



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:09 AM GMT

PDB ID : 3KTK  
Title : Structure of ClpP in complex with ADEP2 in triclinic crystal form  
Authors : Lee, B.-G.; Brotz-Oesterhelt, H.; Song, H.K.  
Deposited on : 2009-11-25  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

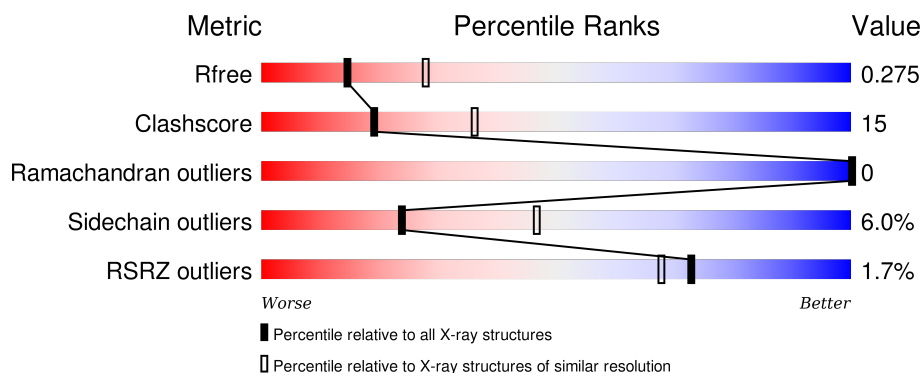
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	199	<div> <div>2%</div> <div>62% 23% • 13%</div> </div>
1	B	199	<div> <div>2%</div> <div>61% 24% • 13%</div> </div>
1	C	199	<div> <div>2%</div> <div>57% 28% • 13%</div> </div>
1	D	199	<div> <div>2%</div> <div>63% 23% • 13%</div> </div>
1	E	199	<div> <div>2%</div> <div>64% 22% • 13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	199	
1	G	199	
1	H	199	
1	I	199	
1	J	199	
1	K	199	
1	L	199	
1	M	199	
1	N	199	
2	O	7	
2	1	7	
2	O	7	
2	P	7	
2	Q	7	
2	R	7	
2	S	7	
2	T	7	
2	U	7	
2	V	7	
2	W	7	
2	X	7	
2	Y	7	
2	Z	7	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 19732 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	B	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	C	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	D	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	E	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	F	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	G	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	H	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	I	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	J	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	K	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	L	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	M	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			
1	N	174	Total	C	N	O	S	0	0	0
			1325	838	223	257	7			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	HIS	-	EXPRESSION TAG	UNP P80244

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Chain	Residue	Modelled	Actual	Comment	Reference
A	198	HIS	-	EXPRESSION TAG	UNP P80244
A	199	HIS	-	EXPRESSION TAG	UNP P80244
B	197	HIS	-	EXPRESSION TAG	UNP P80244
B	198	HIS	-	EXPRESSION TAG	UNP P80244
B	199	HIS	-	EXPRESSION TAG	UNP P80244
C	197	HIS	-	EXPRESSION TAG	UNP P80244
C	198	HIS	-	EXPRESSION TAG	UNP P80244
C	199	HIS	-	EXPRESSION TAG	UNP P80244
D	197	HIS	-	EXPRESSION TAG	UNP P80244
D	198	HIS	-	EXPRESSION TAG	UNP P80244
D	199	HIS	-	EXPRESSION TAG	UNP P80244
E	197	HIS	-	EXPRESSION TAG	UNP P80244
E	198	HIS	-	EXPRESSION TAG	UNP P80244
E	199	HIS	-	EXPRESSION TAG	UNP P80244
F	197	HIS	-	EXPRESSION TAG	UNP P80244
F	198	HIS	-	EXPRESSION TAG	UNP P80244
F	199	HIS	-	EXPRESSION TAG	UNP P80244
G	197	HIS	-	EXPRESSION TAG	UNP P80244
G	198	HIS	-	EXPRESSION TAG	UNP P80244
G	199	HIS	-	EXPRESSION TAG	UNP P80244
H	197	HIS	-	EXPRESSION TAG	UNP P80244
H	198	HIS	-	EXPRESSION TAG	UNP P80244
H	199	HIS	-	EXPRESSION TAG	UNP P80244
I	197	HIS	-	EXPRESSION TAG	UNP P80244
I	198	HIS	-	EXPRESSION TAG	UNP P80244
I	199	HIS	-	EXPRESSION TAG	UNP P80244
J	197	HIS	-	EXPRESSION TAG	UNP P80244
J	198	HIS	-	EXPRESSION TAG	UNP P80244
J	199	HIS	-	EXPRESSION TAG	UNP P80244
K	197	HIS	-	EXPRESSION TAG	UNP P80244
K	198	HIS	-	EXPRESSION TAG	UNP P80244
K	199	HIS	-	EXPRESSION TAG	UNP P80244
L	197	HIS	-	EXPRESSION TAG	UNP P80244
L	198	HIS	-	EXPRESSION TAG	UNP P80244
L	199	HIS	-	EXPRESSION TAG	UNP P80244
M	197	HIS	-	EXPRESSION TAG	UNP P80244
M	198	HIS	-	EXPRESSION TAG	UNP P80244
M	199	HIS	-	EXPRESSION TAG	UNP P80244
N	197	HIS	-	EXPRESSION TAG	UNP P80244
N	198	HIS	-	EXPRESSION TAG	UNP P80244
N	199	HIS	-	EXPRESSION TAG	UNP P80244

- Molecule 2 is a protein called Acyldepsipeptide 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	P	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	Q	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	R	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	S	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	T	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	U	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	V	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	W	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	X	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	Y	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	Z	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	0	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			
2	1	7	Total	C	F	N	O	0	0	0
			57	41	2	6	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
O	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
O	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
P	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
P	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
P	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
Q	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
Q	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
Q	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
R	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
R	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
R	5	YCP	MAA	SEE REMARK 999	NOR NOR01131

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Chain	Residue	Modelled	Actual	Comment	Reference
S	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
S	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
S	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
T	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
T	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
T	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
U	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
U	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
U	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
V	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
V	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
V	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
W	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
W	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
W	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
X	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
X	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
X	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
Y	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
Y	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
Y	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
Z	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
Z	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
Z	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
0	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
0	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
0	5	YCP	MAA	SEE REMARK 999	NOR NOR01131
1	1	CXP	OTT	SEE REMARK 999	NOR NOR01131
1	2	WFP	PHE	SEE REMARK 999	NOR NOR01131
1	5	YCP	MAA	SEE REMARK 999	NOR NOR01131

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	36	Total O 36 36	0	0
3	B	23	Total O 23 23	0	0
3	C	35	Total O 35 35	0	0
3	D	28	Total O 28 28	0	0

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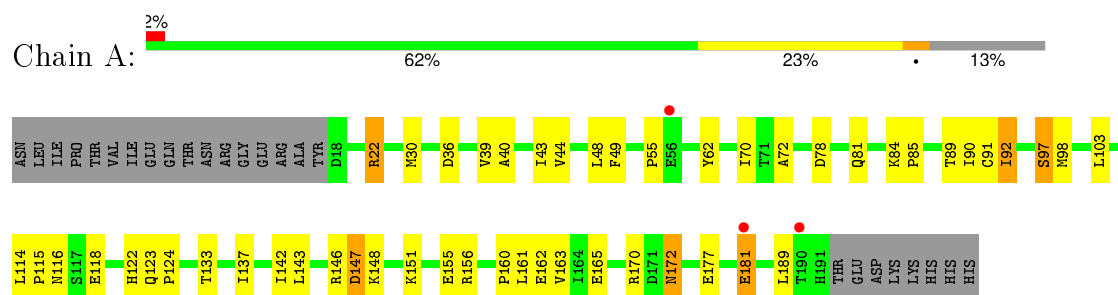
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	33	Total 33	O 33	0	0
3	F	27	Total 27	O 27	0	0
3	G	27	Total 27	O 27	0	0
3	Q	1	Total 1	O 1	0	0
3	T	1	Total 1	O 1	0	0
3	H	25	Total 25	O 25	0	0
3	I	26	Total 26	O 26	0	0
3	J	26	Total 26	O 26	0	0
3	K	24	Total 24	O 24	0	0
3	L	26	Total 26	O 26	0	0
3	M	22	Total 22	O 22	0	0
3	N	24	Total 24	O 24	0	0



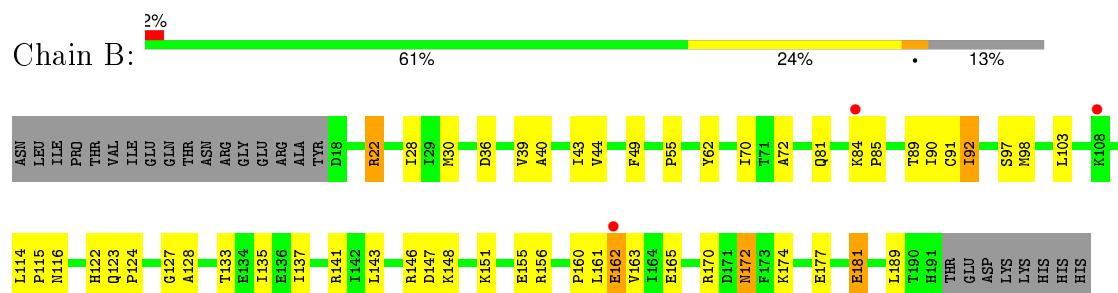
### 3 Residue-property plots [i](#)

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

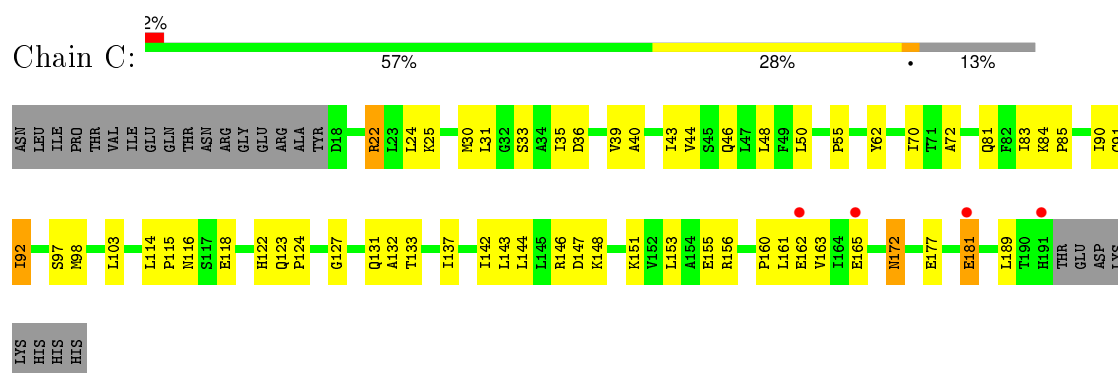
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

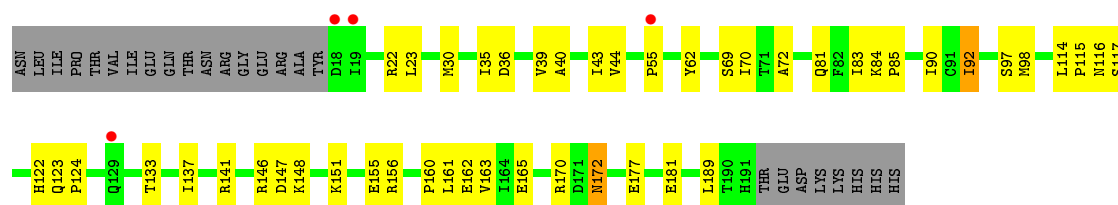


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

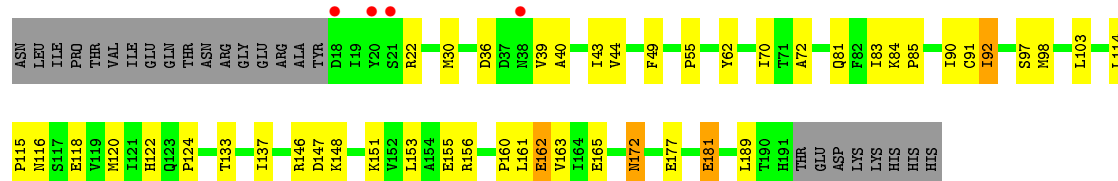


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

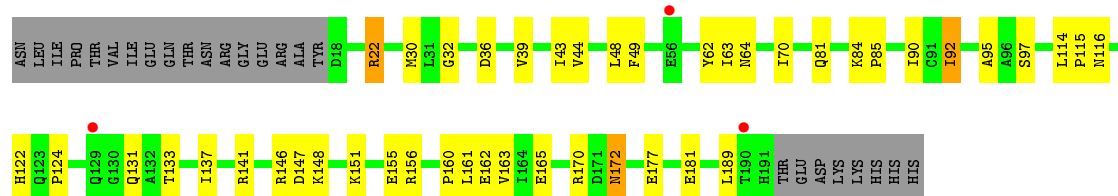




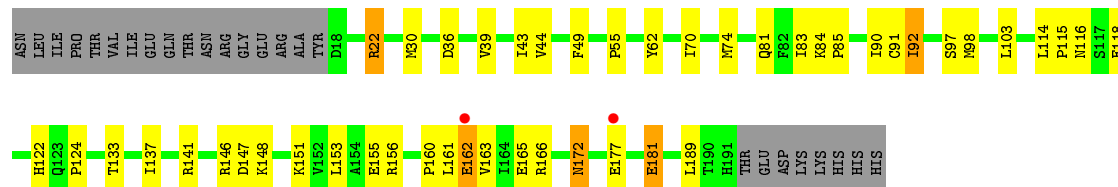
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



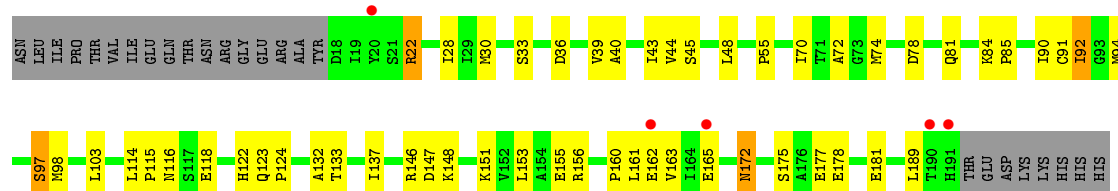
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



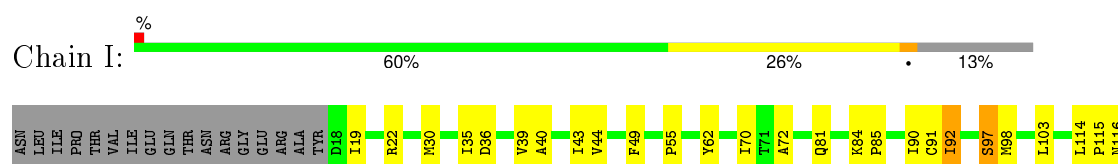
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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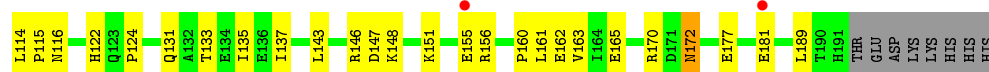
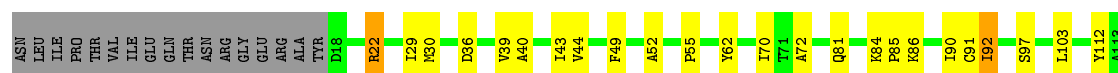
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



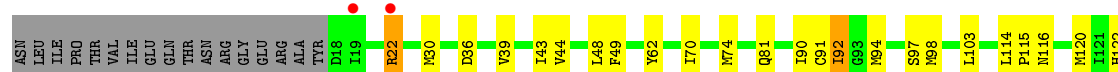
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



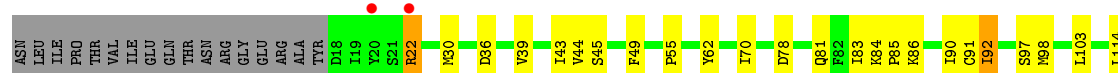
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



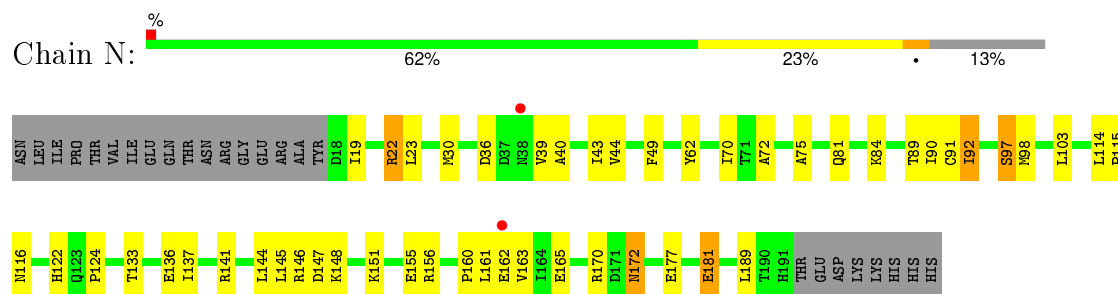
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 2: Acyldepsipeptide 2



- Molecule 2: Acyldepsipeptide 2



- Molecule 2: Acyldepsipeptide 2



- Molecule 2: Acyldepsipeptide 2



- Molecule 2: Acyldepsipeptide 2



- Molecule 2: Acyldepsipeptide 2




- Molecule 2: Acyldepsipeptide 2

Chain U:  29% 71%



- Molecule 2: Acyldepsipeptide 2

Chain V:  14% 86%



- Molecule 2: Acyldepsipeptide 2

Chain W:  29% 71%



- Molecule 2: Acyldepsipeptide 2

Chain X:  57% 43%

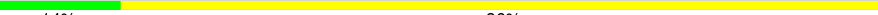


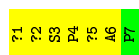
- Molecule 2: Acyldepsipeptide 2

Chain Y:  29% 71%




- Molecule 2: Acyldepsipeptide 2

Chain Z:  14% 86%



- Molecule 2: Acyldepsipeptide 2

Chain 0:  57% 43%



- Molecule 2: Acyldepsipeptide 2

Chain 1:  29% 71%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.17Å 97.24Å 100.03Å 71.51° 73.89° 77.30°	Depositor
Resolution (Å)	50.00 – 2.60 47.88 – 2.59	Depositor EDS
% Data completeness (in resolution range)	85.5 (50.00-2.60) 87.2 (47.88-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.269 , 0.294 0.277 , 0.275	Depositor DCC
$R_{free}$ test set	4870 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.0	EDS
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 97656 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	19732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CXP, WFP, YCP, MP8

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	0.38	0/1340	0.56	0/1806
1	B	0.37	0/1340	0.56	0/1806
1	C	0.37	0/1340	0.57	0/1806
1	D	0.38	0/1340	0.56	0/1806
1	E	0.38	0/1340	0.56	0/1806
1	F	0.38	0/1340	0.56	0/1806
1	G	0.37	0/1340	0.56	0/1806
1	H	0.38	0/1340	0.57	0/1806
1	I	0.37	0/1340	0.56	0/1806
1	J	0.38	0/1340	0.56	0/1806
1	K	0.37	0/1340	0.56	0/1806
1	L	0.37	0/1340	0.56	0/1806
1	M	0.39	0/1340	0.57	0/1806
1	N	0.37	0/1340	0.56	0/1806
2	O	2.66	1/17 (5.9%)	1.96	0/21
2	1	2.62	3/17 (17.6%)	1.97	0/21
2	O	2.86	3/17 (17.6%)	1.81	0/21
2	P	2.62	1/17 (5.9%)	1.90	0/21
2	Q	2.56	2/17 (11.8%)	1.95	0/21
2	R	2.65	1/17 (5.9%)	1.79	0/21
2	S	2.66	3/17 (17.6%)	2.07	0/21
2	T	2.79	3/17 (17.6%)	1.92	0/21
2	U	2.79	3/17 (17.6%)	1.84	0/21
2	V	2.73	3/17 (17.6%)	1.86	0/21
2	W	2.86	3/17 (17.6%)	1.68	0/21
2	X	2.69	1/17 (5.9%)	1.87	0/21
2	Y	2.85	3/17 (17.6%)	1.91	0/21
2	Z	2.62	2/17 (11.8%)	1.89	0/21
All	All	0.48	32/18998 (0.2%)	0.59	0/25578

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	4	PRO	N-CA	5.78	1.57	1.47
2	T	3	SER	C-N	5.76	1.45	1.34
2	0	3	SER	C-N	5.73	1.45	1.34
2	X	3	SER	C-N	5.71	1.45	1.34
2	O	4	PRO	CA-C	5.68	1.64	1.52
2	P	3	SER	C-N	5.67	1.45	1.34
2	Y	3	SER	C-N	5.66	1.45	1.34
2	V	4	PRO	N-CA	5.60	1.56	1.47
2	Y	4	PRO	CA-C	5.58	1.64	1.52
2	T	4	PRO	N-CA	5.55	1.56	1.47
2	U	4	PRO	CA-C	5.53	1.64	1.52
2	O	4	PRO	N-CA	5.53	1.56	1.47
2	V	3	SER	C-N	5.52	1.44	1.34
2	R	3	SER	C-N	5.46	1.44	1.34
2	1	3	SER	C-N	5.37	1.44	1.34
2	T	4	PRO	CA-C	5.34	1.63	1.52
2	S	3	SER	C-N	5.30	1.44	1.34
2	1	4	PRO	N-CA	5.29	1.56	1.47
2	V	4	PRO	CA-C	5.28	1.63	1.52
2	Q	4	PRO	N-CA	5.26	1.56	1.47
2	W	3	SER	C-N	5.21	1.44	1.34
2	Q	3	SER	C-N	5.21	1.44	1.34
2	Y	4	PRO	N-CA	5.18	1.56	1.47
2	U	3	SER	C-N	5.17	1.44	1.34
2	W	4	PRO	N-CA	5.14	1.55	1.47
2	Z	3	SER	C-N	5.13	1.44	1.34
2	O	3	SER	C-N	5.08	1.44	1.34
2	1	4	PRO	CA-C	5.08	1.62	1.52
2	W	4	PRO	CA-C	5.05	1.62	1.52
2	U	4	PRO	N-CA	5.05	1.55	1.47
2	S	4	PRO	CA-C	5.04	1.62	1.52
2	Z	4	PRO	N-CA	5.04	1.55	1.47

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	1325	0	1364	56	0
1	B	1325	0	1364	53	0
1	C	1325	0	1364	62	0
1	D	1325	0	1364	49	0
1	E	1325	0	1364	47	0
1	F	1325	0	1364	44	0
1	G	1325	0	1364	46	0
1	H	1325	0	1364	52	0
1	I	1325	0	1364	60	0
1	J	1325	0	1364	54	0
1	K	1325	0	1364	50	0
1	L	1325	0	1364	40	0
1	M	1325	0	1364	53	0
1	N	1325	0	1364	54	0
2	O	57	0	55	2	0
2	1	57	0	55	3	0
2	O	57	0	55	3	0
2	P	57	0	55	2	0
2	Q	57	0	55	1	0
2	R	57	0	55	3	0
2	S	57	0	55	4	0
2	T	57	0	55	1	0
2	U	57	0	55	4	0
2	V	57	0	55	4	0
2	W	57	0	55	3	0
2	X	57	0	55	2	0
2	Y	57	0	55	3	0
2	Z	57	0	55	5	0
3	A	36	0	0	5	0
3	B	23	0	0	4	0
3	C	35	0	0	13	0
3	D	28	0	0	8	0
3	E	33	0	0	5	0
3	F	27	0	0	5	0
3	G	27	0	0	4	0
3	H	25	0	0	3	0
3	I	26	0	0	12	0
3	J	26	0	0	4	0
3	K	24	0	0	8	0
3	L	26	0	0	2	0
3	M	22	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	24	0	0	9	0
3	Q	1	0	0	0	0
3	T	1	0	0	0	0
All	All	19732	0	19866	594	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 15.

All (594) 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:I:170:ARG:HD2	3:I:481:HOH:O	1.66	0.95
1:H:92:ILE:HD11	1:N:44:VAL:HG21	1.50	0.93
1:A:170:ARG:HD2	3:A:295:HOH:O	1.69	0.92
1:I:72:ALA:HB3	3:I:395:HOH:O	1.70	0.91
1:C:31:LEU:HD11	3:C:346:HOH:O	1.74	0.88
1:F:44:VAL:HG21	1:G:92:ILE:HD11	1.55	0.88
1:B:44:VAL:HG21	1:C:92:ILE:HD11	1.55	0.87
1:M:120:MET:SD	3:M:448:HOH:O	2.33	0.86
1:K:177:GLU:O	1:K:181:GLU:HG2	1.77	0.84
1:A:177:GLU:O	1:A:181:GLU:HG2	1.77	0.84
1:D:44:VAL:HG21	1:E:92:ILE:HD11	1.59	0.84
1:I:177:GLU:O	1:I:181:GLU:HG2	1.77	0.84
1:F:177:GLU:O	1:F:181:GLU:HG2	1.77	0.83
1:G:177:GLU:O	1:G:181:GLU:HG2	1.78	0.83
1:I:44:VAL:HG21	1:J:92:ILE:HD11	1.58	0.82
1:J:177:GLU:O	1:J:181:GLU:HG2	1.80	0.82
1:H:177:GLU:O	1:H:181:GLU:HG2	1.79	0.82
1:D:177:GLU:O	1:D:181:GLU:HG2	1.80	0.82
3:C:530:HOH:O	1:J:170:ARG:HD2	1.80	0.81
1:C:177:GLU:O	1:C:181:GLU:HG2	1.78	0.81
1:M:171:ASP:HA	3:M:448:HOH:O	1.80	0.81
1:L:177:GLU:O	1:L:181:GLU:HG2	1.80	0.80
1:A:161:LEU:O	1:A:165:GLU:HG3	1.81	0.80
1:C:46:GLN:HB3	3:C:445:HOH:O	1.79	0.80
1:B:177:GLU:O	1:B:181:GLU:HG2	1.80	0.80
1:N:177:GLU:O	1:N:181:GLU:HG2	1.80	0.79
1:I:121:ILE:HG23	3:I:401:HOH:O	1.81	0.79
1:M:177:GLU:O	1:M:181:GLU:HG2	1.82	0.79
1:K:44:VAL:HG21	1:L:92:ILE:HD11	1.64	0.79
1:M:161:LEU:O	1:M:165:GLU:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:LEU:O	1:H:165:GLU:HG3	1.82	0.78
1:E:177:GLU:O	1:E:181:GLU:HG2	1.83	0.77
1:C:161:LEU:O	1:C:165:GLU:HG3	1.84	0.77
1:B:44:VAL:HG11	1:C:92:ILE:HD12	1.67	0.77
1:L:94:MET:SD	3:L:584:HOH:O	2.43	0.77
1:A:92:ILE:HD11	1:G:44:VAL:HG21	1.66	0.76
1:H:22:ARG:HH11	1:N:49:PHE:HE1	1.34	0.76
1:E:44:VAL:HG21	1:F:92:ILE:HD11	1.66	0.76
1:C:165:GLU:HB3	3:C:218:HOH:O	1.85	0.76
1:K:161:LEU:O	1:K:165:GLU:HG3	1.86	0.75
1:B:161:LEU:O	1:B:165:GLU:HG3	1.86	0.75
1:E:162:GLU:HB2	3:E:223:HOH:O	1.87	0.75
1:J:44:VAL:HG21	1:K:92:ILE:HD11	1.69	0.75
1:F:156:ARG:HD2	3:F:225:HOH:O	1.85	0.75
1:I:156:ARG:HD2	3:I:245:HOH:O	1.87	0.74
1:I:161:LEU:O	1:I:165:GLU:HG3	1.87	0.74
1:G:161:LEU:O	1:G:165:GLU:HG3	1.88	0.73
1:F:161:LEU:O	1:F:165:GLU:HG3	1.88	0.73
1:F:63:ILE:HG22	3:F:265:HOH:O	1.88	0.73
1:A:44:VAL:HG21	1:B:92:ILE:HD11	1.69	0.73
1:G:70:ILE:HD11	1:G:124:PRO:HB3	1.69	0.73
1:M:86:LYS:HE2	3:M:430:HOH:O	1.89	0.73
1:K:44:VAL:HG11	1:L:92:ILE:HD12	1.70	0.73
3:G:575:HOH:O	1:M:170:ARG:HD2	1.88	0.73
1:C:44:VAL:HG21	1:D:92:ILE:HD11	1.72	0.72
1:L:161:LEU:O	1:L:165:GLU:HG3	1.88	0.72
1:E:161:LEU:O	1:E:165:GLU:HG3	1.90	0.71
1:M:122:HIS:HB3	3:M:448:HOH:O	1.88	0.71
1:L:44:VAL:HG21	1:M:92:ILE:HD11	1.70	0.71
1:A:148:LYS:HD2	1:B:116:ASN:HD22	1.55	0.71
1:M:70:ILE:HD11	1:M:124:PRO:HB3	1.72	0.71
1:C:35:ILE:HG12	3:C:346:HOH:O	1.91	0.71
1:C:70:ILE:HD11	1:C:124:PRO:HB3	1.72	0.71
1:M:148:LYS:HD2	1:N:116:ASN:HD22	1.55	0.71
1:C:24:LEU:HD11	3:C:445:HOH:O	1.91	0.70
1:D:70:ILE:HD11	1:D:124:PRO:HB3	1.73	0.70
1:I:44:VAL:HG11	1:J:92:ILE:HD12	1.71	0.70
1:H:92:ILE:HD12	1:N:44:VAL:HG11	1.72	0.70
1:F:44:VAL:HG11	1:G:92:ILE:HD12	1.74	0.70
1:K:44:VAL:HG11	1:L:92:ILE:CD1	2.22	0.69
1:L:70:ILE:HD11	1:L:124:PRO:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:161:LEU:O	1:J:165:GLU:HG3	1.92	0.69
1:L:120:MET:N	3:L:584:HOH:O	2.23	0.69
1:K:81:GLN:NE2	1:K:156:ARG:HH22	1.90	0.69
1:E:148:LYS:HD2	1:F:116:ASN:HD22	1.56	0.69
1:K:70:ILE:HD11	1:K:124:PRO:HB3	1.75	0.69
1:F:81:GLN:NE2	1:F:156:ARG:HH22	1.91	0.69
1:N:161:LEU:O	1:N:165:GLU:HG3	1.92	0.69
1:M:81:GLN:NE2	1:M:156:ARG:HH22	1.91	0.69
1:B:70:ILE:HD11	1:B:124:PRO:HB3	1.75	0.68
1:J:162:GLU:HB2	3:J:222:HOH:O	1.93	0.68
1:D:161:LEU:O	1:D:165:GLU:HG3	1.93	0.68
1:M:44:VAL:HG21	1:N:92:ILE:HD11	1.75	0.68
1:E:120:MET:SD	3:E:227:HOH:O	2.50	0.68
1:E:70:ILE:HD11	1:E:124:PRO:HB3	1.74	0.68
1:F:70:ILE:HD11	1:F:124:PRO:HB3	1.75	0.68
1:F:170:ARG:HD2	3:N:504:HOH:O	1.92	0.68
1:B:44:VAL:HG11	1:C:92:ILE:CD1	2.23	0.68
1:D:81:GLN:NE2	1:D:156:ARG:HH22	1.92	0.68
1:I:70:ILE:HD11	1:I:124:PRO:HB3	1.76	0.68
1:F:181:GLU:HB3	3:F:386:HOH:O	1.95	0.67
3:B:491:HOH:O	1:K:170:ARG:HD2	1.93	0.67
1:B:81:GLN:NE2	1:B:156:ARG:HH22	1.93	0.67
1:A:70:ILE:HD11	1:A:124:PRO:HB3	1.76	0.67
1:D:72:ALA:HB3	3:D:457:HOH:O	1.94	0.66
1:J:44:VAL:HG11	1:K:92:ILE:HD12	1.78	0.66
1:N:144:LEU:HG	3:N:490:HOH:O	1.96	0.66
1:N:70:ILE:HD11	1:N:124:PRO:HB3	1.76	0.66
1:G:160:PRO:HG2	1:G:163:VAL:HG23	1.77	0.66
1:H:70:ILE:HD11	1:H:124:PRO:HB3	1.77	0.66
1:C:33:SER:O	3:C:346:HOH:O	2.13	0.66
1:K:29:ILE:HA	3:K:493:HOH:O	1.94	0.66
1:N:81:GLN:NE2	1:N:156:ARG:HH22	1.94	0.66
1:C:81:GLN:NE2	1:C:156:ARG:HH22	1.93	0.65
1:G:162:GLU:HB2	3:G:251:HOH:O	1.96	0.65
1:H:22:ARG:NH1	1:N:49:PHE:HE1	1.93	0.65
1:H:81:GLN:NE2	1:H:156:ARG:HH22	1.95	0.65
1:D:44:VAL:HG11	1:E:92:ILE:HD12	1.78	0.65
1:K:86:LYS:HD3	3:K:397:HOH:O	1.96	0.65
1:N:145:LEU:HD23	3:N:258:HOH:O	1.97	0.64
1:I:81:GLN:NE2	1:I:156:ARG:HH22	1.94	0.64
1:N:160:PRO:HG2	1:N:163:VAL:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:LEU:HD22	2:V:1:CXP:O2	1.98	0.64
1:L:81:GLN:NE2	1:L:156:ARG:HH22	1.95	0.64
1:I:119:VAL:HG12	3:I:401:HOH:O	1.97	0.63
1:A:160:PRO:HG2	1:A:163:VAL:HG23	1.80	0.63
1:I:44:VAL:HG11	1:J:92:ILE:CD1	2.28	0.63
1:J:70:ILE:HD11	1:J:124:PRO:HB3	1.81	0.63
1:K:160:PRO:HG2	1:K:163:VAL:HG23	1.81	0.63
1:A:48:LEU:HB3	2:O:1:CXP:H72	1.79	0.62
1:N:90:ILE:HD11	2:1:6:ALA:HB1	1.81	0.62
1:F:160:PRO:HG2	1:F:163:VAL:HG23	1.81	0.62
1:A:81:GLN:NE2	1:A:156:ARG:HH22	1.97	0.62
1:H:160:PRO:HG2	1:H:163:VAL:HG23	1.80	0.62
1:E:81:GLN:NE2	1:E:156:ARG:HH22	1.97	0.62
1:A:98:MET:HB2	3:A:244:HOH:O	1.99	0.62
1:C:35:ILE:CG1	3:C:346:HOH:O	2.47	0.61
1:J:44:VAL:HG11	1:K:92:ILE:CD1	2.30	0.61
1:B:160:PRO:HG2	1:B:163:VAL:HG23	1.81	0.61
1:E:49:PHE:HE1	1:F:22:ARG:HH11	1.48	0.61
1:H:44:VAL:HG21	1:I:92:ILE:HD11	1.81	0.61
1:C:160:PRO:HG2	1:C:163:VAL:HG23	1.82	0.61
1:B:49:PHE:HE1	1:C:22:ARG:HH11	1.49	0.61
1:E:156:ARG:HD2	3:E:275:HOH:O	2.00	0.60
1:M:151:LYS:O	1:M:155:GLU:HG3	2.01	0.60
1:G:151:LYS:O	1:G:155:GLU:HG3	2.01	0.60
1:G:156:ARG:HD2	3:G:486:HOH:O	2.02	0.60
1:A:90:ILE:HD11	2:P:6:ALA:HB1	1.84	0.60
1:E:151:LYS:O	1:E:155:GLU:HG3	2.01	0.60
1:I:146:ARG:NH1	3:I:503:HOH:O	2.35	0.60
1:C:151:LYS:O	1:C:155:GLU:HG3	2.01	0.60
1:I:160:PRO:HG2	1:I:163:VAL:HG23	1.83	0.60
1:I:162:GLU:HB2	3:I:407:HOH:O	2.01	0.60
1:B:151:LYS:O	1:B:155:GLU:HG3	2.02	0.60
1:A:92:ILE:HD12	1:G:44:VAL:HG11	1.83	0.60
1:B:90:ILE:HD11	2:O:6:ALA:HB1	1.83	0.60
1:A:172:ASN:HD22	1:A:172:ASN:C	2.05	0.60
1:L:151:LYS:O	1:L:155:GLU:HG3	2.02	0.60
1:I:90:ILE:HD11	2:V:6:ALA:HB1	1.84	0.59
1:G:81:GLN:NE2	1:G:156:ARG:HH22	1.99	0.59
1:D:160:PRO:HG2	1:D:163:VAL:HG23	1.84	0.59
1:J:48:LEU:HB3	2:Z:1:CXP:H72	1.84	0.59
1:M:160:PRO:HG2	1:M:163:VAL:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:ILE:HD11	2:Z:6:ALA:HB1	1.83	0.59
2:V:1:CXP:H82	2:V:7:MP8:HD	1.84	0.59
1:E:160:PRO:HG2	1:E:163:VAL:HG23	1.84	0.59
1:L:160:PRO:HG2	1:L:163:VAL:HG23	1.84	0.58
1:G:166:ARG:HD2	3:G:276:HOH:O	2.03	0.58
1:A:49:PHE:HE1	1:B:22:ARG:HH11	1.49	0.58
1:C:172:ASN:HD22	1:C:172:ASN:C	2.06	0.58
1:F:90:ILE:HD11	2:Q:6:ALA:HB1	1.84	0.58
1:I:151:LYS:O	1:I:155:GLU:HG3	2.03	0.58
1:C:44:VAL:HG11	1:D:92:ILE:HD12	1.84	0.58
1:I:172:ASN:HD22	1:I:172:ASN:C	2.07	0.58
1:A:151:LYS:O	1:A:155:GLU:HG3	2.03	0.58
1:H:151:LYS:O	1:H:155:GLU:HG3	2.04	0.58
1:B:162:GLU:HB2	3:B:213:HOH:O	2.04	0.57
1:J:81:GLN:NE2	1:J:156:ARG:HH22	2.02	0.57
1:F:49:PHE:HE1	1:G:22:ARG:NH1	2.02	0.57
1:F:148:LYS:HD2	1:G:116:ASN:HD22	1.69	0.57
1:I:160:PRO:HB2	3:I:407:HOH:O	2.04	0.57
1:K:151:LYS:O	1:K:155:GLU:HG3	2.05	0.57
1:L:148:LYS:HD2	1:M:116:ASN:HD22	1.69	0.56
1:I:35:ILE:HG22	3:I:395:HOH:O	2.04	0.56
1:B:133:THR:H	1:J:123:GLN:HE22	1.53	0.56
1:N:151:LYS:O	1:N:155:GLU:HG3	2.06	0.56
1:F:151:LYS:O	1:F:155:GLU:HG3	2.06	0.56
1:H:172:ASN:C	1:H:172:ASN:HD22	2.08	0.56
1:H:92:ILE:CD1	1:N:44:VAL:HG11	2.35	0.56
1:D:151:LYS:O	1:D:155:GLU:HG3	2.06	0.56
1:C:132:ALA:HB3	1:I:123:GLN:HE21	1.71	0.56
1:C:123:GLN:HE22	1:I:133:THR:H	1.54	0.56
1:L:44:VAL:HG11	1:M:92:ILE:HD12	1.88	0.55
1:J:148:LYS:HD2	1:K:116:ASN:HD22	1.71	0.55
1:J:160:PRO:HG2	1:J:163:VAL:HG23	1.87	0.55
1:D:90:ILE:HD11	2:S:6:ALA:HB1	1.87	0.55
1:L:172:ASN:C	1:L:172:ASN:HD22	2.08	0.55
1:E:44:VAL:HG11	1:F:92:ILE:HD12	1.87	0.55
1:C:44:VAL:HG11	1:D:92:ILE:CD1	2.36	0.55
1:J:151:LYS:O	1:J:155:GLU:HG3	2.07	0.55
1:M:172:ASN:C	1:M:172:ASN:HD22	2.08	0.55
1:C:123:GLN:NE2	1:I:133:THR:H	2.05	0.55
1:F:44:VAL:HG11	1:G:92:ILE:CD1	2.36	0.55
1:I:36:ASP:OD1	1:I:39:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:ARG:HD2	3:K:233:HOH:O	2.07	0.55
1:K:170:ARG:NH1	3:K:351:HOH:O	2.40	0.55
1:D:172:ASN:C	1:D:172:ASN:HD22	2.10	0.55
1:F:49:PHE:HE1	1:G:22:ARG:HH11	1.54	0.54
1:J:49:PHE:HE1	1:K:22:ARG:HH11	1.53	0.54
1:D:44:VAL:HG11	1:E:92:ILE:CD1	2.36	0.54
1:C:50:LEU:HG	3:C:445:HOH:O	2.05	0.54
1:J:114:LEU:HD11	2:Y:2:WFP:CZ	2.37	0.54
1:B:128:ALA:O	1:J:127:GLY:HA2	2.08	0.54
1:K:172:ASN:HD22	1:K:172:ASN:C	2.11	0.54
1:A:147:ASP:OD1	3:A:220:HOH:O	2.18	0.54
1:G:160:PRO:HG2	1:G:163:VAL:CG2	2.37	0.54
1:M:124:PRO:HD2	1:M:146:ARG:HG3	1.90	0.53
1:H:160:PRO:HG2	1:H:163:VAL:CG2	2.38	0.53
1:G:172:ASN:HD22	1:G:172:ASN:C	2.11	0.53
1:A:44:VAL:HG11	1:B:92:ILE:HD12	1.91	0.53
1:G:124:PRO:HD2	1:G:146:ARG:HG3	1.91	0.53
1:F:148:LYS:HD2	1:G:116:ASN:ND2	2.23	0.53
1:D:69:SER:N	3:D:457:HOH:O	2.42	0.53
1:M:39:VAL:O	1:M:43:ILE:HG12	2.09	0.53
1:A:123:GLN:HE22	1:K:133:THR:H	1.55	0.53
1:I:124:PRO:HD2	1:I:146:ARG:HG3	1.90	0.53
1:B:170:ARG:HG2	3:K:351:HOH:O	2.09	0.53
2:R:1:CXP:H82	2:R:7:MP8:HD	1.91	0.53
1:J:124:PRO:HD2	1:J:146:ARG:HG3	1.90	0.53
1:H:74:MET:HE3	1:I:116:ASN:HB3	1.90	0.53
1:E:124:PRO:HD2	1:E:146:ARG:HG3	1.90	0.53
1:F:124:PRO:HD2	1:F:146:ARG:HG3	1.90	0.53
1:N:160:PRO:HG2	1:N:163:VAL:CG2	2.38	0.53
1:A:160:PRO:HG2	1:A:163:VAL:CG2	2.39	0.52
1:B:133:THR:H	1:J:123:GLN:NE2	2.07	0.52
1:K:81:GLN:NE2	3:K:232:HOH:O	2.42	0.52
1:N:124:PRO:HD2	1:N:146:ARG:HG3	1.91	0.52
1:B:160:PRO:HG2	1:B:163:VAL:CG2	2.39	0.52
1:D:170:ARG:HD2	3:D:508:HOH:O	2.08	0.52
1:B:172:ASN:C	1:B:172:ASN:HD22	2.13	0.52
1:H:28:ILE:HD11	2:W:7:MP8:HE	1.92	0.52
1:E:70:ILE:HG12	1:E:98:MET:HE1	1.90	0.52
1:F:160:PRO:HG2	1:F:163:VAL:CG2	2.40	0.52
1:B:124:PRO:HD2	1:B:146:ARG:HG3	1.92	0.52
1:A:116:ASN:HD22	1:G:148:LYS:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:HD2	1:A:146:ARG:HG3	1.92	0.52
1:B:28:ILE:HD11	2:O:7:MP8:HE	1.91	0.52
1:D:141:ARG:NE	1:E:118:GLU:OE1	2.41	0.52
1:N:36:ASP:OD1	1:N:39:VAL:HG23	2.10	0.52
1:K:160:PRO:HG2	1:K:163:VAL:CG2	2.39	0.51
1:N:172:ASN:HD22	1:N:172:ASN:C	2.12	0.51
1:H:124:PRO:HD2	1:H:146:ARG:HG3	1.93	0.51
1:N:23:LEU:HD23	2:1:1:CXP:H51	1.92	0.51
1:H:22:ARG:NH1	1:N:49:PHE:CE1	2.77	0.51
1:A:148:LYS:HD2	1:B:116:ASN:ND2	2.24	0.51
1:C:70:ILE:HG12	1:C:98:MET:HE1	1.92	0.51
1:J:172:ASN:C	1:J:172:ASN:HD22	2.14	0.51
1:L:124:PRO:HD2	1:L:146:ARG:HG3	1.92	0.51
1:D:146:ARG:CZ	3:D:440:HOH:O	2.59	0.51
1:H:116:ASN:HD22	1:N:148:LYS:HD2	1.75	0.51
1:C:160:PRO:HG2	1:C:163:VAL:CG2	2.40	0.51
1:C:22:ARG:NE	3:C:329:HOH:O	2.43	0.51
1:A:92:ILE:CD1	1:G:44:VAL:HG11	2.41	0.50
1:B:90:ILE:N	1:B:90:ILE:HD12	2.26	0.50
1:H:165:GLU:HB3	3:H:217:HOH:O	2.11	0.50
1:M:151:LYS:HB3	3:M:308:HOH:O	2.11	0.50
1:J:90:ILE:HD11	2:Y:6:ALA:HB1	1.93	0.50
1:J:166:ARG:HD2	3:J:263:HOH:O	2.12	0.50
1:M:160:PRO:HG2	1:M:163:VAL:CG2	2.42	0.50
1:C:36:ASP:OD1	1:C:39:VAL:HG23	2.11	0.50
1:E:114:LEU:HD11	2:T:2:WFP:CZ	2.41	0.50
1:E:172:ASN:C	1:E:172:ASN:HD22	2.14	0.50
1:N:75:ALA:HA	3:N:250:HOH:O	2.10	0.50
1:G:90:ILE:HD11	2:U:6:ALA:HB1	1.93	0.50
1:L:177:GLU:H	1:L:177:GLU:CD	2.15	0.50
1:H:148:LYS:HD2	1:I:116:ASN:HD22	1.76	0.50
1:H:78:ASP:HB3	1:I:114:LEU:HD13	1.93	0.50
1:B:135:ILE:HD12	1:J:142:ILE:HD13	1.94	0.50
1:H:161:LEU:HB2	3:H:495:HOH:O	2.13	0.49
1:N:145:LEU:HA	3:N:258:HOH:O	2.11	0.49
1:E:146:ARG:CZ	3:E:399:HOH:O	2.60	0.49
1:H:118:GLU:OE1	1:N:141:ARG:NE	2.45	0.49
1:G:115:PRO:HD3	1:G:189:LEU:O	2.13	0.49
1:M:177:GLU:CD	1:M:177:GLU:H	2.15	0.49
1:K:124:PRO:HD2	1:K:146:ARG:HG3	1.94	0.49
1:A:123:GLN:HG2	1:K:131:GLN:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:GLU:H	1:D:177:GLU:CD	2.15	0.49
1:D:70:ILE:HG12	1:D:98:MET:HE1	1.95	0.49
1:K:146:ARG:CZ	3:K:334:HOH:O	2.60	0.49
1:B:36:ASP:OD1	1:B:39:VAL:HG23	2.13	0.49
1:C:124:PRO:HD2	1:C:146:ARG:HG3	1.95	0.49
1:A:70:ILE:HG12	1:A:98:MET:HE3	1.95	0.49
1:C:156:ARG:HD2	3:C:247:HOH:O	2.13	0.49
1:C:132:ALA:HB3	1:I:123:GLN:NE2	2.28	0.48
1:N:136:GLU:HG2	3:N:243:HOH:O	2.13	0.48
1:I:160:PRO:HG2	1:I:163:VAL:CG2	2.43	0.48
1:F:141:ARG:NE	1:G:118:GLU:OE1	2.46	0.48
1:F:172:ASN:HD22	1:F:172:ASN:C	2.15	0.48
1:C:114:LEU:HD11	2:R:2:WFP:CZ	2.43	0.48
1:H:133:THR:O	1:H:137:ILE:HG12	2.12	0.48
1:J:156:ARG:HD2	3:J:413:HOH:O	2.12	0.48
1:C:177:GLU:H	1:C:177:GLU:CD	2.16	0.48
1:M:148:LYS:HD2	1:N:116:ASN:ND2	2.25	0.48
1:D:148:LYS:HD2	1:E:116:ASN:HD22	1.78	0.48
1:D:36:ASP:OD1	1:D:39:VAL:HG23	2.13	0.48
1:I:97:SER:HB3	3:I:239:HOH:O	2.13	0.48
1:D:160:PRO:HG2	1:D:163:VAL:CG2	2.42	0.48
1:B:123:GLN:HE22	1:J:133:THR:H	1.62	0.48
1:D:133:THR:H	1:H:123:GLN:HE22	1.61	0.48
1:E:177:GLU:H	1:E:177:GLU:CD	2.16	0.48
1:M:148:LYS:CD	1:N:116:ASN:HD22	2.24	0.48
1:E:49:PHE:HE1	1:F:22:ARG:NH1	2.11	0.48
1:D:90:ILE:HD12	1:D:90:ILE:N	2.28	0.48
1:M:62:TYR:CE1	1:M:90:ILE:HD13	2.48	0.48
1:A:22:ARG:HH11	1:G:49:PHE:HE1	1.61	0.48
1:J:177:GLU:H	1:J:177:GLU:CD	2.16	0.48
1:D:124:PRO:HD2	1:D:146:ARG:HG3	1.94	0.48
1:J:48:LEU:HD22	2:Z:1:CXP:O2	2.13	0.48
1:E:160:PRO:HG2	1:E:163:VAL:CG2	2.43	0.48
1:F:62:TYR:CE1	1:F:90:ILE:HD13	2.49	0.48
1:A:116:ASN:HB3	1:G:74:MET:HE3	1.96	0.48
1:N:177:GLU:CD	1:N:177:GLU:H	2.17	0.48
1:F:115:PRO:HD3	1:F:189:LEU:O	2.14	0.48
1:B:127:GLY:HA2	1:J:128:ALA:O	2.13	0.48
1:E:120:MET:CE	3:E:227:HOH:O	2.61	0.47
1:B:39:VAL:O	1:B:43:ILE:HG12	2.13	0.47
1:K:52:ALA:CB	2:0:1:CXP:H31	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:49:PHE:HE1	1:N:22:ARG:HH11	1.62	0.47
1:E:44:VAL:HG11	1:F:92:ILE:CD1	2.44	0.47
1:H:116:ASN:ND2	1:N:148:LYS:HD2	2.29	0.47
1:L:62:TYR:CE1	1:L:90:ILE:HD13	2.50	0.47
1:B:148:LYS:HD2	1:C:116:ASN:HD22	1.78	0.47
1:J:70:ILE:HG12	1:J:98:MET:HE1	1.95	0.47
1:H:115:PRO:HD3	1:H:189:LEU:O	2.14	0.47
1:J:115:PRO:HD3	1:J:189:LEU:O	2.15	0.47
1:A:36:ASP:OD1	1:A:39:VAL:HG23	2.14	0.47
1:J:91:CYS:HB2	1:J:103:LEU:HD22	1.97	0.47
1:G:62:TYR:CE1	1:G:90:ILE:HD13	2.49	0.47
1:L:115:PRO:HD3	1:L:189:LEU:O	2.15	0.47
1:D:133:THR:O	1:D:137:ILE:HG12	2.15	0.47
1:H:91:CYS:HB2	1:H:103:LEU:HD22	1.96	0.47
1:N:133:THR:O	1:N:137:ILE:HG12	2.15	0.47
1:K:177:GLU:CD	1:K:177:GLU:H	2.18	0.47
1:G:70:ILE:HG12	1:G:98:MET:HE1	1.97	0.47
1:L:70:ILE:HG12	1:L:98:MET:HE1	1.97	0.47
1:B:133:THR:O	1:B:137:ILE:HG12	2.15	0.47
1:J:62:TYR:CE1	1:J:90:ILE:HD13	2.50	0.47
1:J:39:VAL:O	1:J:43:ILE:HG12	2.15	0.47
1:L:44:VAL:HG11	1:M:92:ILE:CD1	2.45	0.46
1:G:177:GLU:H	1:G:177:GLU:CD	2.19	0.46
1:N:90:ILE:N	1:N:90:ILE:HD12	2.30	0.46
1:L:148:LYS:HD2	1:M:116:ASN:ND2	2.29	0.46
1:H:90:ILE:HD11	2:W:6:ALA:HB1	1.96	0.46
1:L:160:PRO:HG2	1:L:163:VAL:CG2	2.44	0.46
1:C:90:ILE:N	1:C:90:ILE:HD12	2.31	0.46
1:K:112:TYR:CE2	2:Z:5:YCP:HD	2.50	0.46
1:A:148:LYS:CD	1:B:116:ASN:HD22	2.25	0.46
1:H:114:LEU:HD11	2:W:2:WFP:CZ	2.46	0.46
1:B:70:ILE:HG12	1:B:98:MET:HE1	1.97	0.46
1:K:49:PHE:HE1	1:L:22:ARG:HH11	1.63	0.46
1:A:39:VAL:O	1:A:43:ILE:HG12	2.15	0.46
1:D:114:LEU:HD11	2:S:2:WFP:CZ	2.46	0.46
1:F:48:LEU:HD22	2:U:1:CXP:O2	2.16	0.46
1:K:148:LYS:HD2	1:L:116:ASN:HD22	1.79	0.46
1:C:91:CYS:HB2	1:C:103:LEU:HD22	1.98	0.46
1:A:177:GLU:CD	1:A:177:GLU:H	2.19	0.46
1:H:177:GLU:H	1:H:177:GLU:CD	2.18	0.46
1:I:49:PHE:HE1	1:J:22:ARG:HH11	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:153:LEU:HD23	1:J:153:LEU:HA	1.84	0.46
1:M:133:THR:O	1:M:137:ILE:HG12	2.15	0.46
1:I:91:CYS:HB2	1:I:103:LEU:HD22	1.97	0.46
1:B:123:GLN:NE2	1:J:133:THR:H	2.14	0.46
1:C:48:LEU:HD22	2:S:1:CXP:O2	2.15	0.46
1:H:97:SER:HB3	3:H:341:HOH:O	2.16	0.46
1:K:90:ILE:N	1:K:90:ILE:HD12	2.31	0.46
1:C:115:PRO:HD3	1:C:189:LEU:O	2.15	0.46
1:D:148:LYS:HD2	1:E:116:ASN:ND2	2.31	0.46
1:D:117:SER:HA	3:D:238:HOH:O	2.15	0.46
1:A:115:PRO:HD3	1:A:189:LEU:O	2.16	0.46
1:G:49:PHE:HA	2:P:1:CXP:H31	1.98	0.45
1:I:177:GLU:CD	1:I:177:GLU:H	2.20	0.45
1:H:44:VAL:HG11	1:I:92:ILE:HD12	1.99	0.45
1:F:141:ARG:HD3	3:F:315:HOH:O	2.15	0.45
1:H:153:LEU:HA	1:H:153:LEU:HD23	1.82	0.45
1:B:141:ARG:NE	1:C:118:GLU:OE1	2.48	0.45
1:M:44:VAL:HG11	1:N:92:ILE:HD12	1.98	0.45
1:A:49:PHE:HE1	1:B:22:ARG:NH1	2.14	0.45
1:J:160:PRO:HG2	1:J:163:VAL:CG2	2.46	0.45
1:M:36:ASP:OD1	1:M:39:VAL:HG23	2.17	0.45
1:B:91:CYS:HB2	1:B:103:LEU:HD22	1.98	0.45
1:D:115:PRO:HD3	1:D:189:LEU:O	2.16	0.45
1:F:36:ASP:OD1	1:F:39:VAL:HG23	2.16	0.45
1:H:39:VAL:O	1:H:43:ILE:HG12	2.17	0.45
1:M:78:ASP:HB3	1:N:114:LEU:HD13	1.99	0.45
1:B:177:GLU:H	1:B:177:GLU:CD	2.20	0.45
1:L:74:MET:HE3	1:M:116:ASN:HB3	1.98	0.45
1:M:133:THR:HG21	1:N:170:ARG:HD3	1.99	0.45
1:N:39:VAL:O	1:N:43:ILE:HG12	2.16	0.45
1:H:36:ASP:OD1	1:H:39:VAL:HG23	2.17	0.45
1:E:133:THR:O	1:E:137:ILE:HG12	2.16	0.45
1:D:62:TYR:CE1	1:D:90:ILE:HD13	2.52	0.45
1:J:122:HIS:CG	3:J:224:HOH:O	2.68	0.45
1:A:91:CYS:HB2	1:A:103:LEU:HD22	1.97	0.45
1:D:92:ILE:O	1:D:92:ILE:HG23	2.17	0.45
1:C:90:ILE:HD11	2:R:6:ALA:HB1	1.99	0.45
2:U:1:CXP:H62	2:U:1:CXP:H82	1.88	0.45
1:L:36:ASP:OD1	1:L:39:VAL:HG23	2.17	0.45
1:E:91:CYS:HB2	1:E:103:LEU:HD22	1.99	0.45
1:E:115:PRO:HD3	1:E:189:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:LEU:HB3	2:X:1:CXP:H72	1.98	0.45
1:B:174:LYS:HG2	3:B:373:HOH:O	2.17	0.45
2:Y:1:CXP:H81	2:Y:1:CXP:H62	1.80	0.45
1:E:153:LEU:HD23	1:E:153:LEU:HA	1.86	0.45
1:I:62:TYR:CE1	1:I:90:ILE:HD13	2.51	0.44
1:G:133:THR:O	1:G:137:ILE:HG12	2.16	0.44
1:K:62:TYR:CE1	1:K:90:ILE:HD13	2.52	0.44
1:I:114:LEU:HD23	1:I:189:LEU:HB2	1.98	0.44
1:C:131:GLN:HA	1:I:125:LEU:HD23	1.99	0.44
1:L:133:THR:O	1:L:137:ILE:HG12	2.18	0.44
1:F:177:GLU:CD	1:F:177:GLU:H	2.21	0.44
1:E:148:LYS:HD2	1:F:116:ASN:ND2	2.26	0.44
1:C:39:VAL:O	1:C:43:ILE:HG12	2.18	0.44
1:K:114:LEU:HD11	2:Z:2:WFP:CZ	2.47	0.44
1:A:123:GLN:CD	1:K:131:GLN:HB3	2.38	0.44
1:L:90:ILE:HD11	2:0:6:ALA:HB1	1.99	0.44
1:G:39:VAL:O	1:G:43:ILE:HG12	2.17	0.44
1:F:131:GLN:NE2	1:M:123:GLN:HG2	2.31	0.44
1:B:40:ALA:HB2	1:B:72:ALA:HB1	1.99	0.44
1:E:36:ASP:OD1	1:E:39:VAL:HG23	2.17	0.44
1:L:148:LYS:CD	1:M:116:ASN:HD22	2.30	0.44
1:F:114:LEU:HD23	1:F:189:LEU:HB2	2.00	0.44
1:I:148:LYS:HD2	1:J:116:ASN:HD22	1.83	0.44
1:D:35:ILE:HG22	3:D:457:HOH:O	2.17	0.44
1:F:39:VAL:O	1:F:43:ILE:HG12	2.18	0.44
1:C:142:ILE:HD13	1:I:135:ILE:HD12	1.99	0.44
1:N:115:PRO:HD3	1:N:189:LEU:O	2.18	0.44
1:F:133:THR:H	1:M:123:GLN:HE22	1.65	0.44
1:H:94:MET:HG2	3:N:335:HOH:O	2.17	0.44
1:A:146:ARG:CZ	3:A:220:HOH:O	2.66	0.44
1:B:115:PRO:HD3	1:B:189:LEU:O	2.18	0.44
1:D:40:ALA:HB2	1:D:72:ALA:HB1	2.00	0.44
1:C:127:GLY:HA2	1:I:128:ALA:O	2.18	0.44
1:C:148:LYS:HD2	1:D:116:ASN:HD22	1.83	0.44
1:A:133:THR:O	1:A:137:ILE:HG12	2.18	0.44
1:G:114:LEU:HD23	1:G:189:LEU:HB2	2.00	0.43
1:D:114:LEU:HD23	1:D:189:LEU:HB2	2.00	0.43
1:A:114:LEU:HD23	1:A:189:LEU:HB2	2.00	0.43
1:K:55:PRO:HA	1:K:85:PRO:HG3	1.99	0.43
1:M:91:CYS:HB2	1:M:103:LEU:HD22	1.99	0.43
1:A:172:ASN:C	1:A:172:ASN:ND2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:VAL:O	1:I:43:ILE:HG12	2.18	0.43
1:K:40:ALA:HB2	1:K:72:ALA:HB1	2.00	0.43
1:C:133:THR:O	1:C:137:ILE:HG12	2.17	0.43
1:M:115:PRO:HD3	1:M:189:LEU:O	2.18	0.43
1:A:142:ILE:HD13	1:K:135:ILE:HD12	2.00	0.43
1:F:95:ALA:HB2	3:F:265:HOH:O	2.17	0.43
1:C:143:LEU:CD2	1:C:146:ARG:HH21	2.32	0.43
1:J:114:LEU:HD23	1:J:189:LEU:HB2	2.00	0.43
1:L:91:CYS:HB2	1:L:103:LEU:HD22	2.00	0.43
1:A:143:LEU:CD2	1:A:146:ARG:HH21	2.32	0.43
1:A:116:ASN:ND2	1:G:148:LYS:HD2	2.34	0.43
1:I:115:PRO:HD3	1:I:189:LEU:O	2.19	0.43
1:I:49:PHE:HE1	1:J:22:ARG:NH1	2.16	0.43
1:C:22:ARG:CZ	3:C:329:HOH:O	2.67	0.43
1:I:141:ARG:NE	1:J:118:GLU:OE1	2.50	0.43
1:B:98:MET:HB2	3:B:319:HOH:O	2.19	0.43
1:C:40:ALA:HB2	1:C:72:ALA:HB1	1.99	0.43
1:N:91:CYS:HB2	1:N:103:LEU:HD22	2.01	0.43
1:M:143:LEU:CD2	1:M:146:ARG:HH21	2.32	0.43
1:A:97:SER:HB3	3:A:244:HOH:O	2.19	0.43
1:A:78:ASP:HB3	1:B:114:LEU:HD13	2.01	0.43
1:K:39:VAL:O	1:K:43:ILE:HG12	2.19	0.43
1:K:115:PRO:HD3	1:K:189:LEU:O	2.19	0.43
1:E:90:ILE:HD12	1:E:90:ILE:N	2.33	0.43
1:E:92:ILE:HG23	1:E:92:ILE:O	2.18	0.42
1:I:70:ILE:HG12	1:I:98:MET:HE1	2.01	0.42
1:B:89:THR:C	1:B:90:ILE:HD12	2.39	0.42
1:K:36:ASP:OD1	1:K:39:VAL:HG23	2.19	0.42
1:J:55:PRO:HA	1:J:85:PRO:HG3	2.01	0.42
1:G:83:ILE:HB	1:G:85:PRO:HD2	2.01	0.42
1:A:44:VAL:HG11	1:B:92:ILE:CD1	2.49	0.42
1:C:123:GLN:HE21	1:I:132:ALA:HB3	1.84	0.42
1:C:62:TYR:CE1	1:C:90:ILE:HD13	2.54	0.42
1:B:114:LEU:HD23	1:B:189:LEU:HB2	2.01	0.42
1:N:40:ALA:HB2	1:N:72:ALA:HB1	2.01	0.42
1:N:97:SER:HB3	3:N:214:HOH:O	2.19	0.42
1:K:133:THR:O	1:K:137:ILE:HG12	2.19	0.42
1:E:114:LEU:HD23	1:E:189:LEU:HB2	2.01	0.42
1:H:114:LEU:HD23	1:H:189:LEU:HB2	2.01	0.42
1:G:36:ASP:OD1	1:G:39:VAL:HG23	2.18	0.42
1:M:114:LEU:HD23	1:M:189:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:TYR:CE1	1:E:90:ILE:HD13	2.54	0.42
1:G:84:LYS:N	1:G:84:LYS:HD2	2.35	0.42
1:F:84:LYS:N	1:F:85:PRO:CD	2.82	0.42
1:N:181:GLU:H	1:N:181:GLU:HG2	1.71	0.42
1:M:83:ILE:HB	1:M:85:PRO:HD2	2.00	0.42
1:L:39:VAL:O	1:L:43:ILE:HG12	2.19	0.42
1:E:40:ALA:HB2	1:E:72:ALA:HB1	2.01	0.42
1:N:84:LYS:N	1:N:84:LYS:HD2	2.34	0.42
1:I:35:ILE:CG2	3:I:395:HOH:O	2.65	0.42
1:J:90:ILE:N	1:J:90:ILE:HD12	2.34	0.42
1:F:133:THR:O	1:F:137:ILE:HG12	2.20	0.42
1:I:55:PRO:HA	1:I:85:PRO:HG3	2.01	0.42
1:H:45:SER:HB3	1:I:19:ILE:HG13	2.01	0.42
1:L:153:LEU:HA	1:L:153:LEU:HD23	1.82	0.42
1:C:153:LEU:HA	1:C:153:LEU:HD23	1.83	0.42
1:J:40:ALA:HB2	1:J:72:ALA:HB1	2.01	0.42
1:D:70:ILE:HG12	1:D:98:MET:CE	2.48	0.42
1:C:114:LEU:HD23	1:C:189:LEU:HB2	2.01	0.42
1:K:91:CYS:HB2	1:K:103:LEU:HD22	2.01	0.42
1:M:70:ILE:HG12	1:M:98:MET:HE1	2.02	0.42
1:A:62:TYR:CE1	1:A:90:ILE:HD13	2.55	0.42
1:C:83:ILE:HB	1:C:85:PRO:HD2	2.00	0.42
1:E:84:LYS:HD2	1:E:84:LYS:N	2.35	0.42
1:K:92:ILE:O	1:K:92:ILE:HG23	2.20	0.42
1:N:144:LEU:HA	1:N:144:LEU:HD23	1.94	0.42
1:G:114:LEU:HD11	2:U:2:WFP:CZ	2.49	0.42
1:N:114:LEU:HD23	1:N:189:LEU:HB2	2.01	0.42
1:J:84:LYS:N	1:J:85:PRO:CD	2.83	0.42
1:H:45:SER:HB3	1:I:19:ILE:CG1	2.49	0.42
1:C:25:LYS:HE2	3:C:333:HOH:O	2.20	0.42
1:N:70:ILE:HG12	1:N:98:MET:HE1	2.01	0.41
1:I:133:THR:O	1:I:137:ILE:HG12	2.20	0.41
1:D:39:VAL:O	1:D:43:ILE:HG12	2.20	0.41
1:M:133:THR:HG21	1:N:170:ARG:CD	2.50	0.41
1:G:84:LYS:N	1:G:85:PRO:CD	2.83	0.41
1:C:84:LYS:N	1:C:85:PRO:CD	2.83	0.41
1:D:84:LYS:HD2	1:D:84:LYS:N	2.35	0.41
1:K:114:LEU:HD23	1:K:189:LEU:HB2	2.02	0.41
1:L:92:ILE:HG23	1:L:92:ILE:O	2.20	0.41
1:L:143:LEU:CD2	1:L:146:ARG:HH21	2.33	0.41
1:I:98:MET:HB2	3:I:239:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:LEU:HD11	2:V:2:WFP:CZ	2.50	0.41
1:D:124:PRO:HA	3:D:269:HOH:O	2.20	0.41
1:A:90:ILE:N	1:A:90:ILE:HD12	2.34	0.41
1:L:114:LEU:HD23	1:L:189:LEU:HB2	2.02	0.41
1:G:91:CYS:HB2	1:G:103:LEU:HD22	2.03	0.41
1:G:153:LEU:HA	1:G:153:LEU:HD23	1.87	0.41
1:A:84:LYS:N	1:A:85:PRO:CD	2.83	0.41
1:K:143:LEU:CD2	1:K:146:ARG:HH21	2.33	0.41
1:H:172:ASN:ND2	1:H:172:ASN:C	2.74	0.41
1:N:114:LEU:HD11	2:1:2:WFP:CZ	2.51	0.41
1:E:84:LYS:N	1:E:85:PRO:CD	2.84	0.41
1:D:84:LYS:HD3	3:D:309:HOH:O	2.20	0.41
1:K:81:GLN:HG3	3:K:232:HOH:O	2.21	0.41
1:N:62:TYR:CE1	1:N:90:ILE:HD13	2.56	0.41
1:M:90:ILE:HD11	2:X:6:ALA:HB1	2.02	0.41
1:J:36:ASP:OD1	1:J:39:VAL:HG23	2.20	0.41
1:D:23:LEU:HD23	2:S:1:CXP:H51	2.02	0.41
1:C:84:LYS:N	1:C:84:LYS:HD2	2.36	0.41
1:H:55:PRO:HA	1:H:85:PRO:HG3	2.02	0.41
1:J:144:LEU:HA	1:J:144:LEU:HD23	1.95	0.41
1:A:123:GLN:NE2	1:K:133:THR:H	2.18	0.41
1:L:90:ILE:HD12	1:L:90:ILE:N	2.35	0.41
1:C:55:PRO:HA	1:C:85:PRO:HG3	2.02	0.41
1:D:83:ILE:HB	1:D:85:PRO:HD2	2.02	0.41
1:H:33:SER:HA	3:N:387:HOH:O	2.21	0.41
1:B:55:PRO:HA	1:B:85:PRO:HG3	2.03	0.41
1:A:116:ASN:HD22	1:G:148:LYS:CD	2.34	0.41
1:J:133:THR:O	1:J:137:ILE:HG12	2.20	0.41
1:M:49:PHE:HE1	1:N:22:ARG:NH1	2.19	0.41
1:K:84:LYS:N	1:K:85:PRO:CD	2.83	0.41
1:H:84:LYS:N	1:H:84:LYS:HD2	2.35	0.41
1:A:70:ILE:HG12	1:A:98:MET:CE	2.51	0.41
1:J:143:LEU:CD2	1:J:146:ARG:HH21	2.33	0.41
1:I:92:ILE:O	1:I:92:ILE:HG23	2.20	0.41
1:G:55:PRO:HA	1:G:85:PRO:HG3	2.03	0.41
1:M:55:PRO:HA	1:M:85:PRO:HG3	2.02	0.41
1:E:83:ILE:HB	1:E:85:PRO:HD2	2.03	0.41
1:B:84:LYS:N	1:B:85:PRO:CD	2.84	0.41
1:L:49:PHE:HE1	1:M:22:ARG:HH11	1.68	0.41
1:C:144:LEU:HA	1:C:144:LEU:HD23	1.94	0.41
1:H:40:ALA:HB2	1:H:72:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:92:ILE:HG23	1:J:92:ILE:O	2.21	0.41
1:B:49:PHE:HE1	1:C:22:ARG:NH1	2.17	0.41
1:B:62:TYR:CE1	1:B:90:ILE:HD13	2.56	0.41
1:E:55:PRO:HA	1:E:85:PRO:HG3	2.02	0.41
1:D:123:GLN:HE21	1:H:132:ALA:HB3	1.85	0.41
1:A:40:ALA:HB2	1:A:72:ALA:HB1	2.03	0.41
1:A:118:GLU:OE1	1:G:141:ARG:NE	2.53	0.41
1:I:153:LEU:HA	1:I:153:LEU:HD23	1.85	0.41
1:M:92:ILE:O	1:M:92:ILE:HG23	2.21	0.40
1:H:70:ILE:HG12	1:H:98:MET:HE1	2.03	0.40
1:A:89:THR:C	1:A:90:ILE:HD12	2.42	0.40
1:D:55:PRO:HA	1:D:85:PRO:HG3	2.03	0.40
1:F:32:GLY:HA2	1:F:64:ASN:O	2.20	0.40
1:I:40:ALA:HB2	1:I:72:ALA:HB1	2.02	0.40
1:E:181:GLU:HG2	1:E:181:GLU:H	1.72	0.40
1:I:84:LYS:N	1:I:85:PRO:CD	2.85	0.40
1:L:141:ARG:NE	1:M:118:GLU:OE1	2.53	0.40
1:C:181:GLU:HG2	1:C:181:GLU:H	1.70	0.40
1:E:44:VAL:HG21	1:F:92:ILE:CD1	2.45	0.40
1:E:39:VAL:O	1:E:43:ILE:HG12	2.21	0.40
1:I:84:LYS:N	1:I:84:LYS:HD2	2.37	0.40
1:D:84:LYS:N	1:D:85:PRO:CD	2.85	0.40
1:A:55:PRO:HA	1:A:85:PRO:HG3	2.03	0.40
1:H:175:SER:OG	1:H:178:GLU:HG3	2.21	0.40
1:B:143:LEU:CD2	1:B:146:ARG:HH21	2.35	0.40
1:N:89:THR:C	1:N:90:ILE:HD12	2.41	0.40
1:D:133:THR:H	1:H:123:GLN:NE2	2.18	0.40
1:H:90:ILE:N	1:H:90:ILE:HD12	2.37	0.40
1:M:133:THR:CG2	1:N:170:ARG:HD3	2.51	0.40
1:M:84:LYS:N	1:M:85:PRO:CD	2.84	0.40
1:M:45:SER:HB3	1:N:19:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/199 (86%)	168 (98%)	4 (2%)	0	100	100
1	B	172/199 (86%)	167 (97%)	5 (3%)	0	100	100
1	C	172/199 (86%)	168 (98%)	4 (2%)	0	100	100
1	D	172/199 (86%)	168 (98%)	4 (2%)	0	100	100
1	E	172/199 (86%)	168 (98%)	4 (2%)	0	100	100
1	F	172/199 (86%)	168 (98%)	4 (2%)	0	100	100
1	G	172/199 (86%)	168 (98%)	4 (2%)	0	100	100
1	H	172/199 (86%)	167 (97%)	5 (3%)	0	100	100
1	I	172/199 (86%)	168 (98%)	4 (2%)	0	100	100
1	J	172/199 (86%)	169 (98%)	3 (2%)	0	100	100
1	K	172/199 (86%)	169 (98%)	3 (2%)	0	100	100
1	L	172/199 (86%)	168 (98%)	4 (2%)	0	100	100
1	M	172/199 (86%)	167 (97%)	5 (3%)	0	100	100
1	N	172/199 (86%)	168 (98%)	4 (2%)	0	100	100
2	O	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	1	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	O	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	P	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Q	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	R	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	S	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	T	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	U	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	V	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	W	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	X	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Y	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
2	Z	3/7 (43%)	2 (67%)	1 (33%)	0	100	100
All	All	2450/2884 (85%)	2379 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	141/165 (86%)	132 (94%)	9 (6%)	22	43
1	B	141/165 (86%)	132 (94%)	9 (6%)	22	43
1	C	141/165 (86%)	132 (94%)	9 (6%)	22	43
1	D	141/165 (86%)	133 (94%)	8 (6%)	25	49
1	E	141/165 (86%)	132 (94%)	9 (6%)	22	43
1	F	141/165 (86%)	133 (94%)	8 (6%)	25	49
1	G	141/165 (86%)	132 (94%)	9 (6%)	22	43
1	H	141/165 (86%)	133 (94%)	8 (6%)	25	49
1	I	141/165 (86%)	133 (94%)	8 (6%)	25	49
1	J	141/165 (86%)	132 (94%)	9 (6%)	22	43
1	K	141/165 (86%)	133 (94%)	8 (6%)	25	49
1	L	141/165 (86%)	132 (94%)	9 (6%)	22	43
1	M	141/165 (86%)	132 (94%)	9 (6%)	22	43
1	N	141/165 (86%)	132 (94%)	9 (6%)	22	43
2	O	2/2 (100%)	2 (100%)	0	100	100
2	1	2/2 (100%)	2 (100%)	0	100	100
2	O	2/2 (100%)	2 (100%)	0	100	100
2	P	2/2 (100%)	2 (100%)	0	100	100
2	Q	2/2 (100%)	2 (100%)	0	100	100
2	R	2/2 (100%)	2 (100%)	0	100	100
2	S	2/2 (100%)	2 (100%)	0	100	100
2	T	2/2 (100%)	2 (100%)	0	100	100
2	U	2/2 (100%)	2 (100%)	0	100	100
2	V	2/2 (100%)	2 (100%)	0	100	100
2	W	2/2 (100%)	2 (100%)	0	100	100
2	X	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y	2/2 (100%)	2 (100%)	0	100	100
2	Z	2/2 (100%)	2 (100%)	0	100	100
All	All	2002/2338 (86%)	1881 (94%)	121 (6%)	24	47

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	30	MET
1	A	92	ILE
1	A	97	SER
1	A	122	HIS
1	A	147	ASP
1	A	162	GLU
1	A	172	ASN
1	A	181	GLU
1	B	22	ARG
1	B	30	MET
1	B	92	ILE
1	B	97	SER
1	B	122	HIS
1	B	147	ASP
1	B	162	GLU
1	B	172	ASN
1	B	181	GLU
1	C	22	ARG
1	C	30	MET
1	C	92	ILE
1	C	97	SER
1	C	122	HIS
1	C	147	ASP
1	C	162	GLU
1	C	172	ASN
1	C	181	GLU
1	D	22	ARG
1	D	30	MET
1	D	92	ILE
1	D	97	SER
1	D	122	HIS
1	D	147	ASP
1	D	162	GLU

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Mol	Chain	Res	Type
1	D	172	ASN
1	E	22	ARG
1	E	30	MET
1	E	92	ILE
1	E	97	SER
1	E	122	HIS
1	E	147	ASP
1	E	162	GLU
1	E	172	ASN
1	E	181	GLU
1	F	22	ARG
1	F	30	MET
1	F	92	ILE
1	F	97	SER
1	F	122	HIS
1	F	147	ASP
1	F	162	GLU
1	F	172	ASN
1	G	22	ARG
1	G	30	MET
1	G	92	ILE
1	G	97	SER
1	G	122	HIS
1	G	147	ASP
1	G	162	GLU
1	G	172	ASN
1	G	181	GLU
1	H	22	ARG
1	H	30	MET
1	H	92	ILE
1	H	97	SER
1	H	122	HIS
1	H	147	ASP
1	H	162	GLU
1	H	172	ASN
1	I	22	ARG
1	I	30	MET
1	I	92	ILE
1	I	97	SER
1	I	122	HIS
1	I	147	ASP
1	I	162	GLU

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Mol	Chain	Res	Type
1	I	172	ASN
1	J	22	ARG
1	J	30	MET
1	J	92	ILE
1	J	97	SER
1	J	122	HIS
1	J	147	ASP
1	J	162	GLU
1	J	172	ASN
1	J	181	GLU
1	K	22	ARG
1	K	30	MET
1	K	92	ILE
1	K	97	SER
1	K	122	HIS
1	K	147	ASP
1	K	162	GLU
1	K	172	ASN
1	L	22	ARG
1	L	30	MET
1	L	92	ILE
1	L	97	SER
1	L	122	HIS
1	L	147	ASP
1	L	162	GLU
1	L	172	ASN
1	L	181	GLU
1	M	22	ARG
1	M	30	MET
1	M	92	ILE
1	M	97	SER
1	M	122	HIS
1	M	147	ASP
1	M	162	GLU
1	M	172	ASN
1	M	181	GLU
1	N	22	ARG
1	N	30	MET
1	N	92	ILE
1	N	97	SER
1	N	122	HIS
1	N	147	ASP

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Mol	Chain	Res	Type
1	N	162	GLU
1	N	172	ASN
1	N	181	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	116	ASN
1	A	123	GLN
1	A	172	ASN
1	B	81	GLN
1	B	116	ASN
1	B	123	GLN
1	B	172	ASN
1	C	81	GLN
1	C	116	ASN
1	C	123	GLN
1	C	172	ASN
1	D	81	GLN
1	D	116	ASN
1	D	123	GLN
1	D	172	ASN
1	E	81	GLN
1	E	116	ASN
1	E	123	GLN
1	E	172	ASN
1	F	81	GLN
1	F	116	ASN
1	F	123	GLN
1	F	172	ASN
1	G	81	GLN
1	G	116	ASN
1	G	123	GLN
1	G	172	ASN
1	H	81	GLN
1	H	116	ASN
1	H	123	GLN
1	H	172	ASN
1	I	81	GLN
1	I	116	ASN
1	I	123	GLN

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Mol	Chain	Res	Type
1	I	172	ASN
1	J	81	GLN
1	J	116	ASN
1	J	123	GLN
1	J	172	ASN
1	K	81	GLN
1	K	116	ASN
1	K	123	GLN
1	K	172	ASN
1	L	81	GLN
1	L	116	ASN
1	L	123	GLN
1	L	172	ASN
1	M	81	GLN
1	M	116	ASN
1	M	123	GLN
1	M	172	ASN
1	N	81	GLN
1	N	116	ASN
1	N	123	GLN
1	N	172	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

42 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
2	WFP	0	2	2	12,13,14	4.16	7 (58%)	14,17,19	1.99	5 (35%)
2	YCP	0	5	2	6,8,9	1.46	1 (16%)	5,9,11	2.75	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MP8	0	7	2	7,8,9	0.69	0	5,10,12	1.51	1 (20%)
2	WFP	1	2	2	12,13,14	3.90	7 (58%)	14,17,19	1.91	5 (35%)
2	YCP	1	5	2	6,8,9	1.33	0	5,9,11	2.72	1 (20%)
2	MP8	1	7	2	7,8,9	0.94	0	5,10,12	1.47	1 (20%)
2	WFP	O	2	2	12,13,14	3.86	7 (58%)	14,17,19	1.82	5 (35%)
2	YCP	O	5	2	6,8,9	1.45	1 (16%)	5,9,11	2.73	1 (20%)
2	MP8	O	7	2	7,8,9	0.97	1 (14%)	5,10,12	1.43	1 (20%)
2	WFP	P	2	2	12,13,14	3.99	7 (58%)	14,17,19	1.87	5 (35%)
2	YCP	P	5	2	6,8,9	1.31	0	5,9,11	2.72	1 (20%)
2	MP8	P	7	2	7,8,9	0.94	0	5,10,12	1.45	1 (20%)
2	WFP	Q	2	2	12,13,14	3.88	7 (58%)	14,17,19	1.84	5 (35%)
2	YCP	Q	5	2	6,8,9	1.36	1 (16%)	5,9,11	2.80	1 (20%)
2	MP8	Q	7	2	7,8,9	0.88	0	5,10,12	1.43	1 (20%)
2	WFP	R	2	2	12,13,14	3.99	7 (58%)	14,17,19	1.93	5 (35%)
2	YCP	R	5	2	6,8,9	1.35	0	5,9,11	2.80	1 (20%)
2	MP8	R	7	2	7,8,9	0.97	0	5,10,12	1.41	1 (20%)
2	WFP	S	2	2	12,13,14	4.10	7 (58%)	14,17,19	1.95	5 (35%)
2	YCP	S	5	2	6,8,9	1.37	1 (16%)	5,9,11	2.75	1 (20%)
2	MP8	S	7	2	7,8,9	0.80	0	5,10,12	1.44	1 (20%)
2	WFP	T	2	2	12,13,14	4.09	6 (50%)	14,17,19	1.81	5 (35%)
2	YCP	T	5	2	6,8,9	1.27	0	5,9,11	2.77	1 (20%)
2	MP8	T	7	2	7,8,9	0.83	0	5,10,12	1.65	1 (20%)
2	WFP	U	2	2	12,13,14	4.05	6 (50%)	14,17,19	1.86	5 (35%)
2	YCP	U	5	2	6,8,9	1.30	0	5,9,11	2.75	1 (20%)
2	MP8	U	7	2	7,8,9	0.80	0	5,10,12	1.48	1 (20%)
2	WFP	V	2	2	12,13,14	3.93	7 (58%)	14,17,19	1.89	5 (35%)
2	YCP	V	5	2	6,8,9	1.37	1 (16%)	5,9,11	2.78	1 (20%)
2	MP8	V	7	2	7,8,9	0.89	0	5,10,12	1.46	1 (20%)
2	WFP	W	2	2	12,13,14	3.79	6 (50%)	14,17,19	1.72	5 (35%)
2	YCP	W	5	2	6,8,9	1.33	1 (16%)	5,9,11	2.80	1 (20%)
2	MP8	W	7	2	7,8,9	1.00	1 (14%)	5,10,12	1.33	1 (20%)
2	WFP	X	2	2	12,13,14	3.99	7 (58%)	14,17,19	1.90	5 (35%)
2	YCP	X	5	2	6,8,9	1.36	1 (16%)	5,9,11	2.80	1 (20%)
2	MP8	X	7	2	7,8,9	0.86	0	5,10,12	1.30	1 (20%)
2	WFP	Y	2	2	12,13,14	3.91	7 (58%)	14,17,19	1.86	5 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	YCP	Y	5	2	6,8,9	1.31	0	5,9,11	2.79	1 (20%)
2	MP8	Y	7	2	7,8,9	0.98	0	5,10,12	1.23	0
2	WFP	Z	2	2	12,13,14	3.81	7 (58%)	14,17,19	1.87	5 (35%)
2	YCP	Z	5	2	6,8,9	1.37	1 (16%)	5,9,11	2.75	1 (20%)
2	MP8	Z	7	2	7,8,9	0.73	0	5,10,12	1.40	1 (20%)

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
2	WFP	0	2	2	-	0/4/6/8	0/1/1/1
2	YCP	0	5	2	-	0/1/10/12	0/1/1/1
2	MP8	0	7	2	-	0/0/11/13	0/1/1/1
2	WFP	1	2	2	-	0/4/6/8	0/1/1/1
2	YCP	1	5	2	-	0/1/10/12	0/1/1/1
2	MP8	1	7	2	-	0/0/11/13	0/1/1/1
2	WFP	O	2	2	-	0/4/6/8	0/1/1/1
2	YCP	O	5	2	-	0/1/10/12	0/1/1/1
2	MP8	O	7	2	-	0/0/11/13	0/1/1/1
2	WFP	P	2	2	-	0/4/6/8	0/1/1/1
2	YCP	P	5	2	-	0/1/10/12	0/1/1/1
2	MP8	P	7	2	-	0/0/11/13	0/1/1/1
2	WFP	Q	2	2	-	0/4/6/8	0/1/1/1
2	YCP	Q	5	2	-	0/1/10/12	0/1/1/1
2	MP8	Q	7	2	-	0/0/11/13	0/1/1/1
2	WFP	R	2	2	-	0/4/6/8	0/1/1/1
2	YCP	R	5	2	-	0/1/10/12	0/1/1/1
2	MP8	R	7	2	-	0/0/11/13	0/1/1/1
2	WFP	S	2	2	-	0/4/6/8	0/1/1/1
2	YCP	S	5	2	-	0/1/10/12	0/1/1/1
2	MP8	S	7	2	-	0/0/11/13	0/1/1/1
2	WFP	T	2	2	-	0/4/6/8	0/1/1/1
2	YCP	T	5	2	-	0/1/10/12	0/1/1/1
2	MP8	T	7	2	-	0/0/11/13	0/1/1/1
2	WFP	U	2	2	-	0/4/6/8	0/1/1/1
2	YCP	U	5	2	-	0/1/10/12	0/1/1/1
2	MP8	U	7	2	-	0/0/11/13	0/1/1/1
2	WFP	V	2	2	-	0/4/6/8	0/1/1/1
2	YCP	V	5	2	-	0/1/10/12	0/1/1/1
2	MP8	V	7	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WFP	W	2	2	-	0/4/6/8	0/1/1/1
2	YCP	W	5	2	-	0/1/10/12	0/1/1/1
2	MP8	W	7	2	-	0/0/11/13	0/1/1/1
2	WFP	X	2	2	-	0/4/6/8	0/1/1/1
2	YCP	X	5	2	-	0/1/10/12	0/1/1/1
2	MP8	X	7	2	-	0/0/11/13	0/1/1/1
2	WFP	Y	2	2	-	0/4/6/8	0/1/1/1
2	YCP	Y	5	2	-	0/1/10/12	0/1/1/1
2	MP8	Y	7	2	-	0/0/11/13	0/1/1/1
2	WFP	Z	2	2	-	0/4/6/8	0/1/1/1
2	YCP	Z	5	2	-	0/1/10/12	0/1/1/1
2	MP8	Z	7	2	-	0/0/11/13	0/1/1/1

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	5	YCP	CG-CB	2.02	1.58	1.53
2	X	5	YCP	CG-CB	2.02	1.58	1.53
2	Z	5	YCP	CG-CB	2.03	1.58	1.53
2	W	7	MP8	CA-N	2.04	1.50	1.47
2	O	7	MP8	CA-N	2.05	1.50	1.47
2	S	5	YCP	CG-CB	2.09	1.58	1.53
2	V	5	YCP	CG-CB	2.10	1.58	1.53
2	Y	2	WFP	CB-CA	2.10	1.58	1.53
2	Q	5	YCP	CG-CB	2.13	1.58	1.53
2	S	2	WFP	CB-CA	2.15	1.58	1.53
2	1	2	WFP	CB-CA	2.18	1.58	1.53
2	Q	2	WFP	CB-CA	2.18	1.58	1.53
2	O	5	YCP	CG-CB	2.18	1.59	1.53
2	O	2	WFP	CB-CA	2.24	1.58	1.53
2	P	2	WFP	CB-CA	2.38	1.58	1.53
2	0	2	WFP	CB-CA	2.38	1.58	1.53
2	X	2	WFP	CB-CA	2.40	1.58	1.53
2	0	5	YCP	CG-CB	2.44	1.59	1.53
2	Z	2	WFP	CB-CA	2.52	1.59	1.53
2	V	2	WFP	CB-CA	2.57	1.59	1.53
2	R	2	WFP	CB-CA	2.69	1.59	1.53
2	W	2	WFP	CD1-CE1	4.21	1.44	1.37
2	Q	2	WFP	CD1-CE1	4.25	1.45	1.37
2	Z	2	WFP	CD1-CE1	4.38	1.45	1.37
2	Z	2	WFP	CZ-CE1	4.38	1.45	1.37
2	T	2	WFP	CD1-CE1	4.40	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	2	WFP	CD1-CE1	4.41	1.45	1.37
2	V	2	WFP	CD1-CE1	4.51	1.45	1.37
2	U	2	WFP	CD2-CG	4.52	1.47	1.39
2	1	2	WFP	CD2-CG	4.55	1.47	1.39
2	Z	2	WFP	CD2-CG	4.57	1.47	1.39
2	Y	2	WFP	CD2-CG	4.58	1.47	1.39
2	P	2	WFP	CD2-CG	4.64	1.47	1.39
2	W	2	WFP	CD2-CG	4.65	1.47	1.39
2	R	2	WFP	CD1-CE1	4.66	1.45	1.37
2	Y	2	WFP	CD1-CE1	4.68	1.45	1.37
2	O	2	WFP	CD2-CG	4.75	1.47	1.39
2	S	2	WFP	CD1-CE1	4.79	1.45	1.37
2	R	2	WFP	CD2-CG	4.80	1.47	1.39
2	X	2	WFP	CZ-CE1	4.81	1.46	1.37
2	P	2	WFP	CD1-CE1	4.82	1.46	1.37
2	W	2	WFP	CZ-CE1	4.83	1.46	1.37
2	U	2	WFP	CD1-CE1	4.85	1.46	1.37
2	S	2	WFP	CD2-CG	4.88	1.47	1.39
2	Q	2	WFP	CD2-CG	4.88	1.47	1.39
2	O	2	WFP	CZ-CE1	4.92	1.46	1.37
2	0	2	WFP	CD1-CE1	4.94	1.46	1.37
2	X	2	WFP	CD2-CG	4.96	1.48	1.39
2	Q	2	WFP	CZ-CE1	4.98	1.46	1.37
2	1	2	WFP	CD1-CE1	5.01	1.46	1.37
2	V	2	WFP	CZ-CE1	5.02	1.46	1.37
2	V	2	WFP	CD2-CG	5.05	1.48	1.39
2	0	2	WFP	CD2-CG	5.14	1.48	1.39
2	1	2	WFP	CZ-CE1	5.15	1.46	1.37
2	R	2	WFP	CZ-CE1	5.18	1.46	1.37
2	P	2	WFP	CD2-CE2	5.19	1.46	1.37
2	X	2	WFP	CD1-CE1	5.19	1.46	1.37
2	T	2	WFP	CD2-CG	5.20	1.48	1.39
2	P	2	WFP	CZ-CE1	5.28	1.46	1.37
2	Y	2	WFP	CZ-CE1	5.29	1.46	1.37
2	T	2	WFP	CZ-CE1	5.30	1.46	1.37
2	Y	2	WFP	CD2-CE2	5.31	1.46	1.37
2	U	2	WFP	CZ-CE1	5.34	1.46	1.37
2	S	2	WFP	CZ-CE1	5.39	1.47	1.37
2	V	2	WFP	CD2-CE2	5.39	1.47	1.37
2	1	2	WFP	CD2-CE2	5.53	1.47	1.37
2	W	2	WFP	CD2-CE2	5.59	1.47	1.37
2	Q	2	WFP	CD2-CE2	5.59	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	2	WFP	CZ-CE1	5.64	1.47	1.37
2	U	2	WFP	CD2-CE2	5.74	1.47	1.37
2	W	2	WFP	CD1-CG	5.75	1.49	1.39
2	O	2	WFP	CD1-CG	5.75	1.49	1.39
2	R	2	WFP	CD2-CE2	5.77	1.47	1.37
2	O	2	WFP	CZ-CE2	5.77	1.47	1.37
2	Z	2	WFP	CZ-CE2	5.78	1.47	1.37
2	X	2	WFP	CD1-CG	5.92	1.49	1.39
2	Z	2	WFP	CD1-CG	5.93	1.49	1.39
2	1	2	WFP	CZ-CE2	5.95	1.48	1.37
2	X	2	WFP	CD2-CE2	5.98	1.48	1.37
2	Q	2	WFP	CZ-CE2	5.98	1.48	1.37
2	Z	2	WFP	CD2-CE2	5.98	1.48	1.37
2	1	2	WFP	CD1-CG	6.00	1.49	1.39
2	X	2	WFP	CZ-CE2	6.00	1.48	1.37
2	R	2	WFP	CD1-CG	6.02	1.50	1.39
2	T	2	WFP	CD2-CE2	6.03	1.48	1.37
2	W	2	WFP	CZ-CE2	6.04	1.48	1.37
2	Y	2	WFP	CD1-CG	6.04	1.50	1.39
2	0	2	WFP	CD1-CG	6.06	1.50	1.39
2	O	2	WFP	CD2-CE2	6.08	1.48	1.37
2	V	2	WFP	CZ-CE2	6.10	1.48	1.37
2	V	2	WFP	CD1-CG	6.15	1.50	1.39
2	Q	2	WFP	CD1-CG	6.17	1.50	1.39
2	S	2	WFP	CD2-CE2	6.18	1.48	1.37
2	P	2	WFP	CD1-CG	6.20	1.50	1.39
2	S	2	WFP	CD1-CG	6.22	1.50	1.39
2	0	2	WFP	CD2-CE2	6.26	1.48	1.37
2	Y	2	WFP	CZ-CE2	6.27	1.48	1.37
2	R	2	WFP	CZ-CE2	6.32	1.48	1.37
2	T	2	WFP	CD1-CG	6.33	1.50	1.39
2	T	2	WFP	CZ-CE2	6.38	1.48	1.37
2	0	2	WFP	CZ-CE2	6.39	1.48	1.37
2	U	2	WFP	CZ-CE2	6.45	1.48	1.37
2	S	2	WFP	CZ-CE2	6.49	1.48	1.37
2	U	2	WFP	CD1-CG	6.51	1.50	1.39
2	P	2	WFP	CZ-CE2	6.69	1.49	1.37

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2	WFP	CD1-CE1-CZ	-3.34	119.11	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	2	WFP	CD1-CE1-CZ	-3.32	119.13	123.52
2	P	2	WFP	CD1-CE1-CZ	-3.30	119.16	123.52
2	S	2	WFP	CD1-CE1-CZ	-3.20	119.30	123.52
2	0	2	WFP	CD1-CE1-CZ	-3.19	119.31	123.52
2	Y	2	WFP	CD1-CE1-CZ	-3.19	119.31	123.52
2	R	2	WFP	CD1-CE1-CZ	-3.18	119.32	123.52
2	V	2	WFP	CD1-CE1-CZ	-3.18	119.33	123.52
2	Q	2	WFP	CD1-CE1-CZ	-3.00	119.56	123.52
2	X	2	WFP	CD1-CE1-CZ	-2.95	119.62	123.52
2	Z	2	WFP	CD1-CE1-CZ	-2.89	119.70	123.52
2	T	2	WFP	CD1-CE1-CZ	-2.89	119.70	123.52
2	0	2	WFP	CD2-CE2-CZ	-2.84	119.77	123.52
2	O	2	WFP	CD1-CE1-CZ	-2.78	119.85	123.52
2	W	2	WFP	CD1-CE1-CZ	-2.68	119.99	123.52
2	O	2	WFP	CD2-CE2-CZ	-2.54	120.17	123.52
2	S	2	WFP	CD2-CE2-CZ	-2.52	120.20	123.52
2	P	2	WFP	CD2-CE2-CZ	-2.39	120.37	123.52
2	R	2	WFP	CD2-CE2-CZ	-2.38	120.37	123.52
2	X	2	WFP	CD2-CE2-CZ	-2.36	120.41	123.52
2	Y	2	WFP	CD2-CE2-CZ	-2.36	120.41	123.52
2	W	2	WFP	CD2-CE2-CZ	-2.33	120.44	123.52
2	V	2	WFP	CD2-CE2-CZ	-2.32	120.46	123.52
2	T	2	WFP	CD2-CE2-CZ	-2.26	120.54	123.52
2	Z	2	WFP	CD2-CE2-CZ	-2.25	120.55	123.52
2	Q	2	WFP	CD2-CE2-CZ	-2.24	120.57	123.52
2	U	2	WFP	CD2-CE2-CZ	-2.20	120.62	123.52
2	1	2	WFP	CD2-CE2-CZ	-2.18	120.65	123.52
2	X	7	MP8	CB-CG-CD	2.12	105.04	102.21
2	W	7	MP8	CB-CG-CD	2.14	105.06	102.21
2	O	2	WFP	F1-CE1-CD1	2.20	121.15	118.22
2	R	7	MP8	CB-CG-CD	2.32	105.31	102.21
2	O	7	MP8	CB-CG-CD	2.36	105.36	102.21
2	U	7	MP8	CB-CG-CD	2.48	105.52	102.21
2	Z	7	MP8	CB-CG-CD	2.49	105.53	102.21
2	U	2	WFP	CG-CD1-CE1	2.52	120.93	118.84
2	Q	7	MP8	CB-CG-CD	2.52	105.57	102.21
2	Q	2	WFP	CG-CD1-CE1	2.55	120.96	118.84
2	W	2	WFP	F1-CE1-CD1	2.57	121.64	118.22
2	W	2	WFP	CE2-CZ-CE1	2.59	120.03	116.07
2	V	2	WFP	CG-CD1-CE1	2.61	121.01	118.84
2	S	7	MP8	CB-CG-CD	2.62	105.70	102.21
2	T	2	WFP	CG-CD1-CE1	2.62	121.02	118.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	2	WFP	CG-CD1-CE1	2.64	121.04	118.84
2	V	7	MP8	CB-CG-CD	2.66	105.75	102.21
2	0	7	MP8	CB-CG-CD	2.70	105.81	102.21
2	P	2	WFP	F1-CE1-CD1	2.70	121.81	118.22
2	P	2	WFP	CG-CD1-CE1	2.71	121.09	118.84
2	O	2	WFP	CG-CD1-CE1	2.72	121.10	118.84
2	1	7	MP8	CB-CG-CD	2.73	105.84	102.21
2	P	7	MP8	CB-CG-CD	2.73	105.84	102.21
2	Y	2	WFP	F1-CE1-CD1	2.74	121.87	118.22
2	T	7	MP8	CB-CG-CD	2.75	105.87	102.21
2	Q	2	WFP	F1-CE1-CD1	2.76	121.89	118.22
2	Y	2	WFP	CG-CD1-CE1	2.76	121.14	118.84
2	T	2	WFP	F1-CE1-CD1	2.79	121.94	118.22
2	Y	2	WFP	CE2-CZ-CE1	2.79	120.33	116.07
2	0	2	WFP	F1-CE1-CD1	2.80	121.95	118.22
2	0	2	WFP	CG-CD1-CE1	2.80	121.17	118.84
2	Z	2	WFP	CE2-CZ-CE1	2.80	120.35	116.07
2	X	2	WFP	CG-CD1-CE1	2.81	121.17	118.84
2	R	2	WFP	F1-CE1-CD1	2.82	121.97	118.22
2	R	2	WFP	CE2-CZ-CE1	2.82	120.38	116.07
2	O	2	WFP	CE2-CZ-CE1	2.83	120.38	116.07
2	X	2	WFP	CE2-CZ-CE1	2.84	120.40	116.07
2	T	2	WFP	CE2-CZ-CE1	2.84	120.41	116.07
2	1	2	WFP	CE2-CZ-CE1	2.86	120.43	116.07
2	Z	2	WFP	F1-CE1-CD1	2.87	122.05	118.22
2	P	2	WFP	CE2-CZ-CE1	2.87	120.45	116.07
2	1	2	WFP	CG-CD1-CE1	2.91	121.26	118.84
2	V	2	WFP	F1-CE1-CD1	2.93	122.12	118.22
2	Q	2	WFP	CE2-CZ-CE1	2.94	120.55	116.07
2	S	2	WFP	F1-CE1-CD1	2.94	122.14	118.22
2	S	2	WFP	CE2-CZ-CE1	2.94	120.56	116.07
2	U	2	WFP	CE2-CZ-CE1	2.95	120.58	116.07
2	X	2	WFP	F1-CE1-CD1	3.02	122.24	118.22
2	S	2	WFP	CG-CD1-CE1	3.03	121.36	118.84
2	1	2	WFP	F1-CE1-CD1	3.04	122.28	118.22
2	V	2	WFP	CE2-CZ-CE1	3.07	120.75	116.07
2	Z	2	WFP	CG-CD1-CE1	3.08	121.40	118.84
2	0	2	WFP	CE2-CZ-CE1	3.13	120.84	116.07
2	R	2	WFP	CG-CD1-CE1	3.15	121.46	118.84
2	U	2	WFP	F1-CE1-CD1	3.17	122.45	118.22
2	1	5	YCP	CD-CG-CB	5.71	123.41	111.44
2	Z	5	YCP	CD-CG-CB	5.73	123.45	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	5	YCP	CD-CG-CB	5.73	123.46	111.44
2	O	5	YCP	CD-CG-CB	5.75	123.50	111.44
2	P	5	YCP	CD-CG-CB	5.76	123.51	111.44
2	U	5	YCP	CD-CG-CB	5.77	123.53	111.44
2	0	5	YCP	CD-CG-CB	5.78	123.55	111.44
2	R	5	YCP	CD-CG-CB	5.82	123.63	111.44
2	T	5	YCP	CD-CG-CB	5.84	123.68	111.44
2	V	5	YCP	CD-CG-CB	5.86	123.72	111.44
2	W	5	YCP	CD-CG-CB	5.87	123.74	111.44
2	Q	5	YCP	CD-CG-CB	5.88	123.77	111.44
2	Y	5	YCP	CD-CG-CB	5.88	123.77	111.44
2	X	5	YCP	CD-CG-CB	5.91	123.82	111.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	2	WFP	1	0
2	O	7	MP8	1	0
2	R	2	WFP	1	0
2	R	7	MP8	1	0
2	S	2	WFP	1	0
2	T	2	WFP	1	0
2	U	2	WFP	1	0
2	V	2	WFP	1	0
2	V	7	MP8	1	0
2	W	2	WFP	1	0
2	W	7	MP8	1	0
2	Y	2	WFP	1	0
2	Z	2	WFP	1	0
2	Z	5	YCP	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	174/199 (87%)	0.13	3 (1%) 73 68	14, 30, 52, 74	0
1	B	174/199 (87%)	0.18	3 (1%) 73 68	15, 31, 53, 73	0
1	C	174/199 (87%)	0.12	4 (2%) 64 57	14, 30, 52, 73	0
1	D	174/199 (87%)	0.13	4 (2%) 64 57	14, 30, 53, 73	0
1	E	174/199 (87%)	0.21	4 (2%) 64 57	14, 30, 52, 73	0
1	F	174/199 (87%)	0.07	3 (1%) 73 68	15, 31, 52, 74	0
1	G	174/199 (87%)	0.07	2 (1%) 82 79	15, 30, 52, 73	0
1	H	174/199 (87%)	0.22	5 (2%) 55 48	15, 30, 52, 72	0
1	I	174/199 (87%)	0.05	1 (0%) 90 88	15, 30, 52, 74	0
1	J	174/199 (87%)	0.10	0 100 100	13, 30, 53, 73	0
1	K	174/199 (87%)	0.13	2 (1%) 82 79	15, 30, 52, 73	0
1	L	174/199 (87%)	0.08	3 (1%) 73 68	15, 30, 52, 73	0
1	M	174/199 (87%)	0.14	5 (2%) 55 48	12, 30, 53, 73	0
1	N	174/199 (87%)	0.05	2 (1%) 82 79	13, 31, 52, 72	0
2	O	3/7 (42%)	-0.14	0 100 100	45, 45, 47, 48	0
2	1	3/7 (42%)	0.28	0 100 100	44, 44, 49, 49	0
2	O	3/7 (42%)	0.09	0 100 100	48, 48, 51, 53	0
2	P	3/7 (42%)	0.48	0 100 100	41, 41, 42, 45	0
2	Q	3/7 (42%)	0.41	0 100 100	42, 42, 44, 47	0
2	R	3/7 (42%)	0.42	0 100 100	52, 52, 53, 55	0
2	S	3/7 (42%)	0.71	1 (33%) 0 0	40, 40, 43, 45	0
2	T	3/7 (42%)	-0.18	0 100 100	44, 44, 46, 46	0
2	U	3/7 (42%)	-0.07	0 100 100	34, 34, 36, 38	0
2	V	3/7 (42%)	0.55	0 100 100	44, 44, 46, 47	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
2	W	3/7 (42%)	-0.24	0	100	100	41, 41, 42, 43	0
2	X	3/7 (42%)	0.27	0	100	100	46, 46, 47, 48	0
2	Y	3/7 (42%)	0.19	0	100	100	40, 40, 41, 43	0
2	Z	3/7 (42%)	0.48	0	100	100	37, 37, 39, 47	0
All	All	2478/2884 (85%)	0.12	42 (1%)	73	68	12, 30, 53, 74	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	162	GLU	4.0
1	C	165	GLU	4.0
1	E	21	SER	3.4
1	M	191	HIS	3.4
1	H	165	GLU	3.4
1	H	162	GLU	3.2
1	L	19	ILE	3.2
1	I	129	GLN	3.1
1	M	162	GLU	3.0
1	M	20	TYR	2.7
1	F	129	GLN	2.7
1	K	181	GLU	2.7
1	D	129	GLN	2.7
1	F	56	GLU	2.7
1	A	56	GLU	2.6
1	E	38	ASN	2.6
1	H	190	THR	2.6
1	H	20	TYR	2.5
1	N	38	ASN	2.5
1	D	18	ASP	2.5
1	C	162	GLU	2.5
1	B	108	LYS	2.4
1	E	18	ASP	2.4
2	S	4	PRO	2.4
1	H	191	HIS	2.3
1	K	155	GLU	2.3
1	L	22	ARG	2.3
1	C	191	HIS	2.3
1	A	190	THR	2.2
1	M	22	ARG	2.2
1	G	162	GLU	2.2
1	B	84	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	20	TYR	2.1
1	C	181	GLU	2.1
1	B	162	GLU	2.1
1	D	19	ILE	2.1
1	D	55	PRO	2.1
1	L	162	GLU	2.0
1	F	190	THR	2.0
1	G	177	GLU	2.0
1	M	190	THR	2.0
1	A	181	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	WFP	Y	2	13/14	0.93	0.17	-	20,24,37,39	0
2	WFP	V	2	13/14	0.91	0.19	-	35,36,45,47	0
2	WFP	T	2	13/14	0.91	0.15	-	29,33,42,43	0
2	YCP	T	5	8/9	0.91	0.23	-	45,45,46,47	0
2	WFP	R	2	13/14	0.93	0.20	-	44,45,49,50	0
2	MP8	Z	7	8/9	0.93	0.15	-	42,43,45,45	0
2	YCP	U	5	8/9	0.93	0.21	-	34,36,37,37	0
2	MP8	O	7	8/9	0.94	0.20	-	43,44,47,50	0
2	MP8	R	7	8/9	0.94	0.22	-	53,55,56,57	0
2	MP8	S	7	8/9	0.93	0.22	-	40,41,42,42	0
2	YCP	R	5	8/9	0.90	0.19	-	53,53,53,54	0
2	MP8	O	7	8/9	0.94	0.14	-	50,50,51,51	0
2	WFP	O	2	13/14	0.92	0.18	-	31,33,42,42	0
2	WFP	1	2	13/14	0.89	0.21	-	34,35,40,41	0
2	YCP	S	5	8/9	0.82	0.22	-	41,42,42,42	0
2	WFP	Z	2	13/14	0.93	0.23	-	37,39,42,43	0
2	MP8	Y	7	8/9	0.94	0.21	-	40,43,45,46	0
2	MP8	T	7	8/9	0.96	0.17	-	43,43,44,44	0
2	MP8	V	7	8/9	0.94	0.25	-	44,45,46,46	0
2	YCP	X	5	8/9	0.89	0.22	-	46,46,46,46	0
2	MP8	P	7	8/9	0.96	0.23	-	42,43,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MP8	W	7	8/9	0.97	0.15	-	36,36,38,38	0
2	WFP	X	2	13/14	0.94	0.17	-	41,43,45,45	0
2	YCP	O	5	8/9	0.83	0.30	-	45,47,48,48	0
2	WFP	P	2	13/14	0.92	0.17	-	32,33,37,38	0
2	WFP	Q	2	13/14	0.89	0.19	-	37,38,42,43	0
2	WFP	W	2	13/14	0.94	0.17	-	33,36,42,43	0
2	MP8	X	7	8/9	0.92	0.27	-	47,48,49,49	0
2	WFP	S	2	13/14	0.89	0.20	-	42,44,45,45	0
2	WFP	O	2	13/14	0.88	0.20	-	35,37,43,43	0
2	YCP	V	5	8/9	0.89	0.19	-	47,47,47,50	0
2	YCP	O	5	8/9	0.74	0.21	-	53,53,53,54	0
2	MP8	1	7	8/9	0.94	0.25	-	48,50,50,51	0
2	YCP	Z	5	8/9	0.91	0.17	-	39,41,44,45	0
2	YCP	P	5	8/9	0.86	0.20	-	43,44,45,45	0
2	YCP	1	5	8/9	0.91	0.19	-	50,52,52,52	0
2	YCP	Y	5	8/9	0.89	0.25	-	42,43,44,47	0
2	YCP	Q	5	8/9	0.84	0.20	-	44,44,46,47	0
2	YCP	W	5	8/9	0.91	0.19	-	43,44,44,46	0
2	MP8	U	7	8/9	0.96	0.15	-	29,30,32,33	0
2	MP8	Q	7	8/9	0.95	0.15	-	39,40,41,41	0
2	WFP	U	2	13/14	0.90	0.19	-	28,30,34,37	0

### 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.