



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 07:43 PM UTC

PDB ID : 8SE8 / pdb_00008se8
Title : HTRA-1 PD/SA bound to CKP 1G10
Authors : Ultsch, M.H.
Deposited on : 2023-04-08
Resolution : 3.18 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
Mogul : 2022.3.0, CSD as543be (2022)
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

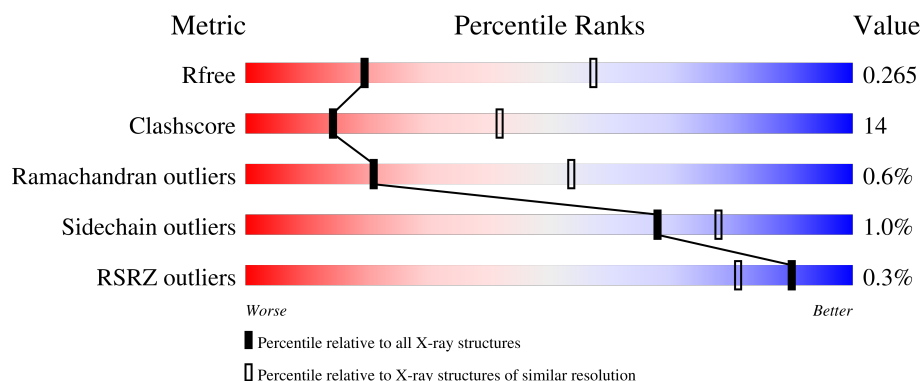
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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.



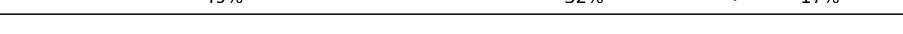
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	 62% 19% 19%
1	B	240	 54% 26% 20%
1	C	240	 63% 18% 19%
1	D	240	 55% 25% 18%
1	E	240	 59% 17% 23%

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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	41	
2	H	41	
2	I	41	
2	J	41	
2	N	41	
2	O	41	
2	P	41	
2	T	41	
2	U	41	
2	V	41	
2	X	41	
2	Y	41	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18768 atoms, of which 8 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	195	Total	C	N	O		0	0	0
			1387	882	237	268				
1	B	192	Total	C	N	O		0	0	0
			1382	876	233	273				
1	C	195	Total	C	N	O		0	0	0
			1391	886	236	269				
1	D	197	Total	C	N	O	S	0	0	0
			1369	871	230	267	1			
1	E	184	Total	C	N	O		0	0	0
			1199	755	207	237				
1	F	195	Total	C	N	O		0	0	0
			1324	834	226	264				
1	K	184	Total	C	N	O		0	0	0
			1237	779	206	252				
1	L	197	Total	C	N	O	S	0	0	0
			1308	821	224	262	1			
1	M	200	Total	C	N	O		0	0	0
			1336	842	230	264				
1	Q	191	Total	C	N	O		0	0	0
			1285	807	220	258				
1	R	195	Total	C	N	O		0	0	0
			1378	878	231	269				
1	S	190	Total	C	N	O		0	0	0
			1271	797	217	257				

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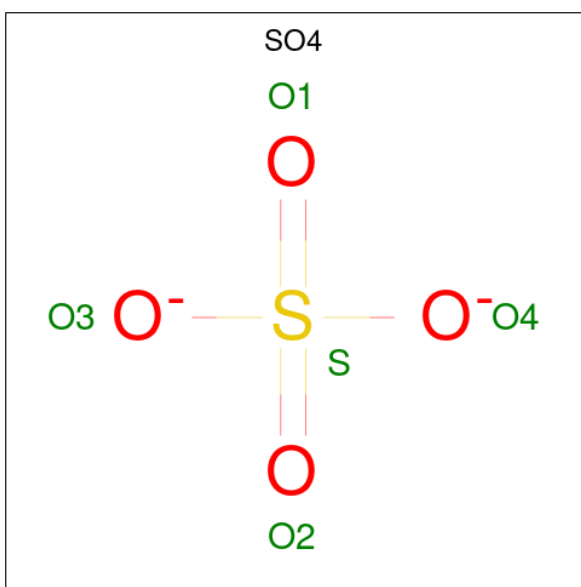
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Chain	Residue	Modelled	Actual	Comment	Reference
S	155	PRO	-	expression tag	UNP Q92743
S	156	ARG	-	expression tag	UNP Q92743
S	157	GLY	-	expression tag	UNP Q92743
S	158	SER	-	expression tag	UNP Q92743
S	159	HIS	-	expression tag	UNP Q92743
S	160	MET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

- Molecule 2 is a protein called Cysteine knot peptide.

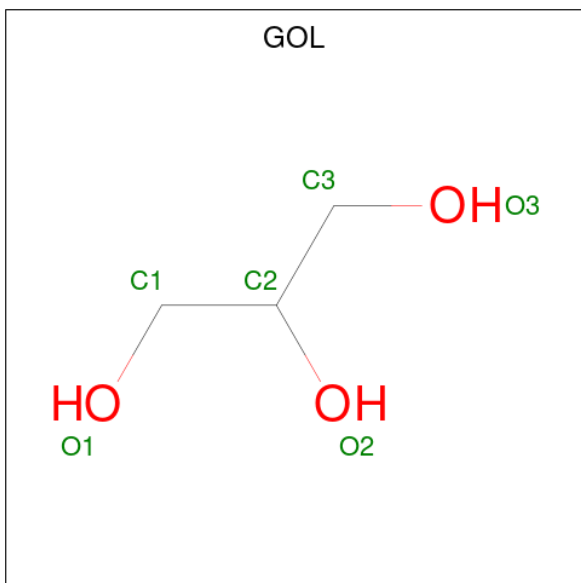
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	32	Total	C	N	O	S	0	0	0
			212	127	37	42	6			
2	X	37	Total	C	N	O	S	0	0	0
			266	164	45	51	6			
2	Y	38	Total	C	N	O	S	0	0	0
			269	165	45	53	6			
2	G	35	Total	C	N	O	S	0	0	0
			237	145	43	43	6			
2	H	35	Total	C	N	O	S	0	0	0
			232	142	40	44	6			
2	J	34	Total	C	N	O	S	0	0	0
			231	142	39	44	6			
2	N	36	Total	C	N	O	S	0	0	0
			254	157	44	47	6			
2	O	37	Total	C	N	O	S	0	0	0
			245	148	42	49	6			
2	P	32	Total	C	N	O	S	0	0	0
			218	134	37	41	6			
2	T	34	Total	C	N	O	S	0	0	0
			229	140	40	43	6			
2	U	36	Total	C	N	O	S	0	0	0
			243	148	41	48	6			
2	V	32	Total	C	N	O	S	0	0	0
			226	139	38	43	6			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	Y	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		

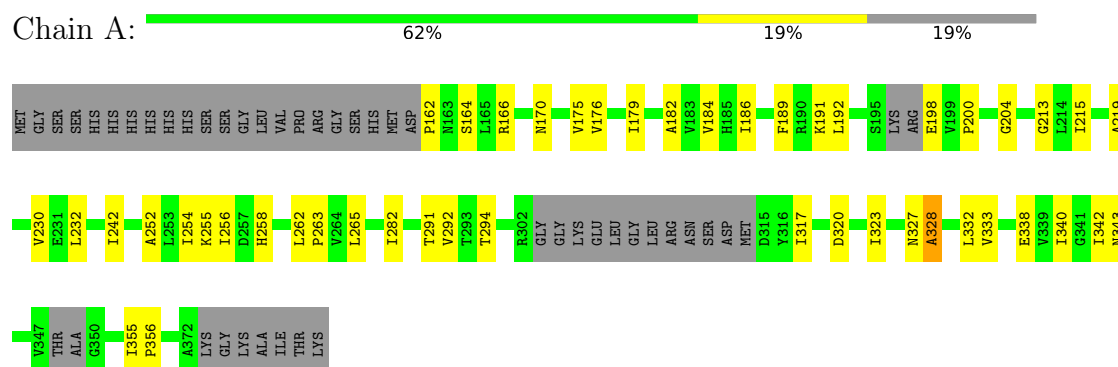
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			1	1		
5	M	1	Total	O	0	0
			1	1		
5	O	2	Total	O	0	0
			2	2		
5	V	1	Total	O	0	0
			1	1		

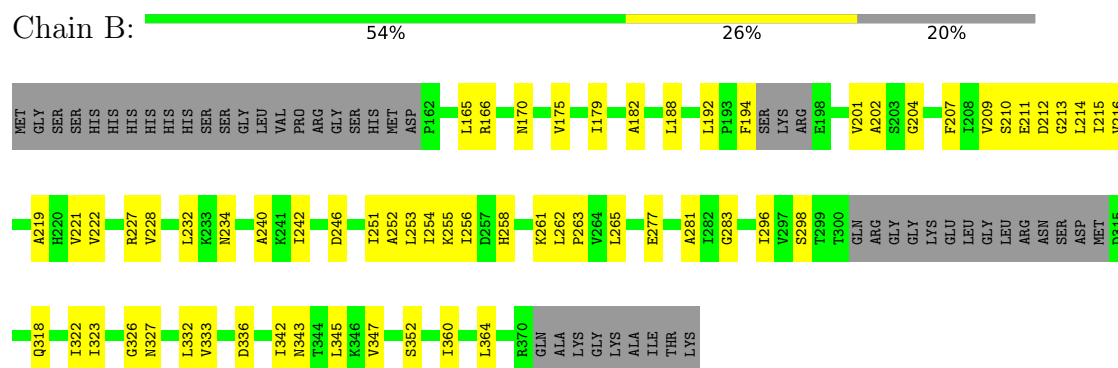
3 Residue-property plots [i](#)

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.

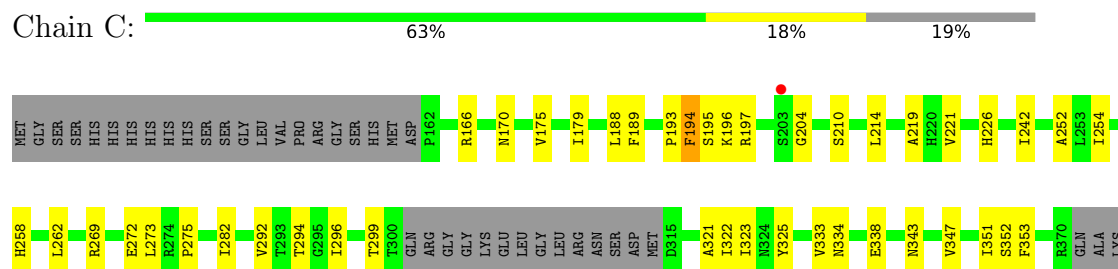
• Molecule 1: Serine protease HTRA1



• Molecule 1: Serine protease HTRA1



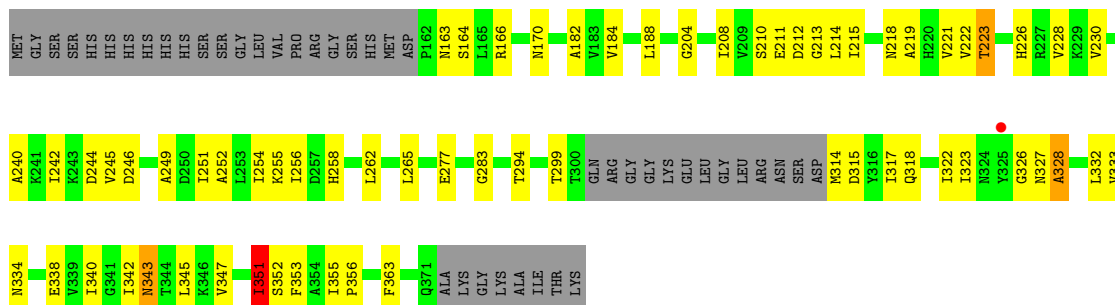
• Molecule 1: Serine protease HTRA1



GLY
LYS
ALA
ILE
THR
LYS

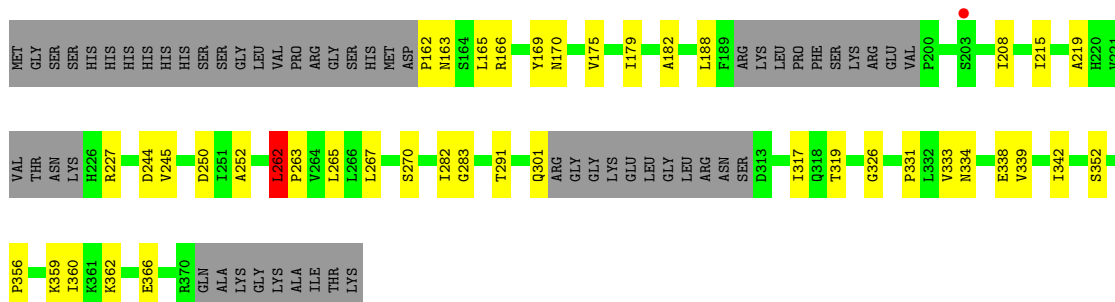
• Molecule 1: Serine protease HTRA1

Chain D:  55% 25% 18%



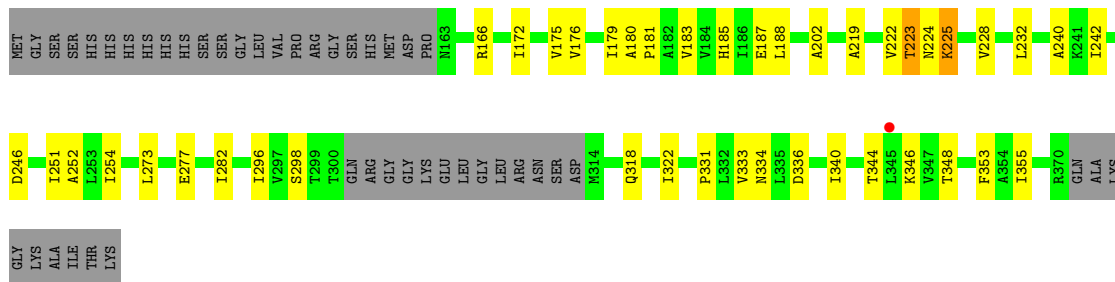
• Molecule 1: Serine protease HTRA1

Chain E:  59% 17% 23%



• Molecule 1: Serine protease HTRA1

Chain F:  64% 17% 19%

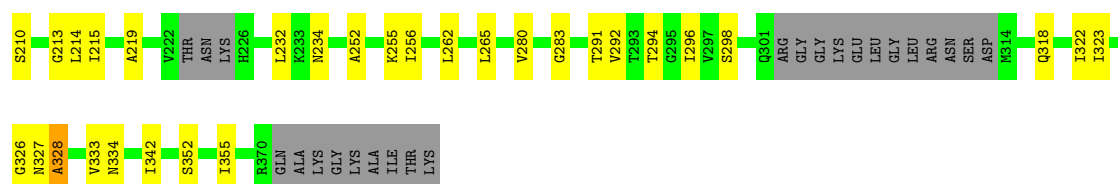


GLY
LYS
ALA
ILE
THR
LYS

• Molecule 1: Serine protease HTRA1

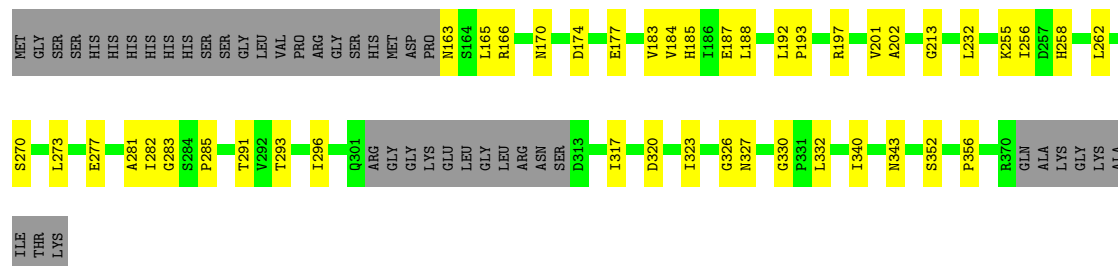
Chain K:  59% 18% 23%





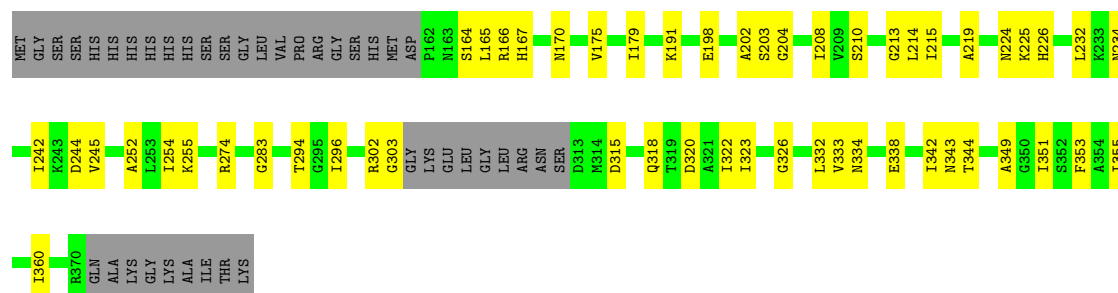
• Molecule 1: Serine protease HTRA1

Chain L: 64% 18% 18%



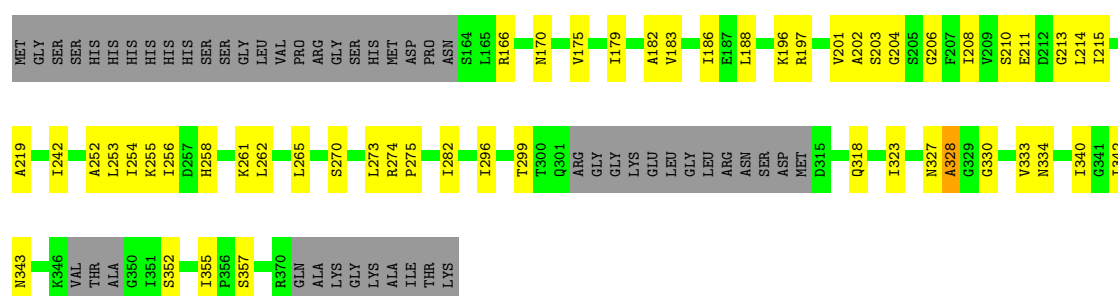
• Molecule 1: Serine protease HTRA1

Chain M: 61% 22% 17%



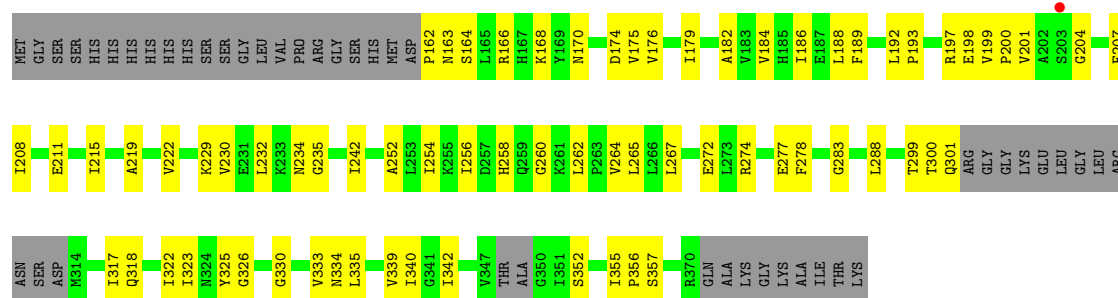
• Molecule 1: Serine protease HTRA1

Chain Q: 58% 21% 20%



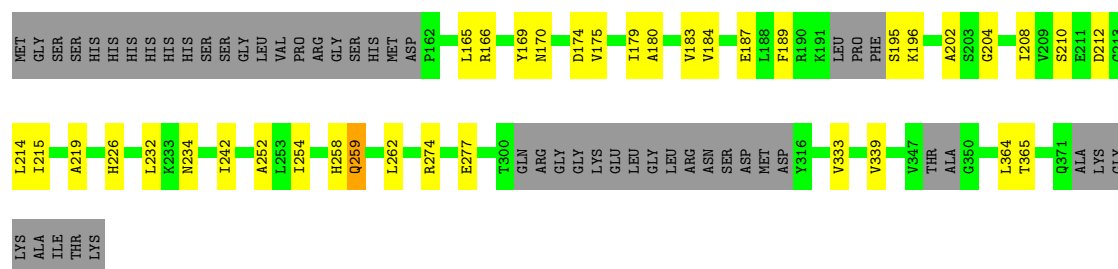
• Molecule 1: Serine protease HTRA1

Chain R: 52% 29% 19%



- Molecule 1: Serine protease HTRA1

Chain S: 64% 15% 21%



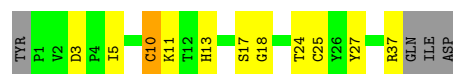
- Molecule 2: Cysteine knot peptide

Chain I: 2% 61% 15% 22%



- Molecule 2: Cysteine knot peptide

Chain X: 63% 24% 10%



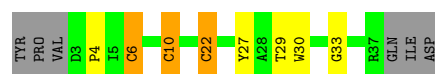
- Molecule 2: Cysteine knot peptide

Chain Y: 44% 46% 7%

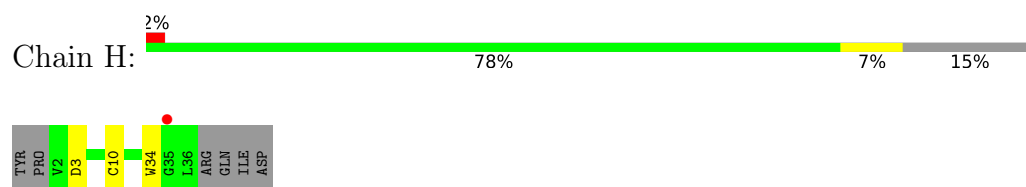


- Molecule 2: Cysteine knot peptide

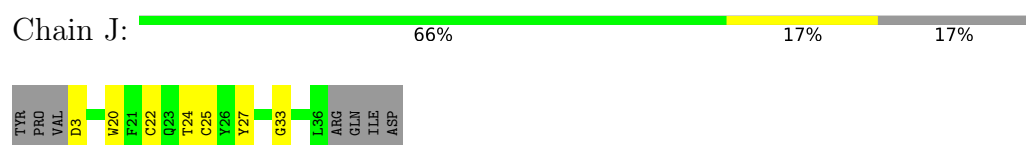
Chain G: 66% 12% 7% 15%



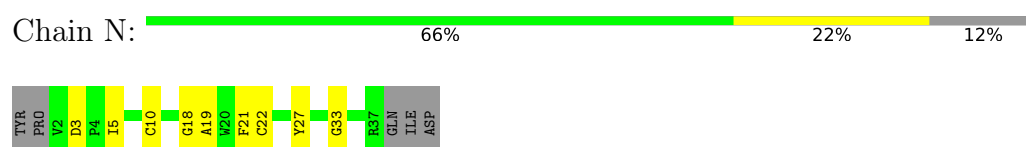
- Molecule 2: Cysteine knot peptide



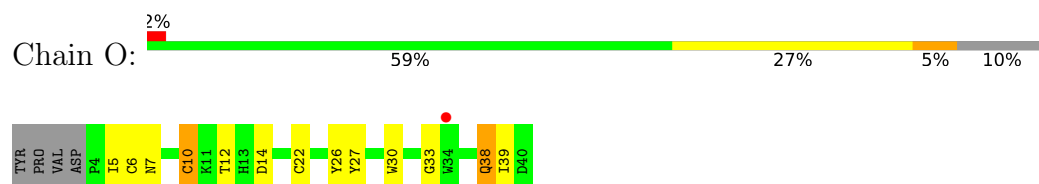
- Molecule 2: Cysteine knot peptide



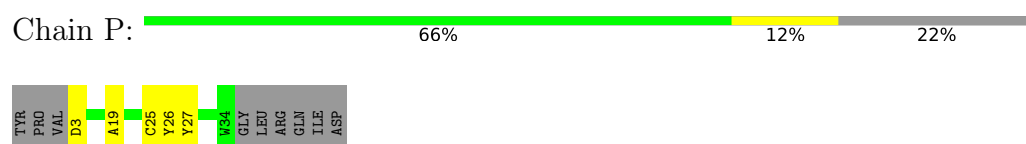
- Molecule 2: Cysteine knot peptide



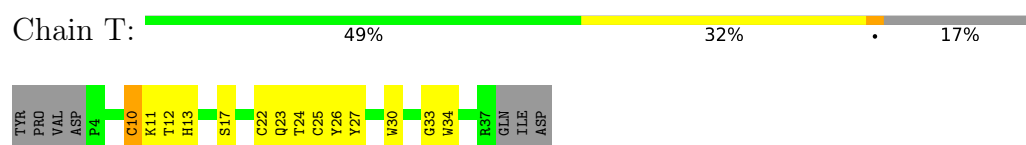
- Molecule 2: Cysteine knot peptide



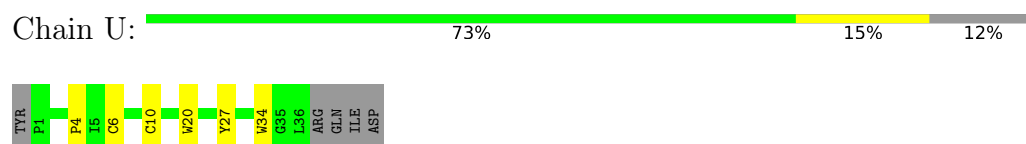
- Molecule 2: Cysteine knot peptide



- 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	120.82Å 155.36Å 173.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.18 19.99 – 3.18	Depositor EDS
% Data completeness (in resolution range)	83.3 (19.99-3.18) 82.9 (19.99-3.18)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.15Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.259 , 0.282 0.260 , 0.265	Depositor DCC
R_{free} test set	2334 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	140.8	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 89.1	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	0.94	EDS
Total number of atoms	18768	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	0.07	0/1410	0.25	0/1927
1	B	0.08	0/1404	0.23	0/1921
1	C	0.07	0/1415	0.23	0/1935
1	D	0.07	0/1394	0.25	0/1915
1	E	0.07	0/1216	0.23	0/1668
1	F	0.07	0/1346	0.23	0/1850
1	K	0.07	0/1253	0.22	0/1721
1	L	0.08	0/1330	0.25	0/1831
1	M	0.09	0/1357	0.23	0/1865
1	Q	0.08	0/1301	0.24	0/1789
1	R	0.08	0/1401	0.24	0/1920
1	S	0.08	0/1290	0.23	0/1768
2	G	0.15	0/245	0.44	0/337
2	H	0.10	0/240	0.40	0/331
2	I	0.14	0/218	0.40	0/299
2	J	0.09	0/239	0.30	0/330
2	N	0.09	0/262	0.33	0/361
2	O	0.09	0/251	0.26	0/344
2	P	0.11	0/226	0.33	0/312
2	T	0.09	0/237	0.37	0/326
2	U	0.08	0/252	0.27	0/348
2	V	0.13	0/234	0.34	0/323
2	X	0.13	0/275	0.38	0/378
2	Y	0.09	0/278	0.31	0/383
All	All	0.08	0/19074	0.26	0/26182

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	262	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1387	0	1291	34	0
1	B	1382	0	1310	47	0
1	C	1391	0	1313	34	0
1	D	1369	0	1241	57	0
1	E	1199	0	1011	31	0
1	F	1324	0	1162	33	0
1	K	1237	0	1075	32	0
1	L	1308	0	1091	32	0
1	M	1336	0	1161	40	0
1	Q	1285	0	1148	40	0
1	R	1378	0	1288	48	0
1	S	1271	0	1083	37	0
2	G	237	0	167	7	0
2	H	232	0	153	3	0
2	I	212	0	152	5	0
2	J	231	0	163	5	0
2	N	254	0	199	6	0
2	O	245	0	180	13	0
2	P	218	0	146	6	0
2	T	229	0	159	12	0
2	U	243	0	174	3	0
2	V	226	0	164	8	0
2	X	266	0	216	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	269	0	207	18	0
3	A	5	0	0	0	0
3	F	5	0	0	0	0
3	P	5	0	0	0	0
3	Y	5	0	0	0	0
4	A	6	8	8	0	0
5	B	1	0	0	0	0
5	M	1	0	0	0	0
5	O	2	0	0	0	0
5	V	1	0	0	0	0
All	All	18760	8	16262	493	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 14.

The worst 5 of 493 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)
2:Y:36:LEU:HD12	2:Y:37:ARG:H	1.33	0.93
1:D:219:ALA:HA	1:D:252:ALA:HB2	1.57	0.84
1:L:193:PRO:HG2	1:L:197:ARG:HA	1.59	0.84
1:D:299:THR:HG22	1:D:318:GLN:HB2	1.61	0.81
1:F:202:ALA:HB1	2:J:27:TYR:HB3	1.62	0.81

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	187/240 (78%)	180 (96%)	6 (3%)	1 (0%)	24 57
1	B	186/240 (78%)	177 (95%)	8 (4%)	1 (0%)	24 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	191/240 (80%)	181 (95%)	8 (4%)	2 (1%)	12	43
1	D	193/240 (80%)	183 (95%)	7 (4%)	3 (2%)	7	34
1	E	176/240 (73%)	169 (96%)	6 (3%)	1 (1%)	21	53
1	F	191/240 (80%)	182 (95%)	7 (4%)	2 (1%)	12	43
1	K	176/240 (73%)	173 (98%)	2 (1%)	1 (1%)	21	53
1	L	193/240 (80%)	183 (95%)	9 (5%)	1 (0%)	24	57
1	M	196/240 (82%)	182 (93%)	14 (7%)	0	100	100
1	Q	185/240 (77%)	176 (95%)	8 (4%)	1 (0%)	24	57
1	R	189/240 (79%)	183 (97%)	6 (3%)	0	100	100
1	S	182/240 (76%)	172 (94%)	9 (5%)	1 (0%)	24	57
2	G	33/41 (80%)	25 (76%)	8 (24%)	0	100	100
2	H	33/41 (80%)	30 (91%)	3 (9%)	0	100	100
2	I	30/41 (73%)	26 (87%)	4 (13%)	0	100	100
2	J	32/41 (78%)	27 (84%)	5 (16%)	0	100	100
2	N	34/41 (83%)	31 (91%)	3 (9%)	0	100	100
2	O	35/41 (85%)	29 (83%)	5 (14%)	1 (3%)	3	21
2	P	30/41 (73%)	26 (87%)	4 (13%)	0	100	100
2	T	32/41 (78%)	27 (84%)	5 (16%)	0	100	100
2	U	34/41 (83%)	28 (82%)	5 (15%)	1 (3%)	3	21
2	V	30/41 (73%)	27 (90%)	3 (10%)	0	100	100
2	X	35/41 (85%)	30 (86%)	5 (14%)	0	100	100
2	Y	36/41 (88%)	28 (78%)	7 (19%)	1 (3%)	4	22
All	All	2639/3372 (78%)	2475 (94%)	147 (6%)	17 (1%)	21	53

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ALA
2	Y	36	LEU
1	D	223	THR
1	D	351	ILE
1	E	262	LEU

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	136/202 (67%)	136 (100%)	0	100	100
1	B	141/202 (70%)	141 (100%)	0	100	100
1	C	138/202 (68%)	138 (100%)	0	100	100
1	D	130/202 (64%)	127 (98%)	3 (2%)	44	68
1	E	97/202 (48%)	97 (100%)	0	100	100
1	F	120/202 (59%)	120 (100%)	0	100	100
1	K	110/202 (54%)	110 (100%)	0	100	100
1	L	109/202 (54%)	109 (100%)	0	100	100
1	M	115/202 (57%)	113 (98%)	2 (2%)	53	72
1	Q	118/202 (58%)	117 (99%)	1 (1%)	73	80
1	R	137/202 (68%)	137 (100%)	0	100	100
1	S	111/202 (55%)	111 (100%)	0	100	100
2	G	19/36 (53%)	16 (84%)	3 (16%)	2	12
2	H	18/36 (50%)	17 (94%)	1 (6%)	19	48
2	I	19/36 (53%)	17 (90%)	2 (10%)	6	25
2	J	20/36 (56%)	20 (100%)	0	100	100
2	N	24/36 (67%)	23 (96%)	1 (4%)	26	56
2	O	22/36 (61%)	21 (96%)	1 (4%)	24	55
2	P	18/36 (50%)	18 (100%)	0	100	100
2	T	19/36 (53%)	18 (95%)	1 (5%)	20	50
2	U	22/36 (61%)	21 (96%)	1 (4%)	24	55
2	V	21/36 (58%)	20 (95%)	1 (5%)	23	53
2	X	27/36 (75%)	26 (96%)	1 (4%)	30	59
2	Y	26/36 (72%)	26 (100%)	0	100	100
All	All	1717/2856 (60%)	1699 (99%)	18 (1%)	68	78

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	256	ILE
2	V	23	GLN
2	U	10	CYS
2	G	22	CYS
2	O	10	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	290	ASN
2	V	7	ASN
2	T	7	ASN
1	F	224	ASN
1	R	218	ASN

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](#)

5 ligands are modelled in this entry.

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	SO4	P	101	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	F	401	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	Y	101	-	4,4,4	0.24	0	6,6,6	0.08	0
4	GOL	A	402	-	5,5,5	0.98	0	5,5,5	1.31	1 (20%)
3	SO4	A	401	-	4,4,4	0.24	0	6,6,6	0.08	0

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
4	GOL	A	402	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	402	GOL	C3-C2-C1	-2.30	103.37	111.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	GOL	C1-C2-C3-O3
4	A	402	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	195/240 (81%)	-0.29	0 100 100	94, 125, 170, 208	0
1	B	192/240 (80%)	-0.28	0 100 100	90, 114, 152, 181	0
1	C	195/240 (81%)	-0.31	1 (0%) 87 75	93, 112, 147, 175	0
1	D	197/240 (82%)	-0.21	1 (0%) 87 75	112, 132, 171, 200	0
1	E	184/240 (76%)	-0.30	1 (0%) 87 75	119, 145, 172, 209	0
1	F	195/240 (81%)	-0.23	1 (0%) 87 75	109, 133, 169, 232	0
1	K	184/240 (76%)	-0.38	0 100 100	116, 135, 152, 170	0
1	L	197/240 (82%)	-0.28	0 100 100	113, 137, 166, 212	0
1	M	200/240 (83%)	-0.31	0 100 100	111, 130, 165, 204	0
1	Q	191/240 (79%)	-0.29	0 100 100	117, 134, 167, 192	0
1	R	195/240 (81%)	-0.26	1 (0%) 87 75	114, 135, 166, 184	0
1	S	190/240 (79%)	-0.27	0 100 100	122, 140, 167, 206	0
2	G	35/41 (85%)	-0.04	0 100 100	136, 158, 177, 187	0
2	H	35/41 (85%)	0.18	1 (2%) 53 34	170, 191, 208, 211	0
2	I	32/41 (78%)	0.19	1 (3%) 51 31	131, 156, 186, 187	0
2	J	34/41 (82%)	0.10	0 100 100	150, 179, 202, 204	0
2	N	36/41 (87%)	0.03	0 100 100	137, 170, 200, 204	0
2	O	37/41 (90%)	0.12	1 (2%) 56 35	159, 193, 241, 257	0
2	P	32/41 (78%)	0.11	0 100 100	133, 153, 169, 170	0
2	T	34/41 (82%)	-0.12	0 100 100	158, 182, 201, 203	0
2	U	36/41 (87%)	-0.11	0 100 100	140, 164, 182, 204	0
2	V	32/41 (78%)	-0.02	0 100 100	163, 191, 209, 215	0
2	X	37/41 (90%)	-0.02	0 100 100	122, 155, 185, 198	0
2	Y	38/41 (92%)	-0.08	0 100 100	113, 140, 169, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2733/3372 (81%)	-0.24	8 (0%) 90 81	90, 136, 186, 257	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	34	TRP	4.2
1	D	325	TYR	3.2
1	C	203	SER	2.6
1	F	345	LEU	2.5
1	R	203	SER	2.4

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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	402	6/6	0.41	0.10	97,97,168,168	0
3	SO4	F	401	5/5	0.78	0.13	148,148,148,148	0
3	SO4	P	101	5/5	0.79	0.09	165,165,165,165	0
3	SO4	Y	101	5/5	0.84	0.19	133,133,133,133	0
3	SO4	A	401	5/5	0.86	0.15	125,125,125,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.