



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 04:49 AM UTC

PDB ID : 8SE7 / pdb_00008se7
Title : HTRA-1 PDSA bound to CKP 1A8
Authors : Ultsch, M.H.; Kirchhofer, D.; Wei, Y.
Deposited on : 2023-04-08
Resolution : 2.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

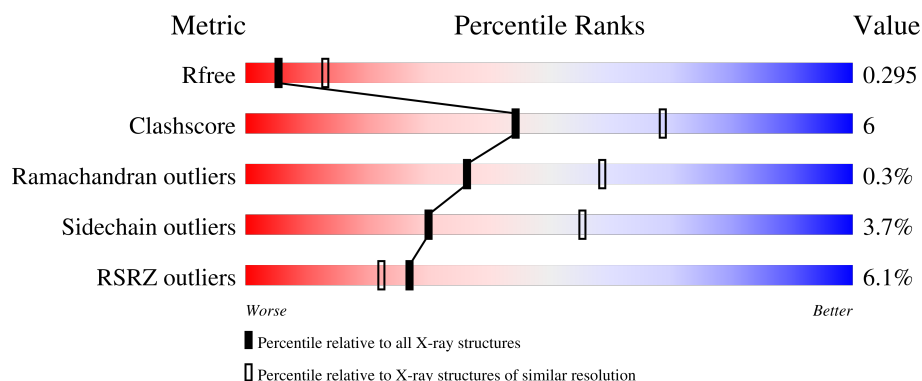
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	5% 70%11%18%
1	B	240	2% 58%19%•21%
1	C	240	5% 68%12%•19%
1	D	240	7% 68%11%20%
1	E	240	8% 60%12%28%

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Mol	Chain	Length	Quality of chain
1	F	240	
1	K	240	
1	L	240	
1	M	240	
1	Q	240	
1	R	240	
1	S	240	
2	G	40	
2	H	40	
2	I	40	
2	J	40	
2	N	40	
2	O	40	
2	P	40	
2	T	40	
2	U	40	
2	V	40	
2	X	40	
2	Y	40	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19018 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 Serine protease HTRA1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	0	0	0
			1393	888	235	270			
1	B	190	Total	C	N	O	0	0	0
			1381	880	232	269			
1	C	195	Total	C	N	O	0	0	0
			1392	885	236	271			
1	D	191	Total	C	N	O	0	0	0
			1362	872	229	261			
1	E	173	Total	C	N	O	0	0	0
			1169	739	200	230			
1	F	197	Total	C	N	O	0	0	0
			1388	876	238	274			
1	K	194	Total	C	N	O	0	1	0
			1377	877	226	274			
1	L	191	Total	C	N	O	0	0	0
			1369	870	231	267			
				S					
			1						
1	M	188	Total	C	N	O	0	0	0
			1307	830	220	257			
1	Q	193	Total	C	N	O	0	0	0
			1308	823	226	259			
1	R	193	Total	C	N	O	0	0	0
			1389	887	234	268			
1	S	191	Total	C	N	O	0	0	0
			1332	848	223	261			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	MET	-	expression tag	UNP Q92743
A	141	GLY	-	expression tag	UNP Q92743
A	142	SER	-	expression tag	UNP Q92743
A	143	SER	-	expression tag	UNP Q92743
A	144	HIS	-	expression tag	UNP Q92743

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Chain	Residue	Modelled	Actual	Comment	Reference
A	145	HIS	-	expression tag	UNP Q92743
A	146	HIS	-	expression tag	UNP Q92743
A	147	HIS	-	expression tag	UNP Q92743
A	148	HIS	-	expression tag	UNP Q92743
A	149	HIS	-	expression tag	UNP Q92743
A	150	SER	-	expression tag	UNP Q92743
A	151	SER	-	expression tag	UNP Q92743
A	152	GLY	-	expression tag	UNP Q92743
A	153	LEU	-	expression tag	UNP Q92743
A	154	VAL	-	expression tag	UNP Q92743
A	155	PRO	-	expression tag	UNP Q92743
A	156	ARG	-	expression tag	UNP Q92743
A	157	GLY	-	expression tag	UNP Q92743
A	158	SER	-	expression tag	UNP Q92743
A	159	HIS	-	expression tag	UNP Q92743
A	160	MET	-	expression tag	UNP Q92743
A	328	ALA	SER	engineered mutation	UNP Q92743
B	140	MET	-	expression tag	UNP Q92743
B	141	GLY	-	expression tag	UNP Q92743
B	142	SER	-	expression tag	UNP Q92743
B	143	SER	-	expression tag	UNP Q92743
B	144	HIS	-	expression tag	UNP Q92743
B	145	HIS	-	expression tag	UNP Q92743
B	146	HIS	-	expression tag	UNP Q92743
B	147	HIS	-	expression tag	UNP Q92743
B	148	HIS	-	expression tag	UNP Q92743
B	149	HIS	-	expression tag	UNP Q92743
B	150	SER	-	expression tag	UNP Q92743
B	151	SER	-	expression tag	UNP Q92743
B	152	GLY	-	expression tag	UNP Q92743
B	153	LEU	-	expression tag	UNP Q92743
B	154	VAL	-	expression tag	UNP Q92743
B	155	PRO	-	expression tag	UNP Q92743
B	156	ARG	-	expression tag	UNP Q92743
B	157	GLY	-	expression tag	UNP Q92743
B	158	SER	-	expression tag	UNP Q92743
B	159	HIS	-	expression tag	UNP Q92743
B	160	MET	-	expression tag	UNP Q92743
B	328	ALA	SER	engineered mutation	UNP Q92743
C	140	MET	-	expression tag	UNP Q92743
C	141	GLY	-	expression tag	UNP Q92743
C	142	SER	-	expression tag	UNP Q92743

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Chain	Residue	Modelled	Actual	Comment	Reference
C	143	SER	-	expression tag	UNP Q92743
C	144	HIS	-	expression tag	UNP Q92743
C	145	HIS	-	expression tag	UNP Q92743
C	146	HIS	-	expression tag	UNP Q92743
C	147	HIS	-	expression tag	UNP Q92743
C	148	HIS	-	expression tag	UNP Q92743
C	149	HIS	-	expression tag	UNP Q92743
C	150	SER	-	expression tag	UNP Q92743
C	151	SER	-	expression tag	UNP Q92743
C	152	GLY	-	expression tag	UNP Q92743
C	153	LEU	-	expression tag	UNP Q92743
C	154	VAL	-	expression tag	UNP Q92743
C	155	PRO	-	expression tag	UNP Q92743
C	156	ARG	-	expression tag	UNP Q92743
C	157	GLY	-	expression tag	UNP Q92743
C	158	SER	-	expression tag	UNP Q92743
C	159	HIS	-	expression tag	UNP Q92743
C	160	MET	-	expression tag	UNP Q92743
C	328	ALA	SER	engineered mutation	UNP Q92743
D	140	MET	-	expression tag	UNP Q92743
D	141	GLY	-	expression tag	UNP Q92743
D	142	SER	-	expression tag	UNP Q92743
D	143	SER	-	expression tag	UNP Q92743
D	144	HIS	-	expression tag	UNP Q92743
D	145	HIS	-	expression tag	UNP Q92743
D	146	HIS	-	expression tag	UNP Q92743
D	147	HIS	-	expression tag	UNP Q92743
D	148	HIS	-	expression tag	UNP Q92743
D	149	HIS	-	expression tag	UNP Q92743
D	150	SER	-	expression tag	UNP Q92743
D	151	SER	-	expression tag	UNP Q92743
D	152	GLY	-	expression tag	UNP Q92743
D	153	LEU	-	expression tag	UNP Q92743
D	154	VAL	-	expression tag	UNP Q92743
D	155	PRO	-	expression tag	UNP Q92743
D	156	ARG	-	expression tag	UNP Q92743
D	157	GLY	-	expression tag	UNP Q92743
D	158	SER	-	expression tag	UNP Q92743
D	159	HIS	-	expression tag	UNP Q92743
D	160	MET	-	expression tag	UNP Q92743
D	328	ALA	SER	engineered mutation	UNP Q92743
E	140	MET	-	expression tag	UNP Q92743

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Chain	Residue	Modelled	Actual	Comment	Reference
E	141	GLY	-	expression tag	UNP Q92743
E	142	SER	-	expression tag	UNP Q92743
E	143	SER	-	expression tag	UNP Q92743
E	144	HIS	-	expression tag	UNP Q92743
E	145	HIS	-	expression tag	UNP Q92743
E	146	HIS	-	expression tag	UNP Q92743
E	147	HIS	-	expression tag	UNP Q92743
E	148	HIS	-	expression tag	UNP Q92743
E	149	HIS	-	expression tag	UNP Q92743
E	150	SER	-	expression tag	UNP Q92743
E	151	SER	-	expression tag	UNP Q92743
E	152	GLY	-	expression tag	UNP Q92743
E	153	LEU	-	expression tag	UNP Q92743
E	154	VAL	-	expression tag	UNP Q92743
E	155	PRO	-	expression tag	UNP Q92743
E	156	ARG	-	expression tag	UNP Q92743
E	157	GLY	-	expression tag	UNP Q92743
E	158	SER	-	expression tag	UNP Q92743
E	159	HIS	-	expression tag	UNP Q92743
E	160	MET	-	expression tag	UNP Q92743
E	328	ALA	SER	engineered mutation	UNP Q92743
F	140	MET	-	expression tag	UNP Q92743
F	141	GLY	-	expression tag	UNP Q92743
F	142	SER	-	expression tag	UNP Q92743
F	143	SER	-	expression tag	UNP Q92743
F	144	HIS	-	expression tag	UNP Q92743
F	145	HIS	-	expression tag	UNP Q92743
F	146	HIS	-	expression tag	UNP Q92743
F	147	HIS	-	expression tag	UNP Q92743
F	148	HIS	-	expression tag	UNP Q92743
F	149	HIS	-	expression tag	UNP Q92743
F	150	SER	-	expression tag	UNP Q92743
F	151	SER	-	expression tag	UNP Q92743
F	152	GLY	-	expression tag	UNP Q92743
F	153	LEU	-	expression tag	UNP Q92743
F	154	VAL	-	expression tag	UNP Q92743
F	155	PRO	-	expression tag	UNP Q92743
F	156	ARG	-	expression tag	UNP Q92743
F	157	GLY	-	expression tag	UNP Q92743
F	158	SER	-	expression tag	UNP Q92743
F	159	HIS	-	expression tag	UNP Q92743
F	160	MET	-	expression tag	UNP Q92743

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Chain	Residue	Modelled	Actual	Comment	Reference
F	328	ALA	SER	engineered mutation	UNP Q92743
K	140	MET	-	expression tag	UNP Q92743
K	141	GLY	-	expression tag	UNP Q92743
K	142	SER	-	expression tag	UNP Q92743
K	143	SER	-	expression tag	UNP Q92743
K	144	HIS	-	expression tag	UNP Q92743
K	145	HIS	-	expression tag	UNP Q92743
K	146	HIS	-	expression tag	UNP Q92743
K	147	HIS	-	expression tag	UNP Q92743
K	148	HIS	-	expression tag	UNP Q92743
K	149	HIS	-	expression tag	UNP Q92743
K	150	SER	-	expression tag	UNP Q92743
K	151	SER	-	expression tag	UNP Q92743
K	152	GLY	-	expression tag	UNP Q92743
K	153	LEU	-	expression tag	UNP Q92743
K	154	VAL	-	expression tag	UNP Q92743
K	155	PRO	-	expression tag	UNP Q92743
K	156	ARG	-	expression tag	UNP Q92743
K	157	GLY	-	expression tag	UNP Q92743
K	158	SER	-	expression tag	UNP Q92743
K	159	HIS	-	expression tag	UNP Q92743
K	160	MET	-	expression tag	UNP Q92743
K	328	ALA	SER	engineered mutation	UNP Q92743
L	140	MET	-	expression tag	UNP Q92743
L	141	GLY	-	expression tag	UNP Q92743
L	142	SER	-	expression tag	UNP Q92743
L	143	SER	-	expression tag	UNP Q92743
L	144	HIS	-	expression tag	UNP Q92743
L	145	HIS	-	expression tag	UNP Q92743
L	146	HIS	-	expression tag	UNP Q92743
L	147	HIS	-	expression tag	UNP Q92743
L	148	HIS	-	expression tag	UNP Q92743
L	149	HIS	-	expression tag	UNP Q92743
L	150	SER	-	expression tag	UNP Q92743
L	151	SER	-	expression tag	UNP Q92743
L	152	GLY	-	expression tag	UNP Q92743
L	153	LEU	-	expression tag	UNP Q92743
L	154	VAL	-	expression tag	UNP Q92743
L	155	PRO	-	expression tag	UNP Q92743
L	156	ARG	-	expression tag	UNP Q92743
L	157	GLY	-	expression tag	UNP Q92743
L	158	SER	-	expression tag	UNP Q92743

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Chain	Residue	Modelled	Actual	Comment	Reference
L	159	HIS	-	expression tag	UNP Q92743
L	160	MET	-	expression tag	UNP Q92743
L	328	ALA	SER	engineered mutation	UNP Q92743
M	140	MET	-	expression tag	UNP Q92743
M	141	GLY	-	expression tag	UNP Q92743
M	142	SER	-	expression tag	UNP Q92743
M	143	SER	-	expression tag	UNP Q92743
M	144	HIS	-	expression tag	UNP Q92743
M	145	HIS	-	expression tag	UNP Q92743
M	146	HIS	-	expression tag	UNP Q92743
M	147	HIS	-	expression tag	UNP Q92743
M	148	HIS	-	expression tag	UNP Q92743
M	149	HIS	-	expression tag	UNP Q92743
M	150	SER	-	expression tag	UNP Q92743
M	151	SER	-	expression tag	UNP Q92743
M	152	GLY	-	expression tag	UNP Q92743
M	153	LEU	-	expression tag	UNP Q92743
M	154	VAL	-	expression tag	UNP Q92743
M	155	PRO	-	expression tag	UNP Q92743
M	156	ARG	-	expression tag	UNP Q92743
M	157	GLY	-	expression tag	UNP Q92743
M	158	SER	-	expression tag	UNP Q92743
M	159	HIS	-	expression tag	UNP Q92743
M	160	MET	-	expression tag	UNP Q92743
M	328	ALA	SER	engineered mutation	UNP Q92743
Q	140	MET	-	expression tag	UNP Q92743
Q	141	GLY	-	expression tag	UNP Q92743
Q	142	SER	-	expression tag	UNP Q92743
Q	143	SER	-	expression tag	UNP Q92743
Q	144	HIS	-	expression tag	UNP Q92743
Q	145	HIS	-	expression tag	UNP Q92743
Q	146	HIS	-	expression tag	UNP Q92743
Q	147	HIS	-	expression tag	UNP Q92743
Q	148	HIS	-	expression tag	UNP Q92743
Q	149	HIS	-	expression tag	UNP Q92743
Q	150	SER	-	expression tag	UNP Q92743
Q	151	SER	-	expression tag	UNP Q92743
Q	152	GLY	-	expression tag	UNP Q92743
Q	153	LEU	-	expression tag	UNP Q92743
Q	154	VAL	-	expression tag	UNP Q92743
Q	155	PRO	-	expression tag	UNP Q92743
Q	156	ARG	-	expression tag	UNP Q92743

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	157	GLY	-	expression tag	UNP Q92743
Q	158	SER	-	expression tag	UNP Q92743
Q	159	HIS	-	expression tag	UNP Q92743
Q	160	MET	-	expression tag	UNP Q92743
Q	328	ALA	SER	engineered mutation	UNP Q92743
R	140	MET	-	expression tag	UNP Q92743
R	141	GLY	-	expression tag	UNP Q92743
R	142	SER	-	expression tag	UNP Q92743
R	143	SER	-	expression tag	UNP Q92743
R	144	HIS	-	expression tag	UNP Q92743
R	145	HIS	-	expression tag	UNP Q92743
R	146	HIS	-	expression tag	UNP Q92743
R	147	HIS	-	expression tag	UNP Q92743
R	148	HIS	-	expression tag	UNP Q92743
R	149	HIS	-	expression tag	UNP Q92743
R	150	SER	-	expression tag	UNP Q92743
R	151	SER	-	expression tag	UNP Q92743
R	152	GLY	-	expression tag	UNP Q92743
R	153	LEU	-	expression tag	UNP Q92743
R	154	VAL	-	expression tag	UNP Q92743
R	155	PRO	-	expression tag	UNP Q92743
R	156	ARG	-	expression tag	UNP Q92743
R	157	GLY	-	expression tag	UNP Q92743
R	158	SER	-	expression tag	UNP Q92743
R	159	HIS	-	expression tag	UNP Q92743
R	160	MET	-	expression tag	UNP Q92743
R	328	ALA	SER	engineered mutation	UNP Q92743
S	140	MET	-	expression tag	UNP Q92743
S	141	GLY	-	expression tag	UNP Q92743
S	142	SER	-	expression tag	UNP Q92743
S	143	SER	-	expression tag	UNP Q92743
S	144	HIS	-	expression tag	UNP Q92743
S	145	HIS	-	expression tag	UNP Q92743
S	146	HIS	-	expression tag	UNP Q92743
S	147	HIS	-	expression tag	UNP Q92743
S	148	HIS	-	expression tag	UNP Q92743
S	149	HIS	-	expression tag	UNP Q92743
S	150	SER	-	expression tag	UNP Q92743
S	151	SER	-	expression tag	UNP Q92743
S	152	GLY	-	expression tag	UNP Q92743
S	153	LEU	-	expression tag	UNP Q92743
S	154	VAL	-	expression tag	UNP Q92743

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Chain	Residue	Modelled	Actual	Comment	Reference
S	155	PRO	-	expression tag	UNP Q92743
S	156	ARG	-	expression tag	UNP Q92743
S	157	GLY	-	expression tag	UNP Q92743
S	158	SER	-	expression tag	UNP Q92743
S	159	HIS	-	expression tag	UNP Q92743
S	160	MET	-	expression tag	UNP Q92743
S	328	ALA	SER	engineered mutation	UNP Q92743

- Molecule 2 is a protein called Cysteine knot peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	32	Total	C	N	O	S	0	0	0
			212	127	37	42	6			
2	X	37	Total	C	N	O	S	0	0	0
			277	174	46	51	6			
2	Y	36	Total	C	N	O	S	0	0	0
			260	159	46	49	6			
2	G	34	Total	C	N	O	S	0	0	0
			240	147	43	44	6			
2	H	33	Total	C	N	O	S	0	0	0
			226	139	38	43	6			
2	J	34	Total	C	N	O	S	0	0	0
			249	159	40	44	6			
2	N	35	Total	C	N	O	S	0	0	0
			267	168	45	48	6			
2	O	34	Total	C	N	O	S	0	0	0
			245	152	42	45	6			
2	P	30	Total	C	N	O	S	0	0	0
			195	118	33	38	6			
2	T	29	Total	C	N	O	S	0	0	0
			197	119	34	38	6			
2	U	33	Total	C	N	O	S	0	0	0
			233	142	39	46	6			
2	V	34	Total	C	N	O	S	0	0	0
			243	153	40	44	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		

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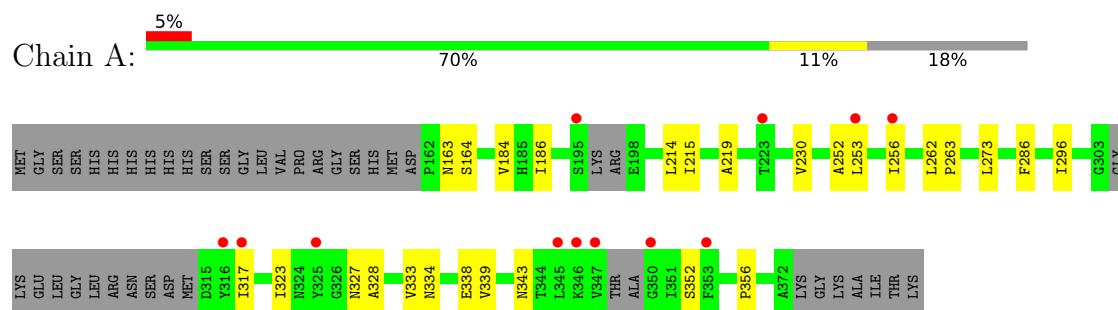
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total 1	O 1	0	0
3	Q	1	Total 1	O 1	0	0
3	R	2	Total 2	O 2	0	0
3	U	1	Total 1	O 1	0	0

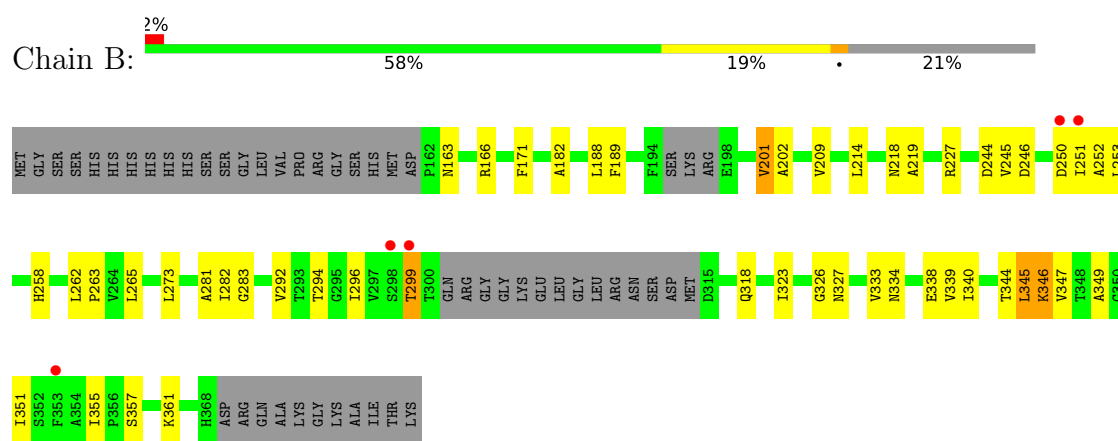
3 Residue-property plots [i](#)

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

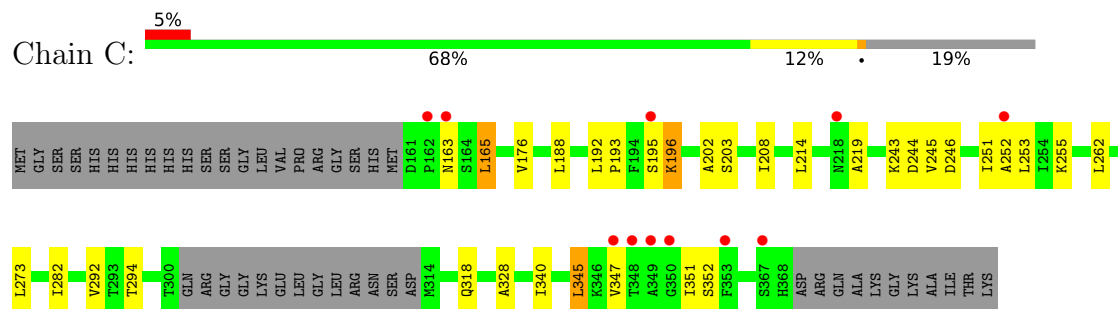
• Molecule 1: Serine protease HTRA1



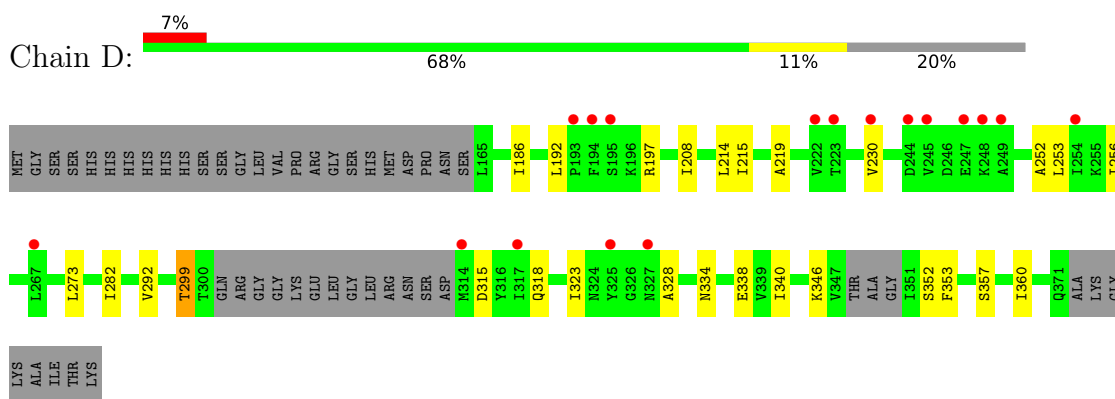
• Molecule 1: Serine protease HTRA1



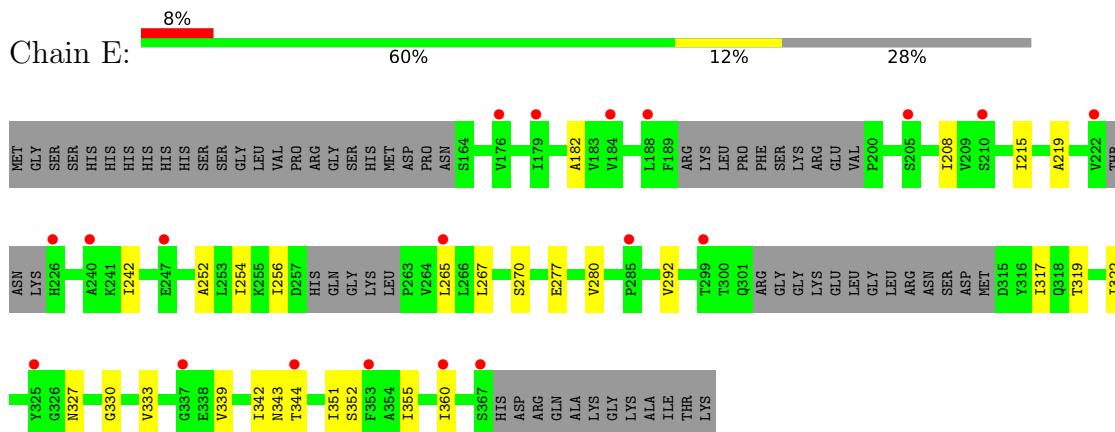
• Molecule 1: Serine protease HTRA1



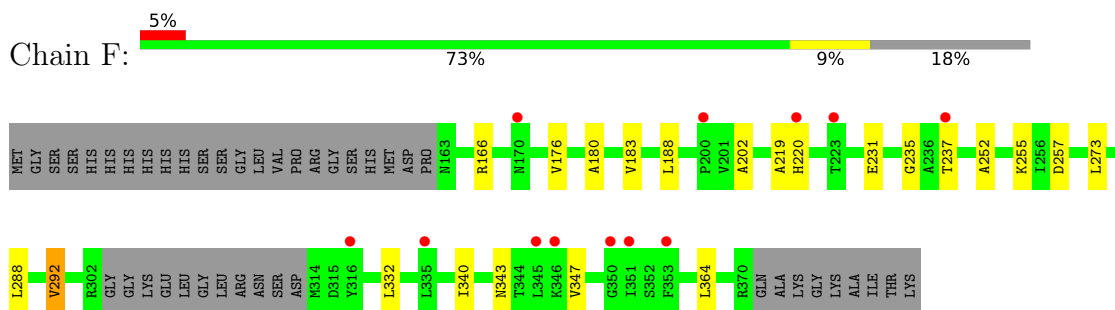
• Molecule 1: Serine protease HTRA1



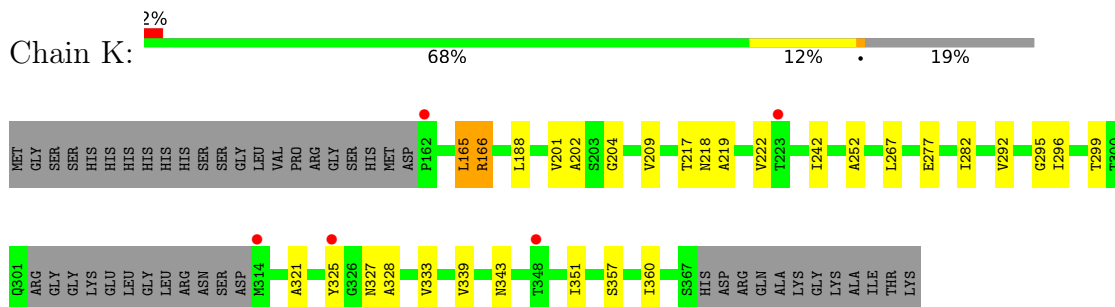
- Molecule 1: Serine protease HTRA1



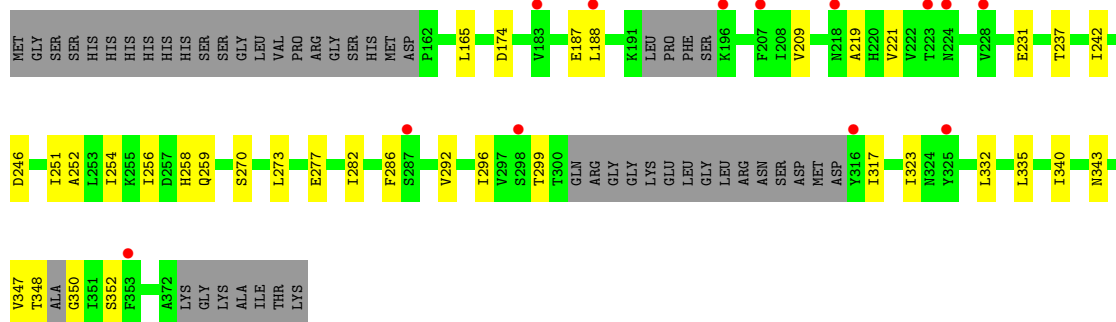
- Molecule 1: Serine protease HTRA1



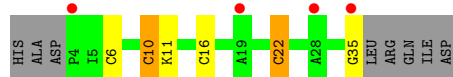
- Molecule 1: Serine protease HTRA1



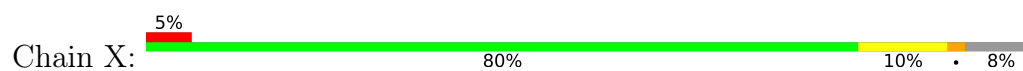
- Molecule 1: Serine protease HTRA1



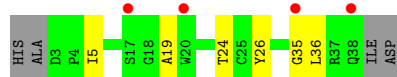
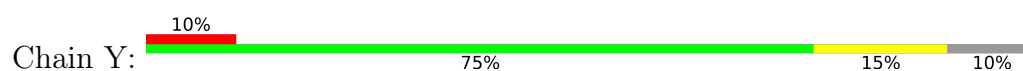
- Molecule 2: Cysteine knot peptide



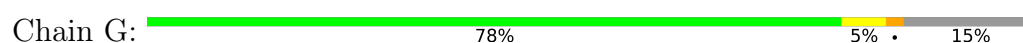
- Molecule 2: Cysteine knot peptide



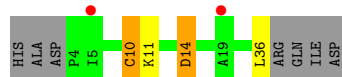
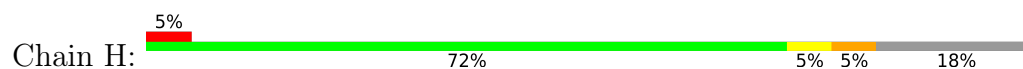
- Molecule 2: Cysteine knot peptide



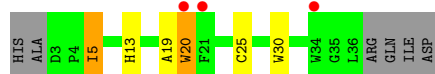
- Molecule 2: Cysteine knot peptide



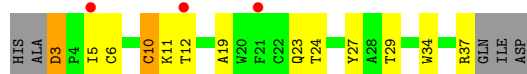
- Molecule 2: Cysteine knot peptide



- Molecule 2: Cysteine knot peptide



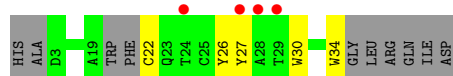
- Molecule 2: Cysteine knot peptide



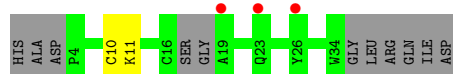
- Molecule 2: Cysteine knot peptide



- Molecule 2: Cysteine knot peptide



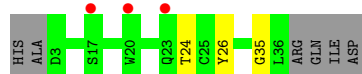
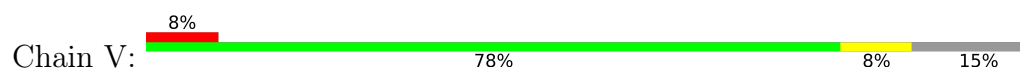
- Molecule 2: Cysteine knot peptide



- Molecule 2: Cysteine knot peptide



- Molecule 2: Cysteine knot peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.03Å 152.72Å 165.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.23 – 2.96 54.23 – 2.96	Depositor EDS
% Data completeness (in resolution range)	77.6 (54.23-2.96) 77.6 (54.23-2.96)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.270 , 0.296 0.271 , 0.295	Depositor DCC
R_{free} test set	1991 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	86.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	19018	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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](#)

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	0.10	0/1416	0.28	0/1937
1	B	0.11	0/1404	0.33	0/1919
1	C	0.11	0/1414	0.30	0/1932
1	D	0.10	0/1385	0.29	0/1895
1	E	0.09	0/1182	0.26	0/1616
1	F	0.09	0/1409	0.27	0/1929
1	K	0.10	0/1398	0.30	0/1917
1	L	0.10	0/1391	0.28	0/1904
1	M	0.09	0/1325	0.28	0/1811
1	Q	0.10	0/1325	0.31	0/1820
1	R	0.10	0/1413	0.27	0/1933
1	S	0.10	0/1351	0.29	0/1848
2	G	0.09	0/248	0.36	0/340
2	H	0.12	0/234	0.39	0/321
2	I	0.10	0/218	0.36	0/299
2	J	0.13	0/260	0.33	0/359
2	N	0.29	0/278	0.42	0/382
2	O	0.19	0/254	0.43	0/347
2	P	0.12	0/200	0.34	0/274
2	T	0.11	0/202	0.32	0/276
2	U	0.08	0/241	0.33	0/331
2	V	0.14	0/253	0.41	0/350
2	X	0.09	0/288	0.32	0/396
2	Y	0.12	0/268	0.34	0/368
All	All	0.11	0/19357	0.30	0/26504

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	1393	0	1303	16	0
1	B	1381	0	1329	26	0
1	C	1392	0	1326	20	0
1	D	1362	0	1279	13	0
1	E	1169	0	1065	14	0
1	F	1388	0	1297	11	0
1	K	1377	0	1296	19	0
1	L	1369	0	1287	17	0
1	M	1307	0	1223	22	0
1	Q	1308	0	1174	15	0
1	R	1389	0	1320	17	0
1	S	1332	0	1235	20	0
2	G	240	0	184	1	0
2	H	226	0	162	2	0
2	I	212	0	152	3	0
2	J	249	0	187	4	0
2	N	267	0	214	7	0
2	O	245	0	187	3	0
2	P	195	0	127	4	0
2	T	197	0	138	1	0
2	U	233	0	176	3	0
2	V	243	0	180	2	0
2	X	277	0	222	3	0
2	Y	260	0	204	3	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	O	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	2	0	0	0	0
3	U	1	0	0	0	0
All	All	19018	0	17267	217	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 6.

The worst 5 of 217 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:258:HIS:HB3	1:L:262:LEU:HD11	1.70	0.73
1:B:171:PHE:HB2	1:C:165:LEU:HD21	1.72	0.70
1:M:188:LEU:HD11	1:M:221:VAL:HG23	1.73	0.69
1:D:214:LEU:HD22	1:D:253:LEU:HD21	1.75	0.67
1:C:246:ASP:HB3	1:C:251:ILE:HG22	1.78	0.66

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	188/240 (78%)	180 (96%)	7 (4%)	1 (0%)	24	49
1	B	184/240 (77%)	170 (92%)	12 (6%)	2 (1%)	11	29
1	C	191/240 (80%)	179 (94%)	11 (6%)	1 (0%)	24	49
1	D	185/240 (77%)	180 (97%)	4 (2%)	1 (0%)	24	49
1	E	163/240 (68%)	158 (97%)	5 (3%)	0	100	100
1	F	193/240 (80%)	185 (96%)	8 (4%)	0	100	100
1	K	191/240 (80%)	186 (97%)	4 (2%)	1 (0%)	24	49
1	L	185/240 (77%)	177 (96%)	6 (3%)	2 (1%)	11	29
1	M	182/240 (76%)	176 (97%)	6 (3%)	0	100	100
1	Q	185/240 (77%)	177 (96%)	8 (4%)	0	100	100
1	R	187/240 (78%)	185 (99%)	2 (1%)	0	100	100
1	S	183/240 (76%)	174 (95%)	8 (4%)	1 (0%)	24	49
2	G	32/40 (80%)	27 (84%)	5 (16%)	0	100	100
2	H	31/40 (78%)	26 (84%)	5 (16%)	0	100	100
2	I	30/40 (75%)	26 (87%)	4 (13%)	0	100	100
2	J	32/40 (80%)	29 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	33/40 (82%)	28 (85%)	5 (15%)	0	100	100
2	O	32/40 (80%)	27 (84%)	5 (16%)	0	100	100
2	P	26/40 (65%)	23 (88%)	3 (12%)	0	100	100
2	T	25/40 (62%)	23 (92%)	2 (8%)	0	100	100
2	U	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
2	V	32/40 (80%)	27 (84%)	5 (16%)	0	100	100
2	X	35/40 (88%)	32 (91%)	3 (9%)	0	100	100
2	Y	34/40 (85%)	28 (82%)	6 (18%)	0	100	100
All	All	2590/3360 (77%)	2453 (95%)	128 (5%)	9 (0%)	36	59

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	346	LYS
1	D	328	ALA
1	K	328	ALA
1	S	347	VAL
1	C	196	LYS

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	138/202 (68%)	138 (100%)	0	100	100
1	B	143/202 (71%)	137 (96%)	6 (4%)	26	53
1	C	139/202 (69%)	135 (97%)	4 (3%)	37	61
1	D	134/202 (66%)	132 (98%)	2 (2%)	57	76
1	E	107/202 (53%)	104 (97%)	3 (3%)	38	62
1	F	137/202 (68%)	134 (98%)	3 (2%)	45	69
1	K	137/202 (68%)	132 (96%)	5 (4%)	31	56
1	L	138/202 (68%)	133 (96%)	5 (4%)	31	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	126/202 (62%)	123 (98%)	3 (2%)	43	67
1	Q	121/202 (60%)	114 (94%)	7 (6%)	18	41
1	R	141/202 (70%)	137 (97%)	4 (3%)	38	62
1	S	128/202 (63%)	124 (97%)	4 (3%)	35	59
2	G	22/34 (65%)	20 (91%)	2 (9%)	9	23
2	H	20/34 (59%)	17 (85%)	3 (15%)	3	8
2	I	19/34 (56%)	16 (84%)	3 (16%)	2	8
2	J	23/34 (68%)	21 (91%)	2 (9%)	9	25
2	N	27/34 (79%)	22 (82%)	5 (18%)	1	4
2	O	23/34 (68%)	20 (87%)	3 (13%)	4	12
2	P	16/34 (47%)	16 (100%)	0	100	100
2	T	18/34 (53%)	18 (100%)	0	100	100
2	U	23/34 (68%)	20 (87%)	3 (13%)	4	12
2	V	22/34 (65%)	22 (100%)	0	100	100
2	X	27/34 (79%)	26 (96%)	1 (4%)	30	55
2	Y	25/34 (74%)	24 (96%)	1 (4%)	28	53
All	All	1854/2832 (66%)	1785 (96%)	69 (4%)	30	55

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	362	LYS
1	R	222	VAL
1	S	299	THR
2	G	37	ARG
2	G	10	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	163	ASN
1	S	218	ASN
1	S	327	ASN
1	R	226	HIS
2	J	13	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	196/240 (81%)	0.61	12 (6%) 27 22	49, 82, 117, 170	0
1	B	190/240 (79%)	0.46	5 (2%) 57 49	46, 63, 92, 115	0
1	C	195/240 (81%)	0.44	11 (5%) 30 25	51, 71, 100, 112	0
1	D	191/240 (79%)	0.64	17 (8%) 15 14	65, 86, 113, 145	0
1	E	173/240 (72%)	0.87	19 (10%) 10 9	77, 105, 133, 146	0
1	F	197/240 (82%)	0.58	12 (6%) 27 22	54, 73, 98, 132	0
1	K	194/240 (80%)	0.43	5 (2%) 57 49	39, 72, 98, 118	1 (0%)
1	L	191/240 (79%)	0.57	10 (5%) 33 28	62, 82, 109, 150	0
1	M	188/240 (78%)	0.61	6 (3%) 50 43	69, 88, 110, 120	0
1	Q	193/240 (80%)	0.79	13 (6%) 24 20	67, 101, 145, 198	0
1	R	193/240 (80%)	0.51	7 (3%) 46 38	60, 77, 104, 125	0
1	S	191/240 (79%)	0.67	13 (6%) 23 20	71, 87, 108, 121	0
2	G	34/40 (85%)	0.43	0 100 100	87, 108, 121, 125	0
2	H	33/40 (82%)	0.98	2 (6%) 27 22	101, 117, 125, 129	0
2	I	32/40 (80%)	0.86	4 (12%) 8 7	96, 120, 141, 145	0
2	J	34/40 (85%)	0.66	3 (8%) 15 14	80, 106, 124, 131	0
2	N	35/40 (87%)	0.61	3 (8%) 16 14	76, 91, 107, 111	0
2	O	34/40 (85%)	0.83	4 (11%) 9 8	87, 109, 116, 118	0
2	P	30/40 (75%)	1.00	4 (13%) 7 7	102, 138, 159, 163	0
2	T	29/40 (72%)	1.20	3 (10%) 12 11	120, 146, 152, 157	0
2	U	33/40 (82%)	0.36	2 (6%) 27 22	71, 90, 103, 105	0
2	V	34/40 (85%)	0.63	3 (8%) 15 14	86, 96, 109, 119	0
2	X	37/40 (92%)	0.67	2 (5%) 31 26	67, 88, 108, 114	0
2	Y	36/40 (90%)	0.71	4 (11%) 10 9	75, 98, 113, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	2693/3360 (80%)	0.62	164 (6%)	27	22	39, 85, 127, 198	1 (0%)

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	360	ILE	4.8
1	E	285	PRO	4.5
1	E	179	ILE	4.4
1	Q	316	TYR	4.4
1	K	223	THR	4.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.