Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:17 AM GMT

PDB ID	:	3HLN
Title	:	Crystal structure of ClpP A153C mutant with inter-heptamer disulfide bonds
Authors	:	Kimber, M.S.; Yu, A.Y.H.; Borg, M.; Chan, H.S.; Houry, W.A.
Deposited on	:	2009-05-27
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

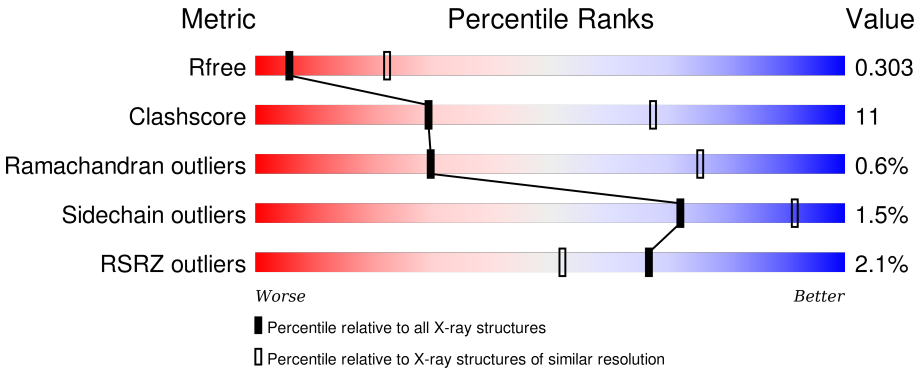
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	1	193	67% 17% • 16%
1	2	193	2% 65% 18% • 16%
1	A	193	3% 62% 20% • 16%
1	B	193	2% 64% 19% • 16%
1	C	193	64% 19% • 16%

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Mol	Chain	Length	Quality of chain
1	D	193	63% 20% 15%
1	E	193	68% 15% 16%
1	F	193	65% 21% 14%
1	G	193	67% 16% 16%
1	H	193	64% 21% 15%
1	I	193	62% 22% 16%
1	J	193	69% 15% 16%
1	K	193	65% 18% 17%
1	L	193	59% 25% 16%
1	M	193	64% 19% 16%
1	N	193	61% 22% 16%
1	O	193	64% 21% 14%
1	P	193	62% 22% 16%
1	Q	193	64% 19% 16%
1	R	193	65% 19% 16%
1	S	193	61% 23% 16%
1	T	193	61% 22% 17%
1	U	193	64% 19% 16%
1	V	193	69% 16% 16%
1	W	193	59% 23% 17%
1	X	193	59% 23% 17%
1	Y	193	67% 17% 16%
1	Z	193	64% 22% 15%

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	CA	Z	215	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35844 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	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	B	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	C	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	D	165	Total	C	N	O	S	0	0	0
			1294	816	225	241	12			
1	E	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	F	166	Total	C	N	O	S	0	0	0
			1308	824	226	246	12			
1	G	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	H	164	Total	C	N	O	S	0	0	0
			1292	814	224	242	12			
1	I	163	Total	C	N	O	S	0	0	0
			1282	808	223	239	12			
1	J	163	Total	C	N	O	S	0	0	0
			1282	808	223	239	12			
1	K	161	Total	C	N	O	S	0	0	0
			1265	797	219	237	12			
1	L	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	M	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	N	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	O	166	Total	C	N	O	S	0	0	0
			1307	825	226	244	12			
1	P	163	Total	C	N	O	S	0	0	0
			1282	808	223	239	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	R	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	S	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	T	161	Total	C	N	O	S	0	0	0
			1265	797	219	237	12			
1	U	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			
1	V	163	Total	C	N	O	S	0	0	0
			1283	809	223	239	12			
1	W	161	Total	C	N	O	S	0	0	0
			1265	797	219	237	12			
1	X	161	Total	C	N	O	S	0	0	0
			1266	798	220	236	12			
1	Y	163	Total	C	N	O	S	0	0	0
			1283	809	223	239	12			
1	Z	165	Total	C	N	O	S	0	0	0
			1299	819	225	243	12			
1	1	163	Total	C	N	O	S	0	0	0
			1283	809	223	239	12			
1	2	162	Total	C	N	O	S	0	0	0
			1275	803	222	238	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	CYS	ALA	ENGINEERED	UNP P0A6G7
B	139	CYS	ALA	ENGINEERED	UNP P0A6G7
C	139	CYS	ALA	ENGINEERED	UNP P0A6G7
D	139	CYS	ALA	ENGINEERED	UNP P0A6G7
E	139	CYS	ALA	ENGINEERED	UNP P0A6G7
F	139	CYS	ALA	ENGINEERED	UNP P0A6G7
G	139	CYS	ALA	ENGINEERED	UNP P0A6G7
H	139	CYS	ALA	ENGINEERED	UNP P0A6G7
I	139	CYS	ALA	ENGINEERED	UNP P0A6G7
J	139	CYS	ALA	ENGINEERED	UNP P0A6G7
K	139	CYS	ALA	ENGINEERED	UNP P0A6G7
L	139	CYS	ALA	ENGINEERED	UNP P0A6G7
M	139	CYS	ALA	ENGINEERED	UNP P0A6G7
N	139	CYS	ALA	ENGINEERED	UNP P0A6G7
O	139	CYS	ALA	ENGINEERED	UNP P0A6G7

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Chain	Residue	Modelled	Actual	Comment	Reference
P	139	CYS	ALA	ENGINEERED	UNP P0A6G7
Q	139	CYS	ALA	ENGINEERED	UNP P0A6G7
R	139	CYS	ALA	ENGINEERED	UNP P0A6G7
S	139	CYS	ALA	ENGINEERED	UNP P0A6G7
T	139	CYS	ALA	ENGINEERED	UNP P0A6G7
U	139	CYS	ALA	ENGINEERED	UNP P0A6G7
V	139	CYS	ALA	ENGINEERED	UNP P0A6G7
W	139	CYS	ALA	ENGINEERED	UNP P0A6G7
X	139	CYS	ALA	ENGINEERED	UNP P0A6G7
Y	139	CYS	ALA	ENGINEERED	UNP P0A6G7
Z	139	CYS	ALA	ENGINEERED	UNP P0A6G7
1	139	CYS	ALA	ENGINEERED	UNP P0A6G7
2	139	CYS	ALA	ENGINEERED	UNP P0A6G7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

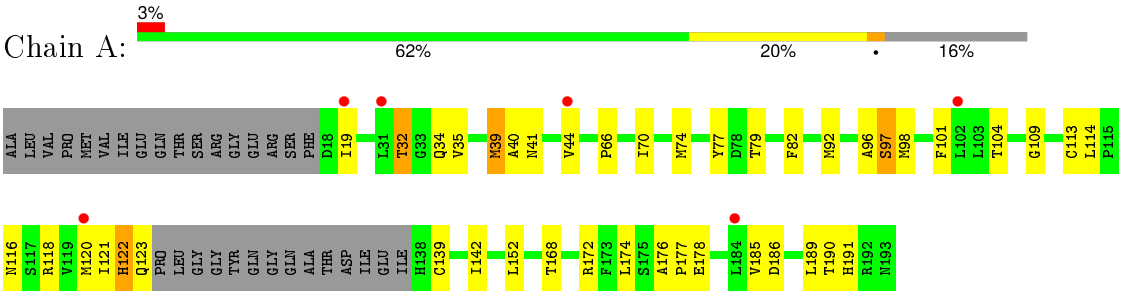
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	3	Total Ca 3 3	0	0
2	1	1	Total Ca 1 1	0	0
2	E	2	Total Ca 2 2	0	0
2	I	2	Total Ca 2 2	0	0
2	V	1	Total Ca 1 1	0	0
2	Z	1	Total Ca 1 1	0	0
2	T	1	Total Ca 1 1	0	0
2	2	1	Total Ca 1 1	0	0
2	M	1	Total Ca 1 1	0	0

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.

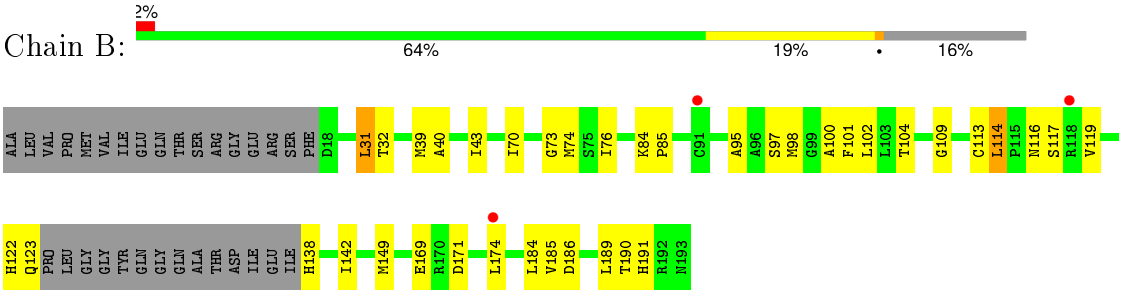
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



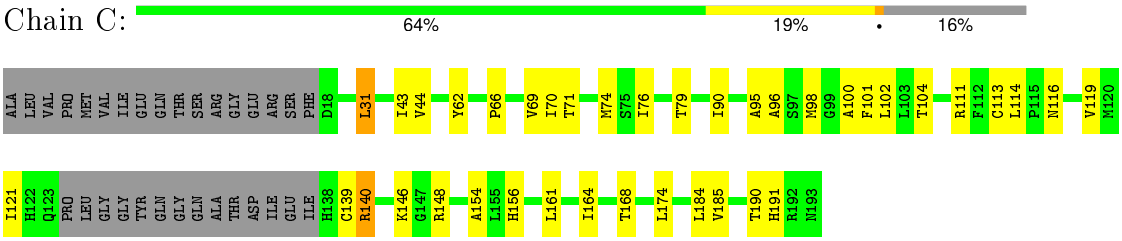
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



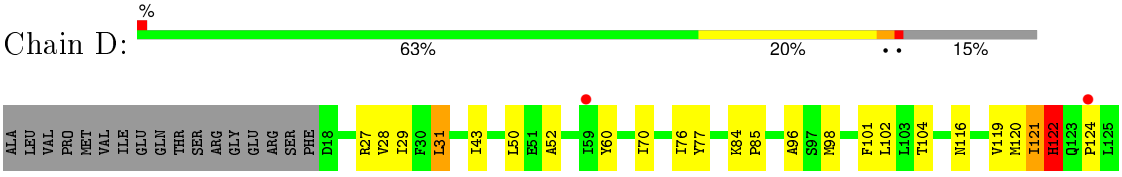
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



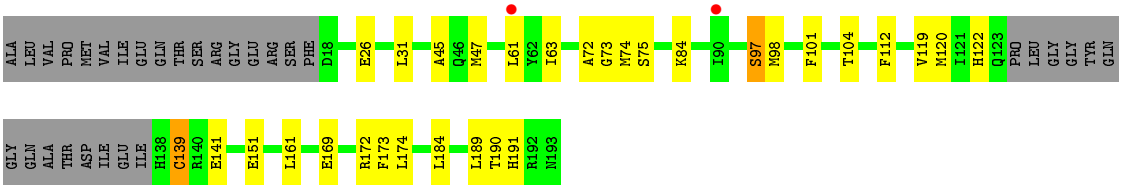
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



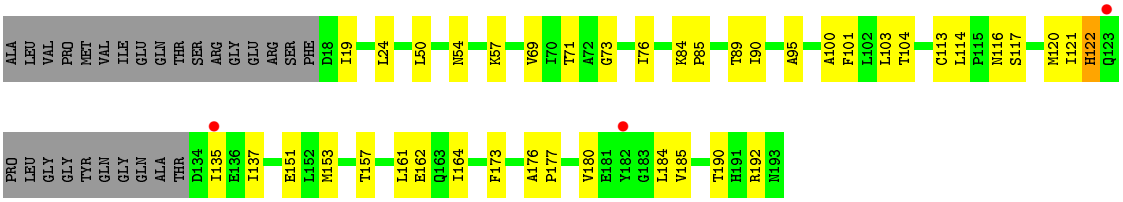
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



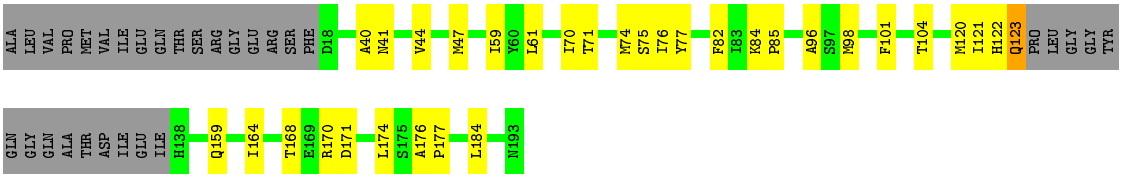
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



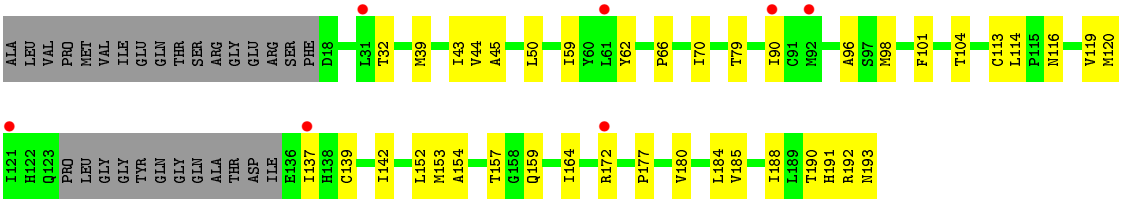
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



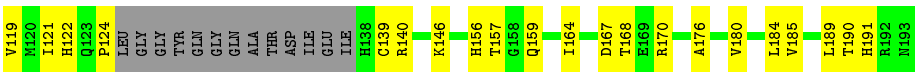
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



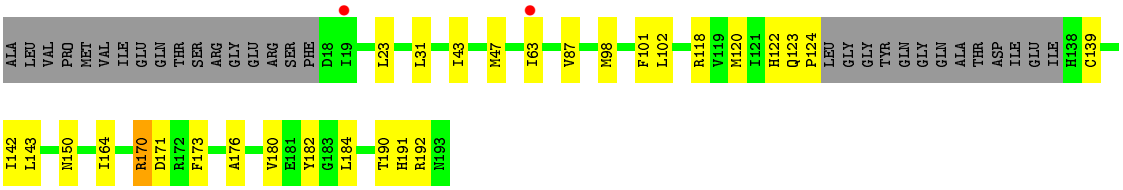
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



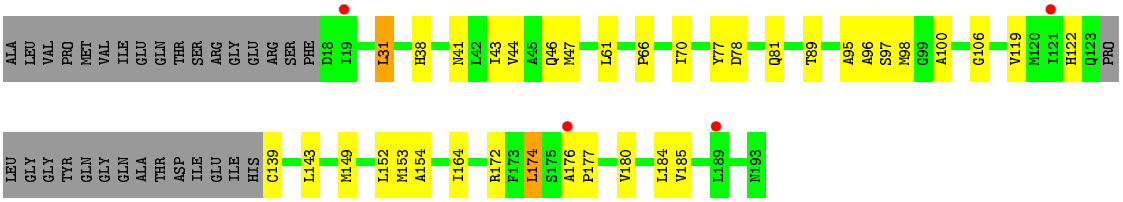
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



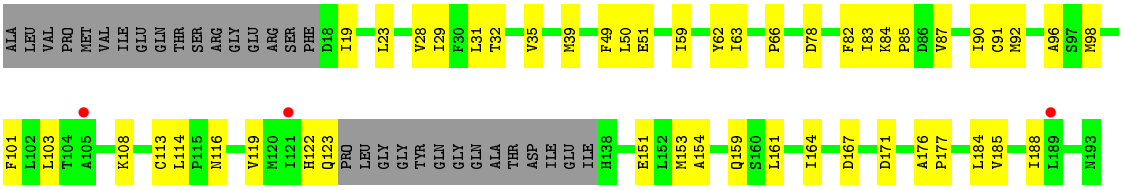
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



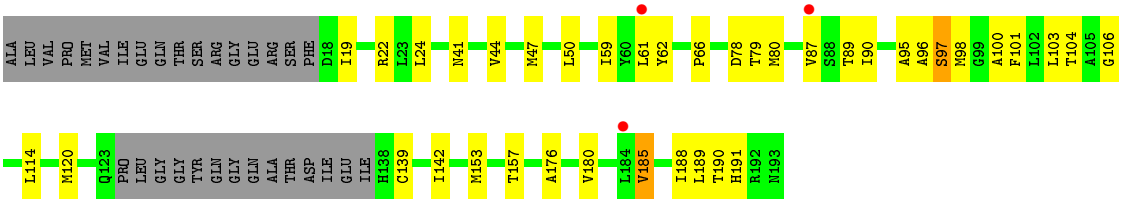
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



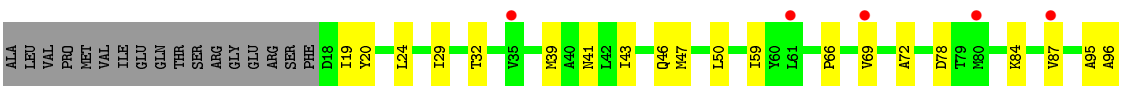
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

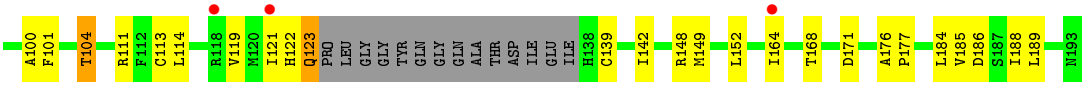
Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

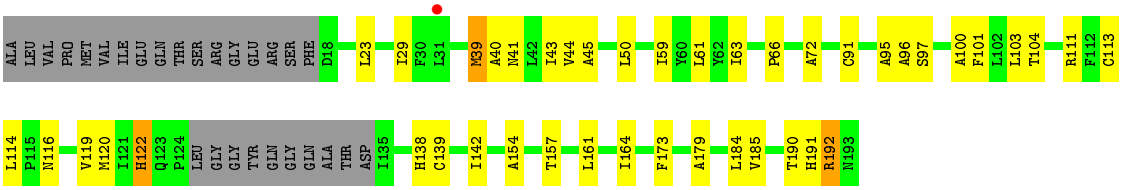
Chain N:





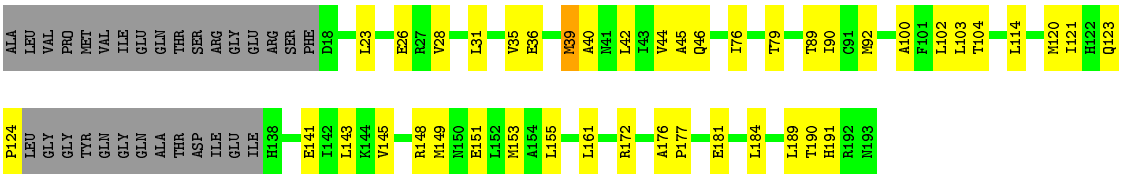
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain O:



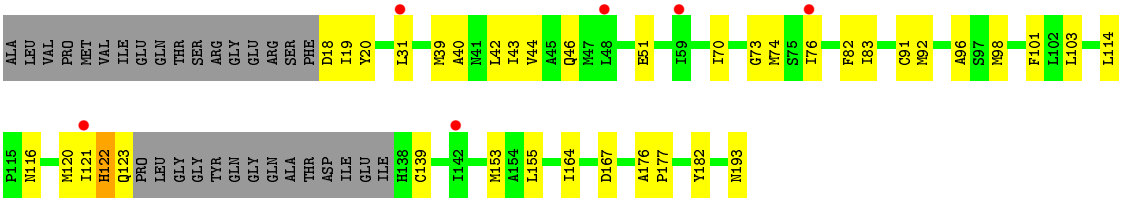
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain P:



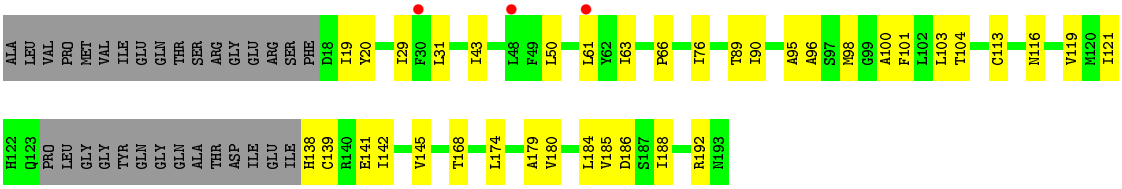
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q:



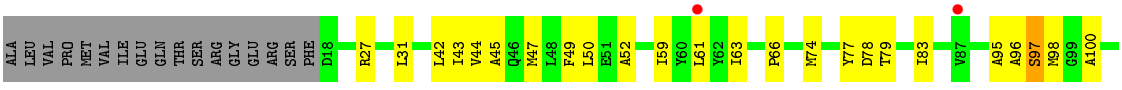
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

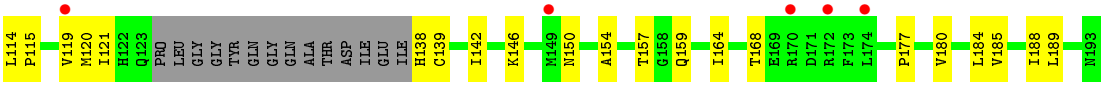
Chain R:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

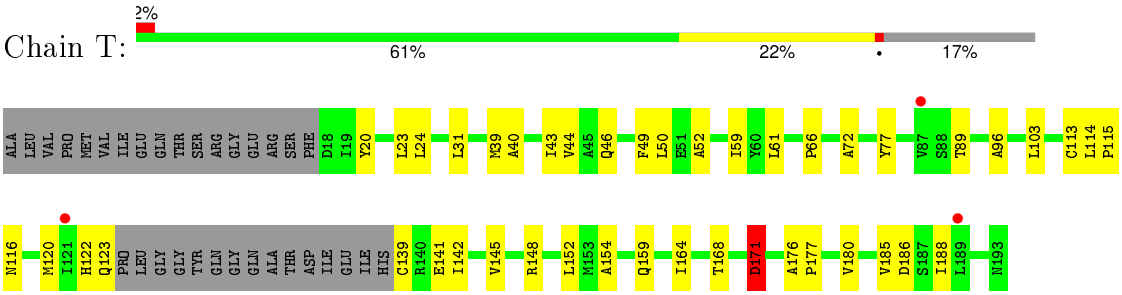
Chain S:





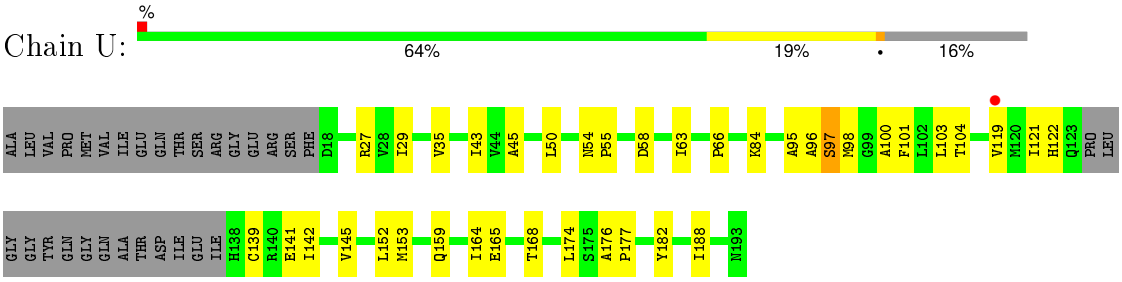
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T:



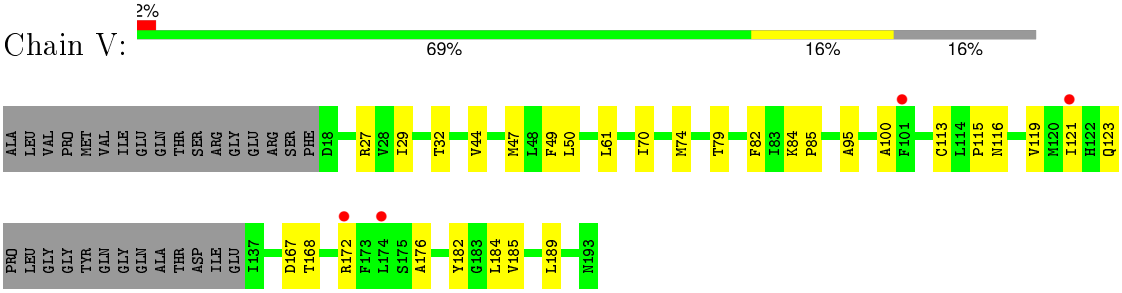
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain U:



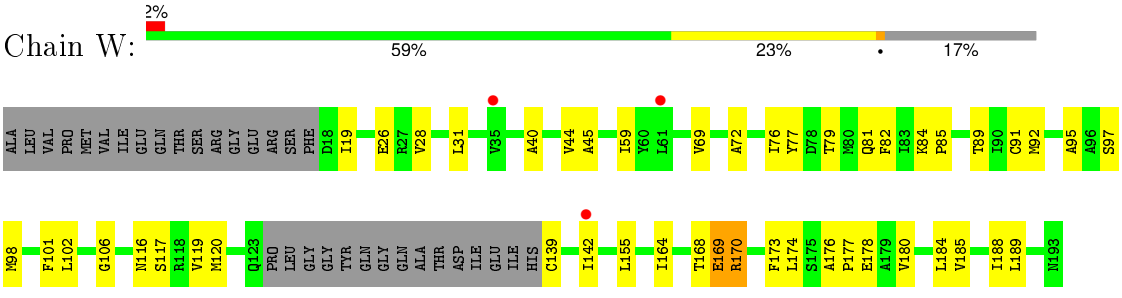
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:



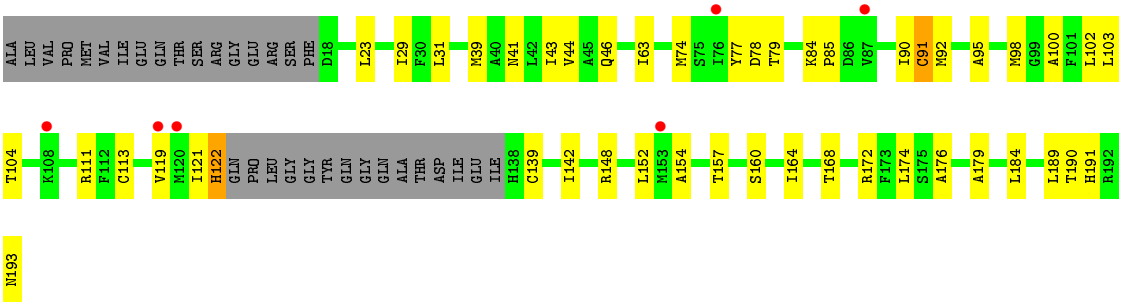
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain W:



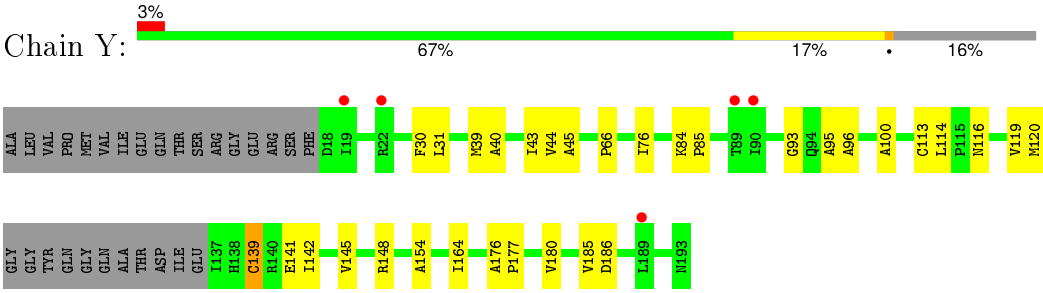
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X:



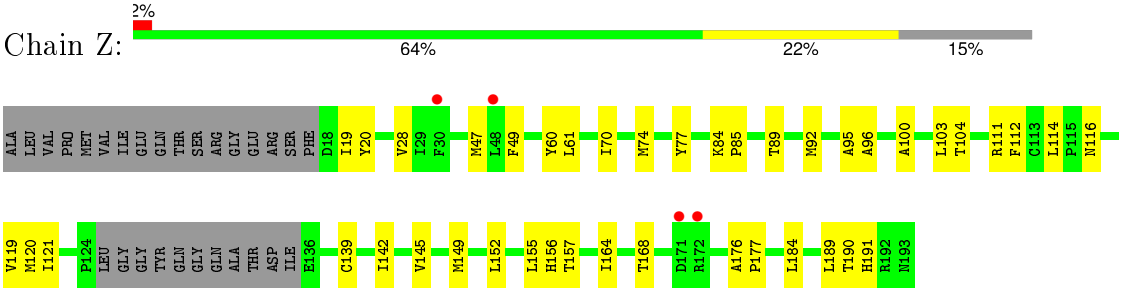
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y:



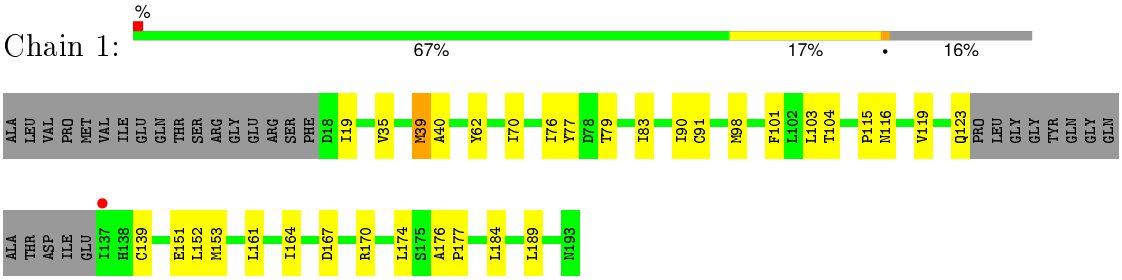
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:



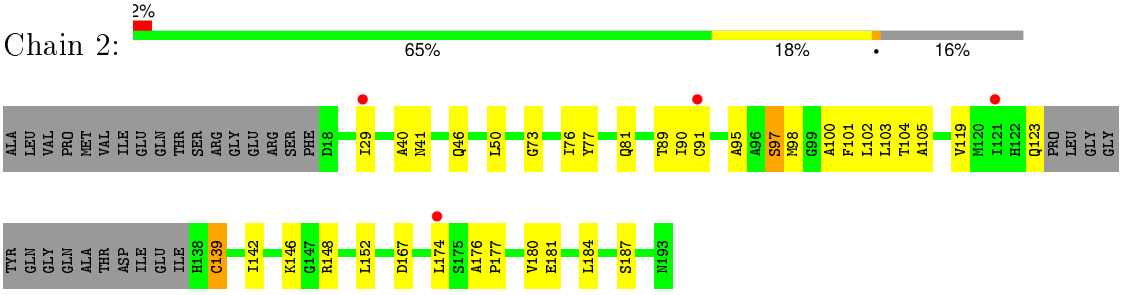
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain 1:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain 2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.30Å 182.30Å 476.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.22 – 3.20 42.21 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (42.22-3.20) 97.5 (42.21-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.253 0.271 , 0.303	Depositor DCC
R_{free} test set	7451 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	105.3	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.4	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 148224 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	35844	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA

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	1	0.37	0/1302	0.52	0/1750
1	2	0.39	0/1294	0.57	0/1739
1	A	0.38	0/1294	0.53	0/1739
1	B	0.40	0/1294	0.57	0/1739
1	C	0.36	0/1294	0.55	0/1739
1	D	0.40	0/1314	0.58	0/1767
1	E	0.36	0/1294	0.58	0/1739
1	F	0.37	0/1327	0.54	0/1784
1	G	0.35	0/1294	0.54	0/1739
1	H	0.34	0/1311	0.50	0/1762
1	I	0.37	0/1302	0.53	0/1751
1	J	0.38	0/1302	0.55	0/1751
1	K	0.35	0/1283	0.55	0/1724
1	L	0.35	0/1294	0.53	0/1739
1	M	0.34	0/1294	0.50	0/1739
1	N	0.35	0/1294	0.51	0/1739
1	O	0.41	0/1327	0.57	0/1785
1	P	0.36	0/1302	0.54	0/1751
1	Q	0.36	0/1294	0.53	0/1739
1	R	0.35	0/1294	0.49	0/1739
1	S	0.37	0/1294	0.51	0/1739
1	T	0.36	0/1283	0.50	0/1724
1	U	0.38	0/1294	0.52	0/1739
1	V	0.37	0/1302	0.53	0/1750
1	W	0.38	0/1283	0.53	0/1724
1	X	0.35	0/1285	0.53	0/1727
1	Y	0.38	0/1302	0.55	0/1750
1	Z	0.40	0/1319	0.55	0/1774
All	All	0.37	0/36366	0.54	0/48881

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	W	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	170	ARG	Peptide
1	W	170	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1283	0	1296	24	0
1	2	1275	0	1284	29	0
1	A	1275	0	1284	36	0
1	B	1275	0	1284	28	0
1	C	1275	0	1284	32	0
1	D	1294	0	1305	33	0
1	E	1275	0	1284	25	0
1	F	1308	0	1316	33	0
1	G	1275	0	1284	29	0
1	H	1292	0	1301	45	0
1	I	1282	0	1291	37	0
1	J	1282	0	1291	21	0
1	K	1265	0	1277	30	0
1	L	1275	0	1284	37	0
1	M	1275	0	1284	35	0
1	N	1275	0	1284	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1307	0	1320	43	0
1	P	1282	0	1291	44	0
1	Q	1275	0	1284	34	0
1	R	1275	0	1285	25	0
1	S	1275	0	1284	35	0
1	T	1265	0	1277	32	0
1	U	1275	0	1285	30	0
1	V	1283	0	1295	29	0
1	W	1265	0	1278	38	0
1	X	1266	0	1276	40	0
1	Y	1283	0	1295	30	0
1	Z	1299	0	1309	38	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
2	E	2	0	0	0	0
2	I	2	0	0	0	0
2	J	3	0	0	0	0
2	M	1	0	0	0	0
2	T	1	0	0	0	0
2	V	1	0	0	0	0
2	Z	1	0	0	0	0
All	All	35844	0	36112	813	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 11.

All (813) 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:103:LEU:HD11	1:I:185:VAL:CG1	1.94	0.98
1:A:139:CYS:O	1:A:142:ILE:HG22	1.62	0.98
1:C:104:THR:HG22	1:C:156:HIS:HB3	1.48	0.95
1:U:176:ALA:HB1	1:U:188:ILE:HD12	1.49	0.93
1:I:103:LEU:HD11	1:I:185:VAL:HG12	1.51	0.93
1:Z:119:VAL:HG11	1:Z:184:LEU:HD13	1.51	0.93
1:V:119:VAL:HG11	1:V:184:LEU:HD22	1.49	0.92
1:N:121:ILE:HG12	1:N:168:THR:HG22	1.51	0.92
1:D:31:LEU:CD2	1:D:43:ILE:HD13	1.99	0.92
1:H:70:ILE:HA	1:H:98:MET:HE3	1.52	0.91
1:H:157:THR:HG21	1:H:164:ILE:HD11	1.52	0.89
1:D:31:LEU:HD22	1:D:43:ILE:CD1	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LEU:HD22	1:D:43:ILE:HD13	1.54	0.88
1:X:104:THR:HG22	1:X:184:LEU:O	1.73	0.88
1:W:164:ILE:O	1:W:168:THR:HG22	1.74	0.85
1:V:116:ASN:ND2	1:2:152:LEU:HD11	1.91	0.85
1:V:44:VAL:HG21	1:W:92:MET:HE1	1.61	0.83
1:C:31:LEU:HD22	1:C:43:ILE:HD13	1.61	0.83
1:V:121:ILE:HD11	1:V:184:LEU:HD11	1.61	0.82
1:N:139:CYS:O	1:N:142:ILE:HG22	1.79	0.81
1:R:180:VAL:HG21	1:R:188:ILE:HD12	1.61	0.81
1:Z:121:ILE:HG22	1:Z:168:THR:HG22	1.63	0.81
1:I:103:LEU:CD1	1:I:185:VAL:HG12	2.10	0.81
1:J:31:LEU:HD23	1:J:43:ILE:CD1	2.11	0.80
1:N:164:ILE:O	1:N:168:THR:HG23	1.80	0.79
1:T:50:LEU:HD13	1:T:59:ILE:HD12	1.64	0.79
1:F:69:VAL:HG12	1:F:71:THR:HG22	1.65	0.78
1:B:138:HIS:O	1:B:142:ILE:HD13	1.83	0.78
1:M:50:LEU:HD13	1:M:59:ILE:HD12	1.64	0.77
1:V:32:THR:OG1	1:2:41:ASN:ND2	2.18	0.77
1:S:31:LEU:HD12	1:S:63:ILE:HG23	1.67	0.76
1:Y:44:VAL:HG11	1:Z:92:MET:HE2	1.65	0.76
1:X:44:VAL:HG22	1:X:79:THR:HG21	1.66	0.76
1:E:31:LEU:HD12	1:E:63:ILE:HG23	1.66	0.76
1:S:50:LEU:HD13	1:S:59:ILE:HD12	1.68	0.76
1:1:119:VAL:HG11	1:1:184:LEU:HD13	1.66	0.76
1:D:122:HIS:HB2	1:D:168:THR:O	1.86	0.76
1:X:154:ALA:HB2	1:X:164:ILE:HD13	1.68	0.76
1:P:121:ILE:HD13	1:P:153:MET:HE1	1.69	0.75
1:V:116:ASN:HD21	1:2:152:LEU:HD11	1.52	0.74
1:C:31:LEU:HD22	1:C:43:ILE:CD1	2.16	0.74
1:H:96:ALA:HB1	1:H:120:MET:HE2	1.69	0.74
1:O:44:VAL:HG11	1:P:92:MET:CE	2.17	0.74
1:Y:95:ALA:HB3	1:Y:119:VAL:HG22	1.70	0.74
1:F:69:VAL:CG1	1:F:71:THR:HG22	2.17	0.73
1:S:74:MET:HE2	1:T:116:ASN:HB2	1.70	0.73
1:R:138:HIS:O	1:R:142:ILE:HD13	1.89	0.73
1:U:139:CYS:O	1:U:142:ILE:HG22	1.89	0.72
1:X:139:CYS:HA	1:X:142:ILE:HG22	1.69	0.72
1:D:122:HIS:CB	1:D:168:THR:O	2.37	0.72
1:Z:121:ILE:CG2	1:Z:168:THR:HG22	2.19	0.72
1:W:44:VAL:HG22	1:W:79:THR:HG21	1.70	0.72
1:W:119:VAL:HG11	1:W:184:LEU:HD13	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:ILE:H	1:G:70:ILE:HD12	1.56	0.71
1:H:139:CYS:O	1:H:142:ILE:HG22	1.91	0.70
1:D:121:ILE:O	1:D:122:HIS:HB3	1.89	0.70
1:R:104:THR:HB	1:R:184:LEU:HD23	1.74	0.69
1:L:119:VAL:HG11	1:L:184:LEU:HD13	1.73	0.69
1:K:119:VAL:HG11	1:K:184:LEU:HD13	1.73	0.69
1:A:96:ALA:HB1	1:A:120:MET:HE2	1.74	0.69
1:S:74:MET:HE2	1:T:116:ASN:CB	2.21	0.69
1:M:176:ALA:HB1	1:M:188:ILE:HG23	1.73	0.69
1:O:138:HIS:O	1:O:142:ILE:HD13	1.92	0.69
1:I:31:LEU:HD22	1:I:43:ILE:CD1	2.23	0.69
1:2:119:VAL:HG11	1:2:184:LEU:HD13	1.73	0.69
1:Z:139:CYS:HA	1:Z:142:ILE:HG22	1.76	0.68
1:J:31:LEU:HD23	1:J:43:ILE:HD11	1.76	0.68
1:I:103:LEU:CD1	1:I:185:VAL:CG1	2.70	0.68
1:P:44:VAL:HG22	1:P:79:THR:HG21	1.74	0.68
1:H:50:LEU:HD13	1:H:59:ILE:HD12	1.76	0.68
1:N:122:HIS:NE2	1:N:171:ASP:HA	2.09	0.67
1:H:70:ILE:HG23	1:H:98:MET:CE	2.24	0.67
1:A:174:LEU:HD22	1:A:178:GLU:HB3	1.75	0.67
1:X:119:VAL:HG11	1:X:184:LEU:HD13	1.76	0.67
1:N:29:ILE:HD11	1:N:50:LEU:HD11	1.77	0.67
1:V:82:PHE:CE1	1:W:189:LEU:HD22	2.30	0.67
1:C:104:THR:CG2	1:C:156:HIS:HB3	2.23	0.67
1:H:119:VAL:HG11	1:H:184:LEU:HD21	1.77	0.67
1:J:150:ASN:HD22	1:J:164:ILE:HG22	1.60	0.67
1:Z:104:THR:HG22	1:Z:156:HIS:HB3	1.75	0.66
1:O:44:VAL:HG21	1:P:92:MET:HE1	1.76	0.66
1:Q:46:GLN:HA	1:R:19:ILE:HD11	1.76	0.66
1:O:154:ALA:HA	1:O:164:ILE:CD1	2.26	0.66
1:T:120:MET:HE3	1:T:171:ASP:CB	2.24	0.66
1:R:113:CYS:SG	1:R:185:VAL:HG21	2.36	0.66
1:W:97:SER:OG	1:W:98:MET:N	2.29	0.65
1:G:174:LEU:HD22	1:G:184:LEU:HD12	1.77	0.65
1:F:135:ILE:HD12	1:I:146:LYS:HD2	1.78	0.65
1:S:42:LEU:HD12	1:T:20:TYR:OH	1.97	0.65
1:K:77:TYR:OH	1:K:152:LEU:HD22	1.97	0.65
1:Z:114:LEU:HD23	1:Z:189:LEU:HB3	1.78	0.64
1:J:120:MET:HB2	1:J:173:PHE:CD1	2.33	0.64
1:J:31:LEU:HD12	1:J:63:ILE:HG23	1.79	0.64
1:P:121:ILE:HD11	1:P:184:LEU:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:59:ILE:HD11	1:N:87:VAL:HG22	1.80	0.64
1:C:98:MET:HE3	1:C:101:PHE:CD2	2.33	0.64
1:E:139:CYS:SG	1:J:143:LEU:HD11	2.37	0.64
1:X:119:VAL:HG11	1:X:184:LEU:CD1	2.28	0.64
1:Z:77:TYR:OH	1:Z:152:LEU:HD22	1.98	0.63
1:C:104:THR:HG23	1:C:111:ARG:NH1	2.14	0.63
1:O:44:VAL:HG11	1:P:92:MET:HE1	1.79	0.63
1:1:153:MET:HB3	1:1:164:ILE:HD13	1.80	0.63
1:Y:45:ALA:HB1	1:Z:19:ILE:HG21	1.80	0.63
1:H:190:THR:HG22	1:H:191:HIS:CD2	2.33	0.63
1:R:174:LEU:HD23	1:R:179:ALA:HA	1.79	0.63
1:A:41:ASN:ND2	1:B:32:THR:HG21	2.12	0.63
1:I:104:THR:HG22	1:I:156:HIS:HB3	1.81	0.63
1:H:62:TYR:CE1	1:H:90:ILE:HD12	2.33	0.63
1:Y:44:VAL:HG11	1:Z:92:MET:CE	2.28	0.63
1:S:138:HIS:O	1:S:142:ILE:HD13	1.98	0.63
1:P:46:GLN:HG3	1:Q:19:ILE:HD13	1.81	0.62
1:U:35:VAL:HG12	1:U:35:VAL:O	1.99	0.62
1:N:123:GLN:HE22	1:N:149:MET:HE2	1.64	0.62
1:D:31:LEU:HD22	1:D:43:ILE:HD11	1.80	0.62
1:H:153:MET:O	1:H:157:THR:HG22	1.99	0.62
1:S:44:VAL:HG13	1:S:79:THR:HG21	1.82	0.62
1:P:76:ILE:O	1:P:79:THR:HG22	1.99	0.62
1:X:95:ALA:O	1:X:100:ALA:HB2	2.00	0.62
1:V:121:ILE:HG22	1:V:168:THR:HG22	1.82	0.62
1:L:62:TYR:CE2	1:L:90:ILE:HG21	2.35	0.62
1:W:139:CYS:N	1:W:142:ILE:HD13	2.15	0.62
1:Z:95:ALA:O	1:Z:100:ALA:HB2	2.00	0.62
1:C:174:LEU:HD12	1:C:184:LEU:CD1	2.30	0.62
1:S:50:LEU:CD1	1:S:59:ILE:HD12	2.29	0.62
1:D:176:ALA:HB1	1:D:188:ILE:HD12	1.82	0.62
1:Y:154:ALA:HA	1:Y:164:ILE:HD11	1.81	0.62
1:X:31:LEU:HD23	1:X:43:ILE:CD1	2.30	0.62
1:M:66:PRO:HA	1:M:96:ALA:HB3	1.82	0.62
1:I:70:ILE:HD11	1:I:124:PRO:HG3	1.81	0.61
1:K:44:VAL:HG11	1:L:92:MET:CE	2.30	0.61
1:K:153:MET:HG2	1:K:164:ILE:HD13	1.82	0.61
1:A:70:ILE:HD11	1:A:123:GLN:HE22	1.65	0.61
1:M:180:VAL:HG21	1:M:188:ILE:HG13	1.82	0.61
1:Q:70:ILE:HD12	1:Q:98:MET:SD	2.40	0.61
1:G:122:HIS:O	1:G:123:GLN:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:98:MET:HE2	1:X:102:LEU:HD12	1.82	0.61
1:X:154:ALA:HB2	1:X:164:ILE:CD1	2.30	0.61
1:B:98:MET:O	1:B:102:LEU:HD23	2.01	0.61
1:A:101:PHE:O	1:A:104:THR:HG22	2.01	0.61
1:H:157:THR:HG23	1:H:159:GLN:H	1.66	0.61
1:R:180:VAL:HG21	1:R:188:ILE:CD1	2.29	0.60
1:X:31:LEU:HD23	1:X:43:ILE:HD13	1.82	0.60
1:A:66:PRO:HA	1:A:96:ALA:HB3	1.83	0.60
1:T:139:CYS:O	1:T:142:ILE:HG22	2.01	0.60
1:D:101:PHE:O	1:D:104:THR:HG22	2.02	0.60
1:C:76:ILE:HG22	1:C:102:LEU:HD22	1.83	0.60
1:Z:190:THR:HG22	1:Z:191:HIS:CD2	2.36	0.60
1:Z:89:THR:HG21	1:Z:103:LEU:O	2.01	0.59
1:Y:154:ALA:HA	1:Y:164:ILE:CD1	2.33	0.59
1:A:121:ILE:HD12	1:A:168:THR:HG22	1.84	0.59
1:J:98:MET:HE3	1:J:101:PHE:HB3	1.85	0.59
1:F:101:PHE:HA	1:F:153:MET:HE1	1.83	0.59
1:1:151:GLU:HG2	1:1:161:LEU:HD21	1.84	0.59
1:1:40:ALA:HA	1:1:76:ILE:HD11	1.83	0.59
1:W:76:ILE:O	1:W:79:THR:HG22	2.03	0.58
1:U:27:ARG:HD3	1:U:58:ASP:O	2.03	0.58
1:U:164:ILE:HD13	1:U:182:TYR:OH	2.02	0.58
1:I:40:ALA:HB1	1:I:76:ILE:HD11	1.83	0.58
1:P:35:VAL:HA	1:P:39:MET:SD	2.43	0.58
1:V:119:VAL:HG11	1:V:184:LEU:CD2	2.27	0.58
1:R:139:CYS:HG	1:W:139:CYS:HG	1.51	0.58
1:H:66:PRO:O	1:H:96:ALA:HB3	2.04	0.58
1:C:104:THR:HG22	1:C:156:HIS:CB	2.29	0.58
1:2:142:ILE:HD11	1:2:146:LYS:NZ	2.19	0.58
1:L:78:ASP:HB3	1:M:114:LEU:HD13	1.85	0.57
1:R:139:CYS:SG	1:W:139:CYS:SG	3.01	0.57
1:C:31:LEU:CD2	1:C:43:ILE:HD13	2.33	0.57
1:L:153:MET:HB3	1:L:164:ILE:HG21	1.87	0.57
1:J:190:THR:HG22	1:J:191:HIS:CD2	2.39	0.57
1:P:190:THR:HG22	1:P:191:HIS:CD2	2.39	0.57
1:K:152:LEU:HD11	1:L:116:ASN:HD21	1.70	0.57
1:F:104:THR:HG21	1:F:153:MET:CE	2.34	0.57
1:K:70:ILE:HD11	1:K:149:MET:SD	2.43	0.57
1:J:139:CYS:HA	1:J:142:ILE:HG22	1.86	0.57
1:O:39:MET:HE1	1:O:43:ILE:HD12	1.87	0.57
1:X:98:MET:HE2	1:X:102:LEU:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:153:MET:O	1:M:157:THR:HG23	2.05	0.57
1:X:190:THR:HG23	1:X:191:HIS:H	1.68	0.57
1:S:154:ALA:HB2	1:S:164:ILE:HG13	1.87	0.56
1:Y:176:ALA:HB3	1:Y:177:PRO:CD	2.35	0.56
1:C:44:VAL:HG13	1:C:79:THR:HG21	1.86	0.56
1:X:172:ARG:HD3	1:X:174:LEU:HD21	1.87	0.56
1:J:190:THR:HG23	1:P:181:GLU:HA	1.87	0.56
1:T:50:LEU:CD1	1:T:59:ILE:HD12	2.35	0.56
1:D:96:ALA:HB1	1:D:120:MET:HE3	1.86	0.56
1:E:97:SER:OG	1:E:98:MET:N	2.39	0.56
1:E:31:LEU:CD1	1:E:63:ILE:HG23	2.35	0.56
1:1:91:CYS:HB2	1:1:103:LEU:HD22	1.87	0.56
1:K:41:ASN:ND2	1:L:32:THR:OG1	2.38	0.56
1:C:174:LEU:HD12	1:C:184:LEU:HD12	1.88	0.56
1:Y:139:CYS:HA	1:Y:142:ILE:HG22	1.86	0.56
1:A:74:MET:HE2	1:B:116:ASN:CB	2.36	0.56
1:G:101:PHE:O	1:G:104:THR:HG22	2.05	0.56
1:P:100:ALA:O	1:P:104:THR:HG22	2.06	0.56
1:C:104:THR:OG1	1:C:184:LEU:HD23	2.06	0.56
1:2:81:GLN:HE22	1:2:105:ALA:HB1	1.71	0.56
1:S:31:LEU:HD23	1:S:43:ILE:HD11	1.88	0.55
1:E:45:ALA:HB3	1:F:19:ILE:HD12	1.88	0.55
1:W:45:ALA:O	1:X:23:LEU:HD11	2.06	0.55
1:K:172:ARG:HG3	1:K:174:LEU:HD13	1.87	0.55
1:T:120:MET:HE3	1:T:171:ASP:HB2	1.87	0.55
1:A:113:CYS:SG	1:A:185:VAL:HG21	2.47	0.55
1:K:152:LEU:HD11	1:L:116:ASN:ND2	2.21	0.55
1:E:98:MET:HE3	1:E:101:PHE:CD2	2.41	0.55
1:A:74:MET:HE2	1:B:116:ASN:HB2	1.89	0.55
1:T:154:ALA:HB1	1:T:159:GLN:O	2.07	0.55
1:R:89:THR:HB	1:R:103:LEU:HD12	1.88	0.55
1:L:29:ILE:HD11	1:L:50:LEU:HD12	1.88	0.55
1:2:104:THR:HB	1:2:184:LEU:CD2	2.37	0.55
1:W:98:MET:HE2	1:W:102:LEU:HD11	1.89	0.55
1:D:119:VAL:HG11	1:D:184:LEU:HD13	1.87	0.55
1:A:96:ALA:CB	1:A:120:MET:HE2	2.36	0.55
1:P:44:VAL:HG21	1:Q:92:MET:HE3	1.89	0.55
1:M:50:LEU:CD1	1:M:59:ILE:HD12	2.36	0.55
1:O:154:ALA:CA	1:O:164:ILE:CD1	2.85	0.55
1:Q:40:ALA:O	1:Q:76:ILE:HD11	2.07	0.55
1:B:190:THR:HG22	1:B:191:HIS:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:159:GLN:NE2	1:U:182:TYR:CE1	2.74	0.55
1:D:27:ARG:HG2	1:D:50:LEU:HD22	1.88	0.54
1:A:96:ALA:HB1	1:A:120:MET:CE	2.37	0.54
1:1:62:TYR:CZ	1:1:90:ILE:HD12	2.43	0.54
1:T:43:ILE:HA	1:T:46:GLN:HE21	1.72	0.54
1:Y:40:ALA:O	1:Y:44:VAL:HG23	2.07	0.54
1:X:74:MET:HE2	1:Y:116:ASN:HB2	1.88	0.54
1:D:28:VAL:HG22	1:D:60:TYR:HB2	1.88	0.54
1:R:98:MET:HE3	1:R:101:PHE:CD2	2.43	0.54
1:H:152:LEU:HD11	1:I:116:ASN:ND2	2.22	0.54
1:F:90:ILE:HD12	1:F:90:ILE:N	2.23	0.54
1:W:176:ALA:HB1	1:W:188:ILE:HD12	1.89	0.54
1:O:29:ILE:HG21	1:O:43:ILE:HG23	1.89	0.54
1:E:45:ALA:CB	1:F:19:ILE:HD12	2.37	0.54
1:P:31:LEU:CD2	1:P:39:MET:HE1	2.38	0.54
1:A:109:GLY:N	1:A:186:ASP:OD2	2.35	0.54
1:U:153:MET:HG2	1:U:164:ILE:HD12	1.89	0.54
1:O:190:THR:HG23	1:O:191:HIS:H	1.73	0.54
1:S:47:MET:CE	1:S:61:LEU:HD22	2.38	0.53
1:X:122:HIS:HA	1:X:168:THR:HG23	1.88	0.53
1:F:121:ILE:O	1:F:122:HIS:CB	2.56	0.53
1:D:122:HIS:HB3	1:D:168:THR:O	2.07	0.53
1:A:41:ASN:ND2	1:B:32:THR:CG2	2.71	0.53
1:T:164:ILE:O	1:T:168:THR:HG22	2.08	0.53
1:A:32:THR:OG1	1:G:41:ASN:ND2	2.41	0.53
1:A:172:ARG:NH1	1:A:174:LEU:HD21	2.24	0.53
1:H:114:LEU:HD23	1:N:78:ASP:CB	2.39	0.53
1:E:172:ARG:HG3	1:E:174:LEU:HD11	1.90	0.53
1:S:114:LEU:HD12	1:S:189:LEU:HB3	1.90	0.53
1:Y:31:LEU:HD23	1:Y:43:ILE:CD1	2.38	0.53
1:H:50:LEU:CD1	1:H:59:ILE:HD12	2.38	0.53
1:N:50:LEU:HD13	1:N:59:ILE:HG22	1.89	0.53
1:J:120:MET:HB2	1:J:173:PHE:CE1	2.44	0.53
1:V:29:ILE:HD11	1:V:50:LEU:HD12	1.90	0.53
1:Z:119:VAL:CG1	1:Z:184:LEU:HD13	2.33	0.53
1:M:24:LEU:O	1:M:50:LEU:HD21	2.09	0.53
1:U:176:ALA:HB1	1:U:188:ILE:CD1	2.29	0.53
1:2:139:CYS:O	1:2:142:ILE:HG22	2.09	0.53
1:L:159:GLN:HB2	1:L:164:ILE:HD11	1.90	0.53
1:F:176:ALA:HB3	1:F:177:PRO:HD3	1.89	0.53
1:N:66:PRO:HA	1:N:96:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:155:LEU:C	1:Q:155:LEU:HD12	2.30	0.53
1:L:151:GLU:HA	1:L:161:LEU:HD23	1.91	0.53
1:M:50:LEU:HD13	1:M:59:ILE:CD1	2.36	0.52
1:X:160:SER:O	1:X:164:ILE:HD12	2.09	0.52
1:T:120:MET:HE2	1:T:122:HIS:HB3	1.91	0.52
1:X:31:LEU:HD12	1:X:63:ILE:HG23	1.90	0.52
1:O:39:MET:CE	1:O:43:ILE:HD12	2.38	0.52
1:H:44:VAL:HG13	1:H:79:THR:HG21	1.90	0.52
1:T:113:CYS:SG	1:T:185:VAL:HG11	2.49	0.52
1:S:31:LEU:CD1	1:S:63:ILE:HG23	2.37	0.52
1:X:139:CYS:HA	1:X:142:ILE:CG2	2.39	0.52
1:O:154:ALA:HB2	1:O:164:ILE:HD12	1.89	0.52
1:F:104:THR:HG21	1:F:153:MET:HE2	1.90	0.52
1:K:139:CYS:O	1:K:143:LEU:HD22	2.09	0.52
1:Z:74:MET:HE2	1:1:116:ASN:CB	2.40	0.52
1:S:47:MET:HE2	1:S:61:LEU:HD22	1.90	0.52
1:L:91:CYS:HB2	1:L:103:LEU:HD13	1.91	0.52
1:W:84:LYS:HZ2	1:X:193:ASN:HA	1.74	0.52
1:I:140:ARG:NH2	1:O:161:LEU:HD12	2.24	0.52
1:K:176:ALA:HB3	1:K:177:PRO:HD3	1.91	0.52
1:I:113:CYS:SG	1:I:185:VAL:HG11	2.50	0.52
1:L:84:LYS:N	1:L:85:PRO:HD2	2.25	0.52
1:A:189:LEU:HD22	1:G:82:PHE:CE1	2.45	0.52
1:K:38:HIS:CE1	1:L:32:THR:HG22	2.44	0.52
1:G:121:ILE:CG2	1:G:168:THR:HG22	2.40	0.52
1:I:31:LEU:HD22	1:I:43:ILE:HD13	1.92	0.52
1:C:148:ARG:HE	1:D:116:ASN:HD21	1.56	0.52
1:L:119:VAL:CG1	1:L:184:LEU:HD13	2.40	0.51
1:Q:39:MET:O	1:Q:43:ILE:HD12	2.10	0.51
1:K:97:SER:OG	1:K:98:MET:N	2.44	0.51
1:O:119:VAL:HG11	1:O:184:LEU:CD2	2.40	0.51
1:A:121:ILE:HD12	1:A:168:THR:CG2	2.40	0.51
1:P:89:THR:HB	1:P:103:LEU:HD12	1.92	0.51
1:2:29:ILE:HD11	1:2:50:LEU:HD11	1.92	0.51
1:J:182:TYR:HD2	1:J:184:LEU:HD22	1.75	0.51
1:O:154:ALA:HA	1:O:164:ILE:HD11	1.91	0.51
1:A:92:MET:HE1	1:G:44:VAL:HG11	1.92	0.51
1:1:70:ILE:HD11	1:1:123:GLN:NE2	2.25	0.51
1:R:61:LEU:HD23	1:R:63:ILE:HD11	1.91	0.51
1:V:182:TYR:HD2	1:V:184:LEU:HD12	1.76	0.51
1:H:114:LEU:HD23	1:N:78:ASP:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ALA:HB1	1:E:26:GLU:OE2	2.10	0.51
1:N:121:ILE:CG1	1:N:168:THR:HG22	2.32	0.51
1:M:180:VAL:CG2	1:M:185:VAL:HG23	2.40	0.51
1:N:24:LEU:HD23	1:N:50:LEU:HD21	1.93	0.51
1:2:101:PHE:O	1:2:104:THR:HG22	2.10	0.51
1:B:190:THR:HG22	1:B:191:HIS:CD2	2.45	0.51
1:E:190:THR:HG22	1:E:191:HIS:CD2	2.45	0.51
1:C:154:ALA:HB2	1:C:164:ILE:HG13	1.93	0.51
1:Y:66:PRO:O	1:Y:96:ALA:HB3	2.11	0.51
1:N:50:LEU:HD13	1:N:59:ILE:CG2	2.41	0.51
1:Y:180:VAL:HG13	1:Y:186:ASP:O	2.10	0.51
1:V:113:CYS:SG	1:V:185:VAL:HG21	2.51	0.51
1:2:29:ILE:HD12	1:2:46:GLN:HB3	1.93	0.51
1:S:27:ARG:HG2	1:S:50:LEU:HD22	1.93	0.51
1:L:176:ALA:HB1	1:L:188:ILE:HG13	1.93	0.51
1:A:190:THR:HG22	1:A:191:HIS:CD2	2.45	0.51
1:O:113:CYS:SG	1:O:185:VAL:HG11	2.51	0.51
1:B:31:LEU:HD12	1:B:31:LEU:C	2.32	0.51
1:Y:95:ALA:O	1:Y:100:ALA:HB2	2.11	0.51
1:Z:89:THR:HG22	1:Z:111:ARG:HB3	1.92	0.51
1:X:148:ARG:HH11	1:Y:116:ASN:HD21	1.58	0.51
1:K:172:ARG:HD2	1:K:174:LEU:HD11	1.93	0.50
1:K:153:MET:CG	1:K:164:ILE:HD13	2.41	0.50
1:H:137:ILE:HD12	1:I:170:ARG:HD2	1.92	0.50
1:C:66:PRO:HA	1:C:96:ALA:HB3	1.93	0.50
1:M:190:THR:HG23	1:M:191:HIS:H	1.76	0.50
1:D:98:MET:HE2	1:D:102:LEU:HD11	1.93	0.50
1:I:113:CYS:SG	1:I:185:VAL:HG21	2.50	0.50
1:H:154:ALA:HA	1:H:157:THR:HG22	1.92	0.50
1:Z:70:ILE:HD12	1:Z:149:MET:HE1	1.92	0.50
1:N:119:VAL:HG11	1:N:184:LEU:HD13	1.92	0.50
1:K:77:TYR:O	1:K:81:GLN:NE2	2.45	0.50
1:Z:19:ILE:HG22	1:Z:20:TYR:N	2.25	0.50
1:Q:74:MET:HE2	1:R:116:ASN:HB2	1.92	0.50
1:G:74:MET:HE3	1:G:77:TYR:HB3	1.94	0.50
1:A:77:TYR:OH	1:A:152:LEU:HD22	2.12	0.50
1:X:41:ASN:HD21	1:Y:30:PHE:HD1	1.58	0.50
1:B:70:ILE:HG23	1:B:149:MET:CE	2.41	0.50
1:N:101:PHE:O	1:N:104:THR:HG22	2.12	0.50
1:I:190:THR:HG22	1:I:191:HIS:CD2	2.47	0.50
1:C:121:ILE:HD11	1:C:184:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:174:LEU:HD12	1:1:184:LEU:HD12	1.94	0.50
1:U:121:ILE:O	1:U:122:HIS:HB3	2.11	0.50
1:W:59:ILE:HD13	1:W:85:PRO:HB2	1.92	0.50
1:O:66:PRO:HA	1:O:96:ALA:HB3	1.94	0.50
1:B:114:LEU:O	1:B:117:SER:OG	2.28	0.50
1:A:74:MET:HE3	1:A:77:TYR:HB3	1.94	0.50
1:D:98:MET:HE3	1:D:102:LEU:HG	1.93	0.50
1:2:40:ALA:HA	1:2:76:ILE:HD11	1.94	0.50
1:A:39:MET:HG3	1:A:40:ALA:N	2.27	0.50
1:G:59:ILE:HD12	1:G:85:PRO:HB2	1.94	0.50
1:J:118:ARG:HG2	1:J:173:PHE:CD1	2.46	0.49
1:T:113:CYS:SG	1:T:185:VAL:HG21	2.52	0.49
1:C:190:THR:HG22	1:C:191:HIS:CD2	2.47	0.49
1:U:98:MET:HE3	1:U:101:PHE:HD2	1.78	0.49
1:T:31:LEU:HB2	1:T:61:LEU:HD11	1.93	0.49
1:2:176:ALA:O	1:2:180:VAL:HG23	2.12	0.49
1:J:47:MET:HE1	1:J:87:VAL:HG21	1.93	0.49
1:U:119:VAL:HG13	1:U:174:LEU:HB2	1.93	0.49
1:P:39:MET:HE2	1:P:40:ALA:HA	1.93	0.49
1:V:74:MET:HE2	1:W:116:ASN:HB2	1.95	0.49
1:P:148:ARG:HD3	1:Q:116:ASN:HD21	1.77	0.49
1:F:73:GLY:HA2	1:F:76:ILE:HD12	1.94	0.49
1:Z:157:THR:CG2	1:Z:184:LEU:HD23	2.43	0.49
1:H:104:THR:HB	1:H:184:LEU:HD12	1.94	0.49
1:Y:39:MET:O	1:Y:43:ILE:HD12	2.12	0.49
1:G:96:ALA:HB1	1:G:120:MET:HE1	1.94	0.49
1:R:29:ILE:HD11	1:R:50:LEU:HD12	1.93	0.49
1:V:167:ASP:HB3	1:V:172:ARG:NH1	2.28	0.49
1:C:31:LEU:HD21	1:C:76:ILE:HD13	1.95	0.49
1:M:44:VAL:HG13	1:M:79:THR:HG21	1.93	0.49
1:S:31:LEU:HD23	1:S:43:ILE:CD1	2.42	0.49
1:U:141:GLU:O	1:U:145:VAL:HG23	2.12	0.49
1:O:116:ASN:ND2	1:U:152:LEU:HD11	2.27	0.49
1:S:97:SER:OG	1:S:98:MET:N	2.46	0.49
1:I:51:GLU:OE2	1:J:192:ARG:NE	2.45	0.49
1:V:44:VAL:HG13	1:V:79:THR:HG21	1.95	0.49
1:P:31:LEU:HD21	1:P:39:MET:HE1	1.93	0.49
1:F:120:MET:HB2	1:F:173:PHE:CD1	2.48	0.49
1:B:40:ALA:HA	1:B:76:ILE:HD11	1.95	0.49
1:F:157:THR:HG22	1:F:184:LEU:HA	1.93	0.49
1:D:31:LEU:HD23	1:D:43:ILE:HD13	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:CYS:O	1:C:140:ARG:C	2.52	0.48
1:I:103:LEU:HD11	1:I:185:VAL:HG11	1.91	0.48
1:Y:45:ALA:HB1	1:Z:19:ILE:CG2	2.42	0.48
1:S:157:THR:HG22	1:S:184:LEU:HA	1.94	0.48
1:R:90:ILE:N	1:R:90:ILE:HD12	2.28	0.48
1:M:97:SER:OG	1:M:98:MET:N	2.46	0.48
1:X:44:VAL:HG22	1:X:79:THR:CG2	2.38	0.48
1:1:151:GLU:CG	1:1:161:LEU:HD21	2.42	0.48
1:F:121:ILE:O	1:F:122:HIS:HB3	2.14	0.48
1:X:78:ASP:HB3	1:Y:114:LEU:HB3	1.95	0.48
1:2:119:VAL:HG11	1:2:184:LEU:CD1	2.42	0.48
1:P:36:GLU:O	1:P:39:MET:HG3	2.14	0.48
1:B:109:GLY:N	1:B:186:ASP:OD2	2.46	0.48
1:T:40:ALA:CB	1:T:72:ALA:HB1	2.43	0.48
1:R:180:VAL:HG13	1:R:186:ASP:O	2.12	0.48
1:Q:98:MET:HE3	1:Q:101:PHE:HD2	1.78	0.48
1:P:114:LEU:HD13	1:P:189:LEU:HB2	1.95	0.48
1:L:82:PHE:CE1	1:M:189:LEU:HD21	2.49	0.48
1:V:82:PHE:HE1	1:W:189:LEU:HD22	1.76	0.48
1:K:44:VAL:HG11	1:L:92:MET:HE3	1.95	0.48
1:O:39:MET:HE2	1:O:40:ALA:HA	1.95	0.48
1:O:120:MET:HE2	1:O:122:HIS:HB3	1.94	0.48
1:H:116:ASN:ND2	1:N:152:LEU:HD11	2.29	0.48
1:Q:91:CYS:HB2	1:Q:103:LEU:HD22	1.95	0.48
1:W:69:VAL:HG13	1:W:72:ALA:CB	2.44	0.48
1:F:137:ILE:HD12	1:G:170:ARG:CZ	2.44	0.48
1:S:66:PRO:HA	1:S:96:ALA:HB3	1.96	0.48
1:Y:176:ALA:HB3	1:Y:177:PRO:HD2	1.94	0.48
1:D:52:ALA:CB	1:E:26:GLU:OE2	2.61	0.48
1:L:23:LEU:HD12	1:L:28:VAL:HG11	1.96	0.48
1:Z:49:PHE:CB	1:1:19:ILE:HD11	2.43	0.48
1:M:78:ASP:HB3	1:N:114:LEU:HD12	1.94	0.48
1:O:44:VAL:HG11	1:P:92:MET:HE3	1.95	0.48
1:G:70:ILE:HD12	1:G:70:ILE:N	2.27	0.48
1:Z:74:MET:HE2	1:1:116:ASN:HB3	1.96	0.48
1:A:92:MET:HB3	1:A:114:LEU:HD12	1.94	0.48
1:E:119:VAL:HG11	1:E:184:LEU:HD13	1.95	0.48
1:D:77:TYR:OH	1:D:152:LEU:HD12	2.14	0.48
1:1:35:VAL:HA	1:1:39:MET:SD	2.54	0.48
1:F:54:ASN:HD21	1:F:57:LYS:HG3	1.78	0.48
1:U:176:ALA:HB3	1:U:177:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:154:ALA:CA	1:Y:164:ILE:CD1	2.92	0.48
1:I:40:ALA:CB	1:I:76:ILE:HD11	2.44	0.48
1:L:59:ILE:HB	1:L:87:VAL:HG22	1.96	0.48
1:Q:164:ILE:HD13	1:Q:182:TYR:OH	2.14	0.48
1:A:19:ILE:N	1:A:19:ILE:HD12	2.28	0.48
1:Z:112:PHE:CG	1:Z:189:LEU:HD13	2.49	0.48
1:F:137:ILE:HD12	1:G:170:ARG:NE	2.29	0.48
1:V:70:ILE:HD11	1:V:123:GLN:OE1	2.14	0.48
1:B:113:CYS:SG	1:B:185:VAL:HG21	2.53	0.48
1:I:176:ALA:O	1:I:180:VAL:HG23	2.14	0.48
1:B:74:MET:HE2	1:C:116:ASN:HB2	1.95	0.48
1:2:104:THR:HB	1:2:184:LEU:HD23	1.96	0.47
1:E:98:MET:HE3	1:E:101:PHE:HD2	1.79	0.47
1:B:70:ILE:HG23	1:B:149:MET:HE1	1.96	0.47
1:S:119:VAL:HG11	1:S:184:LEU:HD22	1.96	0.47
1:N:69:VAL:HG12	1:N:72:ALA:H	1.79	0.47
1:G:47:MET:CE	1:G:61:LEU:HD13	2.44	0.47
1:T:49:PHE:O	1:T:52:ALA:HB3	2.13	0.47
1:Q:121:ILE:HG21	1:Q:153:MET:HE1	1.96	0.47
1:P:120:MET:HE2	1:P:172:ARG:N	2.29	0.47
1:2:97:SER:OG	1:2:98:MET:N	2.44	0.47
1:C:98:MET:HE3	1:C:101:PHE:HD2	1.78	0.47
1:W:180:VAL:HG22	1:W:185:VAL:HG23	1.96	0.47
1:I:95:ALA:HB3	1:I:119:VAL:HG22	1.95	0.47
1:X:74:MET:HE2	1:Y:116:ASN:CB	2.45	0.47
1:B:122:HIS:O	1:B:123:GLN:HB3	2.14	0.47
1:I:114:LEU:HD13	1:I:189:LEU:HB2	1.95	0.47
1:D:70:ILE:HD13	1:D:145:VAL:HG11	1.96	0.47
1:Q:96:ALA:HB1	1:Q:120:MET:HE2	1.96	0.47
1:H:101:PHE:HD1	1:H:153:MET:HE2	1.79	0.47
1:J:150:ASN:ND2	1:J:164:ILE:HG22	2.29	0.47
1:Z:145:VAL:HG12	1:Z:149:MET:HE1	1.96	0.47
1:Z:104:THR:HG21	1:Z:157:THR:CG2	2.44	0.47
1:H:96:ALA:CB	1:H:120:MET:HE2	2.43	0.47
1:I:104:THR:HG23	1:I:184:LEU:O	2.14	0.47
1:P:89:THR:C	1:P:90:ILE:HD12	2.34	0.47
1:E:47:MET:CE	1:E:61:LEU:HD22	2.44	0.47
1:Y:141:GLU:O	1:Y:145:VAL:HG13	2.15	0.47
1:A:35:VAL:HA	1:A:39:MET:SD	2.55	0.47
1:Q:96:ALA:HB1	1:Q:120:MET:CE	2.44	0.47
1:N:111:ARG:N	1:N:186:ASP:OD2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:GLU:HA	1:E:161:LEU:HD13	1.96	0.47
1:C:161:LEU:HD13	1:C:161:LEU:O	2.15	0.47
1:V:49:PHE:CB	1:W:19:ILE:HD11	2.44	0.47
1:I:121:ILE:HG22	1:I:168:THR:HG22	1.97	0.47
1:F:180:VAL:HG22	1:F:185:VAL:HG23	1.97	0.47
1:U:176:ALA:HB3	1:U:177:PRO:CD	2.45	0.47
1:K:47:MET:HE1	1:K:61:LEU:HD22	1.96	0.47
1:P:151:GLU:HA	1:P:161:LEU:HD13	1.96	0.47
1:O:50:LEU:HD12	1:O:59:ILE:HD12	1.97	0.47
1:N:29:ILE:HD11	1:N:50:LEU:CD1	2.42	0.47
1:A:92:MET:CE	1:G:44:VAL:HG11	2.45	0.47
1:1:98:MET:HE3	1:1:101:PHE:CD2	2.50	0.47
1:V:115:PRO:O	1:V:176:ALA:HB2	2.15	0.47
1:S:78:ASP:HB3	1:T:114:LEU:HD23	1.96	0.47
1:M:101:PHE:O	1:M:104:THR:HG22	2.15	0.47
1:H:154:ALA:HA	1:H:157:THR:CG2	2.45	0.46
1:O:157:THR:HG22	1:O:184:LEU:HA	1.96	0.46
1:L:31:LEU:HD12	1:L:39:MET:CE	2.45	0.46
1:T:177:PRO:HA	1:T:188:ILE:HD11	1.97	0.46
1:H:66:PRO:HA	1:H:96:ALA:HB3	1.97	0.46
1:P:177:PRO:O	1:P:181:GLU:HG3	2.15	0.46
1:S:154:ALA:HB2	1:S:164:ILE:CG1	2.45	0.46
1:Q:74:MET:HE2	1:R:116:ASN:CB	2.46	0.46
1:P:148:ARG:HD3	1:Q:116:ASN:ND2	2.31	0.46
1:E:47:MET:HE2	1:E:61:LEU:HD22	1.97	0.46
1:P:151:GLU:O	1:P:155:LEU:HD23	2.16	0.46
1:1:115:PRO:HD3	1:1:189:LEU:O	2.15	0.46
1:W:98:MET:HE3	1:W:101:PHE:CD2	2.51	0.46
1:G:104:THR:HB	1:G:184:LEU:HD23	1.96	0.46
1:Q:98:MET:HE3	1:Q:101:PHE:CD2	2.50	0.46
1:H:152:LEU:HD11	1:I:116:ASN:HD21	1.80	0.46
1:E:141:GLU:HG3	1:F:173:PHE:HB2	1.98	0.46
1:Z:47:MET:CE	1:Z:61:LEU:HD22	2.46	0.46
1:L:154:ALA:HB2	1:L:164:ILE:CG1	2.46	0.46
1:P:143:LEU:HD21	1:Y:139:CYS:HB3	1.97	0.46
1:L:50:LEU:HD13	1:L:59:ILE:HG23	1.97	0.46
1:C:146:LYS:HE2	1:C:168:THR:HG21	1.98	0.46
1:D:29:ILE:HG21	1:D:43:ILE:HG23	1.97	0.46
1:P:39:MET:HE2	1:P:40:ALA:CA	2.45	0.46
1:O:40:ALA:HB2	1:O:72:ALA:HB1	1.98	0.46
1:Y:142:ILE:HD12	1:Y:145:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:95:ALA:O	1:V:100:ALA:HB2	2.16	0.46
1:I:29:ILE:HD11	1:I:50:LEU:HD12	1.96	0.46
1:H:120:MET:HA	1:H:172:ARG:O	2.16	0.46
1:S:45:ALA:O	1:T:23:LEU:HD11	2.14	0.46
1:2:90:ILE:HD12	1:2:90:ILE:N	2.30	0.46
1:X:174:LEU:HD12	1:X:184:LEU:HD13	1.98	0.46
1:E:101:PHE:O	1:E:104:THR:HG22	2.16	0.46
1:N:24:LEU:O	1:N:24:LEU:HD23	2.16	0.46
1:W:69:VAL:HG13	1:W:72:ALA:HB3	1.98	0.46
1:W:82:PHE:CE1	1:X:189:LEU:HD22	2.50	0.46
1:X:91:CYS:HB2	1:X:103:LEU:HD22	1.97	0.46
1:D:157:THR:HA	1:D:183:GLY:O	2.16	0.46
1:O:45:ALA:O	1:P:23:LEU:HD11	2.16	0.46
1:O:29:ILE:HG22	1:O:61:LEU:CD1	2.46	0.46
1:S:96:ALA:HB2	1:S:120:MET:HE3	1.98	0.46
1:G:47:MET:HE3	1:G:61:LEU:HD13	1.97	0.46
1:U:27:ARG:HB3	1:U:50:LEU:HD22	1.98	0.45
1:S:74:MET:HE3	1:S:77:TYR:HB3	1.98	0.45
1:P:141:GLU:O	1:P:145:VAL:HG23	2.17	0.45
1:H:113:CYS:SG	1:H:185:VAL:HG11	2.56	0.45
1:U:95:ALA:O	1:U:100:ALA:HB2	2.16	0.45
1:O:111:ARG:C	1:O:185:VAL:HG23	2.36	0.45
1:1:101:PHE:O	1:1:104:THR:HG22	2.15	0.45
1:L:49:PHE:HB3	1:M:19:ILE:HD11	1.99	0.45
1:M:47:MET:CE	1:M:61:LEU:HD22	2.46	0.45
1:N:113:CYS:SG	1:N:185:VAL:HG21	2.56	0.45
1:G:40:ALA:HA	1:G:76:ILE:HD11	1.99	0.45
1:G:98:MET:HE3	1:G:101:PHE:CD2	2.52	0.45
1:I:157:THR:HG22	1:I:184:LEU:HA	1.98	0.45
1:K:154:ALA:N	1:K:164:ILE:HD12	2.31	0.45
1:G:159:GLN:HB2	1:G:164:ILE:CD1	2.46	0.45
1:B:101:PHE:O	1:B:104:THR:HG22	2.16	0.45
1:S:180:VAL:HG22	1:S:185:VAL:HG23	1.99	0.45
1:D:138:HIS:O	1:D:142:ILE:HD13	2.17	0.45
1:N:95:ALA:O	1:N:100:ALA:HB2	2.16	0.45
1:U:139:CYS:SG	1:1:139:CYS:SG	3.15	0.45
1:I:40:ALA:CA	1:I:76:ILE:HD11	2.46	0.45
1:P:176:ALA:HB3	1:P:177:PRO:HD3	1.99	0.45
1:T:141:GLU:O	1:T:145:VAL:HG23	2.16	0.45
1:H:32:THR:OG1	1:N:41:ASN:ND2	2.50	0.45
1:Q:92:MET:HB3	1:Q:114:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLY:CA	1:B:186:ASP:OD2	2.64	0.45
1:T:40:ALA:O	1:T:44:VAL:HG23	2.17	0.45
1:W:120:MET:CE	1:W:173:PHE:CD2	2.99	0.45
1:D:161:LEU:O	1:D:162:GLU:C	2.54	0.45
1:O:157:THR:CG2	1:O:184:LEU:HD13	2.47	0.45
1:B:84:LYS:HB2	1:B:85:PRO:HD3	1.99	0.45
1:H:39:MET:O	1:H:43:ILE:HD13	2.16	0.45
1:A:70:ILE:HD11	1:A:123:GLN:NE2	2.30	0.45
1:B:95:ALA:O	1:B:100:ALA:HB2	2.17	0.45
1:T:77:TYR:OH	1:T:152:LEU:HD22	2.17	0.45
1:M:47:MET:HE1	1:M:61:LEU:HD22	1.99	0.45
1:M:139:CYS:HA	1:M:142:ILE:HG22	1.98	0.45
1:L:98:MET:HE3	1:L:101:PHE:HD2	1.82	0.45
1:P:26:GLU:HB2	1:P:28:VAL:HG23	1.99	0.45
1:H:96:ALA:HB1	1:H:120:MET:CE	2.43	0.45
1:I:167:ASP:O	1:I:170:ARG:O	2.35	0.45
1:Q:121:ILE:O	1:Q:122:HIS:CB	2.65	0.45
1:1:79:THR:O	1:1:83:ILE:HG23	2.16	0.45
1:R:95:ALA:O	1:R:100:ALA:HB2	2.17	0.45
1:F:114:LEU:O	1:F:117:SER:OG	2.30	0.45
1:U:66:PRO:HA	1:U:96:ALA:HB3	1.98	0.45
1:M:50:LEU:HB3	1:M:59:ILE:HD11	1.98	0.44
1:J:98:MET:HE2	1:J:102:LEU:HG	1.98	0.44
1:F:101:PHE:HA	1:F:153:MET:CE	2.45	0.44
1:U:101:PHE:O	1:U:104:THR:HG22	2.17	0.44
1:N:113:CYS:O	1:N:188:ILE:HG23	2.16	0.44
1:F:151:GLU:HA	1:F:161:LEU:HD13	1.99	0.44
1:H:192:ARG:HB3	1:N:84:LYS:HG2	1.99	0.44
1:W:174:LEU:HD22	1:W:178:GLU:HB3	1.99	0.44
1:Z:164:ILE:O	1:Z:168:THR:HG23	2.16	0.44
1:U:139:CYS:HA	1:U:142:ILE:HG22	1.99	0.44
1:R:119:VAL:HG11	1:R:184:LEU:HD13	2.00	0.44
1:W:176:ALA:O	1:W:180:VAL:HG23	2.17	0.44
1:C:69:VAL:HG12	1:C:71:THR:HB	1.99	0.44
1:G:176:ALA:HB3	1:G:177:PRO:HD3	1.99	0.44
1:W:77:TYR:O	1:W:81:GLN:HG2	2.17	0.44
1:E:112:PHE:CD1	1:E:189:LEU:HD13	2.53	0.44
1:U:165:GLU:HA	1:U:168:THR:HG22	2.00	0.44
1:Y:113:CYS:SG	1:Y:185:VAL:HG21	2.57	0.44
1:L:63:ILE:HD12	1:L:63:ILE:N	2.32	0.44
1:C:70:ILE:O	1:C:74:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:TYR:CZ	1:H:90:ILE:HD12	2.51	0.44
1:S:154:ALA:HB1	1:S:159:GLN:O	2.18	0.44
1:U:98:MET:HE3	1:U:101:PHE:CD2	2.52	0.44
1:H:180:VAL:HG22	1:H:185:VAL:HG23	1.99	0.44
1:K:31:LEU:HD22	1:K:43:ILE:HD12	1.99	0.44
1:L:113:CYS:SG	1:L:185:VAL:HG21	2.57	0.44
1:R:121:ILE:HB	1:R:168:THR:HG22	1.99	0.44
1:M:62:TYR:CE2	1:M:90:ILE:HG21	2.52	0.44
1:O:190:THR:HG23	1:O:191:HIS:N	2.32	0.44
1:2:176:ALA:HB3	1:2:177:PRO:CD	2.48	0.44
1:Q:121:ILE:HD11	1:Q:167:ASP:HB3	2.00	0.44
1:1:77:TYR:OH	1:1:152:LEU:HD22	2.17	0.44
1:S:74:MET:HE3	1:S:74:MET:HA	1.99	0.44
1:O:95:ALA:O	1:O:100:ALA:HB2	2.18	0.44
1:J:123:GLN:HA	1:J:124:PRO:HD3	1.83	0.44
1:Z:176:ALA:N	1:Z:177:PRO:HD2	2.32	0.44
1:D:84:LYS:N	1:D:85:PRO:CD	2.81	0.44
1:C:113:CYS:SG	1:C:185:VAL:HG21	2.58	0.44
1:R:141:GLU:O	1:R:145:VAL:HG23	2.18	0.44
1:Z:49:PHE:HB2	1:1:19:ILE:HD11	1.99	0.44
1:2:73:GLY:O	1:2:102:LEU:HD21	2.18	0.44
1:L:122:HIS:O	1:L:123:GLN:HB2	2.18	0.44
1:1:167:ASP:O	1:1:170:ARG:O	2.35	0.44
1:W:91:CYS:SG	1:W:95:ALA:HB2	2.58	0.44
1:A:82:PHE:CE1	1:B:189:LEU:HD22	2.53	0.44
1:I:30:PHE:CD1	1:I:62:TYR:HB2	2.53	0.44
1:M:89:THR:OG1	1:M:103:LEU:HD12	2.18	0.44
1:W:169:GLU:HG3	1:W:170:ARG:HG2	1.99	0.44
1:C:119:VAL:HG11	1:C:184:LEU:HD13	1.99	0.43
1:E:73:GLY:HA3	1:E:98:MET:HE2	2.00	0.43
1:X:121:ILE:O	1:X:122:HIS:HB3	2.18	0.43
1:H:137:ILE:HD12	1:I:170:ARG:CD	2.48	0.43
1:K:46:GLN:HG3	1:L:19:ILE:HD13	2.00	0.43
1:K:95:ALA:O	1:K:100:ALA:HB2	2.18	0.43
1:N:19:ILE:HG23	1:N:20:TYR:N	2.33	0.43
1:F:89:THR:HB	1:F:103:LEU:HD12	1.99	0.43
1:G:122:HIS:CG	1:G:123:GLN:N	2.86	0.43
1:2:89:THR:C	1:2:90:ILE:HD12	2.38	0.43
1:Q:42:LEU:HD22	1:R:20:TYR:OH	2.18	0.43
1:B:39:MET:O	1:B:43:ILE:HD12	2.18	0.43
1:X:90:ILE:HD12	1:X:90:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:CYS:HB2	1:O:103:LEU:CD2	2.48	0.43
1:V:182:TYR:CD2	1:V:184:LEU:HD12	2.52	0.43
1:H:190:THR:HG22	1:H:191:HIS:HD2	1.82	0.43
1:F:153:MET:HG2	1:F:164:ILE:HD12	1.99	0.43
1:O:104:THR:HB	1:O:184:LEU:HD12	2.00	0.43
1:L:49:PHE:CE1	1:M:22:ARG:HG2	2.53	0.43
1:W:120:MET:HE1	1:W:173:PHE:CD2	2.53	0.43
1:2:142:ILE:HD11	1:2:146:LYS:HZ1	1.81	0.43
1:U:119:VAL:CG1	1:U:174:LEU:HB2	2.48	0.43
1:2:91:CYS:HB2	1:2:103:LEU:HD22	2.00	0.43
1:2:98:MET:HE3	1:2:101:PHE:CD2	2.54	0.43
1:Z:104:THR:HG21	1:Z:157:THR:HG22	2.00	0.43
1:O:139:CYS:SG	1:Z:139:CYS:SG	3.06	0.43
1:F:104:THR:HG21	1:F:153:MET:HE3	2.00	0.43
1:L:176:ALA:N	1:L:177:PRO:HD2	2.33	0.43
1:B:122:HIS:O	1:B:123:GLN:CB	2.66	0.43
1:L:98:MET:HE3	1:L:101:PHE:CD2	2.52	0.43
1:K:78:ASP:HB3	1:L:114:LEU:HD23	2.00	0.43
1:M:80:MET:HG2	1:M:87:VAL:HG11	2.01	0.43
1:B:76:ILE:HB	1:B:102:LEU:HD11	2.01	0.43
1:P:42:LEU:HD12	1:Q:20:TYR:CE2	2.53	0.43
1:O:154:ALA:CB	1:O:164:ILE:HD12	2.49	0.43
1:T:89:THR:HB	1:T:103:LEU:HD12	2.00	0.43
1:L:29:ILE:HD11	1:L:50:LEU:CD1	2.48	0.43
1:W:176:ALA:N	1:W:177:PRO:HD2	2.33	0.43
1:D:139:CYS:HB3	1:K:143:LEU:HD21	2.01	0.43
1:I:94:GLN:HA	1:I:118:ARG:O	2.19	0.43
1:L:51:GLU:OE1	1:L:83:ILE:HG22	2.18	0.43
1:E:84:LYS:HG2	1:F:192:ARG:HG2	2.00	0.43
1:K:66:PRO:HA	1:K:96:ALA:HB3	2.01	0.43
1:Y:119:VAL:CG1	1:Y:120:MET:N	2.82	0.42
1:V:27:ARG:HG2	1:V:50:LEU:HD22	2.00	0.42
1:Q:121:ILE:CG2	1:Q:153:MET:HE1	2.49	0.42
1:F:113:CYS:SG	1:F:185:VAL:HG21	2.58	0.42
1:D:153:MET:HG2	1:D:164:ILE:HD12	2.00	0.42
1:H:70:ILE:HG23	1:H:98:MET:HE1	2.00	0.42
1:K:174:LEU:HD23	1:K:184:LEU:HD12	2.01	0.42
1:G:121:ILE:HG22	1:G:168:THR:HA	2.01	0.42
1:2:95:ALA:O	1:2:100:ALA:HB2	2.19	0.42
1:B:119:VAL:HG11	1:B:184:LEU:HD13	2.00	0.42
1:R:66:PRO:HA	1:R:96:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:77:TYR:OH	1:X:152:LEU:HD22	2.19	0.42
1:Z:112:PHE:CD1	1:Z:189:LEU:HD13	2.54	0.42
1:I:140:ARG:HH22	1:O:161:LEU:HD12	1.84	0.42
1:O:119:VAL:HG11	1:O:184:LEU:HD21	2.01	0.42
1:H:137:ILE:HD12	1:I:170:ARG:CG	2.49	0.42
1:A:97:SER:OG	1:A:98:MET:N	2.50	0.42
1:H:45:ALA:O	1:I:23:LEU:HD11	2.19	0.42
1:A:118:ARG:HE	1:G:71:THR:HG22	1.83	0.42
1:U:29:ILE:HG21	1:U:43:ILE:HG23	2.02	0.42
1:D:96:ALA:HB1	1:D:120:MET:CE	2.50	0.42
1:T:176:ALA:N	1:T:177:PRO:HD2	2.34	0.42
1:O:91:CYS:HB2	1:O:103:LEU:HD22	2.00	0.42
1:V:121:ILE:CG2	1:V:168:THR:HG22	2.49	0.42
1:D:31:LEU:HD21	1:D:76:ILE:HD13	2.02	0.42
1:Q:44:VAL:HG23	1:Q:76:ILE:HD13	2.01	0.42
1:J:47:MET:HE1	1:J:87:VAL:CG2	2.49	0.42
1:Q:153:MET:HB3	1:Q:164:ILE:HD12	2.02	0.42
1:V:115:PRO:HD3	1:V:189:LEU:O	2.20	0.42
1:C:95:ALA:O	1:C:100:ALA:HB2	2.19	0.42
1:M:41:ASN:ND2	1:N:32:THR:OG1	2.52	0.42
1:I:19:ILE:CG2	1:I:20:TYR:N	2.83	0.42
1:Q:176:ALA:N	1:Q:177:PRO:HD2	2.34	0.42
1:S:146:LYS:NZ	1:S:150:ASN:HD21	2.17	0.42
1:X:104:THR:HA	1:X:111:ARG:HD2	2.02	0.42
1:T:120:MET:HE3	1:T:171:ASP:CA	2.49	0.42
1:E:173:PHE:C	1:E:174:LEU:HD12	2.39	0.42
1:S:177:PRO:HA	1:S:188:ILE:HD11	2.02	0.42
1:O:23:LEU:HD11	1:U:45:ALA:O	2.19	0.42
1:M:50:LEU:CB	1:M:59:ILE:HD11	2.49	0.42
1:P:76:ILE:CG2	1:P:102:LEU:HD22	2.50	0.42
1:S:66:PRO:O	1:S:96:ALA:HB3	2.19	0.42
1:Q:18:ASP:OD2	1:Q:18:ASP:C	2.58	0.42
1:Z:157:THR:HG22	1:Z:184:LEU:HD23	2.00	0.42
1:H:114:LEU:HD23	1:N:78:ASP:HB3	2.02	0.42
1:L:31:LEU:HD11	1:L:35:VAL:HG22	2.00	0.42
1:R:43:ILE:HB	1:R:76:ILE:HD11	2.00	0.42
1:T:120:MET:HE2	1:T:122:HIS:CG	2.55	0.42
1:K:70:ILE:HD11	1:K:149:MET:HE1	2.02	0.42
1:U:97:SER:OG	1:U:98:MET:N	2.50	0.42
1:2:176:ALA:N	1:2:177:PRO:HD2	2.35	0.42
1:C:62:TYR:HA	1:C:90:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:26:GLU:HB2	1:W:28:VAL:HG23	2.01	0.42
1:N:59:ILE:CD1	1:N:87:VAL:HG22	2.48	0.42
1:N:123:GLN:HE21	1:N:123:GLN:HB2	1.71	0.42
1:S:47:MET:HB3	1:S:83:ILE:HD13	2.01	0.42
1:M:89:THR:HB	1:M:103:LEU:HD12	2.02	0.42
1:O:63:ILE:HD12	1:O:103:LEU:HA	2.02	0.42
1:D:190:THR:HG23	1:D:191:HIS:H	1.85	0.42
1:A:44:VAL:HG13	1:A:79:THR:OG1	2.20	0.42
1:M:95:ALA:O	1:M:100:ALA:HB2	2.19	0.42
1:B:73:GLY:HA3	1:B:98:MET:HE2	2.02	0.41
1:W:91:CYS:HG	1:W:117:SER:HG	1.68	0.41
1:L:66:PRO:HA	1:L:96:ALA:HB3	2.02	0.41
1:N:43:ILE:HA	1:N:46:GLN:HE21	1.85	0.41
1:G:84:LYS:N	1:G:85:PRO:CD	2.83	0.41
1:X:176:ALA:O	1:X:179:ALA:HB3	2.20	0.41
1:K:89:THR:HG23	1:K:106:GLY:HA3	2.03	0.41
1:E:74:MET:CE	1:F:116:ASN:HB3	2.50	0.41
1:W:155:LEU:HD23	1:W:155:LEU:C	2.41	0.41
1:J:176:ALA:O	1:J:180:VAL:HG23	2.21	0.41
1:V:47:MET:CE	1:V:61:LEU:HD22	2.50	0.41
1:M:180:VAL:HG22	1:M:185:VAL:HG23	2.01	0.41
1:M:189:LEU:HD23	1:M:189:LEU:C	2.40	0.41
1:Q:51:GLU:OE1	1:Q:83:ILE:HG22	2.20	0.41
1:J:122:HIS:CE1	1:J:170:ARG:HA	2.55	0.41
1:Z:84:LYS:N	1:Z:85:PRO:HD2	2.35	0.41
1:D:176:ALA:N	1:D:177:PRO:HD2	2.35	0.41
1:P:145:VAL:O	1:P:149:MET:HG2	2.19	0.41
1:M:89:THR:CB	1:M:103:LEU:HD12	2.51	0.41
1:K:180:VAL:HG22	1:K:185:VAL:HG13	2.03	0.41
1:O:192:ARG:HB3	1:U:84:LYS:HG3	2.02	0.41
1:X:157:THR:HG22	1:X:184:LEU:HA	2.03	0.41
1:P:45:ALA:HB3	1:Q:19:ILE:HD11	2.03	0.41
1:O:39:MET:HE2	1:O:39:MET:C	2.41	0.41
1:Z:28:VAL:HG22	1:Z:60:TYR:HB2	2.02	0.41
1:T:24:LEU:HD11	1:T:50:LEU:HD11	2.03	0.41
1:2:174:LEU:HD12	1:2:184:LEU:HD12	2.02	0.41
1:P:45:ALA:CB	1:Q:19:ILE:HD12	2.51	0.41
1:O:101:PHE:O	1:O:104:THR:HG22	2.21	0.41
1:T:148:ARG:HH11	1:T:152:LEU:HD11	1.84	0.41
1:P:123:GLN:N	1:P:124:PRO:HD3	2.36	0.41
1:N:176:ALA:HB3	1:N:177:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:49:PHE:O	1:S:52:ALA:HB3	2.21	0.41
1:Y:148:ARG:HE	1:Z:116:ASN:ND2	2.19	0.41
1:X:139:CYS:CA	1:X:142:ILE:HG22	2.46	0.41
1:2:177:PRO:O	1:2:181:GLU:HG3	2.20	0.41
1:S:121:ILE:HB	1:S:168:THR:HG22	2.03	0.41
1:H:154:ALA:CA	1:H:157:THR:HG22	2.50	0.41
1:V:44:VAL:HG11	1:W:92:MET:CE	2.51	0.41
1:P:92:MET:HE2	1:P:92:MET:HB2	1.85	0.41
1:C:174:LEU:CD1	1:C:184:LEU:HD12	2.51	0.41
1:C:76:ILE:CG2	1:C:102:LEU:HD22	2.48	0.41
1:P:76:ILE:HG22	1:P:102:LEU:HD22	2.02	0.41
1:G:123:GLN:HB2	1:G:123:GLN:HE21	1.60	0.41
1:P:39:MET:HG3	1:P:40:ALA:N	2.36	0.41
1:P:176:ALA:HB3	1:P:177:PRO:CD	2.51	0.41
1:K:70:ILE:HD11	1:K:149:MET:CE	2.51	0.41
1:O:119:VAL:HG11	1:O:184:LEU:HD23	2.02	0.41
1:O:179:ALA:HB1	1:O:185:VAL:HG12	2.03	0.41
1:Z:49:PHE:CG	1:1:19:ILE:HD11	2.55	0.41
1:F:95:ALA:O	1:F:100:ALA:HB2	2.21	0.41
1:H:177:PRO:N	1:H:188:ILE:HD11	2.36	0.41
1:T:122:HIS:CG	1:T:123:GLN:N	2.88	0.41
1:Y:43:ILE:HG21	1:Y:76:ILE:HG23	2.03	0.41
1:M:89:THR:HG23	1:M:106:GLY:HA3	2.02	0.41
1:W:89:THR:HG23	1:W:106:GLY:HA3	2.02	0.41
1:Y:84:LYS:N	1:Y:85:PRO:HD2	2.36	0.41
1:1:62:TYR:CE1	1:1:90:ILE:HD12	2.56	0.40
1:E:120:MET:CE	1:E:173:PHE:CE1	3.04	0.40
1:Q:82:PHE:CZ	1:R:192:ARG:HD2	2.56	0.40
1:X:84:LYS:HB2	1:X:85:PRO:HD3	2.02	0.40
1:F:162:GLU:OE1	1:F:162:GLU:N	2.51	0.40
1:H:70:ILE:HG23	1:H:98:MET:HE3	2.02	0.40
1:M:180:VAL:CG2	1:M:188:ILE:HG13	2.49	0.40
1:V:74:MET:HE2	1:W:116:ASN:CB	2.51	0.40
1:1:176:ALA:N	1:1:177:PRO:HD2	2.37	0.40
1:U:63:ILE:HD12	1:U:103:LEU:HA	2.03	0.40
1:2:77:TYR:OH	1:2:152:LEU:HD22	2.22	0.40
1:Q:73:GLY:HA3	1:Q:98:MET:HE2	2.03	0.40
1:B:98:MET:HG3	1:B:102:LEU:HD23	2.02	0.40
1:A:121:ILE:O	1:A:122:HIS:HB3	2.22	0.40
1:N:114:LEU:HD13	1:N:189:LEU:O	2.22	0.40
1:T:66:PRO:O	1:T:96:ALA:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:N	1:A:177:PRO:HD2	2.37	0.40
1:E:72:ALA:O	1:E:75:SER:OG	2.39	0.40
1:S:95:ALA:O	1:S:100:ALA:HB2	2.21	0.40
1:P:45:ALA:HB1	1:Q:19:ILE:HD12	2.04	0.40
1:A:116:ASN:HB2	1:G:74:MET:HE2	2.04	0.40
1:H:116:ASN:ND2	1:N:148:ARG:HE	2.18	0.40
1:X:91:CYS:SG	1:X:92:MET:N	2.95	0.40
1:X:29:ILE:HD13	1:X:46:GLN:HB2	2.02	0.40
1:I:159:GLN:HB2	1:I:164:ILE:HD11	2.02	0.40
1:F:84:LYS:N	1:F:85:PRO:CD	2.85	0.40
1:U:54:ASN:HD22	1:U:55:PRO:HD2	1.87	0.40
1:Z:96:ALA:HB1	1:Z:120:MET:HE1	2.04	0.40
1:V:116:ASN:HD21	1:2:148:ARG:CZ	2.34	0.40
1:W:40:ALA:O	1:W:44:VAL:HG23	2.21	0.40
1:N:47:MET:HG2	1:N:59:ILE:HD12	2.02	0.40
1:X:31:LEU:HD22	1:X:39:MET:CE	2.51	0.40
1:M:96:ALA:HB1	1:M:120:MET:CE	2.51	0.40
1:G:121:ILE:HG22	1:G:168:THR:HG22	2.02	0.40
1:V:84:LYS:HB3	1:V:85:PRO:HD3	2.02	0.40
1:F:24:LEU:HD12	1:F:50:LEU:HD21	2.02	0.40
1:T:180:VAL:HG13	1:T:186:ASP:O	2.20	0.40
1:H:193:ASN:N	1:H:193:ASN:HD22	2.17	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	1	159/193 (82%)	155 (98%)	4 (2%)	0	100	100
1	2	158/193 (82%)	154 (98%)	3 (2%)	1 (1%)	30	75
1	A	158/193 (82%)	151 (96%)	5 (3%)	2 (1%)	15	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	158/193 (82%)	148 (94%)	8 (5%)	2 (1%)	15	59
1	C	158/193 (82%)	152 (96%)	5 (3%)	1 (1%)	30	75
1	D	161/193 (83%)	150 (93%)	8 (5%)	3 (2%)	10	50
1	E	158/193 (82%)	149 (94%)	8 (5%)	1 (1%)	30	75
1	F	162/193 (84%)	155 (96%)	6 (4%)	1 (1%)	30	75
1	G	158/193 (82%)	149 (94%)	8 (5%)	1 (1%)	30	75
1	H	160/193 (83%)	151 (94%)	9 (6%)	0	100	100
1	I	159/193 (82%)	150 (94%)	9 (6%)	0	100	100
1	J	159/193 (82%)	147 (92%)	12 (8%)	0	100	100
1	K	157/193 (81%)	146 (93%)	10 (6%)	1 (1%)	30	75
1	L	158/193 (82%)	148 (94%)	9 (6%)	1 (1%)	30	75
1	M	158/193 (82%)	146 (92%)	11 (7%)	1 (1%)	30	75
1	N	158/193 (82%)	147 (93%)	11 (7%)	0	100	100
1	O	162/193 (84%)	151 (93%)	9 (6%)	2 (1%)	16	60
1	P	159/193 (82%)	151 (95%)	8 (5%)	0	100	100
1	Q	158/193 (82%)	151 (96%)	6 (4%)	1 (1%)	30	75
1	R	158/193 (82%)	147 (93%)	11 (7%)	0	100	100
1	S	158/193 (82%)	144 (91%)	12 (8%)	2 (1%)	15	59
1	T	157/193 (81%)	150 (96%)	5 (3%)	2 (1%)	15	59
1	U	158/193 (82%)	146 (92%)	11 (7%)	1 (1%)	30	75
1	V	159/193 (82%)	150 (94%)	9 (6%)	0	100	100
1	W	157/193 (81%)	148 (94%)	8 (5%)	1 (1%)	30	75
1	X	157/193 (81%)	144 (92%)	13 (8%)	0	100	100
1	Y	159/193 (82%)	147 (92%)	11 (7%)	1 (1%)	30	75
1	Z	161/193 (83%)	147 (91%)	14 (9%)	0	100	100
All	All	4442/5404 (82%)	4174 (94%)	243 (6%)	25 (1%)	30	75

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	122	HIS
1	Q	122	HIS
1	B	169	GLU

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Mol	Chain	Res	Type
1	E	97	SER
1	M	97	SER
1	O	192	ARG
1	S	97	SER
1	A	97	SER
1	C	140	ARG
1	D	124	PRO
1	F	122	HIS
1	G	171	ASP
1	U	97	SER
1	W	169	GLU
1	2	97	SER
1	A	122	HIS
1	B	97	SER
1	D	162	GLU
1	L	108	LYS
1	O	97	SER
1	S	115	PRO
1	T	171	ASP
1	K	122	HIS
1	T	115	PRO
1	Y	93	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	140/164 (85%)	139 (99%)	1 (1%)	88 97
1	2	139/164 (85%)	135 (97%)	4 (3%)	50 83
1	A	139/164 (85%)	136 (98%)	3 (2%)	60 87
1	B	139/164 (85%)	135 (97%)	4 (3%)	50 83
1	C	139/164 (85%)	137 (99%)	2 (1%)	74 92
1	D	141/164 (86%)	136 (96%)	5 (4%)	43 80
1	E	139/164 (85%)	136 (98%)	3 (2%)	60 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	143/164 (87%)	142 (99%)	1 (1%)	88 97
1	G	139/164 (85%)	137 (99%)	2 (1%)	74 92
1	H	141/164 (86%)	141 (100%)	0	100 100
1	I	140/164 (85%)	136 (97%)	4 (3%)	50 83
1	J	140/164 (85%)	138 (99%)	2 (1%)	74 92
1	K	138/164 (84%)	136 (99%)	2 (1%)	74 92
1	L	139/164 (85%)	137 (99%)	2 (1%)	74 92
1	M	139/164 (85%)	138 (99%)	1 (1%)	88 97
1	N	139/164 (85%)	136 (98%)	3 (2%)	60 87
1	O	143/164 (87%)	138 (96%)	5 (4%)	43 80
1	P	140/164 (85%)	139 (99%)	1 (1%)	88 97
1	Q	139/164 (85%)	135 (97%)	4 (3%)	50 83
1	R	139/164 (85%)	138 (99%)	1 (1%)	88 97
1	S	139/164 (85%)	138 (99%)	1 (1%)	88 97
1	T	138/164 (84%)	136 (99%)	2 (1%)	74 92
1	U	139/164 (85%)	139 (100%)	0	100 100
1	V	140/164 (85%)	140 (100%)	0	100 100
1	W	138/164 (84%)	137 (99%)	1 (1%)	88 97
1	X	138/164 (84%)	135 (98%)	3 (2%)	60 87
1	Y	140/164 (85%)	138 (99%)	2 (1%)	74 92
1	Z	142/164 (87%)	141 (99%)	1 (1%)	88 97
All	All	3909/4592 (85%)	3849 (98%)	60 (2%)	72 91

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	34	GLN
1	A	39	MET
1	B	31	LEU
1	B	114	LEU
1	B	171	ASP
1	B	174	LEU
1	C	31	LEU
1	C	114	LEU

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Mol	Chain	Res	Type
1	D	31	LEU
1	D	121	ILE
1	D	122	HIS
1	D	139	CYS
1	D	171	ASP
1	E	122	HIS
1	E	139	CYS
1	E	169	GLU
1	F	190	THR
1	G	75	SER
1	G	123	GLN
1	I	31	LEU
1	I	36	GLU
1	I	122	HIS
1	I	139	CYS
1	J	23	LEU
1	J	171	ASP
1	K	31	LEU
1	K	174	LEU
1	L	167	ASP
1	L	171	ASP
1	M	185	VAL
1	N	39	MET
1	N	104	THR
1	N	123	GLN
1	O	39	MET
1	O	41	ASN
1	O	114	LEU
1	O	122	HIS
1	O	173	PHE
1	P	39	MET
1	Q	31	LEU
1	Q	123	GLN
1	Q	139	CYS
1	Q	193	ASN
1	R	31	LEU
1	S	139	CYS
1	T	39	MET
1	T	171	ASP
1	W	31	LEU
1	X	91	CYS
1	X	113	CYS

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Mol	Chain	Res	Type
1	X	122	HIS
1	Y	123	GLN
1	Y	139	CYS
1	Z	155	LEU
1	1	39	MET
1	2	123	GLN
1	2	139	CYS
1	2	167	ASP
1	2	187	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	122	HIS
1	A	123	GLN
1	A	156	HIS
1	A	191	HIS
1	A	193	ASN
1	B	34	GLN
1	B	41	ASN
1	B	94	GLN
1	B	191	HIS
1	C	34	GLN
1	C	41	ASN
1	C	81	GLN
1	C	116	ASN
1	C	163	GLN
1	D	41	ASN
1	D	116	ASN
1	D	122	HIS
1	D	156	HIS
1	D	163	GLN
1	E	34	GLN
1	E	41	ASN
1	E	94	GLN
1	E	123	GLN
1	E	156	HIS
1	F	41	ASN
1	F	54	ASN
1	G	41	ASN
1	G	123	GLN

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Mol	Chain	Res	Type
1	H	41	ASN
1	H	116	ASN
1	H	193	ASN
1	I	34	GLN
1	I	41	ASN
1	I	116	ASN
1	I	122	HIS
1	I	123	GLN
1	I	163	GLN
1	I	193	ASN
1	J	34	GLN
1	J	41	ASN
1	J	116	ASN
1	J	122	HIS
1	J	150	ASN
1	J	163	GLN
1	K	34	GLN
1	K	41	ASN
1	K	81	GLN
1	K	116	ASN
1	K	123	GLN
1	L	34	GLN
1	L	116	ASN
1	M	41	ASN
1	M	81	GLN
1	N	41	ASN
1	N	54	ASN
1	N	123	GLN
1	O	34	GLN
1	O	116	ASN
1	O	163	GLN
1	O	191	HIS
1	P	123	GLN
1	Q	41	ASN
1	Q	116	ASN
1	Q	191	HIS
1	Q	193	ASN
1	R	41	ASN
1	R	150	ASN
1	S	41	ASN
1	S	150	ASN
1	T	34	GLN

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Mol	Chain	Res	Type
1	T	41	ASN
1	T	46	GLN
1	T	81	GLN
1	T	116	ASN
1	U	41	ASN
1	U	54	ASN
1	U	163	GLN
1	V	41	ASN
1	V	116	ASN
1	V	156	HIS
1	W	163	GLN
1	X	41	ASN
1	X	116	ASN
1	X	138	HIS
1	Y	38	HIS
1	Y	41	ASN
1	Y	116	ASN
1	Y	123	GLN
1	Y	193	ASN
1	Z	116	ASN
1	Z	156	HIS
1	1	41	ASN
1	2	41	ASN
1	2	81	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	1	163/193 (84%)	0.46	1 (0%)	90	84	111, 117, 125, 128	0
1	2	162/193 (83%)	0.56	4 (2%)	61	47	107, 115, 122, 126	0
1	A	162/193 (83%)	0.51	6 (3%)	45	30	104, 112, 122, 125	0
1	B	162/193 (83%)	0.45	3 (1%)	70	55	103, 112, 122, 124	0
1	C	162/193 (83%)	0.44	0	100	100	100, 110, 121, 127	0
1	D	165/193 (85%)	0.54	2 (1%)	81	69	102, 111, 123, 132	0
1	E	162/193 (83%)	0.58	2 (1%)	81	69	107, 114, 124, 128	0
1	F	166/193 (86%)	0.51	3 (1%)	71	58	106, 112, 124, 129	0
1	G	162/193 (83%)	0.49	0	100	100	110, 117, 125, 129	0
1	H	164/193 (84%)	0.41	7 (4%)	39	25	118, 123, 129, 134	0
1	I	163/193 (84%)	0.53	4 (2%)	61	47	112, 118, 125, 131	0
1	J	163/193 (84%)	0.44	2 (1%)	81	69	109, 113, 120, 123	0
1	K	161/193 (83%)	0.50	4 (2%)	61	47	112, 117, 125, 128	0
1	L	162/193 (83%)	0.42	3 (1%)	70	55	113, 120, 129, 135	0
1	M	162/193 (83%)	0.32	3 (1%)	70	55	117, 122, 128, 132	0
1	N	162/193 (83%)	0.37	8 (4%)	33	20	116, 124, 130, 134	0
1	O	166/193 (86%)	0.47	1 (0%)	90	84	104, 112, 126, 135	0
1	P	163/193 (84%)	0.43	0	100	100	112, 117, 124, 130	0
1	Q	162/193 (83%)	0.41	6 (3%)	45	30	118, 123, 130, 132	0
1	R	162/193 (83%)	0.38	3 (1%)	70	55	121, 125, 132, 135	0
1	S	162/193 (83%)	0.46	7 (4%)	39	25	117, 122, 127, 130	0
1	T	161/193 (83%)	0.42	3 (1%)	70	55	116, 122, 129, 134	0
1	U	162/193 (83%)	0.51	1 (0%)	90	84	108, 118, 127, 132	0
1	V	163/193 (84%)	0.48	4 (2%)	61	47	105, 115, 125, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	W	161/193 (83%)	0.45	3 (1%)	70	55	111, 116, 122, 126	0
1	X	161/193 (83%)	0.50	6 (3%)	45	30	106, 116, 124, 126	0
1	Y	163/193 (84%)	0.51	5 (3%)	52	38	101, 109, 117, 124	0
1	Z	165/193 (85%)	0.46	4 (2%)	62	47	107, 117, 130, 136	0
All	All	4554/5404 (84%)	0.46	95 (2%)	67	52	100, 117, 127, 136	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	87	VAL	4.2
1	S	172	ARG	3.5
1	1	137	ILE	3.5
1	F	135	ILE	3.0
1	T	87	VAL	2.9
1	R	61	LEU	2.9
1	S	61	LEU	2.9
1	V	121	ILE	2.9
1	N	61	LEU	2.9
1	Y	189	LEU	2.8
1	X	120	MET	2.8
1	V	172	ARG	2.7
1	X	119	VAL	2.7
1	H	137	ILE	2.7
1	N	164	ILE	2.7
1	O	31	LEU	2.6
1	I	89	THR	2.6
1	X	76	ILE	2.6
1	Y	22	ARG	2.6
1	I	90	ILE	2.5
1	T	121	ILE	2.5
1	Q	142	ILE	2.5
1	B	174	LEU	2.5
1	L	189	LEU	2.5
1	Y	19	ILE	2.4
1	F	123	GLN	2.4
1	A	102	LEU	2.4
1	Q	121	ILE	2.4
1	Z	172	ARG	2.4
1	B	118	ARG	2.4
1	X	153	MET	2.4
1	A	44	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	61	LEU	2.4
1	Q	31	LEU	2.4
1	K	189	LEU	2.3
1	U	119	VAL	2.3
1	W	142	ILE	2.3
1	Z	30	PHE	2.3
1	W	61	LEU	2.3
1	I	61	LEU	2.3
1	X	87	VAL	2.3
1	S	170	ARG	2.3
1	M	87	VAL	2.3
1	Q	48	LEU	2.3
1	H	172	ARG	2.3
1	A	120	MET	2.3
1	H	31	LEU	2.3
1	2	29	ILE	2.3
1	N	69	VAL	2.2
1	M	184	LEU	2.2
1	N	118	ARG	2.2
1	A	184	LEU	2.2
1	K	19	ILE	2.2
1	S	87	VAL	2.2
1	L	105	ALA	2.2
1	Z	48	LEU	2.2
1	D	124	PRO	2.2
1	2	174	LEU	2.2
1	S	119	VAL	2.2
1	B	91	CYS	2.2
1	S	174	LEU	2.2
1	X	108	LYS	2.2
1	E	90	ILE	2.2
1	N	35	VAL	2.2
1	T	189	LEU	2.2
1	H	90	ILE	2.2
1	N	121	ILE	2.2
1	V	101	PHE	2.1
1	2	121	ILE	2.1
1	Q	76	ILE	2.1
1	2	91	CYS	2.1
1	J	63	ILE	2.1
1	Y	90	ILE	2.1
1	F	182	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	30	PHE	2.1
1	Y	89	THR	2.1
1	K	176	ALA	2.1
1	D	59	ILE	2.1
1	H	121	ILE	2.1
1	A	31	LEU	2.1
1	A	19	ILE	2.1
1	J	19	ILE	2.1
1	M	61	LEU	2.1
1	Q	59	ILE	2.1
1	W	35	VAL	2.1
1	K	121	ILE	2.1
1	L	121	ILE	2.0
1	E	61	LEU	2.0
1	Z	171	ASP	2.0
1	I	59	ILE	2.0
1	V	174	LEU	2.0
1	N	80	MET	2.0
1	R	48	LEU	2.0
1	H	92	MET	2.0
1	S	149	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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^{th} 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^2)	Q<0.9
2	CA	Z	215	1/1	0.21	0.42	2.80	182,182,182,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	E	218	1/1	0.50	0.31	0.79	155,155,155,155	0
2	CA	J	219	1/1	0.53	0.25	0.21	173,173,173,173	0
2	CA	I	204	1/1	0.54	0.20	-1.16	129,129,129,129	0
2	CA	I	203	1/1	0.87	0.12	-2.25	125,125,125,125	0
2	CA	M	220	1/1	0.62	0.33	-	176,176,176,176	0
2	CA	E	217	1/1	0.94	0.28	-	162,162,162,162	0
2	CA	1	205	1/1	0.75	0.31	-	154,154,154,154	0
2	CA	T	201	1/1	0.92	0.37	-	162,162,162,162	0
2	CA	J	206	1/1	0.92	0.22	-	109,109,109,109	0
2	CA	2	216	1/1	0.46	0.28	-	186,186,186,186	0
2	CA	V	221	1/1	0.82	0.18	-	177,177,177,177	0
2	CA	J	202	1/1	0.69	0.33	-	176,176,176,176	0

6.5 Other polymers (i)

There are no such residues in this entry.