Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 03:56 PM EDT

PDB ID	:	6BBF
Title	:	The CRAC channel Orai in an open conformation; H206A gain-of-function mutation
Authors	:	Long, S.B.; Hou, X.; Burstein, S.
Deposited on	:	2017-10-18
Resolution	:	6.71 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:

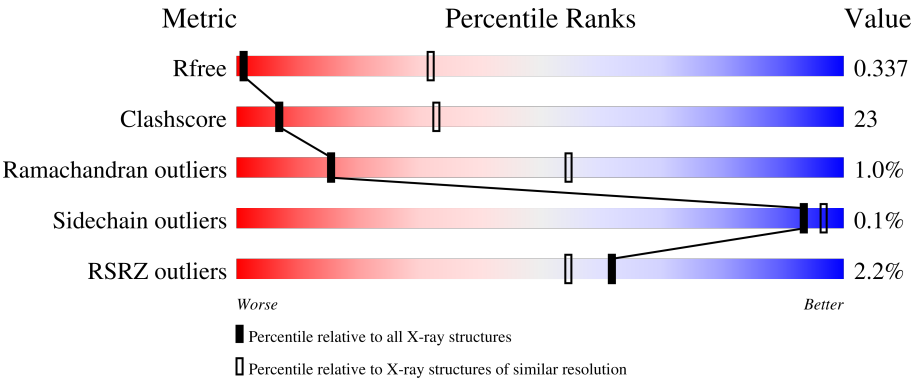
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 6.71 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}	130704	1002 (9.50-3.90)
Clashscore	141614	1066 (9.50-3.90)
Ramachandran outliers	138981	1000 (9.50-3.90)
Sidechain outliers	138945	1000 (9.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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 <=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	214	45% 24% 30%
1	B	214	48% 21% 30%
1	C	214	42% 28% 30%
1	D	214	44% 25% 30%
1	E	214	49% 21% 30%

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Mol	Chain	Length	Quality of chain
1	F	214	47% 23% 30%
1	G	214	5% 46% 23% 30%
1	H	214	46% 23% 30%
1	I	214	2% 41% 29% 30%
1	J	214	4% 44% 25% 30%
1	K	214	2% 48% 21% 30%
1	L	214	2% 44% 25% 30%
1	M	214	3% 42% 28% 30%
1	N	214	43% 27% 30%
1	O	214	43% 26% 30%
1	P	214	42% 27% 30%
1	Q	214	42% 27% 30%
1	R	214	44% 25% 30%
1	S	214	3% 42% 27% 30%
1	T	214	5% 43% 27% 30%
1	U	214	2% 44% 25% 30%
1	V	214	3% 43% 27% 30%
1	W	214	3% 40% 29% 30%
1	X	214	43% 27% 30%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 27120 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 Calcium release-activated calcium channel protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	B	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	C	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	D	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	E	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	F	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	G	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	H	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	I	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	J	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	K	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	L	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	M	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	N	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	O	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	P	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	R	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	S	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	T	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	U	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	V	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	W	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			
1	X	150	Total	C	N	O	S	0	0	0
			1130	753	176	190	11			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ALA	HIS	engineered mutation	UNP Q9U6B8
A	224	SER	CYS	engineered mutation	UNP Q9U6B8
A	283	THR	CYS	engineered mutation	UNP Q9U6B8
A	342	GLU	-	expression tag	UNP Q9U6B8
A	343	GLY	-	expression tag	UNP Q9U6B8
A	344	GLU	-	expression tag	UNP Q9U6B8
A	345	GLU	-	expression tag	UNP Q9U6B8
A	346	PHE	-	expression tag	UNP Q9U6B8
B	206	ALA	HIS	engineered mutation	UNP Q9U6B8
B	224	SER	CYS	engineered mutation	UNP Q9U6B8
B	283	THR	CYS	engineered mutation	UNP Q9U6B8
B	342	GLU	-	expression tag	UNP Q9U6B8
B	343	GLY	-	expression tag	UNP Q9U6B8
B	344	GLU	-	expression tag	UNP Q9U6B8
B	345	GLU	-	expression tag	UNP Q9U6B8
B	346	PHE	-	expression tag	UNP Q9U6B8
C	206	ALA	HIS	engineered mutation	UNP Q9U6B8
C	224	SER	CYS	engineered mutation	UNP Q9U6B8
C	283	THR	CYS	engineered mutation	UNP Q9U6B8
C	342	GLU	-	expression tag	UNP Q9U6B8
C	343	GLY	-	expression tag	UNP Q9U6B8
C	344	GLU	-	expression tag	UNP Q9U6B8
C	345	GLU	-	expression tag	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	346	PHE	-	expression tag	UNP Q9U6B8
D	206	ALA	HIS	engineered mutation	UNP Q9U6B8
D	224	SER	CYS	engineered mutation	UNP Q9U6B8
D	283	THR	CYS	engineered mutation	UNP Q9U6B8
D	342	GLU	-	expression tag	UNP Q9U6B8
D	343	GLY	-	expression tag	UNP Q9U6B8
D	344	GLU	-	expression tag	UNP Q9U6B8
D	345	GLU	-	expression tag	UNP Q9U6B8
D	346	PHE	-	expression tag	UNP Q9U6B8
E	206	ALA	HIS	engineered mutation	UNP Q9U6B8
E	224	SER	CYS	engineered mutation	UNP Q9U6B8
E	283	THR	CYS	engineered mutation	UNP Q9U6B8
E	342	GLU	-	expression tag	UNP Q9U6B8
E	343	GLY	-	expression tag	UNP Q9U6B8
E	344	GLU	-	expression tag	UNP Q9U6B8
E	345	GLU	-	expression tag	UNP Q9U6B8
E	346	PHE	-	expression tag	UNP Q9U6B8
F	206	ALA	HIS	engineered mutation	UNP Q9U6B8
F	224	SER	CYS	engineered mutation	UNP Q9U6B8
F	283	THR	CYS	engineered mutation	UNP Q9U6B8
F	342	GLU	-	expression tag	UNP Q9U6B8
F	343	GLY	-	expression tag	UNP Q9U6B8
F	344	GLU	-	expression tag	UNP Q9U6B8
F	345	GLU	-	expression tag	UNP Q9U6B8
F	346	PHE	-	expression tag	UNP Q9U6B8
G	206	ALA	HIS	engineered mutation	UNP Q9U6B8
G	224	SER	CYS	engineered mutation	UNP Q9U6B8
G	283	THR	CYS	engineered mutation	UNP Q9U6B8
G	342	GLU	-	expression tag	UNP Q9U6B8
G	343	GLY	-	expression tag	UNP Q9U6B8
G	344	GLU	-	expression tag	UNP Q9U6B8
G	345	GLU	-	expression tag	UNP Q9U6B8
G	346	PHE	-	expression tag	UNP Q9U6B8
H	206	ALA	HIS	engineered mutation	UNP Q9U6B8
H	224	SER	CYS	engineered mutation	UNP Q9U6B8
H	283	THR	CYS	engineered mutation	UNP Q9U6B8
H	342	GLU	-	expression tag	UNP Q9U6B8
H	343	GLY	-	expression tag	UNP Q9U6B8
H	344	GLU	-	expression tag	UNP Q9U6B8
H	345	GLU	-	expression tag	UNP Q9U6B8
H	346	PHE	-	expression tag	UNP Q9U6B8
I	206	ALA	HIS	engineered mutation	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	224	SER	CYS	engineered mutation	UNP Q9U6B8
I	283	THR	CYS	engineered mutation	UNP Q9U6B8
I	342	GLU	-	expression tag	UNP Q9U6B8
I	343	GLY	-	expression tag	UNP Q9U6B8
I	344	GLU	-	expression tag	UNP Q9U6B8
I	345	GLU	-	expression tag	UNP Q9U6B8
I	346	PHE	-	expression tag	UNP Q9U6B8
J	206	ALA	HIS	engineered mutation	UNP Q9U6B8
J	224	SER	CYS	engineered mutation	UNP Q9U6B8
J	283	THR	CYS	engineered mutation	UNP Q9U6B8
J	342	GLU	-	expression tag	UNP Q9U6B8
J	343	GLY	-	expression tag	UNP Q9U6B8
J	344	GLU	-	expression tag	UNP Q9U6B8
J	345	GLU	-	expression tag	UNP Q9U6B8
J	346	PHE	-	expression tag	UNP Q9U6B8
K	206	ALA	HIS	engineered mutation	UNP Q9U6B8
K	224	SER	CYS	engineered mutation	UNP Q9U6B8
K	283	THR	CYS	engineered mutation	UNP Q9U6B8
K	342	GLU	-	expression tag	UNP Q9U6B8
K	343	GLY	-	expression tag	UNP Q9U6B8
K	344	GLU	-	expression tag	UNP Q9U6B8
K	345	GLU	-	expression tag	UNP Q9U6B8
K	346	PHE	-	expression tag	UNP Q9U6B8
L	206	ALA	HIS	engineered mutation	UNP Q9U6B8
L	224	SER	CYS	engineered mutation	UNP Q9U6B8
L	283	THR	CYS	engineered mutation	UNP Q9U6B8
L	342	GLU	-	expression tag	UNP Q9U6B8
L	343	GLY	-	expression tag	UNP Q9U6B8
L	344	GLU	-	expression tag	UNP Q9U6B8
L	345	GLU	-	expression tag	UNP Q9U6B8
L	346	PHE	-	expression tag	UNP Q9U6B8
M	206	ALA	HIS	engineered mutation	UNP Q9U6B8
M	224	SER	CYS	engineered mutation	UNP Q9U6B8
M	283	THR	CYS	engineered mutation	UNP Q9U6B8
M	342	GLU	-	expression tag	UNP Q9U6B8
M	343	GLY	-	expression tag	UNP Q9U6B8
M	344	GLU	-	expression tag	UNP Q9U6B8
M	345	GLU	-	expression tag	UNP Q9U6B8
M	346	PHE	-	expression tag	UNP Q9U6B8
N	206	ALA	HIS	engineered mutation	UNP Q9U6B8
N	224	SER	CYS	engineered mutation	UNP Q9U6B8
N	283	THR	CYS	engineered mutation	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
N	342	GLU	-	expression tag	UNP Q9U6B8
N	343	GLY	-	expression tag	UNP Q9U6B8
N	344	GLU	-	expression tag	UNP Q9U6B8
N	345	GLU	-	expression tag	UNP Q9U6B8
N	346	PHE	-	expression tag	UNP Q9U6B8
O	206	ALA	HIS	engineered mutation	UNP Q9U6B8
O	224	SER	CYS	engineered mutation	UNP Q9U6B8
O	283	THR	CYS	engineered mutation	UNP Q9U6B8
O	342	GLU	-	expression tag	UNP Q9U6B8
O	343	GLY	-	expression tag	UNP Q9U6B8
O	344	GLU	-	expression tag	UNP Q9U6B8
O	345	GLU	-	expression tag	UNP Q9U6B8
O	346	PHE	-	expression tag	UNP Q9U6B8
P	206	ALA	HIS	engineered mutation	UNP Q9U6B8
P	224	SER	CYS	engineered mutation	UNP Q9U6B8
P	283	THR	CYS	engineered mutation	UNP Q9U6B8
P	342	GLU	-	expression tag	UNP Q9U6B8
P	343	GLY	-	expression tag	UNP Q9U6B8
P	344	GLU	-	expression tag	UNP Q9U6B8
P	345	GLU	-	expression tag	UNP Q9U6B8
P	346	PHE	-	expression tag	UNP Q9U6B8
Q	206	ALA	HIS	engineered mutation	UNP Q9U6B8
Q	224	SER	CYS	engineered mutation	UNP Q9U6B8
Q	283	THR	CYS	engineered mutation	UNP Q9U6B8
Q	342	GLU	-	expression tag	UNP Q9U6B8
Q	343	GLY	-	expression tag	UNP Q9U6B8
Q	344	GLU	-	expression tag	UNP Q9U6B8
Q	345	GLU	-	expression tag	UNP Q9U6B8
Q	346	PHE	-	expression tag	UNP Q9U6B8
R	206	ALA	HIS	engineered mutation	UNP Q9U6B8
R	224	SER	CYS	engineered mutation	UNP Q9U6B8
R	283	THR	CYS	engineered mutation	UNP Q9U6B8
R	342	GLU	-	expression tag	UNP Q9U6B8
R	343	GLY	-	expression tag	UNP Q9U6B8
R	344	GLU	-	expression tag	UNP Q9U6B8
R	345	GLU	-	expression tag	UNP Q9U6B8
R	346	PHE	-	expression tag	UNP Q9U6B8
S	206	ALA	HIS	engineered mutation	UNP Q9U6B8
S	224	SER	CYS	engineered mutation	UNP Q9U6B8
S	283	THR	CYS	engineered mutation	UNP Q9U6B8
S	342	GLU	-	expression tag	UNP Q9U6B8
S	343	GLY	-	expression tag	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
S	344	GLU	-	expression tag	UNP Q9U6B8
S	345	GLU	-	expression tag	UNP Q9U6B8
S	346	PHE	-	expression tag	UNP Q9U6B8
T	206	ALA	HIS	engineered mutation	UNP Q9U6B8
T	224	SER	CYS	engineered mutation	UNP Q9U6B8
T	283	THR	CYS	engineered mutation	UNP Q9U6B8
T	342	GLU	-	expression tag	UNP Q9U6B8
T	343	GLY	-	expression tag	UNP Q9U6B8
T	344	GLU	-	expression tag	UNP Q9U6B8
T	345	GLU	-	expression tag	UNP Q9U6B8
T	346	PHE	-	expression tag	UNP Q9U6B8
U	206	ALA	HIS	engineered mutation	UNP Q9U6B8
U	224	SER	CYS	engineered mutation	UNP Q9U6B8
U	283	THR	CYS	engineered mutation	UNP Q9U6B8
U	342	GLU	-	expression tag	UNP Q9U6B8
U	343	GLY	-	expression tag	UNP Q9U6B8
U	344	GLU	-	expression tag	UNP Q9U6B8
U	345	GLU	-	expression tag	UNP Q9U6B8
U	346	PHE	-	expression tag	UNP Q9U6B8
V	206	ALA	HIS	engineered mutation	UNP Q9U6B8
V	224	SER	CYS	engineered mutation	UNP Q9U6B8
V	283	THR	CYS	engineered mutation	UNP Q9U6B8
V	342	GLU	-	expression tag	UNP Q9U6B8
V	343	GLY	-	expression tag	UNP Q9U6B8
V	344	GLU	-	expression tag	UNP Q9U6B8
V	345	GLU	-	expression tag	UNP Q9U6B8
V	346	PHE	-	expression tag	UNP Q9U6B8
W	206	ALA	HIS	engineered mutation	UNP Q9U6B8
W	224	SER	CYS	engineered mutation	UNP Q9U6B8
W	283	THR	CYS	engineered mutation	UNP Q9U6B8
W	342	GLU	-	expression tag	UNP Q9U6B8
W	343	GLY	-	expression tag	UNP Q9U6B8
W	344	GLU	-	expression tag	UNP Q9U6B8
W	345	GLU	-	expression tag	UNP Q9U6B8
W	346	PHE	-	expression tag	UNP Q9U6B8
X	206	ALA	HIS	engineered mutation	UNP Q9U6B8
X	224	SER	CYS	engineered mutation	UNP Q9U6B8
X	283	THR	CYS	engineered mutation	UNP Q9U6B8
X	342	GLU	-	expression tag	UNP Q9U6B8
X	343	GLY	-	expression tag	UNP Q9U6B8
X	344	GLU	-	expression tag	UNP Q9U6B8
X	345	GLU	-	expression tag	UNP Q9U6B8

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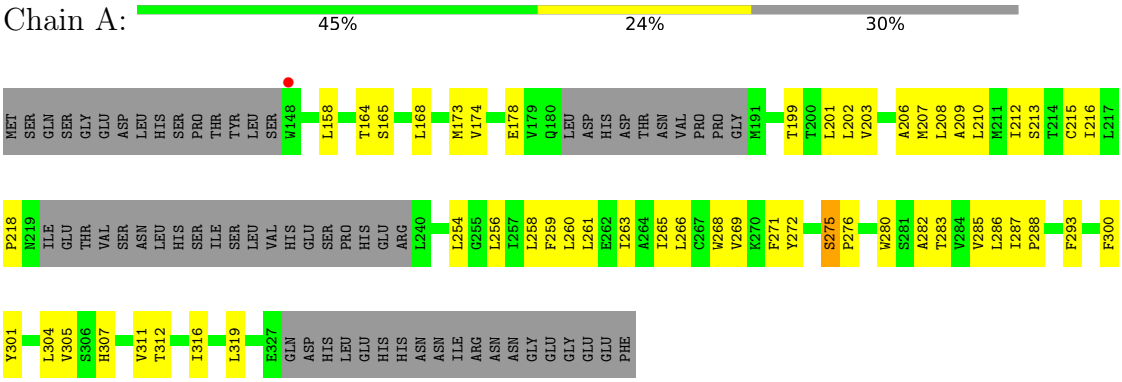
Chain	Residue	Modelled	Actual	Comment	Reference
X	346	PHE	-	expression tag	UNP Q9U6B8

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.

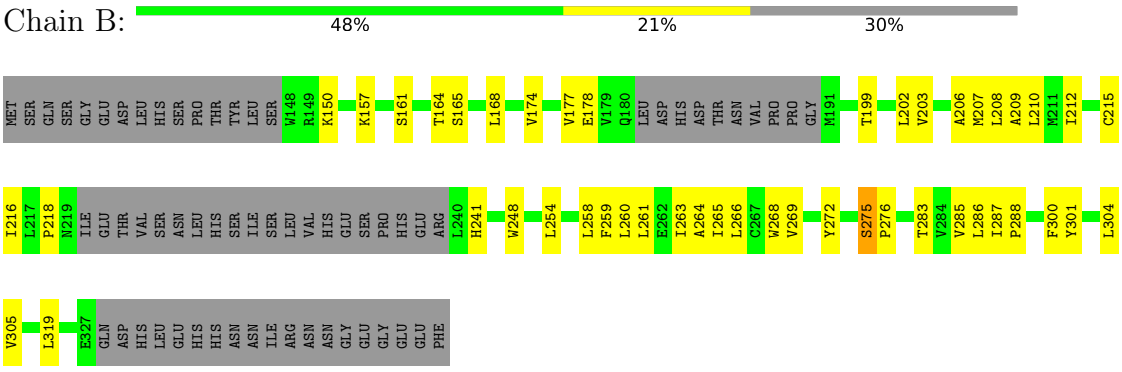
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain A:



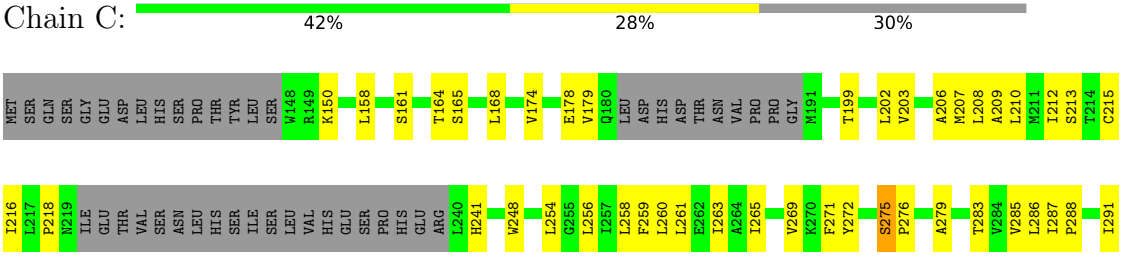
• Molecule 1: Calcium release-activated calcium channel protein 1

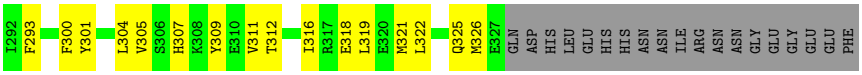
Chain B:



• Molecule 1: Calcium release-activated calcium channel protein 1

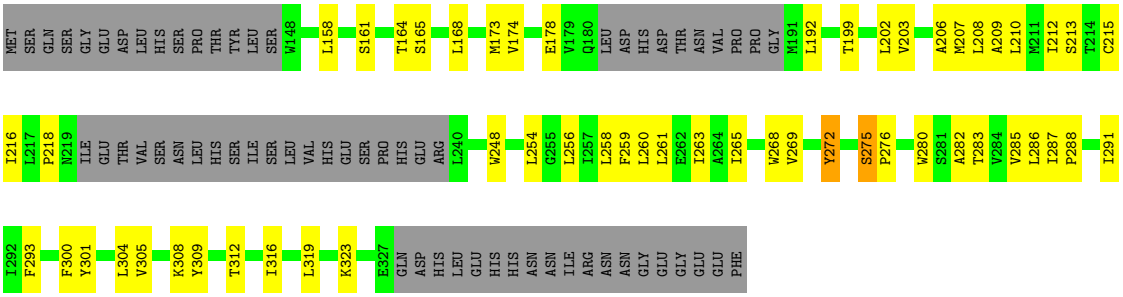
Chain C:





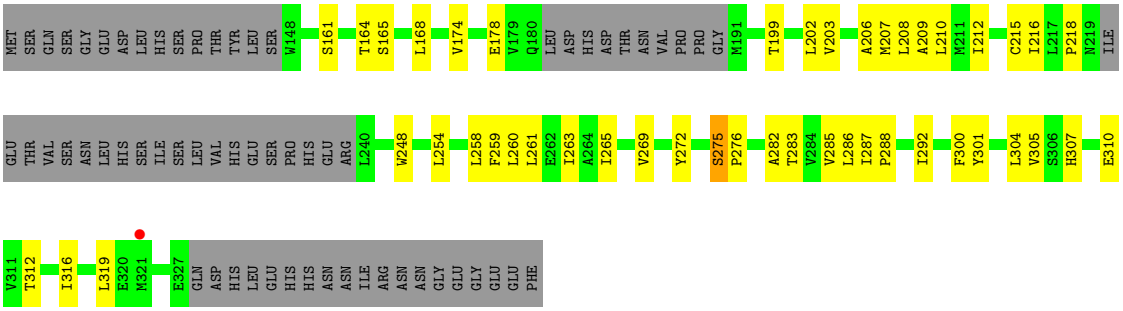
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain D:



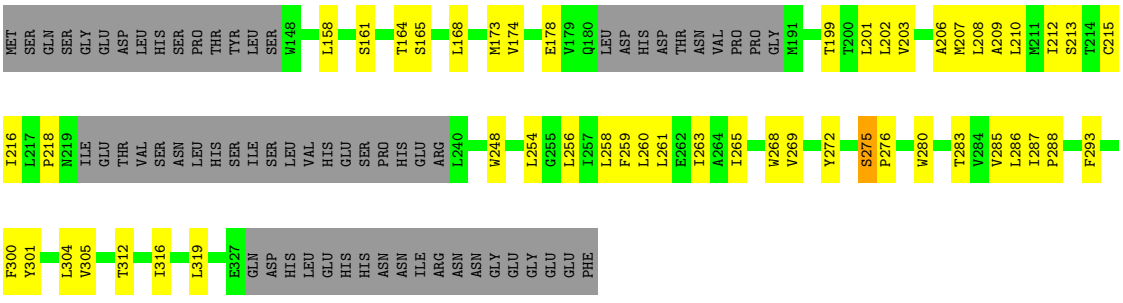
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain E:



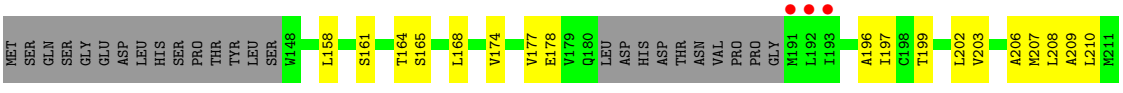
• Molecule 1: Calcium release-activated calcium channel protein 1

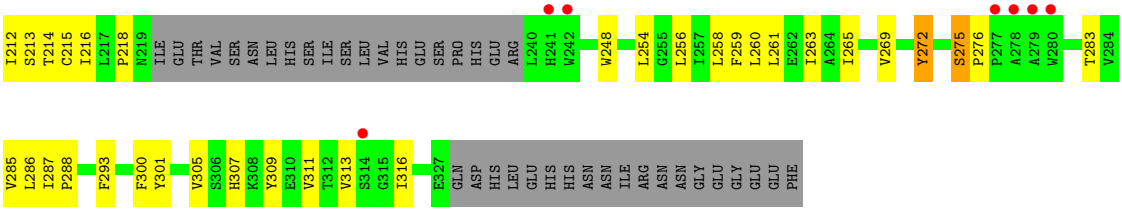
Chain F:



• Molecule 1: Calcium release-activated calcium channel protein 1

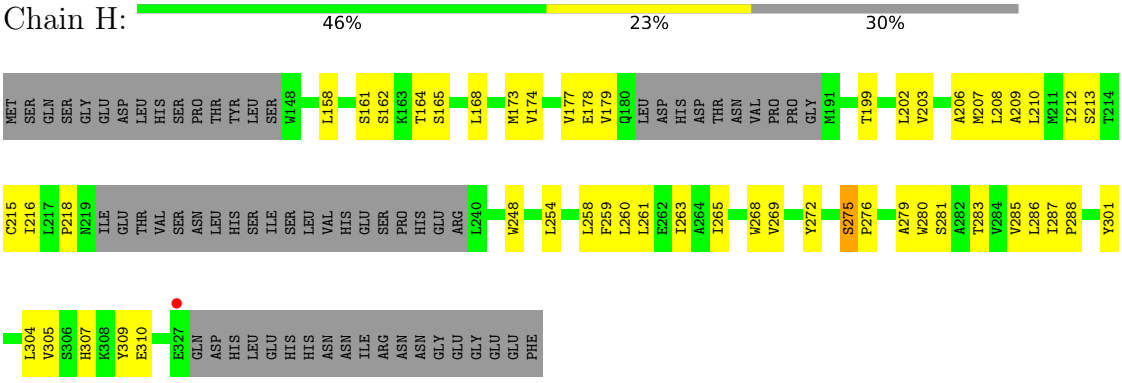
Chain G:





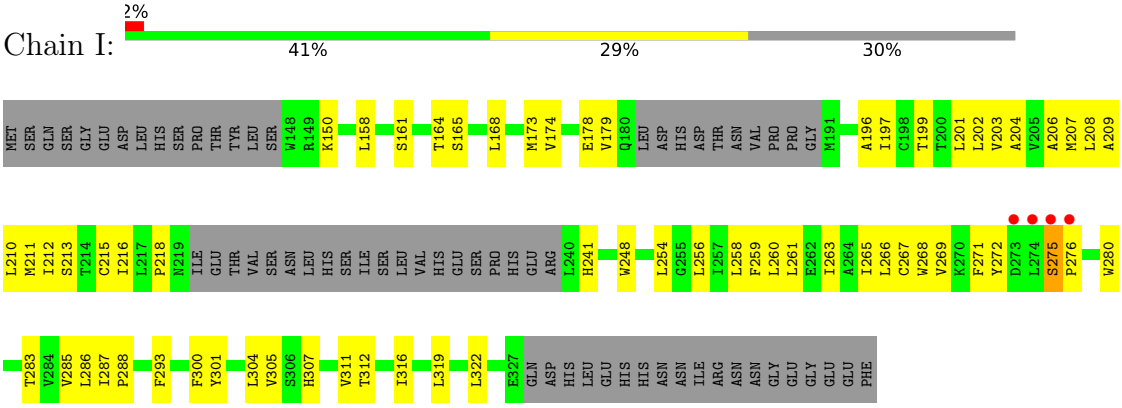
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain H:



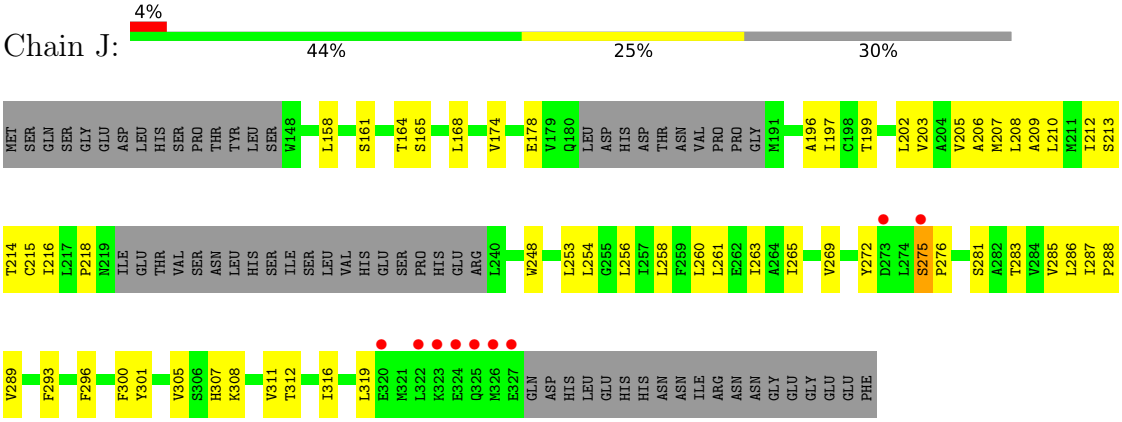
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain I:



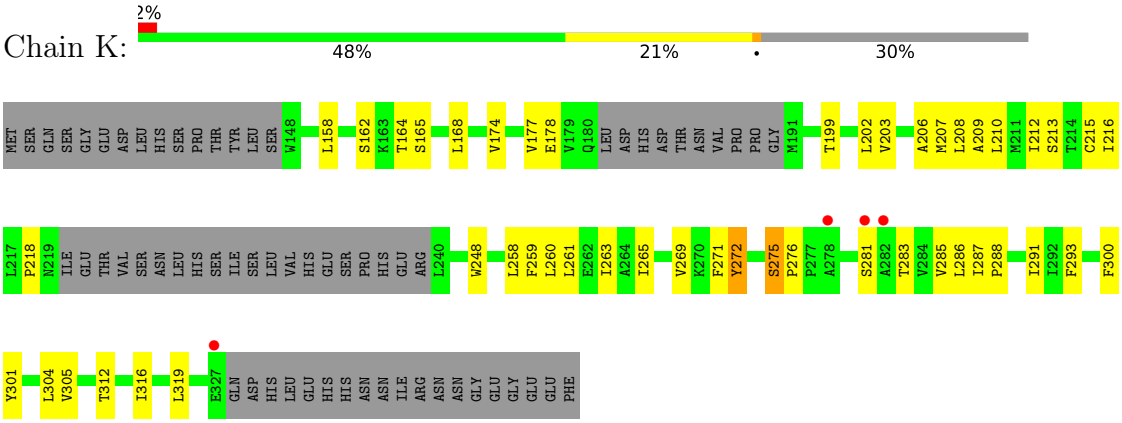
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain J:



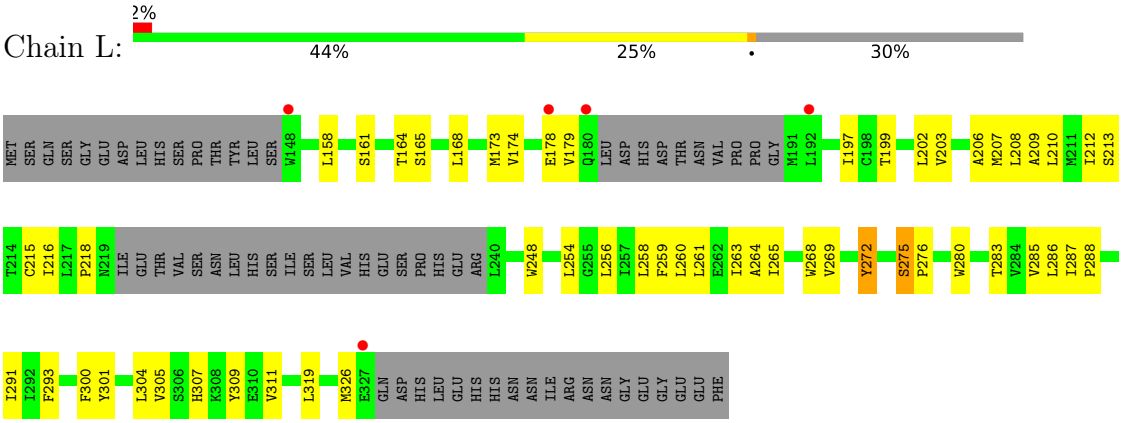
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain K:



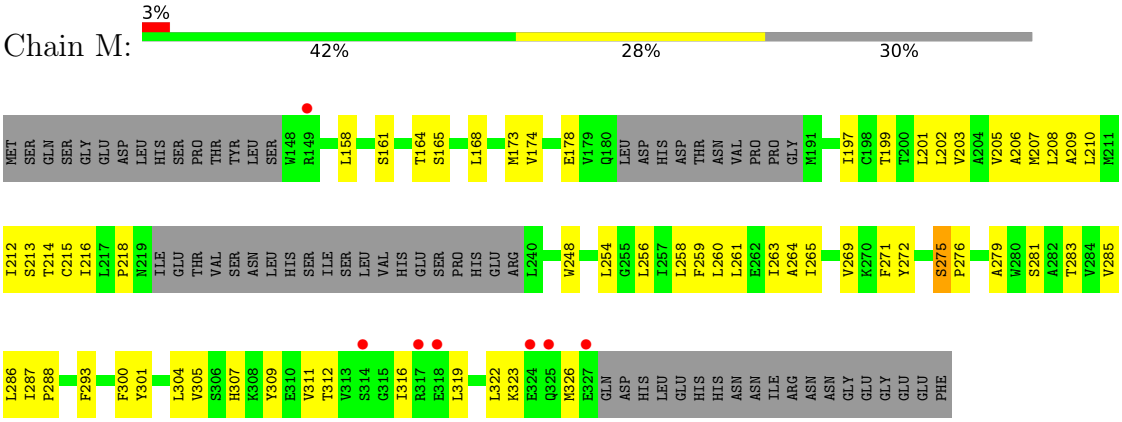
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain L:



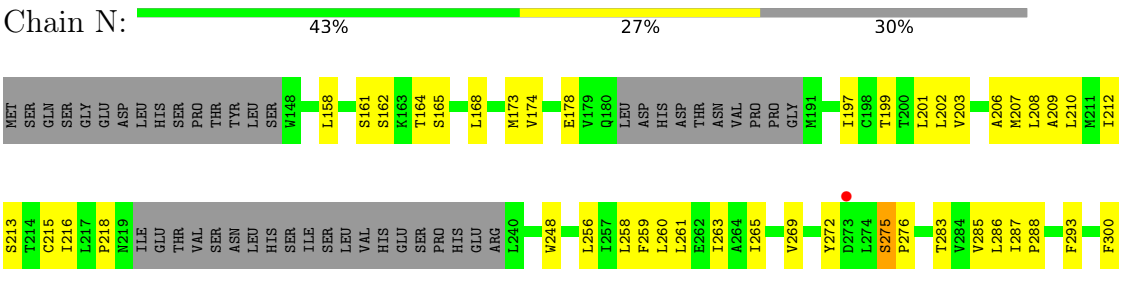
• Molecule 1: Calcium release-activated calcium channel protein 1

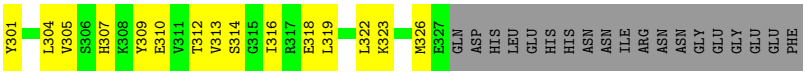
Chain M:



• Molecule 1: Calcium release-activated calcium channel protein 1

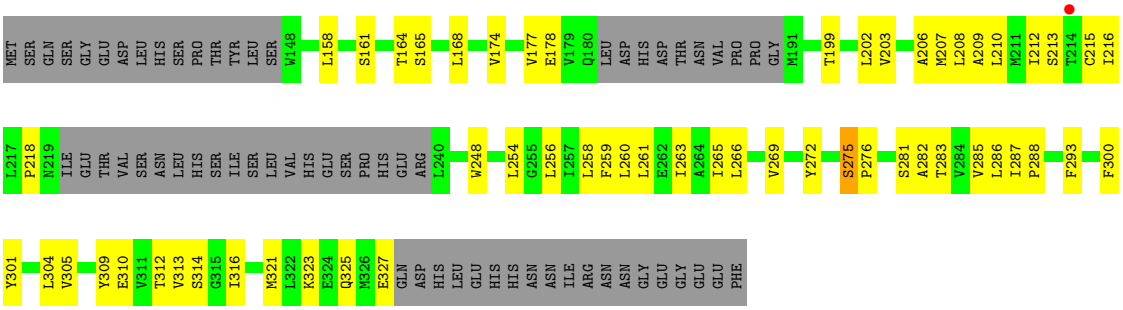
Chain N:





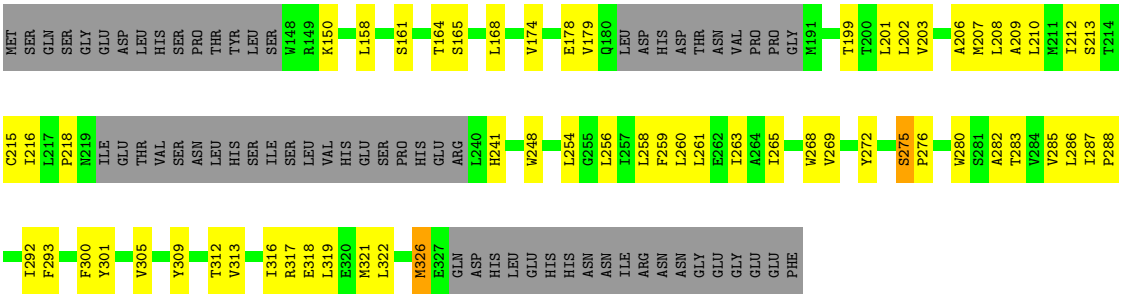
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain O:



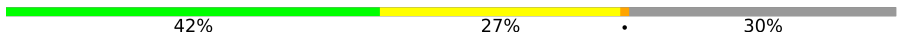
• Molecule 1: Calcium release-activated calcium channel protein 1

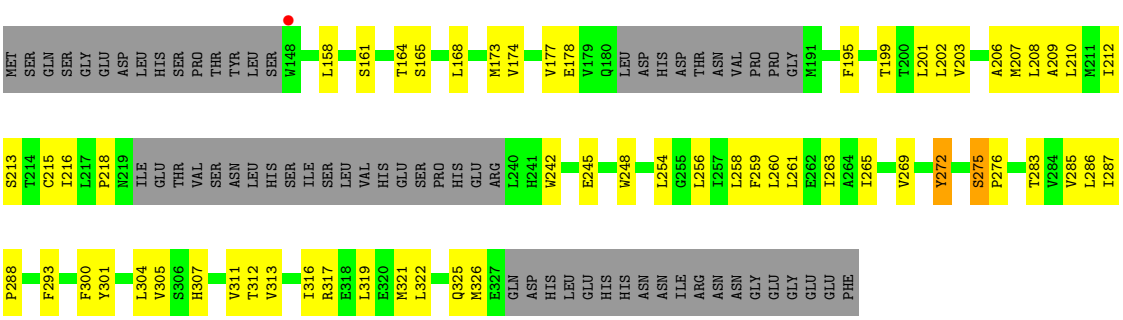
Chain P:



• Molecule 1: Calcium release-activated calcium channel protein 1

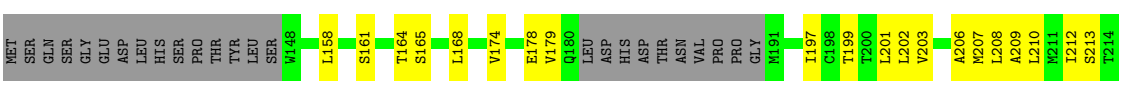
Chain Q:

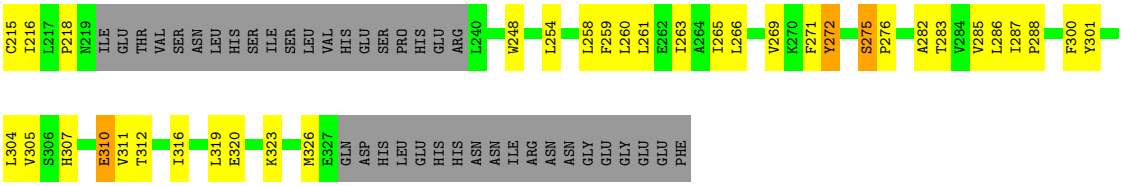




• Molecule 1: Calcium release-activated calcium channel protein 1

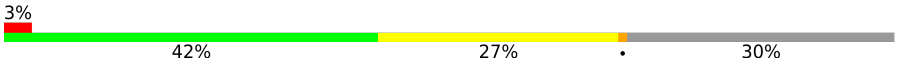
Chain R:

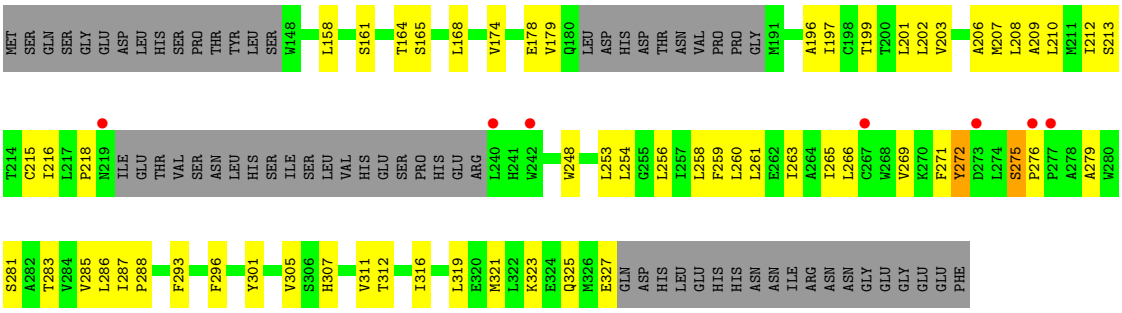




• Molecule 1: Calcium release-activated calcium channel protein 1

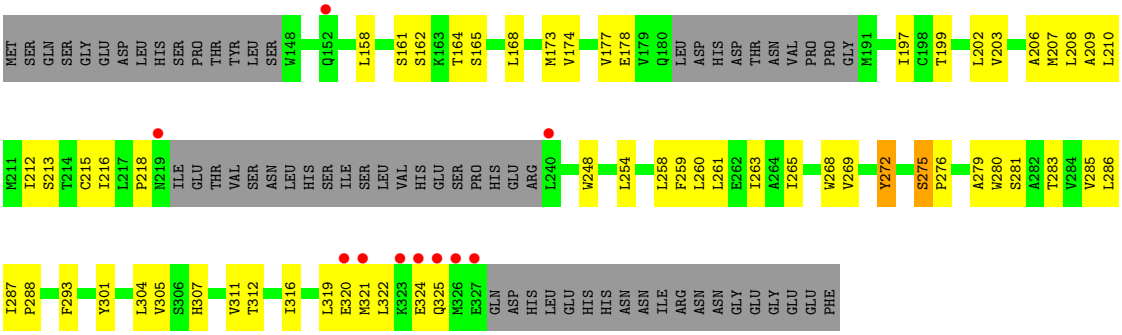
Chain S:





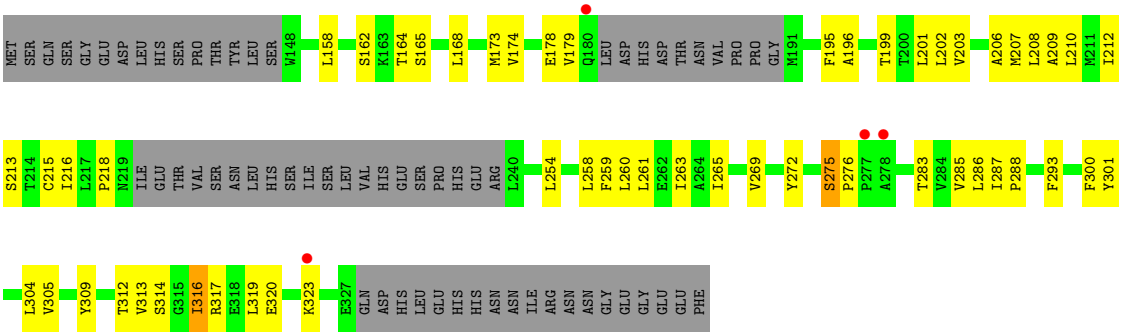
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain T:



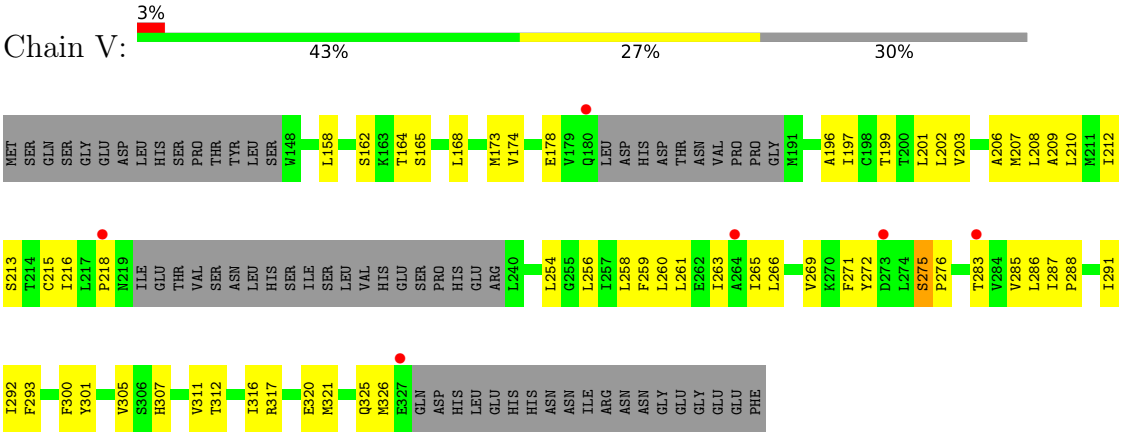
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain U:



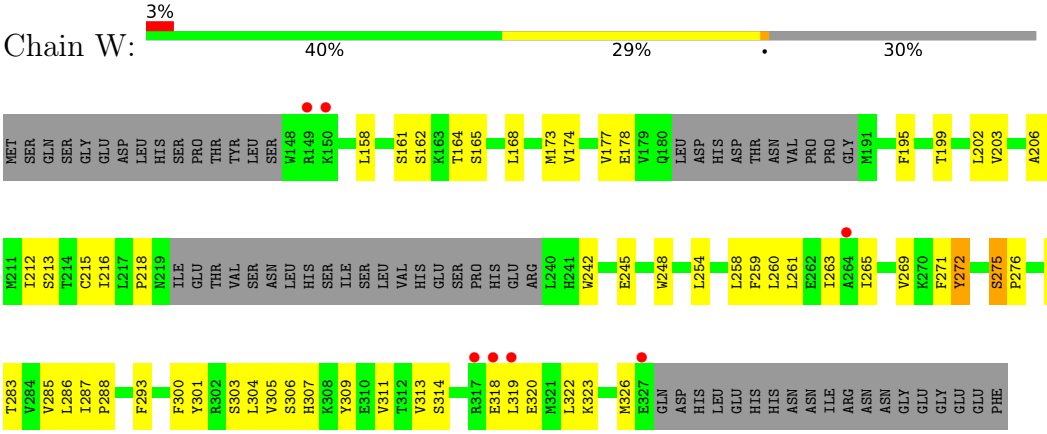
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain V:



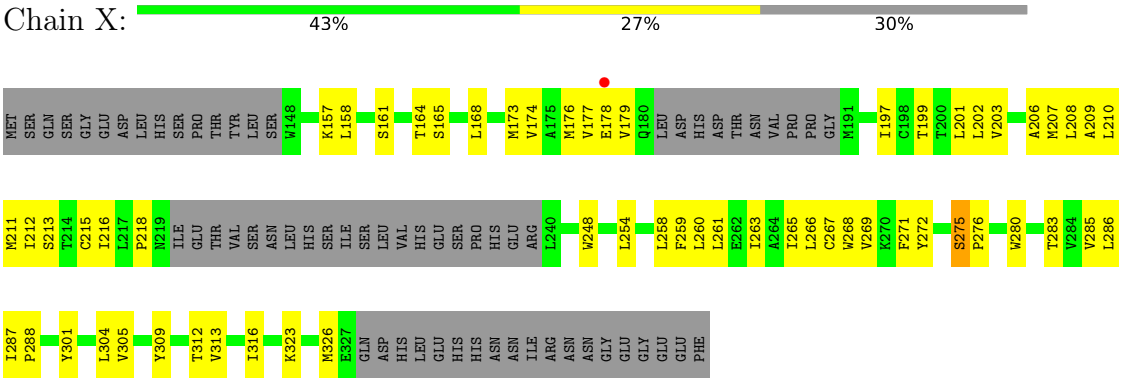
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain W:



• Molecule 1: Calcium release-activated calcium channel protein 1

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	262.34Å 262.34Å 220.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 6.71 19.98 – 6.71	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.98-6.71) 99.5 (19.98-6.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 6.98Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.312 , 0.337 0.312 , 0.337	Depositor DCC
R_{free} test set	1302 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å^2)	655.8	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 551.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.044 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	27120	wwPDB-VP
Average B, all atoms (Å^2)	722.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.30	0/1155	0.48	0/1571
1	B	0.30	0/1155	0.48	0/1571
1	C	0.31	0/1155	0.48	0/1571
1	D	0.30	0/1155	0.48	0/1571
1	E	0.30	0/1155	0.48	0/1571
1	F	0.30	0/1155	0.48	0/1571
1	G	0.30	0/1155	0.48	0/1571
1	H	0.30	0/1155	0.48	0/1571
1	I	0.30	0/1155	0.48	0/1571
1	J	0.30	0/1155	0.48	0/1571
1	K	0.31	0/1155	0.48	0/1571
1	L	0.30	0/1155	0.48	0/1571
1	M	0.30	0/1155	0.48	0/1571
1	N	0.30	0/1155	0.48	0/1571
1	O	0.31	0/1155	0.48	0/1571
1	P	0.30	0/1155	0.48	0/1571
1	Q	0.30	0/1155	0.48	0/1571
1	R	0.30	0/1155	0.48	0/1571
1	S	0.30	0/1155	0.48	0/1571
1	T	0.30	0/1155	0.48	0/1571
1	U	0.30	0/1155	0.48	0/1571
1	V	0.30	0/1155	0.48	0/1571
1	W	0.30	0/1155	0.48	0/1571
1	X	0.30	0/1155	0.48	0/1571
All	All	0.30	0/27720	0.48	0/37704

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1130	0	1141	59	0
1	B	1130	0	1141	52	0
1	C	1130	0	1141	73	0
1	D	1130	0	1141	70	0
1	E	1130	0	1141	48	0
1	F	1130	0	1141	58	0
1	G	1130	0	1141	50	0
1	H	1130	0	1141	55	0
1	I	1130	0	1141	65	0
1	J	1130	0	1141	61	0
1	K	1130	0	1141	55	0
1	L	1130	0	1141	55	0
1	M	1130	0	1141	76	0
1	N	1130	0	1141	76	0
1	O	1130	0	1141	55	0
1	P	1130	0	1141	62	0
1	Q	1130	0	1141	67	0
1	R	1130	0	1141	59	0
1	S	1130	0	1141	66	0
1	T	1130	0	1141	66	0
1	U	1130	0	1141	69	0
1	V	1130	0	1141	67	0
1	W	1130	0	1141	63	0
1	X	1130	0	1141	64	0
All	All	27120	0	27384	1246	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 23.

All (1246) 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:X:161:SER:HB2	1:X:248:TRP:HE1	1.09	1.11
1:F:319:LEU:HD12	1:Q:316:ILE:HG23	1.44	0.99
1:C:316:ILE:HG22	1:N:316:ILE:HA	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:ILE:HG22	1:W:319:LEU:HD13	1.45	0.97
1:J:197:ILE:HG23	1:K:285:VAL:HG21	1.45	0.97
1:U:215:CYS:HB2	1:V:300:PHE:CE2	2.00	0.96
1:V:158:LEU:HG	1:V:213:SER:HB3	1.48	0.94
1:F:319:LEU:HB3	1:Q:312:THR:HG23	1.49	0.93
1:N:322:LEU:HG	1:N:326:MET:HE1	1.52	0.92
1:R:316:ILE:HA	1:R:319:LEU:HD12	1.51	0.92
1:F:312:THR:HA	1:Q:319:LEU:HD22	1.50	0.92
1:E:316:ILE:HG22	1:R:316:ILE:HG22	1.52	0.91
1:X:161:SER:HB2	1:X:248:TRP:NE1	1.87	0.90
1:B:319:LEU:HD22	1:O:312:THR:HG23	1.54	0.89
1:D:312:THR:HA	1:M:319:LEU:HD22	1.51	0.89
1:V:165:SER:HB3	1:V:206:ALA:HB1	1.53	0.88
1:A:312:THR:HG23	1:P:319:LEU:HD22	1.54	0.88
1:A:165:SER:HB3	1:A:206:ALA:HB1	1.57	0.87
1:D:319:LEU:HD22	1:M:312:THR:HA	1.57	0.87
1:S:197:ILE:HG23	1:T:285:VAL:HG21	1.57	0.86
1:I:319:LEU:HD22	1:U:312:THR:HA	1.56	0.86
1:E:319:LEU:HD12	1:R:316:ILE:HG23	1.56	0.86
1:C:319:LEU:HD22	1:N:312:THR:HA	1.58	0.86
1:C:316:ILE:HG23	1:N:319:LEU:HD12	1.57	0.85
1:X:323:LYS:HA	1:X:326:MET:HE2	1.56	0.85
1:J:312:THR:HA	1:T:319:LEU:HD13	1.58	0.83
1:G:165:SER:HB3	1:G:206:ALA:HB1	1.60	0.83
1:N:165:SER:HB3	1:N:206:ALA:HB1	1.61	0.83
1:S:165:SER:HB3	1:S:206:ALA:HB1	1.59	0.83
1:F:165:SER:HB3	1:F:206:ALA:HB1	1.59	0.82
1:K:165:SER:HB3	1:K:206:ALA:HB1	1.61	0.82
1:T:165:SER:HB3	1:T:206:ALA:HB1	1.62	0.82
1:I:165:SER:HB3	1:I:206:ALA:HB1	1.62	0.82
1:O:165:SER:HB3	1:O:206:ALA:HB1	1.59	0.82
1:W:165:SER:HB3	1:W:206:ALA:HB1	1.62	0.82
1:U:165:SER:HB3	1:U:206:ALA:HB1	1.62	0.81
1:A:319:LEU:HB3	1:P:312:THR:HG23	1.62	0.81
1:M:165:SER:HB3	1:M:206:ALA:HB1	1.63	0.81
1:D:319:LEU:HB3	1:M:312:THR:HG23	1.62	0.80
1:J:165:SER:HB3	1:J:206:ALA:HB1	1.64	0.80
1:D:316:ILE:HG23	1:M:319:LEU:HD12	1.63	0.79
1:V:256:LEU:HD13	1:V:293:PHE:HZ	1.47	0.79
1:L:165:SER:HB3	1:L:206:ALA:HB1	1.63	0.78
1:I:206:ALA:O	1:I:210:LEU:HG	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:209:ALA:HA	1:H:212:ILE:HD12	1.66	0.78
1:F:319:LEU:CD1	1:Q:316:ILE:HG23	2.13	0.78
1:I:322:LEU:HD23	1:U:312:THR:OG1	1.83	0.78
1:H:165:SER:HB3	1:H:206:ALA:HB1	1.65	0.77
1:U:209:ALA:HA	1:U:212:ILE:HD12	1.64	0.77
1:D:165:SER:HB3	1:D:206:ALA:HB1	1.65	0.77
1:L:256:LEU:HD13	1:L:293:PHE:HZ	1.50	0.76
1:P:165:SER:HB3	1:P:206:ALA:HB1	1.68	0.76
1:A:158:LEU:HG	1:A:213:SER:HB3	1.67	0.76
1:X:165:SER:HB3	1:X:206:ALA:HB1	1.68	0.76
1:B:206:ALA:O	1:B:210:LEU:HG	1.86	0.76
1:F:316:ILE:HG22	1:Q:316:ILE:HG22	1.68	0.76
1:V:158:LEU:HG	1:V:213:SER:CB	2.16	0.76
1:Q:165:SER:HB3	1:Q:206:ALA:HB1	1.65	0.76
1:K:208:LEU:HD12	1:K:209:ALA:N	2.01	0.75
1:M:208:LEU:HD12	1:M:209:ALA:N	2.01	0.75
1:K:215:CYS:HB2	1:L:300:PHE:CE2	2.21	0.75
1:H:208:LEU:HD12	1:H:209:ALA:N	2.02	0.75
1:S:209:ALA:HA	1:S:212:ILE:HD12	1.69	0.75
1:V:197:ILE:HG23	1:W:285:VAL:HG21	1.69	0.75
1:B:208:LEU:HD12	1:B:209:ALA:N	2.02	0.75
1:F:209:ALA:HA	1:F:212:ILE:HD12	1.69	0.75
1:K:206:ALA:O	1:K:210:LEU:HG	1.87	0.75
1:C:208:LEU:HD12	1:C:209:ALA:N	2.02	0.74
1:E:316:ILE:HG23	1:R:319:LEU:HD13	1.68	0.74
1:I:208:LEU:HD12	1:I:209:ALA:N	2.03	0.74
1:K:209:ALA:HA	1:K:212:ILE:HD12	1.67	0.74
1:P:208:LEU:HD12	1:P:209:ALA:N	2.02	0.74
1:T:209:ALA:HA	1:T:212:ILE:HD12	1.67	0.74
1:M:206:ALA:O	1:M:210:LEU:HG	1.88	0.74
1:O:209:ALA:HA	1:O:212:ILE:HD12	1.69	0.74
1:X:206:ALA:O	1:X:210:LEU:HG	1.87	0.74
1:L:209:ALA:HA	1:L:212:ILE:HD12	1.68	0.74
1:N:209:ALA:HA	1:N:212:ILE:HD12	1.68	0.74
1:Q:206:ALA:O	1:Q:210:LEU:HG	1.87	0.74
1:L:206:ALA:O	1:L:210:LEU:HG	1.88	0.74
1:F:208:LEU:HD12	1:F:209:ALA:N	2.03	0.74
1:A:300:PHE:CE2	1:F:215:CYS:HB2	2.23	0.73
1:G:197:ILE:HG23	1:H:285:VAL:HG21	1.70	0.73
1:W:314:SER:O	1:W:318:GLU:HG2	1.88	0.73
1:C:312:THR:HA	1:N:319:LEU:HD22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:LEU:HD12	1:J:209:ALA:N	2.03	0.73
1:Q:208:LEU:HD12	1:Q:209:ALA:N	2.03	0.73
1:R:209:ALA:HA	1:R:212:ILE:HD12	1.70	0.73
1:O:206:ALA:O	1:O:210:LEU:HG	1.87	0.73
1:E:209:ALA:HA	1:E:212:ILE:HD12	1.69	0.73
1:I:209:ALA:HA	1:I:212:ILE:HD12	1.70	0.73
1:B:165:SER:HB3	1:B:206:ALA:HB1	1.71	0.73
1:N:206:ALA:O	1:N:210:LEU:HG	1.88	0.73
1:D:209:ALA:HA	1:D:212:ILE:HD12	1.70	0.73
1:E:208:LEU:HD12	1:E:209:ALA:N	2.03	0.73
1:T:208:LEU:HD12	1:T:209:ALA:N	2.03	0.73
1:Q:312:THR:O	1:Q:316:ILE:HG12	1.88	0.73
1:B:209:ALA:HA	1:B:212:ILE:HD12	1.71	0.73
1:D:312:THR:O	1:M:319:LEU:HD13	1.88	0.73
1:A:208:LEU:HD12	1:A:209:ALA:N	2.04	0.73
1:C:206:ALA:O	1:C:210:LEU:HG	1.88	0.73
1:J:209:ALA:HA	1:J:212:ILE:HD12	1.70	0.73
1:O:208:LEU:HD12	1:O:209:ALA:N	2.04	0.73
1:Q:209:ALA:HA	1:Q:212:ILE:HD12	1.71	0.72
1:R:165:SER:HB3	1:R:206:ALA:HB1	1.70	0.72
1:W:209:ALA:HA	1:W:212:ILE:HD12	1.69	0.72
1:D:206:ALA:O	1:D:210:LEU:HG	1.88	0.72
1:M:209:ALA:HA	1:M:212:ILE:HD12	1.71	0.72
1:U:208:LEU:HD12	1:U:209:ALA:N	2.03	0.72
1:M:256:LEU:HD13	1:M:293:PHE:HZ	1.54	0.72
1:D:208:LEU:HD12	1:D:209:ALA:N	2.05	0.72
1:C:209:ALA:HA	1:C:212:ILE:HD12	1.72	0.72
1:E:206:ALA:O	1:E:210:LEU:HG	1.90	0.72
1:F:316:ILE:HA	1:Q:316:ILE:HG22	1.71	0.72
1:G:209:ALA:HA	1:G:212:ILE:HD12	1.70	0.72
1:G:256:LEU:HD13	1:G:293:PHE:HZ	1.53	0.72
1:R:208:LEU:HD12	1:R:209:ALA:N	2.04	0.72
1:X:209:ALA:HA	1:X:212:ILE:HD12	1.70	0.72
1:C:165:SER:HB3	1:C:206:ALA:HB1	1.70	0.72
1:F:312:THR:HG23	1:Q:319:LEU:HB3	1.70	0.72
1:X:161:SER:CB	1:X:248:TRP:HE1	1.95	0.72
1:P:209:ALA:HA	1:P:212:ILE:HD12	1.72	0.71
1:V:208:LEU:HD12	1:V:209:ALA:N	2.05	0.71
1:K:158:LEU:HG	1:K:213:SER:HB3	1.72	0.71
1:P:206:ALA:O	1:P:210:LEU:HG	1.89	0.71
1:X:208:LEU:HD12	1:X:209:ALA:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ALA:O	1:A:210:LEU:HG	1.91	0.71
1:F:206:ALA:O	1:F:210:LEU:HG	1.89	0.71
1:T:206:ALA:O	1:T:210:LEU:HG	1.90	0.71
1:R:206:ALA:O	1:R:210:LEU:HG	1.91	0.71
1:N:208:LEU:HD12	1:N:209:ALA:N	2.05	0.71
1:H:158:LEU:HG	1:H:213:SER:HB3	1.71	0.71
1:A:319:LEU:HD22	1:P:312:THR:HG23	1.73	0.71
1:U:158:LEU:HG	1:U:213:SER:HB3	1.71	0.71
1:S:158:LEU:HG	1:S:213:SER:HB3	1.73	0.70
1:S:206:ALA:O	1:S:210:LEU:HG	1.91	0.70
1:L:208:LEU:HD12	1:L:209:ALA:N	2.05	0.70
1:N:314:SER:O	1:N:318:GLU:HG2	1.90	0.70
1:G:208:LEU:HD12	1:G:209:ALA:N	2.05	0.70
1:S:208:LEU:HD12	1:S:209:ALA:N	2.06	0.70
1:V:206:ALA:O	1:V:210:LEU:HG	1.90	0.70
1:D:316:ILE:HG23	1:M:319:LEU:CD1	2.21	0.70
1:W:206:ALA:O	1:W:210:LEU:HG	1.92	0.70
1:X:323:LYS:HA	1:X:326:MET:CE	2.22	0.70
1:N:312:THR:O	1:N:316:ILE:HG12	1.92	0.70
1:A:209:ALA:HA	1:A:212:ILE:HD12	1.72	0.70
1:E:161:SER:HB2	1:E:248:TRP:HE1	1.56	0.70
1:J:206:ALA:O	1:J:210:LEU:HG	1.91	0.70
1:H:206:ALA:O	1:H:210:LEU:HG	1.90	0.69
1:J:319:LEU:HD22	1:T:312:THR:HG23	1.73	0.69
1:M:300:PHE:CE2	1:R:215:CYS:HB2	2.27	0.69
1:F:158:LEU:HG	1:F:213:SER:HB3	1.74	0.69
1:I:319:LEU:HD12	1:U:316:ILE:HG23	1.73	0.69
1:S:179:VAL:CG1	1:X:177:VAL:HB	2.21	0.69
1:T:197:ILE:HG23	1:U:285:VAL:HG21	1.73	0.69
1:W:158:LEU:HG	1:W:213:SER:HB3	1.73	0.69
1:W:208:LEU:HD12	1:W:209:ALA:N	2.07	0.69
1:Q:177:VAL:HB	1:R:179:VAL:HG13	1.73	0.69
1:C:312:THR:O	1:N:319:LEU:HD13	1.92	0.69
1:E:165:SER:HB3	1:E:206:ALA:HB1	1.72	0.69
1:J:312:THR:OG1	1:T:319:LEU:HD22	1.93	0.69
1:U:312:THR:O	1:U:316:ILE:HG12	1.92	0.69
1:G:206:ALA:O	1:G:210:LEU:HG	1.93	0.69
1:D:215:CYS:HB2	1:E:300:PHE:CE2	2.28	0.69
1:A:285:VAL:O	1:A:288:PRO:HD2	1.94	0.68
1:O:158:LEU:HG	1:O:213:SER:HB3	1.76	0.68
1:D:285:VAL:O	1:D:288:PRO:HD2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:209:ALA:HA	1:V:212:ILE:HD12	1.74	0.68
1:V:215:CYS:HB2	1:W:300:PHE:CE2	2.28	0.68
1:C:316:ILE:HG23	1:N:319:LEU:CD1	2.23	0.68
1:Q:285:VAL:O	1:Q:288:PRO:HD2	1.94	0.68
1:L:158:LEU:HG	1:L:213:SER:HB3	1.74	0.68
1:U:206:ALA:O	1:U:210:LEU:HG	1.93	0.67
1:G:300:PHE:CE2	1:L:215:CYS:HB2	2.28	0.67
1:O:208:LEU:O	1:O:212:ILE:HG13	1.95	0.67
1:S:165:SER:HB3	1:S:206:ALA:CB	2.25	0.67
1:W:208:LEU:O	1:W:212:ILE:HG13	1.95	0.67
1:J:256:LEU:HD13	1:J:293:PHE:HZ	1.58	0.67
1:V:165:SER:HB3	1:V:206:ALA:CB	2.24	0.66
1:Q:208:LEU:O	1:Q:212:ILE:HG13	1.96	0.66
1:G:208:LEU:O	1:G:212:ILE:HG13	1.95	0.66
1:H:208:LEU:O	1:H:212:ILE:HG13	1.95	0.66
1:J:208:LEU:O	1:J:212:ILE:HG13	1.96	0.66
1:K:165:SER:HB3	1:K:206:ALA:CB	2.25	0.66
1:I:208:LEU:O	1:I:212:ILE:HG13	1.96	0.65
1:A:208:LEU:O	1:A:212:ILE:HG13	1.95	0.65
1:H:173:MET:HE3	1:I:263:ILE:HD13	1.78	0.65
1:B:272:TYR:O	1:B:276:PRO:HG3	1.97	0.65
1:B:207:MET:HA	1:B:210:LEU:HD12	1.79	0.65
1:N:165:SER:HB3	1:N:206:ALA:CB	2.26	0.65
1:T:158:LEU:HG	1:T:213:SER:HB3	1.79	0.65
1:O:165:SER:HB3	1:O:206:ALA:CB	2.27	0.65
1:W:165:SER:HB3	1:W:206:ALA:CB	2.26	0.65
1:G:158:LEU:HG	1:G:213:SER:HB3	1.78	0.65
1:F:165:SER:HB3	1:F:206:ALA:CB	2.26	0.65
1:L:165:SER:HB3	1:L:206:ALA:CB	2.27	0.65
1:H:158:LEU:HG	1:H:213:SER:CB	2.26	0.65
1:T:165:SER:HB3	1:T:206:ALA:CB	2.26	0.64
1:U:165:SER:HB3	1:U:206:ALA:CB	2.26	0.64
1:A:165:SER:HB3	1:A:206:ALA:CB	2.25	0.64
1:E:285:VAL:O	1:E:288:PRO:HD2	1.97	0.64
1:H:165:SER:HB3	1:H:206:ALA:CB	2.28	0.64
1:M:165:SER:HB3	1:M:206:ALA:CB	2.28	0.64
1:V:208:LEU:O	1:V:212:ILE:HG13	1.97	0.64
1:K:319:LEU:HB3	1:S:312:THR:HG23	1.78	0.64
1:F:285:VAL:O	1:F:288:PRO:HD2	1.98	0.64
1:N:285:VAL:O	1:N:288:PRO:HD2	1.98	0.64
1:J:319:LEU:HD13	1:T:312:THR:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:208:LEU:O	1:M:212:ILE:HG13	1.98	0.64
1:S:281:SER:HB2	1:X:197:ILE:HG12	1.80	0.64
1:K:208:LEU:O	1:K:212:ILE:HG13	1.97	0.64
1:I:165:SER:HB3	1:I:206:ALA:CB	2.28	0.63
1:K:285:VAL:O	1:K:288:PRO:HD2	1.98	0.63
1:S:208:LEU:O	1:S:212:ILE:HG13	1.97	0.63
1:U:208:LEU:O	1:U:212:ILE:HG13	1.97	0.63
1:U:272:TYR:O	1:U:276:PRO:HG3	1.98	0.63
1:R:208:LEU:O	1:R:212:ILE:HG13	1.98	0.63
1:C:312:THR:HG23	1:N:319:LEU:HD22	1.81	0.63
1:D:208:LEU:O	1:D:212:ILE:HG13	1.98	0.63
1:I:319:LEU:CD1	1:U:316:ILE:HG23	2.29	0.63
1:P:215:CYS:HB2	1:Q:300:PHE:CE2	2.34	0.63
1:F:208:LEU:O	1:F:212:ILE:HG13	1.98	0.63
1:J:158:LEU:HG	1:J:213:SER:HB3	1.80	0.63
1:Q:177:VAL:HB	1:R:179:VAL:CG1	2.29	0.63
1:T:208:LEU:O	1:T:212:ILE:HG13	1.98	0.63
1:N:201:LEU:HD21	1:O:285:VAL:HG22	1.81	0.63
1:C:285:VAL:O	1:C:288:PRO:HD2	1.98	0.63
1:D:316:ILE:HG22	1:M:316:ILE:HA	1.81	0.63
1:B:208:LEU:O	1:B:212:ILE:HG13	1.98	0.62
1:L:208:LEU:O	1:L:212:ILE:HG13	1.98	0.62
1:J:285:VAL:O	1:J:288:PRO:HD2	1.99	0.62
1:N:208:LEU:O	1:N:212:ILE:HG13	1.99	0.62
1:W:173:MET:SD	1:X:266:LEU:CD1	2.87	0.62
1:C:316:ILE:HG22	1:N:316:ILE:HG22	1.81	0.62
1:I:196:ALA:HB3	1:J:281:SER:OG	1.99	0.62
1:Q:165:SER:HB3	1:Q:206:ALA:CB	2.29	0.62
1:C:208:LEU:O	1:C:212:ILE:HG13	2.00	0.62
1:L:285:VAL:O	1:L:288:PRO:HD2	1.99	0.62
1:O:285:VAL:O	1:O:288:PRO:HD2	1.99	0.62
1:X:208:LEU:O	1:X:212:ILE:HG13	1.98	0.62
1:C:322:LEU:O	1:C:326:MET:HB2	1.98	0.62
1:M:285:VAL:O	1:M:288:PRO:HD2	1.99	0.62
1:X:165:SER:HB3	1:X:206:ALA:CB	2.29	0.62
1:D:165:SER:HB3	1:D:206:ALA:CB	2.29	0.62
1:E:208:LEU:O	1:E:212:ILE:HG13	1.98	0.62
1:K:272:TYR:O	1:K:276:PRO:HG3	2.00	0.62
1:G:165:SER:HB3	1:G:206:ALA:CB	2.29	0.62
1:P:285:VAL:O	1:P:288:PRO:HD2	1.99	0.62
1:W:285:VAL:O	1:W:288:PRO:HD2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MET:CE	1:B:263:ILE:HD13	2.30	0.62
1:F:316:ILE:HG23	1:Q:319:LEU:CD1	2.30	0.62
1:K:158:LEU:HG	1:K:213:SER:CB	2.29	0.62
1:S:158:LEU:HG	1:S:213:SER:CB	2.30	0.62
1:A:256:LEU:HD13	1:A:293:PHE:HZ	1.64	0.61
1:C:319:LEU:HB3	1:N:312:THR:HG23	1.80	0.61
1:H:173:MET:CE	1:I:263:ILE:HD13	2.30	0.61
1:B:285:VAL:O	1:B:288:PRO:HD2	2.00	0.61
1:L:158:LEU:HG	1:L:213:SER:CB	2.31	0.61
1:U:158:LEU:HG	1:U:213:SER:CB	2.29	0.61
1:A:173:MET:HE3	1:B:263:ILE:HD13	1.82	0.61
1:S:307:HIS:O	1:S:311:VAL:HG23	2.00	0.61
1:A:260:LEU:O	1:A:263:ILE:HG22	2.00	0.61
1:C:161:SER:HB2	1:C:248:TRP:HE1	1.65	0.61
1:B:161:SER:HB2	1:B:248:TRP:HE1	1.64	0.61
1:H:285:VAL:O	1:H:288:PRO:HD2	2.00	0.61
1:Q:307:HIS:O	1:Q:311:VAL:HG23	2.01	0.61
1:D:312:THR:HG23	1:M:319:LEU:HB3	1.83	0.61
1:W:158:LEU:HG	1:W:213:SER:CB	2.30	0.61
1:D:168:LEU:HD22	1:D:259:PHE:CZ	2.36	0.61
1:L:268:TRP:CZ3	1:L:280:TRP:HA	2.36	0.61
1:R:285:VAL:O	1:R:288:PRO:HD2	2.01	0.60
1:U:285:VAL:O	1:U:288:PRO:HD2	2.02	0.60
1:F:319:LEU:HD12	1:Q:316:ILE:CG2	2.28	0.60
1:D:312:THR:OG1	1:M:322:LEU:HD23	2.00	0.60
1:N:158:LEU:HG	1:N:213:SER:HB3	1.82	0.60
1:P:208:LEU:O	1:P:212:ILE:HG13	2.00	0.60
1:I:285:VAL:O	1:I:288:PRO:HD2	2.00	0.60
1:K:319:LEU:CD1	1:S:316:ILE:HG23	2.31	0.60
1:X:285:VAL:O	1:X:288:PRO:HD2	2.02	0.60
1:P:207:MET:HA	1:P:210:LEU:HD12	1.83	0.60
1:K:319:LEU:HD12	1:S:316:ILE:HG23	1.82	0.60
1:X:312:THR:O	1:X:316:ILE:HG12	2.00	0.60
1:N:215:CYS:HB2	1:O:300:PHE:CE2	2.37	0.60
1:C:319:LEU:CD1	1:N:316:ILE:HG23	2.32	0.60
1:C:272:TYR:O	1:C:276:PRO:HG3	2.02	0.59
1:N:168:LEU:HD22	1:N:259:PHE:CZ	2.37	0.59
1:J:207:MET:HA	1:J:210:LEU:HD12	1.83	0.59
1:T:158:LEU:HG	1:T:213:SER:CB	2.33	0.59
1:X:168:LEU:HD22	1:X:259:PHE:CZ	2.37	0.59
1:W:177:VAL:HB	1:X:179:VAL:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HG	1:A:213:SER:CB	2.31	0.59
1:I:158:LEU:HG	1:I:213:SER:HB3	1.85	0.59
1:B:165:SER:HB3	1:B:206:ALA:CB	2.32	0.59
1:E:165:SER:HB3	1:E:206:ALA:CB	2.32	0.59
1:R:161:SER:HB2	1:R:248:TRP:HE1	1.67	0.59
1:X:215:CYS:O	1:X:218:PRO:HD2	2.02	0.59
1:T:285:VAL:O	1:T:288:PRO:HD2	2.02	0.59
1:S:179:VAL:HG13	1:X:177:VAL:HB	1.83	0.59
1:R:165:SER:HB3	1:R:206:ALA:CB	2.32	0.58
1:C:165:SER:HB3	1:C:206:ALA:CB	2.32	0.58
1:H:207:MET:HA	1:H:210:LEU:HD12	1.85	0.58
1:M:215:CYS:HB2	1:N:300:PHE:CE2	2.38	0.58
1:V:207:MET:HA	1:V:210:LEU:HD12	1.85	0.58
1:C:307:HIS:O	1:C:311:VAL:HG23	2.04	0.58
1:C:312:THR:O	1:C:316:ILE:HG12	2.02	0.58
1:P:165:SER:HB3	1:P:206:ALA:CB	2.31	0.58
1:N:256:LEU:HD13	1:N:293:PHE:HZ	1.68	0.58
1:Q:272:TYR:O	1:Q:276:PRO:HG3	2.04	0.58
1:S:285:VAL:O	1:S:288:PRO:HD2	2.04	0.58
1:C:207:MET:HA	1:C:210:LEU:HD12	1.86	0.58
1:E:207:MET:HA	1:E:210:LEU:HD12	1.84	0.57
1:E:319:LEU:CD1	1:R:316:ILE:HG23	2.28	0.57
1:I:215:CYS:O	1:I:218:PRO:HD2	2.04	0.57
1:M:285:VAL:HG22	1:R:201:LEU:HD21	1.85	0.57
1:R:207:MET:HA	1:R:210:LEU:HD12	1.87	0.57
1:J:165:SER:HB3	1:J:206:ALA:CB	2.32	0.57
1:U:201:LEU:HD21	1:V:285:VAL:HG22	1.85	0.57
1:A:168:LEU:HD22	1:A:259:PHE:CZ	2.39	0.57
1:T:319:LEU:HD23	1:T:322:LEU:HD23	1.85	0.57
1:N:207:MET:HA	1:N:210:LEU:HD12	1.87	0.57
1:X:207:MET:HA	1:X:210:LEU:HD12	1.86	0.57
1:S:312:THR:O	1:S:316:ILE:HG12	2.05	0.57
1:V:285:VAL:O	1:V:288:PRO:HD2	2.04	0.57
1:X:272:TYR:O	1:X:276:PRO:HG3	2.05	0.57
1:G:285:VAL:O	1:G:288:PRO:HD2	2.03	0.57
1:L:256:LEU:HD13	1:L:293:PHE:CZ	2.36	0.57
1:Q:256:LEU:HD13	1:Q:293:PHE:HZ	1.70	0.57
1:B:150:LYS:O	1:B:241:HIS:NE2	2.30	0.56
1:C:215:CYS:O	1:C:218:PRO:HD2	2.05	0.56
1:I:319:LEU:HB3	1:U:312:THR:HG23	1.87	0.56
1:Q:161:SER:HB2	1:Q:248:TRP:HE1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:SER:HB2	1:E:248:TRP:NE1	2.21	0.56
1:F:168:LEU:HD22	1:F:259:PHE:CZ	2.40	0.56
1:V:168:LEU:HD22	1:V:259:PHE:CZ	2.40	0.56
1:A:272:TYR:O	1:A:276:PRO:HG3	2.05	0.56
1:D:260:LEU:O	1:D:263:ILE:HG22	2.05	0.56
1:E:215:CYS:HB2	1:F:300:PHE:CE2	2.41	0.56
1:E:319:LEU:HD22	1:R:312:THR:HG23	1.87	0.56
1:F:158:LEU:HG	1:F:213:SER:CB	2.36	0.56
1:E:312:THR:HG23	1:R:319:LEU:HB3	1.87	0.56
1:S:285:VAL:CG2	1:X:201:LEU:HD21	2.36	0.56
1:T:207:MET:HA	1:T:210:LEU:HD12	1.88	0.56
1:W:309:TYR:O	1:W:313:VAL:HG23	2.05	0.56
1:E:199:THR:O	1:E:203:VAL:HG23	2.05	0.56
1:W:177:VAL:HB	1:X:179:VAL:CG1	2.36	0.56
1:A:215:CYS:HB2	1:B:300:PHE:CE2	2.41	0.56
1:G:158:LEU:HG	1:G:213:SER:CB	2.36	0.56
1:D:309:TYR:HB2	1:M:326:MET:HE3	1.87	0.56
1:K:207:MET:HA	1:K:210:LEU:HD12	1.87	0.56
1:F:316:ILE:HG23	1:Q:319:LEU:HD13	1.87	0.55
1:U:215:CYS:O	1:U:218:PRO:HD2	2.05	0.55
1:C:215:CYS:HB2	1:D:300:PHE:CE2	2.42	0.55
1:I:207:MET:HA	1:I:210:LEU:HD12	1.88	0.55
1:J:215:CYS:O	1:J:218:PRO:HD2	2.06	0.55
1:M:207:MET:HA	1:M:210:LEU:HD12	1.87	0.55
1:N:199:THR:O	1:N:203:VAL:HG23	2.07	0.55
1:W:272:TYR:O	1:W:276:PRO:HG3	2.06	0.55
1:B:168:LEU:HD22	1:B:259:PHE:CZ	2.41	0.55
1:G:207:MET:HA	1:G:210:LEU:HD12	1.88	0.55
1:P:322:LEU:HG	1:P:326:MET:SD	2.46	0.55
1:R:199:THR:O	1:R:203:VAL:HG23	2.07	0.55
1:V:207:MET:C	1:W:293:PHE:HE2	2.09	0.55
1:C:312:THR:HG23	1:N:319:LEU:HB3	1.87	0.55
1:E:168:LEU:HD22	1:E:259:PHE:CZ	2.41	0.55
1:T:199:THR:O	1:T:203:VAL:HG23	2.06	0.55
1:F:260:LEU:O	1:F:263:ILE:HG22	2.07	0.55
1:P:161:SER:HB2	1:P:248:TRP:HE1	1.72	0.55
1:R:287:ILE:HB	1:R:288:PRO:HD3	1.89	0.55
1:D:207:MET:HA	1:D:210:LEU:HD12	1.89	0.55
1:J:319:LEU:HD22	1:T:312:THR:CG2	2.36	0.55
1:B:287:ILE:HB	1:B:288:PRO:HD3	1.89	0.55
1:L:199:THR:O	1:L:203:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:207:MET:HA	1:Q:210:LEU:HD12	1.89	0.55
1:J:199:THR:O	1:J:203:VAL:HG23	2.06	0.54
1:O:199:THR:O	1:O:203:VAL:HG23	2.07	0.54
1:F:256:LEU:HD13	1:F:293:PHE:HZ	1.72	0.54
1:I:260:LEU:O	1:I:263:ILE:HG22	2.07	0.54
1:L:207:MET:HA	1:L:210:LEU:HD12	1.90	0.54
1:P:272:TYR:O	1:P:276:PRO:HG3	2.08	0.54
1:J:158:LEU:HG	1:J:213:SER:CB	2.37	0.54
1:O:207:MET:HA	1:O:210:LEU:HD12	1.88	0.54
1:R:307:HIS:HA	1:R:310:GLU:HB3	1.90	0.54
1:C:316:ILE:HG22	1:N:316:ILE:CA	2.26	0.54
1:D:312:THR:HG23	1:M:319:LEU:HD22	1.90	0.54
1:E:312:THR:HA	1:R:319:LEU:HD22	1.89	0.54
1:J:312:THR:HA	1:T:319:LEU:CD1	2.32	0.54
1:N:283:THR:O	1:N:286:LEU:HB3	2.08	0.54
1:A:283:THR:O	1:A:286:LEU:HB3	2.08	0.54
1:A:285:VAL:C	1:A:288:PRO:HD2	2.28	0.54
1:J:283:THR:O	1:J:286:LEU:HB3	2.08	0.54
1:M:272:TYR:O	1:M:276:PRO:HG3	2.08	0.54
1:B:161:SER:HB2	1:B:248:TRP:NE1	2.23	0.54
1:C:316:ILE:CG2	1:N:316:ILE:HA	2.28	0.54
1:F:199:THR:O	1:F:203:VAL:HG23	2.07	0.54
1:F:272:TYR:O	1:F:276:PRO:HG3	2.07	0.54
1:F:207:MET:HA	1:F:210:LEU:HD12	1.90	0.54
1:I:199:THR:O	1:I:203:VAL:HG23	2.08	0.54
1:S:256:LEU:HD13	1:S:293:PHE:HZ	1.72	0.54
1:M:199:THR:O	1:M:203:VAL:HG23	2.07	0.54
1:O:168:LEU:HD22	1:O:259:PHE:CZ	2.42	0.54
1:A:285:VAL:HG22	1:F:201:LEU:HD21	1.90	0.53
1:D:283:THR:O	1:D:286:LEU:HB3	2.07	0.53
1:L:319:LEU:HD22	1:X:312:THR:HG23	1.89	0.53
1:N:265:ILE:O	1:N:269:VAL:HG23	2.08	0.53
1:Q:199:THR:O	1:Q:203:VAL:HG23	2.08	0.53
1:V:199:THR:O	1:V:203:VAL:HG23	2.07	0.53
1:C:258:LEU:O	1:C:261:LEU:HB3	2.09	0.53
1:G:215:CYS:O	1:G:218:PRO:HD2	2.08	0.53
1:G:265:ILE:O	1:G:269:VAL:HG23	2.08	0.53
1:H:199:THR:O	1:H:203:VAL:HG23	2.08	0.53
1:C:318:GLU:O	1:C:321:MET:HB2	2.09	0.53
1:F:283:THR:O	1:F:286:LEU:HB3	2.07	0.53
1:J:312:THR:HG23	1:T:319:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:256:LEU:HD13	1:V:293:PHE:CZ	2.36	0.53
1:Q:285:VAL:C	1:Q:288:PRO:HD2	2.28	0.53
1:S:168:LEU:HD22	1:S:259:PHE:CZ	2.43	0.53
1:W:287:ILE:HB	1:W:288:PRO:HD3	1.90	0.53
1:G:263:ILE:HD13	1:L:173:MET:CE	2.38	0.53
1:L:265:ILE:O	1:L:269:VAL:HG23	2.07	0.53
1:M:158:LEU:HG	1:M:213:SER:HB3	1.91	0.53
1:M:287:ILE:HB	1:M:288:PRO:HD3	1.89	0.53
1:Q:215:CYS:O	1:Q:218:PRO:HD2	2.09	0.53
1:I:316:ILE:HG23	1:U:319:LEU:HD13	1.90	0.53
1:M:264:ALA:CB	1:M:286:LEU:HD22	2.39	0.53
1:U:168:LEU:HD22	1:U:259:PHE:CZ	2.43	0.53
1:V:265:ILE:O	1:V:269:VAL:HG23	2.07	0.53
1:W:215:CYS:O	1:W:218:PRO:HD2	2.07	0.53
1:X:283:THR:O	1:X:286:LEU:HB3	2.09	0.53
1:A:173:MET:SD	1:B:266:LEU:CD1	2.97	0.53
1:D:312:THR:CA	1:M:319:LEU:HD22	2.31	0.53
1:F:258:LEU:O	1:F:261:LEU:HB3	2.09	0.53
1:F:285:VAL:C	1:F:288:PRO:HD2	2.29	0.53
1:I:258:LEU:O	1:I:261:LEU:HB3	2.09	0.53
1:S:179:VAL:HG12	1:X:177:VAL:HB	1.90	0.53
1:X:287:ILE:HB	1:X:288:PRO:HD3	1.91	0.53
1:A:207:MET:HA	1:A:210:LEU:HD12	1.90	0.53
1:D:215:CYS:O	1:D:218:PRO:HD2	2.09	0.53
1:G:316:ILE:CG2	1:W:319:LEU:HD13	2.30	0.53
1:I:211:MET:CE	1:J:296:PHE:HD2	2.22	0.53
1:R:260:LEU:O	1:R:263:ILE:HG22	2.09	0.53
1:S:208:LEU:N	1:T:293:PHE:HE2	2.06	0.53
1:T:287:ILE:HB	1:T:288:PRO:HD3	1.91	0.53
1:U:199:THR:O	1:U:203:VAL:HG23	2.09	0.53
1:A:319:LEU:HB3	1:P:312:THR:CG2	2.34	0.52
1:D:285:VAL:C	1:D:288:PRO:HD2	2.29	0.52
1:D:287:ILE:HB	1:D:288:PRO:HD3	1.91	0.52
1:E:283:THR:O	1:E:286:LEU:HB3	2.09	0.52
1:G:199:THR:O	1:G:203:VAL:HG23	2.08	0.52
1:O:158:LEU:HG	1:O:213:SER:CB	2.39	0.52
1:U:207:MET:HA	1:U:210:LEU:HD12	1.91	0.52
1:A:258:LEU:O	1:A:261:LEU:HB3	2.09	0.52
1:D:258:LEU:O	1:D:261:LEU:HB3	2.09	0.52
1:D:319:LEU:CB	1:M:312:THR:HG23	2.35	0.52
1:K:215:CYS:HB2	1:L:300:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:THR:O	1:D:203:VAL:HG23	2.09	0.52
1:E:287:ILE:HB	1:E:288:PRO:HD3	1.91	0.52
1:G:168:LEU:HD22	1:G:259:PHE:CZ	2.45	0.52
1:J:161:SER:HB2	1:J:248:TRP:HE1	1.74	0.52
1:P:309:TYR:O	1:P:313:VAL:HG23	2.10	0.52
1:S:283:THR:O	1:S:286:LEU:HB3	2.10	0.52
1:U:195:PHE:CD2	1:V:271:PHE:HZ	2.27	0.52
1:V:258:LEU:O	1:V:261:LEU:HB3	2.09	0.52
1:G:287:ILE:HB	1:G:288:PRO:HD3	1.90	0.52
1:H:177:VAL:HB	1:I:179:VAL:CG1	2.40	0.52
1:H:215:CYS:O	1:H:218:PRO:HD2	2.10	0.52
1:P:287:ILE:HB	1:P:288:PRO:HD3	1.91	0.52
1:T:283:THR:O	1:T:286:LEU:HB3	2.09	0.52
1:V:287:ILE:HB	1:V:288:PRO:HD3	1.92	0.52
1:X:199:THR:O	1:X:203:VAL:HG23	2.08	0.52
1:M:168:LEU:HD22	1:M:259:PHE:CZ	2.45	0.52
1:A:287:ILE:HB	1:A:288:PRO:HD3	1.92	0.52
1:D:256:LEU:HD13	1:D:293:PHE:HZ	1.74	0.52
1:K:199:THR:O	1:K:203:VAL:HG23	2.08	0.52
1:P:199:THR:O	1:P:203:VAL:HG23	2.09	0.52
1:R:168:LEU:HD22	1:R:259:PHE:CZ	2.44	0.52
1:X:265:ILE:O	1:X:269:VAL:HG23	2.09	0.52
1:C:287:ILE:HB	1:C:288:PRO:HD3	1.91	0.52
1:J:287:ILE:HB	1:J:288:PRO:HD3	1.92	0.52
1:N:287:ILE:HB	1:N:288:PRO:HD3	1.92	0.52
1:R:283:THR:O	1:R:286:LEU:HB3	2.10	0.52
1:S:207:MET:HA	1:S:210:LEU:HD12	1.91	0.52
1:K:168:LEU:HD22	1:K:259:PHE:CZ	2.45	0.52
1:Q:258:LEU:O	1:Q:261:LEU:HB3	2.10	0.52
1:I:268:TRP:CZ3	1:I:280:TRP:HA	2.44	0.52
1:K:287:ILE:HB	1:K:288:PRO:HD3	1.92	0.52
1:N:258:LEU:O	1:N:261:LEU:HB3	2.10	0.52
1:Q:265:ILE:O	1:Q:269:VAL:HG23	2.10	0.52
1:T:272:TYR:O	1:T:276:PRO:HG3	2.10	0.52
1:U:265:ILE:O	1:U:269:VAL:HG23	2.10	0.52
1:A:319:LEU:CB	1:P:312:THR:HG23	2.37	0.52
1:H:209:ALA:HA	1:H:212:ILE:CD1	2.39	0.52
1:H:287:ILE:HB	1:H:288:PRO:HD3	1.90	0.52
1:K:285:VAL:C	1:K:288:PRO:HD2	2.31	0.52
1:L:287:ILE:HB	1:L:288:PRO:HD3	1.92	0.52
1:S:287:ILE:HB	1:S:288:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:THR:O	1:H:286:LEU:HB3	2.10	0.51
1:X:258:LEU:O	1:X:261:LEU:HB3	2.10	0.51
1:A:199:THR:O	1:A:203:VAL:HG23	2.10	0.51
1:G:177:VAL:HB	1:H:179:VAL:HG13	1.91	0.51
1:M:260:LEU:O	1:M:263:ILE:HG22	2.09	0.51
1:N:158:LEU:HG	1:N:213:SER:CB	2.41	0.51
1:Q:283:THR:O	1:Q:286:LEU:HB3	2.09	0.51
1:F:265:ILE:O	1:F:269:VAL:HG23	2.10	0.51
1:I:265:ILE:O	1:I:269:VAL:HG23	2.10	0.51
1:J:285:VAL:C	1:J:288:PRO:HD2	2.31	0.51
1:L:285:VAL:C	1:L:288:PRO:HD2	2.31	0.51
1:Q:287:ILE:HB	1:Q:288:PRO:HD3	1.92	0.51
1:W:199:THR:O	1:W:203:VAL:HG23	2.10	0.51
1:M:256:LEU:HD13	1:M:293:PHE:CZ	2.42	0.51
1:S:203:VAL:O	1:S:207:MET:HG2	2.10	0.51
1:U:287:ILE:HB	1:U:288:PRO:HD3	1.91	0.51
1:W:168:LEU:HD22	1:W:259:PHE:CZ	2.45	0.51
1:W:320:GLU:HA	1:W:323:LYS:HB3	1.93	0.51
1:C:260:LEU:O	1:C:263:ILE:HG22	2.11	0.51
1:C:265:ILE:O	1:C:269:VAL:HG23	2.11	0.51
1:P:283:THR:O	1:P:286:LEU:HB3	2.10	0.51
1:F:287:ILE:HB	1:F:288:PRO:HD3	1.93	0.51
1:K:215:CYS:O	1:K:218:PRO:HD2	2.11	0.51
1:K:319:LEU:HD22	1:S:312:THR:HG23	1.93	0.51
1:O:215:CYS:HB2	1:P:300:PHE:CE2	2.46	0.51
1:O:258:LEU:O	1:O:261:LEU:HB3	2.11	0.51
1:R:258:LEU:O	1:R:261:LEU:HB3	2.10	0.51
1:S:199:THR:O	1:S:203:VAL:HG23	2.09	0.51
1:V:173:MET:HE2	1:W:263:ILE:HD13	1.93	0.51
1:B:258:LEU:O	1:B:261:LEU:HB3	2.10	0.51
1:E:272:TYR:O	1:E:276:PRO:HG3	2.11	0.51
1:E:285:VAL:C	1:E:288:PRO:HD2	2.31	0.51
1:I:158:LEU:HG	1:I:213:SER:CB	2.40	0.51
1:K:258:LEU:O	1:K:261:LEU:HB3	2.11	0.51
1:L:319:LEU:CB	1:X:316:ILE:HG23	2.41	0.51
1:O:287:ILE:HB	1:O:288:PRO:HD3	1.91	0.51
1:P:201:LEU:HD21	1:Q:285:VAL:HG22	1.93	0.51
1:P:265:ILE:O	1:P:269:VAL:HG23	2.11	0.51
1:P:285:VAL:C	1:P:288:PRO:HD2	2.31	0.51
1:T:212:ILE:O	1:T:216:ILE:HG13	2.11	0.51
1:T:321:MET:HB3	1:T:325:GLN:HE21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:203:VAL:O	1:U:207:MET:HG2	2.11	0.51
1:E:258:LEU:O	1:E:261:LEU:HB3	2.11	0.51
1:E:260:LEU:O	1:E:263:ILE:HG22	2.11	0.51
1:L:168:LEU:HD22	1:L:259:PHE:CZ	2.45	0.51
1:M:197:ILE:HG23	1:N:285:VAL:HG21	1.92	0.51
1:S:265:ILE:O	1:S:269:VAL:HG23	2.11	0.51
1:X:164:THR:O	1:X:168:LEU:HG	2.11	0.51
1:B:199:THR:O	1:B:203:VAL:HG23	2.10	0.51
1:B:260:LEU:O	1:B:263:ILE:HG22	2.10	0.51
1:C:161:SER:HB2	1:C:248:TRP:NE1	2.25	0.51
1:C:164:THR:O	1:C:168:LEU:HG	2.11	0.51
1:D:319:LEU:HD12	1:M:316:ILE:HG23	1.93	0.51
1:H:161:SER:HB2	1:H:248:TRP:HE1	1.76	0.51
1:I:285:VAL:C	1:I:288:PRO:HD2	2.31	0.51
1:K:209:ALA:HA	1:K:212:ILE:CD1	2.41	0.51
1:O:283:THR:O	1:O:286:LEU:HB3	2.10	0.51
1:V:164:THR:O	1:V:168:LEU:HG	2.11	0.51
1:V:307:HIS:O	1:V:311:VAL:HG23	2.11	0.51
1:X:260:LEU:O	1:X:263:ILE:HG22	2.11	0.51
1:C:285:VAL:C	1:C:288:PRO:HD2	2.31	0.50
1:D:161:SER:HB2	1:D:248:TRP:HE1	1.76	0.50
1:H:164:THR:O	1:H:168:LEU:HG	2.11	0.50
1:M:283:THR:O	1:M:286:LEU:HB3	2.10	0.50
1:T:177:VAL:HB	1:U:179:VAL:HG13	1.92	0.50
1:T:215:CYS:HB2	1:U:300:PHE:CE2	2.46	0.50
1:U:215:CYS:HB2	1:V:300:PHE:CD2	2.43	0.50
1:B:215:CYS:O	1:B:218:PRO:HD2	2.11	0.50
1:I:164:THR:O	1:I:168:LEU:HG	2.11	0.50
1:O:164:THR:O	1:O:168:LEU:HG	2.12	0.50
1:Q:260:LEU:O	1:Q:263:ILE:HG22	2.11	0.50
1:W:164:THR:O	1:W:168:LEU:HG	2.12	0.50
1:P:260:LEU:O	1:P:263:ILE:HG22	2.10	0.50
1:Q:173:MET:SD	1:R:266:LEU:CD1	3.00	0.50
1:R:164:THR:O	1:R:168:LEU:HG	2.12	0.50
1:W:207:MET:HA	1:W:210:LEU:HD12	1.92	0.50
1:A:164:THR:O	1:A:168:LEU:HG	2.11	0.50
1:D:268:TRP:CZ3	1:D:280:TRP:HA	2.46	0.50
1:E:215:CYS:O	1:E:218:PRO:HD2	2.11	0.50
1:J:316:ILE:HG22	1:T:316:ILE:HG22	1.93	0.50
1:N:285:VAL:C	1:N:288:PRO:HD2	2.31	0.50
1:P:258:LEU:O	1:P:261:LEU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:265:ILE:O	1:W:269:VAL:HG23	2.12	0.50
1:D:265:ILE:O	1:D:269:VAL:HG23	2.11	0.50
1:E:265:ILE:O	1:E:269:VAL:HG23	2.12	0.50
1:I:287:ILE:HB	1:I:288:PRO:HD3	1.92	0.50
1:P:164:THR:O	1:P:168:LEU:HG	2.12	0.50
1:S:201:LEU:HD21	1:T:285:VAL:HG22	1.94	0.50
1:L:164:THR:O	1:L:168:LEU:HG	2.12	0.50
1:O:256:LEU:HD13	1:O:293:PHE:HZ	1.76	0.50
1:O:285:VAL:C	1:O:288:PRO:HD2	2.32	0.50
1:Q:158:LEU:HG	1:Q:213:SER:HB3	1.93	0.50
1:S:164:THR:O	1:S:168:LEU:HG	2.11	0.50
1:S:196:ALA:HB3	1:T:281:SER:OG	2.12	0.50
1:B:164:THR:O	1:B:168:LEU:HG	2.11	0.50
1:C:258:LEU:HA	1:C:261:LEU:HB3	1.94	0.50
1:H:258:LEU:HA	1:H:261:LEU:HB3	1.94	0.50
1:L:215:CYS:O	1:L:218:PRO:HD2	2.12	0.50
1:L:283:THR:O	1:L:286:LEU:HB3	2.12	0.50
1:M:164:THR:O	1:M:168:LEU:HG	2.11	0.50
1:N:164:THR:O	1:N:168:LEU:HG	2.11	0.50
1:Q:164:THR:O	1:Q:168:LEU:HG	2.12	0.50
1:S:258:LEU:O	1:S:261:LEU:HB3	2.11	0.50
1:T:168:LEU:HD22	1:T:259:PHE:CZ	2.47	0.50
1:W:258:LEU:HA	1:W:261:LEU:HB3	1.93	0.50
1:E:164:THR:O	1:E:168:LEU:HG	2.11	0.50
1:I:203:VAL:O	1:I:207:MET:HG2	2.12	0.50
1:J:164:THR:O	1:J:168:LEU:HG	2.11	0.50
1:K:164:THR:O	1:K:168:LEU:HG	2.11	0.50
1:L:258:LEU:O	1:L:261:LEU:HB3	2.11	0.50
1:O:321:MET:O	1:O:325:GLN:HG3	2.11	0.50
1:S:260:LEU:O	1:S:263:ILE:HG22	2.12	0.50
1:U:283:THR:O	1:U:286:LEU:HB3	2.12	0.50
1:V:208:LEU:N	1:W:293:PHE:HE2	2.10	0.50
1:A:201:LEU:HD21	1:B:285:VAL:HG22	1.93	0.50
1:C:199:THR:O	1:C:203:VAL:HG23	2.12	0.50
1:D:312:THR:HG23	1:M:319:LEU:CB	2.42	0.50
1:J:260:LEU:O	1:J:263:ILE:HG22	2.12	0.50
1:M:258:LEU:O	1:M:261:LEU:HB3	2.11	0.50
1:K:260:LEU:O	1:K:263:ILE:HG22	2.12	0.49
1:P:168:LEU:HD22	1:P:259:PHE:CZ	2.47	0.49
1:V:258:LEU:HA	1:V:261:LEU:HB3	1.94	0.49
1:W:173:MET:SD	1:X:266:LEU:HD11	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:TYR:O	1:H:276:PRO:HG3	2.11	0.49
1:K:212:ILE:O	1:K:216:ILE:HG13	2.11	0.49
1:O:265:ILE:O	1:O:269:VAL:HG23	2.12	0.49
1:U:285:VAL:C	1:U:288:PRO:HD2	2.32	0.49
1:X:285:VAL:C	1:X:288:PRO:HD2	2.32	0.49
1:G:164:THR:O	1:G:168:LEU:HG	2.11	0.49
1:M:285:VAL:C	1:M:288:PRO:HD2	2.32	0.49
1:V:285:VAL:C	1:V:288:PRO:HD2	2.33	0.49
1:B:285:VAL:C	1:B:288:PRO:HD2	2.33	0.49
1:C:150:LYS:O	1:C:241:HIS:NE2	2.44	0.49
1:D:272:TYR:O	1:D:276:PRO:HG3	2.12	0.49
1:H:203:VAL:O	1:H:207:MET:HG2	2.12	0.49
1:J:212:ILE:O	1:J:216:ILE:HG13	2.12	0.49
1:L:258:LEU:HA	1:L:261:LEU:HB3	1.95	0.49
1:Q:258:LEU:HA	1:Q:261:LEU:HB3	1.95	0.49
1:U:212:ILE:O	1:U:216:ILE:HG13	2.13	0.49
1:C:158:LEU:HG	1:C:213:SER:HB3	1.95	0.49
1:H:285:VAL:C	1:H:288:PRO:HD2	2.33	0.49
1:M:158:LEU:HG	1:M:213:SER:CB	2.42	0.49
1:R:272:TYR:O	1:R:276:PRO:HG3	2.12	0.49
1:S:285:VAL:C	1:S:288:PRO:HD2	2.32	0.49
1:T:285:VAL:C	1:T:288:PRO:HD2	2.33	0.49
1:W:283:THR:O	1:W:286:LEU:HB3	2.12	0.49
1:C:319:LEU:HD12	1:N:316:ILE:HG23	1.93	0.49
1:F:164:THR:O	1:F:168:LEU:HG	2.11	0.49
1:T:164:THR:O	1:T:168:LEU:HG	2.11	0.49
1:U:164:THR:O	1:U:168:LEU:HG	2.12	0.49
1:V:283:THR:O	1:V:286:LEU:HB3	2.12	0.49
1:W:203:VAL:O	1:W:207:MET:HG2	2.12	0.49
1:G:283:THR:O	1:G:286:LEU:HB3	2.13	0.49
1:J:258:LEU:O	1:J:261:LEU:HB3	2.13	0.49
1:O:260:LEU:O	1:O:263:ILE:HG22	2.12	0.49
1:P:215:CYS:O	1:P:218:PRO:HD2	2.12	0.49
1:R:323:LYS:O	1:R:326:MET:HB3	2.13	0.49
1:W:285:VAL:C	1:W:288:PRO:HD2	2.32	0.49
1:D:164:THR:O	1:D:168:LEU:HG	2.11	0.49
1:J:215:CYS:HB2	1:K:300:PHE:CE2	2.47	0.49
1:P:158:LEU:HG	1:P:213:SER:HB3	1.95	0.49
1:R:265:ILE:O	1:R:269:VAL:HG23	2.12	0.49
1:V:173:MET:CE	1:W:263:ILE:HD13	2.43	0.49
1:V:201:LEU:HD21	1:W:285:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:O	1:A:269:VAL:HG23	2.12	0.49
1:C:168:LEU:HD22	1:C:259:PHE:CZ	2.48	0.49
1:T:268:TRP:CZ3	1:T:280:TRP:HA	2.48	0.49
1:V:158:LEU:CG	1:V:213:SER:HB3	2.33	0.49
1:N:322:LEU:HG	1:N:326:MET:CE	2.35	0.48
1:W:258:LEU:O	1:W:261:LEU:HB3	2.13	0.48
1:C:283:THR:O	1:C:286:LEU:HB3	2.14	0.48
1:G:258:LEU:O	1:G:261:LEU:HB3	2.13	0.48
1:H:258:LEU:O	1:H:261:LEU:HB3	2.13	0.48
1:J:203:VAL:O	1:J:207:MET:HG2	2.12	0.48
1:Q:313:VAL:O	1:Q:317:ARG:HB2	2.13	0.48
1:U:207:MET:C	1:V:293:PHE:HE2	2.15	0.48
1:U:209:ALA:HA	1:U:212:ILE:CD1	2.40	0.48
1:X:215:CYS:C	1:X:218:PRO:HD2	2.34	0.48
1:L:212:ILE:O	1:L:216:ILE:HG13	2.13	0.48
1:T:173:MET:HE3	1:U:263:ILE:HD13	1.96	0.48
1:T:202:LEU:HD23	1:T:202:LEU:O	2.13	0.48
1:B:177:VAL:HB	1:C:179:VAL:HG13	1.95	0.48
1:D:158:LEU:HG	1:D:213:SER:HB3	1.95	0.48
1:G:285:VAL:C	1:G:288:PRO:HD2	2.34	0.48
1:K:283:THR:O	1:K:286:LEU:HB3	2.12	0.48
1:M:215:CYS:O	1:M:218:PRO:HD2	2.13	0.48
1:V:203:VAL:O	1:V:207:MET:HG2	2.14	0.48
1:W:307:HIS:O	1:W:311:VAL:HG23	2.14	0.48
1:F:215:CYS:O	1:F:218:PRO:HD2	2.13	0.48
1:L:209:ALA:HA	1:L:212:ILE:CD1	2.42	0.48
1:N:173:MET:SD	1:O:266:LEU:CD1	3.02	0.48
1:R:258:LEU:HA	1:R:261:LEU:HB3	1.96	0.48
1:S:208:LEU:N	1:T:293:PHE:CE2	2.82	0.48
1:A:174:VAL:O	1:A:178:GLU:HG2	2.14	0.48
1:B:319:LEU:CD1	1:O:316:ILE:HG23	2.43	0.48
1:R:320:GLU:HA	1:R:323:LYS:HB3	1.95	0.48
1:S:258:LEU:HA	1:S:261:LEU:HB3	1.95	0.48
1:U:174:VAL:O	1:U:178:GLU:HG2	2.14	0.48
1:X:174:VAL:O	1:X:178:GLU:HG2	2.14	0.48
1:B:209:ALA:HA	1:B:212:ILE:CD1	2.43	0.48
1:D:323:LYS:HG3	1:M:309:TYR:HE1	1.78	0.48
1:F:212:ILE:O	1:F:216:ILE:HG13	2.14	0.48
1:H:202:LEU:HD12	1:H:258:LEU:HB3	1.96	0.48
1:I:161:SER:HB2	1:I:248:TRP:HE1	1.79	0.48
1:L:174:VAL:O	1:L:178:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:264:ALA:CB	1:L:286:LEU:HD22	2.43	0.48
1:N:260:LEU:O	1:N:263:ILE:HG22	2.14	0.48
1:R:215:CYS:O	1:R:218:PRO:HD2	2.14	0.48
1:V:174:VAL:O	1:V:178:GLU:HG2	2.14	0.48
1:C:275:SER:N	1:C:276:PRO:HD3	2.29	0.48
1:D:174:VAL:O	1:D:178:GLU:HG2	2.14	0.48
1:D:316:ILE:HA	1:M:316:ILE:HG22	1.95	0.48
1:I:215:CYS:C	1:I:218:PRO:HD2	2.34	0.48
1:O:174:VAL:O	1:O:178:GLU:HG2	2.14	0.48
1:O:272:TYR:O	1:O:276:PRO:HG3	2.14	0.48
1:P:275:SER:N	1:P:276:PRO:HD3	2.29	0.48
1:R:285:VAL:C	1:R:288:PRO:HD2	2.33	0.48
1:S:174:VAL:O	1:S:178:GLU:HG2	2.14	0.48
1:B:275:SER:N	1:B:276:PRO:HD3	2.29	0.48
1:D:275:SER:N	1:D:276:PRO:HD3	2.29	0.48
1:H:177:VAL:HB	1:I:179:VAL:HG13	1.94	0.48
1:Q:174:VAL:O	1:Q:178:GLU:HG2	2.14	0.48
1:R:161:SER:HB2	1:R:248:TRP:NE1	2.29	0.48
1:T:174:VAL:O	1:T:178:GLU:HG2	2.14	0.48
1:W:161:SER:HB2	1:W:248:TRP:HE1	1.78	0.48
1:J:308:LYS:HE3	1:T:322:LEU:HD21	1.96	0.48
1:U:301:TYR:O	1:U:305:VAL:HG23	2.14	0.48
1:X:212:ILE:O	1:X:216:ILE:HG13	2.14	0.48
1:G:203:VAL:O	1:G:207:MET:HG2	2.13	0.47
1:H:260:LEU:O	1:H:263:ILE:HG22	2.14	0.47
1:J:312:THR:HG23	1:T:319:LEU:HD13	1.96	0.47
1:K:275:SER:N	1:K:276:PRO:HD3	2.29	0.47
1:N:174:VAL:O	1:N:178:GLU:HG2	2.14	0.47
1:O:209:ALA:HA	1:O:212:ILE:CD1	2.42	0.47
1:T:275:SER:N	1:T:276:PRO:HD3	2.29	0.47
1:D:258:LEU:HA	1:D:261:LEU:HB3	1.95	0.47
1:D:309:TYR:HE1	1:M:323:LYS:HG3	1.79	0.47
1:E:209:ALA:HA	1:E:212:ILE:CD1	2.42	0.47
1:H:168:LEU:HD22	1:H:259:PHE:CZ	2.48	0.47
1:H:265:ILE:O	1:H:269:VAL:HG23	2.13	0.47
1:I:174:VAL:O	1:I:178:GLU:HG2	2.14	0.47
1:L:260:LEU:O	1:L:263:ILE:HG22	2.13	0.47
1:L:275:SER:N	1:L:276:PRO:HD3	2.29	0.47
1:T:301:TYR:O	1:T:305:VAL:HG23	2.14	0.47
1:W:275:SER:N	1:W:276:PRO:HD3	2.29	0.47
1:F:258:LEU:HA	1:F:261:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:258:LEU:HA	1:U:261:LEU:HB3	1.96	0.47
1:W:174:VAL:O	1:W:178:GLU:HG2	2.14	0.47
1:H:173:MET:SD	1:I:266:LEU:CD1	3.02	0.47
1:R:174:VAL:O	1:R:178:GLU:HG2	2.14	0.47
1:V:275:SER:N	1:V:276:PRO:HD3	2.30	0.47
1:D:319:LEU:HD13	1:M:312:THR:O	2.14	0.47
1:K:312:THR:HG23	1:S:319:LEU:HB3	1.94	0.47
1:O:275:SER:N	1:O:276:PRO:HD3	2.29	0.47
1:O:310:GLU:OE1	1:O:314:SER:HB2	2.14	0.47
1:Q:275:SER:N	1:Q:276:PRO:HD3	2.29	0.47
1:U:258:LEU:O	1:U:261:LEU:HB3	2.14	0.47
1:C:174:VAL:O	1:C:178:GLU:HG2	2.14	0.47
1:G:258:LEU:HA	1:G:261:LEU:HB3	1.95	0.47
1:J:174:VAL:O	1:J:178:GLU:HG2	2.14	0.47
1:M:174:VAL:O	1:M:178:GLU:HG2	2.14	0.47
1:P:258:LEU:HA	1:P:261:LEU:HB3	1.97	0.47
1:Q:168:LEU:HD22	1:Q:259:PHE:CZ	2.49	0.47
1:T:265:ILE:O	1:T:269:VAL:HG23	2.14	0.47
1:U:195:PHE:HD2	1:V:271:PHE:HZ	1.62	0.47
1:V:215:CYS:O	1:V:218:PRO:HD2	2.14	0.47
1:X:275:SER:N	1:X:276:PRO:HD3	2.29	0.47
1:A:215:CYS:O	1:A:218:PRO:HD2	2.14	0.47
1:D:319:LEU:HB3	1:M:312:THR:CG2	2.38	0.47
1:F:174:VAL:O	1:F:178:GLU:HG2	2.14	0.47
1:G:174:VAL:O	1:G:178:GLU:HG2	2.14	0.47
1:J:196:ALA:HB3	1:K:281:SER:OG	2.15	0.47
1:J:265:ILE:O	1:J:269:VAL:HG23	2.15	0.47
1:J:275:SER:N	1:J:276:PRO:HD3	2.30	0.47
1:K:174:VAL:O	1:K:178:GLU:HG2	2.14	0.47
1:K:258:LEU:HA	1:K:261:LEU:HB3	1.95	0.47
1:L:203:VAL:O	1:L:207:MET:HG2	2.14	0.47
1:M:203:VAL:O	1:M:207:MET:HG2	2.15	0.47
1:M:264:ALA:HB2	1:M:286:LEU:HD22	1.96	0.47
1:N:275:SER:N	1:N:276:PRO:HD3	2.29	0.47
1:O:258:LEU:HA	1:O:261:LEU:HB3	1.97	0.47
1:S:215:CYS:O	1:S:218:PRO:HD2	2.15	0.47
1:S:271:PHE:HZ	1:X:176:MET:HE2	1.80	0.47
1:T:215:CYS:O	1:T:218:PRO:HD2	2.14	0.47
1:X:258:LEU:HA	1:X:261:LEU:HB3	1.96	0.47
1:A:275:SER:N	1:A:276:PRO:HD3	2.29	0.47
1:C:203:VAL:O	1:C:207:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:CYS:C	1:C:218:PRO:HD2	2.35	0.47
1:G:260:LEU:O	1:G:263:ILE:HG22	2.13	0.47
1:O:301:TYR:O	1:O:305:VAL:HG23	2.14	0.47
1:Q:158:LEU:HG	1:Q:213:SER:CB	2.45	0.47
1:Q:322:LEU:O	1:Q:326:MET:HB2	2.15	0.47
1:S:275:SER:N	1:S:276:PRO:HD3	2.29	0.47
1:S:321:MET:O	1:S:325:GLN:HG3	2.14	0.47
1:T:258:LEU:O	1:T:261:LEU:HB3	2.15	0.47
1:A:319:LEU:CD1	1:P:316:ILE:HG23	2.44	0.47
1:E:174:VAL:O	1:E:178:GLU:HG2	2.14	0.47
1:G:275:SER:N	1:G:276:PRO:HD3	2.30	0.47
1:H:275:SER:N	1:H:276:PRO:HD3	2.30	0.47
1:P:174:VAL:O	1:P:178:GLU:HG2	2.14	0.47
1:Q:203:VAL:O	1:Q:207:MET:HG2	2.15	0.47
1:Q:209:ALA:HA	1:Q:212:ILE:CD1	2.43	0.47
1:U:275:SER:N	1:U:276:PRO:HD3	2.29	0.47
1:M:265:ILE:O	1:M:269:VAL:HG23	2.14	0.47
1:M:275:SER:N	1:M:276:PRO:HD3	2.29	0.47
1:T:161:SER:HB2	1:T:248:TRP:HE1	1.79	0.47
1:B:174:VAL:O	1:B:178:GLU:HG2	2.14	0.46
1:E:275:SER:N	1:E:276:PRO:HD3	2.29	0.46
1:F:316:ILE:HG23	1:Q:319:LEU:HD12	1.97	0.46
1:F:319:LEU:HB3	1:Q:312:THR:CG2	2.34	0.46
1:H:268:TRP:HA	1:H:279:ALA:HB1	1.97	0.46
1:I:201:LEU:HG	1:J:285:VAL:HG21	1.97	0.46
1:P:212:ILE:O	1:P:216:ILE:HG13	2.15	0.46
1:R:275:SER:N	1:R:276:PRO:HD3	2.29	0.46
1:S:212:ILE:O	1:S:216:ILE:HG13	2.15	0.46
1:U:215:CYS:C	1:U:218:PRO:HD2	2.35	0.46
1:V:260:LEU:O	1:V:263:ILE:HG22	2.15	0.46
1:D:312:THR:CG2	1:M:319:LEU:HB3	2.44	0.46
1:E:258:LEU:HA	1:E:261:LEU:HB3	1.96	0.46
1:I:173:MET:HE3	1:J:263:ILE:HD13	1.95	0.46
1:I:258:LEU:HA	1:I:261:LEU:HB3	1.97	0.46
1:K:265:ILE:O	1:K:269:VAL:HG23	2.15	0.46
1:M:161:SER:HB2	1:M:248:TRP:HE1	1.80	0.46
1:M:201:LEU:HD21	1:N:285:VAL:HG22	1.97	0.46
1:O:215:CYS:O	1:O:218:PRO:HD2	2.15	0.46
1:R:301:TYR:O	1:R:305:VAL:HG23	2.15	0.46
1:W:212:ILE:O	1:W:216:ILE:HG13	2.15	0.46
1:H:174:VAL:O	1:H:178:GLU:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:212:ILE:O	1:I:216:ILE:HG13	2.15	0.46
1:P:256:LEU:HD13	1:P:293:PHE:HZ	1.81	0.46
1:P:316:ILE:HG13	1:P:317:ARG:N	2.29	0.46
1:S:209:ALA:HA	1:S:212:ILE:CD1	2.44	0.46
1:V:208:LEU:N	1:W:293:PHE:CE2	2.84	0.46
1:D:209:ALA:HA	1:D:212:ILE:CD1	2.44	0.46
1:E:202:LEU:HD12	1:E:258:LEU:HB3	1.97	0.46
1:G:177:VAL:HB	1:H:179:VAL:CG1	2.46	0.46
1:G:272:TYR:O	1:G:276:PRO:HG3	2.15	0.46
1:I:283:THR:O	1:I:286:LEU:HB3	2.16	0.46
1:J:253:LEU:HD11	1:J:293:PHE:HE1	1.81	0.46
1:J:301:TYR:O	1:J:305:VAL:HG23	2.16	0.46
1:W:195:PHE:CD2	1:X:271:PHE:HZ	2.32	0.46
1:A:266:LEU:CD1	1:F:173:MET:SD	3.03	0.46
1:B:207:MET:HA	1:B:210:LEU:CD1	2.45	0.46
1:B:301:TYR:O	1:B:305:VAL:HG23	2.16	0.46
1:I:215:CYS:HB2	1:J:300:PHE:CE2	2.51	0.46
1:N:212:ILE:O	1:N:216:ILE:HG13	2.16	0.46
1:N:215:CYS:O	1:N:218:PRO:HD2	2.16	0.46
1:A:201:LEU:HD21	1:B:285:VAL:CG2	2.46	0.46
1:B:319:LEU:HD12	1:O:316:ILE:HG23	1.97	0.46
1:E:212:ILE:O	1:E:216:ILE:HG13	2.15	0.46
1:J:215:CYS:C	1:J:218:PRO:HD2	2.35	0.46
1:J:256:LEU:HD13	1:J:293:PHE:CZ	2.45	0.46
1:L:307:HIS:O	1:L:311:VAL:HG23	2.15	0.46
1:N:309:TYR:O	1:N:313:VAL:HG23	2.16	0.46
1:O:212:ILE:O	1:O:216:ILE:HG13	2.15	0.46
1:T:260:LEU:O	1:T:263:ILE:HG22	2.14	0.46
1:B:212:ILE:O	1:B:216:ILE:HG13	2.15	0.46
1:F:275:SER:N	1:F:276:PRO:HD3	2.29	0.46
1:F:316:ILE:HG22	1:Q:316:ILE:CG2	2.43	0.46
1:G:196:ALA:HB3	1:H:281:SER:OG	2.16	0.46
1:J:258:LEU:HA	1:J:261:LEU:HB3	1.97	0.46
1:W:215:CYS:C	1:W:218:PRO:HD2	2.36	0.46
1:B:215:CYS:HB2	1:C:300:PHE:CE2	2.51	0.46
1:D:282:ALA:O	1:D:285:VAL:HG12	2.16	0.46
1:H:301:TYR:O	1:H:305:VAL:HG23	2.16	0.46
1:V:317:ARG:O	1:V:320:GLU:HB3	2.16	0.46
1:E:202:LEU:HA	1:E:258:LEU:HD13	1.97	0.46
1:S:323:LYS:O	1:S:327:GLU:HG3	2.15	0.46
1:X:268:TRP:CH2	1:X:280:TRP:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:MET:CE	1:E:263:ILE:HD13	2.46	0.45
1:D:212:ILE:O	1:D:216:ILE:HG13	2.16	0.45
1:N:258:LEU:HA	1:N:261:LEU:HB3	1.97	0.45
1:R:310:GLU:HG3	1:R:311:VAL:N	2.31	0.45
1:X:268:TRP:CZ3	1:X:280:TRP:HA	2.51	0.45
1:C:322:LEU:HD23	1:N:312:THR:OG1	2.15	0.45
1:G:161:SER:HB2	1:G:248:TRP:HE1	1.80	0.45
1:I:275:SER:N	1:I:276:PRO:HD3	2.30	0.45
1:K:202:LEU:HD12	1:K:258:LEU:HB3	1.99	0.45
1:K:202:LEU:O	1:K:202:LEU:HD23	2.16	0.45
1:K:203:VAL:O	1:K:207:MET:HG2	2.15	0.45
1:G:209:ALA:HA	1:G:212:ILE:CD1	2.43	0.45
1:W:209:ALA:HA	1:W:212:ILE:CD1	2.43	0.45
1:C:316:ILE:HG23	1:N:319:LEU:HB2	1.98	0.45
1:I:211:MET:HE3	1:J:296:PHE:HD2	1.81	0.45
1:U:202:LEU:O	1:U:202:LEU:HD23	2.17	0.45
1:B:258:LEU:HA	1:B:261:LEU:HB3	1.97	0.45
1:C:326:MET:HE3	1:N:309:TYR:HB2	1.99	0.45
1:G:263:ILE:HD13	1:L:173:MET:HE3	1.97	0.45
1:N:301:TYR:O	1:N:305:VAL:HG23	2.16	0.45
1:O:177:VAL:HB	1:P:179:VAL:HG13	1.99	0.45
1:S:208:LEU:HA	1:T:293:PHE:CE2	2.52	0.45
1:V:162:SER:HA	1:V:210:LEU:CD2	2.46	0.45
1:C:316:ILE:CG2	1:N:319:LEU:HB2	2.47	0.45
1:F:202:LEU:HA	1:F:258:LEU:HD13	1.98	0.45
1:Q:215:CYS:HB2	1:R:300:PHE:CE2	2.51	0.45
1:S:254:LEU:C	1:S:254:LEU:HD23	2.37	0.45
1:S:272:TYR:O	1:S:276:PRO:HG3	2.16	0.45
1:V:301:TYR:O	1:V:305:VAL:HG23	2.17	0.45
1:C:158:LEU:HG	1:C:213:SER:CB	2.46	0.45
1:C:212:ILE:O	1:C:216:ILE:HG13	2.16	0.45
1:D:319:LEU:CD1	1:M:316:ILE:HG23	2.47	0.45
1:H:215:CYS:HB2	1:I:300:PHE:CE2	2.51	0.45
1:L:272:TYR:O	1:L:276:PRO:HG3	2.16	0.45
1:C:326:MET:HE3	1:N:309:TYR:CA	2.47	0.45
1:E:301:TYR:O	1:E:305:VAL:HG23	2.16	0.45
1:F:268:TRP:CZ3	1:F:280:TRP:HA	2.52	0.45
1:G:215:CYS:C	1:G:218:PRO:HD2	2.37	0.45
1:Q:161:SER:HB2	1:Q:248:TRP:NE1	2.32	0.45
1:Q:301:TYR:O	1:Q:305:VAL:HG23	2.17	0.45
1:W:260:LEU:O	1:W:263:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:158:LEU:HG	1:P:213:SER:CB	2.47	0.45
1:T:209:ALA:HA	1:T:212:ILE:CD1	2.44	0.45
1:U:260:LEU:O	1:U:263:ILE:HG22	2.17	0.45
1:H:309:TYR:HD1	1:V:326:MET:HE2	1.81	0.44
1:M:214:THR:HG23	1:N:248:TRP:CH2	2.52	0.44
1:S:161:SER:HB2	1:S:248:TRP:HE1	1.81	0.44
1:W:301:TYR:O	1:W:305:VAL:HG23	2.17	0.44
1:B:268:TRP:HZ3	1:B:283:THR:HB	1.82	0.44
1:I:307:HIS:O	1:I:311:VAL:HG23	2.17	0.44
1:Q:215:CYS:C	1:Q:218:PRO:HD2	2.37	0.44
1:R:282:ALA:O	1:R:285:VAL:HG12	2.17	0.44
1:X:202:LEU:HD23	1:X:202:LEU:O	2.18	0.44
1:I:301:TYR:O	1:I:305:VAL:HG23	2.17	0.44
1:P:202:LEU:HA	1:P:258:LEU:HD13	1.99	0.44
1:U:162:SER:HA	1:U:210:LEU:CD2	2.48	0.44
1:U:309:TYR:O	1:U:313:VAL:HG23	2.18	0.44
1:V:212:ILE:O	1:V:216:ILE:HG13	2.17	0.44
1:C:326:MET:HE3	1:N:309:TYR:HA	2.00	0.44
1:I:168:LEU:HD22	1:I:259:PHE:CZ	2.51	0.44
1:J:202:LEU:HD12	1:J:258:LEU:HB3	1.98	0.44
1:S:207:MET:C	1:T:293:PHE:HE2	2.21	0.44
1:D:215:CYS:C	1:D:218:PRO:HD2	2.38	0.44
1:F:209:ALA:HA	1:F:212:ILE:CD1	2.44	0.44
1:L:309:TYR:HD1	1:X:326:MET:SD	2.40	0.44
1:M:301:TYR:O	1:M:305:VAL:HG23	2.18	0.44
1:W:271:PHE:HB2	1:W:279:ALA:HB2	1.99	0.44
1:A:258:LEU:HA	1:A:261:LEU:HB3	1.98	0.44
1:P:161:SER:HB2	1:P:248:TRP:NE1	2.31	0.44
1:S:281:SER:HB2	1:X:197:ILE:CG1	2.46	0.44
1:S:301:TYR:O	1:S:305:VAL:HG23	2.18	0.44
1:V:312:THR:O	1:V:316:ILE:HG12	2.17	0.44
1:X:301:TYR:O	1:X:305:VAL:HG23	2.16	0.44
1:A:209:ALA:HA	1:A:212:ILE:CD1	2.46	0.44
1:A:212:ILE:O	1:A:216:ILE:HG13	2.17	0.44
1:K:301:TYR:O	1:K:305:VAL:HG23	2.17	0.44
1:A:316:ILE:HG23	1:P:319:LEU:CD1	2.48	0.44
1:D:254:LEU:C	1:D:254:LEU:HD23	2.38	0.44
1:F:202:LEU:HD12	1:F:258:LEU:HB3	2.00	0.44
1:G:212:ILE:O	1:G:216:ILE:HG13	2.18	0.44
1:M:202:LEU:HD12	1:M:258:LEU:HB3	1.99	0.44
1:O:203:VAL:O	1:O:207:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:TYR:O	1:A:305:VAL:HG23	2.18	0.44
1:A:312:THR:OG1	1:P:322:LEU:HD23	2.18	0.44
1:J:214:THR:HG23	1:K:248:TRP:CH2	2.53	0.44
1:K:215:CYS:C	1:K:218:PRO:HD2	2.39	0.44
1:L:202:LEU:HD12	1:L:258:LEU:HB3	1.99	0.44
1:M:212:ILE:O	1:M:216:ILE:HG13	2.18	0.44
1:N:307:HIS:HA	1:N:310:GLU:HB3	1.99	0.44
1:Q:202:LEU:HA	1:Q:258:LEU:HD13	2.00	0.44
1:T:258:LEU:HA	1:T:261:LEU:HB3	1.98	0.44
1:V:202:LEU:HA	1:V:258:LEU:HD13	2.00	0.44
1:B:215:CYS:C	1:B:218:PRO:HD2	2.39	0.43
1:E:316:ILE:CG2	1:R:316:ILE:HG22	2.36	0.43
1:I:204:ALA:CB	1:J:289:VAL:HG11	2.48	0.43
1:K:202:LEU:HA	1:K:258:LEU:HD13	2.00	0.43
1:L:202:LEU:HA	1:L:258:LEU:HD13	2.00	0.43
1:M:258:LEU:HA	1:M:261:LEU:HB3	1.98	0.43
1:O:254:LEU:HD23	1:O:254:LEU:C	2.38	0.43
1:P:203:VAL:O	1:P:207:MET:HG2	2.17	0.43
1:S:202:LEU:HD12	1:S:258:LEU:HB3	2.00	0.43
1:S:253:LEU:HD11	1:S:293:PHE:HE1	1.83	0.43
1:T:162:SER:HA	1:T:210:LEU:CD2	2.48	0.43
1:T:202:LEU:HA	1:T:258:LEU:HD13	2.00	0.43
1:U:314:SER:O	1:U:317:ARG:HB3	2.17	0.43
1:B:283:THR:O	1:B:286:LEU:HB3	2.17	0.43
1:G:285:VAL:HG21	1:L:197:ILE:HG23	2.00	0.43
1:I:202:LEU:HA	1:I:258:LEU:HD13	1.99	0.43
1:I:256:LEU:HD13	1:I:293:PHE:HZ	1.84	0.43
1:K:316:ILE:HG22	1:S:316:ILE:HG22	2.00	0.43
1:M:281:SER:HB2	1:R:197:ILE:CG1	2.48	0.43
1:Q:201:LEU:HD21	1:R:285:VAL:HG22	1.99	0.43
1:T:254:LEU:C	1:T:254:LEU:HD23	2.38	0.43
1:A:304:LEU:C	1:A:304:LEU:HD23	2.39	0.43
1:G:307:HIS:O	1:G:311:VAL:HG23	2.18	0.43
1:M:202:LEU:HA	1:M:258:LEU:HD13	1.99	0.43
1:N:173:MET:CE	1:O:263:ILE:HD13	2.48	0.43
1:U:254:LEU:C	1:U:254:LEU:HD23	2.38	0.43
1:B:202:LEU:HA	1:B:258:LEU:HD13	1.99	0.43
1:C:202:LEU:HD12	1:C:258:LEU:HB3	2.00	0.43
1:C:319:LEU:HB3	1:N:312:THR:CG2	2.46	0.43
1:C:319:LEU:CB	1:N:312:THR:HG23	2.47	0.43
1:C:322:LEU:HG	1:C:326:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:LEU:O	1:D:308:LYS:HG2	2.18	0.43
1:F:301:TYR:O	1:F:305:VAL:HG23	2.18	0.43
1:G:202:LEU:HA	1:G:258:LEU:HD13	2.00	0.43
1:N:201:LEU:HD21	1:O:285:VAL:CG2	2.46	0.43
1:T:177:VAL:HB	1:U:179:VAL:CG1	2.48	0.43
1:A:282:ALA:O	1:A:285:VAL:HG12	2.19	0.43
1:N:202:LEU:HA	1:N:258:LEU:HD13	1.99	0.43
1:O:282:ALA:O	1:O:285:VAL:HG12	2.18	0.43
1:U:316:ILE:HG12	1:U:316:ILE:H	1.64	0.43
1:E:282:ALA:O	1:E:285:VAL:HG12	2.19	0.43
1:F:316:ILE:CG2	1:Q:316:ILE:HG22	2.44	0.43
1:P:202:LEU:HD12	1:P:258:LEU:HB3	2.00	0.43
1:Q:254:LEU:HD23	1:Q:254:LEU:C	2.39	0.43
1:T:203:VAL:O	1:T:207:MET:HG2	2.18	0.43
1:B:265:ILE:O	1:B:269:VAL:HG23	2.18	0.43
1:H:215:CYS:C	1:H:218:PRO:HD2	2.38	0.43
1:H:268:TRP:CZ3	1:H:280:TRP:HA	2.53	0.43
1:L:161:SER:HB2	1:L:248:TRP:HE1	1.84	0.43
1:L:301:TYR:O	1:L:305:VAL:HG23	2.18	0.43
1:R:212:ILE:O	1:R:216:ILE:HG13	2.18	0.43
1:S:202:LEU:HA	1:S:258:LEU:HD13	2.00	0.43
1:S:271:PHE:HB2	1:S:279:ALA:HB2	2.00	0.43
1:T:320:GLU:O	1:T:324:GLU:HB3	2.19	0.43
1:B:157:LYS:CB	1:B:248:TRP:CD2	3.01	0.43
1:E:304:LEU:C	1:E:304:LEU:HD23	2.39	0.43
1:H:212:ILE:O	1:H:216:ILE:HG13	2.19	0.43
1:I:254:LEU:C	1:I:254:LEU:HD23	2.38	0.43
1:A:254:LEU:C	1:A:254:LEU:HD23	2.39	0.43
1:F:215:CYS:C	1:F:218:PRO:HD2	2.40	0.43
1:I:150:LYS:O	1:I:241:HIS:NE2	2.48	0.43
1:I:319:LEU:HD22	1:U:312:THR:CA	2.39	0.43
1:J:202:LEU:HA	1:J:258:LEU:HD13	2.00	0.43
1:J:307:HIS:O	1:J:311:VAL:HG23	2.19	0.43
1:O:202:LEU:HD12	1:O:258:LEU:HB3	2.01	0.43
1:P:268:TRP:CZ3	1:P:280:TRP:HA	2.54	0.43
1:R:158:LEU:HG	1:R:213:SER:HB3	2.01	0.43
1:A:319:LEU:CD2	1:P:312:THR:HG23	2.45	0.43
1:I:202:LEU:HD23	1:I:202:LEU:O	2.19	0.43
1:K:207:MET:HB3	1:L:293:PHE:CE2	2.53	0.43
1:P:209:ALA:HA	1:P:212:ILE:CD1	2.44	0.43
1:U:195:PHE:HD2	1:V:271:PHE:CZ	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:157:LYS:HA	1:X:248:TRP:CZ2	2.53	0.43
1:N:272:TYR:O	1:N:276:PRO:HG3	2.19	0.42
1:R:202:LEU:HA	1:R:258:LEU:HD13	2.00	0.42
1:S:266:LEU:CD1	1:X:173:MET:SD	3.07	0.42
1:X:202:LEU:HD12	1:X:258:LEU:HB3	2.01	0.42
1:X:202:LEU:HA	1:X:258:LEU:HD13	2.01	0.42
1:H:202:LEU:HA	1:H:258:LEU:HD13	2.01	0.42
1:N:209:ALA:HA	1:N:212:ILE:CD1	2.43	0.42
1:U:202:LEU:HD12	1:U:258:LEU:HB3	2.00	0.42
1:C:202:LEU:HA	1:C:258:LEU:HD13	2.00	0.42
1:E:215:CYS:C	1:E:218:PRO:HD2	2.39	0.42
1:F:304:LEU:C	1:F:304:LEU:HD23	2.40	0.42
1:I:197:ILE:HG12	1:J:281:SER:HB2	2.01	0.42
1:M:271:PHE:HB2	1:M:279:ALA:HB2	1.99	0.42
1:O:161:SER:HB2	1:O:248:TRP:HE1	1.85	0.42
1:V:196:ALA:HB3	1:W:281:SER:OG	2.18	0.42
1:V:207:MET:C	1:W:293:PHE:CE2	2.91	0.42
1:W:254:LEU:C	1:W:254:LEU:HD23	2.39	0.42
1:W:303:SER:O	1:W:306:SER:HB3	2.20	0.42
1:X:158:LEU:HG	1:X:213:SER:HB3	2.01	0.42
1:H:254:LEU:C	1:H:254:LEU:HD23	2.40	0.42
1:L:215:CYS:C	1:L:218:PRO:HD2	2.39	0.42
1:O:202:LEU:HA	1:O:258:LEU:HD13	2.00	0.42
1:O:309:TYR:O	1:O:313:VAL:HG23	2.20	0.42
1:T:215:CYS:C	1:T:218:PRO:HD2	2.40	0.42
1:B:268:TRP:CZ3	1:B:283:THR:HB	2.54	0.42
1:C:256:LEU:HD13	1:C:293:PHE:HZ	1.84	0.42
1:H:158:LEU:CG	1:H:213:SER:HB3	2.46	0.42
1:I:209:ALA:HA	1:I:212:ILE:CD1	2.44	0.42
1:M:215:CYS:C	1:M:218:PRO:HD2	2.40	0.42
1:Q:212:ILE:O	1:Q:216:ILE:HG13	2.19	0.42
1:C:309:TYR:OH	1:N:323:LYS:HG3	2.20	0.42
1:K:207:MET:CB	1:L:293:PHE:HE2	2.33	0.42
1:X:304:LEU:C	1:X:304:LEU:HD23	2.40	0.42
1:B:203:VAL:O	1:B:207:MET:HG2	2.20	0.42
1:C:301:TYR:O	1:C:305:VAL:HG23	2.20	0.42
1:G:301:TYR:O	1:G:305:VAL:HG23	2.20	0.42
1:I:316:ILE:HG22	1:U:316:ILE:HG22	2.02	0.42
1:K:162:SER:HA	1:K:210:LEU:CD2	2.49	0.42
1:P:150:LYS:O	1:P:241:HIS:NE2	2.47	0.42
1:U:320:GLU:HA	1:U:323:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:321:MET:SD	1:V:325:GLN:NE2	2.92	0.42
1:C:304:LEU:HD23	1:C:304:LEU:C	2.40	0.42
1:D:304:LEU:C	1:D:304:LEU:HD23	2.40	0.42
1:G:202:LEU:HD12	1:G:258:LEU:HB3	2.00	0.42
1:L:304:LEU:C	1:L:304:LEU:HD23	2.39	0.42
1:N:197:ILE:CG1	1:O:281:SER:HB2	2.50	0.42
1:R:202:LEU:HD12	1:R:258:LEU:HB3	2.00	0.42
1:V:215:CYS:C	1:V:218:PRO:HD2	2.40	0.42
1:A:202:LEU:HA	1:A:258:LEU:HD13	2.00	0.42
1:O:215:CYS:HB2	1:P:300:PHE:CZ	2.55	0.42
1:P:254:LEU:C	1:P:254:LEU:HD23	2.40	0.42
1:P:275:SER:N	1:P:276:PRO:CD	2.83	0.42
1:Q:275:SER:N	1:Q:276:PRO:CD	2.83	0.42
1:X:254:LEU:C	1:X:254:LEU:HD23	2.40	0.42
1:B:275:SER:N	1:B:276:PRO:CD	2.83	0.42
1:B:304:LEU:C	1:B:304:LEU:HD23	2.40	0.42
1:D:268:TRP:CH2	1:D:280:TRP:HA	2.55	0.42
1:D:301:TYR:O	1:D:305:VAL:HG23	2.19	0.42
1:E:254:LEU:HD23	1:E:254:LEU:C	2.40	0.42
1:E:307:HIS:HA	1:E:310:GLU:HB3	2.02	0.42
1:H:304:LEU:HD23	1:H:304:LEU:C	2.41	0.42
1:I:304:LEU:C	1:I:304:LEU:HD23	2.41	0.42
1:O:323:LYS:O	1:O:327:GLU:HG3	2.20	0.42
1:R:209:ALA:HA	1:R:212:ILE:CD1	2.44	0.42
1:W:242:TRP:O	1:W:245:GLU:HB3	2.20	0.42
1:A:215:CYS:C	1:A:218:PRO:HD2	2.39	0.41
1:B:254:LEU:C	1:B:254:LEU:HD23	2.40	0.41
1:D:202:LEU:HA	1:D:258:LEU:HD13	2.01	0.41
1:F:161:SER:HB2	1:F:248:TRP:HE1	1.85	0.41
1:I:202:LEU:HD12	1:I:258:LEU:HB3	2.02	0.41
1:J:254:LEU:HD23	1:J:254:LEU:C	2.40	0.41
1:K:207:MET:HB3	1:L:293:PHE:HE2	1.84	0.41
1:R:215:CYS:C	1:R:218:PRO:HD2	2.41	0.41
1:C:271:PHE:HB2	1:C:279:ALA:HB2	2.02	0.41
1:C:275:SER:N	1:C:276:PRO:CD	2.83	0.41
1:I:268:TRP:CH2	1:I:280:TRP:HA	2.55	0.41
1:J:202:LEU:HD23	1:J:202:LEU:O	2.20	0.41
1:Q:202:LEU:HD12	1:Q:258:LEU:HB3	2.02	0.41
1:R:254:LEU:C	1:R:254:LEU:HD23	2.39	0.41
1:B:202:LEU:HD12	1:B:258:LEU:HB3	2.02	0.41
1:C:316:ILE:CG2	1:N:316:ILE:HG22	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:254:LEU:C	1:F:254:LEU:HD23	2.41	0.41
1:G:214:THR:HG23	1:H:248:TRP:CH2	2.55	0.41
1:H:309:TYR:CD1	1:V:326:MET:HG2	2.55	0.41
1:M:275:SER:N	1:M:276:PRO:CD	2.83	0.41
1:Q:304:LEU:C	1:Q:304:LEU:HD23	2.40	0.41
1:T:275:SER:N	1:T:276:PRO:CD	2.83	0.41
1:U:202:LEU:HA	1:U:258:LEU:HD13	2.02	0.41
1:D:316:ILE:CG2	1:M:319:LEU:HD12	2.42	0.41
1:D:319:LEU:HD22	1:M:312:THR:CA	2.40	0.41
1:G:256:LEU:HD13	1:G:293:PHE:CZ	2.43	0.41
1:M:254:LEU:C	1:M:254:LEU:HD23	2.40	0.41
1:M:304:LEU:HD23	1:M:304:LEU:C	2.41	0.41
1:P:318:GLU:O	1:P:321:MET:HB2	2.19	0.41
1:Q:242:TRP:O	1:Q:245:GLU:HB3	2.21	0.41
1:U:173:MET:SD	1:V:266:LEU:CD1	3.08	0.41
1:V:202:LEU:HD12	1:V:258:LEU:HB3	2.02	0.41
1:J:205:VAL:HG21	1:J:254:LEU:HD22	2.02	0.41
1:Q:321:MET:O	1:Q:325:GLN:HG3	2.20	0.41
1:R:203:VAL:O	1:R:207:MET:HG2	2.21	0.41
1:V:209:ALA:HA	1:V:212:ILE:CD1	2.45	0.41
1:W:304:LEU:C	1:W:304:LEU:HD23	2.40	0.41
1:A:260:LEU:O	1:A:263:ILE:CG2	2.68	0.41
1:C:326:MET:HE3	1:N:309:TYR:CB	2.50	0.41
1:G:309:TYR:O	1:G:313:VAL:HG23	2.21	0.41
1:H:173:MET:HE2	1:I:263:ILE:HB	2.01	0.41
1:I:312:THR:HA	1:U:319:LEU:HD22	2.01	0.41
1:P:301:TYR:O	1:P:305:VAL:HG23	2.20	0.41
1:S:271:PHE:CZ	1:X:176:MET:HE2	2.55	0.41
1:U:304:LEU:C	1:U:304:LEU:HD23	2.41	0.41
1:D:192:LEU:HD12	1:D:192:LEU:N	2.36	0.41
1:K:287:ILE:O	1:K:291:ILE:HG13	2.21	0.41
1:N:304:LEU:HD23	1:N:304:LEU:C	2.41	0.41
1:P:215:CYS:C	1:P:218:PRO:HD2	2.40	0.41
1:R:275:SER:N	1:R:276:PRO:CD	2.84	0.41
1:R:304:LEU:HD23	1:R:304:LEU:C	2.41	0.41
1:S:296:PHE:HD2	1:X:211:MET:CE	2.34	0.41
1:U:196:ALA:HB2	1:V:271:PHE:CE2	2.55	0.41
1:W:282:ALA:O	1:W:285:VAL:HG12	2.21	0.41
1:A:307:HIS:O	1:A:311:VAL:HG23	2.20	0.41
1:D:203:VAL:O	1:D:207:MET:HG2	2.21	0.41
1:K:275:SER:N	1:K:276:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:275:SER:N	1:N:276:PRO:CD	2.83	0.41
1:P:288:PRO:O	1:P:292:ILE:HG13	2.21	0.41
1:T:173:MET:CE	1:U:263:ILE:HD13	2.51	0.41
1:W:162:SER:HA	1:W:210:LEU:CD2	2.51	0.41
1:W:260:LEU:HG	1:W:286:LEU:HD13	2.02	0.41
1:X:267:CYS:O	1:X:271:PHE:CD2	2.74	0.41
1:A:268:TRP:CZ3	1:A:280:TRP:HA	2.56	0.41
1:C:321:MET:O	1:C:325:GLN:HG3	2.20	0.41
1:D:202:LEU:HD12	1:D:258:LEU:HB3	2.03	0.41
1:D:275:SER:N	1:D:276:PRO:CD	2.84	0.41
1:D:287:ILE:O	1:D:291:ILE:HG13	2.21	0.41
1:F:212:ILE:HG22	1:F:216:ILE:CD1	2.51	0.41
1:G:202:LEU:HD23	1:G:202:LEU:O	2.21	0.41
1:G:254:LEU:C	1:G:254:LEU:HD23	2.41	0.41
1:H:162:SER:HA	1:H:210:LEU:CD2	2.50	0.41
1:J:161:SER:HB2	1:J:248:TRP:NE1	2.35	0.41
1:K:304:LEU:C	1:K:304:LEU:HD23	2.40	0.41
1:L:275:SER:N	1:L:276:PRO:CD	2.84	0.41
1:L:287:ILE:O	1:L:291:ILE:HG13	2.21	0.41
1:M:202:LEU:O	1:M:202:LEU:HD23	2.21	0.41
1:M:209:ALA:HA	1:M:212:ILE:CD1	2.44	0.41
1:O:304:LEU:C	1:O:304:LEU:HD23	2.41	0.41
1:O:323:LYS:O	1:O:327:GLU:CD	2.59	0.41
1:Q:173:MET:HB2	1:Q:173:MET:HE3	1.96	0.41
1:S:215:CYS:C	1:S:218:PRO:HD2	2.41	0.41
1:S:275:SER:N	1:S:276:PRO:CD	2.84	0.41
1:U:207:MET:CB	1:V:293:PHE:HE2	2.33	0.41
1:V:287:ILE:O	1:V:291:ILE:HG13	2.20	0.41
1:X:209:ALA:HA	1:X:212:ILE:CD1	2.44	0.41
1:X:275:SER:N	1:X:276:PRO:CD	2.83	0.41
1:A:275:SER:N	1:A:276:PRO:CD	2.83	0.41
1:D:173:MET:HB2	1:D:173:MET:HE2	1.96	0.41
1:F:212:ILE:HA	1:F:215:CYS:SG	2.61	0.41
1:M:205:VAL:O	1:M:208:LEU:HG	2.21	0.41
1:N:162:SER:HA	1:N:210:LEU:CD2	2.51	0.41
1:N:202:LEU:HD12	1:N:258:LEU:HB3	2.02	0.41
1:P:212:ILE:HG22	1:P:216:ILE:CD1	2.50	0.41
1:T:307:HIS:O	1:T:311:VAL:HG23	2.21	0.41
1:A:271:PHE:O	1:A:275:SER:N	2.53	0.40
1:C:287:ILE:O	1:C:291:ILE:HG13	2.21	0.40
1:F:202:LEU:HD23	1:F:202:LEU:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:275:SER:N	1:H:276:PRO:CD	2.84	0.40
1:I:267:CYS:O	1:I:271:PHE:CD2	2.74	0.40
1:M:307:HIS:O	1:M:311:VAL:HG23	2.21	0.40
1:N:215:CYS:C	1:N:218:PRO:HD2	2.41	0.40
1:P:319:LEU:HD23	1:P:319:LEU:HA	1.94	0.40
1:W:322:LEU:O	1:W:326:MET:HB2	2.20	0.40
1:A:202:LEU:HD12	1:A:258:LEU:HB3	2.02	0.40
1:E:316:ILE:CG2	1:R:319:LEU:HD13	2.46	0.40
1:H:307:HIS:HA	1:H:310:GLU:HB3	2.04	0.40
1:L:254:LEU:C	1:L:254:LEU:HD23	2.42	0.40
1:O:215:CYS:C	1:O:218:PRO:HD2	2.41	0.40
1:T:304:LEU:HD23	1:T:304:LEU:C	2.41	0.40
1:U:210:LEU:HD12	1:V:256:LEU:CD2	2.51	0.40
1:V:207:MET:HA	1:V:210:LEU:CD1	2.50	0.40
1:E:275:SER:N	1:E:276:PRO:CD	2.84	0.40
1:E:288:PRO:O	1:E:292:ILE:HG13	2.22	0.40
1:F:203:VAL:O	1:F:207:MET:HG2	2.21	0.40
1:G:275:SER:N	1:G:276:PRO:CD	2.85	0.40
1:K:271:PHE:O	1:K:275:SER:N	2.55	0.40
1:O:275:SER:N	1:O:276:PRO:CD	2.84	0.40
1:Q:195:PHE:CD2	1:R:271:PHE:HZ	2.39	0.40
1:S:285:VAL:HG21	1:X:201:LEU:HD21	2.02	0.40
1:T:207:MET:CB	1:U:293:PHE:HE2	2.34	0.40
1:V:254:LEU:HD23	1:V:254:LEU:C	2.41	0.40
1:V:275:SER:N	1:V:276:PRO:CD	2.84	0.40
1:W:202:LEU:O	1:W:202:LEU:HD23	2.21	0.40
1:A:312:THR:CG2	1:P:319:LEU:HD22	2.39	0.40
1:B:264:ALA:CB	1:B:286:LEU:HD22	2.52	0.40
1:C:254:LEU:C	1:C:254:LEU:HD23	2.41	0.40
1:D:158:LEU:HG	1:D:213:SER:CB	2.51	0.40
1:J:158:LEU:HD23	1:J:158:LEU:C	2.42	0.40
1:O:158:LEU:HD23	1:O:158:LEU:C	2.42	0.40
1:P:158:LEU:C	1:P:158:LEU:HD23	2.42	0.40
1:V:158:LEU:C	1:V:158:LEU:HD23	2.42	0.40
1:V:288:PRO:O	1:V:292:ILE:HG13	2.22	0.40
1:W:202:LEU:HA	1:W:258:LEU:HD13	2.03	0.40
1:W:275:SER:N	1:W:276:PRO:CD	2.84	0.40
1:X:309:TYR:O	1:X:313:VAL:HG23	2.21	0.40
1:A:173:MET:HE2	1:B:263:ILE:HD13	2.02	0.40
1:F:275:SER:N	1:F:276:PRO:CD	2.84	0.40
1:H:158:LEU:C	1:H:158:LEU:HD23	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:312:THR:HG21	1:U:323:LYS:HB2	2.02	0.40
1:J:207:MET:CB	1:K:293:PHE:HE2	2.34	0.40
1:K:158:LEU:HD23	1:K:158:LEU:C	2.42	0.40
1:K:177:VAL:HB	1:L:179:VAL:HG13	2.03	0.40
1:L:326:MET:HE3	1:X:309:TYR:HA	2.03	0.40
1:M:158:LEU:HD23	1:M:158:LEU:C	2.42	0.40
1:M:173:MET:HB2	1:M:173:MET:HE3	1.95	0.40
1:N:161:SER:HB2	1:N:248:TRP:HE1	1.86	0.40
1:P:282:ALA:O	1:P:285:VAL:HG12	2.21	0.40
1:Q:158:LEU:C	1:Q:158:LEU:HD23	2.42	0.40
1:S:253:LEU:CD1	1:S:293:PHE:HE1	2.35	0.40
1:T:268:TRP:HA	1:T:279:ALA:HB1	2.02	0.40
1:U:275:SER:N	1:U:276:PRO:CD	2.84	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	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	B	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	C	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	D	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	E	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	F	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	G	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	H	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	I	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	J	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	L	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	M	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	N	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	O	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	P	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	Q	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	R	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	S	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	T	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	U	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
1	V	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	W	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	11	46
1	X	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22	63
All	All	3456/5136 (67%)	3360 (97%)	60 (2%)	36 (1%)	15	54

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	272	TYR
1	J	272	TYR
1	W	272	TYR
1	D	272	TYR
1	I	272	TYR
1	K	272	TYR
1	L	272	TYR
1	S	272	TYR
1	T	272	TYR
1	V	272	TYR
1	C	275	SER
1	F	275	SER
1	M	275	SER
1	N	275	SER
1	R	272	TYR
1	A	275	SER
1	B	275	SER
1	D	275	SER

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Mol	Chain	Res	Type
1	E	275	SER
1	G	275	SER
1	H	275	SER
1	I	275	SER
1	J	275	SER
1	K	275	SER
1	L	275	SER
1	O	275	SER
1	P	275	SER
1	Q	272	TYR
1	Q	275	SER
1	R	275	SER
1	S	275	SER
1	T	275	SER
1	U	275	SER
1	V	275	SER
1	W	275	SER
1	X	275	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/189 (61%)	115 (100%)	0	100	100
1	B	115/189 (61%)	115 (100%)	0	100	100
1	C	115/189 (61%)	115 (100%)	0	100	100
1	D	115/189 (61%)	115 (100%)	0	100	100
1	E	115/189 (61%)	115 (100%)	0	100	100
1	F	115/189 (61%)	115 (100%)	0	100	100
1	G	115/189 (61%)	115 (100%)	0	100	100
1	H	115/189 (61%)	115 (100%)	0	100	100
1	I	115/189 (61%)	115 (100%)	0	100	100
1	J	115/189 (61%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	115/189 (61%)	115 (100%)	0	100 100
1	L	115/189 (61%)	115 (100%)	0	100 100
1	M	115/189 (61%)	115 (100%)	0	100 100
1	N	115/189 (61%)	115 (100%)	0	100 100
1	O	115/189 (61%)	115 (100%)	0	100 100
1	P	115/189 (61%)	114 (99%)	1 (1%)	78 87
1	Q	115/189 (61%)	115 (100%)	0	100 100
1	R	115/189 (61%)	114 (99%)	1 (1%)	78 87
1	S	115/189 (61%)	115 (100%)	0	100 100
1	T	115/189 (61%)	115 (100%)	0	100 100
1	U	115/189 (61%)	114 (99%)	1 (1%)	78 87
1	V	115/189 (61%)	115 (100%)	0	100 100
1	W	115/189 (61%)	115 (100%)	0	100 100
1	X	115/189 (61%)	115 (100%)	0	100 100
All	All	2760/4536 (61%)	2757 (100%)	3 (0%)	93 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	326	MET
1	R	310	GLU
1	U	316	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	325	GLN
1	Q	325	GLN
1	T	325	GLN
1	V	325	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	A	150/214 (70%)	-0.31	1 (0%) 87 82	584, 646, 758, 811	0
1	B	150/214 (70%)	-0.37	0 100 100	598, 671, 767, 807	0
1	C	150/214 (70%)	-0.45	0 100 100	581, 656, 730, 754	0
1	D	150/214 (70%)	-0.56	0 100 100	549, 611, 728, 776	0
1	E	150/214 (70%)	-0.40	1 (0%) 87 82	523, 568, 843, 918	0
1	F	150/214 (70%)	-0.57	0 100 100	543, 575, 708, 752	0
1	G	150/214 (70%)	0.15	10 (6%) 17 18	592, 781, 885, 905	0
1	H	150/214 (70%)	-0.07	1 (0%) 87 82	585, 712, 910, 931	0
1	I	150/214 (70%)	-0.15	4 (2%) 54 48	252, 719, 907, 986	0
1	J	150/214 (70%)	0.14	9 (6%) 21 21	609, 771, 916, 967	0
1	K	150/214 (70%)	-0.14	4 (2%) 54 48	617, 778, 945, 962	0
1	L	150/214 (70%)	-0.09	5 (3%) 46 41	607, 778, 851, 884	0
1	M	150/214 (70%)	-0.33	7 (4%) 31 30	635, 696, 790, 832	0
1	N	150/214 (70%)	-0.50	1 (0%) 87 82	646, 684, 747, 771	0
1	O	150/214 (70%)	-0.23	1 (0%) 87 82	640, 710, 788, 825	0
1	P	150/214 (70%)	-0.49	0 100 100	584, 643, 785, 850	0
1	Q	150/214 (70%)	-0.48	1 (0%) 87 82	565, 633, 752, 815	0
1	R	150/214 (70%)	-0.45	0 100 100	613, 699, 815, 878	0
1	S	150/214 (70%)	-0.02	7 (4%) 31 30	679, 746, 880, 973	0
1	T	150/214 (70%)	0.29	10 (6%) 17 18	20, 764, 884, 971	0
1	U	150/214 (70%)	-0.19	4 (2%) 54 48	740, 830, 912, 950	0
1	V	150/214 (70%)	0.07	6 (4%) 38 34	731, 835, 900, 932	0
1	W	150/214 (70%)	0.12	7 (4%) 31 30	711, 814, 948, 981	0
1	X	150/214 (70%)	-0.25	1 (0%) 87 82	674, 741, 884, 952	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	3600/5136 (70%)	-0.22	80 (2%) 62 54	20, 712, 880, 986	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	324	GLU	7.2
1	T	325	GLN	6.7
1	T	324	GLU	6.2
1	T	327	GLU	5.9
1	I	274	LEU	5.2
1	J	325	GLN	4.8
1	T	326	MET	4.7
1	I	275	SER	4.4
1	J	327	GLU	4.3
1	K	327	GLU	3.9
1	J	323	LYS	3.8
1	T	321	MET	3.7
1	G	193	ILE	3.6
1	J	273	ASP	3.4
1	T	323	LYS	3.3
1	W	327	GLU	3.2
1	L	180	GLN	3.2
1	G	278	ALA	3.2
1	I	273	ASP	3.1
1	V	327	GLU	3.1
1	K	281	SER	2.9
1	L	327	GLU	2.9
1	J	322	LEU	2.8
1	U	278	ALA	2.8
1	X	178	GLU	2.8
1	V	264	ALA	2.7
1	T	219	ASN	2.7
1	G	242	TRP	2.7
1	G	192	LEU	2.7
1	V	180	GLN	2.7
1	M	327	GLU	2.6
1	S	219	ASN	2.6
1	I	276	PRO	2.6
1	Q	148	TRP	2.6
1	M	325	GLN	2.5
1	L	192	LEU	2.5
1	W	317	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	U	180	GLN	2.5
1	S	273	ASP	2.5
1	W	264	ALA	2.4
1	W	318	GLU	2.4
1	W	150	LYS	2.4
1	G	280	TRP	2.4
1	S	240	LEU	2.4
1	K	278	ALA	2.4
1	V	273	ASP	2.4
1	H	327	GLU	2.4
1	S	277	PRO	2.4
1	S	276	PRO	2.3
1	M	149	ARG	2.3
1	M	324	GLU	2.3
1	G	279	ALA	2.3
1	A	148	TRP	2.2
1	L	178	GLU	2.2
1	K	282	ALA	2.2
1	G	314	SER	2.2
1	M	317	ARG	2.2
1	J	326	MET	2.2
1	T	152	GLN	2.2
1	U	277	PRO	2.2
1	N	273	ASP	2.2
1	V	218	PRO	2.2
1	J	275	SER	2.1
1	W	149	ARG	2.1
1	S	242	TRP	2.1
1	J	320	GLU	2.1
1	U	323	LYS	2.1
1	V	283	THR	2.1
1	G	277	PRO	2.1
1	T	240	LEU	2.1
1	W	319	LEU	2.1
1	L	148	TRP	2.1
1	G	191	MET	2.1
1	G	241	HIS	2.1
1	M	318	GLU	2.1
1	T	320	GLU	2.1
1	M	314	SER	2.1
1	S	267	CYS	2.0
1	E	321	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	214	THR	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 monosaccharides 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.