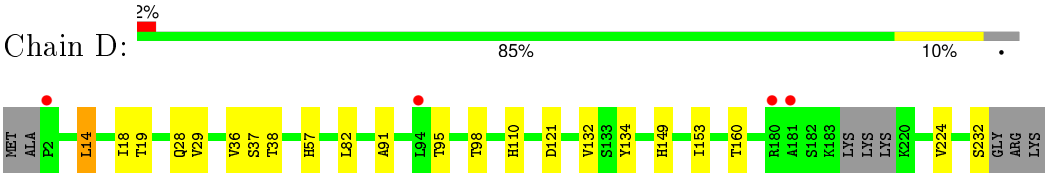
- Molecule 1: NS3 protease

Chain C:



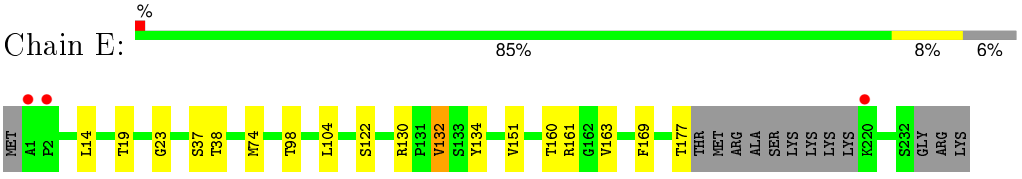
- Molecule 1: NS3 protease

Chain D:



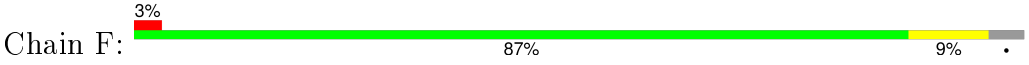
- Molecule 1: NS3 protease

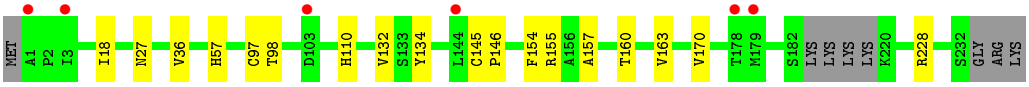
Chain E:



- Molecule 1: NS3 protease

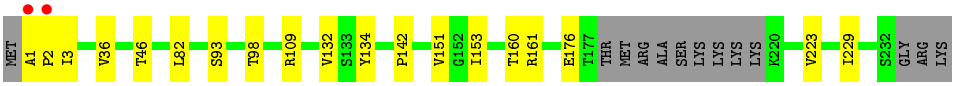
Chain F:





• Molecule 1: NS3 protease

Chain G:



• Molecule 1: NS3 protease

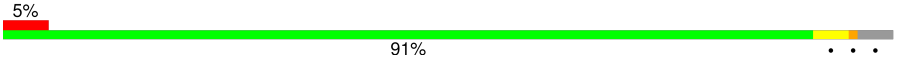
Chain H:

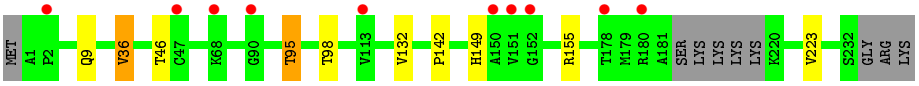
• Molecule 1: NS3 protease

Chain J:

• Molecule 1: NS3 protease

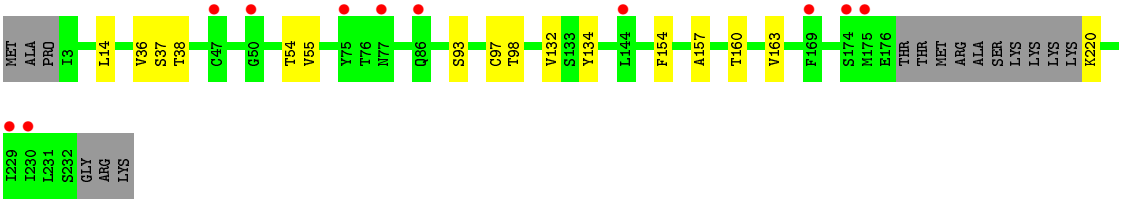
Chain K:





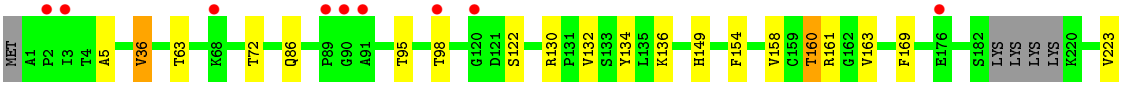
• Molecule 1: NS3 protease

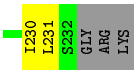
Chain L:



• Molecule 1: NS3 protease

Chain M:




I230
L231
S232
GLY
ARG
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	140.69Å 143.20Å 240.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.84 49.12 – 2.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-2.84) 99.7 (49.12-2.84)	Depositor EDS
R_{merge}	13.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.267 0.214 , 0.258	Depositor DCC
R_{free} test set	997 reflections (1.77%)	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[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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

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:HD11	1:D:18:ILE:HD13	1.96	0.48
1:B:18:ILE:HG12	1:D:18:ILE:HD13	1.95	0.48
1:C:27:ASN:HD22	1:F:27:ASN:HD22	1.60	0.48
1:K:155:ARG:HG2	3:K:302:3EO:C39	2.45	0.47
1:A:27:ASN:HD22	1:A:27:ASN:N	2.12	0.47
1:H:5:ALA:HB2	1:H:231:LEU:HD23	1.96	0.47
1:D:82:LEU:CD1	1:D:153:ILE:HD11	2.44	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:L:154:PHE:CE2	3:L:302:3EO:H13	2.51	0.46
1:K:46:THR:HG21	1:K:142:PRO:HB3	1.96	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:F:97:CYS:HG	2:F:301:ZN:ZN	1.24	0.45
1:B:14:LEU:HG	1:C:17:ILE:HG21	1.98	0.45
1:D:57:HIS:HB2	3:D:302:3EO:H40	1.99	0.45
1:C:157:ALA:HB3	3:C:302:3EO:H28	1.99	0.44
1:A:114:ILE:HG23	1:A:130:ARG:NH1	2.32	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: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:G:82:LEU:CD1	1:G:153:ILE:HD11	2.47	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:F:160:THR:O	1:F:163:VAL:HG12	2.18	0.43
1:C:5:ALA:HB2	1:C:231:LEU:HD23	2.01	0.43
1:L:160:THR:O	1:L:163:VAL:HG12	2.19	0.42
1:C:140:GLY:HA2	1:C:153:ILE:HD12	2.01	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:N	1:J:230:ILE:HD12	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: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:110:HIS:O	1:A:111:ALA:HB3	2.21	0.41
1:M:154:PHE:CE2	3:M:302:3EO:H13	2.56	0.41
1:K:9:GLN:OE1	1:L:220:LYS:N	2.54	0.41
1:A:63:THR:HG22	1:A:72:THR:HA	2.02	0.41
1:D:14:LEU:HD11	1:E:14:LEU:CD1	2.51	0.41
1:H:161:ARG:HG2	1:M:158:VAL:HG13	2.02	0.41
1:J:29:VAL:HG11	1:J:91:ALA:HB2	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:M:160:THR:O	1:M:163:VAL:HG12	2.21	0.40
1:E:122:SER:HB2	1:E:169:PHE:O	2.21	0.40
1:C:14:LEU:HB3	1:F:18:ILE:HD11	2.02	0.40

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%)	34	67
1	F	191/203 (94%)	185 (97%)	6 (3%)	0	100	100
1	G	186/203 (92%)	181 (97%)	4 (2%)	1 (0%)	34	67
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%)	56	86

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%)	40 73
1	B	158/165 (96%)	150 (95%)	8 (5%)	29 61
1	C	159/165 (96%)	154 (97%)	5 (3%)	47 79
1	D	159/165 (96%)	152 (96%)	7 (4%)	35 68
1	E	154/165 (93%)	149 (97%)	5 (3%)	46 79
1	F	158/165 (96%)	155 (98%)	3 (2%)	65 89
1	G	154/165 (93%)	148 (96%)	6 (4%)	39 72
1	H	157/165 (95%)	155 (99%)	2 (1%)	76 93
1	J	158/165 (96%)	152 (96%)	6 (4%)	40 73
1	K	157/165 (95%)	154 (98%)	3 (2%)	65 89
1	L	152/165 (92%)	148 (97%)	4 (3%)	54 84
1	M	158/165 (96%)	152 (96%)	6 (4%)	40 73
All	All	1882/1980 (95%)	1821 (97%)	61 (3%)	46 79

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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 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	-	51,58,58	2.25	9 (17%)	57,89,89	1.84	14 (24%)
3	3EO	B	302	-	51,58,58	2.22	10 (19%)	57,89,89	2.12	15 (26%)
3	3EO	C	302	-	51,58,58	2.19	10 (19%)	57,89,89	2.15	15 (26%)
3	3EO	D	302	-	51,58,58	2.24	9 (17%)	57,89,89	1.97	15 (26%)
3	3EO	E	302	-	51,58,58	2.19	10 (19%)	57,89,89	2.01	14 (24%)
3	3EO	F	302	-	51,58,58	2.20	9 (17%)	57,89,89	1.93	15 (26%)
3	3EO	G	302	-	51,58,58	2.25	9 (17%)	57,89,89	2.16	17 (29%)
3	3EO	H	302	-	51,58,58	2.22	10 (19%)	57,89,89	2.18	17 (29%)
3	3EO	J	302	-	51,58,58	2.17	9 (17%)	57,89,89	2.15	17 (29%)
3	3EO	K	302	-	51,58,58	2.24	9 (17%)	57,89,89	2.29	16 (28%)
3	3EO	L	302	-	51,58,58	2.28	9 (17%)	57,89,89	2.11	16 (28%)
3	3EO	M	302	-	51,58,58	2.17	9 (17%)	57,89,89	2.08	18 (31%)

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	-	-	0/42/85/85	0/4/7/7
3	3EO	B	302	-	-	0/42/85/85	0/4/7/7
3	3EO	C	302	-	-	0/42/85/85	0/4/7/7
3	3EO	D	302	-	-	0/42/85/85	0/4/7/7
3	3EO	E	302	-	-	0/42/85/85	0/4/7/7
3	3EO	F	302	-	-	0/42/85/85	0/4/7/7
3	3EO	G	302	-	-	0/42/85/85	0/4/7/7
3	3EO	H	302	-	-	0/42/85/85	0/4/7/7
3	3EO	J	302	-	-	0/42/85/85	0/4/7/7
3	3EO	K	302	-	-	0/42/85/85	0/4/7/7
3	3EO	L	302	-	-	0/42/85/85	0/4/7/7
3	3EO	M	302	-	-	0/42/85/85	0/4/7/7

All (112) 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	D	302	3EO	C3-C4	-3.00	1.51	1.55
3	M	302	3EO	C3-C4	-2.85	1.51	1.55
3	F	302	3EO	C3-C4	-2.77	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	3EO	C3-C4	-2.75	1.51	1.55
3	H	302	3EO	C3-C4	-2.72	1.52	1.55
3	J	302	3EO	C3-C4	-2.71	1.52	1.55
3	E	302	3EO	C3-C4	-2.71	1.52	1.55
3	L	302	3EO	C3-C4	-2.70	1.52	1.55
3	K	302	3EO	C3-C4	-2.67	1.52	1.55
3	C	302	3EO	C3-C4	-2.61	1.52	1.55
3	B	302	3EO	C3-C4	-2.56	1.52	1.55
3	G	302	3EO	C3-C4	-2.50	1.52	1.55
3	E	302	3EO	C41-C36	-2.15	1.38	1.41
3	C	302	3EO	C34-C36	-2.03	1.39	1.42
3	B	302	3EO	C41-C36	-2.01	1.38	1.41
3	H	302	3EO	C19-N18	2.07	1.49	1.45
3	E	302	3EO	C43-N45	2.09	1.34	1.31
3	H	302	3EO	C43-N45	2.24	1.34	1.31
3	D	302	3EO	C6-N9	2.29	1.39	1.35
3	C	302	3EO	C43-N45	2.31	1.34	1.31
3	B	302	3EO	C6-N9	2.41	1.39	1.35
3	F	302	3EO	C6-N9	2.43	1.39	1.35
3	J	302	3EO	C43-N45	2.43	1.35	1.31
3	G	302	3EO	C43-N45	2.44	1.35	1.31
3	A	302	3EO	C43-N45	2.47	1.35	1.31
3	F	302	3EO	C43-N45	2.48	1.35	1.31
3	L	302	3EO	C43-N45	2.52	1.35	1.31
3	G	302	3EO	C6-N9	2.57	1.39	1.35
3	K	302	3EO	C43-N45	2.57	1.35	1.31
3	D	302	3EO	C43-N45	2.59	1.35	1.31
3	B	302	3EO	C43-N45	2.60	1.35	1.31
3	C	302	3EO	C6-N9	2.70	1.40	1.35
3	G	302	3EO	C37-N38	2.71	1.37	1.33
3	B	302	3EO	C37-N38	2.78	1.38	1.33
3	J	302	3EO	C6-N9	2.79	1.40	1.35
3	M	302	3EO	C43-N45	2.89	1.35	1.31
3	M	302	3EO	C31-C30	2.89	1.57	1.50
3	G	302	3EO	C31-C30	2.90	1.57	1.50
3	L	302	3EO	C37-N38	2.91	1.38	1.33
3	A	302	3EO	C31-C30	2.92	1.57	1.50
3	H	302	3EO	C6-N9	2.92	1.40	1.35
3	D	302	3EO	C37-N38	2.93	1.38	1.33
3	E	302	3EO	C6-N9	2.94	1.40	1.35
3	K	302	3EO	C31-C30	2.96	1.57	1.50
3	H	302	3EO	C31-C30	2.96	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	3EO	C31-C30	2.97	1.57	1.50
3	D	302	3EO	C31-C30	2.97	1.57	1.50
3	C	302	3EO	C37-N38	2.98	1.38	1.33
3	M	302	3EO	C6-N9	2.98	1.40	1.35
3	L	302	3EO	C31-C30	3.01	1.57	1.50
3	M	302	3EO	C37-N38	3.03	1.38	1.33
3	E	302	3EO	C31-C30	3.05	1.57	1.50
3	F	302	3EO	C31-C30	3.08	1.58	1.50
3	K	302	3EO	C37-N38	3.08	1.38	1.33
3	K	302	3EO	C6-N9	3.08	1.40	1.35
3	J	302	3EO	C31-C30	3.08	1.58	1.50
3	L	302	3EO	C6-N9	3.10	1.40	1.35
3	C	302	3EO	C31-C30	3.10	1.58	1.50
3	H	302	3EO	C37-N38	3.13	1.38	1.33
3	A	302	3EO	C6-N9	3.15	1.40	1.35
3	F	302	3EO	C37-N38	3.17	1.38	1.33
3	E	302	3EO	C37-N38	3.18	1.38	1.33
3	H	302	3EO	C20-C16	3.22	1.53	1.50
3	M	302	3EO	C20-C16	3.28	1.53	1.50
3	A	302	3EO	C37-N38	3.28	1.39	1.33
3	J	302	3EO	C37-N38	3.29	1.39	1.33
3	A	302	3EO	C20-C16	3.41	1.53	1.50
3	K	302	3EO	C20-C16	3.56	1.53	1.50
3	E	302	3EO	C20-C16	3.63	1.53	1.50
3	B	302	3EO	C20-C16	3.66	1.54	1.50
3	J	302	3EO	C20-C16	3.70	1.54	1.50
3	G	302	3EO	C20-C16	3.71	1.54	1.50
3	C	302	3EO	C20-C16	3.81	1.54	1.50
3	F	302	3EO	C20-C16	3.89	1.54	1.50
3	L	302	3EO	C20-C16	3.93	1.54	1.50
3	D	302	3EO	C20-C16	3.98	1.54	1.50
3	F	302	3EO	C21-C19	4.27	1.55	1.51
3	C	302	3EO	C21-C19	4.43	1.55	1.51
3	A	302	3EO	C21-C19	4.50	1.55	1.51
3	D	302	3EO	C21-C19	4.74	1.55	1.51
3	E	302	3EO	C21-C19	4.77	1.55	1.51
3	L	302	3EO	C21-C19	4.79	1.55	1.51
3	H	302	3EO	C21-C19	4.82	1.55	1.51
3	M	302	3EO	C21-C19	4.84	1.55	1.51
3	J	302	3EO	C21-C19	4.88	1.55	1.51
3	G	302	3EO	C21-C19	5.02	1.56	1.51
3	B	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	K	302	3EO	C21-C19	5.45	1.56	1.51

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	302	3EO	O27-S25-O28	-6.10	108.34	120.31
3	E	302	3EO	O27-S25-O28	-6.09	108.37	120.31
3	B	302	3EO	O27-S25-O28	-6.04	108.46	120.31
3	C	302	3EO	O27-S25-O28	-6.02	108.49	120.31
3	J	302	3EO	O27-S25-O28	-5.91	108.72	120.31
3	H	302	3EO	O27-S25-O28	-5.86	108.82	120.31
3	G	302	3EO	O27-S25-O28	-5.80	108.92	120.31
3	D	302	3EO	O27-S25-O28	-5.61	109.30	120.31
3	C	302	3EO	C30-C31-C26	-5.55	57.14	60.19
3	K	302	3EO	O27-S25-O28	-5.50	109.52	120.31
3	E	302	3EO	C30-C31-C26	-5.48	57.18	60.19
3	L	302	3EO	C30-C31-C26	-5.45	57.19	60.19
3	F	302	3EO	C30-C31-C26	-5.36	57.24	60.19
3	A	302	3EO	C30-C31-C26	-5.34	57.25	60.19
3	M	302	3EO	C30-C31-C26	-5.26	57.30	60.19
3	A	302	3EO	O27-S25-O28	-5.21	110.09	120.31
3	G	302	3EO	C30-C31-C26	-5.18	57.34	60.19
3	C	302	3EO	C46-C47-C48	-5.13	121.63	129.21
3	M	302	3EO	O27-S25-O28	-5.12	110.27	120.31
3	D	302	3EO	C30-C31-C26	-5.09	57.39	60.19
3	J	302	3EO	C30-C31-C26	-5.09	57.39	60.19
3	H	302	3EO	C30-C31-C26	-5.06	57.41	60.19
3	B	302	3EO	C30-C31-C26	-5.00	57.44	60.19
3	K	302	3EO	C30-C31-C26	-5.00	57.44	60.19
3	K	302	3EO	C46-C47-C48	-4.97	121.86	129.21
3	B	302	3EO	C46-C47-C48	-4.95	121.88	129.21
3	L	302	3EO	C46-C47-C48	-4.90	121.97	129.21
3	J	302	3EO	C46-C47-C48	-4.82	122.08	129.21
3	F	302	3EO	C46-C47-C48	-4.82	122.08	129.21
3	G	302	3EO	C46-C47-C48	-4.81	122.10	129.21
3	L	302	3EO	C19-N18-C7	-4.78	115.15	123.32
3	H	302	3EO	C46-C47-C48	-4.76	122.18	129.21
3	M	302	3EO	C46-C47-C48	-4.67	122.31	129.21
3	A	302	3EO	C46-C47-C48	-4.63	122.36	129.21
3	F	302	3EO	O27-S25-O28	-4.52	111.45	120.31
3	M	302	3EO	C19-N18-C7	-4.41	115.78	123.32
3	D	302	3EO	C46-C47-C48	-4.41	122.69	129.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	302	3EO	C19-N18-C7	-4.39	115.81	123.32
3	G	302	3EO	C19-N18-C7	-4.37	115.84	123.32
3	J	302	3EO	C19-N18-C7	-4.31	115.95	123.32
3	F	302	3EO	C19-N18-C7	-4.30	115.97	123.32
3	H	302	3EO	C19-N18-C7	-4.25	116.06	123.32
3	E	302	3EO	C46-C47-C48	-4.21	122.99	129.21
3	K	302	3EO	C19-N18-C7	-4.19	116.15	123.32
3	E	302	3EO	C19-N18-C7	-4.11	116.30	123.32
3	B	302	3EO	C10-N9-C11	-3.92	108.00	115.72
3	B	302	3EO	C19-N18-C7	-3.87	116.70	123.32
3	C	302	3EO	C34-C36-N38	-3.64	119.35	122.90
3	M	302	3EO	C10-N9-C11	-3.53	108.76	115.72
3	K	302	3EO	C35-C37-N38	-3.48	119.49	122.24
3	M	302	3EO	C35-C37-N38	-3.41	119.54	122.24
3	L	302	3EO	C10-N9-C11	-3.38	109.06	115.72
3	J	302	3EO	C34-C36-N38	-3.37	119.61	122.90
3	E	302	3EO	C10-N9-C11	-3.36	109.10	115.72
3	E	302	3EO	C35-C37-N38	-3.24	119.67	122.24
3	H	302	3EO	C10-N9-C11	-3.22	109.37	115.72
3	J	302	3EO	C10-N9-C11	-3.20	109.41	115.72
3	D	302	3EO	C34-C36-N38	-3.19	119.78	122.90
3	H	302	3EO	C34-C36-N38	-3.19	119.79	122.90
3	B	302	3EO	C34-C36-N38	-3.19	119.79	122.90
3	K	302	3EO	C34-C36-N38	-3.15	119.82	122.90
3	H	302	3EO	C35-C37-N38	-3.15	119.74	122.24
3	G	302	3EO	C35-C37-N38	-3.13	119.76	122.24
3	L	302	3EO	C34-C36-N38	-3.11	119.86	122.90
3	F	302	3EO	C35-C37-N38	-3.08	119.80	122.24
3	J	302	3EO	C35-C37-N38	-3.07	119.81	122.24
3	C	302	3EO	C10-N9-C11	-3.03	109.76	115.72
3	C	302	3EO	C19-N18-C7	-2.96	118.26	123.32
3	A	302	3EO	C19-N18-C7	-2.90	118.36	123.32
3	C	302	3EO	C12-C13-C14	-2.85	102.74	113.86
3	G	302	3EO	C34-C36-N38	-2.84	120.13	122.90
3	G	302	3EO	C10-N9-C11	-2.82	110.17	115.72
3	K	302	3EO	C10-N9-C11	-2.80	110.21	115.72
3	M	302	3EO	C34-C36-N38	-2.73	120.23	122.90
3	L	302	3EO	C35-C37-N38	-2.69	120.11	122.24
3	F	302	3EO	C34-C36-N38	-2.68	120.28	122.90
3	B	302	3EO	C12-C13-C14	-2.64	103.56	113.86
3	B	302	3EO	C35-C37-N38	-2.63	120.16	122.24
3	A	302	3EO	C34-C36-N38	-2.59	120.37	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	302	3EO	C12-C13-C14	-2.58	103.81	113.86
3	M	302	3EO	C12-C13-C14	-2.51	104.07	113.86
3	E	302	3EO	C34-C36-N38	-2.49	120.47	122.90
3	D	302	3EO	C35-C37-N38	-2.49	120.27	122.24
3	C	302	3EO	C35-C37-N38	-2.42	120.33	122.24
3	E	302	3EO	C12-C13-C14	-2.41	104.45	113.86
3	M	302	3EO	O51-C42-C41	-2.39	118.61	124.62
3	F	302	3EO	O51-C42-C41	-2.35	118.70	124.62
3	G	302	3EO	C20-C19-C22	-2.31	112.72	117.09
3	J	302	3EO	C12-C13-C14	-2.26	105.05	113.86
3	L	302	3EO	O51-C42-C41	-2.25	118.95	124.62
3	H	302	3EO	C12-C13-C14	-2.24	105.10	113.86
3	A	302	3EO	C35-C37-N38	-2.23	120.48	122.24
3	E	302	3EO	O51-C42-C41	-2.22	119.04	124.62
3	L	302	3EO	C12-C13-C14	-2.21	105.23	113.86
3	G	302	3EO	O51-C42-C41	-2.18	119.15	124.62
3	K	302	3EO	O51-C42-C41	-2.17	119.15	124.62
3	H	302	3EO	O51-C42-C41	-2.17	119.16	124.62
3	G	302	3EO	C29-C26-C31	-2.04	111.98	116.94
3	M	302	3EO	O17-C7-N18	-2.02	116.64	120.97
3	A	302	3EO	C10-N9-C11	-2.01	111.76	115.72
3	F	302	3EO	O8-C6-C4	-2.01	115.94	120.09
3	D	302	3EO	O32-C33-C34	2.00	120.46	114.91
3	M	302	3EO	C29-C26-C30	2.05	121.92	116.94
3	D	302	3EO	C42-C41-C36	2.05	120.36	119.14
3	J	302	3EO	C4-C6-N9	2.05	123.66	119.47
3	M	302	3EO	C48-C47-N45	2.06	123.86	120.26
3	J	302	3EO	C48-C47-N45	2.06	123.87	120.26
3	B	302	3EO	C29-C26-C30	2.12	122.10	116.94
3	H	302	3EO	C48-C47-N45	2.13	123.98	120.26
3	L	302	3EO	C52-O51-C42	2.14	122.53	117.51
3	A	302	3EO	C37-N38-C36	2.17	119.61	118.00
3	J	302	3EO	C52-O51-C42	2.19	122.65	117.51
3	M	302	3EO	C52-O51-C42	2.21	122.70	117.51
3	J	302	3EO	C35-C37-C43	2.25	122.84	120.18
3	F	302	3EO	C48-C47-N45	2.25	124.20	120.26
3	C	302	3EO	C48-C47-N45	2.34	124.35	120.26
3	A	302	3EO	C42-C41-C36	2.37	120.55	119.14
3	K	302	3EO	C52-O51-C42	2.38	123.09	117.51
3	A	302	3EO	C21-C20-C16	2.39	124.56	119.32
3	L	302	3EO	C48-C47-N45	2.40	124.46	120.26
3	H	302	3EO	C52-O51-C42	2.41	123.15	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	302	3EO	O27-S25-C26	2.44	109.44	107.56
3	G	302	3EO	C52-O51-C42	2.47	123.29	117.51
3	E	302	3EO	O27-S25-C26	2.50	109.49	107.56
3	B	302	3EO	C52-O51-C42	2.51	123.40	117.51
3	D	302	3EO	C4-C6-N9	2.54	124.64	119.47
3	D	302	3EO	C1-O32-C33	2.55	126.67	118.22
3	G	302	3EO	C1-O32-C33	2.58	126.78	118.22
3	B	302	3EO	C1-O32-C33	2.59	126.81	118.22
3	A	302	3EO	C1-O32-C33	2.60	126.85	118.22
3	M	302	3EO	C35-C37-C43	2.62	123.27	120.18
3	E	302	3EO	C21-C20-C16	2.64	125.12	119.32
3	C	302	3EO	C35-C37-C43	2.68	123.34	120.18
3	C	302	3EO	C1-O32-C33	2.70	127.19	118.22
3	L	302	3EO	C1-O32-C33	2.71	127.19	118.22
3	C	302	3EO	C52-O51-C42	2.71	123.86	117.51
3	M	302	3EO	C21-C20-C16	2.75	125.36	119.32
3	H	302	3EO	C35-C37-C43	2.77	123.45	120.18
3	F	302	3EO	C4-C6-N9	2.78	125.13	119.47
3	L	302	3EO	C21-C20-C16	2.78	125.42	119.32
3	L	302	3EO	O27-S25-C26	2.80	109.72	107.56
3	M	302	3EO	C1-O32-C33	2.80	127.50	118.22
3	D	302	3EO	C21-C20-C16	2.81	125.48	119.32
3	A	302	3EO	C4-C6-N9	2.81	125.20	119.47
3	K	302	3EO	C35-C37-C43	2.83	123.52	120.18
3	G	302	3EO	C21-C20-C16	2.85	125.57	119.32
3	F	302	3EO	C1-O32-C33	2.87	127.72	118.22
3	K	302	3EO	C21-C19-N18	2.93	121.92	117.84
3	D	302	3EO	C52-O51-C42	2.93	124.38	117.51
3	J	302	3EO	C1-O32-C33	2.94	127.98	118.22
3	C	302	3EO	C21-C20-C16	2.95	125.80	119.32
3	K	302	3EO	C1-O32-C33	2.96	128.03	118.22
3	H	302	3EO	C21-C20-C16	2.96	125.82	119.32
3	E	302	3EO	C52-O51-C42	3.00	124.53	117.51
3	B	302	3EO	C21-C20-C16	3.03	125.97	119.32
3	B	302	3EO	C35-C37-C43	3.04	123.78	120.18
3	E	302	3EO	C1-O32-C33	3.05	128.33	118.22
3	G	302	3EO	C35-C37-C43	3.06	123.80	120.18
3	F	302	3EO	C21-C20-C16	3.08	126.06	119.32
3	A	302	3EO	C52-O51-C42	3.12	124.80	117.51
3	H	302	3EO	C1-O32-C33	3.13	128.60	118.22
3	F	302	3EO	C52-O51-C42	3.18	124.95	117.51
3	A	302	3EO	O27-S25-C26	3.24	110.06	107.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	302	3EO	C35-C37-C43	3.25	124.02	120.18
3	D	302	3EO	C37-N38-C36	3.29	120.44	118.00
3	J	302	3EO	O28-S25-C26	3.29	110.10	107.56
3	F	302	3EO	C37-N38-C36	3.38	120.51	118.00
3	D	302	3EO	O28-S25-C26	3.61	110.35	107.56
3	J	302	3EO	C21-C20-C16	3.62	127.26	119.32
3	E	302	3EO	C37-N38-C36	3.69	120.74	118.00
3	F	302	3EO	O27-S25-C26	3.72	110.43	107.56
3	H	302	3EO	O28-S25-C26	3.78	110.48	107.56
3	L	302	3EO	C37-N38-C36	3.96	120.94	118.00
3	B	302	3EO	C37-N38-C36	3.96	120.94	118.00
3	M	302	3EO	C37-N38-C36	4.00	120.97	118.00
3	C	302	3EO	O27-S25-C26	4.11	110.74	107.56
3	G	302	3EO	C37-N38-C36	4.19	121.11	118.00
3	B	302	3EO	O27-S25-C26	4.20	110.80	107.56
3	M	302	3EO	O27-S25-C26	4.20	110.80	107.56
3	J	302	3EO	C37-N38-C36	4.26	121.16	118.00
3	H	302	3EO	C37-N38-C36	4.27	121.17	118.00
3	J	302	3EO	O27-S25-C26	4.29	110.87	107.56
3	K	302	3EO	O27-S25-C26	4.35	110.92	107.56
3	K	302	3EO	C21-C20-C16	4.41	129.00	119.32
3	K	302	3EO	C37-N38-C36	4.47	121.32	118.00
3	G	302	3EO	O28-S25-C26	4.48	111.02	107.56
3	H	302	3EO	O27-S25-C26	4.59	111.11	107.56
3	C	302	3EO	C37-N38-C36	4.60	121.42	118.00
3	K	302	3EO	O28-S25-C26	5.23	111.61	107.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 41 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	302	3EO	5	0
3	K	302	3EO	2	0
3	L	302	3EO	3	0
3	M	302	3EO	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	194/203 (95%)	-0.08	0 100 100	48, 64, 91, 123	0
1	B	196/203 (96%)	-0.13	3 (1%) 76 69	43, 60, 85, 117	0
1	C	196/203 (96%)	0.03	2 (1%) 84 78	47, 62, 92, 113	0
1	D	195/203 (96%)	-0.00	4 (2%) 67 57	47, 64, 92, 124	0
1	E	190/203 (93%)	-0.01	3 (1%) 74 67	42, 63, 97, 122	0
1	F	195/203 (96%)	0.16	6 (3%) 52 41	45, 67, 104, 130	0
1	G	190/203 (93%)	0.02	2 (1%) 82 76	40, 64, 91, 126	0
1	H	193/203 (95%)	-0.08	5 (2%) 59 49	48, 74, 111, 135	0
1	J	196/203 (96%)	-0.02	3 (1%) 76 69	50, 72, 97, 120	0
1	K	194/203 (95%)	0.40	10 (5%) 31 21	55, 84, 114, 142	0
1	L	187/203 (92%)	0.45	11 (5%) 26 17	54, 87, 113, 130	0
1	M	195/203 (96%)	0.23	9 (4%) 36 26	46, 70, 105, 129	0
All	All	2321/2436 (95%)	0.08	58 (2%) 61 50	40, 69, 107, 142	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	174	SER	5.4
1	M	90	GLY	4.9
1	G	1	ALA	4.6
1	L	230	ILE	4.6
1	M	2	PRO	4.2
1	F	178	THR	4.2
1	B	1	ALA	4.1
1	J	181	ALA	4.0
1	L	144	LEU	3.9
1	K	151	VAL	3.8
1	C	182	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	98	THR	3.5
1	D	181	ALA	3.4
1	L	75	TYR	3.4
1	L	50	GLY	3.3
1	F	3	ILE	3.3
1	L	175	MET	3.2
1	F	179	MET	3.2
1	K	152	GLY	3.1
1	H	8	GLN	2.9
1	F	144	LEU	2.8
1	H	182	SER	2.8
1	L	229	ILE	2.8
1	M	89	PRO	2.7
1	D	2	PRO	2.7
1	C	1	ALA	2.7
1	B	181	ALA	2.7
1	M	3	ILE	2.6
1	F	1	ALA	2.5
1	D	94	LEU	2.5
1	E	220	LYS	2.5
1	H	3	ILE	2.5
1	K	68	LYS	2.5
1	K	113	VAL	2.5
1	G	2	PRO	2.5
1	K	150	ALA	2.5
1	M	120	GLY	2.4
1	K	178	THR	2.4
1	L	86	GLN	2.4
1	E	1	ALA	2.4
1	B	234	ARG	2.3
1	L	47	CYS	2.3
1	M	91	ALA	2.3
1	K	180	ARG	2.3
1	H	6	TYR	2.3
1	M	176	GLU	2.3
1	J	75	TYR	2.2
1	E	2	PRO	2.2
1	D	180	ARG	2.2
1	K	90	GLY	2.2
1	M	68	LYS	2.2
1	K	2	PRO	2.1
1	L	77	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	103	ASP	2.1
1	H	174	SER	2.1
1	J	180	ARG	2.1
1	K	47	CYS	2.0
1	L	169	PHE	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 carbohydrates 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. 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	3EO	G	302	52/52	0.98	0.20	1.08	47,51,55,55	0
3	3EO	B	302	52/52	0.97	0.19	0.72	41,51,55,56	0
2	ZN	B	301	1/1	0.99	0.18	0.65	77,77,77,77	0
3	3EO	A	302	52/52	0.97	0.18	0.63	43,49,51,53	0
3	3EO	J	302	52/52	0.95	0.20	0.59	55,59,64,65	0
2	ZN	D	301	1/1	0.94	0.16	0.49	94,94,94,94	0
3	3EO	E	302	52/52	0.97	0.18	0.46	45,51,56,57	0
3	3EO	L	302	52/52	0.95	0.21	0.33	63,66,74,74	0
3	3EO	K	302	52/52	0.94	0.19	0.14	59,64,72,73	0
2	ZN	H	301	1/1	0.89	0.15	0.14	120,120,120,120	0
3	3EO	H	302	52/52	0.97	0.17	0.06	51,55,58,59	0
3	3EO	M	302	52/52	0.95	0.18	0.04	45,56,70,71	0
3	3EO	D	302	52/52	0.97	0.18	-0.01	46,53,60,61	0
3	3EO	F	302	52/52	0.96	0.17	-0.13	49,53,58,59	0
2	ZN	J	301	1/1	0.96	0.14	-0.27	92,92,92,92	0
3	3EO	C	302	52/52	0.97	0.17	-0.29	48,56,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CL	A	303	1/1	0.93	0.17	-0.48	55,55,55,55	0
2	ZN	E	301	1/1	0.99	0.11	-0.76	53,53,53,53	0
4	CL	F	303	1/1	0.83	0.14	-0.80	69,69,69,69	0
4	CL	B	303	1/1	0.87	0.14	-0.87	68,68,68,68	0
2	ZN	A	301	1/1	0.98	0.10	-0.92	80,80,80,80	0
2	ZN	M	301	1/1	0.99	0.10	-1.19	77,77,77,77	0
2	ZN	C	301	1/1	0.97	0.11	-1.23	86,86,86,86	0
2	ZN	G	301	1/1	0.97	0.09	-1.55	85,85,85,85	0
2	ZN	L	301	1/1	0.94	0.10	-2.24	120,120,120,120	0
2	ZN	F	301	1/1	0.96	0.10	-2.34	96,96,96,96	0
2	ZN	K	301	1/1	0.91	0.09	-2.44	123,123,123,123	0
4	CL	H	303	1/1	0.93	0.09	-	59,59,59,59	0
4	CL	F	304	1/1	0.86	0.08	-	62,62,62,62	0
4	CL	C	304	1/1	0.89	0.17	-	64,64,64,64	0
4	CL	C	303	1/1	0.96	0.11	-	55,55,55,55	0
4	CL	F	305	1/1	0.93	0.10	-	55,55,55,55	0
4	CL	M	303	1/1	0.92	0.17	-	54,54,54,54	0
4	CL	E	303	1/1	0.96	0.17	-	46,46,46,46	0
4	CL	E	304	1/1	0.89	0.09	-	59,59,59,59	0

6.5 Other polymers

There are no such residues in this entry.