Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 07:40 am BST

PDB ID	:	5E7S
Title	:	Hexameric structure of a LonA protease domain in active state
Authors	:	Lin, C.-C.; Su, S.-C.; Chang, C.-I.
Deposited on	:	2015-10-13
Resolution	:	3.03 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11
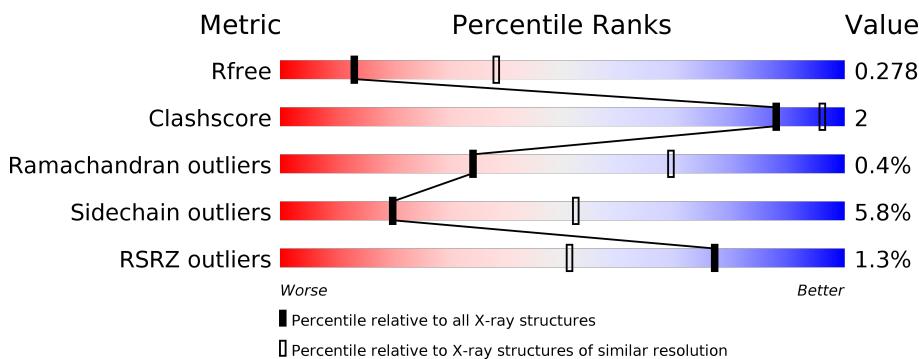
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.03 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		2
Ramachandran outliers		0.4%
Sidechain outliers		5.8%
RSRZ outliers		1.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	298	90% 6% ·
1	B	298	2% 89% 7% ·
1	C	298	% 87% 9% · ·
1	D	298	% 88% 7% · ·
1	E	298	2% 89% 7% · ·
1	F	298	% 89% 7% · ·

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Mol	Chain	Length	Quality of chain
1	G	298	2% 89% 8%
1	H	298	% 88% 7%
1	I	298	2% 86% 10%
1	J	298	% 90% 7%
1	K	298	2% 88% 8%
1	L	298	% 82% 9% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 26298 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 Lon protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total 2199	C 1393	N 380	O 418	S 8	0	0	0
1	B	288	Total 2199	C 1393	N 380	O 418	S 8	0	0	0
1	C	287	Total 2192	C 1388	N 379	O 417	S 8	0	0	0
1	D	289	Total 2206	C 1398	N 381	O 419	S 8	0	0	0
1	E	288	Total 2202	C 1396	N 380	O 418	S 8	0	0	0
1	F	287	Total 2192	C 1388	N 379	O 417	S 8	0	0	0
1	G	289	Total 2206	C 1398	N 381	O 419	S 8	0	0	0
1	H	287	Total 2198	C 1392	N 379	O 419	S 8	0	1	0
1	I	287	Total 2192	C 1388	N 379	O 417	S 8	0	0	0
1	J	289	Total 2206	C 1398	N 381	O 419	S 8	0	0	0
1	K	288	Total 2199	C 1393	N 380	O 418	S 8	0	0	0
1	L	276	Total 2107	C 1337	N 364	O 399	S 7	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	490	MET	-	expression tag	UNP A0A059VAZ3
A	782	HIS	-	expression tag	UNP A0A059VAZ3
A	783	HIS	-	expression tag	UNP A0A059VAZ3
A	784	HIS	-	expression tag	UNP A0A059VAZ3
A	785	HIS	-	expression tag	UNP A0A059VAZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	786	HIS	-	expression tag	UNP A0A059VAZ3
A	787	HIS	-	expression tag	UNP A0A059VAZ3
B	490	MET	-	expression tag	UNP A0A059VAZ3
B	782	HIS	-	expression tag	UNP A0A059VAZ3
B	783	HIS	-	expression tag	UNP A0A059VAZ3
B	784	HIS	-	expression tag	UNP A0A059VAZ3
B	785	HIS	-	expression tag	UNP A0A059VAZ3
B	786	HIS	-	expression tag	UNP A0A059VAZ3
B	787	HIS	-	expression tag	UNP A0A059VAZ3
C	490	MET	-	expression tag	UNP A0A059VAZ3
C	782	HIS	-	expression tag	UNP A0A059VAZ3
C	783	HIS	-	expression tag	UNP A0A059VAZ3
C	784	HIS	-	expression tag	UNP A0A059VAZ3
C	785	HIS	-	expression tag	UNP A0A059VAZ3
C	786	HIS	-	expression tag	UNP A0A059VAZ3
C	787	HIS	-	expression tag	UNP A0A059VAZ3
D	490	MET	-	expression tag	UNP A0A059VAZ3
D	782	HIS	-	expression tag	UNP A0A059VAZ3
D	783	HIS	-	expression tag	UNP A0A059VAZ3
D	784	HIS	-	expression tag	UNP A0A059VAZ3
D	785	HIS	-	expression tag	UNP A0A059VAZ3
D	786	HIS	-	expression tag	UNP A0A059VAZ3
D	787	HIS	-	expression tag	UNP A0A059VAZ3
E	490	MET	-	expression tag	UNP A0A059VAZ3
E	782	HIS	-	expression tag	UNP A0A059VAZ3
E	783	HIS	-	expression tag	UNP A0A059VAZ3
E	784	HIS	-	expression tag	UNP A0A059VAZ3
E	785	HIS	-	expression tag	UNP A0A059VAZ3
E	786	HIS	-	expression tag	UNP A0A059VAZ3
E	787	HIS	-	expression tag	UNP A0A059VAZ3
F	490	MET	-	expression tag	UNP A0A059VAZ3
F	782	HIS	-	expression tag	UNP A0A059VAZ3
F	783	HIS	-	expression tag	UNP A0A059VAZ3
F	784	HIS	-	expression tag	UNP A0A059VAZ3
F	785	HIS	-	expression tag	UNP A0A059VAZ3
F	786	HIS	-	expression tag	UNP A0A059VAZ3
F	787	HIS	-	expression tag	UNP A0A059VAZ3
G	490	MET	-	expression tag	UNP A0A059VAZ3
G	782	HIS	-	expression tag	UNP A0A059VAZ3
G	783	HIS	-	expression tag	UNP A0A059VAZ3
G	784	HIS	-	expression tag	UNP A0A059VAZ3
G	785	HIS	-	expression tag	UNP A0A059VAZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	786	HIS	-	expression tag	UNP A0A059VAZ3
G	787	HIS	-	expression tag	UNP A0A059VAZ3
H	490	MET	-	expression tag	UNP A0A059VAZ3
H	782	HIS	-	expression tag	UNP A0A059VAZ3
H	783	HIS	-	expression tag	UNP A0A059VAZ3
H	784	HIS	-	expression tag	UNP A0A059VAZ3
H	785	HIS	-	expression tag	UNP A0A059VAZ3
H	786	HIS	-	expression tag	UNP A0A059VAZ3
H	787	HIS	-	expression tag	UNP A0A059VAZ3
I	490	MET	-	expression tag	UNP A0A059VAZ3
I	782	HIS	-	expression tag	UNP A0A059VAZ3
I	783	HIS	-	expression tag	UNP A0A059VAZ3
I	784	HIS	-	expression tag	UNP A0A059VAZ3
I	785	HIS	-	expression tag	UNP A0A059VAZ3
I	786	HIS	-	expression tag	UNP A0A059VAZ3
I	787	HIS	-	expression tag	UNP A0A059VAZ3
J	490	MET	-	expression tag	UNP A0A059VAZ3
J	782	HIS	-	expression tag	UNP A0A059VAZ3
J	783	HIS	-	expression tag	UNP A0A059VAZ3
J	784	HIS	-	expression tag	UNP A0A059VAZ3
J	785	HIS	-	expression tag	UNP A0A059VAZ3
J	786	HIS	-	expression tag	UNP A0A059VAZ3
J	787	HIS	-	expression tag	UNP A0A059VAZ3
K	490	MET	-	expression tag	UNP A0A059VAZ3
K	782	HIS	-	expression tag	UNP A0A059VAZ3
K	783	HIS	-	expression tag	UNP A0A059VAZ3
K	784	HIS	-	expression tag	UNP A0A059VAZ3
K	785	HIS	-	expression tag	UNP A0A059VAZ3
K	786	HIS	-	expression tag	UNP A0A059VAZ3
K	787	HIS	-	expression tag	UNP A0A059VAZ3
L	490	MET	-	expression tag	UNP A0A059VAZ3
L	782	HIS	-	expression tag	UNP A0A059VAZ3
L	783	HIS	-	expression tag	UNP A0A059VAZ3
L	784	HIS	-	expression tag	UNP A0A059VAZ3
L	785	HIS	-	expression tag	UNP A0A059VAZ3
L	786	HIS	-	expression tag	UNP A0A059VAZ3
L	787	HIS	-	expression tag	UNP A0A059VAZ3

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Lon protease
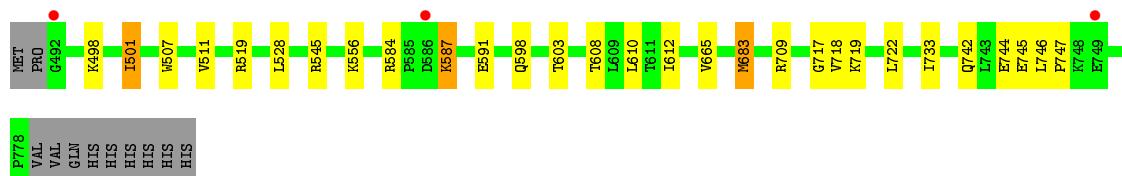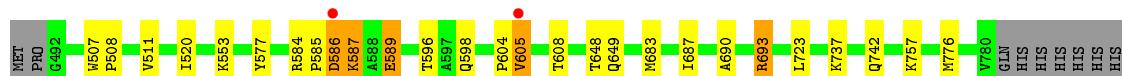
- Molecule 1: Lon protease

- Molecule 1: Lon protease

- Molecule 1: Lon protease

- Molecule 1: Lon protease

• Molecule 1: Lon protease

Chain F:

• Molecule 1: Lon protease

Chain G:

• Molecule 1: Lon protease

Chain H:

• Molecule 1: Lon protease

Chain I:

• Molecule 1: Lon protease

Chain J:

• Molecule 1: Lon protease

Chain K:

V779 VAL GLN HIS HIS HIS HIS HIS

• Molecule 1: Lon protease

Chain L:

%

82% 9% • 7%

MET PRO G492 E497 I501 A502 L506 W507 P508 K509 Q510 V511 R512 GLU SER GLY MET GLU GLY ARG ILE E521 V522 G548 K549 I550 K553 K556 F557 TRP LEU GLU GLY ALA W563 E564 G565 L566 R567 T568 I569 Y577 L578 K587 W602 T608 L625 Q649

V665 R693 L723 L746 P747 K748 E749 V750 L751 E773 P777 P778 V779 V780 GLN HIS HIS HIS HIS HIS
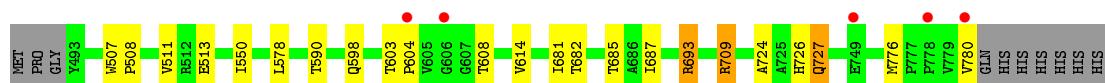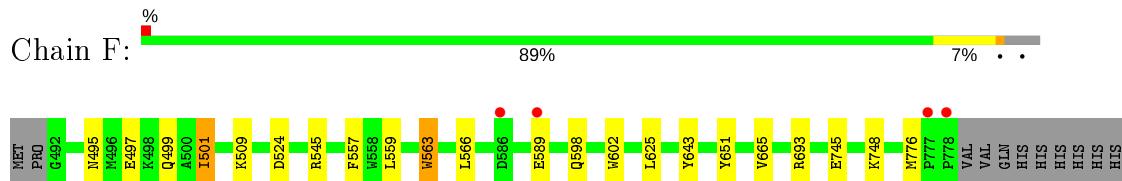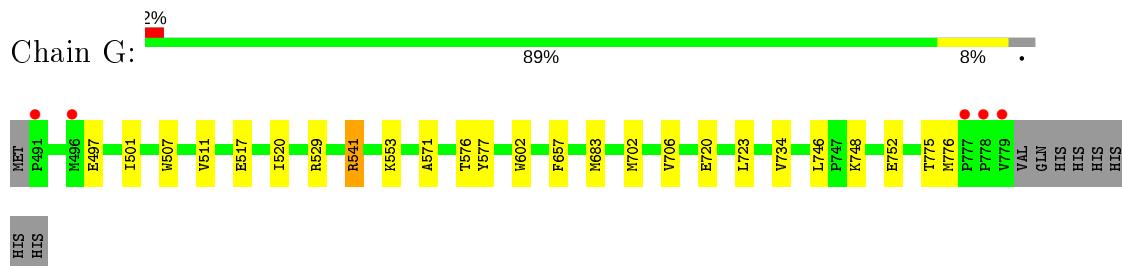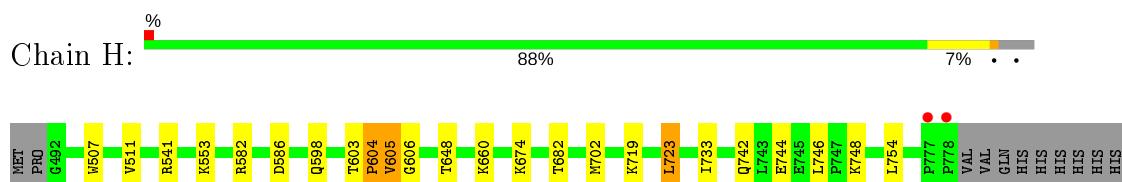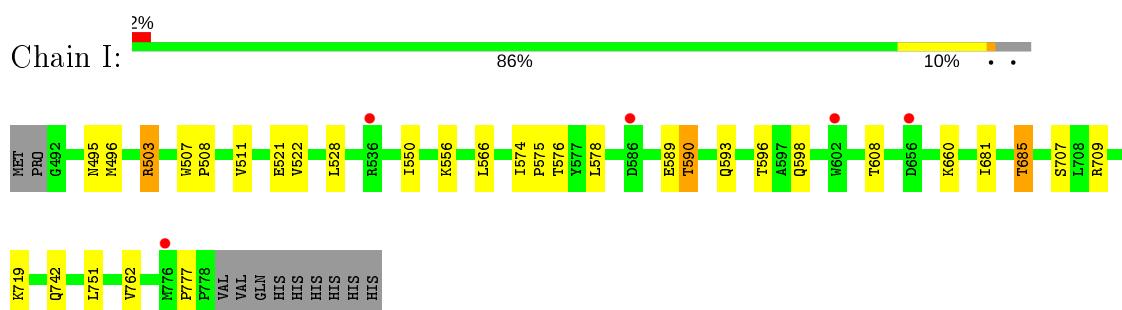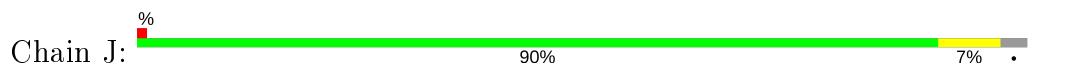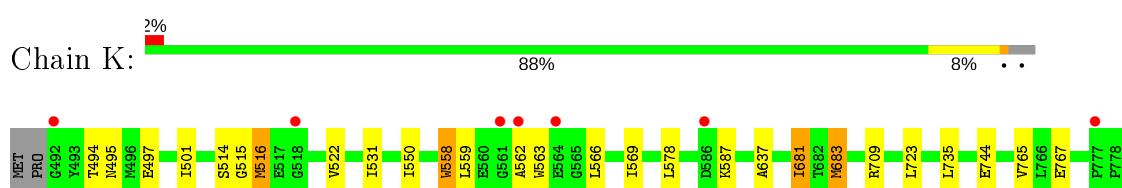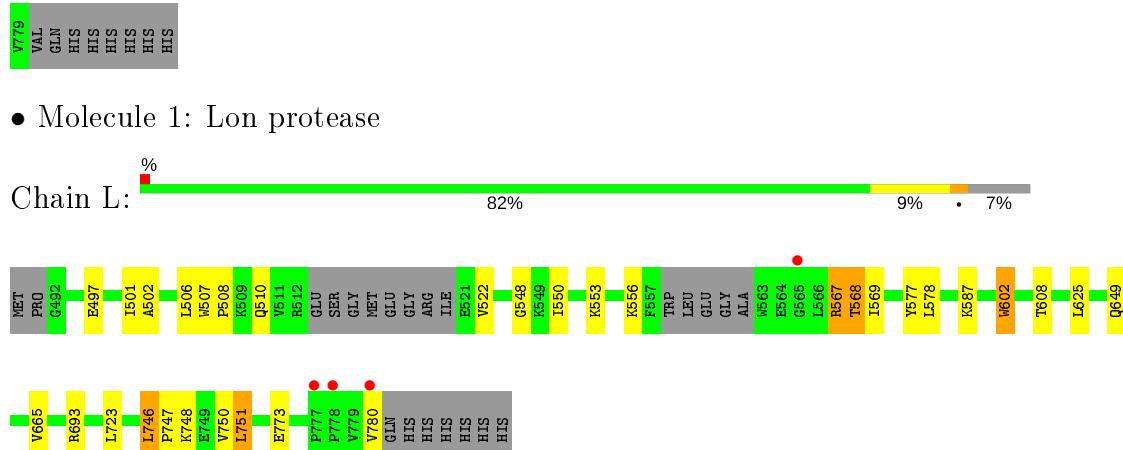
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	116.31Å 212.79Å 178.92Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	20.00 – 3.03 19.86 – 3.03	Depositor EDS
% Data completeness (in resolution range)	90.5 (20.00-3.03) 90.9 (19.86-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.227 , 0.279 0.226 , 0.278	Depositor DCC
R_{free} test set	3798 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	63.1	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 18.3	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	26298	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.27	0/2241	0.49	0/3040
1	B	0.27	0/2241	0.50	0/3040
1	C	0.28	0/2234	0.52	0/3030
1	D	0.27	0/2248	0.48	0/3050
1	E	0.26	0/2244	0.49	0/3045
1	F	0.27	0/2234	0.48	0/3030
1	G	0.27	0/2249	0.51	0/3051
1	H	0.27	0/2243	0.49	0/3042
1	I	0.27	0/2234	0.50	0/3030
1	J	0.28	0/2248	0.51	0/3050
1	K	0.29	0/2241	0.51	0/3040
1	L	0.28	0/2145	0.51	0/2909
All	All	0.27	0/26802	0.50	0/36357

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2199	0	2240	5	0
1	B	2199	0	2240	14	0
1	C	2192	0	2231	14	0
1	D	2206	0	2249	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2202	0	2246	10	0
1	F	2192	0	2231	5	0
1	G	2206	0	2248	10	0
1	H	2198	0	2237	8	0
1	I	2192	0	2231	8	0
1	J	2206	0	2249	5	0
1	K	2199	0	2240	9	0
1	L	2107	0	2156	12	0
All	All	26298	0	26798	107	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 2.

All (107) 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:B:637:ALA:HB2	1:B:683:MET:CE	1.97	0.93
1:B:637:ALA:HB2	1:B:683:MET:HE3	1.51	0.89
1:K:558:TRP:HZ3	1:K:562:ALA:HA	1.41	0.86
1:B:637:ALA:CB	1:B:683:MET:CE	2.67	0.71
1:H:604:PRO:HA	1:H:605:VAL:C	2.10	0.70
1:C:722:LEU:HD11	1:C:733:ILE:HG21	1.74	0.69
1:K:637:ALA:HB2	1:K:683:MET:HE1	1.73	0.69
1:C:665:VAL:HG11	1:C:683:MET:CE	2.23	0.68
1:D:604:PRO:O	1:D:605:VAL:HG22	1.96	0.66
1:K:637:ALA:HB2	1:K:683:MET:CE	2.26	0.65
1:I:681:ILE:O	1:I:685:THR:OG1	2.15	0.65
1:H:605:VAL:HG13	1:H:606:GLY:H	1.63	0.63
1:A:669:ASP:O	1:A:674:LYS:NZ	2.31	0.63
1:I:503:ARG:NH2	1:I:522:VAL:O	2.30	0.63
1:E:507:TRP:O	1:E:511:VAL:HG23	1.98	0.63
1:D:507:TRP:O	1:D:511:VAL:HG23	2.00	0.62
1:I:507:TRP:O	1:I:511:VAL:HG23	2.02	0.59
1:G:507:TRP:O	1:G:511:VAL:HG23	2.01	0.59
1:B:612:ILE:HG21	1:B:683:MET:HG3	1.85	0.58
1:C:665:VAL:HG11	1:C:683:MET:HE2	1.84	0.58
1:E:681:ILE:O	1:E:685:THR:OG1	2.12	0.58
1:K:558:TRP:CZ3	1:K:562:ALA:HA	2.31	0.57
1:D:585:PRO:HB2	1:D:586:ASP:HA	1.86	0.56
1:E:603:THR:HB	1:E:604:PRO:CD	2.36	0.56
1:C:612:ILE:HG21	1:C:683:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:665:VAL:HG11	1:C:683:MET:HE1	1.87	0.55
1:F:497:GLU:O	1:F:501:ILE:HG22	2.07	0.54
1:D:585:PRO:CB	1:D:586:ASP:HA	2.36	0.54
1:C:584:ARG:CZ	1:C:587:LYS:HB3	2.37	0.54
1:B:507:TRP:O	1:B:511:VAL:HG23	2.10	0.52
1:C:584:ARG:HB3	1:C:591:GLU:HB3	1.91	0.52
1:G:541:ARG:H	1:G:541:ARG:CD	2.24	0.51
1:D:553:LYS:HG2	1:D:577:TYR:HA	1.92	0.51
1:J:609:LEU:HD21	1:J:728:ALA:HB1	1.91	0.51
1:B:637:ALA:CA	1:B:683:MET:CE	2.88	0.50
1:C:717:GLY:O	1:C:719:LYS:N	2.45	0.50
1:E:507:TRP:HB3	1:E:508:PRO:HD3	1.92	0.50
1:C:498:LYS:HA	1:C:501:ILE:CD1	2.42	0.49
1:K:550:ILE:HG13	1:K:578:LEU:HD21	1.94	0.49
1:B:637:ALA:CB	1:B:683:MET:HE2	2.41	0.49
1:J:609:LEU:HD21	1:J:728:ALA:CB	2.42	0.49
1:L:747:PRO:HD2	1:L:750:VAL:HB	1.93	0.49
1:B:747:PRO:O	1:B:749:GLU:N	2.45	0.48
1:C:665:VAL:CG1	1:C:683:MET:HE1	2.43	0.48
1:L:746:LEU:HB2	1:L:751:LEU:CD1	2.44	0.48
1:C:584:ARG:NH2	1:C:587:LYS:O	2.46	0.48
1:L:510:GLN:HG3	1:L:548:GLY:HA2	1.96	0.48
1:D:683:MET:O	1:D:687:ILE:HG13	2.14	0.48
1:H:604:PRO:HA	1:H:605:VAL:O	2.13	0.47
1:B:613:GLU:OE2	1:C:709:ARG:NH1	2.48	0.47
1:L:502:ALA:HA	1:L:506:LEU:HB2	1.96	0.47
1:E:614:VAL:HG11	1:E:687:ILE:HA	1.97	0.47
1:A:497:GLU:O	1:A:501:ILE:HG13	2.15	0.46
1:G:529:ARG:NH1	1:G:571:ALA:O	2.48	0.46
1:K:681:ILE:HD12	1:K:765:VAL:HG21	1.97	0.46
1:G:541:ARG:H	1:G:541:ARG:HD3	1.80	0.46
1:I:550:ILE:HG13	1:I:578:LEU:HD21	1.96	0.46
1:B:519:ARG:HD3	1:B:558:TRP:CZ3	2.50	0.46
1:D:596:THR:HG21	1:E:709:ARG:HD3	1.97	0.46
1:F:693:ARG:HG3	1:F:776:MET:HB2	1.98	0.46
1:D:507:TRP:HB3	1:D:508:PRO:HD3	1.98	0.45
1:E:550:ILE:HG13	1:E:578:LEU:HD21	1.98	0.45
1:B:637:ALA:HA	1:B:683:MET:CE	2.46	0.45
1:E:603:THR:HB	1:E:604:PRO:HD2	1.98	0.45
1:B:637:ALA:CA	1:B:683:MET:HE1	2.47	0.45
1:D:587:LYS:O	1:D:589:GLU:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:693:ARG:HG3	1:E:776:MET:HB2	1.97	0.45
1:I:507:TRP:HB3	1:I:508:PRO:HD3	1.97	0.45
1:G:553:LYS:HG2	1:G:577:TYR:HA	1.99	0.45
1:D:690:ALA:O	1:D:693:ARG:NH1	2.50	0.44
1:E:724:ALA:HA	1:E:727:GLN:HE22	1.81	0.44
1:L:550:ILE:HG13	1:L:578:LEU:HD21	1.99	0.44
1:J:499:GLN:NE2	1:J:524:ASP:O	2.50	0.44
1:I:596:THR:HG21	1:J:709:ARG:HD3	1.99	0.43
1:F:557:PHE:HB3	1:F:563:TRP:HH2	1.83	0.43
1:H:507:TRP:O	1:H:511:VAL:HG23	2.18	0.43
1:L:567:ARG:O	1:L:568:THR:OG1	2.27	0.43
1:K:514:SER:O	1:K:516:MET:N	2.50	0.43
1:D:693:ARG:HG3	1:D:776:MET:HB2	2.00	0.43
1:L:507:TRP:HB3	1:L:508:PRO:HD3	2.00	0.43
1:A:586:ASP:N	1:A:586:ASP:OD1	2.51	0.43
1:G:497:GLU:O	1:G:501:ILE:HG13	2.18	0.43
1:G:541:ARG:HD3	1:G:541:ARG:N	2.32	0.43
1:A:550:ILE:HG13	1:A:578:LEU:HD21	2.00	0.43
1:L:522:VAL:HG12	1:L:569:ILE:HB	2.01	0.43
1:A:679:ALA:O	1:A:683:MET:HG2	2.19	0.42
1:H:733:ILE:HD12	1:H:754:LEU:HD13	2.01	0.42
1:K:522:VAL:HG12	1:K:569:ILE:HB	2.00	0.42
1:H:603:THR:O	1:H:606:GLY:N	2.52	0.42
1:B:614:VAL:HG11	1:B:687:ILE:HA	2.00	0.42
1:I:589:GLU:O	1:I:590:THR:HB	2.20	0.42
1:C:584:ARG:NH2	1:C:587:LYS:HB3	2.34	0.42
1:H:682:THR:HA	1:H:702:MET:SD	2.60	0.41
1:B:637:ALA:HA	1:B:683:MET:HE1	2.02	0.41
1:C:507:TRP:O	1:C:511:VAL:HG23	2.21	0.41
1:G:775:THR:HG23	1:G:776:MET:HG3	2.02	0.41
1:J:613:GLU:OE2	1:K:709:ARG:NH1	2.53	0.41
1:L:497:GLU:O	1:L:501:ILE:HG13	2.20	0.41
1:I:574:ILE:N	1:I:575:PRO:CD	2.83	0.41
1:H:719:LYS:O	1:H:723:LEU:HD23	2.20	0.41
1:L:602:TRP:CD1	1:L:602:TRP:C	2.93	0.41
1:L:553:LYS:HG2	1:L:577:TYR:HA	2.03	0.41
1:F:643:TYR:HH	1:F:651:TYR:HH	1.67	0.40
1:F:625:LEU:HD23	1:F:665:VAL:HB	2.02	0.40
1:G:511:VAL:HG12	1:G:517:GLU:HA	2.03	0.40
1:G:702:MET:HB3	1:G:734:VAL:HB	2.04	0.40
1:L:625:LEU:HD23	1:L:665:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/298 (96%)	277 (97%)	9 (3%)	0	100	100
1	B	286/298 (96%)	276 (96%)	10 (4%)	0	100	100
1	C	285/298 (96%)	272 (95%)	11 (4%)	2 (1%)	22	57
1	D	287/298 (96%)	278 (97%)	7 (2%)	2 (1%)	22	57
1	E	286/298 (96%)	277 (97%)	9 (3%)	0	100	100
1	F	285/298 (96%)	279 (98%)	6 (2%)	0	100	100
1	G	287/298 (96%)	274 (96%)	12 (4%)	1 (0%)	41	74
1	H	286/298 (96%)	275 (96%)	9 (3%)	2 (1%)	22	57
1	I	285/298 (96%)	275 (96%)	9 (3%)	1 (0%)	34	69
1	J	287/298 (96%)	279 (97%)	7 (2%)	1 (0%)	41	74
1	K	286/298 (96%)	274 (96%)	11 (4%)	1 (0%)	41	74
1	L	270/298 (91%)	258 (96%)	10 (4%)	2 (1%)	22	57
All	All	3416/3576 (96%)	3294 (96%)	110 (3%)	12 (0%)	34	69

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	718	VAL
1	D	605	VAL
1	G	602	TRP
1	H	605	VAL
1	K	515	GLY
1	L	568	THR
1	D	584	ARG
1	I	590	THR
1	L	567	ARG

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Mol	Chain	Res	Type
1	C	747	PRO
1	H	604	PRO
1	J	772	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/239 (96%)	219 (96%)	10 (4%)	28	63
1	B	229/239 (96%)	218 (95%)	11 (5%)	25	60
1	C	228/239 (95%)	213 (93%)	15 (7%)	16	47
1	D	230/239 (96%)	217 (94%)	13 (6%)	20	53
1	E	230/239 (96%)	220 (96%)	10 (4%)	29	63
1	F	228/239 (95%)	214 (94%)	14 (6%)	18	50
1	G	230/239 (96%)	219 (95%)	11 (5%)	25	60
1	H	229/239 (96%)	216 (94%)	13 (6%)	20	53
1	I	228/239 (95%)	208 (91%)	20 (9%)	10	34
1	J	230/239 (96%)	216 (94%)	14 (6%)	18	50
1	K	229/239 (96%)	212 (93%)	17 (7%)	13	42
1	L	221/239 (92%)	209 (95%)	12 (5%)	22	55
All	All	2741/2868 (96%)	2581 (94%)	160 (6%)	20	52

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	504	GLN
1	A	567	ARG
1	A	622	LYS
1	A	650	ASP
1	A	702	MET
1	A	711	LYS
1	A	723	LEU

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Mol	Chain	Res	Type
1	A	737	LYS
1	A	749	GLU
1	A	751	LEU
1	B	496	MET
1	B	541	ARG
1	B	549	LYS
1	B	589	GLU
1	B	610	LEU
1	B	650	ASP
1	B	683	MET
1	B	693	ARG
1	B	723	LEU
1	B	744	GLU
1	B	779	VAL
1	C	501	ILE
1	C	519	ARG
1	C	528	LEU
1	C	545	ARG
1	C	556	LYS
1	C	587	LYS
1	C	598	GLN
1	C	603	THR
1	C	608	THR
1	C	610	LEU
1	C	683	MET
1	C	742	GLN
1	C	744	GLU
1	C	745	GLU
1	C	746	LEU
1	D	520	ILE
1	D	586	ASP
1	D	587	LYS
1	D	589	GLU
1	D	598	GLN
1	D	608	THR
1	D	648	THR
1	D	649	GLN
1	D	693	ARG
1	D	723	LEU
1	D	737	LYS
1	D	742	GLN
1	D	757	LYS

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Mol	Chain	Res	Type
1	E	513	GLU
1	E	590	THR
1	E	598	GLN
1	E	608	THR
1	E	682	THR
1	E	693	ARG
1	E	709	ARG
1	E	726	HIS
1	E	727	GLN
1	E	780	VAL
1	F	495	ASN
1	F	499	GLN
1	F	501	ILE
1	F	509	LYS
1	F	524	ASP
1	F	545	ARG
1	F	559	LEU
1	F	563	TRP
1	F	566	LEU
1	F	589	GLU
1	F	598	GLN
1	F	602	TRP
1	F	745	GLU
1	F	748	LYS
1	G	520	ILE
1	G	541	ARG
1	G	576	THR
1	G	657	PHE
1	G	683	MET
1	G	706	VAL
1	G	720	GLU
1	G	723	LEU
1	G	746	LEU
1	G	748	LYS
1	G	752	GLU
1	H	541	ARG
1	H	553	LYS
1	H	582	ARG
1	H	586	ASP
1	H	598	GLN
1	H	648	THR
1	H	660	LYS

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Mol	Chain	Res	Type
1	H	674	LYS
1	H	723	LEU
1	H	742	GLN
1	H	744	GLU
1	H	746	LEU
1	H	748	LYS
1	I	495	ASN
1	I	496	MET
1	I	503	ARG
1	I	521	GLU
1	I	528	LEU
1	I	556	LYS
1	I	566	LEU
1	I	576	THR
1	I	593	GLN
1	I	598	GLN
1	I	608	THR
1	I	660	LYS
1	I	685	THR
1	I	707	SER
1	I	709	ARG
1	I	719	LYS
1	I	742	GLN
1	I	751	LEU
1	I	762	VAL
1	I	777	PRO
1	J	495	ASN
1	J	497	GLU
1	J	511	VAL
1	J	541	ARG
1	J	546	GLU
1	J	593	GLN
1	J	602	TRP
1	J	707	SER
1	J	722	LEU
1	J	723	LEU
1	J	746	LEU
1	J	754	LEU
1	J	755	GLU
1	J	756	ILE
1	K	494	THR
1	K	495	ASN

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Mol	Chain	Res	Type
1	K	497	GLU
1	K	501	ILE
1	K	516	MET
1	K	531	ILE
1	K	558	TRP
1	K	559	LEU
1	K	563	TRP
1	K	566	LEU
1	K	587	LYS
1	K	681	ILE
1	K	683	MET
1	K	723	LEU
1	K	735	LEU
1	K	744	GLU
1	K	767	GLU
1	L	556	LYS
1	L	587	LYS
1	L	602	TRP
1	L	608	THR
1	L	649	GLN
1	L	693	ARG
1	L	723	LEU
1	L	746	LEU
1	L	748	LYS
1	L	751	LEU
1	L	773	GLU
1	L	780	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	ASN
1	A	647	HIS
1	A	742	GLN
1	B	495	ASN
1	C	598	GLN
1	C	638	GLN
1	C	742	GLN
1	D	495	ASN
1	D	598	GLN
1	D	742	GLN
1	E	495	ASN

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Mol	Chain	Res	Type
1	E	727	GLN
1	G	598	GLN
1	H	593	GLN
1	H	598	GLN
1	H	638	GLN
1	I	495	ASN
1	J	495	ASN
1	J	593	GLN
1	J	598	GLN
1	K	495	ASN
1	K	598	GLN
1	K	742	GLN
1	L	495	ASN
1	L	598	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (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	288/298 (96%)	-0.37	0	100	100	37, 62, 84, 101	0
1	B	288/298 (96%)	-0.24	5 (1%)	70	42	39, 68, 99, 117	0
1	C	287/298 (96%)	-0.21	3 (1%)	82	59	40, 72, 103, 122	0
1	D	289/298 (96%)	-0.32	2 (0%)	87	69	38, 63, 86, 108	0
1	E	288/298 (96%)	-0.20	5 (1%)	70	42	38, 69, 102, 121	0
1	F	287/298 (96%)	-0.20	4 (1%)	75	49	38, 68, 97, 116	0
1	G	289/298 (96%)	-0.28	5 (1%)	70	42	38, 69, 95, 108	0
1	H	287/298 (96%)	-0.25	2 (0%)	87	69	40, 71, 92, 103	0
1	I	287/298 (96%)	-0.17	5 (1%)	70	42	39, 80, 101, 110	0
1	J	289/298 (96%)	-0.16	3 (1%)	82	59	40, 81, 103, 115	0
1	K	288/298 (96%)	-0.12	7 (2%)	59	30	41, 83, 117, 134	0
1	L	276/298 (92%)	-0.22	4 (1%)	75	49	40, 71, 98, 119	0
All	All	3443/3576 (96%)	-0.23	45 (1%)	77	51	37, 70, 102, 134	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	562	ALA	5.3
1	E	604	PRO	3.8
1	H	778	PRO	3.4
1	L	565	GLY	3.4
1	E	778	PRO	3.2
1	K	518	GLY	3.2
1	F	778	PRO	3.2
1	E	606	GLY	3.0
1	C	586	ASP	2.9
1	E	780	VAL	2.9
1	B	777	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	586	ASP	2.8
1	H	777	PRO	2.8
1	D	586	ASP	2.8
1	K	564	GLU	2.8
1	I	656	ASP	2.7
1	L	780	VAL	2.7
1	J	604	PRO	2.6
1	B	779	VAL	2.5
1	B	604	PRO	2.5
1	C	749	GLU	2.5
1	I	776	MET	2.5
1	F	586	ASP	2.5
1	G	779	VAL	2.5
1	K	561	GLY	2.4
1	C	492	GLY	2.4
1	L	778	PRO	2.4
1	K	492	GLY	2.3
1	G	491	PRO	2.3
1	K	777	PRO	2.3
1	D	605	VAL	2.3
1	I	586	ASP	2.3
1	F	589	GLU	2.2
1	B	776	MET	2.2
1	I	536	ARG	2.2
1	I	602	TRP	2.2
1	E	749	GLU	2.2
1	L	777	PRO	2.2
1	G	778	PRO	2.1
1	B	745	GLU	2.1
1	F	777	PRO	2.1
1	J	562	ALA	2.1
1	G	777	PRO	2.1
1	J	752	GLU	2.0
1	G	496	MET	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.