



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:19 PM UTC

PDB ID : 3KTK / pdb_00003ktk
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

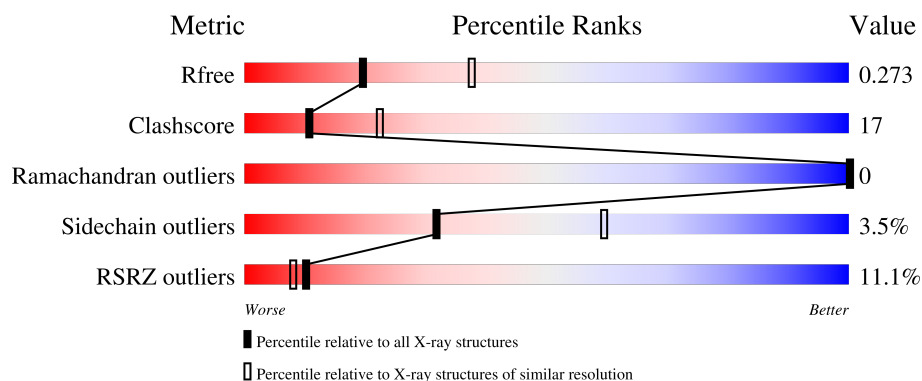
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	199	10% 60% 26% • 13%
1	B	199	9% 59% 26% • 13%
1	C	199	10% 56% 31% • 13%
1	D	199	6% 62% 24% • 13%
1	E	199	12% 63% 23% • 13%

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	WFP	O	2	-	X	-	-
2	WFP	Q	2	-	X	-	-
2	WFP	Z	2	-	X	-	-

2 Entry composition

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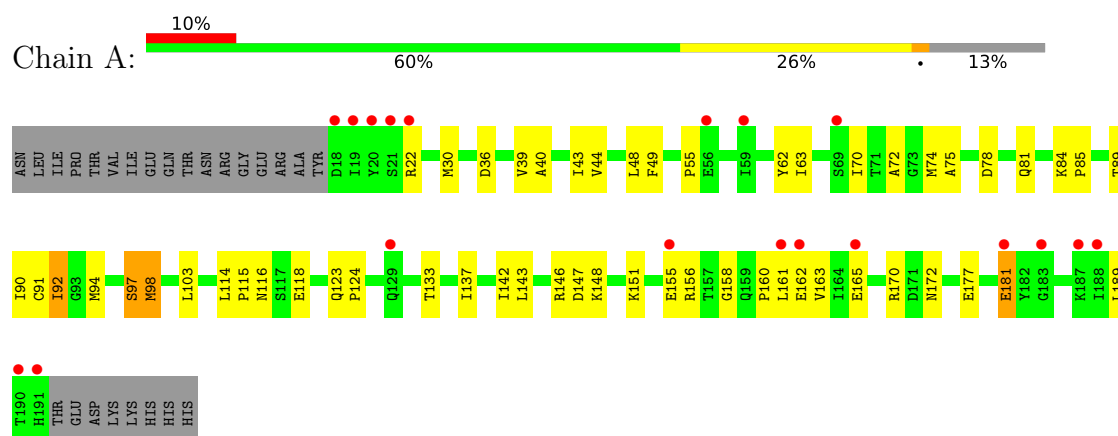
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	33	Total 33	O 33	0	0
3	F	27	Total 27	O 27	0	0
3	G	27	Total 27	O 27	0	0
3	Q	1	Total 1	O 1	0	0
3	T	1	Total 1	O 1	0	0
3	H	25	Total 25	O 25	0	0
3	I	26	Total 26	O 26	0	0
3	J	26	Total 26	O 26	0	0
3	K	24	Total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

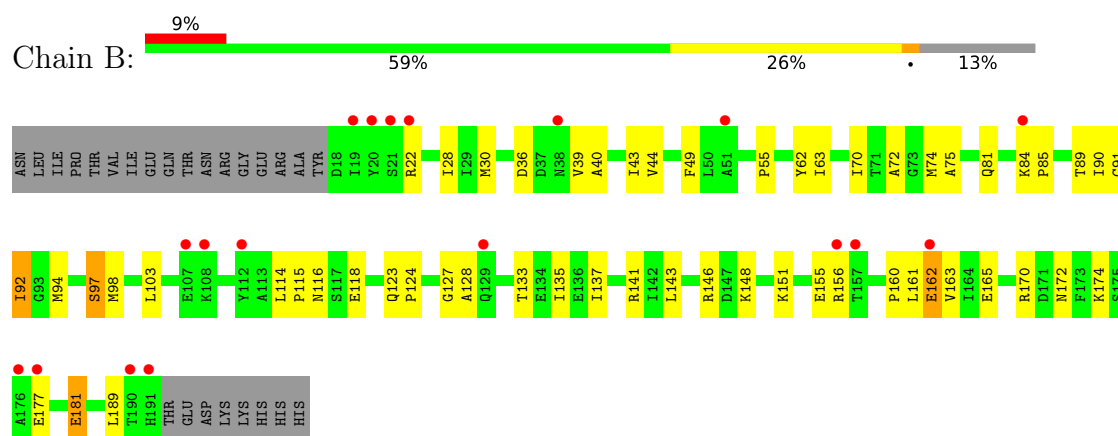
3 Residue-property plots [i](#)

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

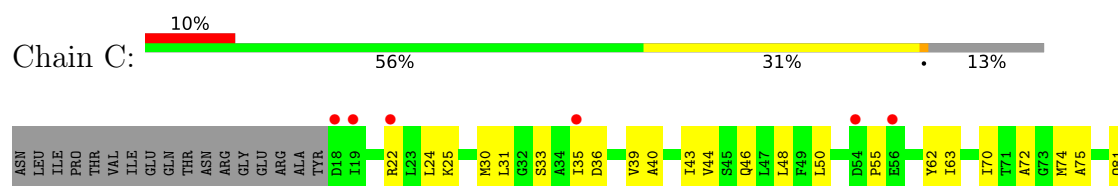
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

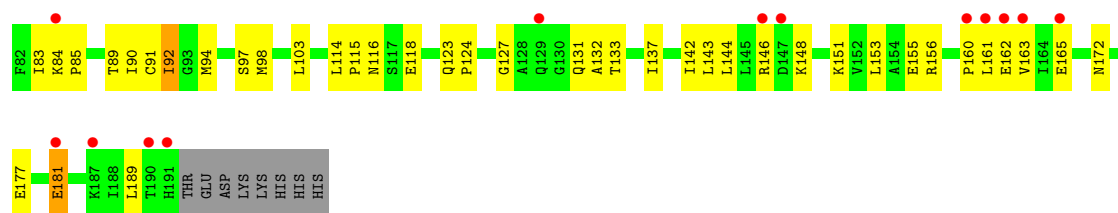


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

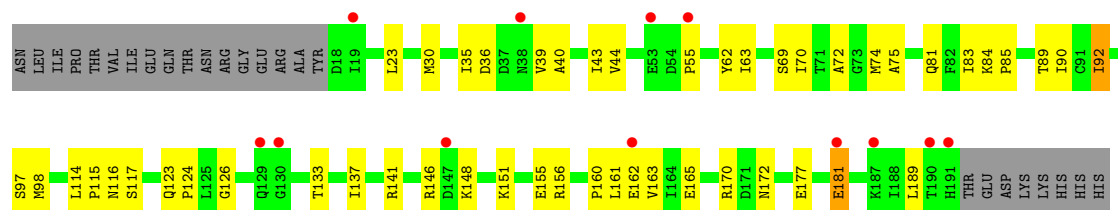


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

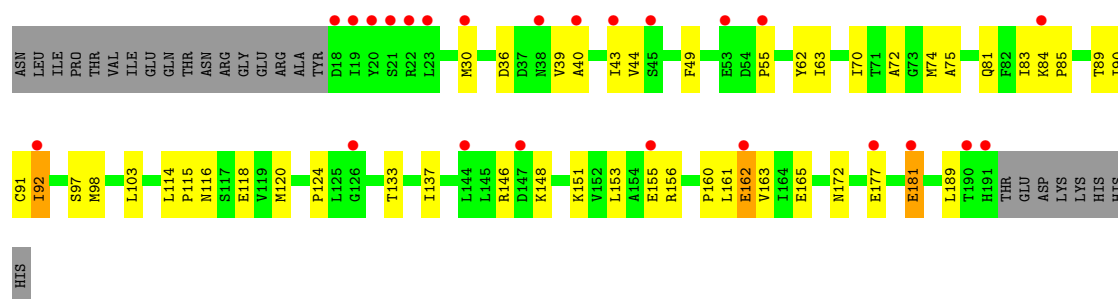




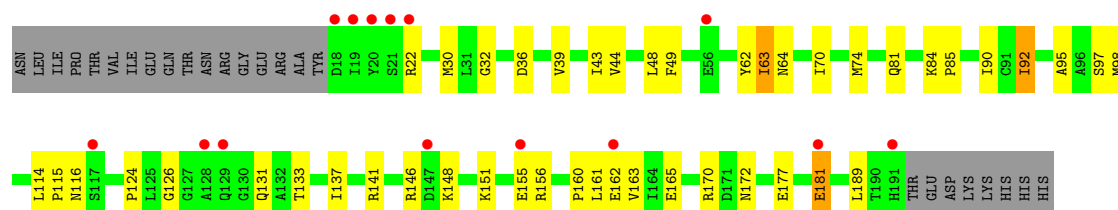
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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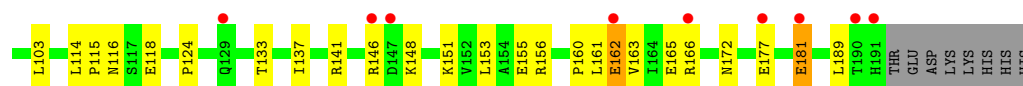


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

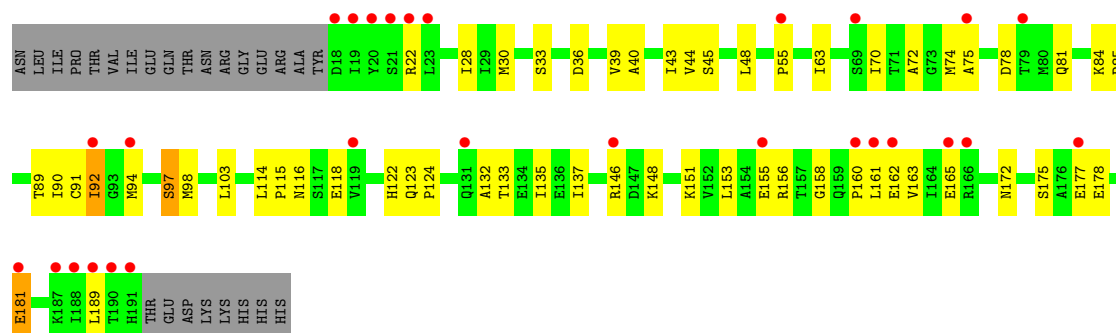


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

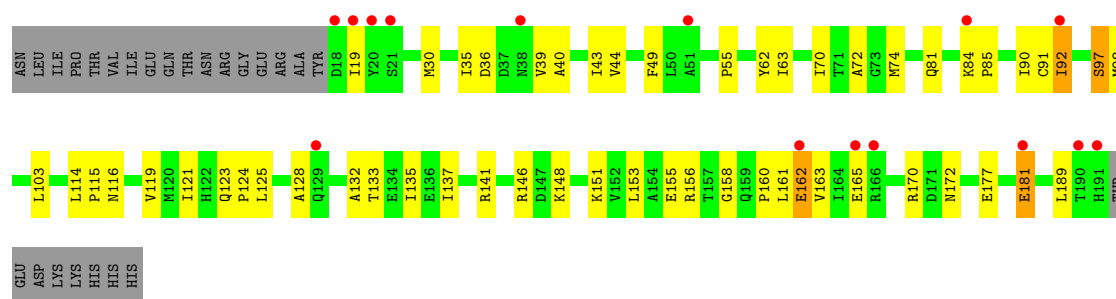




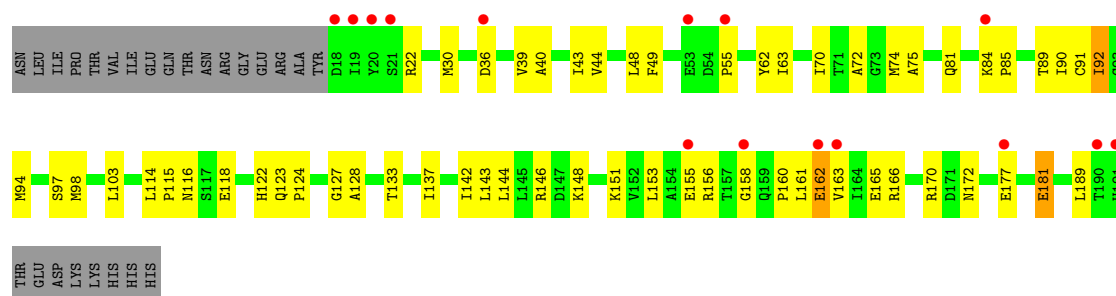
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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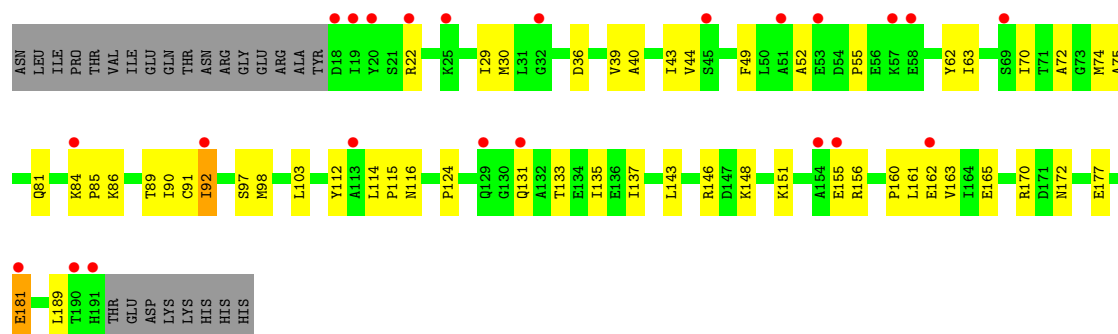


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

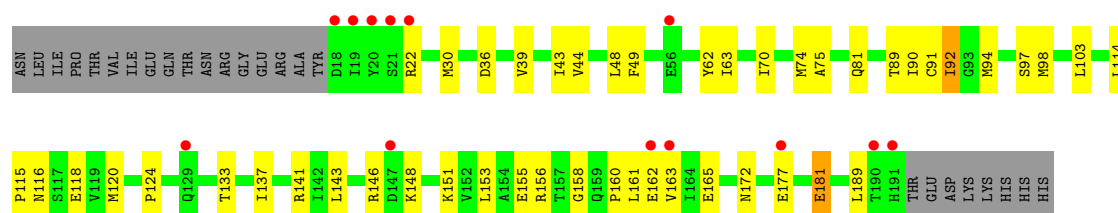


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

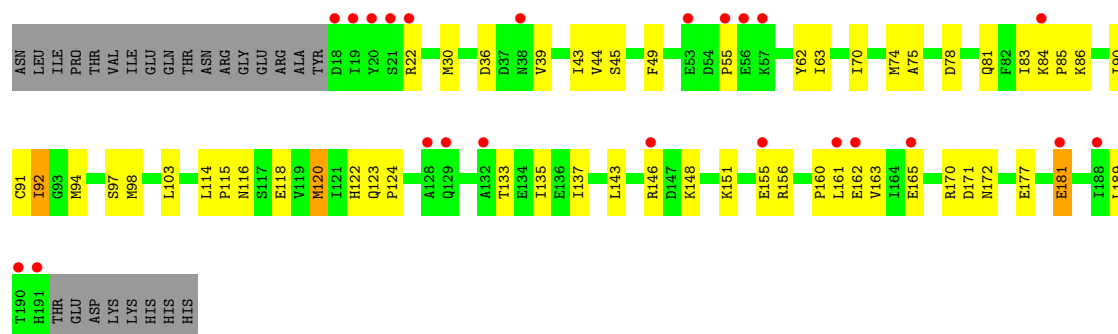




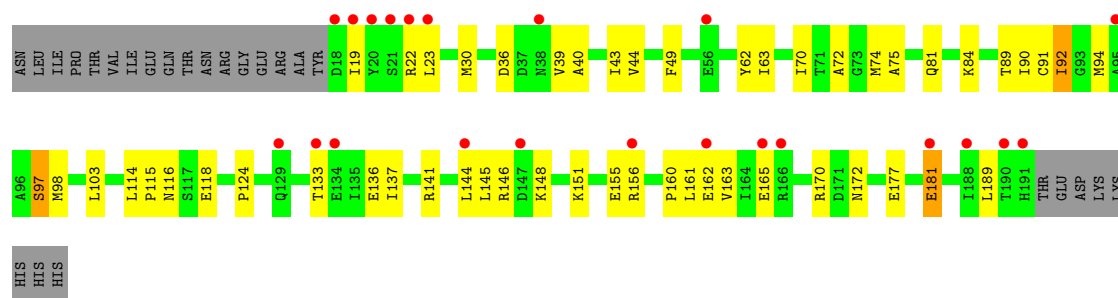
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



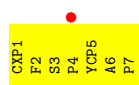
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



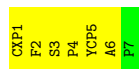
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



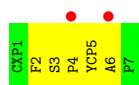
- Molecule 2: Acyldepsipeptide 2



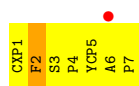
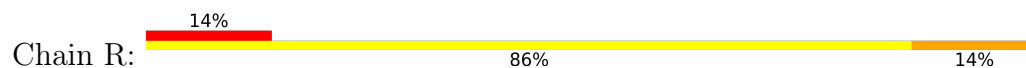
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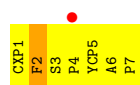
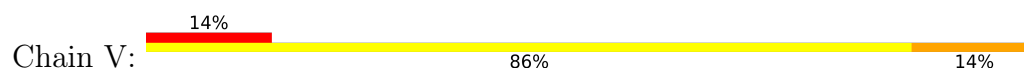
- Molecule 2: Acyldepsipeptide 2



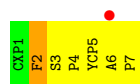
- Molecule 2: Acyldepsipeptide 2



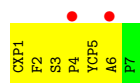
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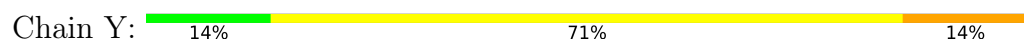
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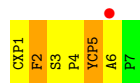
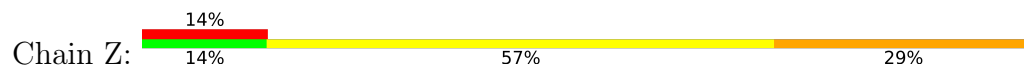
- Molecule 2: Acyldepsipeptide 2



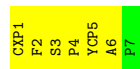
- Molecule 2: Acyldepsipeptide 2



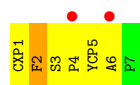
- Molecule 2: Acyldepsipeptide 2



- Molecule 2: Acyldepsipeptide 2



- Molecule 2: Acyldepsipeptide 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.17Å 97.24Å 100.03Å 71.51° 73.89° 77.30°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	85.5 (50.00-2.60) 95.6 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.269 , 0.294 0.271 , 0.273	Depositor DCC
R_{free} test set	4901 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	19732	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YCP, CXP, WFP, 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	0.50	1/1340 (0.1%)	0.89	3/1806 (0.2%)
1	B	0.45	0/1340	0.88	3/1806 (0.2%)
1	C	0.48	0/1340	0.89	2/1806 (0.1%)
1	D	0.46	0/1340	0.89	2/1806 (0.1%)
1	E	0.51	0/1340	0.88	2/1806 (0.1%)
1	F	0.46	0/1340	0.89	1/1806 (0.1%)
1	G	0.49	0/1340	0.89	2/1806 (0.1%)
1	H	0.49	0/1340	0.90	3/1806 (0.2%)
1	I	0.47	0/1340	0.88	2/1806 (0.1%)
1	J	0.47	0/1340	0.89	3/1806 (0.2%)
1	K	0.46	0/1340	0.88	2/1806 (0.1%)
1	L	0.50	0/1340	0.90	3/1806 (0.2%)
1	M	0.52	1/1340 (0.1%)	0.89	2/1806 (0.1%)
1	N	0.47	0/1340	0.88	1/1806 (0.1%)
2	O	2.74	2/17 (11.8%)	2.02	0/21
2	I	2.76	2/17 (11.8%)	1.99	0/21
2	O	2.92	3/17 (17.6%)	1.85	0/21
2	P	2.72	2/17 (11.8%)	1.96	0/21
2	Q	2.67	2/17 (11.8%)	2.02	0/21
2	R	2.72	2/17 (11.8%)	1.86	0/21
2	S	2.81	2/17 (11.8%)	2.16	0/21
2	T	2.88	3/17 (17.6%)	1.97	0/21
2	U	2.84	3/17 (17.6%)	1.87	0/21
2	V	2.82	2/17 (11.8%)	1.92	0/21
2	W	2.91	2/17 (11.8%)	1.74	0/21
2	X	2.79	2/17 (11.8%)	1.94	0/21
2	Y	2.87	3/17 (17.6%)	1.92	0/21
2	Z	2.66	2/17 (11.8%)	1.94	0/21
All	All	0.57	34/18998 (0.2%)	0.91	31/25578 (0.1%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	4	PRO	N-CA	6.68	1.57	1.47
2	T	3	SER	C-N	6.66	1.45	1.34
2	O	3	SER	C-N	6.62	1.45	1.34
2	X	3	SER	C-N	6.60	1.45	1.34
2	P	3	SER	C-N	6.55	1.45	1.34
2	Y	3	SER	C-N	6.53	1.45	1.34
2	V	4	PRO	N-CA	6.48	1.56	1.47
2	T	4	PRO	N-CA	6.43	1.56	1.47
2	O	4	PRO	N-CA	6.40	1.56	1.47
2	V	3	SER	C-N	6.37	1.44	1.34
2	R	3	SER	C-N	6.30	1.44	1.34
2	1	3	SER	C-N	6.19	1.44	1.34
2	1	4	PRO	N-CA	6.12	1.56	1.47
2	S	3	SER	C-N	6.11	1.44	1.34
2	Q	4	PRO	N-CA	6.10	1.56	1.47
2	Y	4	PRO	N-CA	6.01	1.56	1.47
2	W	3	SER	C-N	6.00	1.44	1.34
2	Q	3	SER	C-N	6.00	1.44	1.34
2	W	4	PRO	N-CA	5.96	1.55	1.47
2	U	3	SER	C-N	5.96	1.44	1.34
2	Z	3	SER	C-N	5.91	1.44	1.34
2	U	4	PRO	N-CA	5.85	1.55	1.47
2	O	3	SER	C-N	5.84	1.44	1.34
2	Z	4	PRO	N-CA	5.84	1.55	1.47
2	O	4	PRO	N-CA	5.76	1.55	1.47
2	P	4	PRO	N-CA	5.75	1.55	1.47
2	X	4	PRO	N-CA	5.58	1.55	1.47
2	R	4	PRO	N-CA	5.53	1.55	1.47
1	M	120	MET	SD-CE	-5.41	1.66	1.79
2	O	4	PRO	CA-C	5.37	1.64	1.52
2	Y	4	PRO	CA-C	5.26	1.64	1.52
2	U	4	PRO	CA-C	5.22	1.64	1.52
1	A	98	MET	SD-CE	-5.08	1.66	1.79
2	T	4	PRO	CA-C	5.04	1.63	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	63	ILE	N-CA-C	6.73	117.53	108.11
1	C	63	ILE	N-CA-C	6.49	117.19	108.11
1	G	63	ILE	N-CA-C	6.48	117.19	108.11
1	N	63	ILE	N-CA-C	6.44	117.12	108.11
1	K	63	ILE	N-CA-C	6.40	117.07	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	ILE	N-CA-C	6.36	117.02	108.11
1	H	63	ILE	N-CA-C	6.33	116.97	108.11
1	L	63	ILE	N-CA-C	6.30	116.92	108.11
1	M	63	ILE	N-CA-C	6.17	116.75	108.11
1	B	63	ILE	N-CA-C	6.10	116.65	108.11
1	L	75	ALA	N-CA-C	-6.04	104.61	111.14
1	I	63	ILE	N-CA-C	6.01	116.53	108.11
1	E	63	ILE	N-CA-C	5.99	116.50	108.11
1	G	75	ALA	N-CA-C	-5.93	104.74	111.14
1	H	75	ALA	N-CA-C	-5.83	104.85	111.14
1	F	63	ILE	N-CA-C	5.78	116.20	108.11
1	A	63	ILE	N-CA-C	5.71	116.10	108.11
1	K	75	ALA	N-CA-C	-5.68	105.08	111.28
1	C	75	ALA	N-CA-C	-5.59	105.10	111.14
1	J	75	ALA	N-CA-C	-5.48	105.39	111.36
1	I	158	GLY	N-CA-C	-5.40	107.91	114.92
1	A	75	ALA	N-CA-C	-5.37	105.32	111.07
1	J	158	GLY	N-CA-C	-5.32	108.00	114.92
1	M	75	ALA	N-CA-C	-5.26	105.54	111.28
1	B	75	ALA	N-CA-C	-5.25	105.64	111.36
1	D	75	ALA	N-CA-C	-5.22	105.67	111.36
1	E	75	ALA	N-CA-C	-5.14	105.75	111.36
1	H	158	GLY	N-CA-C	-5.05	108.35	114.92
1	L	158	GLY	N-CA-C	-5.04	108.37	114.92
1	A	158	GLY	N-CA-C	-5.03	108.38	114.92
1	B	97	SER	CB-CA-C	-5.00	110.79	116.54

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	62	0
1	B	1325	0	1364	57	0
1	C	1325	0	1364	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1325	0	1364	58	0
1	E	1325	0	1364	52	0
1	F	1325	0	1364	48	0
1	G	1325	0	1364	50	0
1	H	1325	0	1364	57	0
1	I	1325	0	1364	65	0
1	J	1325	0	1364	60	0
1	K	1325	0	1364	54	0
1	L	1325	0	1364	47	0
1	M	1325	0	1364	60	0
1	N	1325	0	1364	59	0
2	O	57	0	55	3	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	9	0
3	L	26	0	0	2	0
3	M	22	0	0	5	0
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	653	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 17.

All (653) 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:H:177:GLU:O	1:H:181:GLU:HG2	1.79	0.82
1:J:177:GLU:O	1:J:181:GLU:HG2	1.80	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:156:ARG:HD2	3:F:225:HOH:O	1.85	0.75
1:J:44:VAL:HG21	1:K:92:ILE:HD11	1.69	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:F:161:LEU:O	1:F:165:GLU:HG3	1.88	0.73
1:G:161:LEU:O	1:G: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:A:148:LYS:HD2	1:B:116:ASN:HD22	1.55	0.71
1:L:44:VAL:HG21	1:M:92:ILE:HD11	1.70	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
1:J:161:LEU:O	1:J:165:GLU:HG3	1.92	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:K:81:GLN:NE2	1:K:156:ARG:HH22	1.90	0.69
1:L:120:MET:N	3:L:584:HOH:O	2.23	0.69
1:F:81:GLN:NE2	1:F:156:ARG:HH22	1.91	0.69
1:M:81:GLN:NE2	1:M:156:ARG:HH22	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:161:LEU:O	1:N:165:GLU:HG3	1.92	0.69
1:B:70:ILE:HD11	1:B:124:PRO:HB3	1.75	0.68
1:D:161:LEU:O	1:D:165:GLU:HG3	1.93	0.68
1:J:162:GLU:HB2	3:J:222:HOH:O	1.93	0.68
1:M:44:VAL:HG21	1:N:92:ILE:HD11	1.75	0.68
1:E:70:ILE:HD11	1:E:124:PRO:HB3	1.74	0.68
1:E:120:MET:SD	3:E:227:HOH:O	2.50	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:70:ILE:HD11	1:N:124:PRO:HB3	1.76	0.66
1:N:144:LEU:HG	3:N:490:HOH:O	1.96	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:A:172:ASN:HD22	1:A:172:ASN:C	2.05	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
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:A:160:PRO:HG2	1:A:163:VAL:HG23	1.80	0.63
1:I:119:VAL:HG12	3:I:401:HOH:O	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:PRO:HG2	1:K:163:VAL:HG23	1.81	0.63
1:I:172:ASN:C	1:I:172:ASN:HD22	2.07	0.62
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:C:160:PRO:HG2	1:C:163:VAL:HG23	1.82	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:H:172:ASN:HD22	1:H:172:ASN:C	2.08	0.61
1:C:172:ASN:C	1:C:172:ASN:HD22	2.06	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:G:151:LYS:O	1:G:155:GLU:HG3	2.01	0.60
1:M:151:LYS:O	1:M: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:C:151:LYS:O	1:C:155:GLU:HG3	2.01	0.60
1:I:146:ARG:NH1	3:I:503:HOH:O	2.35	0.60
1:I:160:PRO:HG2	1:I:163:VAL:HG23	1.83	0.60
1:B:151:LYS:O	1:B:155:GLU:HG3	2.02	0.60
1:I:162:GLU:HB2	3:I:407:HOH:O	2.01	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:D:172:ASN:C	1:D:172:ASN:HD22	2.10	0.60
1:L:172:ASN:C	1:L:172:ASN:HD22	2.08	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:D:160:PRO:HG2	1:D:163:VAL:HG23	1.84	0.59
1:G:81:GLN:NE2	1:G:156:ARG:HH22	1.99	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
1:M:172:ASN:HD22	1:M:172:ASN:C	2.08	0.59
1:K:90:ILE:HD11	2:Z:6:ALA:HB1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:PRO:HG2	1:E:163:VAL:HG23	1.84	0.59
1:K:172:ASN:C	1:K:172:ASN:HD22	2.11	0.59
2:V:1:CXP:H82	2:V:7:MP8:HD	1.84	0.59
1:L:160:PRO:HG2	1:L:163:VAL:HG23	1.84	0.58
1:A:49:PHE:HE1	1:B:22:ARG:HH11	1.49	0.58
1:G:166:ARG:HD2	3:G:276:HOH:O	2.03	0.58
1:F:90:ILE:HD11	2:Q:6:ALA:HB1	1.84	0.58
1:G:172:ASN:C	1:G:172:ASN:HD22	2.11	0.58
1:H:74:MET:HE3	1:I:116:ASN:HB3	1.85	0.58
1:I:151:LYS:O	1:I:155:GLU:HG3	2.03	0.58
1:A:151:LYS:O	1:A:155:GLU:HG3	2.03	0.58
1:C:44:VAL:HG11	1:D:92:ILE:HD12	1.84	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:N:172:ASN:C	1:N:172:ASN:HD22	2.12	0.56
1:B:133:THR:H	1:J:123:GLN:HE22	1.53	0.56
1:F:151:LYS:O	1:F:155:GLU:HG3	2.06	0.56
1:I:35:ILE:HG22	3:I:395:HOH:O	2.04	0.56
1:N:151:LYS:O	1:N:155:GLU:HG3	2.06	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:123:GLN:HE22	1:I:133:THR:H	1.54	0.56
1:C:132:ALA:HB3	1:I:123:GLN:HE21	1.71	0.56
1:J:172:ASN:C	1:J:172:ASN:HD22	2.14	0.56
1:B:172:ASN:C	1:B:172:ASN:HD22	2.13	0.55
1:J:148:LYS:HD2	1:K:116:ASN:HD22	1.71	0.55
1:L:44:VAL:HG11	1:M:92:ILE:HD12	1.88	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:C:44:VAL:HG11	1:D:92:ILE:CD1	2.36	0.55
1:E:44:VAL:HG11	1:F:92:ILE:HD12	1.87	0.55
1:J:151:LYS:O	1:J:155:GLU:HG3	2.07	0.55
1:C:123:GLN:NE2	1:I:133:THR:H	2.05	0.55
1:A:70:ILE:HA	1:A:98:MET:HE3	1.87	0.55
1:F:44:VAL:HG11	1:G:92:ILE:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:ASP:OD1	1:I:39:VAL:HG23	2.06	0.55
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:E:172:ASN:C	1:E:172:ASN:HD22	2.14	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:A:116:ASN:CB	1:G:74:MET:HE3	2.38	0.54
1:C:50:LEU:HG	3:C:445:HOH:O	2.05	0.54
1:D:44:VAL:HG11	1:E:92:ILE:CD1	2.36	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:M:177:GLU:CD	1:M:177:GLU:H	2.15	0.54
1:L:177:GLU:CD	1:L:177:GLU:H	2.15	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:D:177:GLU:CD	1:D:177:GLU:H	2.15	0.53
1:H:160:PRO:HG2	1:H:163:VAL:CG2	2.38	0.53
1:M:124:PRO:HD2	1:M:146:ARG:HG3	1.90	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:F:172:ASN:C	1:F:172:ASN:HD22	2.15	0.53
1:B:170:ARG:HG2	3:K:351:HOH:O	2.09	0.53
1:I:124:PRO:HD2	1:I:146:ARG:HG3	1.90	0.53
1:C:177:GLU:H	1:C:177:GLU:CD	2.16	0.53
2:R:1:CXP:H82	2:R:7:MP8:HD	1.91	0.53
1:D:74:MET:HE3	1:E:116:ASN:CG	2.34	0.53
1:E:177:GLU:H	1:E:177:GLU:CD	2.16	0.53
1:J:124:PRO:HD2	1:J:146:ARG:HG3	1.90	0.53
1:J:177:GLU:H	1:J:177:GLU:CD	2.16	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:N:177:GLU:CD	1:N:177:GLU:H	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:MET:HE3	1:I:116:ASN:CB	2.39	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:H:28:ILE:HD11	2:W:7:MP8:HE	1.92	0.52
1:L:74:MET:HE3	1:M:116:ASN:CB	2.40	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:L:74:MET:HE3	1:M:116:ASN:HB3	1.91	0.52
1:A:116:ASN:HD22	1:G:148:LYS:HD2	1.75	0.52
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:177:GLU:CD	1:K:177:GLU:H	2.18	0.51
1:K:160:PRO:HG2	1:K:163:VAL:CG2	2.39	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:A:148:LYS:HD2	1:B:116:ASN:ND2	2.24	0.51
1:G:177:GLU:CD	1:G:177:GLU:H	2.19	0.51
1:H:22:ARG:NH1	1:N:49:PHE:CE1	2.77	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:H:177:GLU:CD	1:H:177:GLU:H	2.18	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:A:116:ASN:HB3	1:G:74:MET:HE3	1.92	0.50
1:B:90:ILE:HD12	1:B:90:ILE:N	2.26	0.50
1:H:165:GLU:HB3	3:H:217: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:L:70:ILE:HA	1:L:98:MET:HE3	1.92	0.50
1:M:151:LYS:HB3	3:M:308:HOH:O	2.11	0.50
1:C:36:ASP:OD1	1:C:39:VAL:HG23	2.11	0.50
1:M:160:PRO:HG2	1:M:163:VAL:CG2	2.42	0.50
1:A:74:MET:HE3	1:B:116:ASN:HB3	1.94	0.50
1:C:70:ILE:HA	1:C:98:MET:HE3	1.93	0.50
1:E:114:LEU:HD11	2:T:2:WFP:CZ	2.41	0.50
1:I:177:GLU:CD	1:I:177:GLU:H	2.20	0.50
1:N:75:ALA:HA	3:N:250:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ILE:HD11	2:U:6:ALA:HB1	1.93	0.50
1:H:78:ASP:HB3	1:I:114:LEU:HD13	1.93	0.50
1:H:148:LYS:HD2	1:I:116:ASN:HD22	1.76	0.50
1:B:177:GLU:CD	1:B:177:GLU:H	2.20	0.50
1:B:135:ILE:HD12	1:J:142:ILE:HD13	1.94	0.50
1:A:177:GLU:CD	1:A:177:GLU:H	2.19	0.49
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:C:74:MET:HE3	1:D:116:ASN:HB3	1.93	0.49
1:G:115:PRO:HD3	1:G:189:LEU:O	2.13	0.49
1:A:123:GLN:HG2	1:K:131:GLN:NE2	2.28	0.49
1:K:124:PRO:HD2	1:K:146:ARG:HG3	1.94	0.49
1:A:123:GLN:CD	1:K:131:GLN:HB3	2.38	0.49
1:M:74:MET:HE3	1:N:116:ASN:HB3	1.95	0.49
1:B:36:ASP:OD1	1:B:39:VAL:HG23	2.13	0.49
1:K:146:ARG:CZ	3:K:334:HOH:O	2.60	0.49
1:C:124:PRO:HD2	1:C:146:ARG:HG3	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:C:114:LEU:HD11	2:R:2:WFP:CZ	2.43	0.48
1:F:141:ARG:NE	1:G:118:GLU:OE1	2.46	0.48
1:H:133:THR:O	1:H:137:ILE:HG12	2.12	0.48
1:I:160:PRO:HG2	1:I:163:VAL:CG2	2.43	0.48
1:K:74:MET:HE2	1:K:148:LYS:HE3	1.94	0.48
1:J:156:ARG:HD2	3:J:413:HOH:O	2.12	0.48
1:D:148:LYS:HD2	1:E:116:ASN:HD22	1.78	0.48
1:M:148:LYS:HD2	1:N:116:ASN:ND2	2.25	0.48
1:D:36:ASP:OD1	1:D:39:VAL:HG23	2.13	0.48
1:A:116:ASN:CG	1:G:74:MET:HE3	2.38	0.48
1:B:70:ILE:HA	1:B:98:MET:HE3	1.96	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:D:160:PRO:HG2	1:D:163:VAL:CG2	2.42	0.48
1:F:177:GLU:CD	1:F:177:GLU:H	2.21	0.48
1:G:70:ILE:HA	1:G:98:MET:HE3	1.95	0.48
1:I:97:SER:HB3	3:I:239:HOH:O	2.13	0.48
1:A:22:ARG:HH11	1:G:49:PHE:HE1	1.61	0.48
1:D:90:ILE:N	1:D:90:ILE:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:PHE:HE1	1:F:22:ARG:NH1	2.11	0.48
1:I:70:ILE:HA	1:I:98:MET:HE3	1.96	0.48
1:M:62:TYR:CE1	1:M:90:ILE:HD13	2.48	0.48
1:M:148:LYS:CD	1:N:116:ASN:HD22	2.24	0.48
1:D:124:PRO:HD2	1:D:146:ARG:HG3	1.94	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:J:48:LEU:HD22	2:Z:1:CXP:O2	2.13	0.48
1:B:127:GLY:HA2	1:J:128:ALA:O	2.13	0.48
1:F:115:PRO:HD3	1:F:189:LEU:O	2.14	0.48
1:B:39:VAL:O	1:B:43:ILE:HG12	2.13	0.47
1:E:120:MET:CE	3:E:227:HOH:O	2.61	0.47
1:K:52:ALA:CB	2:O:1:CXP:H31	2.44	0.47
1:M:49:PHE:HE1	1:N:22:ARG:HH11	1.62	0.47
1:B:89:THR:C	1:B:90:ILE:HD12	2.39	0.47
1:B:148:LYS:HD2	1:C:116:ASN:HD22	1.78	0.47
1:E:44:VAL:HG11	1:F:92:ILE:CD1	2.44	0.47
1:E:70:ILE:HA	1:E:98:MET:HE3	1.96	0.47
1:H:116:ASN:ND2	1:N:148:LYS:HD2	2.29	0.47
1:J:70:ILE:HA	1:J:98:MET:HE3	1.96	0.47
1:L:62:TYR:CE1	1:L:90:ILE:HD13	2.50	0.47
1:H:115:PRO:HD3	1:H:189:LEU:O	2.14	0.47
1:A:36:ASP:OD1	1:A:39:VAL:HG23	2.14	0.47
1:D:74:MET:HE3	1:E:116:ASN:ND2	2.28	0.47
1:J:91:CYS:HB2	1:J:103:LEU:HD22	1.97	0.47
1:J:115:PRO:HD3	1:J:189:LEU:O	2.15	0.47
1:G:62:TYR:CE1	1:G:90:ILE:HD13	2.49	0.47
1:G:74:MET:HE2	1:G:148:LYS:HE3	1.97	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:B:133:THR:O	1:B:137:ILE:HG12	2.15	0.47
1:J:39:VAL:O	1:J:43:ILE:HG12	2.15	0.47
1:J:62:TYR:CE1	1:J:90:ILE:HD13	2.50	0.47
1:E:74:MET:HE2	1:E:148:LYS:HE3	1.96	0.47
1:L:44:VAL:HG11	1:M:92:ILE:CD1	2.45	0.46
1:H:90:ILE:HD11	2:W:6:ALA:HB1	1.96	0.46
1:L:148:LYS:HD2	1:M:116:ASN:ND2	2.29	0.46
1:N:90:ILE:N	1:N:90:ILE:HD12	2.30	0.46
1:C:90:ILE:N	1:C:90:ILE:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:112:TYR:CE2	2:Z:5:YCP:HD	2.50	0.46
1:L:160:PRO:HG2	1:L:163:VAL:CG2	2.44	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: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:C:91:CYS:HB2	1:C:103:LEU:HD22	1.98	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:N:89:THR:C	1:N:90:ILE:HD12	2.41	0.46
1:I:49:PHE:HE1	1:J:22:ARG:HH11	1.63	0.46
1:I:91:CYS:HB2	1:I:103:LEU:HD22	1.97	0.46
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: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:M:172:ASN:C	1:M:172:ASN:ND2	2.74	0.46
1:A:115:PRO:HD3	1:A:189:LEU:O	2.16	0.46
1:C:115:PRO:HD3	1:C:189:LEU:O	2.15	0.46
1:D:70:ILE:HA	1:D:98:MET:HE3	1.98	0.46
1:D:117:SER:HA	3:D:238:HOH:O	2.15	0.46
1:D:148:LYS:HD2	1:E:116:ASN:ND2	2.31	0.46
1:K:70:ILE:HA	1:K:98:MET:HE3	1.98	0.46
1:K:90:ILE:N	1:K:90:ILE:HD12	2.31	0.46
1:G:49:PHE:HA	2:P:1:CXP:H31	1.98	0.45
1:A:74:MET:HE3	1:B:116:ASN:CB	2.47	0.45
1:B:141:ARG:NE	1:C:118:GLU:OE1	2.48	0.45
1:F:141:ARG:HD3	3:F:315:HOH:O	2.15	0.45
1:H:44:VAL:HG11	1:I:92:ILE:HD12	1.99	0.45
1:H:153:LEU:HD23	1:H:153:LEU:HA	1.82	0.45
1:I:74:MET:HE3	1:J:116:ASN:CG	2.41	0.45
1:A:49:PHE:HE1	1:B:22:ARG:NH1	2.14	0.45
1:B:91:CYS:HB2	1:B:103:LEU:HD22	1.98	0.45
1:J:160:PRO:HG2	1:J:163:VAL:CG2	2.46	0.45
1:L:172:ASN:C	1:L:172:ASN:ND2	2.75	0.45
1:M:36:ASP:OD1	1:M:39:VAL:HG23	2.17	0.45
1:M:44:VAL:HG11	1:N:92:ILE:HD12	1.98	0.45
1:A:89:THR:C	1:A:90:ILE:HD12	2.42	0.45
1:D:115:PRO:HD3	1:D:189:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:ASP:OD1	1:F:39:VAL:HG23	2.16	0.45
1:F:74:MET:HE2	1:F:148:LYS:HE3	1.98	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:A:172:ASN:C	1:A:172:ASN:ND2	2.72	0.45
1:M:133:THR:HG21	1:N:170:ARG:HD3	1.99	0.45
1:E:133:THR:O	1:E:137:ILE:HG12	2.16	0.45
1:H:36:ASP:OD1	1:H:39:VAL:HG23	2.17	0.45
1:N:39:VAL:O	1:N:43:ILE:HG12	2.16	0.45
1:A:91:CYS:HB2	1:A:103:LEU:HD22	1.97	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:M:74:MET:HE3	1:N:116:ASN:CB	2.47	0.45
1:C:90:ILE:HD11	2:R:6:ALA:HB1	1.99	0.45
1:D:92:ILE:HG23	1:D:92:ILE:O	2.17	0.45
1:E:91:CYS:HB2	1:E:103:LEU:HD22	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:B:174:LYS:HG2	3:B:373:HOH:O	2.17	0.45
1:E:115:PRO:HD3	1:E:189:LEU:O	2.17	0.45
1:E:153:LEU:HD23	1:E:153:LEU:HA	1.86	0.45
1:L:48:LEU:HB3	2:X:1:CXP:H72	1.98	0.45
1:N:70:ILE:HA	1:N:98:MET:HE3	2.00	0.45
2:Y:1:CXP:H62	2:Y:1:CXP:H81	1.80	0.45
1:E:89:THR:C	1:E:90:ILE:HD12	2.42	0.44
1:G:133:THR:O	1:G:137:ILE:HG12	2.16	0.44
1:I:62:TYR:CE1	1:I:90:ILE:HD13	2.51	0.44
1:C:131:GLN:HA	1:I:125:LEU:HD23	1.99	0.44
1:I:114:LEU:HD23	1:I:189:LEU:HB2	1.98	0.44
1:K:62:TYR:CE1	1:K:90:ILE:HD13	2.52	0.44
1:L:133:THR:O	1:L:137:ILE:HG12	2.18	0.44
1:C:39:VAL:O	1:C:43:ILE:HG12	2.18	0.44
1:E:148:LYS:HD2	1:F:116:ASN:ND2	2.26	0.44
1:K:114:LEU:HD11	2:Z:2:WFP:CZ	2.47	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:F:131:GLN:NE2	1:M:123:GLN:HG2	2.31	0.44
1:G:39:VAL:O	1:G:43:ILE:HG12	2.17	0.44
1:L:90:ILE:HD11	2:O:6:ALA:HB1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:172:ASN:C	1:I:172:ASN:ND2	2.73	0.44
1:L:148:LYS:CD	1:M:116:ASN:HD22	2.30	0.44
1:C:142:ILE:HD13	1:I:135:ILE:HD12	1.99	0.44
1:D:35:ILE:HG22	3:D:457:HOH:O	2.17	0.44
1:D:172:ASN:C	1:D:172:ASN:ND2	2.76	0.44
1:F:39:VAL:O	1:F:43:ILE:HG12	2.18	0.44
1:H:70:ILE:HA	1:H:98:MET:HE3	1.99	0.44
1:L:74:MET:HE3	1:M:116:ASN:CG	2.43	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:N:115:PRO:HD3	1:N:189:LEU:O	2.18	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:A:133:THR:O	1:A:137:ILE:HG12	2.18	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:D:40:ALA:HB2	1:D:72:ALA:HB1	2.00	0.44
1:D:74:MET:HE2	1:D:148:LYS:HE3	2.00	0.44
1:H:89:THR:C	1:H:90:ILE:HD12	2.43	0.44
1:H:172:ASN:C	1:H:172:ASN:ND2	2.74	0.44
1:A:94:MET:HE1	1:A:118:GLU:HG2	2.00	0.43
1:A:114:LEU:HD23	1:A:189:LEU:HB2	2.00	0.43
1:D:114:LEU:HD23	1:D:189:LEU:HB2	2.00	0.43
1:G:114:LEU:HD23	1:G:189:LEU:HB2	2.00	0.43
1:G:172:ASN:C	1:G:172:ASN:ND2	2.76	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:142:ILE:HD13	1:K:135:ILE:HD12	2.00	0.43
1:C:133:THR:O	1:C:137:ILE:HG12	2.17	0.43
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:M:115:PRO:HD3	1:M:189:LEU:O	2.18	0.43
1:C:143:LEU:CD2	1:C:146:ARG:HH21	2.32	0.43
1:F:95:ALA:HB2	3:F:265:HOH:O	2.17	0.43
1:J:114:LEU:HD23	1:J:189:LEU:HB2	2.00	0.43
1:K:89:THR:C	1:K:90:ILE:HD12	2.44	0.43
1:L:91:CYS:HB2	1:L:103:LEU:HD22	2.00	0.43
1:A:116:ASN:ND2	1:G:148:LYS:HD2	2.34	0.43
1:A:143:LEU:CD2	1:A:146:ARG:HH21	2.32	0.43
1:I:115:PRO:HD3	1:I:189:LEU:O	2.19	0.43
1:F:126:GLY:C	1:M:135:ILE:HD11	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:PHE:HE1	1:J:22:ARG:NH1	2.16	0.43
1:L:94:MET:HE1	1:L:118:GLU:HG2	2.01	0.43
1:C:22:ARG:CZ	3:C:329:HOH:O	2.67	0.43
1:C:89:THR:C	1:C:90:ILE:HD12	2.44	0.43
1:I:141:ARG:NE	1:J:118:GLU:OE1	2.50	0.43
3:K:479:HOH:O	1:L:94:MET:HE3	2.19	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:I:74:MET:HE2	1:I:148:LYS:HE3	2.00	0.43
1:N:91:CYS:HB2	1:N:103:LEU:HD22	2.01	0.43
1:A:78:ASP:HB3	1:B:114:LEU:HD13	2.01	0.43
1:A:97:SER:HB3	3:A:244:HOH:O	2.19	0.43
1:K:39:VAL:O	1:K:43:ILE:HG12	2.19	0.43
1:M:143:LEU:CD2	1:M:146:ARG:HH21	2.32	0.43
1:E:90:ILE:HD12	1:E:90:ILE:N	2.33	0.43
1:K:115:PRO:HD3	1:K:189:LEU:O	2.19	0.43
1:D:70:ILE:HG12	1:D:98:MET:HE3	2.01	0.42
1:E:92:ILE:HG23	1:E:92:ILE:O	2.18	0.42
1:G:83:ILE:HB	1:G:85:PRO:HD2	2.01	0.42
1:J:55:PRO:HA	1:J:85:PRO:HG3	2.01	0.42
1:K:36:ASP:OD1	1:K:39:VAL:HG23	2.19	0.42
1:K:172:ASN:C	1:K:172:ASN:ND2	2.76	0.42
1:A:44:VAL:HG11	1:B:92:ILE:CD1	2.49	0.42
1:B:114:LEU:HD23	1:B:189:LEU:HB2	2.01	0.42
1:C:62:TYR:CE1	1:C:90:ILE:HD13	2.54	0.42
1:C:123:GLN:HE21	1:I:132:ALA:HB3	1.84	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:E:62:TYR:CE1	1:E:90:ILE:HD13	2.54	0.42
1:E:114:LEU:HD23	1:E:189:LEU:HB2	2.01	0.42
1:F:84:LYS:N	1:F:85:PRO:CD	2.82	0.42
1:G:36:ASP:OD1	1:G:39:VAL:HG23	2.18	0.42
1:G:84:LYS:N	1:G:84:LYS:HD2	2.35	0.42
1:H:114:LEU:HD23	1:H:189:LEU:HB2	2.01	0.42
1:K:133:THR:O	1:K:137:ILE:HG12	2.19	0.42
1:M:114:LEU:HD23	1:M:189:LEU:HB2	2.01	0.42
1:M:83:ILE:HB	1:M:85:PRO:HD2	2.00	0.42
1:N:181:GLU:HG2	1:N:181:GLU:H	1.71	0.42
1:E:40:ALA:HB2	1:E:72:ALA:HB1	2.01	0.42
1:L:39:VAL:O	1:L:43:ILE:HG12	2.19	0.42
1:N:84:LYS:HD2	1:N:84:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LEU:HD23	1:C:153:LEU:HA	1.83	0.42
1:F:70:ILE:HA	1:F:98:MET:HE3	2.02	0.42
1:F:133:THR:O	1:F:137:ILE:HG12	2.20	0.42
1:H:45:SER:HB3	1:I:19:ILE:HG13	2.01	0.42
1:I:35:ILE:CG2	3:I:395:HOH:O	2.65	0.42
1:I:55:PRO:HA	1:I:85:PRO:HG3	2.01	0.42
1:J:40:ALA:HB2	1:J:72:ALA:HB1	2.01	0.42
1:J:90:ILE:HD12	1:J:90:ILE:N	2.34	0.42
1:L:153:LEU:HD23	1:L:153:LEU:HA	1.82	0.42
1:C:114:LEU:HD23	1:C:189:LEU:HB2	2.01	0.42
1:D:70:ILE:HG12	1:D:98:MET:CE	2.48	0.42
1:D:89:THR:C	1:D:90:ILE:HD12	2.44	0.42
1:K:91:CYS:HB2	1:K:103:LEU:HD22	2.01	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:N	1:E:84:LYS:HD2	2.35	0.42
1:G:114:LEU:HD11	2:U:2:WFP:CZ	2.49	0.42
1:K:92:ILE:HG23	1:K:92:ILE:O	2.20	0.42
1:N:114:LEU:HD23	1:N:189:LEU:HB2	2.01	0.42
1:N:144:LEU:HD23	1:N:144:LEU:HA	1.94	0.42
1:C:25:LYS:HE2	3:C:333:HOH:O	2.20	0.42
1:D:126:GLY:C	1:H:135:ILE:HD11	2.45	0.42
1:H:45:SER:HB3	1:I:19:ILE:CG1	2.49	0.42
1:I:74:MET:HE3	1:J:116:ASN:CB	2.50	0.42
1:J:84:LYS:N	1:J:85:PRO:CD	2.83	0.42
1:C:84:LYS:N	1:C:85:PRO:CD	2.83	0.41
1:C:94:MET:HE1	1:C:118:GLU:HG2	2.02	0.41
1:D:39:VAL:O	1:D:43:ILE:HG12	2.20	0.41
1:D:84:LYS:HD2	1:D:84:LYS:N	2.35	0.41
1:F:172:ASN:C	1:F:172:ASN:ND2	2.78	0.41
1:G:84:LYS:N	1:G:85:PRO:CD	2.83	0.41
1:I:133:THR:O	1:I:137:ILE:HG12	2.20	0.41
1:L:62:TYR:OH	2:O:6:ALA:O	2.35	0.41
1:M:133:THR:HG21	1:N:170:ARG:CD	2.50	0.41
1:C:70:ILE:HG12	1:C:98:MET:CE	2.50	0.41
1:K:114:LEU:HD23	1:K:189:LEU:HB2	2.02	0.41
1:D:74:MET:HE3	1:E:116:ASN:CB	2.50	0.41
1:I:98:MET:HB2	3:I:239:HOH:O	2.19	0.41
1:I:114:LEU:HD11	2:V:2:WFP:CZ	2.50	0.41
1:J:89:THR:C	1:J:90:ILE:HD12	2.44	0.41
1:L:92:ILE:O	1:L:92:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:143:LEU:CD2	1:L:146:ARG:HH21	2.33	0.41
1:A:84:LYS:N	1:A:85:PRO:CD	2.83	0.41
1:A:90:ILE:HD12	1:A:90:ILE:N	2.34	0.41
1:D:124:PRO:HA	3:D:269:HOH:O	2.20	0.41
1:G:91:CYS:HB2	1:G:103:LEU:HD22	2.03	0.41
1:G:153:LEU:HD23	1:G:153:LEU:HA	1.87	0.41
1:L:114:LEU:HD23	1:L:189:LEU:HB2	2.02	0.41
1:N:94:MET:HE1	1:N:118:GLU:HG2	2.03	0.41
1:N:172:ASN:C	1:N:172:ASN:ND2	2.78	0.41
1:D:84:LYS:HD3	3:D:309:HOH:O	2.20	0.41
1:E:84:LYS:N	1:E:85:PRO:CD	2.84	0.41
1:K:143:LEU:CD2	1:K:146:ARG:HH21	2.33	0.41
1:M:94:MET:HE1	1:M:118:GLU:HG2	2.01	0.41
1:N:114:LEU:HD11	2:1:2:WFP:CZ	2.51	0.41
1:C:84:LYS:N	1:C:84:LYS:HD2	2.36	0.41
1:D:23:LEU:HD23	2:S:1:CXP:H51	2.02	0.41
1:H:55:PRO:HA	1:H:85:PRO:HG3	2.02	0.41
1:J:36:ASP:OD1	1:J:39:VAL:HG23	2.20	0.41
1:J:144:LEU:HD23	1:J:144:LEU:HA	1.95	0.41
1:J:172:ASN:C	1:J:172:ASN:ND2	2.78	0.41
1:K:81:GLN:HG3	3:K:232:HOH:O	2.21	0.41
1:M:90:ILE:HD11	2:X:6:ALA:HB1	2.02	0.41
1:N:62:TYR:CE1	1:N:90:ILE:HD13	2.56	0.41
1:A:123:GLN:NE2	1:K:133:THR:H	2.18	0.41
1:B:55:PRO:HA	1:B:85:PRO:HG3	2.03	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:J:74:MET:HE2	1:J:148:LYS:HE3	2.03	0.41
1:L:90:ILE:HD12	1:L:90:ILE:N	2.35	0.41
1:A:116:ASN:HD22	1:G:148:LYS:CD	2.34	0.41
1:C:172:ASN:C	1:C:172:ASN:ND2	2.73	0.41
1:H:84:LYS:HD2	1:H:84:LYS:N	2.35	0.41
1:J:133:THR:O	1:J:137:ILE:HG12	2.20	0.41
1:K:84:LYS:N	1:K:85:PRO:CD	2.83	0.41
1:L:89:THR:C	1:L:90:ILE:HD12	2.46	0.41
1:M:49:PHE:HE1	1:N:22:ARG:NH1	2.19	0.41
1:A:70:ILE:HG12	1:A:98:MET:CE	2.51	0.41
1:A:74:MET:HE2	1:A:148:LYS:HE3	2.03	0.41
1:B:84:LYS:N	1:B:85:PRO:CD	2.84	0.41
1:C:144:LEU:HD23	1:C:144:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ILE:HB	1:E:85:PRO:HD2	2.03	0.41
1:G:55:PRO:HA	1:G:85:PRO:HG3	2.03	0.41
1:H:40:ALA:HB2	1:H:72:ALA:HB1	2.03	0.41
1:I:92:ILE:HG23	1:I:92:ILE:O	2.20	0.41
1:J:94:MET:HE1	1:J:118:GLU:HG2	2.03	0.41
1:J:143:LEU:CD2	1:J:146:ARG:HH21	2.33	0.41
1:L:49:PHE:HE1	1:M:22:ARG:HH11	1.68	0.41
1:M:55:PRO:HA	1:M:85:PRO:HG3	2.02	0.41
1:M:70:ILE:HA	1:M:98:MET:HE3	2.02	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: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:D:123:GLN:HE21	1:H:132:ALA:HB3	1.85	0.41
1:E:55:PRO:HA	1:E:85:PRO:HG3	2.02	0.41
1:I:153:LEU:HD23	1:I:153:LEU:HA	1.85	0.41
1:J:92:ILE:O	1:J:92:ILE:HG23	2.21	0.41
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:M:92:ILE:HG23	1:M:92:ILE:O	2.21	0.40
1:C:70:ILE:HG12	1:C:98:MET:HE3	2.03	0.40
1:E:181:GLU:HG2	1:E:181:GLU:H	1.72	0.40
1:H:122:HIS:C	1:H:122:HIS:CD2	2.99	0.40
1:I:40:ALA:HB2	1:I:72:ALA:HB1	2.02	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:A:55:PRO:HA	1:A:85:PRO:HG3	2.03	0.40
1:B:74:MET:HE2	1:B:148:LYS:HE3	2.03	0.40
1:B:94:MET:HE1	1:B:118:GLU:HG2	2.04	0.40
1:C:181:GLU:HG2	1:C:181:GLU:H	1.70	0.40
1:D:84:LYS:N	1:D:85:PRO:CD	2.85	0.40
1:E:39:VAL:O	1:E:43:ILE:HG12	2.21	0.40
1:E:44:VAL:HG21	1:F:92:ILE:CD1	2.45	0.40
1:H:175:SER:OG	1:H:178:GLU:HG3	2.21	0.40
1:I:84:LYS:N	1:I:84:LYS:HD2	2.37	0.40
1:B:143:LEU:CD2	1:B:146:ARG:HH21	2.35	0.40
1:D:133:THR:H	1:H:123:GLN:NE2	2.18	0.40
1:H:90:ILE:HD12	1:H:90:ILE:N	2.37	0.40
1:H:116:ASN:CG	1:N:74:MET:HE3	2.47	0.40
1:M:45:SER:HB3	1:N:19:ILE:HG13	2.03	0.40
1:M:84:LYS:N	1:M:85:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:133:THR:CG2	1:N:170:ARG:HD3	2.51	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	136 (96%)	5 (4%)	32	59
1	B	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	C	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	D	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	E	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	F	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	G	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	H	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	I	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	J	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	K	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	L	141/165 (86%)	136 (96%)	5 (4%)	32	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	141/165 (86%)	136 (96%)	5 (4%)	32	59
1	N	141/165 (86%)	136 (96%)	5 (4%)	32	59
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
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%)	1932 (96%)	70 (4%)	32	59

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	92	ILE
1	A	97	SER
1	A	162	GLU
1	A	181	GLU
1	B	30	MET
1	B	92	ILE
1	B	97	SER
1	B	162	GLU
1	B	181	GLU
1	C	30	MET
1	C	92	ILE
1	C	97	SER
1	C	162	GLU
1	C	181	GLU

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Mol	Chain	Res	Type
1	D	30	MET
1	D	92	ILE
1	D	97	SER
1	D	162	GLU
1	D	181	GLU
1	E	30	MET
1	E	92	ILE
1	E	97	SER
1	E	162	GLU
1	E	181	GLU
1	F	30	MET
1	F	92	ILE
1	F	97	SER
1	F	162	GLU
1	F	181	GLU
1	G	30	MET
1	G	92	ILE
1	G	97	SER
1	G	162	GLU
1	G	181	GLU
1	H	30	MET
1	H	92	ILE
1	H	97	SER
1	H	162	GLU
1	H	181	GLU
1	I	30	MET
1	I	92	ILE
1	I	97	SER
1	I	162	GLU
1	I	181	GLU
1	J	30	MET
1	J	92	ILE
1	J	97	SER
1	J	162	GLU
1	J	181	GLU
1	K	30	MET
1	K	92	ILE
1	K	97	SER
1	K	162	GLU
1	K	181	GLU
1	L	30	MET
1	L	92	ILE

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Mol	Chain	Res	Type
1	L	97	SER
1	L	162	GLU
1	L	181	GLU
1	M	30	MET
1	M	92	ILE
1	M	97	SER
1	M	162	GLU
1	M	181	GLU
1	N	30	MET
1	N	92	ILE
1	N	97	SER
1	N	162	GLU
1	N	181	GLU

Sometimes 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

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Mol	Chain	Res	Type
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
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	YCP	T	5	2	6,8,9	1.37	1 (16%)	7,9,11	2.57	2 (28%)
2	WFP	O	2	2	12,13,14	4.35	7 (58%)	12,17,19	2.19	5 (41%)
2	WFP	O	2	2	12,13,14	4.03	7 (58%)	12,17,19	2.02	6 (50%)
2	WFP	Z	2	2	12,13,14	3.97	7 (58%)	12,17,19	2.06	6 (50%)
2	MP8	Y	7	2	6,8,9	0.76	0	3,10,12	1.43	0
2	MP8	1	7	2	6,8,9	0.75	0	3,10,12	1.26	0
2	WFP	R	2	2	12,13,14	4.17	7 (58%)	12,17,19	2.11	5 (41%)
2	YCP	O	5	2	6,8,9	1.58	1 (16%)	7,9,11	2.60	2 (28%)
2	YCP	1	5	2	6,8,9	1.43	1 (16%)	7,9,11	2.55	2 (28%)
2	MP8	O	7	2	6,8,9	0.70	0	3,10,12	1.46	0
2	MP8	Z	7	2	6,8,9	0.66	0	3,10,12	1.23	0
2	WFP	P	2	2	12,13,14	4.17	7 (58%)	12,17,19	2.07	5 (41%)
2	MP8	P	7	2	6,8,9	0.72	0	3,10,12	1.15	0
2	MP8	S	7	2	6,8,9	0.66	0	3,10,12	1.11	0
2	YCP	U	5	2	6,8,9	1.41	1 (16%)	7,9,11	2.53	2 (28%)
2	MP8	U	7	2	6,8,9	0.69	0	3,10,12	1.43	0
2	YCP	Z	5	2	6,8,9	1.49	2 (33%)	7,9,11	2.61	2 (28%)
2	MP8	W	7	2	6,8,9	0.76	0	3,10,12	1.45	0
2	YCP	P	5	2	6,8,9	1.43	1 (16%)	7,9,11	2.58	2 (28%)
2	YCP	S	5	2	6,8,9	1.47	1 (16%)	7,9,11	2.61	2 (28%)
2	WFP	U	2	2	12,13,14	4.23	6 (50%)	12,17,19	2.07	5 (41%)
2	MP8	X	7	2	6,8,9	0.66	0	3,10,12	1.38	0
2	MP8	R	7	2	6,8,9	0.72	0	3,10,12	1.22	0
2	WFP	Y	2	2	12,13,14	4.08	7 (58%)	12,17,19	2.06	5 (41%)
2	WFP	Q	2	2	12,13,14	4.05	7 (58%)	12,17,19	2.05	7 (58%)
2	MP8	Q	7	2	6,8,9	0.69	0	3,10,12	1.28	0
2	YCP	R	5	2	6,8,9	1.45	1 (16%)	7,9,11	2.61	2 (28%)
2	WFP	V	2	2	12,13,14	4.10	7 (58%)	12,17,19	2.08	5 (41%)
2	MP8	T	7	2	6,8,9	0.64	0	3,10,12	1.39	0
2	YCP	Y	5	2	6,8,9	1.42	1 (16%)	7,9,11	2.62	2 (28%)
2	MP8	V	7	2	6,8,9	0.69	0	3,10,12	1.07	0
2	WFP	W	2	2	12,13,14	3.96	6 (50%)	12,17,19	1.90	5 (41%)
2	MP8	O	7	2	6,8,9	0.59	0	3,10,12	1.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	YCP	Q	5	2	6,8,9	1.49	2 (33%)	7,9,11	2.69	2 (28%)
2	YCP	V	5	2	6,8,9	1.48	1 (16%)	7,9,11	2.62	2 (28%)
2	WFP	T	2	2	12,13,14	4.27	6 (50%)	12,17,19	2.01	6 (50%)
2	WFP	S	2	2	12,13,14	4.28	7 (58%)	12,17,19	2.16	5 (41%)
2	WFP	1	2	2	12,13,14	4.08	7 (58%)	12,17,19	2.09	5 (41%)
2	YCP	O	5	2	6,8,9	1.57	2 (33%)	7,9,11	2.57	2 (28%)
2	YCP	X	5	2	6,8,9	1.48	2 (33%)	7,9,11	2.68	2 (28%)
2	WFP	X	2	2	12,13,14	4.16	7 (58%)	12,17,19	2.03	5 (41%)
2	YCP	W	5	2	6,8,9	1.44	2 (33%)	7,9,11	2.61	2 (28%)

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	YCP	T	5	2	-	0/1/10/12	0/1/1/1
2	WFP	0	2	2	-	2/5/6/8	0/1/1/1
2	WFP	O	2	2	-	2/5/6/8	0/1/1/1
2	WFP	Z	2	2	-	2/5/6/8	0/1/1/1
2	MP8	Y	7	2	-	0/0/11/13	0/1/1/1
2	MP8	1	7	2	-	0/0/11/13	0/1/1/1
2	WFP	R	2	2	-	2/5/6/8	0/1/1/1
2	YCP	0	5	2	-	0/1/10/12	0/1/1/1
2	YCP	1	5	2	-	0/1/10/12	0/1/1/1
2	MP8	O	7	2	-	0/0/11/13	0/1/1/1
2	MP8	Z	7	2	-	0/0/11/13	0/1/1/1
2	WFP	P	2	2	-	2/5/6/8	0/1/1/1
2	MP8	P	7	2	-	0/0/11/13	0/1/1/1
2	MP8	S	7	2	-	0/0/11/13	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	YCP	Z	5	2	-	0/1/10/12	0/1/1/1
2	MP8	W	7	2	-	0/0/11/13	0/1/1/1
2	YCP	P	5	2	-	0/1/10/12	0/1/1/1
2	YCP	S	5	2	-	0/1/10/12	0/1/1/1
2	WFP	U	2	2	-	1/5/6/8	0/1/1/1
2	MP8	X	7	2	-	0/0/11/13	0/1/1/1
2	MP8	R	7	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WFP	Y	2	2	-	2/5/6/8	0/1/1/1
2	WFP	Q	2	2	-	2/5/6/8	0/1/1/1
2	MP8	Q	7	2	-	0/0/11/13	0/1/1/1
2	YCP	R	5	2	-	0/1/10/12	0/1/1/1
2	WFP	V	2	2	-	2/5/6/8	0/1/1/1
2	MP8	T	7	2	-	0/0/11/13	0/1/1/1
2	YCP	Y	5	2	-	0/1/10/12	0/1/1/1
2	MP8	V	7	2	-	0/0/11/13	0/1/1/1
2	WFP	W	2	2	-	1/5/6/8	0/1/1/1
2	MP8	0	7	2	-	0/0/11/13	0/1/1/1
2	YCP	Q	5	2	-	0/1/10/12	0/1/1/1
2	YCP	V	5	2	-	0/1/10/12	0/1/1/1
2	WFP	T	2	2	-	2/5/6/8	0/1/1/1
2	WFP	S	2	2	-	2/5/6/8	0/1/1/1
2	WFP	1	2	2	-	2/5/6/8	0/1/1/1
2	YCP	O	5	2	-	0/1/10/12	0/1/1/1
2	YCP	X	5	2	-	0/1/10/12	0/1/1/1
2	WFP	X	2	2	-	2/5/6/8	0/1/1/1
2	YCP	W	5	2	-	0/1/10/12	0/1/1/1

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	2	WFP	CZ-CE2	6.99	1.49	1.37
2	U	2	WFP	CD1-CG	6.82	1.50	1.39
2	S	2	WFP	CZ-CE2	6.77	1.48	1.37
2	U	2	WFP	CZ-CE2	6.73	1.48	1.37
2	0	2	WFP	CZ-CE2	6.68	1.48	1.37
2	T	2	WFP	CZ-CE2	6.66	1.48	1.37
2	T	2	WFP	CD1-CG	6.63	1.50	1.39
2	R	2	WFP	CZ-CE2	6.60	1.48	1.37
2	Y	2	WFP	CZ-CE2	6.55	1.48	1.37
2	0	2	WFP	CD2-CE2	6.54	1.48	1.37
2	S	2	WFP	CD1-CG	6.51	1.50	1.39
2	P	2	WFP	CD1-CG	6.49	1.50	1.39
2	Q	2	WFP	CD1-CG	6.46	1.50	1.39
2	S	2	WFP	CD2-CE2	6.45	1.48	1.37
2	V	2	WFP	CD1-CG	6.44	1.50	1.39
2	V	2	WFP	CZ-CE2	6.36	1.48	1.37
2	0	2	WFP	CD1-CG	6.35	1.50	1.39
2	O	2	WFP	CD2-CE2	6.34	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	2	WFP	CD1-CG	6.33	1.50	1.39
2	R	2	WFP	CD1-CG	6.31	1.50	1.39
2	W	2	WFP	CZ-CE2	6.30	1.48	1.37
2	T	2	WFP	CD2-CE2	6.30	1.48	1.37
2	1	2	WFP	CD1-CG	6.28	1.49	1.39
2	X	2	WFP	CZ-CE2	6.26	1.48	1.37
2	Z	2	WFP	CD2-CE2	6.25	1.48	1.37
2	Q	2	WFP	CZ-CE2	6.24	1.48	1.37
2	X	2	WFP	CD2-CE2	6.24	1.48	1.37
2	Z	2	WFP	CD1-CG	6.21	1.49	1.39
2	X	2	WFP	CD1-CG	6.21	1.49	1.39
2	1	2	WFP	CZ-CE2	6.21	1.48	1.37
2	Z	2	WFP	CZ-CE2	6.03	1.47	1.37
2	O	2	WFP	CZ-CE2	6.02	1.47	1.37
2	O	2	WFP	CD1-CG	6.02	1.49	1.39
2	W	2	WFP	CD1-CG	6.02	1.49	1.39
2	R	2	WFP	CD2-CE2	6.02	1.47	1.37
2	U	2	WFP	CD2-CE2	5.99	1.47	1.37
2	0	2	WFP	CZ-CE1	5.88	1.47	1.37
2	Q	2	WFP	CD2-CE2	5.84	1.47	1.37
2	W	2	WFP	CD2-CE2	5.83	1.47	1.37
2	1	2	WFP	CD2-CE2	5.77	1.47	1.37
2	V	2	WFP	CD2-CE2	5.62	1.47	1.37
2	S	2	WFP	CZ-CE1	5.62	1.47	1.37
2	U	2	WFP	CZ-CE1	5.56	1.46	1.37
2	Y	2	WFP	CD2-CE2	5.53	1.46	1.37
2	T	2	WFP	CZ-CE1	5.52	1.46	1.37
2	Y	2	WFP	CZ-CE1	5.52	1.46	1.37
2	P	2	WFP	CZ-CE1	5.50	1.46	1.37
2	T	2	WFP	CD2-CG	5.44	1.48	1.39
2	X	2	WFP	CD1-CE1	5.41	1.46	1.37
2	P	2	WFP	CD2-CE2	5.41	1.46	1.37
2	R	2	WFP	CZ-CE1	5.40	1.46	1.37
2	0	2	WFP	CD2-CG	5.39	1.48	1.39
2	1	2	WFP	CZ-CE1	5.36	1.46	1.37
2	V	2	WFP	CD2-CG	5.29	1.48	1.39
2	V	2	WFP	CZ-CE1	5.23	1.46	1.37
2	1	2	WFP	CD1-CE1	5.22	1.46	1.37
2	X	2	WFP	CD2-CG	5.19	1.48	1.39
2	Q	2	WFP	CZ-CE1	5.19	1.46	1.37
2	0	2	WFP	CD1-CE1	5.14	1.46	1.37
2	O	2	WFP	CZ-CE1	5.13	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	2	WFP	CD2-CG	5.11	1.47	1.39
2	S	2	WFP	CD2-CG	5.11	1.47	1.39
2	U	2	WFP	CD1-CE1	5.05	1.46	1.37
2	W	2	WFP	CZ-CE1	5.03	1.46	1.37
2	R	2	WFP	CD2-CG	5.03	1.47	1.39
2	P	2	WFP	CD1-CE1	5.01	1.46	1.37
2	X	2	WFP	CZ-CE1	5.01	1.46	1.37
2	S	2	WFP	CD1-CE1	4.98	1.45	1.37
2	O	2	WFP	CD2-CG	4.97	1.47	1.39
2	Y	2	WFP	CD1-CE1	4.87	1.45	1.37
2	W	2	WFP	CD2-CG	4.86	1.47	1.39
2	P	2	WFP	CD2-CG	4.86	1.47	1.39
2	R	2	WFP	CD1-CE1	4.85	1.45	1.37
2	Y	2	WFP	CD2-CG	4.80	1.47	1.39
2	Z	2	WFP	CD2-CG	4.78	1.47	1.39
2	1	2	WFP	CD2-CG	4.76	1.47	1.39
2	U	2	WFP	CD2-CG	4.73	1.47	1.39
2	V	2	WFP	CD1-CE1	4.69	1.45	1.37
2	O	2	WFP	CD1-CE1	4.59	1.45	1.37
2	T	2	WFP	CD1-CE1	4.57	1.45	1.37
2	Z	2	WFP	CZ-CE1	4.56	1.45	1.37
2	Z	2	WFP	CD1-CE1	4.55	1.45	1.37
2	Q	2	WFP	CD1-CE1	4.41	1.45	1.37
2	W	2	WFP	CD1-CE1	4.38	1.44	1.37
2	R	2	WFP	CB-CA	2.73	1.59	1.53
2	0	5	YCP	CG-CB	2.62	1.59	1.53
2	V	2	WFP	CB-CA	2.60	1.59	1.53
2	Z	2	WFP	CB-CA	2.55	1.59	1.53
2	X	2	WFP	CB-CA	2.43	1.58	1.53
2	0	2	WFP	CB-CA	2.41	1.58	1.53
2	P	2	WFP	CB-CA	2.41	1.58	1.53
2	O	5	YCP	CG-CB	2.35	1.59	1.53
2	Q	5	YCP	CG-CB	2.29	1.58	1.53
2	O	2	WFP	CB-CA	2.27	1.58	1.53
2	V	5	YCP	CG-CB	2.25	1.58	1.53
2	S	5	YCP	CG-CB	2.25	1.58	1.53
2	Q	2	WFP	CB-CA	2.21	1.58	1.53
2	1	2	WFP	CB-CA	2.21	1.58	1.53
2	Z	5	YCP	CG-CB	2.18	1.58	1.53
2	X	5	YCP	CG-CB	2.18	1.58	1.53
2	W	5	YCP	CG-CB	2.17	1.58	1.53
2	S	2	WFP	CB-CA	2.17	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	5	YCP	CG-CB	2.14	1.58	1.53
2	Y	2	WFP	CB-CA	2.13	1.58	1.53
2	Z	5	YCP	O-C	2.12	1.28	1.20
2	Y	5	YCP	CG-CB	2.12	1.58	1.53
2	1	5	YCP	CG-CB	2.11	1.58	1.53
2	U	5	YCP	CG-CB	2.11	1.58	1.53
2	P	5	YCP	O-C	2.11	1.28	1.20
2	X	5	YCP	O-C	2.10	1.28	1.20
2	R	5	YCP	CG-CB	2.10	1.58	1.53
2	O	5	YCP	O-C	2.10	1.27	1.20
2	Q	5	YCP	O-C	2.03	1.27	1.20
2	W	5	YCP	O-C	2.01	1.27	1.20

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	5	YCP	CD-CG-CB	6.03	123.82	111.42
2	Y	5	YCP	CD-CG-CB	6.01	123.77	111.42
2	Q	5	YCP	CD-CG-CB	6.01	123.77	111.42
2	W	5	YCP	CD-CG-CB	5.99	123.74	111.42
2	V	5	YCP	CD-CG-CB	5.98	123.72	111.42
2	T	5	YCP	CD-CG-CB	5.96	123.68	111.42
2	R	5	YCP	CD-CG-CB	5.94	123.63	111.42
2	0	5	YCP	CD-CG-CB	5.90	123.55	111.42
2	U	5	YCP	CD-CG-CB	5.89	123.53	111.42
2	P	5	YCP	CD-CG-CB	5.88	123.51	111.42
2	O	5	YCP	CD-CG-CB	5.88	123.50	111.42
2	S	5	YCP	CD-CG-CB	5.86	123.46	111.42
2	Z	5	YCP	CD-CG-CB	5.85	123.45	111.42
2	1	5	YCP	CD-CG-CB	5.83	123.41	111.42
2	1	2	WFP	CD1-CE1-CZ	-3.61	119.11	123.50
2	U	2	WFP	CD1-CE1-CZ	-3.59	119.13	123.50
2	P	2	WFP	CD1-CE1-CZ	-3.57	119.16	123.50
2	S	2	WFP	CD1-CE1-CZ	-3.46	119.30	123.50
2	0	2	WFP	CD1-CE1-CZ	-3.45	119.31	123.50
2	Y	2	WFP	CD1-CE1-CZ	-3.45	119.31	123.50
2	R	2	WFP	CD1-CE1-CZ	-3.44	119.32	123.50
2	V	2	WFP	CD1-CE1-CZ	-3.43	119.33	123.50
2	0	2	WFP	CE2-CZ-CE1	3.27	120.84	116.08
2	Q	2	WFP	CD1-CE1-CZ	-3.24	119.56	123.50
2	V	2	WFP	CE2-CZ-CE1	3.21	120.75	116.08
2	X	2	WFP	CD1-CE1-CZ	-3.19	119.62	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	2	WFP	CD1-CE1-CZ	-3.13	119.70	123.50
2	T	2	WFP	CD1-CE1-CZ	-3.13	119.70	123.50
2	R	2	WFP	CG-CD1-CE1	3.11	121.46	118.75
2	U	2	WFP	CE2-CZ-CE1	3.09	120.58	116.08
2	S	2	WFP	CE2-CZ-CE1	3.07	120.56	116.08
2	0	2	WFP	CD2-CE2-CZ	-3.07	119.77	123.50
2	Q	2	WFP	CE2-CZ-CE1	3.07	120.55	116.08
2	Q	5	YCP	CE-N-CA	3.07	118.68	111.75
2	Z	2	WFP	CG-CD1-CE1	3.03	121.40	118.75
2	O	2	WFP	CD1-CE1-CZ	-3.00	119.85	123.50
2	P	2	WFP	CE2-CZ-CE1	3.00	120.45	116.08
2	S	2	WFP	CG-CD1-CE1	2.99	121.36	118.75
2	1	2	WFP	CE2-CZ-CE1	2.99	120.43	116.08
2	T	2	WFP	CE2-CZ-CE1	2.97	120.41	116.08
2	X	2	WFP	CE2-CZ-CE1	2.96	120.40	116.08
2	O	2	WFP	CE2-CZ-CE1	2.95	120.38	116.08
2	R	2	WFP	CE2-CZ-CE1	2.95	120.38	116.08
2	U	2	WFP	F1-CE1-CD1	2.93	122.45	118.28
2	Z	2	WFP	CE2-CZ-CE1	2.93	120.35	116.08
2	Y	2	WFP	CE2-CZ-CE1	2.92	120.33	116.08
2	W	2	WFP	CD1-CE1-CZ	-2.89	119.99	123.50
2	X	5	YCP	CE-N-CA	2.89	118.27	111.75
2	P	5	YCP	CE-N-CA	2.88	118.25	111.75
2	1	2	WFP	CG-CD1-CE1	2.88	121.26	118.75
2	Y	5	YCP	CE-N-CA	2.82	118.12	111.75
2	S	5	YCP	CE-N-CA	2.81	118.11	111.75
2	1	2	WFP	F1-CE1-CD1	2.81	122.28	118.28
2	X	2	WFP	F1-CE1-CD1	2.79	122.24	118.28
2	Z	5	YCP	CE-N-CA	2.78	118.03	111.75
2	X	2	WFP	CG-CD1-CE1	2.78	121.17	118.75
2	V	5	YCP	CE-N-CA	2.78	118.02	111.75
2	0	2	WFP	CG-CD1-CE1	2.77	121.17	118.75
2	0	5	YCP	CE-N-CA	2.76	117.99	111.75
2	O	2	WFP	CD2-CE2-CZ	-2.74	120.17	123.50
2	Y	2	WFP	CG-CD1-CE1	2.74	121.14	118.75
2	S	2	WFP	CD2-CE2-CZ	-2.72	120.20	123.50
2	S	2	WFP	F1-CE1-CD1	2.71	122.14	118.28
2	W	2	WFP	CE2-CZ-CE1	2.71	120.03	116.08
2	V	2	WFP	F1-CE1-CD1	2.70	122.12	118.28
2	T	5	YCP	CE-N-CA	2.70	117.84	111.75
2	O	2	WFP	CG-CD1-CE1	2.69	121.10	118.75
2	1	5	YCP	CE-N-CA	2.69	117.82	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	2	WFP	CG-CD1-CE1	2.68	121.09	118.75
2	Z	2	WFP	F1-CE1-CD1	2.65	122.05	118.28
2	W	2	WFP	CG-CD1-CE1	2.62	121.04	118.75
2	R	2	WFP	F1-CE1-CD1	2.60	121.97	118.28
2	T	2	WFP	CG-CD1-CE1	2.60	121.02	118.75
2	W	5	YCP	CE-N-CA	2.59	117.60	111.75
2	V	2	WFP	CG-CD1-CE1	2.59	121.01	118.75
2	U	5	YCP	CE-N-CA	2.58	117.58	111.75
2	O	2	WFP	F1-CE1-CD1	2.58	121.95	118.28
2	P	2	WFP	CD2-CE2-CZ	-2.58	120.37	123.50
2	R	2	WFP	CD2-CE2-CZ	-2.57	120.37	123.50
2	T	2	WFP	F1-CE1-CD1	2.57	121.94	118.28
2	X	2	WFP	CD2-CE2-CZ	-2.55	120.41	123.50
2	Y	2	WFP	CD2-CE2-CZ	-2.54	120.41	123.50
2	Q	2	WFP	F1-CE1-CD1	2.54	121.89	118.28
2	O	5	YCP	CE-N-CA	2.54	117.48	111.75
2	Q	2	WFP	CG-CD1-CE1	2.54	120.96	118.75
2	Y	2	WFP	F1-CE1-CD1	2.52	121.87	118.28
2	W	2	WFP	CD2-CE2-CZ	-2.52	120.44	123.50
2	U	2	WFP	CG-CD1-CE1	2.50	120.93	118.75
2	V	2	WFP	CD2-CE2-CZ	-2.50	120.46	123.50
2	P	2	WFP	F1-CE1-CD1	2.49	121.81	118.28
2	T	2	WFP	CD2-CE2-CZ	-2.44	120.54	123.50
2	Z	2	WFP	CD2-CE2-CZ	-2.43	120.55	123.50
2	Q	2	WFP	CD2-CE2-CZ	-2.41	120.57	123.50
2	R	5	YCP	CE-N-CA	2.41	117.19	111.75
2	U	2	WFP	CD2-CE2-CZ	-2.37	120.62	123.50
2	W	2	WFP	F1-CE1-CD1	2.36	121.64	118.28
2	1	2	WFP	CD2-CE2-CZ	-2.35	120.65	123.50
2	Q	2	WFP	CB-CG-CD1	-2.22	116.62	120.43
2	O	2	WFP	CB-CG-CD2	2.12	124.06	120.43
2	T	2	WFP	CB-CG-CD1	-2.11	116.80	120.43
2	Z	2	WFP	CB-CG-CD2	2.11	124.06	120.43
2	Q	2	WFP	CB-CG-CD2	2.11	124.05	120.43
2	O	2	WFP	F1-CE1-CD1	2.02	121.15	118.28

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	2	WFP	C-CA-CB-CG
2	R	2	WFP	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	O	2	WFP	N-CA-CB-CG
2	Q	2	WFP	N-CA-CB-CG
2	T	2	WFP	N-CA-CB-CG
2	U	2	WFP	N-CA-CB-CG
2	W	2	WFP	N-CA-CB-CG
2	P	2	WFP	N-CA-CB-CG
2	Q	2	WFP	C-CA-CB-CG
2	R	2	WFP	N-CA-CB-CG
2	S	2	WFP	C-CA-CB-CG
2	S	2	WFP	N-CA-CB-CG
2	V	2	WFP	C-CA-CB-CG
2	V	2	WFP	N-CA-CB-CG
2	X	2	WFP	C-CA-CB-CG
2	X	2	WFP	N-CA-CB-CG
2	Y	2	WFP	C-CA-CB-CG
2	Y	2	WFP	N-CA-CB-CG
2	Z	2	WFP	C-CA-CB-CG
2	Z	2	WFP	N-CA-CB-CG
2	0	2	WFP	C-CA-CB-CG
2	0	2	WFP	N-CA-CB-CG
2	1	2	WFP	C-CA-CB-CG
2	1	2	WFP	N-CA-CB-CG
2	O	2	WFP	C-CA-CB-CG
2	T	2	WFP	C-CA-CB-CG

There are no ring outliers.

14 monomers are involved in 14 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	2	WFP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	174/199 (87%)	0.97	19 (10%) 10 8	14, 30, 52, 74	0
1	B	174/199 (87%)	0.95	18 (10%) 12 9	15, 31, 52, 73	0
1	C	174/199 (87%)	0.99	19 (10%) 10 8	14, 30, 52, 73	0
1	D	174/199 (87%)	0.79	12 (6%) 23 18	14, 30, 53, 73	0
1	E	174/199 (87%)	1.06	24 (13%) 6 5	14, 30, 52, 73	0
1	F	174/199 (87%)	0.89	14 (8%) 18 14	15, 31, 52, 74	0
1	G	174/199 (87%)	0.71	16 (9%) 14 11	15, 30, 52, 73	0
1	H	174/199 (87%)	1.17	28 (16%) 4 3	15, 30, 52, 72	0
1	I	174/199 (87%)	0.79	15 (8%) 16 12	15, 30, 52, 74	0
1	J	174/199 (87%)	0.77	15 (8%) 16 12	13, 30, 53, 73	0
1	K	174/199 (87%)	1.03	23 (13%) 7 5	15, 30, 52, 73	0
1	L	174/199 (87%)	0.74	13 (7%) 20 16	15, 30, 52, 73	0
1	M	174/199 (87%)	0.98	23 (13%) 7 5	12, 30, 53, 73	0
1	N	174/199 (87%)	0.92	22 (12%) 8 6	13, 31, 52, 72	0
2	O	3/7 (42%)	1.24	0 100 100	45, 45, 47, 48	0
2	1	3/7 (42%)	1.80	2 (66%) 0 0	44, 44, 49, 49	0
2	O	3/7 (42%)	1.37	1 (33%) 1 1	48, 48, 51, 53	0
2	P	3/7 (42%)	0.99	0 100 100	41, 41, 42, 45	0
2	Q	3/7 (42%)	2.09	2 (66%) 0 0	42, 42, 44, 47	0
2	R	3/7 (42%)	1.94	1 (33%) 1 1	52, 52, 53, 55	0
2	S	3/7 (42%)	2.27	2 (66%) 0 0	40, 40, 43, 45	0
2	T	3/7 (42%)	1.30	1 (33%) 1 1	44, 44, 46, 46	0
2	U	3/7 (42%)	0.65	0 100 100	34, 34, 36, 38	0
2	V	3/7 (42%)	1.55	1 (33%) 1 1	44, 44, 46, 47	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	3/7 (42%)	1.43	1 (33%) 1 1	41, 41, 42, 43	0
2	X	3/7 (42%)	1.79	2 (66%) 0 0	46, 46, 47, 48	0
2	Y	3/7 (42%)	0.94	0 100 100	40, 40, 41, 43	0
2	Z	3/7 (42%)	1.27	1 (33%) 1 1	37, 37, 39, 47	0
All	All	2478/2884 (85%)	0.92	275 (11%) 10 8	12, 30, 53, 74	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	GLU	6.7
1	H	162	GLU	6.3
1	I	191	HIS	6.2
1	H	191	HIS	5.9
1	M	191	HIS	5.7
1	C	162	GLU	5.6
1	D	191	HIS	5.4
1	M	165	GLU	5.3
1	J	191	HIS	5.3
1	M	162	GLU	5.3
1	H	165	GLU	4.9
1	D	19	ILE	4.8
1	F	129	GLN	4.5
1	H	22	ARG	4.5
1	E	191	HIS	4.4
1	I	20	TYR	4.1
1	N	162	GLU	4.1
1	G	19	ILE	4.1
1	C	191	HIS	4.1
1	E	21	SER	4.1
1	F	20	TYR	4.1
1	A	21	SER	4.1
1	A	165	GLU	4.0
1	E	177	GLU	3.9
1	G	191	HIS	3.9
1	M	18	ASP	3.9
1	N	191	HIS	3.8
1	I	21	SER	3.8
1	A	162	GLU	3.7
1	C	190	THR	3.7
1	L	191	HIS	3.7
1	K	162	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	129	GLN	3.7
1	L	18	ASP	3.7
1	M	181	GLU	3.6
1	M	19	ILE	3.6
1	E	38	ASN	3.6
2	S	4	PRO	3.5
1	B	162	GLU	3.5
1	F	162	GLU	3.5
1	E	18	ASP	3.5
1	A	56	GLU	3.5
1	F	155	GLU	3.5
1	G	177	GLU	3.4
1	F	191	HIS	3.4
1	J	162	GLU	3.4
1	K	191	HIS	3.4
1	K	129	GLN	3.4
1	H	92	ILE	3.4
1	L	21	SER	3.4
1	L	19	ILE	3.3
1	A	181	GLU	3.3
1	G	162	GLU	3.3
1	E	19	ILE	3.3
1	B	190	THR	3.2
1	B	191	HIS	3.2
1	A	155	GLU	3.2
2	Z	6	ALA	3.2
1	C	161	LEU	3.2
1	B	21	SER	3.2
1	K	19	ILE	3.2
1	H	161	LEU	3.1
1	I	19	ILE	3.1
1	J	18	ASP	3.1
1	N	129	GLN	3.1
1	I	18	ASP	3.0
1	M	22	ARG	3.0
1	H	187	LYS	3.0
1	L	190	THR	3.0
1	E	162	GLU	3.0
1	N	95	ALA	3.0
2	Q	6	ALA	3.0
1	J	21	SER	3.0
1	B	108	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	163	VAL	2.9
1	B	84	LYS	2.9
1	D	162	GLU	2.9
1	N	56	GLU	2.9
1	N	181	GLU	2.9
1	H	20	TYR	2.9
1	J	190	THR	2.9
1	H	190	THR	2.9
1	M	190	THR	2.9
1	B	177	GLU	2.9
1	A	190	THR	2.9
1	F	181	GLU	2.8
1	C	160	PRO	2.8
1	F	19	ILE	2.8
1	G	147	ASP	2.8
1	F	21	SER	2.8
1	B	157	THR	2.8
1	L	177	GLU	2.8
1	A	187	LYS	2.8
1	K	84	LYS	2.8
1	H	177	GLU	2.8
1	L	56	GLU	2.8
1	N	21	SER	2.8
1	D	38	ASN	2.8
1	A	18	ASP	2.8
1	B	129	GLN	2.7
1	B	19	ILE	2.7
1	J	177	GLU	2.7
1	K	181	GLU	2.7
2	R	6	ALA	2.7
1	N	22	ARG	2.7
1	N	166	ARG	2.7
1	C	19	ILE	2.7
1	J	19	ILE	2.7
1	M	161	LEU	2.7
1	M	21	SER	2.7
1	A	191	HIS	2.7
1	C	181	GLU	2.7
1	D	181	GLU	2.7
1	G	22	ARG	2.7
1	L	147	ASP	2.7
1	E	45	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	53	GLU	2.7
1	G	190	THR	2.7
1	I	84	LYS	2.7
1	N	18	ASP	2.7
1	M	129	GLN	2.6
1	M	20	TYR	2.6
1	A	69	SER	2.6
1	E	40	ALA	2.6
2	V	4	PRO	2.6
1	E	147	ASP	2.6
1	G	129	GLN	2.6
1	A	19	ILE	2.6
1	E	20	TYR	2.6
1	J	155	GLU	2.6
1	K	155	GLU	2.6
1	C	18	ASP	2.6
1	K	18	ASP	2.6
1	J	20	TYR	2.6
1	F	56	GLU	2.6
1	C	54	ASP	2.6
1	G	53	GLU	2.6
1	H	55	PRO	2.6
1	N	147	ASP	2.5
1	C	187	LYS	2.5
1	L	129	GLN	2.5
1	C	147	ASP	2.5
1	L	22	ARG	2.5
1	J	163	VAL	2.5
1	D	129	GLN	2.5
1	B	22	ARG	2.5
1	F	18	ASP	2.5
1	G	166	ARG	2.5
1	H	19	ILE	2.5
1	M	53	GLU	2.5
1	N	20	TYR	2.5
1	H	160	PRO	2.5
1	N	133	THR	2.5
1	N	23	LEU	2.5
1	G	181	GLU	2.5
1	J	53	GLU	2.5
1	K	45	SER	2.4
1	C	56	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	181	GLU	2.4
1	E	126	GLY	2.4
1	B	20	TYR	2.4
1	B	112	TYR	2.4
1	A	129	GLN	2.4
1	I	190	THR	2.4
1	D	147	ASP	2.4
1	F	147	ASP	2.4
1	M	84	LYS	2.4
1	B	156	ARG	2.4
1	M	146	ARG	2.4
2	T	6	ALA	2.4
1	N	190	THR	2.4
1	E	155	GLU	2.4
1	I	162	GLU	2.4
1	J	158	GLY	2.4
1	A	188	ILE	2.4
1	E	190	THR	2.4
1	K	53	GLU	2.4
1	M	38	ASN	2.3
1	H	181	GLU	2.3
1	I	181	GLU	2.3
1	K	51	ALA	2.3
1	A	59	ILE	2.3
1	A	20	TYR	2.3
1	G	57	LYS	2.3
1	N	134	GLU	2.3
1	H	18	ASP	2.3
1	E	84	LYS	2.3
1	M	57	LYS	2.3
1	H	69	SER	2.3
1	C	22	ARG	2.3
2	Q	4	PRO	2.3
1	K	32	GLY	2.3
2	X	6	ALA	2.3
1	L	20	TYR	2.3
1	L	162	GLU	2.3
1	H	146	ARG	2.3
1	J	36	ASP	2.3
1	H	131	GLN	2.3
1	H	75	ALA	2.2
1	I	51	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	1	6	ALA	2.2
1	B	107	GLU	2.2
1	I	38	ASN	2.2
1	D	55	PRO	2.2
1	A	161	LEU	2.2
1	E	23	LEU	2.2
1	B	51	ALA	2.2
1	N	188	ILE	2.2
1	D	53	GLU	2.2
1	H	79	THR	2.2
1	K	20	TYR	2.2
1	G	23	LEU	2.2
1	D	187	LYS	2.2
1	E	43	ILE	2.2
1	H	188	ILE	2.2
1	G	56	GLU	2.2
1	I	165	GLU	2.2
1	A	22	ARG	2.2
1	C	146	ARG	2.2
1	N	38	ASN	2.2
2	X	4	PRO	2.2
1	F	117	SER	2.2
1	G	18	ASP	2.2
1	H	21	SER	2.2
1	K	25	LYS	2.2
1	H	119	VAL	2.2
1	K	92	ILE	2.2
1	N	19	ILE	2.2
1	K	58	GLU	2.2
1	D	190	THR	2.2
1	G	146	ARG	2.2
2	1	4	PRO	2.2
1	E	92	ILE	2.2
1	K	113	ALA	2.1
2	W	6	ALA	2.1
1	J	55	PRO	2.1
1	C	129	GLN	2.1
1	E	144	LEU	2.1
1	M	132	ALA	2.1
2	S	6	ALA	2.1
1	M	56	GLU	2.1
1	E	22	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	22	ARG	2.1
1	H	166	ARG	2.1
1	E	55	PRO	2.1
1	H	94	MET	2.1
1	H	189	LEU	2.1
1	A	183	GLY	2.1
1	N	165	GLU	2.1
1	D	130	GLY	2.1
1	L	163	VAL	2.1
1	M	188	ILE	2.1
1	K	131	GLN	2.1
1	H	23	LEU	2.1
1	B	38	ASN	2.1
1	C	35	ILE	2.1
1	B	176	ALA	2.0
1	F	128	ALA	2.0
1	M	128	ALA	2.0
1	M	155	GLU	2.0
1	J	84	LYS	2.0
1	K	190	THR	2.0
1	E	30	MET	2.0
1	M	55	PRO	2.0
2	O	4	PRO	2.0
1	N	144	LEU	2.0
1	I	166	ARG	2.0
1	K	22	ARG	2.0
1	H	155	GLU	2.0
1	C	84	LYS	2.0
1	K	57	LYS	2.0
1	K	154	ALA	2.0
1	K	69	SER	2.0
1	I	92	ILE	2.0
1	N	156	ARG	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	YCP	S	5	8/9	0.70	0.18	41,42,42,42	0
2	YCP	O	5	8/9	0.76	0.23	45,47,48,48	0
2	YCP	O	5	8/9	0.77	0.21	53,53,53,54	0
2	YCP	W	5	8/9	0.79	0.18	43,44,44,46	0
2	YCP	Q	5	8/9	0.80	0.17	44,44,46,47	0
2	MP8	X	7	8/9	0.81	0.20	47,48,49,49	0
2	YCP	Y	5	8/9	0.81	0.19	42,43,44,47	0
2	MP8	P	7	8/9	0.81	0.17	42,43,43,44	0
2	MP8	Z	7	8/9	0.82	0.18	42,43,45,45	0
2	YCP	V	5	8/9	0.82	0.17	47,47,47,50	0
2	MP8	V	7	8/9	0.82	0.20	44,45,46,46	0
2	MP8	S	7	8/9	0.82	0.16	40,41,42,42	0
2	YCP	R	5	8/9	0.82	0.20	53,53,53,54	0
2	WFP	O	2	13/14	0.83	0.17	35,37,43,43	0
2	YCP	P	5	8/9	0.83	0.17	43,44,45,45	0
2	MP8	O	7	8/9	0.83	0.19	43,44,47,50	0
2	WFP	Q	2	13/14	0.84	0.15	37,38,42,43	0
2	WFP	Z	2	13/14	0.84	0.15	37,39,42,43	0
2	MP8	Q	7	8/9	0.84	0.15	39,40,41,41	0
2	YCP	Z	5	8/9	0.84	0.12	39,41,44,45	0
2	YCP	T	5	8/9	0.84	0.16	45,45,46,47	0
2	WFP	1	2	13/14	0.85	0.17	34,35,40,41	0
2	WFP	V	2	13/14	0.85	0.15	35,36,45,47	0
2	WFP	S	2	13/14	0.85	0.17	42,44,45,45	0
2	MP8	O	7	8/9	0.85	0.17	50,50,51,51	0
2	YCP	1	5	8/9	0.85	0.16	50,52,52,52	0
2	WFP	U	2	13/14	0.86	0.12	28,30,34,37	0
2	MP8	R	7	8/9	0.86	0.18	53,55,56,57	0
2	YCP	U	5	8/9	0.86	0.16	34,36,37,37	0
2	MP8	1	7	8/9	0.87	0.16	48,50,50,51	0
2	WFP	T	2	13/14	0.87	0.12	29,33,42,43	0
2	WFP	R	2	13/14	0.88	0.15	44,45,49,50	0
2	MP8	Y	7	8/9	0.88	0.15	40,43,45,46	0
2	MP8	U	7	8/9	0.88	0.14	29,30,32,33	0
2	WFP	W	2	13/14	0.88	0.12	33,36,42,43	0
2	WFP	P	2	13/14	0.89	0.12	32,33,37,38	0
2	WFP	X	2	13/14	0.89	0.14	41,43,45,45	0
2	WFP	Y	2	13/14	0.90	0.11	20,24,37,39	0
2	MP8	T	7	8/9	0.90	0.15	43,43,44,44	0
2	WFP	O	2	13/14	0.90	0.13	31,33,42,42	0
2	YCP	X	5	8/9	0.90	0.14	46,46,46,46	0
2	MP8	W	7	8/9	0.91	0.10	36,36,38,38	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.