



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:14 AM UTC

PDB ID : 2P2C / pdb_00002p2c
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

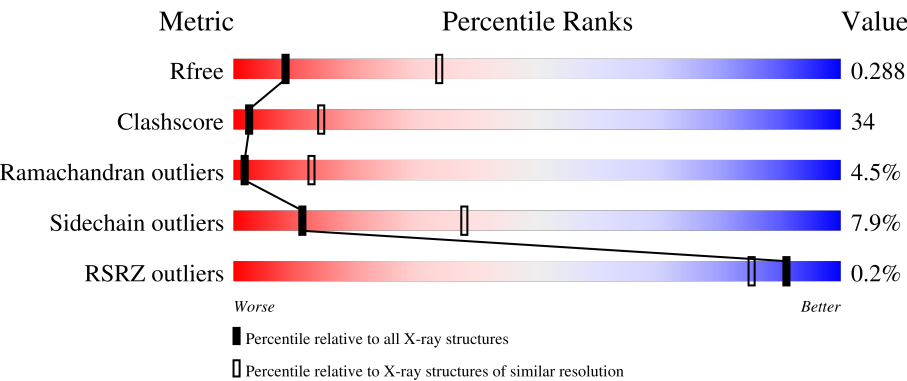
1 Overall quality at a glance i

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.



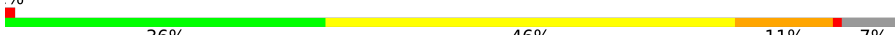
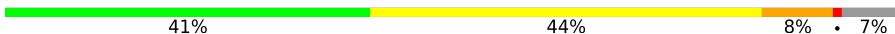
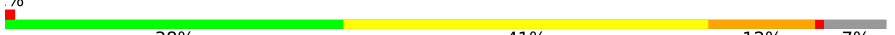
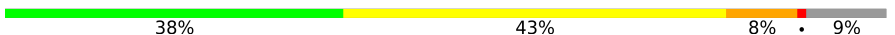
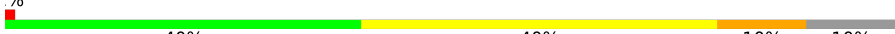
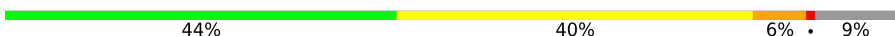
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	169	44% 44% 7% . .
1	C	169	42% 44% 8% . 5%
1	E	169	40% 47% 6% . 5%
1	G	169	45% 42% 7% . 5%
1	I	169	40% 45% 5% . 7%

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

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

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

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

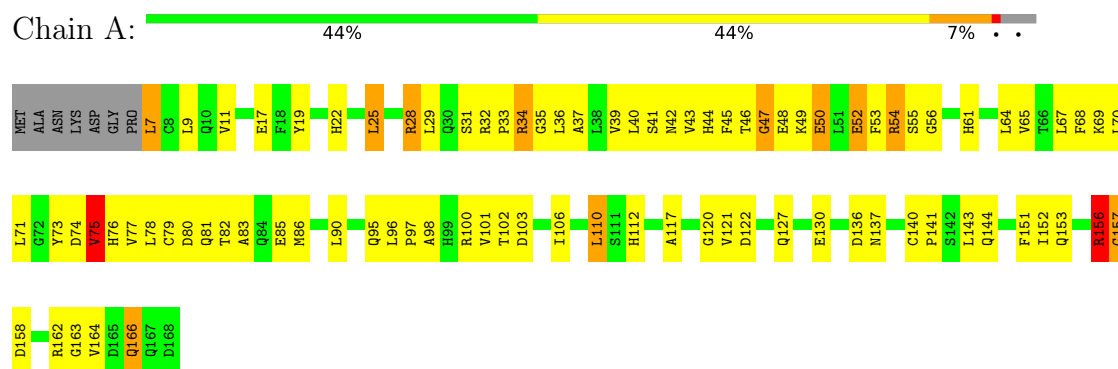
- Molecule 4 is water.

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

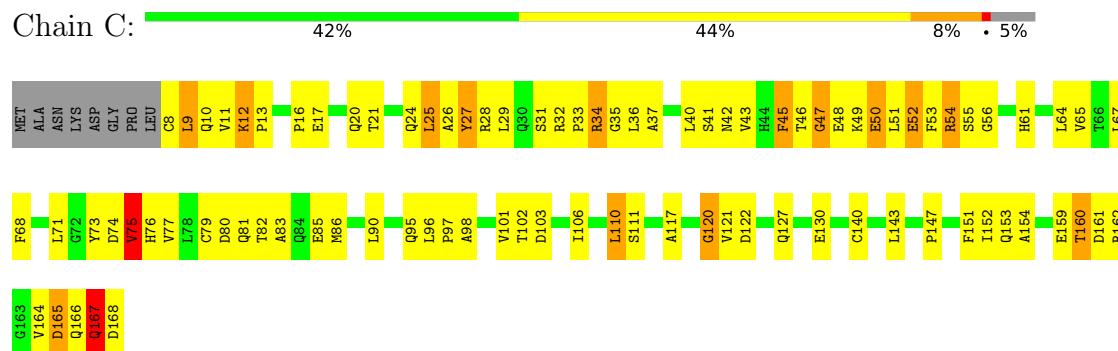
3 Residue-property plots [i](#)

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.

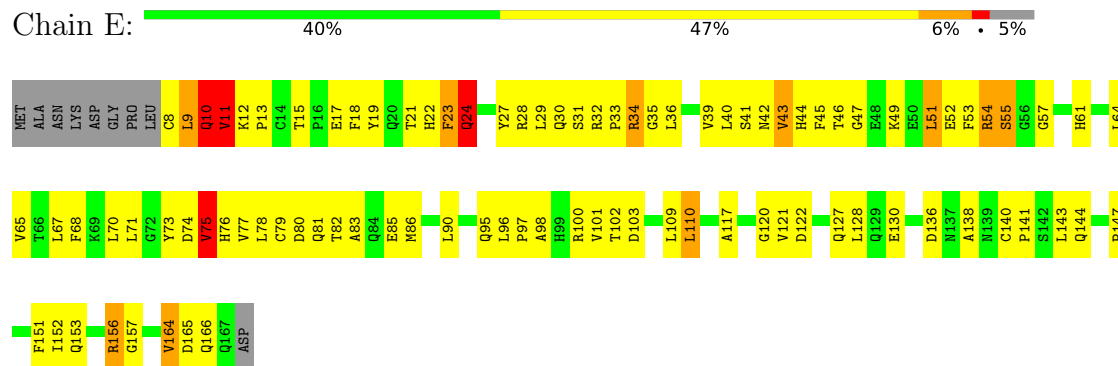
• Molecule 1: Caspase-2



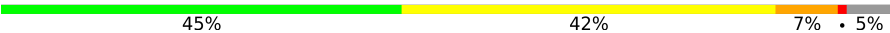
• Molecule 1: Caspase-2

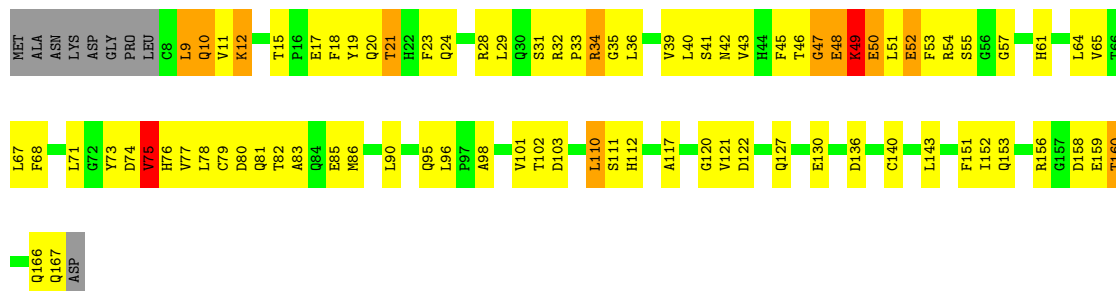


• Molecule 1: Caspase-2

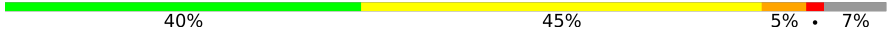


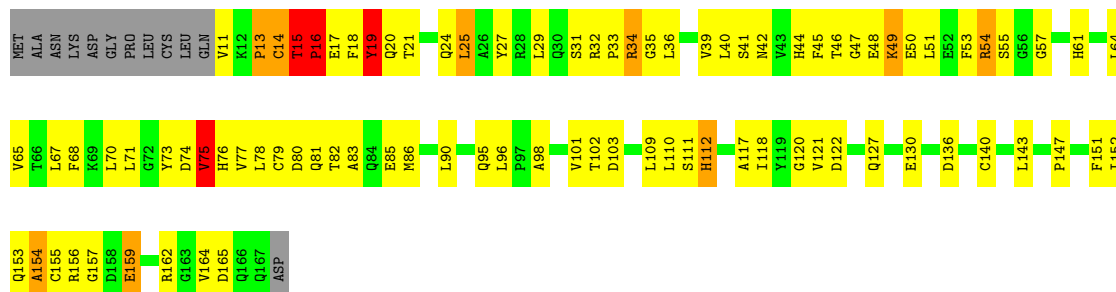
- Molecule 1: Caspase-2

Chain G:  45% 42% 7% • 5%

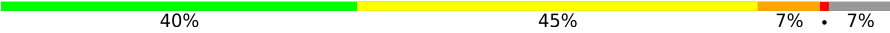


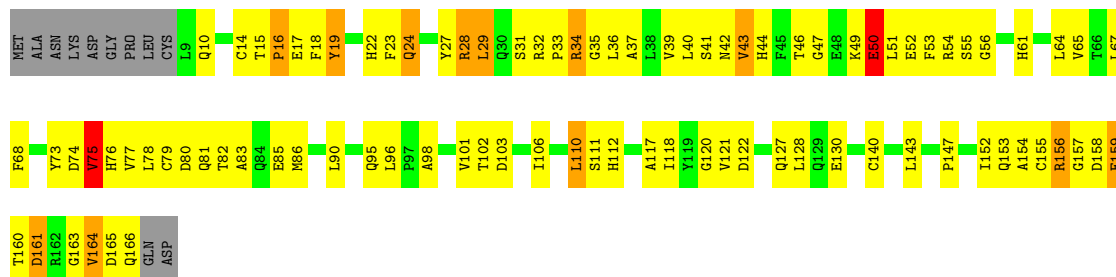
- Molecule 1: Caspase-2

Chain I:  40% 45% 5% • 7%



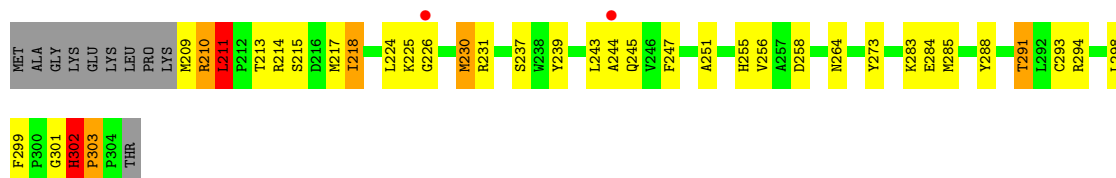
- Molecule 1: Caspase-2

Chain K:  40% 45% 7% • 7%



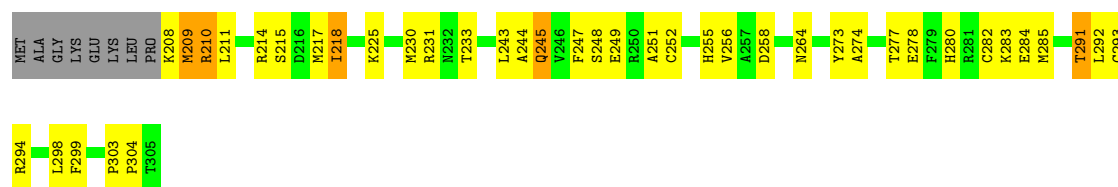
- Molecule 2: Caspase-2

Chain B:  2% 56% 28% 5% • 9%



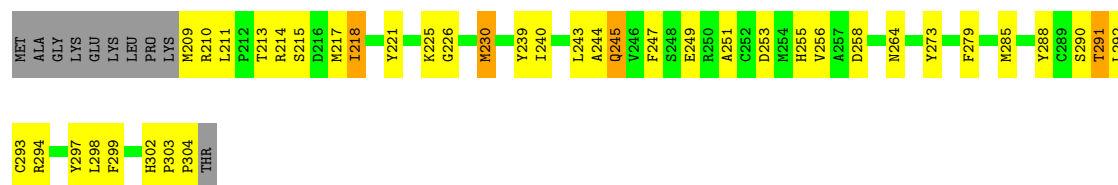
- Molecule 2: Caspase-2

Chain D: 



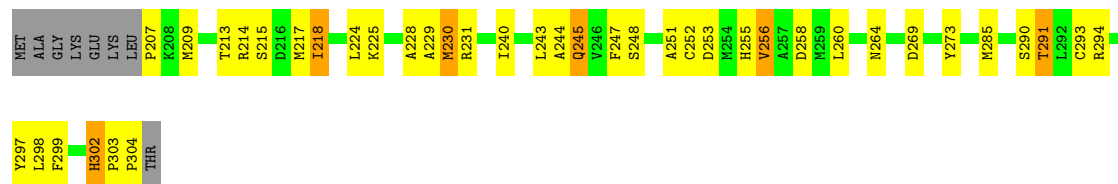
• Molecule 2: Caspase-2

Chain F: 



• Molecule 2: Caspase-2

Chain H: 



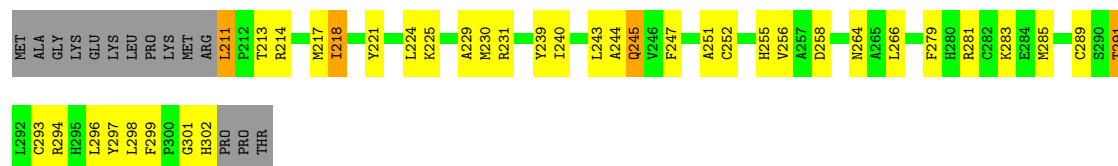
• Molecule 2: Caspase-2

Chain J: 

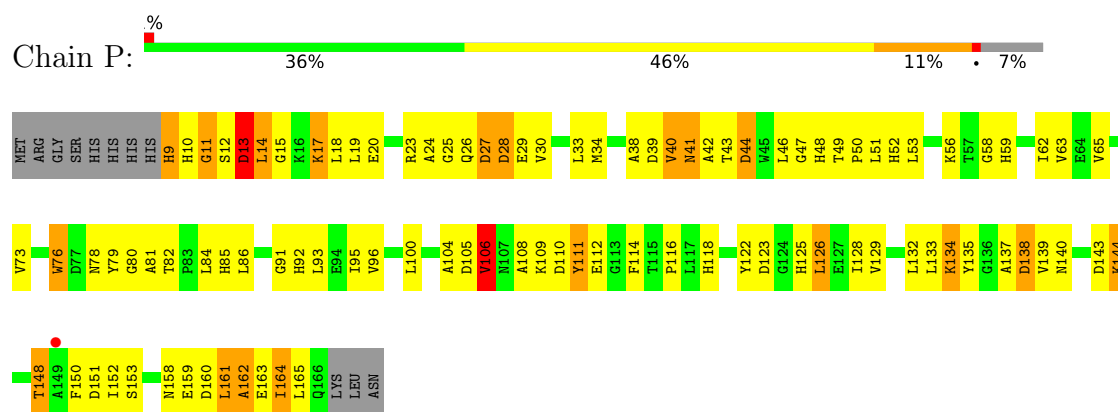


• Molecule 2: Caspase-2

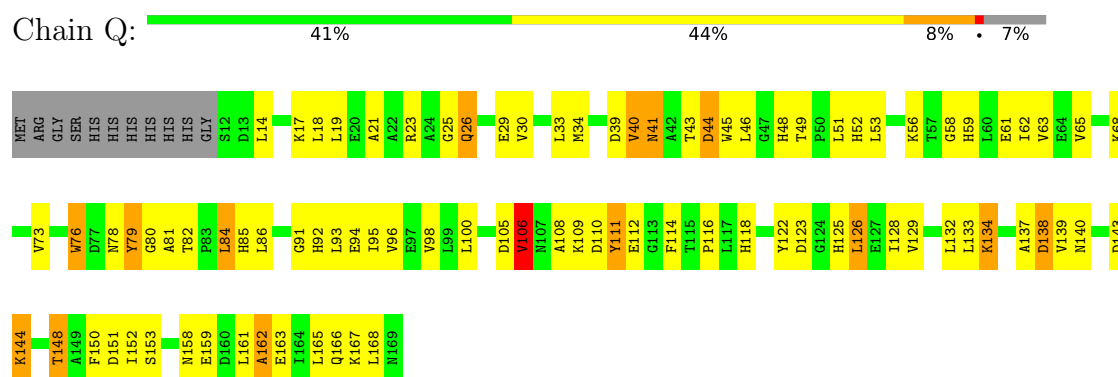
Chain L: 



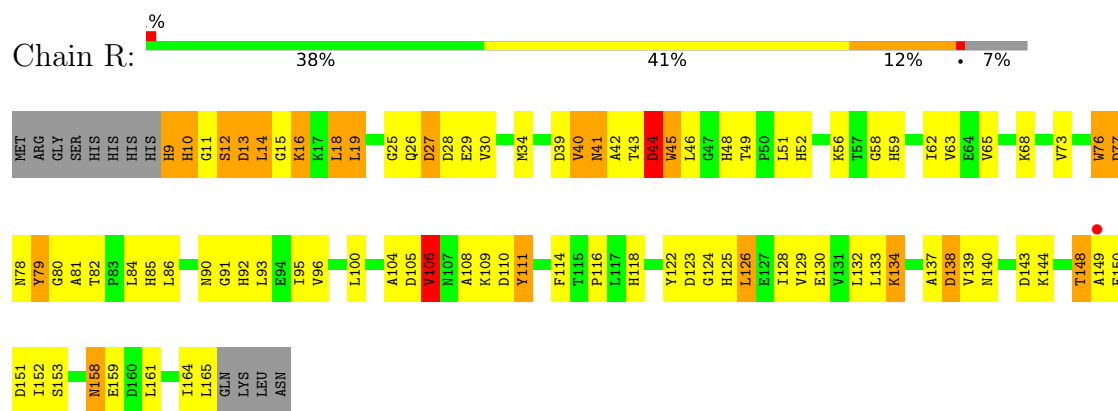
• Molecule 3: Caspase-2



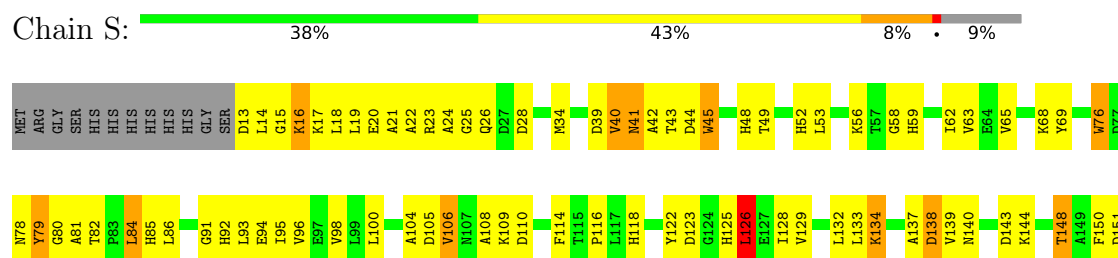
- Molecule 3: Caspase-2



- Molecule 3: Caspase-2

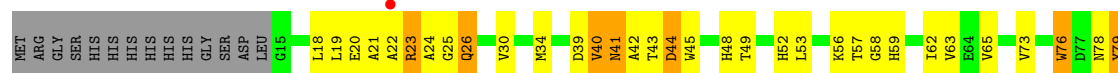


- Molecule 3: Caspase-2

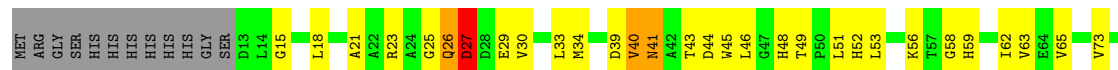




• Molecule 3: Caspase-2



• 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 20.00 – 3.24	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-3.24) 97.8 (20.00-3.24)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	5.90	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.24 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.235 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.50	1/1309 (0.1%)	0.96	6/1769 (0.3%)
1	C	0.50	0/1301	0.99	8/1758 (0.5%)
1	E	0.56	1/1292 (0.1%)	1.03	6/1747 (0.3%)
1	G	0.53	0/1292	0.96	6/1747 (0.3%)
1	I	0.43	0/1269	0.95	3/1716 (0.2%)
1	K	0.43	0/1277	0.95	4/1727 (0.2%)
2	B	0.57	0/778	1.08	7/1047 (0.7%)
2	D	0.49	0/795	0.98	4/1068 (0.4%)
2	F	0.49	0/778	0.97	2/1047 (0.2%)
2	H	0.56	0/795	1.11	5/1069 (0.5%)
2	J	0.43	0/762	1.09	5/1023 (0.5%)
2	L	0.42	0/743	0.96	4/999 (0.4%)
3	P	0.60	2/1231 (0.2%)	0.98	5/1674 (0.3%)
3	Q	0.55	1/1231 (0.1%)	0.92	4/1672 (0.2%)
3	R	0.57	1/1222 (0.1%)	0.95	4/1662 (0.2%)
3	S	0.59	2/1190 (0.2%)	0.93	7/1619 (0.4%)
3	T	0.54	0/1183	0.96	3/1609 (0.2%)
3	U	0.54	1/1199 (0.1%)	0.87	2/1631 (0.1%)
All	All	0.52	9/19647 (0.0%)	0.97	85/26584 (0.3%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	126	LEU	CG-CD2	-7.56	1.27	1.52
3	U	126	LEU	CG-CD2	-7.24	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	LYS	CE-NZ	-6.00	1.31	1.49
3	P	126	LEU	CG-CD2	-5.70	1.33	1.52
3	Q	126	LEU	CG-CD2	-5.29	1.35	1.52
3	P	12	SER	CB-OG	5.20	1.52	1.42
1	E	9	LEU	C-O	5.08	1.31	1.23
3	R	126	LEU	CG-CD2	-5.07	1.35	1.52
3	S	106	VAL	CB-CG1	-5.05	1.35	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	9	LEU	N-CA-C	12.71	126.04	110.41
2	J	274	ALA	CA-C-N	12.28	135.19	119.84
2	J	274	ALA	C-N-CA	12.28	135.19	119.84
2	H	303	PRO	N-CA-C	11.06	124.19	110.70
1	C	152	ILE	N-CA-C	10.21	117.13	106.21
2	B	302	HIS	CA-C-N	9.83	130.51	120.38
2	B	302	HIS	C-N-CA	9.83	130.51	120.38
2	H	291	THR	N-CA-C	-8.54	101.31	112.41
2	H	302	HIS	CA-C-N	8.52	129.15	120.38
2	H	302	HIS	C-N-CA	8.52	129.15	120.38
1	K	157	GLY	N-CA-C	8.49	121.16	110.29
1	G	166	GLN	N-CA-C	8.32	121.79	110.55
1	C	12	LYS	CA-C-N	7.89	128.34	120.52
1	C	12	LYS	C-N-CA	7.89	128.34	120.52
2	D	291	THR	N-CA-C	-7.77	101.73	112.30
3	P	17	LYS	N-CA-C	-7.75	102.84	111.82
3	P	10	HIS	N-CA-C	7.60	120.84	107.61
1	E	28	ARG	N-CA-C	-7.54	98.86	110.10
1	E	10	GLN	N-CA-C	-7.18	95.50	110.80
3	P	24	ALA	N-CA-C	-7.16	104.52	113.18
2	B	291	THR	N-CA-C	-7.15	102.57	112.30
1	I	19	TYR	N-CA-C	-6.87	104.53	113.12
2	J	291	THR	N-CA-C	-6.54	102.67	112.54
2	F	291	THR	N-CA-C	-6.51	103.44	112.30
2	B	303	PRO	N-CA-C	6.49	118.62	110.70
1	A	50	GLU	N-CA-C	-6.26	104.70	112.90
1	A	157	GLY	N-CA-C	6.17	119.62	110.42
3	P	13	ASP	N-CA-C	6.10	123.79	110.80
1	E	156	ARG	N-CA-C	-6.06	105.70	114.12
3	Q	44	ASP	CB-CA-C	-5.90	99.80	111.60
3	R	44	ASP	CB-CA-C	-5.86	99.89	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	79	TYR	N-CA-C	-5.83	106.33	113.50
3	T	144	LYS	CA-CB-CG	5.82	125.75	114.10
3	S	126	LEU	CA-CB-CG	5.71	136.29	116.30
3	S	106	VAL	CG1-CB-CG2	-5.70	98.27	110.80
1	G	75	VAL	N-CA-C	5.66	117.47	108.87
1	C	75	VAL	N-CA-C	5.64	117.44	108.87
1	E	75	VAL	N-CA-C	5.64	117.45	108.87
2	J	290	SER	N-CA-C	5.62	118.39	109.50
1	A	156	ARG	N-CA-C	-5.61	106.32	112.72
1	A	75	VAL	N-CA-C	5.60	117.38	108.87
3	U	79	TYR	N-CA-C	-5.60	106.61	113.50
1	G	12	LYS	CA-C-N	5.54	126.77	119.84
1	G	12	LYS	C-N-CA	5.54	126.77	119.84
2	D	210	ARG	N-CA-C	5.50	117.42	110.33
3	S	44	ASP	CB-CA-C	-5.49	100.63	111.60
3	R	14	LEU	N-CA-C	-5.46	105.33	111.28
3	P	11	GLY	N-CA-C	5.44	126.08	113.18
3	U	126	LEU	CD1-CG-CD2	-5.44	98.84	110.80
1	C	56	GLY	N-CA-C	-5.41	108.17	115.36
1	E	43	VAL	N-CA-C	5.40	116.80	111.67
3	S	45	TRP	N-CA-C	-5.40	106.53	113.01
2	H	229	ALA	N-CA-C	5.38	120.12	113.50
3	T	79	TYR	N-CA-C	-5.37	106.89	113.50
2	D	209	MET	N-CA-C	5.37	117.45	110.53
3	R	79	TYR	N-CA-C	-5.36	106.78	113.38
1	I	75	VAL	N-CA-C	5.36	117.01	108.87
3	S	79	TYR	N-CA-C	-5.35	106.80	113.38
3	R	45	TRP	N-CA-C	-5.35	106.59	113.01
1	K	75	VAL	N-CA-C	5.35	117.00	108.87
1	K	56	GLY	N-CA-C	-5.31	107.99	115.32
3	Q	19	LEU	N-CA-C	5.31	116.75	110.97
2	L	211	LEU	CA-C-N	5.30	125.28	120.03
2	L	211	LEU	C-N-CA	5.30	125.28	120.03
1	A	56	GLY	N-CA-C	-5.25	108.37	115.36
3	S	84	LEU	N-CA-C	-5.25	105.47	111.14
3	S	126	LEU	CD1-CG-CD2	-5.25	99.24	110.80
2	B	210	ARG	N-CA-C	5.21	117.34	109.41
2	B	211	LEU	CA-C-N	5.19	125.47	119.92
2	B	211	LEU	C-N-CA	5.19	125.47	119.92
1	C	152	ILE	CB-CA-C	-5.15	107.45	113.22
1	C	120	GLY	N-CA-C	-5.14	103.72	112.51
2	J	279	PHE	N-CA-C	-5.12	106.88	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	292	LEU	N-CA-C	-5.12	103.77	110.53
2	L	291	THR	N-CA-C	-5.10	104.83	112.54
3	Q	84	LEU	N-CA-C	-5.10	105.63	111.14
2	F	292	LEU	N-CA-C	-5.10	103.80	110.53
3	T	44	ASP	N-CA-CB	5.08	118.69	110.51
1	G	152	ILE	N-CA-C	5.08	114.60	106.88
1	C	45	PHE	N-CA-C	5.05	116.64	108.41
1	I	112	HIS	N-CA-C	-5.05	103.27	110.59
1	A	152	ILE	CB-CA-C	-5.04	106.19	112.45
1	G	50	GLU	N-CA-C	-5.04	108.87	114.62
2	L	279	PHE	N-CA-C	-5.04	106.98	113.23
1	K	46	THR	N-CA-C	5.03	117.73	111.24

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	98	0
1	C	1276	0	1245	96	0
1	E	1267	0	1241	113	0
1	G	1267	0	1241	97	0
1	I	1244	0	1217	108	0
1	K	1252	0	1228	105	0
2	B	760	0	748	48	0
2	D	777	0	768	50	0
2	F	760	0	748	38	0
2	H	776	0	769	41	0
2	J	746	0	734	50	0
2	L	727	0	712	55	0
3	P	1207	0	1162	99	0
3	Q	1209	0	1175	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	1198	0	1154	97	0
3	S	1168	0	1132	92	0
3	T	1161	0	1125	104	0
3	U	1177	0	1140	90	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	1306	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 34.

All (1306) 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
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
2:H:228:ALA:HB3	2:H:230:MET:HE1	1.47	0.94
3:T:25:GLY:HA2	3:T:59:HIS:HD2	1.24	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:17:LYS:HZ2	3:P:33:LEU:HD21	1.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:J:255:HIS:HE1	2:J:258:ASP:CG	1.89	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
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
2:L:255:HIS:HE1	2:L:258:ASP:CG	1.90	0.78
3:U:23:ARG:HB2	3:U:53:LEU:CD1	2.12	0.78
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:17:LYS:NZ	3:P:33:LEU:HD21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:230:MET:HE3	2:F:279:PHE:HD2	1.50	0.75
3:S:163:GLU:C	3:S:164:ILE:HD12	2.10	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
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
2:B:285:MET:HE2	2:D:291:THR:HB	1.71	0.72
3:S:162:ALA:C	3:S:164:ILE:H	1.97	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
3:S:18:LEU:HD23	3:S:19:LEU:HD12	1.72	0.72
3:P:163:GLU:C	3:P:165:LEU:H	1.98	0.71
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: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:P:164:ILE:C	3:P:165:LEU:HD12	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Q:23:ARG:C	3:Q:23:ARG:HD2	2.17	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
2:B:291:THR:HB	2:D:285:MET:HE2	1.75	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:76:TRP:H	3:U:76:TRP:CD1	2.13	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
2:J:255:HIS:CE1	2:J:258:ASP:CG	2.71	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: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
3:Q:76:TRP:CD1	3:Q:76:TRP:H	2.13	0.66
2:F:302:HIS:HA	2:F:303:PRO:C	2.21	0.66
1:K:49:LYS:C	1:K:50:GLU:HG2	2.18	0.66
3:Q:167:LYS:C	3:Q:168:LEU:HD12	2.21	0.65
1:E:27:TYR:CE2	1:E:147:PRO:HB3	2.31	0.65
3:S:49:THR:H	3:S:52:HIS:HB2	1.62	0.65
3:S:76:TRP:CD1	3:S:76:TRP:H	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:PRO:O	1:C:20:GLN:HG2	1.97	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
3:T:76:TRP:H	3:T:76:TRP:CD1	2.15	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:P:76:TRP:H	3:P:76:TRP:CD1	2.15	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:H	3:S:76:TRP:HD1	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)
2:L:255:HIS:CE1	2:L:258:ASP:CG	2.72	0.63
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:CD1	3:U:76:TRP:N	2.64	0.62
1:I:35:GLY:HA2	1:I:102:THR:HB	1.82	0.62
2:J:291:THR:HB	2:L:285:MET:HE2	1.81	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
2:L:229:ALA:C	2:L:230:MET:HE2	2.23	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
1:G:159:GLU:O	1:G:160:THR:C	2.43	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:T:118:HIS:HD1	3:T:143:ASP:HB3	1.65	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
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
1:E:54:ARG:O	1:E:55:SER:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:R:76:TRP:H	3:R:76:TRP:CD1	2.18	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
3:Q:76:TRP:H	3:Q:76:TRP:HD1	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: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:C:26:ALA:O	1:C:27:TYR:C	2.45	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:H	3:U:76:TRP:HD1	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
1:G:95:GLN:O	1:G:96:LEU:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:14:CYS:HB2	1:K:18:PHE:HB2	1.84	0.59
2:B:230:MET:HE3	2:B:230:MET:HA	1.83	0.59
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:T:161:LEU:C	3:T:163:GLU:H	2.09	0.59
3:S:13:ASP:O	3:S:16:LYS:HG2	2.03	0.59
3:T:76:TRP:H	3:T:76:TRP:HD1	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:R:11:GLY:O	3:R:12:SER:C	2.46	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:25:GLY:O	3:Q:26:GLN:C	2.46	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
1:E:53:PHE:C	1:E:55:SER:H	2.11	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:U:46:LEU:C	3:U:78:ASN:OD1	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:76:TRP:H	3:P:76:TRP:HD1	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
2:L:211:LEU:N	2:L:211:LEU:HD12	2.19	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
1:A:95:GLN:O	1:A:96:LEU:C	2.47	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
2:F:285:MET:HE2	2:H:291:THR:HB	1.85	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
2:H:228:ALA:CB	2:H:230:MET:HE1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:76:HIS:O	1:K:77:VAL:HG13	2.05	0.57
1:K:81:GLN:C	1:K:121:VAL:HG22	2.30	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:C:95:GLN:O	1:C:96:LEU:C	2.48	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
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
1:G:19:TYR:CD1	1:G:19:TYR:C	2.83	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:E:95:GLN:O	1:E:96:LEU:C	2.48	0.56
1:I:81:GLN:O	1:I:121:VAL:HG22	2.05	0.56
2:D:293:CYS:C	2:D:294:ARG:HG3	2.31	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
3:T:34:MET:HE3	3:T:34:MET:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:230:MET:HE2	2:L:230:MET:N	2.21	0.55
3:R:76:TRP:H	3:R:76:TRP:HD1	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
3:P:14:LEU:CG	3:P:38:ALA:HA	2.34	0.55
1:C:76:HIS:O	1:C:77:VAL:HG13	2.06	0.55
1:C:81:GLN:C	1:C:121:VAL:HG22	2.31	0.55
3:Q:105:ASP:HB3	3:Q:108:ALA:HB2	1.89	0.55
2:H:293:CYS:C	2:H:294:ARG:HG3	2.32	0.55
2:J:255:HIS:ND1	2:J:258:ASP:HB2	2.22	0.55
2:H:245:GLN:HG3	3:S:45:TRP:HB2	1.88	0.55
1:I:19:TYR:CD1	1:I:19:TYR:C	2.84	0.55
2:L:218:ILE:O	2:L:218:ILE:HG23	2.07	0.55
3:Q:161:LEU:C	3:Q:163:GLU:H	2.14	0.55
1:I:95:GLN:O	1:I:96:LEU:C	2.50	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:G:81:GLN:C	1:G:121:VAL:HG22	2.32	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
3:T:40:VAL:HG22	3:T:40:VAL:O	2.05	0.55
1:C:8:CYS:HA	1:C:10:GLN:HE22	1.72	0.55
3:Q:34:MET:HA	3:Q:34:MET:HE3	1.89	0.55
3:T:23:ARG:HD2	3:T:23:ARG:O	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:GLN:O	1:E:121:VAL:HG22	2.06	0.55
1:E:80:ASP:HA	1:E:121:VAL:HG11	1.89	0.54
1:A:46:THR:O	1:A:47:GLY:C	2.50	0.54
1:A:163:GLY:C	2:D:210:ARG:NH1	2.65	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:P:139:VAL:HG22	3:P:139:VAL:O	2.06	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:A:19:TYR:CD1	1:A:19:TYR:C	2.85	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:80:GLY:HA3	3:T:111:TYR:HD1	1.72	0.54
3:T:118:HIS:ND1	3:T:143:ASP:HB3	2.22	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
1:A:71:LEU:HD22	2:B:298:LEU:HD13	1.90	0.54
1:A:81:GLN:C	1:A:121:VAL:HG22	2.33	0.54
3:P:34:MET:HE3	3:P:34:MET:HA	1.89	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:84:LEU:HD23	3:Q:116:PRO:HG2	1.90	0.54
3:T:23:ARG:NH1	3:T:57:THR:HG22	2.23	0.54
1:K:156:ARG:HH21	2:L:224:LEU:C	2.15	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
3:R:118:HIS:HD1	3:R:143:ASP:HB3	1.73	0.53
1:I:71:LEU:HD22	2:J:298:LEU:HD13	1.90	0.53
1:I:81:GLN:C	1:I:121:VAL:HG22	2.33	0.53
1:C:27:TYR:HD2	1:C:147:PRO:HD3	1.65	0.53
2:D:255:HIS:CE1	2:D:258:ASP:CG	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:H:255:HIS:CE1	2:H:258:ASP:CG	2.86	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
1:E:81:GLN:C	1:E:121:VAL:HG22	2.34	0.53
3:R:25:GLY:CA	3:R:59:HIS:CD2	2.91	0.53
1:G:19:TYR:C	1:G:21:THR:H	2.16	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
3:P:13:ASP:CG	3:P:14:LEU:N	2.66	0.53
3:P:29:GLU:N	3:P:29:GLU:CD	2.66	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:T:39:ASP:C	3:T:41:ASN:H	2.17	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
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
2:J:293:CYS:C	2:J:294:ARG:HG3	2.34	0.53
1:E:46:THR:OG1	1:E:47:GLY:N	2.41	0.53
2:F:293:CYS:C	2:F:294:ARG:HG3	2.34	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:95:GLN:O	1:K:96:LEU:C	2.51	0.52
1:K:44:HIS:N	1:K:80:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:156:ARG:NH2	2:L:224:LEU:C	2.67	0.52
1:A:100:ARG:HD2	3:S:159:GLU:CD	2.35	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
2:L:293:CYS:C	2:L:294:ARG:HG3	2.35	0.52
2:D:225:LYS:HD3	2:D:225:LYS:C	2.34	0.52
1:E:19:TYR:C	1:E:21:THR:H	2.17	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
2:F:291:THR:HB	2:H:285:MET:HE2	1.90	0.52
3:P:163:GLU:C	3:P:165:LEU:N	2.67	0.52
1:C:12:LYS:O	2:D:252:CYS:HB3	2.09	0.52
2:D:230:MET:HE2	2:D:282:CYS:SG	2.50	0.52
3:R:25:GLY:HA2	3:R:62:ILE:CD1	2.40	0.52
3:R:39:ASP:C	3:R:41:ASN:H	2.18	0.52
3:S:139:VAL:O	3:S:139:VAL:HG22	2.08	0.52
1:I:42:ASN:C	1:I:54:ARG:HH21	2.18	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: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
3:U:58:GLY:HA2	3:U:92:HIS:HD2	1.74	0.52
3:U:148:THR:C	3:U:150:PHE:H	2.18	0.52
2:B:293:CYS:C	2:B:294:ARG:HG3	2.35	0.52
1:G:153:GLN:NE2	2:H:240:ILE:HG12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:136:ASP:HB2	2:J:213:THR:O	2.10	0.51
3:P:159:GLU:C	3:P:161:LEU:H	2.18	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:A:163:GLY:C	2:D:210:ARG:HH11	2.19	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:R:138:ASP:C	3:R:140:ASN:H	2.19	0.51
2:J:225:LYS:HD3	2:J:225:LYS:C	2.36	0.51
3:P:138:ASP:C	3:P:140:ASN:H	2.19	0.51
3:S:34:MET:HE3	3:S:34:MET:HA	1.93	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
3:P:39:ASP:C	3:P:41:ASN:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:T:125:HIS:HB3	3:T:128:ILE:HG13	1.93	0.50
2:L:225:LYS:HD3	2:L:225:LYS:C	2.37	0.50
1:A:120:GLY:C	1:A:122:ASP:N	2.68	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:K:29:LEU:N	1:K:29:LEU:CD2	2.75	0.50
1:K:160:THR:O	1:K:161:ASP:C	2.55	0.50
2:B:255:HIS:CE1	2:B:258:ASP:CG	2.88	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
3:S:39:ASP:C	3:S:41:ASN:H	2.19	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
2:J:214:ARG:HG3	2:J:217:MET:HE3	1.93	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:161:LEU:C	3:Q:163:GLU:N	2.69	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: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
3:S:40:VAL:O	3:S:40:VAL:HG22	2.12	0.50
3:S:163:GLU:O	3:S:164:ILE:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:27:ASP:OD1	3:U:62:ILE:HG12	2.11	0.50
2:B:298:LEU:O	2:B:299:PHE:C	2.54	0.49
3:Q:23:ARG:HD2	3:Q:23:ARG:O	2.11	0.49
1:G:42:ASN:ND2	1:G:120:GLY:HA2	2.27	0.49
2:H:225:LYS:HD3	2:H:225:LYS:C	2.37	0.49
3:S:138:ASP:C	3:S:140:ASN:H	2.19	0.49
1:A:40:LEU:HD11	1:A:86:MET:HG2	1.94	0.49
3:P:18:LEU:O	3:P:19:LEU:C	2.54	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:39:ASP:C	3:U:41:ASN:H	2.21	0.49
3:U:118:HIS:ND1	3:U:143:ASP:HB3	2.26	0.49
3:U:148:THR:C	3:U:150:PHE:N	2.67	0.49
3:Q:122:TYR:CE1	3:Q:152:ILE:HD12	2.47	0.49
2:F:230:MET:HE3	2:F:279:PHE:CD2	2.40	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
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
2:B:211:LEU:HA	2:D:283:LYS:HE3	1.94	0.49
1:E:153:GLN:HE22	2:F:239:TYR:HB3	1.76	0.49
2:F:225:LYS:C	2:F:225:LYS:HD3	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Q:139:VAL:HG22	3:Q:139:VAL:O	2.12	0.49
1:G:54:ARG:HG3	1:G:112:HIS:NE2	2.28	0.49
3:S:133:LEU:HA	3:S:137:ALA:CB	2.42	0.49
1:K:23:PHE:O	1:K:24:GLN:C	2.56	0.49
2:L:298:LEU:O	2:L:299:PHE:C	2.56	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:E:120:GLY:C	1:E:122:ASP:N	2.69	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
2:B:225:LYS:HD3	2:B:225:LYS:C	2.38	0.48
3:Q:39:ASP:C	3:Q:41:ASN:H	2.21	0.48
2:F:210:ARG:O	2:F:211:LEU:HD23	2.12	0.48
1:I:120:GLY:C	1:I:122:ASP:N	2.70	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:19:TYR:C	1:E:21:THR:N	2.69	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:T:161:LEU:C	3:T:163:GLU:N	2.70	0.48
3:P:40:VAL:HG22	3:P:40:VAL:O	2.13	0.48
1:E:110:LEU:HA	1:E:153:GLN:O	2.13	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:Q:118:HIS:ND1	3:Q:143:ASP:HB3	2.27	0.48
2:F:214:ARG:HG3	2:F:217:MET:HE3	1.95	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
3:P:148:THR:C	3:P:150:PHE:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:164:VAL:CG2	2:L:213:THR:HA	2.43	0.48
2:J:298:LEU:O	2:J:299:PHE:C	2.56	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
2:D:298:LEU:O	2:D:299:PHE:C	2.55	0.48
1:E:45:PHE:CD2	1:E:51:LEU:HG	2.49	0.48
2:F:255:HIS:CE1	2:F:258:ASP:CG	2.91	0.48
3:R:34:MET:HE3	3:R:34:MET:HA	1.95	0.48
3:S:13:ASP:O	3:S:15:GLY:N	2.46	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
3:R:12:SER:C	3:R:14:LEU:H	2.21	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
3:R:148:THR:C	3:R:150:PHE:N	2.70	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:G:47:GLY:O	1:G:48:GLU:C	2.57	0.48
1:I:47:GLY:C	1:I:49:LYS:H	2.21	0.48
3:T:19:LEU:HD11	3:T:42:ALA:C	2.39	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:138:ASP:C	3:Q:140:ASN:H	2.21	0.48
3:Q:161:LEU:O	3:Q:163:GLU:N	2.46	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:G:46:THR:O	1:G:47:GLY:O	2.32	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
2:D:214:ARG:HG3	2:D:217:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:22:ALA:C	3:T:24:ALA:H	2.22	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
2:F:298:LEU:O	2:F:299:PHE:C	2.57	0.47
1:G:11:VAL:HG22	2:H:248:SER:HA	1.97	0.47
2:H:214:ARG:HG3	2:H:217:MET:HE3	1.95	0.47
1:I:112:HIS:HA	1:I:155:CYS:HG	1.79	0.47
3:P:46:LEU:C	3:P:78:ASN:ND2	2.71	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:214:ARG:HG3	2:B:217:MET:HE3	1.96	0.47
3:P:46:LEU:O	3:P:78:ASN:ND2	2.47	0.47
3:P:160:ASP:C	3:P:161:LEU:HD22	2.40	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:T:148:THR:C	3:T:150:PHE:H	2.23	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
3:T:148:THR:C	3:T:150:PHE:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:80:GLY:HA3	3:U:111:TYR:HD1	1.80	0.47
3:P:159:GLU:C	3:P:161:LEU:N	2.73	0.46
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:148:THR:C	3:S:150:PHE:N	2.71	0.46
1:I:80:ASP:HA	1:I:121:VAL:CG1	2.44	0.46
1:K:22:HIS:O	1:K:23:PHE:C	2.59	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
1:I:41:SER:HA	1:I:110:LEU:O	2.15	0.46
1:I:140:CYS:SG	1:I:140:CYS:O	2.73	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
3:U:138:ASP:C	3:U:140:ASN:H	2.23	0.46
1:A:28:ARG:HG3	1:A:28:ARG:HH11	1.80	0.46
1:C:120:GLY:C	1:C:122:ASP:N	2.71	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
3:T:138:ASP:C	3:T:140:ASN:H	2.22	0.46
1:K:49:LYS:HD2	1:K:50:GLU:H	1.80	0.46
3:P:100:LEU:HD23	3:P:104:ALA:HB3	1.97	0.46
2:H:298:LEU:O	2:H:299:PHE:C	2.58	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:S:148:THR:C	3:S:150:PHE:H	2.24	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:G:55:SER:C	1:G:57:GLY:H	2.22	0.46
1:G:120:GLY:C	1:G:122:ASP:N	2.72	0.46
3:S:162:ALA:C	3:S:164:ILE:N	2.64	0.46
1:I:64:LEU:CD1	1:I:110:LEU:HD21	2.43	0.46
1:I:118:ILE:HG22	1:I:154:ALA:HB2	1.98	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
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:34:MET:HE3	3:U:34:MET:HA	1.97	0.46
3:U:100:LEU:CD2	3:U:106:VAL:HG23	2.35	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:285:MET:CE	2:D:291:THR:HB	2.43	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
1:I:164:VAL:HG12	1:I:165:ASP:H	1.82	0.45
3:U:62:ILE:HA	3:U:65:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:148:THR:C	3:P:150:PHE:H	2.24	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
1:I:47:GLY:C	1:I:49:LYS:N	2.74	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
2:J:230:MET:HE2	2:J:282:CYS:SG	2.57	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
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
3:R:159:GLU:C	3:R:161:LEU:N	2.75	0.45
1:G:79:CYS:O	1:G:80:ASP:C	2.59	0.45
1:A:79:CYS:O	1:A:80:ASP:C	2.59	0.45
3:Q:165:LEU:O	3:Q:167:LYS:N	2.50	0.45
1:E:19:TYR:HH	1:E:30:GLN:CD	2.23	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
3:R:148:THR:C	3:R:150:PHE:H	2.24	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
1:G:36:LEU:CD2	1:G:74:ASP:HB3	2.47	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
1:C:47:GLY:O	1:C:48:GLU:C	2.59	0.45
3:Q:56:LYS:HB2	3:Q:86:LEU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:148:THR:C	3:Q:150:PHE:H	2.25	0.45
3:S:16:LYS:HB3	3:S:42:ALA:HB1	1.99	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: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
1:I:55:SER:C	1:I:57:GLY:H	2.25	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
2:L:214:ARG:HG3	2:L:217:MET:HE3	1.99	0.44
3:P:44:ASP:OD1	3:P:44:ASP:N	2.49	0.44
1:I:40:LEU:C	1:I:40:LEU:HD23	2.42	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
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
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
1:C:53:PHE:O	1:C:53:PHE:CG	2.69	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:Q:148:THR:C	3:Q:150:PHE:N	2.72	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
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: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:39:VAL:O	1:E:39:VAL:HG12	2.18	0.44
1:E:68:PHE:O	1:E:73:TYR:HB2	2.16	0.44
3:R:26:GLN:O	3:R:27:ASP:C	2.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:84:LEU:O	3:Q:85:HIS:C	2.61	0.44
1:G:48:GLU:O	1:G:50:GLU:OE1	2.36	0.44
3:S:138:ASP:C	3:S:140:ASN:N	2.76	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
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
1:C:79:CYS:O	1:C:80:ASP:C	2.61	0.44
3:Q:18:LEU:HD13	3:Q:34:MET:SD	2.58	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:17:LYS:HZ2	3:P:33:LEU:CD2	2.22	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
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
3:P:58:GLY:HA2	3:P:92:HIS:CD2	2.47	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
1:E:166:GLN:NE2	2:H:209:MET:HE2	2.33	0.43
3:R:138:ASP:C	3:R:140:ASN:N	2.75	0.43
1:G:86:MET:O	1:G:90:LEU:HB2	2.18	0.43
1:K:79:CYS:O	1:K:80:ASP:C	2.62	0.43
1:K:163:GLY:C	1:K:164:VAL:HG22	2.44	0.43
3:Q:62:ILE:HA	3:Q:65:VAL:CG1	2.48	0.43
1:E:32:ARG:HA	1:E:33:PRO:C	2.43	0.43
3:R:12:SER:C	3:R:14:LEU:N	2.77	0.43
3:R:82:THR:N	3:R:85:HIS:ND1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:S:163:GLU:O	3:S:163:GLU:HG2	2.18	0.43
3:T:148:THR:O	3:T:152:ILE:HG12	2.18	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
1:G:19:TYR:C	1:G:21:THR:N	2.73	0.43
1:G:40:LEU:C	1:G:40:LEU:HD23	2.43	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
1:A:82:THR:O	1:A:83:ALA:C	2.62	0.43
3:P:138:ASP:C	3:P:140:ASN:N	2.76	0.43
1:C:140:CYS:SG	1:C:140:CYS:O	2.76	0.43
3:Q:138:ASP:C	3:Q:140:ASN:N	2.77	0.43
1:I:79:CYS:O	1:I:80:ASP:C	2.62	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
2:L:211:LEU:N	2:L:211:LEU:CD1	2.80	0.43
1:A:32:ARG:HA	1:A:33:PRO:C	2.44	0.43
1:A:37:ALA:HA	1:A:106:ILE:O	2.19	0.43
3:P:161:LEU:HD22	3:P:161:LEU:N	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
2:B:291:THR:HB	2:D:285:MET:CE	2.44	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
1:K:160:THR:O	1:K:160:THR:HG22	2.19	0.42
3:Q:34:MET:HA	3:Q:34:MET:CE	2.48	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
1:K:32:ARG:HA	1:K:33:PRO:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:120:GLY:C	1:K:122:ASP:N	2.71	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: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:A:120:GLY:C	1:A:122:ASP:H	2.27	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
1:E:17:GLU:C	1:E:19:TYR:H	2.27	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:N	2.78	0.42
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
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
1:G:29:LEU:CD2	1:G:34:ARG:HG2	2.47	0.42
1:I:32:ARG:HA	1:I:33:PRO:C	2.44	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
3:S:13:ASP:C	3:S:15:GLY:N	2.77	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:K:158:ASP:O	1:K:159:GLU:C	2.63	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:C:40:LEU:HD23	1:C:40:LEU:C	2.45	0.42
1:G:32:ARG:HA	1:G:33:PRO:C	2.44	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
3:T:162:ALA:O	3:T:163:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HG12	1:A:54:ARG:HB2	2.02	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: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
1:I:55:SER:C	1:I:57:GLY:N	2.78	0.42
2:B:273:TYR:CB	3:P:79:TYR:CE2	2.90	0.41
1:C:32:ARG:HA	1:C:33:PRO:C	2.44	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
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
1:E:109:LEU:C	1:E:110:LEU:HD12	2.45	0.41
1:A:39:VAL:O	1:A:39:VAL:HG12	2.21	0.41
1:A:86:MET:O	1:A:90:LEU:HB2	2.20	0.41
2:D:303:PRO:HA	2:D:304:PRO:HD3	1.78	0.41
3:Q:159:GLU:OE2	1:E:100:ARG:NH1	2.44	0.41
1:E:79:CYS:O	1:E:80:ASP:C	2.63	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:82:THR:HG23	1:G:85:GLU:OE1	2.20	0.41
3:S:40:VAL:HG11	3:S:69:TYR:O	2.19	0.41
3:S:125:HIS:O	3:S:126:LEU:C	2.63	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
3:U:125:HIS:O	3:U:126:LEU:C	2.63	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:14:LEU:C	3:R:16:LYS:H	2.28	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
2:J:288:TYR:CD1	2:J:288:TYR:C	2.98	0.41
1:A:22:HIS:O	1:A:25:LEU:HD23	2.20	0.41
3:Q:110:ASP:OD1	3:Q:114:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ALA:O	1:E:141:PRO:HD3	2.21	0.41
1:K:15:THR:C	1:K:17:GLU:H	2.28	0.41
3:U:26:GLN:HB3	3:U:29:GLU:CB	2.43	0.41
2:B:288:TYR:CD1	2:B:288:TYR:C	2.98	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
1:C:82:THR:O	1:C:83:ALA:C	2.62	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
1:K:16:PRO:HA	2:L:302:HIS:CE1	2.52	0.41
1:K:82:THR:O	1:K:83:ALA:C	2.64	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
1:C:46:THR:O	1:C:47:GLY:C	2.64	0.41
1:E:35:GLY:HA2	1:E:102:THR:CB	2.48	0.41
1:E:120:GLY:C	1:E:122:ASP:H	2.28	0.41
1:G:54:ARG:NH2	1:G:110:LEU:C	2.79	0.41
1:G:55:SER:C	1:G:57:GLY:N	2.78	0.41
3:S:84:LEU:O	3:S:85:HIS:C	2.64	0.41
1:K:67:LEU:CD2	2:L:244:ALA:HA	2.50	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:27:ASP:O	3:P:28:ASP:C	2.64	0.41
3:P:30:VAL:HG11	3:P:62:ILE:HG23	2.03	0.41
3:P:162:ALA:C	3:P:164:ILE:H	2.28	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:E:82:THR:O	1:E:83:ALA:C	2.64	0.41
1:G:156:ARG:HB2	2:H:224:LEU:O	2.21	0.41
1:I:82:THR:O	1:I:83:ALA:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:285:MET:HE2	2:L:291:THR:HB	2.03	0.41
1:K:15:THR:C	1:K:17:GLU:N	2.79	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
1:I:82:THR:HG23	1:I:85:GLU:OE1	2.21	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
2:B:213:THR:HG1	1:C:161:ASP:CG	2.27	0.40
3:R:159:GLU:C	3:R:161:LEU:H	2.28	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
3:P:152:ILE:HG22	3:P:152:ILE:O	2.21	0.40
3:Q:73:VAL:O	3:Q:73:VAL:HG22	2.20	0.40
1:G:9:LEU:HD23	1:G:10:GLN:N	2.37	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
3:S:78:ASN:N	3:S:78:ASN:ND2	2.68	0.40
1:I:19:TYR:C	1:I:21:THR:H	2.28	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
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
1:C:83:ALA:HA	1:C:86:MET:HE3	2.03	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
3:R:148:THR:O	3:R:150:PHE:N	2.54	0.40
1:G:82:THR:O	1:G:83:ALA:C	2.63	0.40
3:S:148:THR:O	3:S:152:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:239:TYR:O	2:J:243:LEU:HB2	2.21	0.40
3:T:84:LEU:O	3:T:85:HIS:C	2.63	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:245:GLN:CD	3:U:45:TRP:HB2	2.46	0.40
2:L:255:HIS:HB3	2:L:297:TYR:CE1	2.57	0.40
3:U:138:ASP:C	3:U:140:ASN:N	2.78	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:40:LEU:C	1:E:40:LEU:HD23	2.47	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:120:GLY:C	1:I:122:ASP:H	2.29	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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/169 (95%)	135 (84%)	21 (13%)	4 (2%)	4	24
1	C	159/169 (94%)	128 (80%)	26 (16%)	5 (3%)	3	19
1	E	158/169 (94%)	127 (80%)	26 (16%)	5 (3%)	3	19
1	G	158/169 (94%)	128 (81%)	24 (15%)	6 (4%)	2	15
1	I	155/169 (92%)	120 (77%)	28 (18%)	7 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	156/169 (92%)	125 (80%)	21 (14%)	10 (6%)	1	7
2	B	85/106 (80%)	74 (87%)	7 (8%)	4 (5%)	2	12
2	D	96/106 (91%)	89 (93%)	5 (5%)	2 (2%)	5	27
2	F	94/106 (89%)	88 (94%)	4 (4%)	2 (2%)	5	27
2	H	96/106 (91%)	85 (88%)	8 (8%)	3 (3%)	3	19
2	J	92/106 (87%)	83 (90%)	5 (5%)	4 (4%)	2	14
2	L	90/106 (85%)	80 (89%)	7 (8%)	3 (3%)	3	18
3	P	156/169 (92%)	117 (75%)	26 (17%)	13 (8%)	0	4
3	Q	156/169 (92%)	121 (78%)	26 (17%)	9 (6%)	1	9
3	R	155/169 (92%)	124 (80%)	21 (14%)	10 (6%)	1	7
3	S	151/169 (89%)	117 (78%)	27 (18%)	7 (5%)	2	12
3	T	150/169 (89%)	113 (75%)	28 (19%)	9 (6%)	1	8
3	U	152/169 (90%)	119 (78%)	27 (18%)	6 (4%)	2	15
All	All	2419/2664 (91%)	1973 (82%)	337 (14%)	109 (4%)	2	13

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	130 (92%)	12 (8%)	10	34
1	C	141/147 (96%)	131 (93%)	10 (7%)	13	42
1	E	140/147 (95%)	128 (91%)	12 (9%)	10	34
1	G	140/147 (95%)	132 (94%)	8 (6%)	18	49
1	I	137/147 (93%)	127 (93%)	10 (7%)	13	41
1	K	138/147 (94%)	129 (94%)	9 (6%)	15	45
2	B	81/89 (91%)	78 (96%)	3 (4%)	30	59
2	D	83/89 (93%)	80 (96%)	3 (4%)	31	60
2	F	81/89 (91%)	76 (94%)	5 (6%)	16	46
2	H	83/89 (93%)	79 (95%)	4 (5%)	23	53
2	J	79/89 (89%)	78 (99%)	1 (1%)	61	75
2	L	77/89 (86%)	76 (99%)	1 (1%)	61	75
3	P	122/132 (92%)	108 (88%)	14 (12%)	5	23
3	Q	123/132 (93%)	111 (90%)	12 (10%)	7	29
3	R	121/132 (92%)	102 (84%)	19 (16%)	2	12
3	S	118/132 (89%)	104 (88%)	14 (12%)	5	22
3	T	117/132 (89%)	105 (90%)	12 (10%)	7	27
3	U	119/132 (90%)	107 (90%)	12 (10%)	7	28
All	All	2042/2208 (92%)	1881 (92%)	161 (8%)	11	38

All (161) 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	28	ARG
1	A	29	LEU
1	A	34	ARG
1	A	75	VAL
1	A	110	LEU
1	A	156	ARG
1	A	158	ASP
1	A	164	VAL
1	A	166	GLN
2	B	211	LEU
2	B	230	MET
2	B	245	GLN
3	P	9	HIS
3	P	41	ASN
3	P	44	ASP
3	P	76	TRP
3	P	106	VAL
3	P	109	LYS
3	P	123	ASP
3	P	134	LYS
3	P	144	LYS
3	P	148	THR
3	P	151	ASP
3	P	153	SER
3	P	158	ASN
3	P	161	LEU
1	C	9	LEU
1	C	25	LEU
1	C	34	ARG
1	C	50	GLU
1	C	75	VAL
1	C	110	LEU
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

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Mol	Chain	Res	Type
3	Q	17	LYS
3	Q	41	ASN
3	Q	68	LYS
3	Q	76	TRP
3	Q	106	VAL
3	Q	109	LYS
3	Q	123	ASP
3	Q	134	LYS
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	11	VAL
1	E	23	PHE
1	E	24	GLN
1	E	34	ARG
1	E	51	LEU
1	E	52	GLU
1	E	75	VAL
1	E	110	LEU
1	E	164	VAL
2	F	209	MET
2	F	230	MET
2	F	245	GLN
2	F	290	SER
2	F	304	PRO
3	R	9	HIS
3	R	13	ASP
3	R	18	LEU
3	R	19	LEU
3	R	27	ASP
3	R	28	ASP
3	R	41	ASN
3	R	44	ASP
3	R	68	LYS
3	R	76	TRP
3	R	77	ASP
3	R	106	VAL
3	R	109	LYS

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Mol	Chain	Res	Type
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	9	LEU
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	110	LEU
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	68	LYS
3	S	76	TRP
3	S	106	VAL
3	S	109	LYS
3	S	123	ASP
3	S	134	LYS
3	S	144	LYS
3	S	148	THR
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	34	ARG
1	I	51	LEU
1	I	54	ARG
1	I	75	VAL
1	I	159	GLU

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Mol	Chain	Res	Type
2	J	245	GLN
3	T	41	ASN
3	T	44	ASP
3	T	76	TRP
3	T	105	ASP
3	T	106	VAL
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	34	ARG
1	K	43	VAL
1	K	50	GLU
1	K	75	VAL
1	K	110	LEU
1	K	153	GLN
1	K	164	VAL
2	L	245	GLN
3	U	26	GLN
3	U	27	ASP
3	U	41	ASN
3	U	44	ASP
3	U	76	TRP
3	U	106	VAL
3	U	123	ASP
3	U	126	LEU
3	U	134	LYS
3	U	144	LYS
3	U	148	THR
3	U	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	76	HIS
1	A	112	HIS

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Mol	Chain	Res	Type
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	140	ASN
3	P	158	ASN
3	P	166	GLN
1	C	10	GLN
1	C	22	HIS
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	112	HIS
1	E	166	GLN
2	F	245	GLN
2	F	255	HIS
3	R	10	HIS
3	R	36	ASN
3	R	41	ASN
3	R	59	HIS
3	R	78	ASN
3	R	118	HIS
3	R	140	ASN
1	G	10	GLN
1	G	20	GLN
1	G	76	HIS
1	G	92	ASN
1	G	95	GLN
1	G	153	GLN
2	H	245	GLN
2	H	255	HIS

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Mol	Chain	Res	Type
3	S	36	ASN
3	S	41	ASN
3	S	78	ASN
3	S	92	HIS
3	S	118	HIS
3	S	140	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	118	HIS
3	T	140	ASN
3	T	158	ASN
1	K	10	GLN
1	K	76	HIS
1	K	92	ASN
1	K	112	HIS
1	K	145	ASN
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	140	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	162/169 (95%)	-0.35	0 100 100	41, 83, 113, 125	0
1	C	161/169 (95%)	-0.37	0 100 100	37, 81, 105, 121	0
1	E	160/169 (94%)	-0.29	0 100 100	49, 88, 122, 142	0
1	G	160/169 (94%)	-0.31	0 100 100	36, 78, 105, 121	0
1	I	157/169 (92%)	-0.32	0 100 100	52, 91, 142, 160	0
1	K	158/169 (93%)	-0.21	0 100 100	55, 92, 156, 176	0
2	B	96/106 (90%)	-0.43	2 (2%) 63 43	31, 72, 128, 136	0
2	D	98/106 (92%)	-0.35	0 100 100	35, 71, 125, 135	0
2	F	96/106 (90%)	-0.42	0 100 100	29, 73, 127, 136	0
2	H	98/106 (92%)	-0.38	0 100 100	33, 71, 126, 136	0
2	J	94/106 (88%)	-0.33	0 100 100	50, 75, 129, 136	0
2	L	92/106 (86%)	-0.33	0 100 100	49, 74, 122, 137	0
3	P	158/169 (93%)	-0.03	1 (0%) 85 73	57, 106, 181, 191	0
3	Q	158/169 (93%)	-0.09	0 100 100	64, 106, 177, 186	0
3	R	157/169 (92%)	-0.17	1 (0%) 85 73	63, 107, 178, 186	0
3	S	153/169 (90%)	-0.14	0 100 100	67, 110, 177, 186	0
3	T	152/169 (89%)	0.05	1 (0%) 84 70	70, 112, 183, 191	0
3	U	154/169 (91%)	-0.22	0 100 100	66, 110, 182, 196	0
All	All	2464/2664 (92%)	-0.25	5 (0%) 91 85	29, 91, 168, 196	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	149	ALA	3.4
2	B	226	GLY	2.5
3	T	22	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	P	149	ALA	2.1
2	B	244	ALA	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.