Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 09:24 PM EDT

PDB ID	:	2P2C
Title	:	Inhibition of caspase-2 by a designed ankyrin repeat protein (DARPin)
Authors	:	Roschitzki Voser, H.; Briand, C.; Capitani, G.; Gruetter, M.G.
Deposited on	:	2007-03-07
Resolution	:	3.24 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:

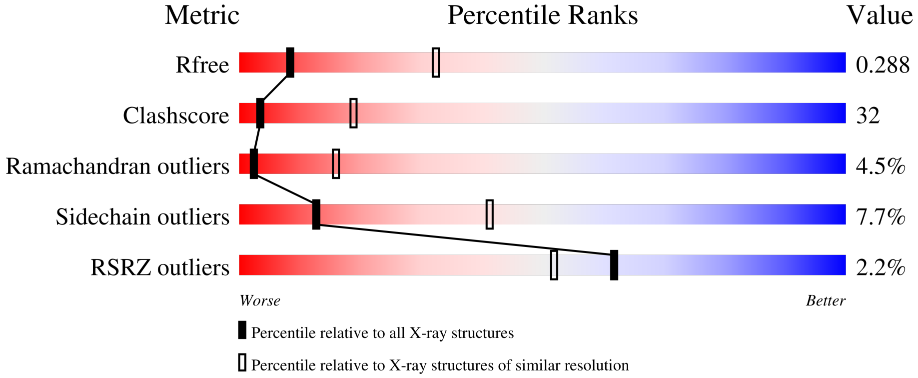
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

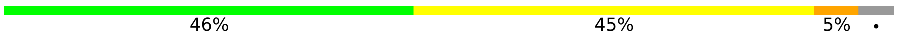
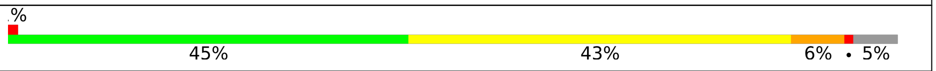
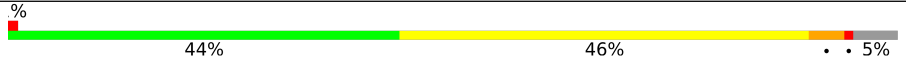
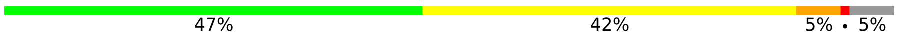
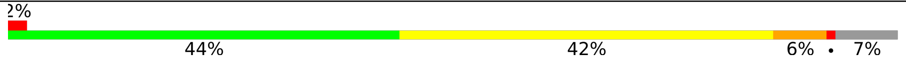
The reported resolution of this entry is 3.24 Å.

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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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	169	
1	C	169	
1	E	169	
1	G	169	
1	I	169	

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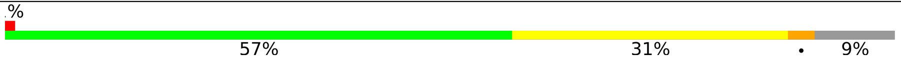
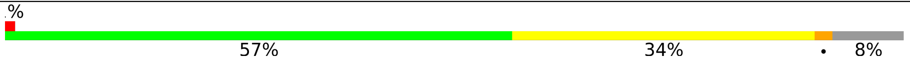
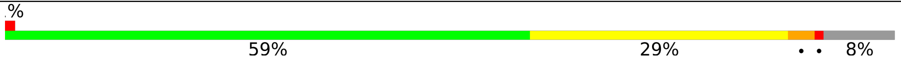
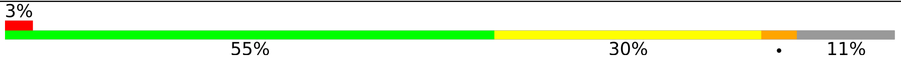
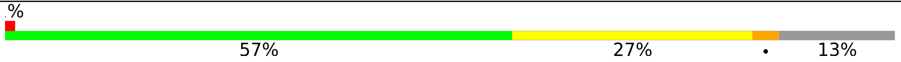
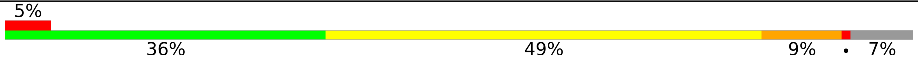
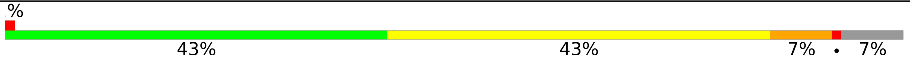
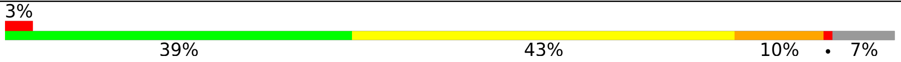
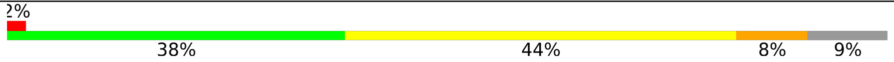
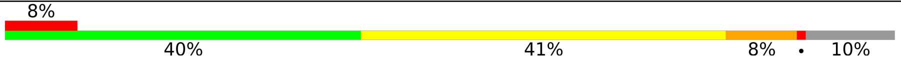
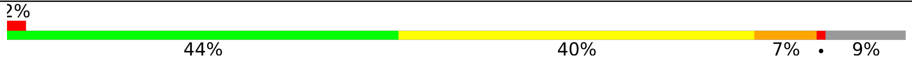
Mol	Chain	Length	Quality of chain
1	K	169	
2	B	106	
2	D	106	
2	F	106	
2	H	106	
2	J	106	
2	L	106	
3	P	169	
3	Q	169	
3	R	169	
3	S	169	
3	T	169	
3	U	169	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19285 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 Caspase-2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	162	Total C N O S 1284 810 223 243 8	0	0	0
1	C	161	Total C N O S 1276 804 222 242 8	0	0	0
1	E	160	Total C N O S 1267 800 221 238 8	0	0	0
1	G	160	Total C N O S 1267 800 221 238 8	0	0	0
1	I	157	Total C N O S 1244 786 217 234 7	0	0	0
1	K	158	Total C N O S 1252 792 218 235 7	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	cloning artifact	UNP P42575
A	1	ALA	-	cloning artifact	UNP P42575
A	7	LEU	VAL	variant	UNP P42575
C	0	MET	-	cloning artifact	UNP P42575
C	1	ALA	-	cloning artifact	UNP P42575
C	7	LEU	VAL	variant	UNP P42575
E	0	MET	-	cloning artifact	UNP P42575
E	1	ALA	-	cloning artifact	UNP P42575
E	7	LEU	VAL	variant	UNP P42575
G	0	MET	-	cloning artifact	UNP P42575
G	1	ALA	-	cloning artifact	UNP P42575
G	7	LEU	VAL	variant	UNP P42575
I	0	MET	-	cloning artifact	UNP P42575
I	1	ALA	-	cloning artifact	UNP P42575
I	7	LEU	VAL	variant	UNP P42575
K	0	MET	-	cloning artifact	UNP P42575
K	1	ALA	-	cloning artifact	UNP P42575

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Chain	Residue	Modelled	Actual	Comment	Reference
K	7	LEU	VAL	variant	UNP P42575

- Molecule 2 is a protein called Caspase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total 760	C 477	N 137	O 134	S 12	0	0	0
2	D	98	Total 777	C 487	N 140	O 138	S 12	0	0	0
2	F	96	Total 760	C 477	N 137	O 134	S 12	0	0	0
2	H	98	Total 776	C 488	N 140	O 136	S 12	0	0	0
2	J	94	Total 746	C 467	N 135	O 132	S 12	0	0	0
2	L	92	Total 727	C 456	N 130	O 130	S 11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	200	MET	-	cloning artifact	UNP P42575
D	200	MET	-	cloning artifact	UNP P42575
F	200	MET	-	cloning artifact	UNP P42575
H	200	MET	-	cloning artifact	UNP P42575
J	200	MET	-	cloning artifact	UNP P42575
L	200	MET	-	cloning artifact	UNP P42575

- Molecule 3 is a protein called Caspase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	158	Total 1207	C 762	N 207	O 237	S 1	0	0	0
3	Q	158	Total 1209	C 764	N 205	O 239	S 1	0	0	0
3	R	157	Total 1198	C 757	N 205	O 235	S 1	0	0	0
3	S	153	Total 1168	C 740	N 197	O 230	S 1	0	0	0
3	T	152	Total 1161	C 735	N 197	O 228	S 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	U	154	1177	745	199	232	1	0	0	0

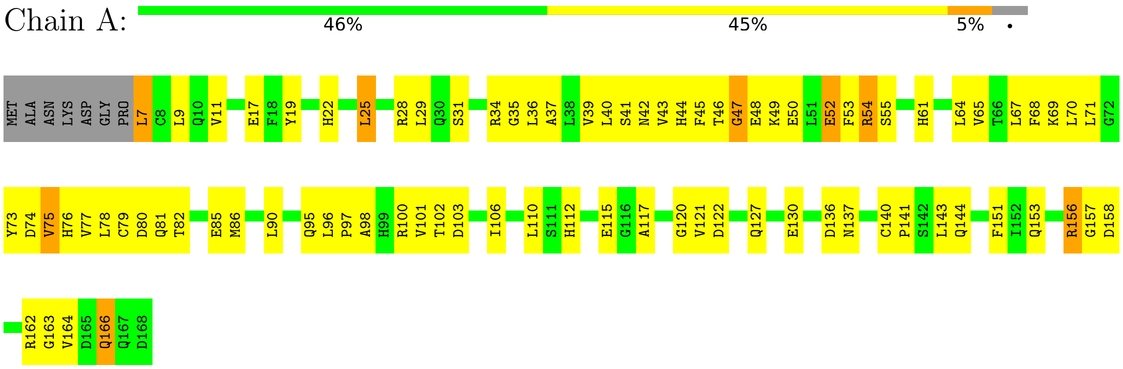
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	4	4	4	0	0
4	P	1	1	1	0	0
4	C	5	5	5	0	0
4	D	5	5	5	0	0
4	Q	2	2	2	0	0
4	E	1	1	1	0	0
4	F	1	1	1	0	0
4	R	1	1	1	0	0
4	G	2	2	2	0	0
4	H	4	4	4	0	0
4	S	1	1	1	0	0
4	I	1	1	1	0	0
4	L	1	1	1	0	0

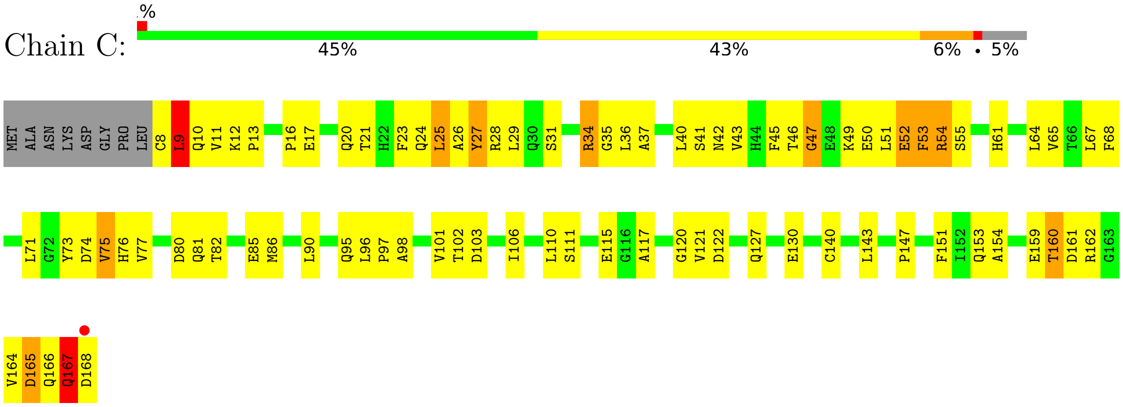
3 Residue-property plots ⓘ

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.

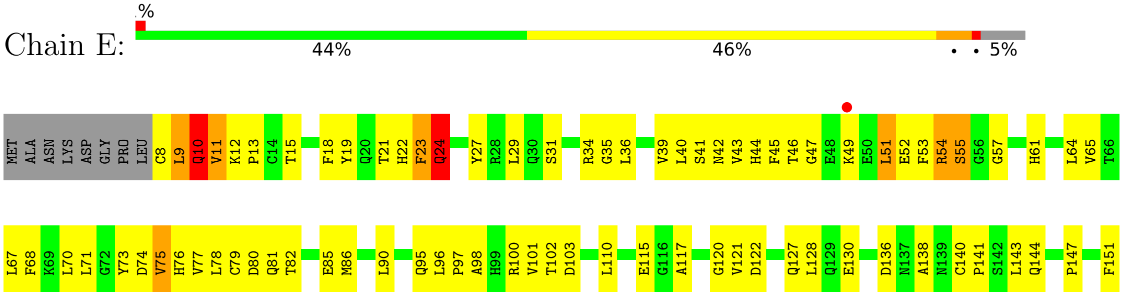
- Molecule 1: Caspase-2

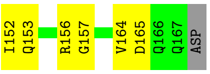


- Molecule 1: Caspase-2



- Molecule 1: Caspase-2



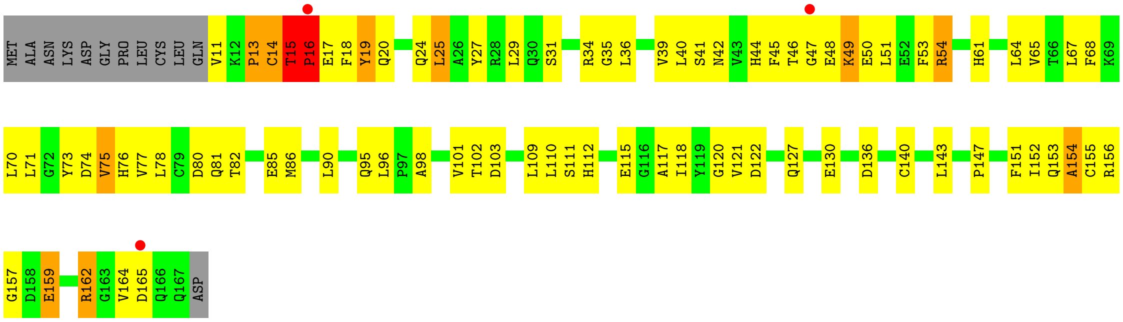


- Molecule 1: Caspase-2

Chain G:

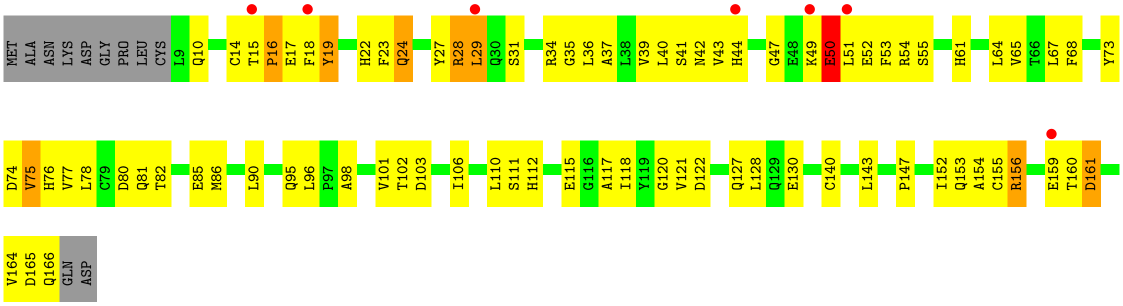
- Molecule 1: Caspase-2

Chain I:



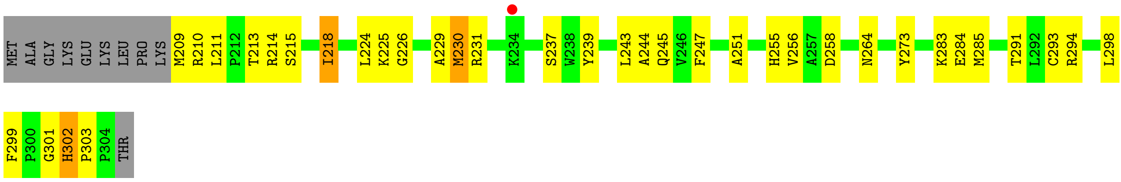
- Molecule 1: Caspase-2

Chain K:

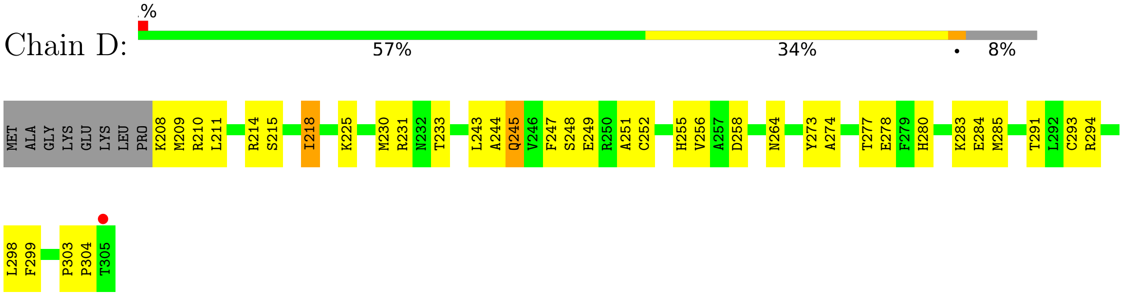


- Molecule 2: Caspase-2

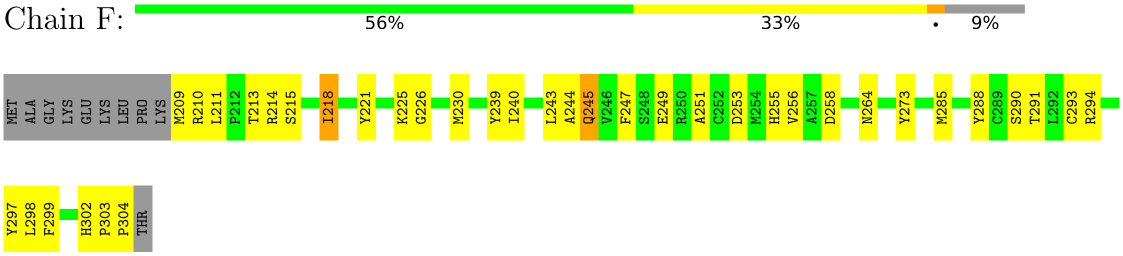
Chain B:



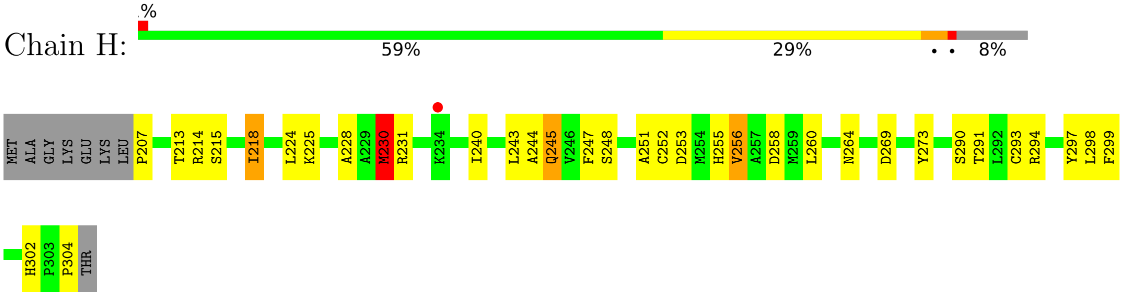
- Molecule 2: Caspase-2



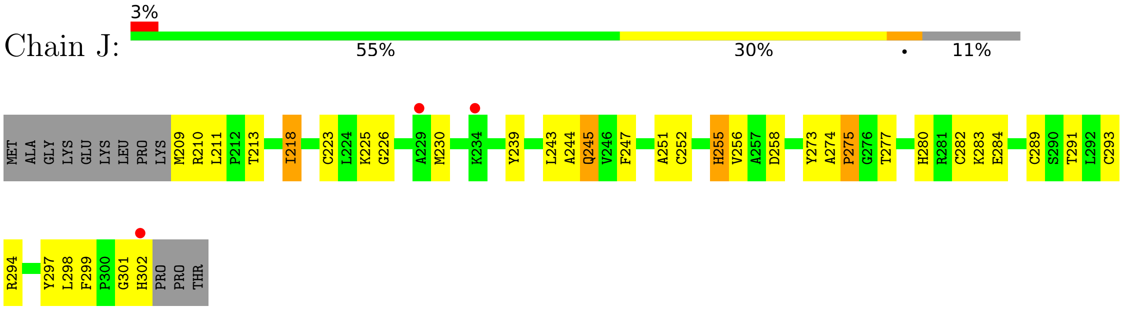
- Molecule 2: Caspase-2



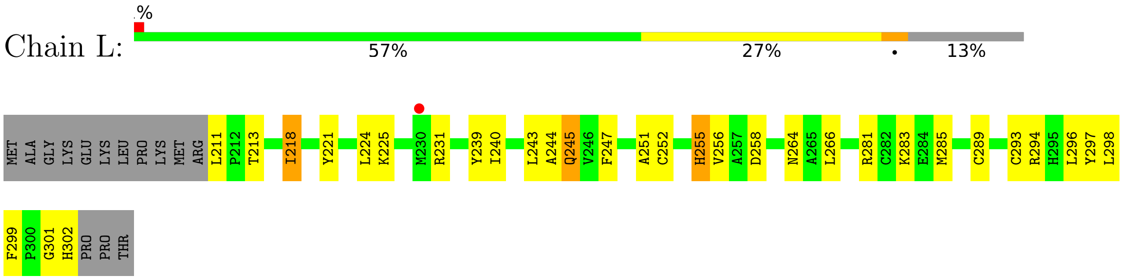
- Molecule 2: Caspase-2



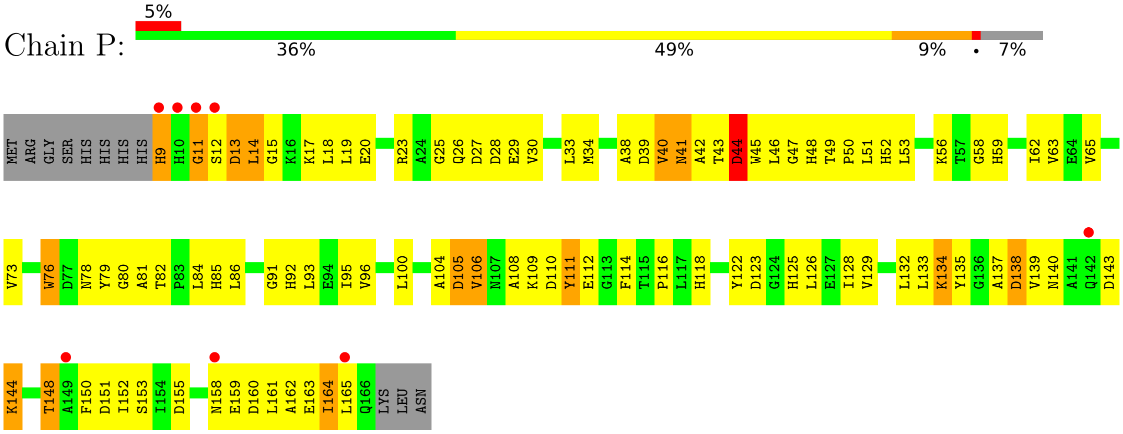
- Molecule 2: Caspase-2



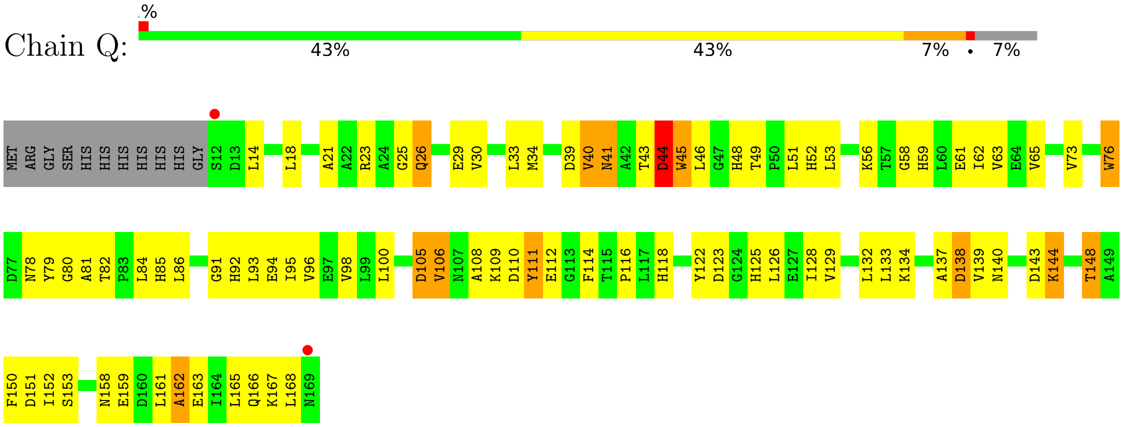
- Molecule 2: Caspase-2



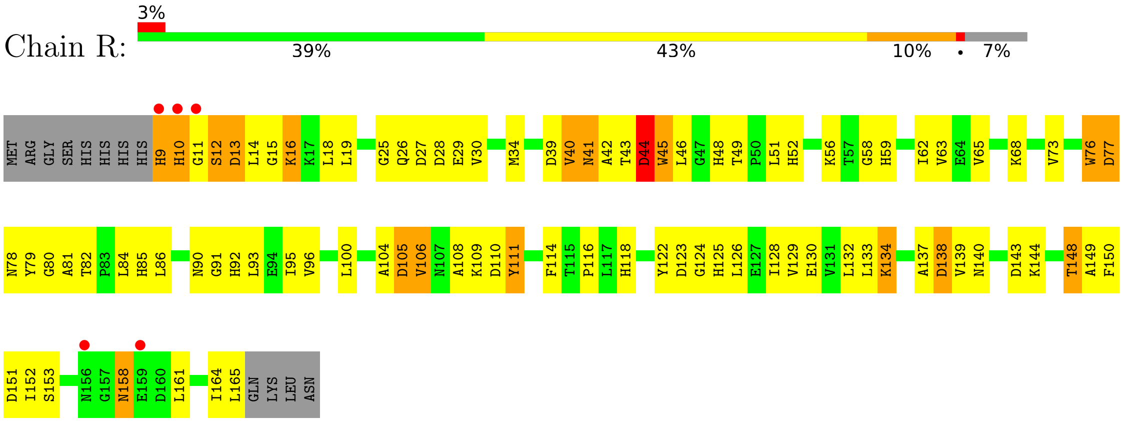
- Molecule 3: Caspase-2



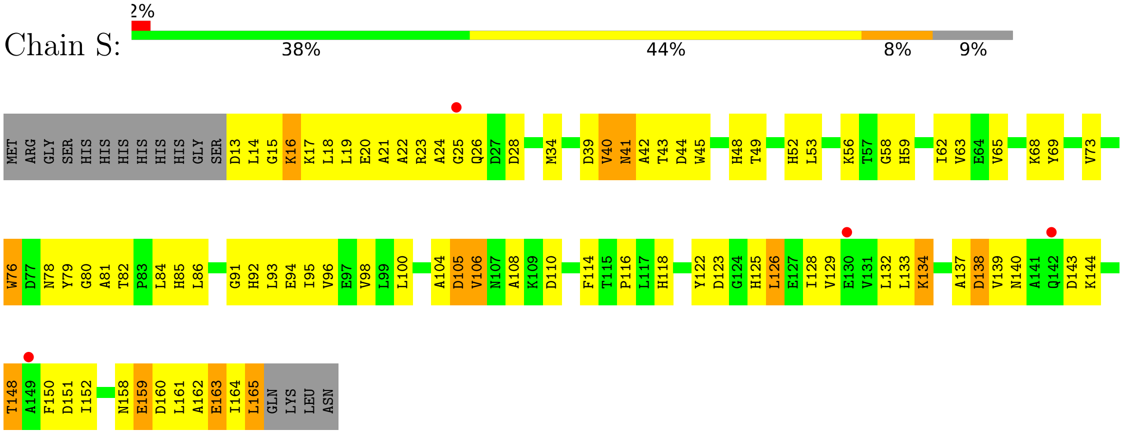
- Molecule 3: Caspase-2



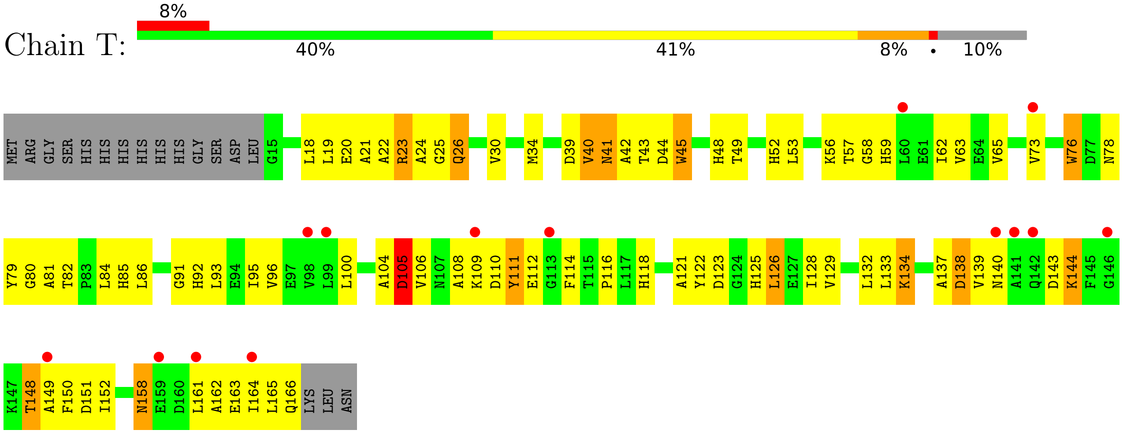
- Molecule 3: Caspase-2



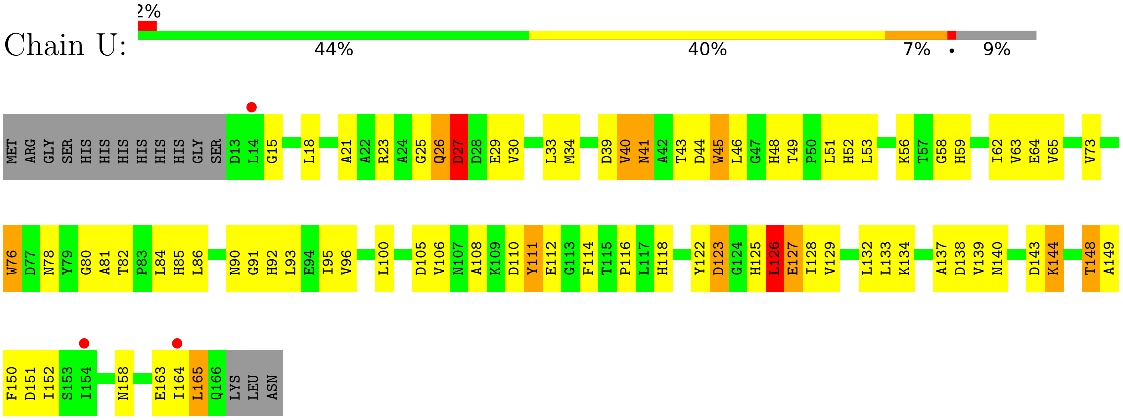
- Molecule 3: Caspase-2



- Molecule 3: Caspase-2



- Molecule 3: Caspase-2



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.02Å 229.21Å 114.93Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	20.00 – 3.24 29.51 – 3.24	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-3.24) 97.6 (29.51-3.24)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	5.90	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.262 , 0.305 0.256 , 0.288	Depositor DCC
R_{free} test set	1026 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å^2)	97.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 24.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.235 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19285	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

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	0.44	1/1309 (0.1%)	0.64	0/1769
1	C	0.38	0/1301	0.63	1/1758 (0.1%)
1	E	0.48	0/1292	0.68	2/1747 (0.1%)
1	G	0.42	0/1292	0.63	0/1747
1	I	0.38	0/1269	0.62	0/1716
1	K	0.39	0/1277	0.62	0/1727
2	B	0.41	0/778	0.63	0/1047
2	D	0.38	0/795	0.63	0/1068
2	F	0.39	0/778	0.65	0/1047
2	H	0.40	0/795	0.66	0/1069
2	J	0.38	0/762	0.64	0/1023
2	L	0.37	0/743	0.59	0/999
3	P	0.54	1/1231 (0.1%)	0.76	2/1674 (0.1%)
3	Q	0.50	0/1231	0.70	1/1672 (0.1%)
3	R	0.51	0/1222	0.73	2/1662 (0.1%)
3	S	0.61	3/1190 (0.3%)	0.78	3/1619 (0.2%)
3	T	0.51	0/1183	0.78	4/1609 (0.2%)
3	U	0.52	2/1199 (0.2%)	0.73	3/1631 (0.2%)
All	All	0.46	7/19647 (0.0%)	0.68	18/26584 (0.1%)

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
2	F	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	106	VAL	CB-CG1	-8.08	1.35	1.52
3	P	12	SER	CB-OG	7.92	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	127	GLU	CD-OE1	-7.16	1.17	1.25
1	A	69	LYS	CE-NZ	-7.09	1.31	1.49
3	S	106	VAL	CB-CG2	-6.92	1.38	1.52
3	S	126	LEU	CG-CD2	-6.55	1.27	1.51
3	U	126	LEU	CG-CD2	-6.27	1.28	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	126	LEU	CA-CB-CG	9.13	136.29	115.30
3	S	106	VAL	CG1-CB-CG2	-7.89	98.27	110.90
3	T	105	ASP	CB-CG-OD1	7.72	125.25	118.30
3	S	126	LEU	CB-CG-CD1	6.77	122.50	111.00
3	T	105	ASP	OD1-CG-OD2	-6.44	111.06	123.30
3	U	126	LEU	CA-CB-CG	6.39	130.01	115.30
3	T	105	ASP	CB-CG-OD2	5.99	123.69	118.30
1	E	10	GLN	N-CA-C	-5.74	95.50	111.00
3	U	151	ASP	CB-CG-OD1	5.69	123.42	118.30
3	T	144	LYS	CA-CB-CG	5.61	125.75	113.40
1	E	9	LEU	N-CA-C	5.57	126.04	111.00
1	C	9	LEU	CA-CB-CG	5.48	127.91	115.30
3	Q	44	ASP	CB-CA-C	-5.30	99.80	110.40
3	U	126	LEU	CB-CG-CD1	5.29	120.00	111.00
3	R	44	ASP	CB-CA-C	-5.26	99.89	110.40
3	P	11	GLY	N-CA-C	5.19	126.08	113.10
3	P	44	ASP	CB-CG-OD2	-5.03	113.78	118.30
3	R	44	ASP	CB-CG-OD2	-5.02	113.79	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	288	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1284	0	1256	95	0
1	C	1276	0	1245	89	0
1	E	1267	0	1241	104	0
1	G	1267	0	1241	93	0
1	I	1244	0	1217	99	0
1	K	1252	0	1228	99	0
2	B	760	0	748	46	0
2	D	777	0	768	48	0
2	F	760	0	748	35	0
2	H	776	0	769	39	0
2	J	746	0	734	47	0
2	L	727	0	712	51	0
3	P	1207	0	1162	95	0
3	Q	1209	0	1175	81	0
3	R	1198	0	1154	89	0
3	S	1168	0	1132	88	0
3	T	1161	0	1125	99	0
3	U	1177	0	1140	86	0
4	B	4	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	4	0	0	1	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	2	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
All	All	19285	0	18795	1225	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 32.

All (1225) 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)
3:T:25:GLY:HA2	3:T:59:HIS:CD2	1.74	1.21
2:J:255:HIS:HE1	2:J:258:ASP:OD2	1.24	1.17
2:L:255:HIS:HE1	2:L:258:ASP:OD2	1.27	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:255:HIS:HE1	2:D:258:ASP:OD2	1.33	1.12
2:H:255:HIS:HE1	2:H:258:ASP:OD2	1.35	1.10
1:E:10:GLN:HG2	1:E:11:VAL:H	1.14	1.10
3:U:23:ARG:HB2	3:U:53:LEU:HD13	1.33	1.10
2:B:255:HIS:HE1	2:B:258:ASP:OD2	1.37	1.06
2:F:255:HIS:HE1	2:F:258:ASP:OD2	1.39	1.05
2:J:255:HIS:CE1	2:J:258:ASP:OD2	2.17	0.98
1:C:159:GLU:HG2	1:C:160:THR:H	1.28	0.98
2:J:273:TYR:HB3	3:T:79:TYR:CE2	1.99	0.95
1:E:43:VAL:HA	1:E:54:ARG:HG3	1.45	0.95
2:L:255:HIS:CE1	2:L:258:ASP:OD2	2.20	0.95
3:T:25:GLY:HA2	3:T:59:HIS:HD2	1.24	0.94
3:U:25:GLY:HA2	3:U:59:HIS:HD2	1.31	0.93
1:A:127:GLN:HB2	1:A:130:GLU:HG2	1.51	0.93
1:E:127:GLN:HB2	1:E:130:GLU:HG2	1.51	0.93
1:I:41:SER:HB2	1:I:54:ARG:HH22	1.31	0.93
1:A:52:GLU:HG2	1:A:53:PHE:H	1.33	0.92
3:T:133:LEU:HD11	3:T:164:ILE:HG22	1.50	0.92
2:D:255:HIS:CE1	2:D:258:ASP:OD2	2.22	0.92
1:G:127:GLN:HB2	1:G:130:GLU:HG2	1.50	0.92
2:B:273:TYR:HB3	3:P:79:TYR:CE2	2.05	0.91
1:I:127:GLN:HB2	1:I:130:GLU:HG2	1.50	0.91
1:E:29:LEU:HD23	2:F:297:TYR:O	1.71	0.91
2:H:273:TYR:HB3	3:S:79:TYR:CE2	2.05	0.91
3:S:16:LYS:HD2	3:S:42:ALA:HB2	1.53	0.91
3:U:25:GLY:HA2	3:U:59:HIS:CD2	2.06	0.91
2:H:255:HIS:CE1	2:H:258:ASP:OD2	2.24	0.90
1:C:127:GLN:HB2	1:C:130:GLU:HG2	1.51	0.90
3:Q:100:LEU:HD21	3:Q:106:VAL:HG23	1.52	0.90
1:K:127:GLN:HB2	1:K:130:GLU:HG2	1.52	0.89
1:C:27:TYR:CD2	1:C:147:PRO:HD3	2.08	0.89
2:D:273:TYR:HB3	3:Q:79:TYR:CE2	2.08	0.89
1:I:15:THR:OG1	2:J:302:HIS:HA	1.73	0.88
3:U:100:LEU:HD21	3:U:106:VAL:HG23	1.55	0.88
2:B:255:HIS:CE1	2:B:258:ASP:OD2	2.26	0.87
2:L:245:GLN:HG3	3:U:45:TRP:HB2	1.55	0.87
3:T:133:LEU:HD11	3:T:164:ILE:CG2	2.04	0.87
1:I:27:TYR:CD1	1:I:147:PRO:HD3	2.09	0.86
1:E:27:TYR:CD2	1:E:147:PRO:HB3	2.11	0.86
2:F:255:HIS:CE1	2:F:258:ASP:OD2	2.27	0.86
3:P:14:LEU:HG	3:P:38:ALA:HA	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:18:LEU:HD11	3:T:30:VAL:HG13	1.56	0.85
1:E:10:GLN:CG	1:E:11:VAL:H	1.88	0.85
3:S:13:ASP:HB3	3:S:16:LYS:HE2	1.59	0.84
1:K:28:ARG:HH11	1:K:28:ARG:HA	1.41	0.84
1:C:17:GLU:O	1:C:21:THR:HG23	1.78	0.84
1:I:109:LEU:HB2	1:I:152:ILE:HD13	1.57	0.83
3:P:19:LEU:HD12	3:P:50:PRO:HG3	1.61	0.83
2:F:273:TYR:HB3	3:R:79:TYR:CE2	2.13	0.83
3:T:100:LEU:HD21	3:T:106:VAL:HG23	1.58	0.83
3:P:25:GLY:HA3	3:P:59:HIS:CE1	2.14	0.83
1:A:100:ARG:CD	3:S:159:GLU:OE2	2.27	0.82
3:Q:125:HIS:O	3:Q:129:VAL:HG23	1.80	0.82
1:I:16:PRO:HA	1:I:19:TYR:HB3	1.60	0.82
1:A:82:THR:HB	1:A:122:ASP:HB2	1.62	0.82
1:K:82:THR:HB	1:K:122:ASP:HB2	1.62	0.82
1:E:43:VAL:HG13	1:E:54:ARG:HB2	1.60	0.81
3:P:100:LEU:HD21	3:P:106:VAL:HG23	1.61	0.81
3:P:17:LYS:HZ2	3:P:33:LEU:HD21	1.43	0.81
1:E:82:THR:HB	1:E:122:ASP:HB2	1.62	0.81
3:U:26:GLN:O	3:U:30:VAL:HG23	1.80	0.81
3:R:100:LEU:HD21	3:R:106:VAL:HG23	1.62	0.81
1:I:14:CYS:HB2	2:J:252:CYS:HB2	1.61	0.81
3:U:26:GLN:HB3	3:U:29:GLU:HB2	1.61	0.81
1:I:112:HIS:HA	1:I:155:CYS:SG	2.20	0.80
1:E:10:GLN:HG2	1:E:11:VAL:N	1.93	0.80
1:I:82:THR:HB	1:I:122:ASP:HB2	1.63	0.80
1:G:82:THR:HB	1:G:122:ASP:HB2	1.63	0.80
3:Q:25:GLY:HA2	3:Q:59:HIS:CD2	2.17	0.80
1:K:156:ARG:HH21	2:L:225:LYS:N	1.80	0.80
1:C:82:THR:HB	1:C:122:ASP:HB2	1.64	0.80
1:E:61:HIS:O	1:E:65:VAL:HG23	1.83	0.79
3:P:17:LYS:NZ	3:P:33:LEU:HD21	1.98	0.79
1:K:52:GLU:HG2	1:K:53:PHE:H	1.47	0.79
1:K:29:LEU:HD22	1:K:29:LEU:H	1.46	0.79
3:P:125:HIS:O	3:P:129:VAL:HG23	1.83	0.79
1:K:14:CYS:HB3	2:L:252:CYS:HB2	1.63	0.79
1:A:166:GLN:HG3	1:A:166:GLN:O	1.81	0.78
2:D:277:THR:HG22	2:D:278:GLU:H	1.48	0.78
1:I:15:THR:OG1	1:I:16:PRO:HD2	1.82	0.78
3:R:125:HIS:O	3:R:129:VAL:HG23	1.83	0.78
3:U:23:ARG:HB2	3:U:53:LEU:CD1	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:163:GLU:HG3	3:U:164:ILE:HG13	1.66	0.78
3:R:19:LEU:HD12	3:R:19:LEU:N	1.98	0.78
3:P:23:ARG:HB2	3:P:53:LEU:HD13	1.66	0.78
3:U:125:HIS:O	3:U:129:VAL:HG23	1.84	0.77
3:Q:14:LEU:HD12	3:Q:14:LEU:H	1.48	0.77
3:S:125:HIS:O	3:S:129:VAL:HG23	1.84	0.76
1:G:153:GLN:HE21	2:H:240:ILE:HG12	1.50	0.76
2:J:255:HIS:HE1	2:J:258:ASP:CG	1.89	0.76
3:R:19:LEU:HD11	3:R:42:ALA:HB3	1.68	0.76
1:K:61:HIS:O	1:K:65:VAL:HG23	1.84	0.76
2:B:273:TYR:HB3	3:P:79:TYR:CD2	2.21	0.76
3:T:125:HIS:O	3:T:129:VAL:HG23	1.86	0.76
1:C:67:LEU:HD22	2:D:244:ALA:HA	1.68	0.75
3:Q:26:GLN:O	3:Q:30:VAL:HG23	1.86	0.75
2:L:281:ARG:NH2	3:U:123:ASP:OD2	2.19	0.75
1:A:100:ARG:HD2	3:S:159:GLU:OE2	1.85	0.75
3:R:12:SER:O	3:R:14:LEU:N	2.20	0.75
3:S:23:ARG:HB3	3:S:53:LEU:HD13	1.67	0.75
1:I:61:HIS:O	1:I:65:VAL:HG23	1.85	0.75
3:P:19:LEU:HD11	3:P:42:ALA:HB3	1.69	0.74
2:D:208:LYS:HE2	2:D:208:LYS:HA	1.67	0.74
1:A:61:HIS:O	1:A:65:VAL:HG23	1.88	0.74
1:C:29:LEU:O	1:C:29:LEU:HD23	1.88	0.74
1:C:50:GLU:HG2	1:C:51:LEU:H	1.50	0.74
1:E:73:TYR:O	1:E:75:VAL:HG12	1.88	0.74
1:I:73:TYR:O	1:I:75:VAL:HG12	1.87	0.74
1:E:27:TYR:HD2	1:E:147:PRO:HB3	1.51	0.73
2:L:255:HIS:HE1	2:L:258:ASP:CG	1.90	0.73
3:R:49:THR:H	3:R:52:HIS:HB2	1.53	0.73
1:K:27:TYR:HB2	1:K:29:LEU:HD13	1.70	0.73
3:U:25:GLY:CA	3:U:59:HIS:CD2	2.72	0.73
1:K:27:TYR:O	1:K:29:LEU:HD22	1.89	0.72
3:U:133:LEU:HA	3:U:137:ALA:HB3	1.71	0.72
1:E:110:LEU:N	1:E:110:LEU:HD12	2.04	0.72
3:R:19:LEU:HD12	3:R:19:LEU:H	1.55	0.72
1:K:73:TYR:O	1:K:75:VAL:HG12	1.90	0.72
1:G:61:HIS:O	1:G:65:VAL:HG23	1.89	0.72
1:I:11:VAL:HG21	1:I:70:LEU:HB2	1.72	0.72
1:C:110:LEU:HD12	1:C:110:LEU:N	2.05	0.72
1:I:25:LEU:HD23	1:I:25:LEU:H	1.53	0.72
2:J:245:GLN:HG3	3:T:45:TRP:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:18:LEU:HD23	3:S:19:LEU:HD12	1.72	0.72
2:H:269:ASP:HB3	3:S:23:ARG:HH12	1.53	0.71
1:C:61:HIS:O	1:C:65:VAL:HG23	1.89	0.71
1:A:97:PRO:HB3	3:S:159:GLU:OE1	1.91	0.71
3:S:163:GLU:C	3:S:164:ILE:HD12	2.10	0.71
3:R:133:LEU:HA	3:R:137:ALA:HB3	1.72	0.71
1:K:34:ARG:HG3	1:K:34:ARG:HH11	1.56	0.71
3:R:76:TRP:HA	3:R:81:ALA:O	1.91	0.70
2:H:273:TYR:HB3	3:S:79:TYR:CD2	2.25	0.70
2:F:273:TYR:HB3	3:R:79:TYR:CD2	2.27	0.70
1:I:127:GLN:HB2	1:I:130:GLU:CG	2.22	0.70
1:A:100:ARG:HD3	3:S:159:GLU:OE2	1.90	0.70
1:K:82:THR:CB	1:K:122:ASP:HB2	2.22	0.70
1:E:27:TYR:CE1	2:F:294:ARG:HB2	2.26	0.70
1:G:67:LEU:HD22	2:H:244:ALA:HA	1.73	0.70
1:A:82:THR:CB	1:A:122:ASP:HB2	2.22	0.69
1:E:82:THR:CB	1:E:122:ASP:HB2	2.22	0.69
1:G:73:TYR:O	1:G:75:VAL:HG12	1.92	0.69
1:I:34:ARG:HG3	1:I:34:ARG:HH11	1.57	0.69
3:P:49:THR:H	3:P:52:HIS:HB2	1.57	0.69
1:I:82:THR:CB	1:I:122:ASP:HB2	2.23	0.69
1:K:127:GLN:HB2	1:K:130:GLU:CG	2.23	0.69
1:K:42:ASN:O	1:K:54:ARG:HD3	1.92	0.69
1:K:110:LEU:HD12	1:K:110:LEU:N	2.07	0.69
3:S:16:LYS:HD2	3:S:42:ALA:CB	2.22	0.69
1:E:10:GLN:CG	1:E:11:VAL:N	2.52	0.69
3:S:19:LEU:HD12	3:S:19:LEU:H	1.57	0.69
3:S:133:LEU:HA	3:S:137:ALA:HB3	1.73	0.69
3:P:58:GLY:CA	3:P:92:HIS:CD2	2.75	0.69
1:A:34:ARG:HH11	1:A:34:ARG:HG3	1.58	0.68
1:C:73:TYR:O	1:C:75:VAL:HG12	1.93	0.68
3:R:15:GLY:O	3:R:16:LYS:HG3	1.93	0.68
1:G:110:LEU:N	1:G:110:LEU:HD12	2.09	0.68
1:I:48:GLU:O	1:I:50:GLU:N	2.26	0.68
3:T:76:TRP:HA	3:T:81:ALA:O	1.93	0.68
1:K:19:TYR:CE2	2:L:302:HIS:HB3	2.29	0.68
3:S:21:ALA:HA	3:S:24:ALA:HB3	1.74	0.68
3:T:58:GLY:CA	3:T:92:HIS:CD2	2.77	0.68
2:D:293:CYS:O	2:D:294:ARG:HG3	1.92	0.68
3:P:58:GLY:CA	3:P:92:HIS:HD2	2.07	0.68
1:G:82:THR:CB	1:G:122:ASP:HB2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLN:HB2	1:A:130:GLU:CG	2.22	0.68
1:A:25:LEU:H	1:A:25:LEU:HD23	1.59	0.68
3:P:58:GLY:HA3	3:P:92:HIS:CD2	2.29	0.68
1:C:82:THR:CB	1:C:122:ASP:HB2	2.24	0.68
1:G:127:GLN:HB2	1:G:130:GLU:CG	2.22	0.68
3:T:23:ARG:HD3	3:T:57:THR:HG21	1.76	0.68
1:G:17:GLU:O	1:G:21:THR:HG22	1.93	0.68
2:J:255:HIS:CE1	2:J:258:ASP:HB2	2.29	0.68
1:A:73:TYR:O	1:A:75:VAL:HG12	1.93	0.68
3:S:162:ALA:C	3:S:164:ILE:H	1.97	0.67
3:S:76:TRP:HA	3:S:81:ALA:O	1.94	0.67
2:J:273:TYR:HB3	3:T:79:TYR:CD2	2.29	0.67
1:E:127:GLN:HB2	1:E:130:GLU:CG	2.24	0.67
1:I:110:LEU:HD12	1:I:110:LEU:N	2.09	0.67
3:T:133:LEU:CD1	3:T:164:ILE:HG22	2.25	0.67
3:P:163:GLU:C	3:P:165:LEU:H	1.98	0.67
1:E:34:ARG:HG3	1:E:34:ARG:HH11	1.59	0.67
3:T:19:LEU:HD21	3:T:42:ALA:O	1.95	0.67
3:T:49:THR:H	3:T:52:HIS:HB2	1.60	0.67
3:T:139:VAL:HG23	3:T:164:ILE:HD12	1.77	0.67
1:C:127:GLN:HB2	1:C:130:GLU:CG	2.23	0.67
3:T:133:LEU:HA	3:T:137:ALA:HB3	1.77	0.67
1:C:34:ARG:HG3	1:C:34:ARG:HH11	1.59	0.67
3:Q:49:THR:H	3:Q:52:HIS:HB2	1.60	0.67
3:Q:133:LEU:HA	3:Q:137:ALA:HB3	1.76	0.67
2:L:255:HIS:CE1	2:L:258:ASP:HB2	2.30	0.67
3:U:163:GLU:HG3	3:U:164:ILE:N	2.08	0.66
3:P:76:TRP:HA	3:P:81:ALA:O	1.95	0.66
3:U:126:LEU:HD23	3:U:126:LEU:H	1.60	0.66
1:A:67:LEU:HD22	2:B:244:ALA:HA	1.78	0.66
3:R:19:LEU:H	3:R:19:LEU:CD1	2.09	0.66
2:H:293:CYS:O	2:H:294:ARG:HG3	1.94	0.66
1:I:151:PHE:CD2	2:J:243:LEU:HD21	2.31	0.66
3:T:129:VAL:HG21	3:T:161:LEU:HD11	1.76	0.66
3:P:133:LEU:HA	3:P:137:ALA:HB3	1.77	0.66
2:F:293:CYS:O	2:F:294:ARG:HG3	1.96	0.66
1:I:64:LEU:HD12	1:I:110:LEU:HD21	1.75	0.66
3:P:164:ILE:C	3:P:165:LEU:HD12	2.16	0.66
3:U:23:ARG:CB	3:U:53:LEU:HD13	2.20	0.66
1:A:110:LEU:HD12	1:A:110:LEU:N	2.10	0.66
1:E:27:TYR:CE2	1:E:147:PRO:HB3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:49:THR:H	3:S:52:HIS:HB2	1.62	0.65
1:C:16:PRO:O	1:C:20:GLN:HG2	1.97	0.65
3:Q:23:ARG:C	3:Q:23:ARG:HD2	2.17	0.65
3:T:58:GLY:HA3	3:T:92:HIS:CD2	2.32	0.65
3:U:49:THR:H	3:U:52:HIS:HB2	1.59	0.65
1:I:156:ARG:HD3	2:J:223:CYS:O	1.96	0.65
2:L:266:LEU:HD22	3:U:45:TRP:CZ3	2.31	0.65
1:E:110:LEU:HG	1:E:153:GLN:HB3	1.78	0.65
3:T:58:GLY:CA	3:T:92:HIS:HD2	2.08	0.65
1:I:109:LEU:HB2	1:I:152:ILE:CD1	2.27	0.65
1:G:15:THR:HB	1:G:18:PHE:HB2	1.79	0.65
3:T:25:GLY:HA2	3:T:59:HIS:NE2	2.10	0.65
3:T:23:ARG:CD	3:T:57:THR:HG21	2.27	0.64
2:J:293:CYS:O	2:J:294:ARG:HG3	1.98	0.64
3:P:17:LYS:O	3:P:20:GLU:HB2	1.97	0.64
3:P:25:GLY:HA3	3:P:59:HIS:ND1	2.12	0.64
1:C:50:GLU:HG2	1:C:51:LEU:N	2.12	0.64
2:D:230:MET:HG2	2:D:284:GLU:OE1	1.98	0.64
1:E:64:LEU:HD12	1:E:110:LEU:HD21	1.77	0.64
1:E:67:LEU:HD22	2:F:244:ALA:HA	1.80	0.64
3:S:76:TRP:CD1	3:S:76:TRP:N	2.64	0.64
3:T:19:LEU:O	3:T:53:LEU:HD12	1.97	0.64
2:L:266:LEU:HD22	3:U:45:TRP:CE3	2.33	0.64
1:A:157:GLY:HA3	2:B:226:GLY:O	1.98	0.64
1:G:34:ARG:HG3	1:G:34:ARG:HH11	1.62	0.64
3:R:14:LEU:HD22	3:R:14:LEU:H	1.62	0.64
3:S:19:LEU:HD11	3:S:42:ALA:HB3	1.79	0.64
3:T:80:GLY:HA3	3:T:111:TYR:CD1	2.33	0.64
1:A:64:LEU:HD12	1:A:110:LEU:HD21	1.78	0.64
3:R:25:GLY:HA3	3:R:59:HIS:CD2	2.33	0.64
3:T:59:HIS:O	3:T:63:VAL:HG23	1.98	0.64
2:L:266:LEU:HB3	3:U:45:TRP:CZ2	2.33	0.64
3:Q:23:ARG:HB3	3:Q:53:LEU:HD13	1.78	0.63
3:R:80:GLY:HA3	3:R:111:TYR:CD1	2.33	0.63
3:T:19:LEU:HD11	3:T:43:THR:N	2.13	0.63
3:S:76:TRP:HD1	3:S:76:TRP:H	1.45	0.63
1:A:44:HIS:HD1	1:A:53:PHE:HE1	1.44	0.63
1:G:29:LEU:HD23	1:G:29:LEU:O	1.98	0.63
1:G:151:PHE:CD1	2:H:243:LEU:HD21	2.34	0.63
1:I:29:LEU:HD23	2:J:298:LEU:HA	1.81	0.63
1:K:43:VAL:HG12	1:K:53:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:58:GLY:CA	3:U:92:HIS:CD2	2.81	0.63
3:Q:80:GLY:HA3	3:Q:111:TYR:CD1	2.34	0.63
3:R:149:ALA:O	3:R:165:LEU:HD11	1.99	0.63
3:R:58:GLY:CA	3:R:92:HIS:CD2	2.82	0.62
1:K:35:GLY:HA2	1:K:102:THR:HB	1.81	0.62
3:U:76:TRP:N	3:U:76:TRP:CD1	2.64	0.62
1:I:35:GLY:HA2	1:I:102:THR:HB	1.82	0.62
1:K:55:SER:O	2:L:231:ARG:HD2	1.99	0.62
1:K:64:LEU:HD12	1:K:110:LEU:HD21	1.80	0.62
3:R:80:GLY:O	3:R:110:ASP:HA	1.99	0.62
3:S:15:GLY:O	3:S:17:LYS:N	2.31	0.62
1:C:153:GLN:O	1:C:153:GLN:NE2	2.32	0.62
3:S:59:HIS:O	3:S:63:VAL:HG23	1.99	0.62
3:T:112:GLU:OE1	3:T:144:LYS:HE2	2.00	0.62
2:J:230:MET:HG2	2:J:284:GLU:OE1	2.00	0.62
1:I:67:LEU:HD22	2:J:244:ALA:HA	1.82	0.62
3:U:56:LYS:HB2	3:U:86:LEU:HD13	1.81	0.62
2:L:293:CYS:O	2:L:294:ARG:HG3	1.99	0.62
1:A:137:ASN:ND2	2:B:211:LEU:HD13	2.15	0.62
2:D:273:TYR:HB3	3:Q:79:TYR:CD2	2.35	0.62
3:S:80:GLY:O	3:S:110:ASP:HA	2.00	0.62
1:I:110:LEU:HG	1:I:153:GLN:HB3	1.82	0.62
3:U:163:GLU:HG3	3:U:164:ILE:H	1.65	0.62
3:Q:58:GLY:CA	3:Q:92:HIS:CD2	2.83	0.62
1:I:15:THR:HG1	2:J:302:HIS:HA	1.63	0.62
1:K:49:LYS:C	1:K:50:GLU:HG2	2.18	0.62
3:R:9:HIS:CD2	3:R:9:HIS:N	2.68	0.61
3:P:80:GLY:HA3	3:P:111:TYR:CD1	2.35	0.61
3:S:63:VAL:HG11	3:S:95:ILE:HG23	1.81	0.61
3:S:129:VAL:HG21	3:S:161:LEU:HD11	1.81	0.61
1:C:151:PHE:CD1	2:D:243:LEU:HD21	2.36	0.61
3:R:161:LEU:O	3:R:165:LEU:HB2	1.99	0.61
2:H:269:ASP:HB3	3:S:23:ARG:NH1	2.14	0.61
2:B:293:CYS:O	2:B:294:ARG:HG3	2.01	0.61
3:P:19:LEU:CD1	3:P:42:ALA:HB3	2.30	0.61
3:Q:76:TRP:CD1	3:Q:76:TRP:N	2.66	0.61
1:K:81:GLN:O	1:K:121:VAL:HG22	2.00	0.61
3:P:15:GLY:O	3:P:19:LEU:HD13	2.01	0.61
2:F:302:HIS:HA	2:F:303:PRO:C	2.21	0.61
1:G:64:LEU:HD12	1:G:110:LEU:HD21	1.82	0.61
1:C:159:GLU:HG2	1:C:160:THR:N	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:76:TRP:HD1	3:Q:76:TRP:H	1.47	0.61
3:R:105:ASP:HB3	3:R:108:ALA:HB2	1.83	0.61
1:I:46:THR:OG1	1:I:47:GLY:N	2.29	0.61
3:T:80:GLY:O	3:T:110:ASP:HA	2.00	0.61
3:P:58:GLY:HA2	3:P:92:HIS:HD2	1.65	0.60
3:Q:167:LYS:C	3:Q:168:LEU:HD12	2.21	0.60
3:U:132:LEU:O	3:U:137:ALA:HB2	2.01	0.60
1:A:11:VAL:HG21	1:A:70:LEU:HB2	1.81	0.60
2:B:283:LYS:HE2	2:D:210:ARG:HB3	1.83	0.60
3:T:82:THR:O	3:T:85:HIS:HB2	2.01	0.60
1:K:29:LEU:HD22	1:K:29:LEU:N	2.15	0.60
3:U:63:VAL:HG11	3:U:95:ILE:HG23	1.82	0.60
3:P:105:ASP:HB3	3:P:108:ALA:HB2	1.83	0.60
3:R:19:LEU:HD11	3:R:42:ALA:CB	2.31	0.60
1:C:159:GLU:CG	1:C:160:THR:H	2.09	0.60
1:E:35:GLY:HA2	1:E:102:THR:HB	1.82	0.60
1:E:51:LEU:N	1:E:51:LEU:HD22	2.17	0.60
3:U:76:TRP:HA	3:U:81:ALA:O	2.01	0.60
1:C:64:LEU:HD12	1:C:110:LEU:HD21	1.82	0.60
1:E:27:TYR:CD2	1:E:147:PRO:HD3	2.36	0.60
1:E:45:PHE:HB2	1:E:51:LEU:HB2	1.84	0.60
2:B:230:MET:O	2:B:237:SER:HA	2.02	0.60
1:C:35:GLY:HA2	1:C:102:THR:HB	1.83	0.60
3:T:63:VAL:HG11	3:T:95:ILE:HG23	1.82	0.60
1:E:12:LYS:HG2	1:E:13:PRO:HD2	1.84	0.60
1:G:81:GLN:O	1:G:121:VAL:HG22	2.02	0.60
3:T:76:TRP:CD1	3:T:76:TRP:N	2.69	0.60
3:U:43:THR:HA	3:U:48:HIS:O	2.02	0.60
3:U:76:TRP:HD1	3:U:76:TRP:H	1.48	0.60
3:U:105:ASP:HB3	3:U:108:ALA:HB2	1.83	0.60
1:A:48:GLU:O	1:A:50:GLU:HG2	2.02	0.60
1:A:35:GLY:HA2	1:A:102:THR:HB	1.82	0.59
1:I:109:LEU:HD12	1:I:152:ILE:HD11	1.84	0.59
1:A:48:GLU:O	1:A:50:GLU:N	2.34	0.59
1:E:34:ARG:NH2	2:F:302:HIS:O	2.35	0.59
3:S:56:LYS:HB2	3:S:86:LEU:HD13	1.84	0.59
1:A:42:ASN:HB3	1:A:45:PHE:CE1	2.36	0.59
3:P:76:TRP:CD1	3:P:76:TRP:N	2.69	0.59
1:E:11:VAL:HG11	1:E:70:LEU:HB3	1.82	0.59
2:J:255:HIS:CE1	2:J:258:ASP:CG	2.71	0.59
1:K:14:CYS:HB2	1:K:18:PHE:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:GLN:HB2	1:C:25:LEU:HD22	1.85	0.59
2:J:289:CYS:HA	2:L:289:CYS:HA	1.85	0.59
3:T:20:GLU:OE1	3:T:20:GLU:N	2.34	0.59
2:B:283:LYS:HE2	2:D:210:ARG:CB	2.33	0.59
3:S:13:ASP:O	3:S:16:LYS:HG2	2.03	0.59
3:T:76:TRP:HD1	3:T:76:TRP:H	1.50	0.59
3:Q:76:TRP:HA	3:Q:81:ALA:O	2.03	0.59
3:P:80:GLY:O	3:P:110:ASP:HA	2.03	0.59
1:C:165:ASP:OD1	1:C:165:ASP:N	2.36	0.59
1:K:16:PRO:HA	2:L:302:HIS:HE1	1.68	0.59
1:A:52:GLU:HG2	1:A:53:PHE:N	2.13	0.58
3:Q:100:LEU:CD2	3:Q:106:VAL:HG23	2.31	0.58
3:T:19:LEU:HD11	3:T:42:ALA:HB1	1.85	0.58
3:U:58:GLY:HA3	3:U:92:HIS:CD2	2.38	0.58
3:Q:59:HIS:O	3:Q:63:VAL:HG23	2.02	0.58
1:G:29:LEU:HD23	1:G:34:ARG:HG2	1.84	0.58
3:T:58:GLY:HA2	3:T:92:HIS:HD2	1.67	0.58
3:T:78:ASN:N	3:T:78:ASN:HD22	2.01	0.58
1:C:81:GLN:O	1:C:121:VAL:HG22	2.03	0.58
3:Q:63:VAL:HG11	3:Q:95:ILE:HG23	1.84	0.58
1:G:35:GLY:HA2	1:G:102:THR:HB	1.84	0.58
1:C:71:LEU:HD22	2:D:298:LEU:HD13	1.84	0.58
2:D:245:GLN:HG3	3:Q:45:TRP:HB2	1.84	0.58
3:Q:92:HIS:O	3:Q:96:VAL:HG23	2.04	0.58
3:R:130:GLU:HG3	3:R:164:ILE:HD12	1.86	0.58
1:I:162:ARG:O	2:J:282:CYS:HA	2.04	0.58
1:C:29:LEU:HD23	1:C:34:ARG:HG2	1.83	0.58
1:E:51:LEU:HD22	1:E:51:LEU:H	1.67	0.58
2:B:264:ASN:ND2	2:D:291:THR:HA	2.19	0.58
3:P:164:ILE:HG22	3:P:164:ILE:O	2.04	0.58
3:Q:43:THR:HA	3:Q:48:HIS:O	2.03	0.58
1:E:27:TYR:CD1	2:F:294:ARG:HB2	2.39	0.58
3:R:76:TRP:CD1	3:R:76:TRP:N	2.70	0.58
3:U:80:GLY:HA3	3:U:111:TYR:CD1	2.39	0.58
3:P:82:THR:O	3:P:85:HIS:HB2	2.03	0.58
3:Q:78:ASN:N	3:Q:78:ASN:HD22	2.00	0.58
1:I:31:SER:HB3	1:I:103:ASP:OD2	2.03	0.58
1:I:76:HIS:O	1:I:77:VAL:HG13	2.04	0.58
1:K:67:LEU:HD22	2:L:244:ALA:HA	1.85	0.58
3:P:63:VAL:HG11	3:P:95:ILE:HG23	1.85	0.58
1:E:71:LEU:HD22	2:F:298:LEU:HD13	1.86	0.58

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
3:P:76:TRP:HD1	3:P:76:TRP:H	1.52	0.57
3:Q:26:GLN:HB3	3:Q:29:GLU:HB3	1.86	0.57
1:E:27:TYR:HD2	1:E:147:PRO:CB	2.17	0.57
1:E:31:SER:HB3	1:E:103:ASP:OD2	2.04	0.57
1:A:45:PHE:HE2	1:A:112:HIS:HB2	1.69	0.57
1:G:159:GLU:O	1:G:160:THR:C	2.43	0.57
2:L:211:LEU:N	2:L:211:LEU:HD12	2.19	0.57
2:L:255:HIS:CE1	2:L:258:ASP:CG	2.72	0.57
3:U:62:ILE:HA	3:U:65:VAL:HG12	1.86	0.57
1:A:31:SER:HB3	1:A:103:ASP:OD2	2.05	0.57
1:A:42:ASN:HB3	1:A:45:PHE:HE1	1.69	0.57
1:K:19:TYR:O	1:K:23:PHE:HB2	2.04	0.57
1:K:29:LEU:H	1:K:29:LEU:CD2	2.17	0.57
1:G:153:GLN:O	1:G:153:GLN:HG3	2.04	0.57
3:P:112:GLU:OE1	3:P:144:LYS:HE2	2.04	0.57
3:R:158:ASN:HB3	3:R:161:LEU:HD22	1.87	0.57
1:G:71:LEU:HD22	2:H:298:LEU:HD13	1.86	0.57
3:T:26:GLN:O	3:T:30:VAL:HG23	2.04	0.57
1:E:165:ASP:OD2	2:H:207:PRO:HG3	2.04	0.57
1:E:18:PHE:CZ	2:F:253:ASP:HA	2.39	0.57
3:R:124:GLY:HA2	3:R:161:LEU:HD21	1.87	0.57
1:K:140:CYS:SG	1:K:143:LEU:HB2	2.45	0.57
3:U:58:GLY:CA	3:U:92:HIS:HD2	2.17	0.57
3:P:132:LEU:O	3:P:137:ALA:HB2	2.04	0.57
1:C:31:SER:HB3	1:C:103:ASP:OD2	2.05	0.57
3:T:23:ARG:HH11	3:T:57:THR:CG2	2.18	0.57
3:T:92:HIS:O	3:T:96:VAL:HG23	2.04	0.57
1:K:156:ARG:HH21	2:L:225:LYS:CA	2.17	0.57
2:L:245:GLN:CG	3:U:45:TRP:HB2	2.29	0.57
1:E:54:ARG:O	1:E:55:SER:C	2.43	0.57
3:R:19:LEU:N	3:R:19:LEU:CD1	2.65	0.57
1:G:31:SER:HB3	1:G:103:ASP:OD2	2.05	0.57
2:H:297:TYR:N	4:H:6:HOH:O	2.35	0.57
3:T:40:VAL:HG22	3:T:40:VAL:O	2.05	0.57
1:K:76:HIS:O	1:K:77:VAL:HG13	2.05	0.57
3:P:118:HIS:HD1	3:P:143:ASP:HB3	1.70	0.56
3:P:160:ASP:O	3:P:164:ILE:HD12	2.05	0.56
1:I:15:THR:OG1	1:I:16:PRO:CD	2.53	0.56
1:A:81:GLN:O	1:A:121:VAL:HG22	2.04	0.56
1:A:54:ARG:HG3	1:A:54:ARG:HH11	1.70	0.56
1:E:43:VAL:HA	1:E:54:ARG:CG	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:PRO:O	1:G:167:GLN:HG2	2.05	0.56
1:E:153:GLN:NE2	2:F:239:TYR:HB3	2.19	0.56
2:H:273:TYR:HB3	3:S:79:TYR:HE2	1.64	0.56
3:S:160:ASP:O	3:S:164:ILE:HD13	2.04	0.56
2:J:301:GLY:O	2:J:302:HIS:HB2	2.05	0.56
3:P:122:TYR:CE1	3:P:152:ILE:HD12	2.40	0.56
3:Q:25:GLY:O	3:Q:62:ILE:HD11	2.04	0.56
3:U:80:GLY:O	3:U:110:ASP:HA	2.05	0.56
1:A:53:PHE:O	1:A:55:SER:N	2.39	0.56
1:A:76:HIS:O	1:A:77:VAL:HG13	2.06	0.56
1:I:81:GLN:O	1:I:121:VAL:HG22	2.05	0.56
1:E:140:CYS:SG	1:E:143:LEU:HB2	2.46	0.56
1:G:50:GLU:HG2	1:G:51:LEU:HG	1.88	0.56
3:S:118:HIS:HD1	3:S:143:ASP:HB3	1.70	0.56
1:C:11:VAL:HG13	1:C:11:VAL:O	2.06	0.56
2:J:301:GLY:O	2:J:302:HIS:CB	2.52	0.56
1:A:34:ARG:HG3	1:A:34:ARG:NH1	2.21	0.56
2:J:209:MET:O	1:K:166:GLN:HG3	2.06	0.56
3:U:25:GLY:CA	3:U:59:HIS:HD2	2.08	0.56
3:Q:153:SER:HB2	3:Q:162:ALA:HB2	1.88	0.56
1:K:31:SER:HB3	1:K:103:ASP:OD2	2.06	0.56
1:A:141:PRO:HB2	1:C:168:ASP:CB	2.36	0.56
3:P:47:GLY:HA3	3:P:78:ASN:HD22	1.71	0.56
3:P:56:LYS:HB2	3:P:86:LEU:HB3	1.86	0.56
3:R:58:GLY:HA3	3:R:92:HIS:CD2	2.41	0.56
1:K:23:PHE:HA	2:L:299:PHE:CZ	2.41	0.56
3:U:82:THR:O	3:U:85:HIS:HB2	2.05	0.56
3:U:164:ILE:O	3:U:165:LEU:HB2	2.06	0.56
1:A:156:ARG:HB2	2:B:224:LEU:O	2.06	0.55
3:Q:58:GLY:HA3	3:Q:92:HIS:CD2	2.41	0.55
3:R:26:GLN:O	3:R:30:VAL:HG23	2.06	0.55
3:T:105:ASP:HB3	3:T:108:ALA:HB2	1.88	0.55
1:K:14:CYS:HB3	2:L:252:CYS:CB	2.32	0.55
1:E:12:LYS:CG	1:E:13:PRO:HD2	2.36	0.55
1:E:157:GLY:HA3	2:F:226:GLY:O	2.06	0.55
3:R:43:THR:HA	3:R:48:HIS:O	2.06	0.55
3:R:132:LEU:O	3:R:137:ALA:HB2	2.06	0.55
1:C:26:ALA:O	1:C:27:TYR:C	2.45	0.55
3:R:76:TRP:HD1	3:R:76:TRP:H	1.54	0.55
1:G:23:PHE:CG	1:G:24:GLN:N	2.74	0.55
3:T:132:LEU:O	3:T:137:ALA:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:14:LEU:CG	3:P:38:ALA:HA	2.34	0.55
3:P:139:VAL:HG22	3:P:139:VAL:O	2.06	0.55
1:C:76:HIS:O	1:C:77:VAL:HG13	2.06	0.55
3:Q:105:ASP:HB3	3:Q:108:ALA:HB2	1.89	0.55
2:J:255:HIS:ND1	2:J:258:ASP:HB2	2.22	0.55
2:H:228:ALA:HB3	2:H:230:MET:HE1	1.87	0.55
2:H:245:GLN:HG3	3:S:45:TRP:HB2	1.88	0.55
2:L:218:ILE:O	2:L:218:ILE:HG23	2.07	0.55
3:Q:34:MET:HA	3:Q:34:MET:HE3	1.89	0.55
1:I:111:SER:O	1:I:154:ALA:HA	2.07	0.55
2:J:255:HIS:CE1	2:J:258:ASP:CB	2.89	0.55
1:I:153:GLN:HG3	1:I:153:GLN:O	2.05	0.55
1:E:27:TYR:CD2	1:E:147:PRO:CB	2.89	0.55
1:E:76:HIS:O	1:E:77:VAL:HG13	2.07	0.55
1:I:44:HIS:CD2	1:I:53:PHE:HE1	2.24	0.55
2:J:283:LYS:HE3	2:L:211:LEU:N	2.22	0.55
1:C:8:CYS:HA	1:C:10:GLN:HE22	1.72	0.55
1:G:95:GLN:O	1:G:96:LEU:C	2.45	0.55
3:T:23:ARG:HD2	3:T:23:ARG:O	2.07	0.55
3:T:118:HIS:ND1	3:T:143:ASP:HB3	2.22	0.55
2:L:255:HIS:CE1	2:L:258:ASP:CB	2.90	0.55
2:B:291:THR:HA	2:D:264:ASN:ND2	2.21	0.55
1:E:81:GLN:O	1:E:121:VAL:HG22	2.06	0.55
2:H:228:ALA:HB3	2:H:230:MET:CE	2.37	0.55
1:E:80:ASP:HA	1:E:121:VAL:HG11	1.89	0.54
1:G:34:ARG:NH2	2:H:302:HIS:O	2.39	0.54
3:T:84:LEU:HD23	3:T:116:PRO:HG2	1.88	0.54
3:Q:118:HIS:HD1	3:Q:143:ASP:HB3	1.72	0.54
1:E:34:ARG:HG3	1:E:34:ARG:NH1	2.22	0.54
3:T:161:LEU:C	3:T:163:GLU:H	2.09	0.54
3:R:82:THR:O	3:R:85:HIS:HB2	2.06	0.54
3:S:82:THR:O	3:S:85:HIS:HB2	2.07	0.54
1:I:34:ARG:HG3	1:I:34:ARG:NH1	2.21	0.54
3:T:56:LYS:HB2	3:T:86:LEU:HD13	1.89	0.54
1:C:34:ARG:HG3	1:C:34:ARG:NH1	2.22	0.54
1:G:76:HIS:O	1:G:77:VAL:HG13	2.07	0.54
3:T:34:MET:HE3	3:T:34:MET:HA	1.89	0.54
3:T:80:GLY:HA3	3:T:111:TYR:HD1	1.72	0.54
3:S:43:THR:HA	3:S:48:HIS:O	2.07	0.54
3:S:84:LEU:HD23	3:S:116:PRO:HG2	1.88	0.54
3:S:105:ASP:HB3	3:S:108:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HD22	2:B:298:LEU:HD13	1.90	0.54
3:Q:153:SER:CB	3:Q:162:ALA:HB2	2.38	0.54
3:T:165:LEU:O	3:T:166:GLN:HB2	2.08	0.54
2:L:247:PHE:O	2:L:251:ALA:HB2	2.07	0.54
3:Q:25:GLY:O	3:Q:26:GLN:C	2.46	0.54
3:Q:84:LEU:HD23	3:Q:116:PRO:HG2	1.90	0.54
3:R:11:GLY:O	3:R:12:SER:C	2.46	0.54
3:T:23:ARG:NH1	3:T:57:THR:HG22	2.23	0.54
3:P:34:MET:HE3	3:P:34:MET:HA	1.89	0.54
1:E:53:PHE:C	1:E:55:SER:H	2.11	0.54
1:E:140:CYS:SG	1:E:140:CYS:O	2.66	0.54
3:S:19:LEU:HD12	3:S:19:LEU:N	2.23	0.54
1:K:80:ASP:HA	1:K:121:VAL:HG11	1.90	0.54
3:R:58:GLY:CA	3:R:92:HIS:HD2	2.21	0.54
2:J:291:THR:HA	2:L:264:ASN:ND2	2.22	0.54
3:P:100:LEU:CD2	3:P:106:VAL:HG23	2.37	0.53
1:I:71:LEU:HD22	2:J:298:LEU:HD13	1.90	0.53
1:C:27:TYR:HD2	1:C:147:PRO:HD3	1.65	0.53
3:R:40:VAL:HG22	3:R:40:VAL:O	2.08	0.53
3:T:18:LEU:HD12	3:T:21:ALA:HB3	1.90	0.53
3:U:46:LEU:C	3:U:78:ASN:OD1	2.46	0.53
3:U:122:TYR:CE1	3:U:152:ILE:HD12	2.44	0.53
3:P:56:LYS:HB2	3:P:86:LEU:HD13	1.89	0.53
3:P:62:ILE:HA	3:P:65:VAL:HG12	1.89	0.53
1:I:42:ASN:ND2	1:I:120:GLY:HA2	2.24	0.53
2:D:277:THR:HG22	2:D:278:GLU:N	2.21	0.53
3:R:25:GLY:CA	3:R:59:HIS:CD2	2.91	0.53
1:I:17:GLU:HA	1:I:17:GLU:OE1	2.07	0.53
1:I:82:THR:OG1	1:I:85:GLU:HG3	2.09	0.53
1:K:29:LEU:O	1:K:29:LEU:HD23	2.07	0.53
2:L:255:HIS:ND1	2:L:258:ASP:HB2	2.24	0.53
2:B:231:ARG:HB2	2:B:231:ARG:CZ	2.37	0.53
2:D:247:PHE:O	2:D:251:ALA:HB2	2.09	0.53
3:Q:132:LEU:O	3:Q:137:ALA:HB2	2.08	0.53
3:S:18:LEU:O	3:S:22:ALA:N	2.30	0.53
2:F:247:PHE:O	2:F:251:ALA:HB2	2.08	0.53
3:R:100:LEU:CD2	3:R:106:VAL:HG23	2.37	0.53
3:U:40:VAL:HG22	3:U:40:VAL:O	2.09	0.53
1:A:80:ASP:HA	1:A:121:VAL:HG11	1.90	0.53
2:B:230:MET:HB2	2:B:284:GLU:OE1	2.09	0.53
1:C:12:LYS:HE3	2:D:249:GLU:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:125:HIS:HB3	3:Q:128:ILE:HG13	1.90	0.53
2:F:218:ILE:HG23	2:F:218:ILE:O	2.09	0.53
1:E:46:THR:OG1	1:E:47:GLY:N	2.41	0.53
3:S:13:ASP:CB	3:S:16:LYS:HE2	2.33	0.53
1:E:54:ARG:O	1:E:57:GLY:N	2.41	0.53
3:R:122:TYR:CE1	3:R:152:ILE:HD12	2.44	0.53
1:I:80:ASP:HA	1:I:121:VAL:HG11	1.91	0.52
1:I:151:PHE:HD2	2:J:243:LEU:HD21	1.73	0.52
1:K:52:GLU:HG2	1:K:53:PHE:N	2.21	0.52
1:K:44:HIS:N	1:K:80:ASP:OD1	2.42	0.52
1:A:95:GLN:O	1:A:96:LEU:C	2.47	0.52
2:B:218:ILE:O	2:B:218:ILE:HG23	2.09	0.52
1:E:80:ASP:CA	1:E:121:VAL:HG11	2.39	0.52
3:R:63:VAL:HG11	3:R:95:ILE:HG23	1.90	0.52
3:P:47:GLY:HA3	3:P:78:ASN:ND2	2.23	0.52
1:C:55:SER:HB2	2:D:233:THR:HG22	1.90	0.52
3:Q:40:VAL:O	3:Q:40:VAL:HG22	2.10	0.52
1:E:136:ASP:HB2	2:F:213:THR:O	2.09	0.52
3:S:78:ASN:N	3:S:78:ASN:HD22	2.07	0.52
1:G:34:ARG:HG3	1:G:34:ARG:NH1	2.24	0.52
2:H:218:ILE:HG23	2:H:218:ILE:O	2.09	0.52
2:J:209:MET:HA	1:K:166:GLN:HE21	1.75	0.52
1:E:82:THR:OG1	1:E:85:GLU:HG3	2.09	0.52
1:K:81:GLN:C	1:K:121:VAL:HG22	2.30	0.52
1:C:12:LYS:O	2:D:252:CYS:HB3	2.09	0.52
1:C:95:GLN:O	1:C:96:LEU:C	2.48	0.52
3:R:25:GLY:HA2	3:R:62:ILE:CD1	2.40	0.52
3:S:139:VAL:O	3:S:139:VAL:HG22	2.08	0.52
3:U:59:HIS:O	3:U:63:VAL:HG23	2.09	0.52
1:C:140:CYS:SG	1:C:143:LEU:HB2	2.50	0.52
2:D:208:LYS:HE2	2:D:208:LYS:CA	2.38	0.52
1:E:164:VAL:HG23	1:E:165:ASP:N	2.25	0.52
2:F:245:GLN:HG3	3:R:45:TRP:HB2	1.92	0.52
2:H:247:PHE:O	2:H:251:ALA:HB2	2.10	0.52
3:S:132:LEU:O	3:S:137:ALA:HB2	2.09	0.52
3:U:112:GLU:OE1	3:U:144:LYS:HE2	2.10	0.52
1:G:19:TYR:CD1	1:G:19:TYR:C	2.83	0.52
1:G:54:ARG:HG3	1:G:112:HIS:CD2	2.45	0.52
3:T:23:ARG:NH1	3:T:57:THR:CG2	2.73	0.52
1:K:40:LEU:HD11	1:K:86:MET:HG2	1.92	0.52
3:U:18:LEU:HA	3:U:33:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:58:GLY:HA2	3:U:92:HIS:HD2	1.74	0.52
1:G:153:GLN:NE2	2:H:240:ILE:HG12	2.24	0.52
3:U:26:GLN:CG	3:U:29:GLU:HG3	2.40	0.52
1:A:140:CYS:SG	1:A:143:LEU:HB2	2.50	0.51
3:Q:58:GLY:CA	3:Q:92:HIS:HD2	2.22	0.51
3:R:44:ASP:HB2	3:R:46:LEU:H	1.75	0.51
3:R:78:ASN:HD22	3:R:78:ASN:N	2.07	0.51
1:E:43:VAL:CG1	1:E:54:ARG:HB2	2.38	0.51
1:E:95:GLN:O	1:E:96:LEU:C	2.48	0.51
1:I:136:ASP:HB2	2:J:213:THR:O	2.10	0.51
1:G:28:ARG:O	1:G:103:ASP:HB3	2.09	0.51
1:G:82:THR:OG1	1:G:85:GLU:HG3	2.09	0.51
1:K:15:THR:OG1	1:K:16:PRO:HD2	2.09	0.51
1:A:52:GLU:OE1	2:B:231:ARG:NH2	2.44	0.51
1:E:156:ARG:HH21	2:F:221:TYR:CB	2.23	0.51
3:R:139:VAL:HG22	3:R:139:VAL:O	2.10	0.51
1:G:54:ARG:NH2	1:G:111:SER:HA	2.26	0.51
3:S:92:HIS:O	3:S:96:VAL:HG23	2.10	0.51
3:T:100:LEU:CD2	3:T:106:VAL:HG23	2.37	0.51
1:K:34:ARG:HG3	1:K:34:ARG:NH1	2.20	0.51
3:S:91:GLY:HA3	3:S:125:HIS:NE2	2.26	0.51
1:I:45:PHE:CD2	1:I:121:VAL:HA	2.45	0.51
1:C:82:THR:OG1	1:C:85:GLU:HG3	2.10	0.51
3:Q:80:GLY:O	3:Q:110:ASP:HA	2.10	0.51
1:G:80:ASP:HA	1:G:121:VAL:HG11	1.92	0.51
1:K:82:THR:OG1	1:K:85:GLU:HG3	2.10	0.51
1:E:144:GLN:OE1	1:G:167:GLN:N	2.44	0.51
3:R:56:LYS:HB2	3:R:86:LEU:HD13	1.93	0.51
3:S:162:ALA:C	3:S:164:ILE:N	2.64	0.51
1:K:80:ASP:CA	1:K:121:VAL:HG11	2.41	0.51
3:S:118:HIS:ND1	3:S:143:ASP:HB3	2.25	0.51
3:S:122:TYR:CE1	3:S:152:ILE:HD12	2.46	0.51
1:K:27:TYR:HB2	1:K:29:LEU:CD1	2.39	0.51
3:P:59:HIS:O	3:P:63:VAL:HG23	2.11	0.51
2:D:218:ILE:HG23	2:D:218:ILE:O	2.10	0.51
1:E:151:PHE:CD1	2:F:243:LEU:HD21	2.46	0.51
1:I:140:CYS:SG	1:I:143:LEU:HB2	2.50	0.51
2:B:247:PHE:O	2:B:251:ALA:HB2	2.11	0.50
1:C:81:GLN:C	1:C:121:VAL:HG22	2.31	0.50
1:G:52:GLU:HG3	1:G:53:PHE:N	2.24	0.50
3:T:133:LEU:HD21	3:T:164:ILE:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:NH1	2:B:225:LYS:N	2.59	0.50
1:C:80:ASP:HA	1:C:121:VAL:HG11	1.92	0.50
1:E:40:LEU:HD11	1:E:86:MET:HG2	1.93	0.50
3:R:133:LEU:HA	3:R:137:ALA:CB	2.41	0.50
1:I:19:TYR:CD1	1:I:19:TYR:C	2.84	0.50
3:T:125:HIS:HB3	3:T:128:ILE:HG13	1.93	0.50
1:E:128:LEU:HD13	1:E:152:ILE:CD1	2.41	0.50
3:R:125:HIS:HB3	3:R:128:ILE:HG13	1.93	0.50
1:I:95:GLN:O	1:I:96:LEU:C	2.50	0.50
1:K:29:LEU:N	1:K:29:LEU:CD2	2.75	0.50
3:P:43:THR:HA	3:P:48:HIS:O	2.11	0.50
3:R:153:SER:OG	3:R:165:LEU:HD13	2.11	0.50
1:I:40:LEU:HD11	1:I:86:MET:HG2	1.93	0.50
3:U:110:ASP:OD1	3:U:114:PHE:HB2	2.12	0.50
3:Q:82:THR:O	3:Q:85:HIS:HB2	2.11	0.50
3:R:10:HIS:CG	3:R:10:HIS:O	2.65	0.50
3:T:43:THR:HA	3:T:48:HIS:O	2.12	0.50
1:K:51:LEU:HD12	1:K:112:HIS:ND1	2.27	0.50
1:A:80:ASP:CA	1:A:121:VAL:HG11	2.42	0.50
3:Q:139:VAL:HG22	3:Q:139:VAL:O	2.12	0.50
1:G:81:GLN:C	1:G:121:VAL:HG22	2.32	0.50
3:S:163:GLU:O	3:S:164:ILE:HD12	2.11	0.50
1:I:15:THR:OG1	2:J:302:HIS:CA	2.52	0.50
3:T:23:ARG:HH11	3:T:57:THR:HG21	1.75	0.50
1:K:39:VAL:HG12	1:K:39:VAL:O	2.12	0.50
1:E:128:LEU:HD13	1:E:152:ILE:HD13	1.92	0.50
3:R:100:LEU:HD23	3:R:104:ALA:HB3	1.93	0.50
1:G:23:PHE:CD1	1:G:24:GLN:N	2.80	0.50
3:S:165:LEU:HD12	3:S:165:LEU:H	1.77	0.50
3:U:133:LEU:HA	3:U:137:ALA:CB	2.39	0.50
3:P:118:HIS:ND1	3:P:143:ASP:HB3	2.27	0.50
3:R:58:GLY:HA2	3:R:92:HIS:HD2	1.76	0.50
1:K:152:ILE:HD12	2:L:221:TYR:CE2	2.47	0.50
1:A:46:THR:O	1:A:47:GLY:C	2.50	0.50
1:A:163:GLY:C	2:D:210:ARG:NH1	2.65	0.50
1:G:42:ASN:HB2	1:G:111:SER:OG	2.12	0.50
1:G:159:GLU:O	1:G:159:GLU:HG3	2.11	0.50
2:H:293:CYS:C	2:H:294:ARG:HG3	2.32	0.50
3:S:40:VAL:O	3:S:40:VAL:HG22	2.12	0.50
3:U:27:ASP:OD1	3:U:62:ILE:HG12	2.11	0.50
3:Q:23:ARG:HD2	3:Q:23:ARG:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ASN:ND2	1:G:120:GLY:HA2	2.27	0.49
1:A:40:LEU:HD11	1:A:86:MET:HG2	1.94	0.49
3:R:77:ASP:OD1	3:R:77:ASP:N	2.44	0.49
1:G:45:PHE:HZ	1:G:111:SER:OG	1.96	0.49
1:G:80:ASP:CA	1:G:121:VAL:HG11	2.42	0.49
2:H:255:HIS:CE1	2:H:258:ASP:HB2	2.47	0.49
3:T:24:ALA:HB3	3:T:26:GLN:HG2	1.94	0.49
3:U:118:HIS:ND1	3:U:143:ASP:HB3	2.26	0.49
1:A:19:TYR:CD1	1:A:19:TYR:C	2.85	0.49
2:D:293:CYS:C	2:D:294:ARG:HG3	2.31	0.49
3:Q:122:TYR:CE1	3:Q:152:ILE:HD12	2.47	0.49
3:Q:161:LEU:C	3:Q:163:GLU:H	2.14	0.49
3:U:93:LEU:HA	3:U:128:ILE:HD13	1.95	0.49
1:A:9:LEU:N	1:A:9:LEU:HD22	2.28	0.49
3:R:80:GLY:HA3	3:R:111:TYR:HD1	1.75	0.49
1:G:15:THR:HG22	1:G:17:GLU:N	2.26	0.49
3:S:25:GLY:O	3:S:26:GLN:HG3	2.11	0.49
1:I:80:ASP:CA	1:I:121:VAL:HG11	2.42	0.49
3:T:62:ILE:HA	3:T:65:VAL:HG12	1.94	0.49
1:K:19:TYR:CE2	2:L:299:PHE:HB3	2.48	0.49
3:P:80:GLY:HA3	3:P:111:TYR:HD1	1.75	0.49
1:C:80:ASP:CA	1:C:121:VAL:HG11	2.43	0.49
1:C:159:GLU:O	1:C:160:THR:HG23	2.13	0.49
3:Q:58:GLY:HA2	3:Q:92:HIS:HD2	1.77	0.49
2:F:291:THR:HA	2:H:264:ASN:ND2	2.27	0.49
1:G:46:THR:OG1	1:G:47:GLY:N	2.44	0.49
1:I:27:TYR:CE1	1:I:147:PRO:HD3	2.47	0.49
1:A:81:GLN:C	1:A:121:VAL:HG22	2.33	0.49
3:Q:80:GLY:HA3	3:Q:111:TYR:HD1	1.75	0.49
3:Q:82:THR:N	3:Q:85:HIS:ND1	2.57	0.49
3:R:84:LEU:HD23	3:R:116:PRO:HG2	1.95	0.49
1:K:156:ARG:HH21	2:L:224:LEU:C	2.15	0.49
2:B:211:LEU:HA	2:D:283:LYS:HE3	1.94	0.49
2:B:285:MET:HE3	2:D:291:THR:HB	1.94	0.49
1:E:153:GLN:HE22	2:F:239:TYR:HB3	1.76	0.49
1:I:36:LEU:CD2	1:I:74:ASP:HB3	2.43	0.49
3:U:139:VAL:O	3:U:139:VAL:HG22	2.13	0.49
1:A:82:THR:OG1	1:A:85:GLU:HG3	2.12	0.49
3:P:18:LEU:HA	3:P:33:LEU:HD13	1.94	0.49
1:C:110:LEU:HG	1:C:153:GLN:HB3	1.94	0.49
1:G:54:ARG:HG3	1:G:112:HIS:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:133:LEU:HA	3:S:137:ALA:CB	2.42	0.49
2:B:285:MET:CE	2:D:291:THR:HB	2.43	0.49
1:C:117:ALA:HB2	1:C:127:GLN:HA	1.95	0.49
2:D:255:HIS:CE1	2:D:258:ASP:HB2	2.47	0.49
3:R:59:HIS:O	3:R:63:VAL:HG23	2.13	0.49
1:E:117:ALA:HB2	1:E:127:GLN:HA	1.95	0.49
1:G:43:VAL:HG12	1:G:53:PHE:HE1	1.76	0.49
1:I:42:ASN:ND2	1:I:81:GLN:O	2.44	0.49
3:U:148:THR:C	3:U:150:PHE:N	2.67	0.49
2:D:255:HIS:CE1	2:D:258:ASP:CG	2.86	0.48
2:F:210:ARG:O	2:F:211:LEU:HD23	2.12	0.48
1:I:81:GLN:C	1:I:121:VAL:HG22	2.33	0.48
2:J:247:PHE:O	2:J:251:ALA:HB2	2.12	0.48
3:U:84:LEU:HD23	3:U:116:PRO:HG2	1.94	0.48
3:U:90:ASN:O	3:U:92:HIS:CE1	2.66	0.48
1:E:80:ASP:HA	1:E:121:VAL:CG1	2.42	0.48
1:E:128:LEU:HD22	1:E:152:ILE:HD11	1.94	0.48
3:T:91:GLY:HA3	3:T:125:HIS:NE2	2.28	0.48
3:P:13:ASP:CG	3:P:14:LEU:N	2.66	0.48
3:P:40:VAL:HG22	3:P:40:VAL:O	2.13	0.48
1:E:81:GLN:C	1:E:121:VAL:HG22	2.34	0.48
1:E:110:LEU:HA	1:E:153:GLN:O	2.13	0.48
1:G:19:TYR:C	1:G:21:THR:H	2.16	0.48
2:H:255:HIS:CE1	2:H:258:ASP:CG	2.86	0.48
3:T:18:LEU:CD1	3:T:30:VAL:HG13	2.38	0.48
1:K:64:LEU:HD11	2:L:240:ILE:HD12	1.96	0.48
3:P:29:GLU:N	3:P:29:GLU:CD	2.66	0.48
3:Q:118:HIS:ND1	3:Q:143:ASP:HB3	2.27	0.48
2:F:264:ASN:ND2	2:H:291:THR:HA	2.28	0.48
1:I:42:ASN:HD22	1:I:120:GLY:HA2	1.78	0.48
1:K:36:LEU:CD2	1:K:74:ASP:HB3	2.43	0.48
1:C:51:LEU:O	1:C:52:GLU:O	2.31	0.48
1:E:36:LEU:HD23	1:E:74:ASP:HB3	1.94	0.48
1:G:40:LEU:HD11	1:G:86:MET:HG2	1.93	0.48
1:I:25:LEU:HD23	1:I:25:LEU:N	2.24	0.48
1:I:164:VAL:CG2	2:L:213:THR:HA	2.43	0.48
3:T:100:LEU:HD23	3:T:104:ALA:HB3	1.95	0.48
1:K:36:LEU:HD23	1:K:74:ASP:HB3	1.94	0.48
1:A:45:PHE:CE2	1:A:112:HIS:HD2	2.32	0.48
1:E:45:PHE:CD2	1:E:51:LEU:HG	2.49	0.48
3:S:13:ASP:O	3:S:15:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:39:ASP:C	3:T:41:ASN:H	2.17	0.48
3:T:139:VAL:HG22	3:T:139:VAL:O	2.13	0.48
1:K:80:ASP:HA	1:K:121:VAL:CG1	2.43	0.48
3:U:126:LEU:HB2	3:U:127:GLU:HG3	1.94	0.48
2:F:293:CYS:C	2:F:294:ARG:HG3	2.34	0.48
1:G:47:GLY:O	1:G:49:LYS:N	2.46	0.48
3:S:18:LEU:CD2	3:S:19:LEU:HD12	2.43	0.48
1:A:110:LEU:HG	1:A:153:GLN:HB3	1.95	0.48
3:P:125:HIS:HB3	3:P:128:ILE:HG13	1.95	0.48
3:R:51:LEU:HD11	3:R:63:VAL:HG13	1.96	0.48
1:G:68:PHE:O	1:G:73:TYR:HB2	2.14	0.48
1:G:80:ASP:HA	1:G:121:VAL:CG1	2.44	0.48
1:I:36:LEU:HD23	1:I:74:ASP:HB3	1.95	0.48
1:A:140:CYS:SG	1:A:140:CYS:O	2.72	0.48
2:B:255:HIS:CE1	2:B:258:ASP:HB2	2.48	0.48
3:P:84:LEU:HD23	3:P:116:PRO:HG2	1.96	0.48
1:K:95:GLN:O	1:K:96:LEU:C	2.51	0.48
2:B:210:ARG:HB3	1:C:165:ASP:HB3	1.95	0.48
1:C:80:ASP:HA	1:C:121:VAL:CG1	2.44	0.48
3:Q:161:LEU:O	3:Q:163:GLU:N	2.46	0.48
2:J:293:CYS:C	2:J:294:ARG:HG3	2.34	0.48
3:T:133:LEU:HA	3:T:137:ALA:CB	2.43	0.48
1:K:15:THR:O	1:K:17:GLU:N	2.46	0.48
1:E:19:TYR:C	1:E:21:THR:H	2.17	0.47
1:G:46:THR:O	1:G:47:GLY:O	2.32	0.47
1:K:156:ARG:NH2	2:L:224:LEU:C	2.67	0.47
2:L:293:CYS:C	2:L:294:ARG:HG3	2.35	0.47
3:U:125:HIS:HB3	3:U:128:ILE:HG13	1.96	0.47
1:A:80:ASP:HA	1:A:121:VAL:CG1	2.44	0.47
1:A:100:ARG:HD2	3:S:159:GLU:CD	2.35	0.47
1:G:43:VAL:HG12	1:G:53:PHE:CE1	2.50	0.47
1:G:43:VAL:HG13	1:G:54:ARG:O	2.14	0.47
1:I:42:ASN:C	1:I:54:ARG:HH21	2.18	0.47
1:I:162:ARG:HG3	1:I:162:ARG:HH11	1.79	0.47
1:K:27:TYR:CB	1:K:29:LEU:HD13	2.43	0.47
2:B:291:THR:HB	2:D:285:MET:CE	2.44	0.47
3:S:19:LEU:H	3:S:19:LEU:CD1	2.25	0.47
1:I:118:ILE:HG22	1:I:154:ALA:CB	2.44	0.47
3:T:122:TYR:CE1	3:T:152:ILE:HD12	2.49	0.47
3:U:46:LEU:O	3:U:78:ASN:OD1	2.32	0.47
1:C:13:PRO:O	2:D:252:CYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:39:ASP:C	3:R:41:ASN:H	2.18	0.47
1:G:11:VAL:HG22	2:H:248:SER:HA	1.97	0.47
1:E:64:LEU:CD1	1:E:110:LEU:HD21	2.45	0.47
1:G:36:LEU:HD23	1:G:74:ASP:HB3	1.97	0.47
1:I:117:ALA:HB2	1:I:127:GLN:HA	1.96	0.47
1:K:156:ARG:NH2	2:L:225:LYS:N	2.57	0.47
1:A:141:PRO:HB2	1:C:168:ASP:HB3	1.97	0.47
1:A:141:PRO:HB2	1:C:168:ASP:HA	1.97	0.47
2:B:293:CYS:C	2:B:294:ARG:HG3	2.35	0.47
3:P:46:LEU:O	3:P:78:ASN:ND2	2.47	0.47
2:D:225:LYS:HD3	2:D:225:LYS:C	2.34	0.47
3:Q:94:GLU:O	3:Q:98:VAL:HG23	2.15	0.47
1:E:18:PHE:CD2	1:E:18:PHE:O	2.68	0.47
1:E:79:CYS:HB2	1:I:44:HIS:CE1	2.50	0.47
1:I:15:THR:HG23	1:I:16:PRO:N	2.29	0.47
3:T:25:GLY:CA	3:T:59:HIS:CD2	2.70	0.47
3:T:82:THR:N	3:T:85:HIS:ND1	2.61	0.47
3:U:49:THR:O	3:U:52:HIS:HB2	2.15	0.47
3:P:82:THR:N	3:P:85:HIS:ND1	2.62	0.47
1:C:25:LEU:HD22	1:C:25:LEU:N	2.30	0.47
1:C:36:LEU:HD23	1:C:74:ASP:HB3	1.97	0.47
1:G:117:ALA:HB2	1:G:127:GLN:HA	1.96	0.47
1:A:117:ALA:HB2	1:A:127:GLN:HA	1.97	0.47
3:P:9:HIS:HD1	3:P:9:HIS:N	2.12	0.47
3:S:125:HIS:HB3	3:S:128:ILE:HG13	1.97	0.47
3:P:92:HIS:O	3:P:96:VAL:HG23	2.15	0.47
3:R:91:GLY:HA3	3:R:125:HIS:NE2	2.29	0.47
1:I:11:VAL:HG21	1:I:70:LEU:CB	2.43	0.47
3:U:80:GLY:HA3	3:U:111:TYR:HD1	1.80	0.47
1:C:40:LEU:HD11	1:C:86:MET:HG2	1.95	0.46
1:E:36:LEU:CD2	1:E:74:ASP:HB3	2.45	0.46
1:E:53:PHE:O	1:E:55:SER:N	2.48	0.46
1:E:64:LEU:HD22	1:E:68:PHE:CE2	2.50	0.46
1:E:128:LEU:CD1	1:E:152:ILE:HD13	2.45	0.46
3:S:34:MET:HE3	3:S:34:MET:HA	1.97	0.46
1:I:80:ASP:HA	1:I:121:VAL:CG1	2.44	0.46
1:I:140:CYS:SG	1:I:140:CYS:O	2.73	0.46
3:P:159:GLU:C	3:P:161:LEU:H	2.18	0.46
3:Q:62:ILE:HA	3:Q:65:VAL:HG12	1.96	0.46
1:E:44:HIS:N	1:E:44:HIS:CD2	2.83	0.46
3:R:56:LYS:HB2	3:R:86:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:41:SER:HA	1:I:110:LEU:O	2.15	0.46
3:T:19:LEU:CD1	3:T:42:ALA:HB1	2.45	0.46
1:K:117:ALA:HB2	1:K:127:GLN:HA	1.98	0.46
1:A:28:ARG:HG3	1:A:28:ARG:HH11	1.80	0.46
1:E:45:PHE:CB	1:E:51:LEU:HB2	2.45	0.46
1:E:98:ALA:O	1:E:101:VAL:HG12	2.15	0.46
3:R:118:HIS:ND1	3:R:143:ASP:HB3	2.30	0.46
3:S:49:THR:O	3:S:52:HIS:HB2	2.16	0.46
3:S:58:GLY:HA3	3:S:92:HIS:CE1	2.51	0.46
1:I:39:VAL:HG12	1:I:39:VAL:O	2.15	0.46
1:K:49:LYS:HD2	1:K:50:GLU:H	1.80	0.46
1:A:163:GLY:C	2:D:210:ARG:HH11	2.19	0.46
3:P:100:LEU:HD23	3:P:104:ALA:HB3	1.97	0.46
3:R:138:ASP:C	3:R:140:ASN:H	2.19	0.46
3:S:94:GLU:O	3:S:98:VAL:HG23	2.16	0.46
1:K:28:ARG:HH11	1:K:28:ARG:CA	2.20	0.46
1:K:98:ALA:O	1:K:101:VAL:HG12	2.15	0.46
1:A:7:LEU:HA	1:A:7:LEU:HD22	1.68	0.46
1:A:136:ASP:HB2	2:B:213:THR:O	2.16	0.46
3:P:138:ASP:C	3:P:140:ASN:H	2.19	0.46
2:D:273:TYR:HB3	3:Q:79:TYR:HE2	1.77	0.46
1:E:42:ASN:ND2	1:E:120:GLY:HA2	2.31	0.46
3:R:110:ASP:OD1	3:R:114:PHE:HB2	2.15	0.46
2:J:225:LYS:HD3	2:J:225:LYS:C	2.36	0.46
3:T:19:LEU:O	3:T:53:LEU:CD1	2.61	0.46
3:T:22:ALA:O	3:T:24:ALA:N	2.49	0.46
3:T:164:ILE:O	3:T:164:ILE:HG13	2.15	0.46
1:K:41:SER:HA	1:K:110:LEU:O	2.14	0.46
1:A:25:LEU:HD23	1:A:25:LEU:N	2.28	0.46
2:B:210:ARG:HB2	1:C:164:VAL:O	2.16	0.46
3:P:110:ASP:OD1	3:P:114:PHE:HB2	2.15	0.46
3:Q:41:ASN:HD22	3:Q:41:ASN:HA	1.56	0.46
1:E:27:TYR:HD2	1:E:147:PRO:CG	2.28	0.46
1:E:54:ARG:NH2	1:E:110:LEU:HB3	2.30	0.46
3:S:62:ILE:HA	3:S:65:VAL:HG12	1.96	0.46
1:A:120:GLY:C	1:A:122:ASP:N	2.68	0.46
2:B:213:THR:OG1	1:C:161:ASP:OD1	2.34	0.46
3:Q:21:ALA:HA	3:Q:26:GLN:OE1	2.16	0.46
3:Q:91:GLY:HA3	3:Q:125:HIS:NE2	2.31	0.46
3:R:30:VAL:HG11	3:R:62:ILE:HG23	1.98	0.46
1:I:64:LEU:CD1	1:I:110:LEU:HD21	2.43	0.46

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:I:118:ILE:HG22	1:I:154:ALA:HB2	1.98	0.46
3:P:39:ASP:C	3:P:41:ASN:H	2.20	0.46
1:C:53:PHE:O	1:C:55:SER:N	2.49	0.46
3:T:73:VAL:O	3:T:73:VAL:HG22	2.16	0.46
1:K:82:THR:HB	1:K:122:ASP:CB	2.41	0.46
1:A:166:GLN:HB3	2:D:211:LEU:HG	1.97	0.46
3:P:93:LEU:HA	3:P:128:ILE:HD13	1.98	0.46
2:J:274:ALA:HA	2:J:275:PRO:HD2	1.56	0.46
2:L:225:LYS:HD3	2:L:225:LYS:C	2.37	0.46
3:U:15:GLY:O	3:U:18:LEU:HB3	2.16	0.46
3:U:26:GLN:HG3	3:U:29:GLU:HG3	1.98	0.46
3:U:100:LEU:CD2	3:U:106:VAL:HG23	2.35	0.46
3:U:148:THR:C	3:U:150:PHE:H	2.18	0.46
3:P:73:VAL:HG22	3:P:73:VAL:O	2.16	0.46
3:P:82:THR:H	3:P:85:HIS:HB2	1.81	0.46
1:C:36:LEU:CD2	1:C:74:ASP:HB3	2.46	0.46
1:C:167:GLN:OE1	1:C:167:GLN:HA	2.15	0.46
1:E:86:MET:O	1:E:90:LEU:HB2	2.16	0.46
1:G:29:LEU:O	1:G:29:LEU:CD2	2.62	0.46
3:S:18:LEU:HD23	3:S:18:LEU:H	1.80	0.46
1:A:36:LEU:CD2	1:A:74:ASP:HB3	2.46	0.45
2:B:255:HIS:CE1	2:B:258:ASP:CG	2.88	0.45
1:C:43:VAL:HG13	1:C:54:ARG:O	2.15	0.45
3:Q:133:LEU:HA	3:Q:137:ALA:CB	2.44	0.45
1:G:19:TYR:O	1:G:21:THR:N	2.50	0.45
3:S:39:ASP:C	3:S:41:ASN:H	2.19	0.45
1:I:164:VAL:HG12	1:I:165:ASP:H	1.82	0.45
1:K:160:THR:O	1:K:161:ASP:C	2.55	0.45
3:U:62:ILE:HA	3:U:65:VAL:CG1	2.46	0.45
3:P:26:GLN:HG2	3:P:29:GLU:OE1	2.17	0.45
3:P:62:ILE:HA	3:P:65:VAL:CG1	2.46	0.45
1:C:46:THR:OG1	1:C:47:GLY:N	2.50	0.45
3:Q:18:LEU:HA	3:Q:33:LEU:HD13	1.98	0.45
1:G:140:CYS:SG	1:G:143:LEU:HB2	2.57	0.45
2:B:301:GLY:O	2:B:302:HIS:CB	2.65	0.45
1:E:41:SER:HA	1:E:110:LEU:O	2.17	0.45
3:R:49:THR:O	3:R:52:HIS:HB2	2.17	0.45
3:S:110:ASP:OD1	3:S:114:PHE:HB2	2.17	0.45
1:K:64:LEU:HD22	1:K:68:PHE:CE2	2.52	0.45
1:A:42:ASN:O	1:A:54:ARG:HG3	2.16	0.45
1:A:44:HIS:ND1	1:A:53:PHE:HE1	2.13	0.45

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
3:Q:161:LEU:C	3:Q:163:GLU:N	2.69	0.45
2:J:273:TYR:CB	3:T:79:TYR:CE2	2.88	0.45
1:A:98:ALA:O	1:A:101:VAL:HG12	2.16	0.45
3:R:14:LEU:N	3:R:14:LEU:HD22	2.29	0.45
1:G:43:VAL:O	1:G:53:PHE:HD1	1.99	0.45
3:U:148:THR:O	3:U:150:PHE:N	2.49	0.45
3:P:163:GLU:O	3:P:165:LEU:N	2.46	0.45
1:E:15:THR:O	1:E:18:PHE:HB3	2.16	0.45
3:R:92:HIS:O	3:R:96:VAL:HG23	2.17	0.45
2:B:298:LEU:O	2:B:299:PHE:C	2.54	0.45
3:Q:165:LEU:O	3:Q:167:LYS:N	2.50	0.45
1:E:77:VAL:O	1:E:78:LEU:HD23	2.17	0.45
3:R:82:THR:H	3:R:85:HIS:HB2	1.82	0.45
3:R:90:ASN:O	3:R:92:HIS:CE1	2.70	0.45
2:J:218:ILE:HG23	2:J:218:ILE:O	2.17	0.45
1:K:77:VAL:O	1:K:78:LEU:HD23	2.16	0.45
1:A:151:PHE:CD1	2:B:243:LEU:HD21	2.52	0.45
3:P:18:LEU:O	3:P:19:LEU:C	2.54	0.45
1:E:120:GLY:C	1:E:122:ASP:N	2.69	0.45
1:G:36:LEU:CD2	1:G:74:ASP:HB3	2.47	0.45
3:S:138:ASP:C	3:S:140:ASN:H	2.19	0.45
3:S:162:ALA:O	3:S:164:ILE:N	2.48	0.45
3:T:110:ASP:OD1	3:T:114:PHE:HB2	2.17	0.45
3:U:30:VAL:HG11	3:U:62:ILE:CG2	2.46	0.45
3:Q:56:LYS:HB2	3:Q:86:LEU:HB3	1.97	0.45
1:E:19:TYR:C	1:E:21:THR:N	2.69	0.45
3:S:16:LYS:HB3	3:S:42:ALA:HB1	1.99	0.45
3:T:161:LEU:C	3:T:163:GLU:N	2.70	0.45
1:A:25:LEU:N	1:A:25:LEU:CD2	2.80	0.45
3:P:19:LEU:CD1	3:P:50:PRO:HG3	2.40	0.45
1:C:53:PHE:O	1:C:53:PHE:CG	2.69	0.45
1:C:75:VAL:HG23	1:C:76:HIS:O	2.17	0.45
3:Q:58:GLY:HA2	3:Q:92:HIS:CD2	2.52	0.45
2:F:255:HIS:CE1	2:F:258:ASP:HB2	2.51	0.45
3:T:25:GLY:CA	3:T:59:HIS:NE2	2.80	0.45
1:A:36:LEU:HD23	1:A:74:ASP:HB3	1.97	0.44
1:A:162:ARG:O	2:D:210:ARG:NH1	2.50	0.44
2:H:225:LYS:HD3	2:H:225:LYS:C	2.37	0.44
1:I:77:VAL:O	1:I:78:LEU:HD23	2.17	0.44
2:J:210:ARG:HB2	2:L:283:LYS:HE2	1.98	0.44
3:U:34:MET:HE3	3:U:34:MET:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:44:ASP:OD1	3:P:44:ASP:N	2.49	0.44
3:T:19:LEU:HD11	3:T:42:ALA:CB	2.46	0.44
1:K:110:LEU:N	1:K:110:LEU:CD1	2.79	0.44
1:C:140:CYS:SG	1:C:140:CYS:O	2.76	0.44
2:F:225:LYS:C	2:F:225:LYS:HD3	2.38	0.44
3:S:82:THR:N	3:S:85:HIS:ND1	2.65	0.44
1:I:17:GLU:H	1:I:20:GLN:HG2	1.82	0.44
3:U:39:ASP:C	3:U:41:ASN:H	2.21	0.44
1:A:41:SER:HA	1:A:110:LEU:O	2.18	0.44
3:P:34:MET:HA	3:P:34:MET:CE	2.46	0.44
3:P:163:GLU:C	3:P:165:LEU:N	2.67	0.44
1:C:111:SER:O	1:C:154:ALA:HA	2.17	0.44
3:Q:112:GLU:OE1	3:Q:144:LYS:HE2	2.17	0.44
3:S:148:THR:C	3:S:150:PHE:N	2.71	0.44
1:I:42:ASN:O	1:I:54:ARG:NE	2.44	0.44
1:I:64:LEU:HD22	1:I:68:PHE:CE2	2.53	0.44
3:T:30:VAL:HG11	3:T:62:ILE:CG2	2.47	0.44
1:K:23:PHE:O	1:K:24:GLN:C	2.56	0.44
2:L:298:LEU:O	2:L:299:PHE:C	2.56	0.44
3:P:91:GLY:HA3	3:P:125:HIS:NE2	2.32	0.44
1:C:68:PHE:O	1:C:73:TYR:HB2	2.18	0.44
1:E:39:VAL:HG12	1:E:39:VAL:O	2.18	0.44
3:R:34:MET:HE3	3:R:34:MET:HA	2.00	0.44
1:G:19:TYR:CD2	2:H:302:HIS:CD2	3.05	0.44
2:H:214:ARG:O	2:H:215:SER:HB3	2.18	0.44
1:C:82:THR:HB	1:C:122:ASP:CB	2.42	0.44
1:E:68:PHE:O	1:E:73:TYR:HB2	2.16	0.44
3:R:73:VAL:HG22	3:R:73:VAL:O	2.17	0.44
1:K:35:GLY:HA2	1:K:102:THR:CB	2.47	0.44
2:B:225:LYS:HD3	2:B:225:LYS:C	2.38	0.44
1:C:64:LEU:HD22	1:C:68:PHE:CE2	2.53	0.44
3:Q:30:VAL:HG11	3:Q:62:ILE:HG23	2.00	0.44
3:Q:39:ASP:C	3:Q:41:ASN:H	2.21	0.44
1:G:48:GLU:O	1:G:50:GLU:OE1	2.36	0.44
3:T:148:THR:C	3:T:150:PHE:N	2.70	0.44
3:T:158:ASN:HD22	3:T:158:ASN:HA	1.57	0.44
1:E:23:PHE:CD1	1:E:24:GLN:N	2.86	0.44
3:R:25:GLY:HA2	3:R:62:ILE:HD11	1.99	0.44
1:G:82:THR:HB	1:G:122:ASP:CB	2.42	0.44
3:U:91:GLY:HA3	3:U:125:HIS:NE2	2.33	0.44
3:P:49:THR:O	3:P:52:HIS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:51:LEU:HD11	3:P:63:VAL:HG13	2.00	0.44
1:C:42:ASN:ND2	1:C:120:GLY:HA2	2.32	0.44
3:Q:18:LEU:HD13	3:Q:34:MET:SD	2.58	0.44
2:J:291:THR:HB	2:L:285:MET:HE3	2.00	0.44
1:A:141:PRO:HB2	1:C:168:ASP:CA	2.48	0.43
2:B:214:ARG:O	2:B:215:SER:HB3	2.18	0.43
3:P:148:THR:C	3:P:150:PHE:N	2.70	0.43
1:C:41:SER:HA	1:C:110:LEU:O	2.17	0.43
3:S:19:LEU:HD11	3:S:42:ALA:CB	2.46	0.43
1:K:75:VAL:HG23	1:K:76:HIS:O	2.17	0.43
1:K:140:CYS:SG	1:K:140:CYS:O	2.75	0.43
1:A:144:GLN:OE1	1:C:166:GLN:HA	2.18	0.43
3:Q:49:THR:O	3:Q:52:HIS:HB2	2.18	0.43
3:Q:148:THR:C	3:Q:150:PHE:N	2.72	0.43
1:E:18:PHE:CE1	1:E:22:HIS:CE1	3.06	0.43
1:G:10:GLN:HE21	1:G:10:GLN:HB2	1.61	0.43
1:G:41:SER:HA	1:G:110:LEU:O	2.17	0.43
1:I:13:PRO:O	1:I:14:CYS:HB2	2.18	0.43
2:J:298:LEU:O	2:J:299:PHE:C	2.56	0.43
3:P:58:GLY:HA2	3:P:92:HIS:CD2	2.47	0.43
2:D:298:LEU:O	2:D:299:PHE:C	2.55	0.43
2:F:255:HIS:CE1	2:F:258:ASP:CG	2.91	0.43
1:I:98:ALA:O	1:I:101:VAL:HG12	2.18	0.43
1:K:165:ASP:N	1:K:165:ASP:OD1	2.51	0.43
1:A:166:GLN:O	1:A:166:GLN:CG	2.59	0.43
1:E:45:PHE:HE1	1:E:54:ARG:HG2	1.82	0.43
1:E:153:GLN:HG2	2:F:240:ILE:HD11	1.99	0.43
3:R:12:SER:C	3:R:14:LEU:H	2.21	0.43
3:R:148:THR:C	3:R:150:PHE:N	2.70	0.43
1:G:86:MET:O	1:G:90:LEU:HB2	2.18	0.43
3:Q:62:ILE:HA	3:Q:65:VAL:CG1	2.48	0.43
3:R:82:THR:N	3:R:85:HIS:ND1	2.66	0.43
1:G:12:LYS:O	2:H:252:CYS:HB3	2.19	0.43
1:I:75:VAL:HG23	1:I:76:HIS:O	2.18	0.43
1:K:37:ALA:HA	1:K:106:ILE:O	2.19	0.43
2:L:239:TYR:O	2:L:243:LEU:HB2	2.18	0.43
1:C:110:LEU:N	1:C:110:LEU:CD1	2.77	0.43
3:Q:44:ASP:HB2	3:Q:46:LEU:H	1.82	0.43
1:G:47:GLY:O	1:G:48:GLU:C	2.57	0.43
3:S:163:GLU:O	3:S:163:GLU:HG2	2.18	0.43
1:I:47:GLY:C	1:I:49:LYS:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:GLY:C	1:I:122:ASP:N	2.70	0.43
3:T:148:THR:O	3:T:152:ILE:HG12	2.18	0.43
1:K:160:THR:O	1:K:160:THR:HG22	2.19	0.43
3:U:18:LEU:O	3:U:21:ALA:HB3	2.18	0.43
2:B:283:LYS:HE2	2:D:210:ARG:HB2	2.00	0.43
3:Q:138:ASP:C	3:Q:140:ASN:H	2.21	0.43
3:S:82:THR:H	3:S:85:HIS:HB2	1.83	0.43
1:K:118:ILE:HG22	1:K:154:ALA:CB	2.48	0.43
1:A:77:VAL:O	1:A:78:LEU:HD23	2.19	0.43
2:B:291:THR:HB	2:D:285:MET:HE3	2.00	0.43
1:I:86:MET:O	1:I:90:LEU:HB2	2.18	0.43
1:K:68:PHE:O	1:K:73:TYR:HB2	2.18	0.43
1:K:86:MET:O	1:K:90:LEU:HB2	2.18	0.43
1:K:120:GLY:C	1:K:122:ASP:N	2.71	0.43
2:L:211:LEU:N	2:L:211:LEU:CD1	2.80	0.43
1:A:37:ALA:HA	1:A:106:ILE:O	2.19	0.43
3:P:161:LEU:N	3:P:161:LEU:HD22	2.34	0.43
1:A:46:THR:OG1	1:A:47:GLY:N	2.50	0.43
1:I:162:ARG:H	1:I:162:ARG:HD2	1.84	0.43
1:A:75:VAL:HG23	1:A:76:HIS:O	2.19	0.42
2:B:209:MET:O	2:B:209:MET:HG3	2.19	0.42
3:R:58:GLY:HA2	3:R:92:HIS:CD2	2.50	0.42
1:G:39:VAL:HG12	1:G:39:VAL:O	2.18	0.42
1:I:68:PHE:O	1:I:73:TYR:HB2	2.18	0.42
3:T:133:LEU:HD21	3:T:164:ILE:HG21	1.99	0.42
3:P:46:LEU:C	3:P:78:ASN:ND2	2.71	0.42
3:Q:34:MET:HA	3:Q:34:MET:CE	2.48	0.42
2:F:298:LEU:O	2:F:299:PHE:C	2.57	0.42
3:S:93:LEU:HA	3:S:128:ILE:HD13	2.01	0.42
1:I:159:GLU:O	1:I:159:GLU:HG3	2.18	0.42
3:T:22:ALA:C	3:T:24:ALA:H	2.22	0.42
1:K:147:PRO:CB	2:L:296:LEU:HD13	2.49	0.42
1:A:54:ARG:HH11	1:A:54:ARG:CG	2.32	0.42
3:P:17:LYS:HZ2	3:P:33:LEU:CD2	2.24	0.42
3:Q:78:ASN:N	3:Q:78:ASN:ND2	2.66	0.42
3:Q:93:LEU:HA	3:Q:128:ILE:HD13	2.01	0.42
1:C:46:THR:O	1:C:47:GLY:O	2.36	0.42
1:C:82:THR:HG23	1:C:85:GLU:OE1	2.19	0.42
3:S:118:HIS:CE1	3:S:143:ASP:HB3	2.54	0.42
1:I:82:THR:HB	1:I:122:ASP:CB	2.42	0.42
3:T:138:ASP:C	3:T:140:ASN:H	2.22	0.42

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:K:15:THR:HG22	1:K:18:PHE:CD2	2.54	0.42
1:K:44:HIS:O	1:K:121:VAL:HG12	2.19	0.42
3:P:160:ASP:C	3:P:161:LEU:HD22	2.40	0.42
2:D:293:CYS:O	2:D:294:ARG:CG	2.65	0.42
3:Q:51:LEU:HD11	3:Q:63:VAL:HG13	2.02	0.42
1:E:75:VAL:HG23	1:E:76:HIS:O	2.19	0.42
2:F:285:MET:HE3	2:H:291:THR:HB	2.02	0.42
1:G:29:LEU:CD2	1:G:34:ARG:HG2	2.47	0.42
1:I:157:GLY:HA3	2:J:226:GLY:O	2.19	0.42
3:T:78:ASN:N	3:T:78:ASN:ND2	2.66	0.42
1:C:35:GLY:HA2	1:C:102:THR:CB	2.49	0.42
2:F:249:GLU:OE2	3:R:9:HIS:HE1	2.02	0.42
1:K:29:LEU:HG	2:L:297:TYR:O	2.19	0.42
1:K:42:ASN:HB2	1:K:111:SER:OG	2.19	0.42
1:K:128:LEU:HD22	1:K:152:ILE:HD13	2.02	0.42
1:A:166:GLN:HB3	2:D:211:LEU:CD1	2.50	0.42
3:P:78:ASN:HD22	3:P:78:ASN:H	1.67	0.42
1:C:9:LEU:CG	1:C:9:LEU:O	2.68	0.42
1:C:98:ALA:O	1:C:101:VAL:HG12	2.19	0.42
3:T:30:VAL:HG11	3:T:62:ILE:HG23	2.01	0.42
3:R:9:HIS:N	3:R:9:HIS:HD2	2.16	0.42
3:R:93:LEU:HA	3:R:128:ILE:HD13	2.02	0.42
2:B:239:TYR:O	2:B:243:LEU:HB2	2.20	0.42
1:G:75:VAL:HG23	1:G:76:HIS:O	2.20	0.42
1:I:153:GLN:O	1:I:153:GLN:CG	2.68	0.42
1:K:22:HIS:O	1:K:23:PHE:C	2.59	0.42
1:A:43:VAL:HG12	1:A:54:ARG:HB2	2.02	0.42
1:C:120:GLY:C	1:C:122:ASP:N	2.71	0.42
3:Q:61:GLU:O	3:Q:65:VAL:HG12	2.20	0.42
2:F:214:ARG:O	2:F:215:SER:HB3	2.20	0.42
1:G:19:TYR:C	1:G:21:THR:N	2.73	0.42
1:G:64:LEU:CD1	1:G:110:LEU:HD21	2.49	0.42
1:G:77:VAL:O	1:G:78:LEU:HD23	2.20	0.42
1:G:98:ALA:O	1:G:101:VAL:HG12	2.20	0.42
2:H:256:VAL:O	2:H:260:LEU:HG	2.20	0.42
3:S:100:LEU:HD23	3:S:104:ALA:HB3	2.01	0.42
2:B:273:TYR:CB	3:P:79:TYR:CE2	2.90	0.41
1:C:37:ALA:HA	1:C:106:ILE:O	2.20	0.41
1:C:86:MET:O	1:C:90:LEU:HB2	2.19	0.41
3:Q:56:LYS:HB2	3:Q:86:LEU:HD13	2.02	0.41
1:G:18:PHE:CZ	2:H:253:ASP:HA	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:273:TYR:CD2	3:T:79:TYR:CD2	3.08	0.41
3:T:58:GLY:HA2	3:T:92:HIS:CD2	2.49	0.41
2:H:298:LEU:O	2:H:299:PHE:C	2.58	0.41
3:T:19:LEU:HD11	3:T:42:ALA:C	2.39	0.41
3:T:148:THR:C	3:T:150:PHE:H	2.23	0.41
1:A:39:VAL:HG12	1:A:39:VAL:O	2.21	0.41
1:A:86:MET:O	1:A:90:LEU:HB2	2.20	0.41
3:P:159:GLU:C	3:P:161:LEU:N	2.73	0.41
2:D:303:PRO:HA	2:D:304:PRO:HD3	1.78	0.41
3:Q:73:VAL:HG22	3:Q:73:VAL:O	2.20	0.41
3:Q:159:GLU:OE2	1:E:100:ARG:NH1	2.44	0.41
3:R:158:ASN:OD1	3:R:161:LEU:HD22	2.21	0.41
1:G:15:THR:HG22	1:G:18:PHE:N	2.35	0.41
1:G:55:SER:C	1:G:57:GLY:H	2.22	0.41
1:G:82:THR:HG23	1:G:85:GLU:OE1	2.20	0.41
1:G:120:GLY:C	1:G:122:ASP:N	2.72	0.41
3:S:40:VAL:HG11	3:S:69:TYR:O	2.19	0.41
3:T:82:THR:H	3:T:85:HIS:HB2	1.86	0.41
3:T:118:HIS:CE1	3:T:143:ASP:HB3	2.55	0.41
3:U:92:HIS:O	3:U:96:VAL:HG23	2.19	0.41
1:A:42:ASN:ND2	1:A:120:GLY:HA2	2.36	0.41
1:A:137:ASN:HB3	2:B:211:LEU:HD11	2.01	0.41
1:E:18:PHE:CD1	1:E:22:HIS:ND1	2.88	0.41
3:R:41:ASN:HD22	3:R:41:ASN:HA	1.54	0.41
1:I:35:GLY:HA2	1:I:102:THR:CB	2.47	0.41
1:A:22:HIS:O	1:A:25:LEU:HD23	2.20	0.41
3:P:148:THR:C	3:P:150:PHE:H	2.24	0.41
3:Q:110:ASP:OD1	3:Q:114:PHE:HB2	2.20	0.41
1:E:138:ALA:O	1:E:141:PRO:HD3	2.21	0.41
3:S:78:ASN:N	3:S:78:ASN:ND2	2.68	0.41
3:U:26:GLN:HB3	3:U:29:GLU:CB	2.43	0.41
1:C:10:GLN:O	2:D:248:SER:HB2	2.21	0.41
1:C:49:LYS:HD2	1:C:49:LYS:HA	1.84	0.41
3:R:51:LEU:CD1	3:R:63:VAL:HG13	2.50	0.41
1:G:15:THR:HG22	1:G:18:PHE:H	1.85	0.41
1:I:42:ASN:ND2	1:I:121:VAL:H	2.18	0.41
3:R:18:LEU:O	3:R:18:LEU:HD12	2.21	0.41
3:R:158:ASN:HD22	3:R:158:ASN:HA	1.59	0.41
3:S:20:GLU:O	3:S:24:ALA:HB2	2.21	0.41
1:I:29:LEU:HD23	2:J:297:TYR:O	2.21	0.41
3:T:118:HIS:O	3:T:121:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:16:PRO:HA	2:L:302:HIS:CE1	2.52	0.41
3:U:51:LEU:HD11	3:U:63:VAL:HG13	2.02	0.41
3:U:139:VAL:CG2	3:U:165:LEU:HD21	2.51	0.41
2:B:229:ALA:O	2:B:230:MET:HE3	2.20	0.41
1:E:35:GLY:HA2	1:E:102:THR:CB	2.48	0.41
3:S:148:THR:C	3:S:150:PHE:H	2.24	0.41
1:K:67:LEU:CD2	2:L:244:ALA:HA	2.50	0.41
1:K:140:CYS:HG	1:K:143:LEU:HB2	1.86	0.41
3:U:82:THR:N	3:U:85:HIS:ND1	2.66	0.41
1:A:64:LEU:HD22	1:A:68:PHE:CE2	2.56	0.41
1:A:163:GLY:O	2:D:210:ARG:NH1	2.54	0.41
3:P:30:VAL:HG11	3:P:62:ILE:HG23	2.03	0.41
1:C:28:ARG:O	1:C:103:ASP:HB3	2.20	0.41
1:C:96:LEU:HA	1:C:97:PRO:HD2	1.85	0.41
2:D:273:TYR:CD2	3:Q:79:TYR:CD2	3.09	0.41
2:D:274:ALA:O	2:D:280:HIS:HB2	2.21	0.41
1:G:156:ARG:HB2	2:H:224:LEU:O	2.21	0.41
1:I:47:GLY:C	1:I:49:LYS:N	2.74	0.41
2:J:211:LEU:CD1	1:K:166:GLN:HG2	2.50	0.41
2:J:274:ALA:O	2:J:280:HIS:HB2	2.21	0.41
1:K:140:CYS:SG	1:K:143:LEU:HD12	2.61	0.41
3:U:25:GLY:HA3	3:U:59:HIS:CD2	2.53	0.41
3:U:30:VAL:HG11	3:U:62:ILE:HG23	2.03	0.41
3:S:73:VAL:HG22	3:S:73:VAL:O	2.21	0.41
1:I:82:THR:HG23	1:I:85:GLU:OE1	2.21	0.41
2:J:291:THR:HB	2:L:285:MET:CE	2.51	0.41
3:U:125:HIS:O	3:U:126:LEU:O	2.38	0.41
1:A:35:GLY:HA2	1:A:102:THR:CB	2.49	0.40
3:R:62:ILE:HA	3:R:65:VAL:HG12	2.03	0.40
1:G:50:GLU:CG	1:G:51:LEU:HG	2.51	0.40
1:G:64:LEU:HD22	1:G:68:PHE:CE2	2.56	0.40
3:S:148:THR:O	3:S:150:PHE:N	2.54	0.40
1:I:44:HIS:O	1:I:121:VAL:HB	2.21	0.40
3:T:93:LEU:HA	3:T:128:ILE:HD13	2.02	0.40
3:U:58:GLY:HA2	3:U:92:HIS:CD2	2.51	0.40
1:A:43:VAL:HA	1:A:54:ARG:HB2	2.02	0.40
1:G:140:CYS:SG	1:G:140:CYS:O	2.80	0.40
2:H:293:CYS:O	2:H:294:ARG:CG	2.67	0.40
1:I:82:THR:CG2	1:I:122:ASP:HB2	2.52	0.40
1:K:82:THR:CG2	1:K:122:ASP:HB2	2.51	0.40
2:B:273:TYR:CD2	3:P:79:TYR:CD2	3.08	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:152:ILE:HG22	3:P:152:ILE:O	2.21	0.40
1:G:9:LEU:HD23	1:G:10:GLN:N	2.37	0.40
1:G:79:CYS:O	1:G:80:ASP:C	2.59	0.40
1:G:136:ASP:HB2	2:H:213:THR:O	2.21	0.40
3:S:62:ILE:HA	3:S:65:VAL:CG1	2.51	0.40
2:L:266:LEU:HD13	3:U:45:TRP:CD2	2.57	0.40
3:U:73:VAL:O	3:U:73:VAL:HG22	2.21	0.40
3:U:127:GLU:HG3	3:U:127:GLU:H	1.31	0.40
1:A:79:CYS:O	1:A:80:ASP:C	2.59	0.40
2:B:273:TYR:CB	3:P:79:TYR:CD2	2.98	0.40
3:P:106:VAL:HG21	3:P:135:TYR:HB2	2.03	0.40
3:P:110:ASP:O	3:P:112:GLU:N	2.54	0.40
2:D:214:ARG:O	2:D:215:SER:HB3	2.22	0.40
3:Q:30:VAL:HG11	3:Q:62:ILE:CG2	2.51	0.40
2:F:285:MET:CE	2:H:291:THR:HB	2.52	0.40
3:R:148:THR:C	3:R:150:PHE:H	2.24	0.40
3:R:148:THR:O	3:R:150:PHE:N	2.54	0.40
3:S:148:THR:O	3:S:152:ILE:HG12	2.21	0.40
2:J:239:TYR:O	2:J:243:LEU:HB2	2.21	0.40
3:T:148:THR:O	3:T:150:PHE:N	2.55	0.40
1:K:82:THR:HG23	1:K:85:GLU:OE1	2.21	0.40
2:L:255:HIS:HB3	2:L:297:TYR:CE1	2.57	0.40
3:U:148:THR:O	3:U:152:ILE:HG12	2.21	0.40
1:A:11:VAL:HG21	1:A:70:LEU:CB	2.49	0.40
1:C:45:PHE:CD1	1:C:45:PHE:N	2.90	0.40
1:C:164:VAL:CG1	1:C:165:ASP:N	2.84	0.40
1:E:96:LEU:HA	1:E:97:PRO:HD2	1.85	0.40
3:R:26:GLN:O	3:R:29:GLU:N	2.49	0.40
3:S:34:MET:HA	3:S:34:MET:CE	2.52	0.40
1:I:164:VAL:HG21	2:L:213:THR:HA	2.03	0.40
3:T:62:ILE:HA	3:T:65:VAL:CG1	2.51	0.40
1:K:64:LEU:HD22	1:K:68:PHE:CZ	2.56	0.40
3:U:138:ASP:C	3:U:140:ASN:H	2.23	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	160/169 (95%)	135 (84%)	21 (13%)	4 (2%)	5	29
1	C	159/169 (94%)	128 (80%)	26 (16%)	5 (3%)	4	24
1	E	158/169 (94%)	127 (80%)	26 (16%)	5 (3%)	4	23
1	G	158/169 (94%)	128 (81%)	24 (15%)	6 (4%)	3	19
1	I	155/169 (92%)	120 (77%)	28 (18%)	7 (4%)	2	16
1	K	156/169 (92%)	125 (80%)	21 (14%)	10 (6%)	1	9
2	B	94/106 (89%)	83 (88%)	7 (7%)	4 (4%)	2	17
2	D	96/106 (91%)	89 (93%)	5 (5%)	2 (2%)	7	33
2	F	94/106 (89%)	88 (94%)	4 (4%)	2 (2%)	7	33
2	H	96/106 (91%)	85 (88%)	8 (8%)	3 (3%)	4	24
2	J	92/106 (87%)	83 (90%)	5 (5%)	4 (4%)	2	17
2	L	90/106 (85%)	80 (89%)	7 (8%)	3 (3%)	4	22
3	P	156/169 (92%)	117 (75%)	26 (17%)	13 (8%)	1	4
3	Q	156/169 (92%)	121 (78%)	26 (17%)	9 (6%)	1	11
3	R	155/169 (92%)	124 (80%)	21 (14%)	10 (6%)	1	8
3	S	151/169 (89%)	117 (78%)	27 (18%)	7 (5%)	2	16
3	T	150/169 (89%)	113 (75%)	28 (19%)	9 (6%)	1	10
3	U	152/169 (90%)	119 (78%)	27 (18%)	6 (4%)	3	19
All	All	2428/2664 (91%)	1982 (82%)	337 (14%)	109 (4%)	2	16

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	52	GLU
3	P	27	ASP
3	P	126	LEU

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Mol	Chain	Res	Type
3	P	162	ALA
1	C	47	GLY
1	C	52	GLU
1	C	54	ARG
3	Q	126	LEU
1	E	54	ARG
3	R	13	ASP
3	R	126	LEU
1	G	158	ASP
3	S	126	LEU
1	I	15	THR
1	I	49	LYS
3	T	26	GLN
3	T	126	LEU
1	K	24	GLN
1	K	50	GLU
1	K	156	ARG
3	U	126	LEU
3	U	165	LEU
1	A	47	GLY
1	A	54	ARG
3	P	11	GLY
3	P	13	ASP
3	P	40	VAL
3	P	134	LYS
3	P	164	ILE
3	Q	40	VAL
3	Q	134	LYS
3	Q	166	GLN
1	E	55	SER
3	R	12	SER
3	R	16	LYS
3	R	40	VAL
1	G	20	GLN
1	G	47	GLY
1	G	48	GLU
1	G	160	THR
2	H	230	MET
3	S	14	LEU
3	S	16	LYS
3	S	40	VAL
3	S	134	LYS

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Mol	Chain	Res	Type
1	I	14	CYS
1	I	154	ALA
3	T	23	ARG
3	T	40	VAL
3	T	134	LYS
1	K	155	CYS
1	K	159	GLU
1	K	161	ASP
3	U	27	ASP
3	U	40	VAL
3	P	28	ASP
3	P	111	TYR
3	P	138	ASP
3	Q	26	GLN
3	Q	111	TYR
3	Q	162	ALA
1	E	24	GLN
1	E	49	LYS
3	R	111	TYR
3	R	134	LYS
3	R	138	ASP
1	G	49	LYS
1	I	16	PRO
1	I	18	PHE
2	J	277	THR
1	K	10	GLN
2	L	301	GLY
3	U	111	TYR
3	P	14	LEU
1	C	167	GLN
3	Q	138	ASP
3	R	10	HIS
3	S	138	ASP
3	S	163	GLU
1	I	13	PRO
3	T	111	TYR
3	T	138	ASP
1	K	16	PRO
1	K	19	TYR
1	K	47	GLY
3	U	149	ALA
2	B	303	PRO

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Mol	Chain	Res	Type
1	C	27	TYR
3	T	162	ALA
2	H	256	VAL
3	T	149	ALA
1	E	11	VAL
2	J	256	VAL
2	J	275	PRO
2	L	218	ILE
2	L	256	VAL
3	R	106	VAL
2	B	218	ILE
2	B	302	HIS
2	D	256	VAL
3	Q	106	VAL
2	F	218	ILE
2	F	256	VAL
2	J	218	ILE
2	B	256	VAL
3	P	106	VAL
2	D	218	ILE
2	H	218	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/147 (97%)	132 (93%)	10 (7%)	15	46
1	C	141/147 (96%)	130 (92%)	11 (8%)	12	41
1	E	140/147 (95%)	131 (94%)	9 (6%)	17	50
1	G	140/147 (95%)	133 (95%)	7 (5%)	24	58
1	I	137/147 (93%)	126 (92%)	11 (8%)	12	40
1	K	138/147 (94%)	131 (95%)	7 (5%)	24	57
2	B	81/89 (91%)	79 (98%)	2 (2%)	47	74
2	D	83/89 (93%)	80 (96%)	3 (4%)	35	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	81/89 (91%)	76 (94%)	5 (6%)	18	51
2	H	83/89 (93%)	78 (94%)	5 (6%)	19	52
2	J	79/89 (89%)	77 (98%)	2 (2%)	47	74
2	L	77/89 (86%)	75 (97%)	2 (3%)	46	74
3	P	122/132 (92%)	107 (88%)	15 (12%)	4	20
3	Q	123/132 (93%)	112 (91%)	11 (9%)	9	34
3	R	121/132 (92%)	103 (85%)	18 (15%)	3	13
3	S	118/132 (89%)	103 (87%)	15 (13%)	4	19
3	T	117/132 (89%)	105 (90%)	12 (10%)	7	27
3	U	119/132 (90%)	106 (89%)	13 (11%)	6	25
All	All	2042/2208 (92%)	1884 (92%)	158 (8%)	13	41

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	17	GLU
1	A	25	LEU
1	A	29	LEU
1	A	75	VAL
1	A	115	GLU
1	A	156	ARG
1	A	158	ASP
1	A	164	VAL
1	A	166	GLN
2	B	230	MET
2	B	245	GLN
3	P	9	HIS
3	P	41	ASN
3	P	44	ASP
3	P	45	TRP
3	P	76	TRP
3	P	105	ASP
3	P	109	LYS
3	P	123	ASP
3	P	134	LYS
3	P	144	LYS
3	P	148	THR

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Mol	Chain	Res	Type
3	P	151	ASP
3	P	153	SER
3	P	155	ASP
3	P	158	ASN
1	C	9	LEU
1	C	23	PHE
1	C	25	LEU
1	C	34	ARG
1	C	53	PHE
1	C	75	VAL
1	C	115	GLU
1	C	160	THR
1	C	162	ARG
1	C	165	ASP
1	C	167	GLN
2	D	209	MET
2	D	231	ARG
2	D	245	GLN
3	Q	41	ASN
3	Q	44	ASP
3	Q	45	TRP
3	Q	76	TRP
3	Q	105	ASP
3	Q	109	LYS
3	Q	123	ASP
3	Q	144	LYS
3	Q	148	THR
3	Q	151	ASP
3	Q	158	ASN
1	E	8	CYS
1	E	9	LEU
1	E	10	GLN
1	E	23	PHE
1	E	24	GLN
1	E	51	LEU
1	E	52	GLU
1	E	75	VAL
1	E	115	GLU
2	F	209	MET
2	F	230	MET
2	F	245	GLN
2	F	290	SER

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Mol	Chain	Res	Type
2	F	304	PRO
3	R	9	HIS
3	R	13	ASP
3	R	27	ASP
3	R	28	ASP
3	R	41	ASN
3	R	44	ASP
3	R	45	TRP
3	R	68	LYS
3	R	76	TRP
3	R	77	ASP
3	R	105	ASP
3	R	109	LYS
3	R	123	ASP
3	R	134	LYS
3	R	144	LYS
3	R	148	THR
3	R	151	ASP
3	R	158	ASN
1	G	10	GLN
1	G	21	THR
1	G	34	ARG
1	G	49	LYS
1	G	52	GLU
1	G	75	VAL
1	G	115	GLU
2	H	230	MET
2	H	231	ARG
2	H	245	GLN
2	H	290	SER
2	H	304	PRO
3	S	28	ASP
3	S	41	ASN
3	S	44	ASP
3	S	68	LYS
3	S	76	TRP
3	S	105	ASP
3	S	106	VAL
3	S	123	ASP
3	S	134	LYS
3	S	144	LYS
3	S	148	THR

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Mol	Chain	Res	Type
3	S	151	ASP
3	S	158	ASN
3	S	159	GLU
3	S	165	LEU
1	I	15	THR
1	I	16	PRO
1	I	19	TYR
1	I	24	GLN
1	I	25	LEU
1	I	51	LEU
1	I	54	ARG
1	I	75	VAL
1	I	115	GLU
1	I	159	GLU
1	I	162	ARG
2	J	245	GLN
2	J	255	HIS
3	T	41	ASN
3	T	44	ASP
3	T	45	TRP
3	T	76	TRP
3	T	105	ASP
3	T	109	LYS
3	T	123	ASP
3	T	126	LEU
3	T	134	LYS
3	T	148	THR
3	T	151	ASP
3	T	158	ASN
1	K	28	ARG
1	K	29	LEU
1	K	50	GLU
1	K	75	VAL
1	K	115	GLU
1	K	153	GLN
1	K	164	VAL
2	L	245	GLN
2	L	255	HIS
3	U	26	GLN
3	U	27	ASP
3	U	41	ASN
3	U	44	ASP

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Mol	Chain	Res	Type
3	U	45	TRP
3	U	64	GLU
3	U	76	TRP
3	U	123	ASP
3	U	126	LEU
3	U	134	LYS
3	U	144	LYS
3	U	148	THR
3	U	158	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	76	HIS
1	A	92	ASN
1	A	112	HIS
1	A	167	GLN
2	B	245	GLN
2	B	255	HIS
3	P	36	ASN
3	P	78	ASN
3	P	118	HIS
3	P	158	ASN
3	P	166	GLN
1	C	10	GLN
1	C	76	HIS
1	C	92	ASN
2	D	245	GLN
2	D	255	HIS
3	Q	36	ASN
3	Q	41	ASN
3	Q	59	HIS
3	Q	78	ASN
3	Q	158	ASN
1	E	44	HIS
1	E	76	HIS
1	E	92	ASN
1	E	153	GLN
2	F	245	GLN
2	F	255	HIS
3	R	36	ASN

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Mol	Chain	Res	Type
3	R	41	ASN
3	R	59	HIS
3	R	78	ASN
3	R	90	ASN
3	R	118	HIS
1	G	10	GLN
1	G	20	GLN
1	G	76	HIS
1	G	92	ASN
1	G	153	GLN
2	H	245	GLN
2	H	255	HIS
3	S	36	ASN
3	S	41	ASN
3	S	78	ASN
3	S	90	ASN
3	S	158	ASN
1	I	24	GLN
1	I	76	HIS
1	I	92	ASN
1	I	145	ASN
2	J	245	GLN
2	J	255	HIS
3	T	36	ASN
3	T	41	ASN
3	T	78	ASN
3	T	90	ASN
3	T	118	HIS
3	T	158	ASN
1	K	10	GLN
1	K	76	HIS
1	K	92	ASN
1	K	112	HIS
1	K	166	GLN
2	L	245	GLN
2	L	255	HIS
2	L	302	HIS
3	U	36	ASN
3	U	41	ASN
3	U	59	HIS
3	U	90	ASN
3	U	158	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	162/169 (95%)	-0.12	0	100	100	41, 83, 113, 125	0
1	C	161/169 (95%)	-0.09	1 (0%)	89	85	37, 81, 105, 121	0
1	E	160/169 (94%)	-0.09	1 (0%)	89	85	49, 88, 122, 142	0
1	G	160/169 (94%)	-0.07	0	100	100	36, 78, 105, 121	0
1	I	157/169 (92%)	-0.08	3 (1%)	66	57	52, 91, 142, 160	0
1	K	158/169 (93%)	0.09	7 (4%)	34	24	55, 92, 156, 176	0
2	B	96/106 (90%)	-0.04	1 (1%)	82	75	31, 72, 128, 136	0
2	D	98/106 (92%)	-0.05	1 (1%)	82	75	35, 71, 125, 135	0
2	F	96/106 (90%)	-0.16	0	100	100	29, 73, 127, 136	0
2	H	98/106 (92%)	-0.02	1 (1%)	82	75	33, 71, 126, 136	0
2	J	94/106 (88%)	-0.05	3 (3%)	47	35	50, 75, 129, 136	0
2	L	92/106 (86%)	-0.14	1 (1%)	80	73	49, 74, 122, 137	0
3	P	158/169 (93%)	0.25	8 (5%)	28	18	57, 106, 181, 191	0
3	Q	158/169 (93%)	0.03	2 (1%)	77	68	64, 106, 177, 186	0
3	R	157/169 (92%)	0.10	5 (3%)	47	35	63, 107, 178, 186	0
3	S	153/169 (90%)	0.13	4 (2%)	56	44	67, 110, 177, 186	0
3	T	152/169 (89%)	0.39	14 (9%)	9	7	70, 112, 183, 191	0
3	U	154/169 (91%)	0.11	3 (1%)	66	57	66, 110, 182, 196	0
All	All	2464/2664 (92%)	0.02	55 (2%)	62	52	29, 91, 168, 196	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	12	SER	7.5
3	Q	169	ASN	6.3
3	R	10	HIS	5.9

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Mol	Chain	Res	Type	RSRZ
3	S	25	GLY	4.7
3	P	11	GLY	4.2
3	R	9	HIS	4.2
1	K	18	PHE	4.2
3	R	159	GLU	3.8
1	C	168	ASP	3.7
1	K	44	HIS	3.6
1	K	29	LEU	3.4
3	P	9	HIS	3.4
3	P	149	ALA	3.4
3	T	142	GLN	3.4
3	T	98	VAL	3.3
3	U	14	LEU	3.3
1	I	47	GLY	3.3
3	S	142	GLN	3.1
2	D	305	THR	3.1
1	I	16	PRO	3.0
3	T	140	ASN	3.0
1	E	49	LYS	3.0
3	Q	12	SER	2.9
3	R	11	GLY	2.8
3	T	60	LEU	2.8
3	P	165	LEU	2.8
2	J	234	LYS	2.8
2	H	234	LYS	2.8
3	P	158	ASN	2.7
3	T	159	GLU	2.7
3	T	113	GLY	2.7
3	T	73	VAL	2.6
3	S	130	GLU	2.6
1	K	15	THR	2.6
3	S	149	ALA	2.6
2	B	234	LYS	2.6
2	J	229	ALA	2.5
3	T	99	LEU	2.5
3	U	164	ILE	2.5
1	I	165	ASP	2.3
1	K	49	LYS	2.3
2	L	230	MET	2.3
3	T	161	LEU	2.3
3	T	141	ALA	2.3
3	R	156	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	T	109	LYS	2.3
3	U	154	ILE	2.2
1	K	51	LEU	2.2
1	K	159	GLU	2.2
3	P	10	HIS	2.2
3	T	149	ALA	2.1
3	P	142	GLN	2.1
3	T	164	ILE	2.1
3	T	146	GLY	2.0
2	J	302	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.