



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:16 PM UTC

PDB ID : 4BI5 / pdb_00004bi5
Title : CRYSTAL STRUCTURE OF A DOUBLE MUTANT (C202A AND C222D) OF TRIOSEPHOSPHATE ISOMERASE FROM GIARDIA LAMBLIA.
Authors : Torres-Larios, A.; Enriquez-Flores, S.; Reyes-Vivas, H.; Oria-Hernandez, J.; Hernandez-Alcantara, G.
Deposited on : 2013-04-09
Resolution : 2.70 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

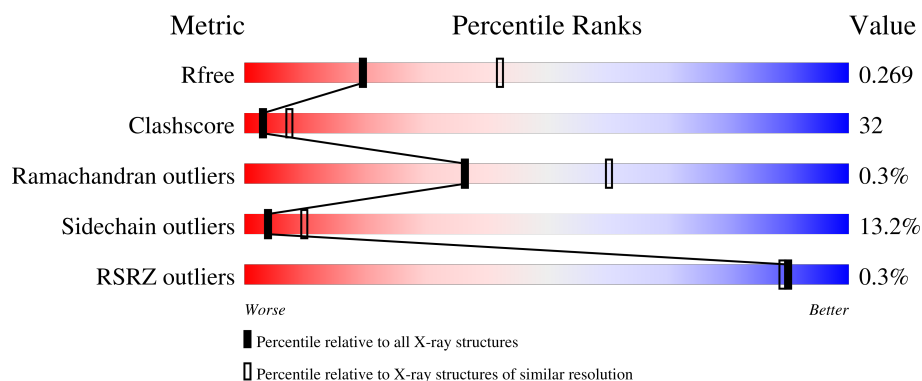
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



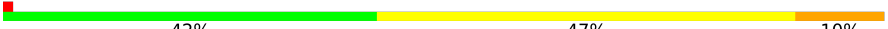
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	255	55% 36% 8%
1	B	255	61% 33% 5%
1	C	255	53% 38% 8%
1	D	255	55% 35% 9%
1	E	255	49% 42% 9%

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Mol	Chain	Length	Quality of chain
1	F	255	
1	G	255	
1	H	255	
1	I	255	
1	J	255	
1	K	255	
1	L	255	
1	M	255	
1	N	255	
1	O	255	
1	P	255	
1	Q	255	
1	R	255	
1	S	255	
1	T	255	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 38560 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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	B	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	C	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	D	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	E	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	F	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	G	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	H	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	I	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	J	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	K	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	L	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	M	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	N	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	O	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	P	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	254	Total 1928	C 1212	N 341	O 364	S 11	0	0	0
1	R	254	Total 1928	C 1212	N 341	O 364	S 11	0	0	0
1	S	254	Total 1928	C 1212	N 341	O 364	S 11	0	0	0
1	T	254	Total 1928	C 1212	N 341	O 364	S 11	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	CYS	engineered mutation	UNP P36186
A	222	ASP	CYS	engineered mutation	UNP P36186
B	202	ALA	CYS	engineered mutation	UNP P36186
B	222	ASP	CYS	engineered mutation	UNP P36186
C	202	ALA	CYS	engineered mutation	UNP P36186
C	222	ASP	CYS	engineered mutation	UNP P36186
D	202	ALA	CYS	engineered mutation	UNP P36186
D	222	ASP	CYS	engineered mutation	UNP P36186
E	202	ALA	CYS	engineered mutation	UNP P36186
E	222	ASP	CYS	engineered mutation	UNP P36186
F	202	ALA	CYS	engineered mutation	UNP P36186
F	222	ASP	CYS	engineered mutation	UNP P36186
G	202	ALA	CYS	engineered mutation	UNP P36186
G	222	ASP	CYS	engineered mutation	UNP P36186
H	202	ALA	CYS	engineered mutation	UNP P36186
H	222	ASP	CYS	engineered mutation	UNP P36186
I	202	ALA	CYS	engineered mutation	UNP P36186
I	222	ASP	CYS	engineered mutation	UNP P36186
J	202	ALA	CYS	engineered mutation	UNP P36186
J	222	ASP	CYS	engineered mutation	UNP P36186
K	202	ALA	CYS	engineered mutation	UNP P36186
K	222	ASP	CYS	engineered mutation	UNP P36186
L	202	ALA	CYS	engineered mutation	UNP P36186
L	222	ASP	CYS	engineered mutation	UNP P36186
M	202	ALA	CYS	engineered mutation	UNP P36186
M	222	ASP	CYS	engineered mutation	UNP P36186
N	202	ALA	CYS	engineered mutation	UNP P36186
N	222	ASP	CYS	engineered mutation	UNP P36186
O	202	ALA	CYS	engineered mutation	UNP P36186
O	222	ASP	CYS	engineered mutation	UNP P36186
P	202	ALA	CYS	engineered mutation	UNP P36186

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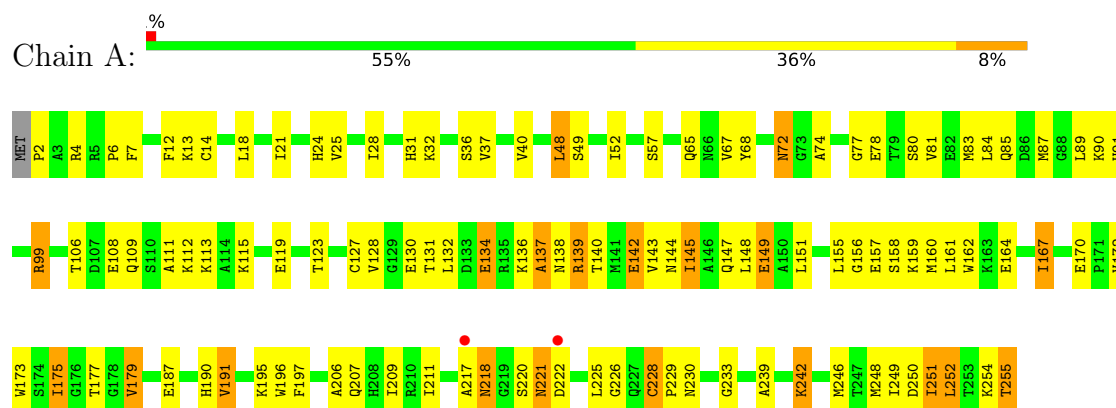
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Chain	Residue	Modelled	Actual	Comment	Reference
P	222	ASP	CYS	engineered mutation	UNP P36186
Q	202	ALA	CYS	engineered mutation	UNP P36186
Q	222	ASP	CYS	engineered mutation	UNP P36186
R	202	ALA	CYS	engineered mutation	UNP P36186
R	222	ASP	CYS	engineered mutation	UNP P36186
S	202	ALA	CYS	engineered mutation	UNP P36186
S	222	ASP	CYS	engineered mutation	UNP P36186
T	202	ALA	CYS	engineered mutation	UNP P36186
T	222	ASP	CYS	engineered mutation	UNP P36186

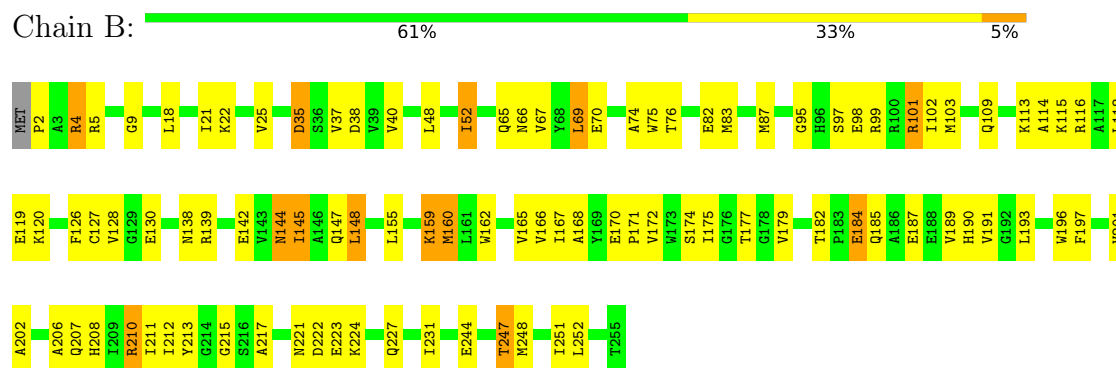
3 Residue-property plots [i](#)

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.

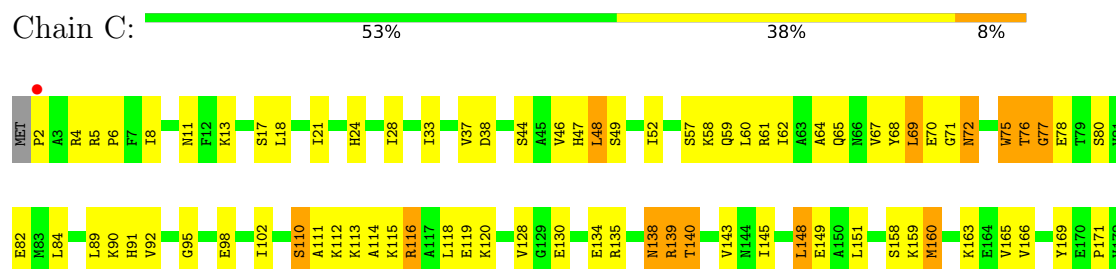
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



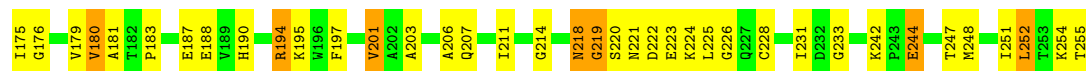
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE





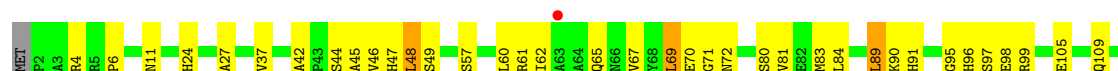
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain D: 55% 35% 9%



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain E: 49% 42% 9%



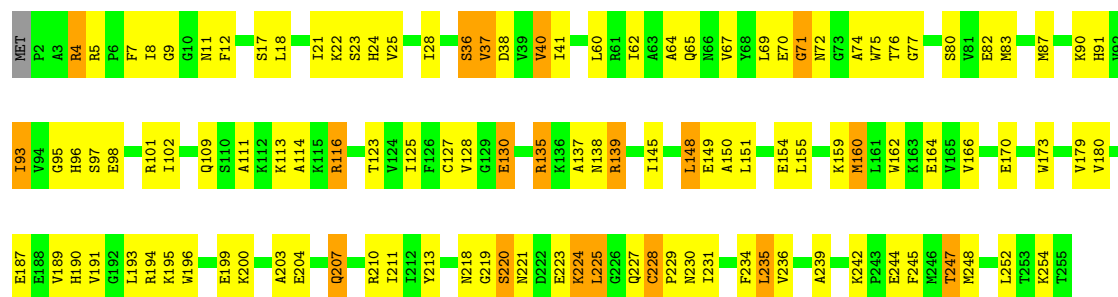
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain F: 57% 36% 6%



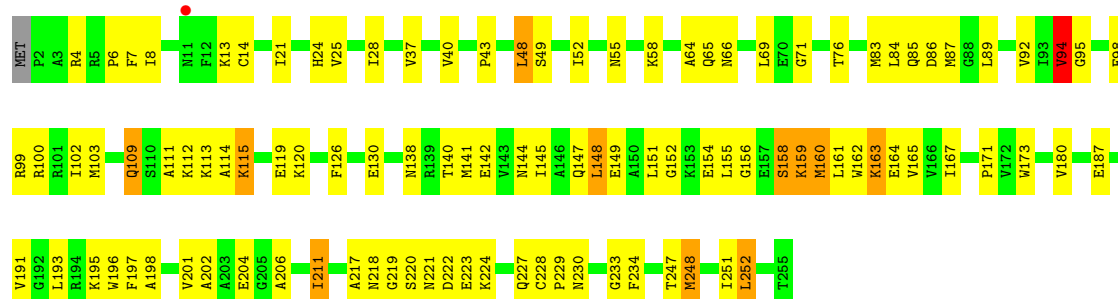
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain G: 55% 38% 7%



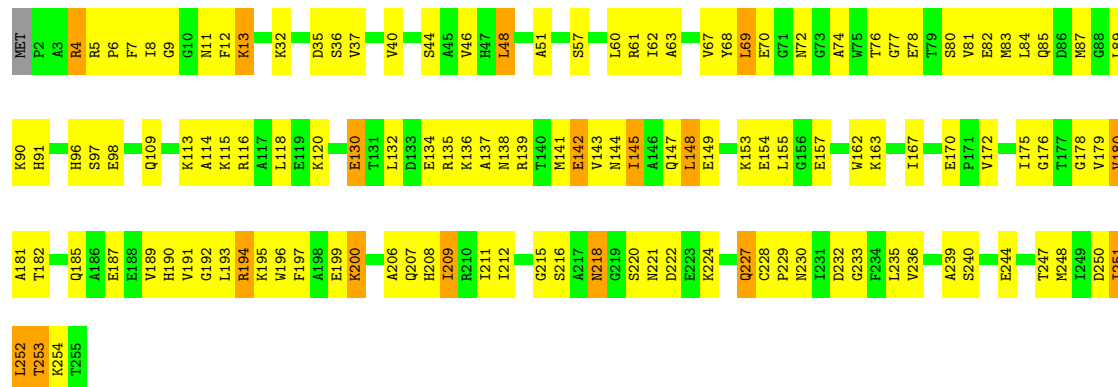
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain H: 59% 36%



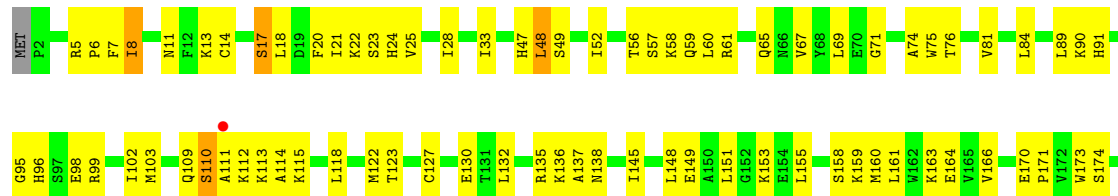
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain I: 49% 44% 7%



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

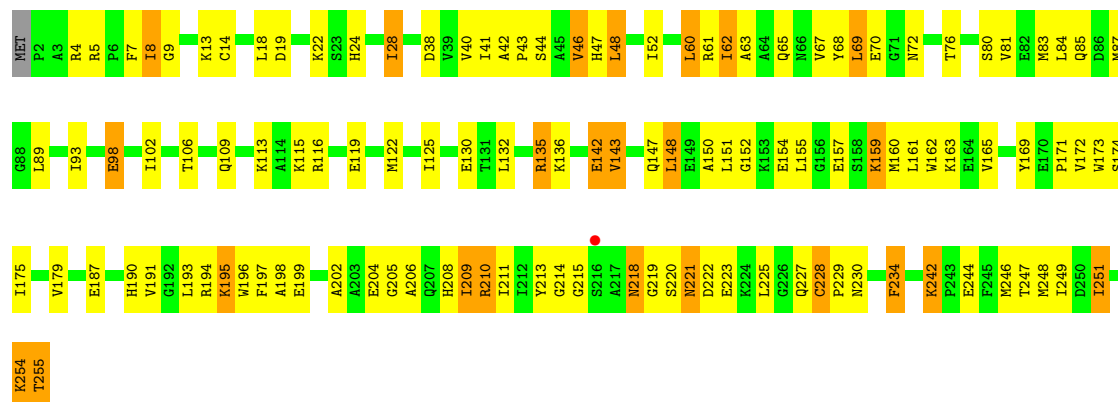
Chain J: 54% 42%





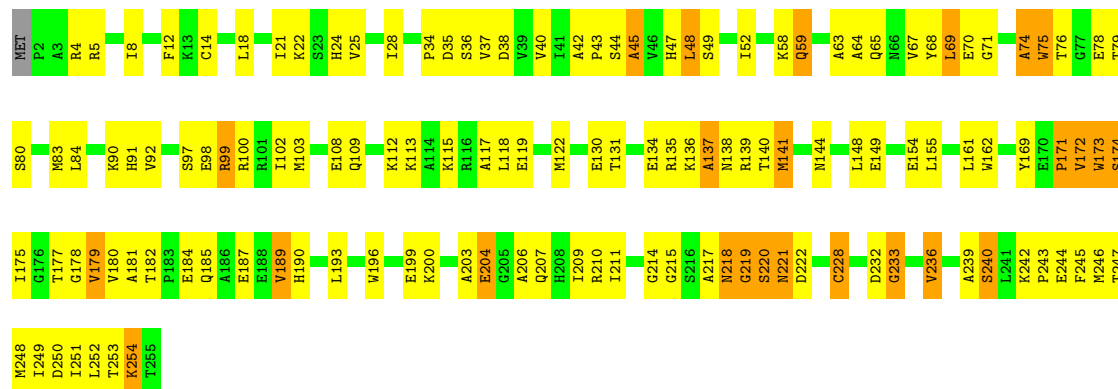
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain K: 53% 38% 9%



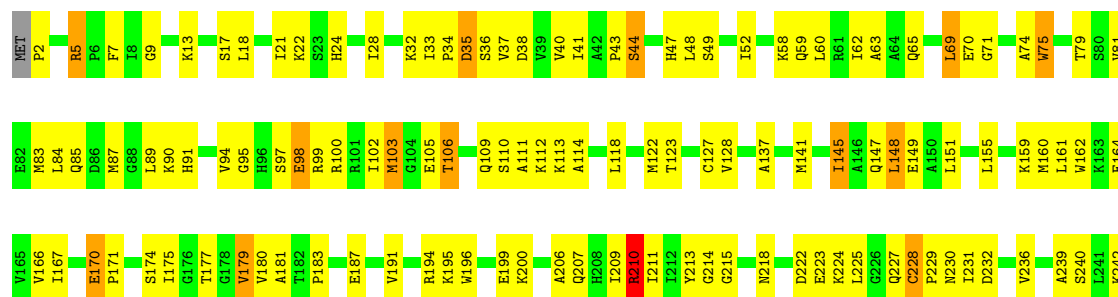
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain L: 47% 42% 10%



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

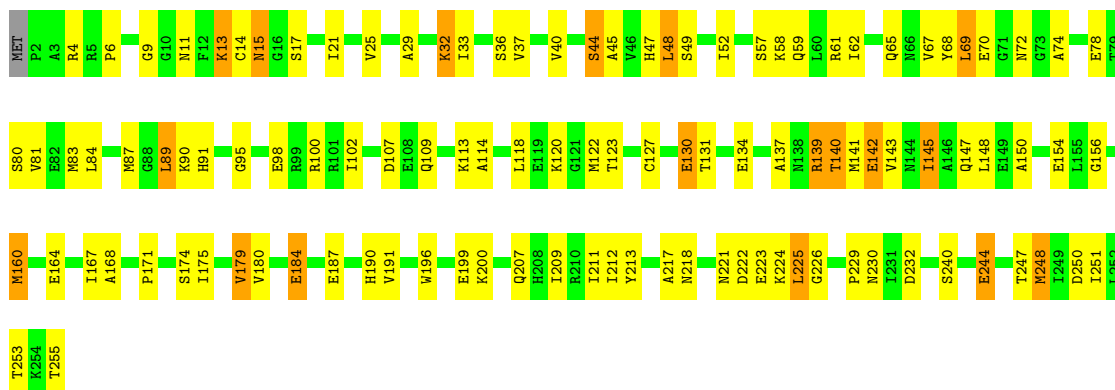
Chain M: 49% 44% 5%





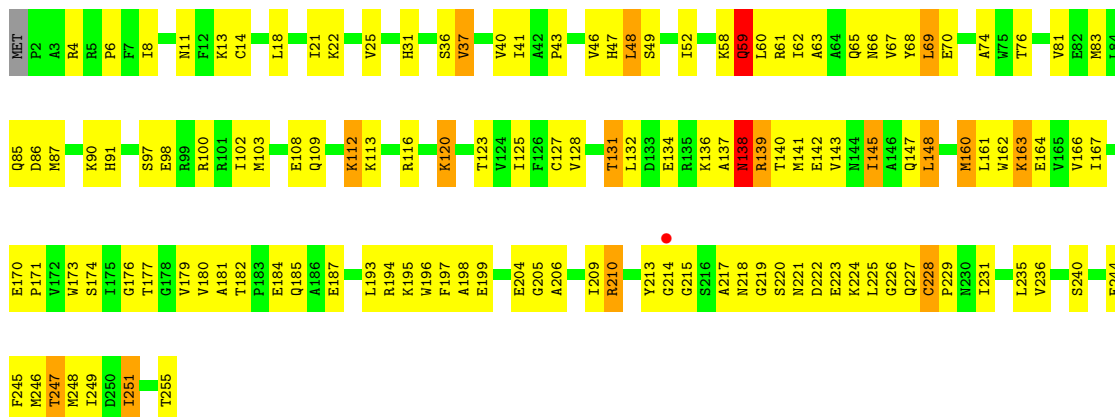
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain N: 56% 36% 7%



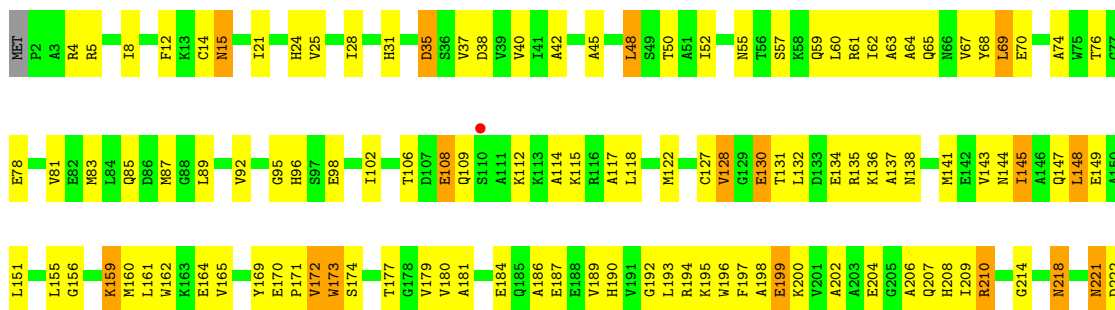
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain O: 48% 45% 6%



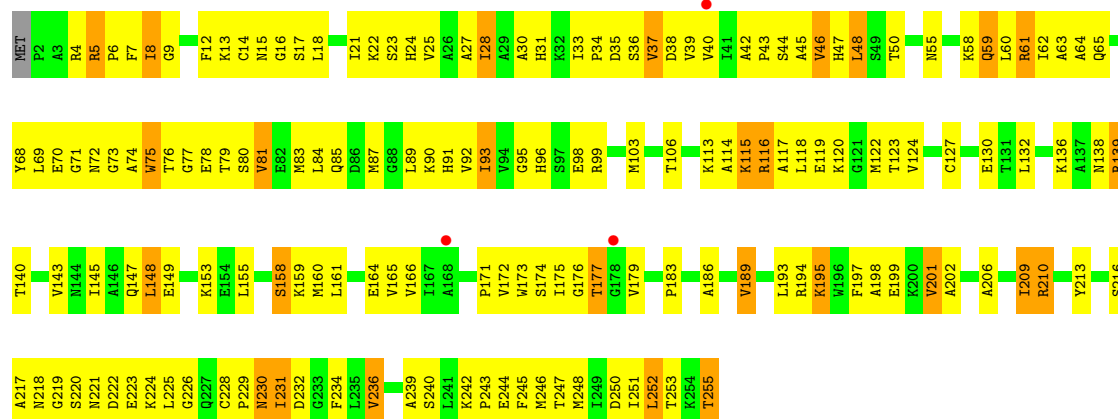
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain P: 48% 44% 7%

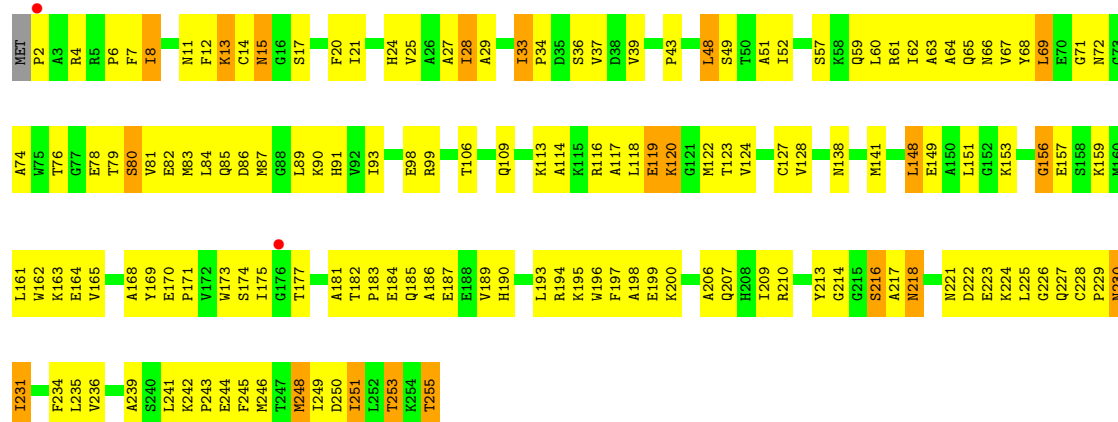




• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

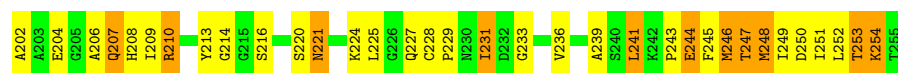


• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

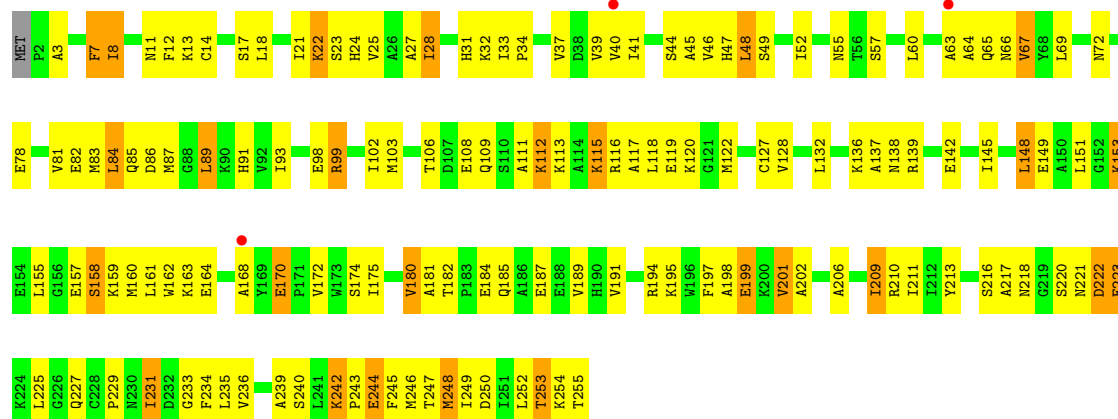


• Molecule 1: TRIOSEPHOSPHATE ISOMERASE





• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	105.22Å 131.57Å 132.55Å 115.73° 89.81° 90.24°	Depositor
Resolution (Å)	78.87 – 2.70 78.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.0 (78.87-2.70) 79.8 (78.87-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.239 , 0.272 0.236 , 0.269	Depositor DCC
R_{free} test set	8804 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.418 for h,-k,-l 0.197 for -h,-l,-k 0.197 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38560	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.63	0/1960	0.88	6/2644 (0.2%)
1	B	0.69	2/1960 (0.1%)	0.84	0/2644
1	C	0.70	4/1960 (0.2%)	0.93	8/2644 (0.3%)
1	D	0.52	0/1960	0.86	6/2644 (0.2%)
1	E	0.78	1/1960 (0.1%)	0.89	3/2644 (0.1%)
1	F	0.62	2/1960 (0.1%)	0.89	3/2644 (0.1%)
1	G	0.69	1/1960 (0.1%)	0.89	8/2644 (0.3%)
1	H	0.72	4/1960 (0.2%)	0.84	1/2644 (0.0%)
1	I	0.48	0/1960	0.85	0/2644
1	J	0.56	1/1960 (0.1%)	0.86	0/2644
1	K	0.42	0/1960	0.87	4/2644 (0.2%)
1	L	0.72	3/1960 (0.2%)	0.99	11/2644 (0.4%)
1	M	0.43	1/1960 (0.1%)	0.80	2/2644 (0.1%)
1	N	0.36	0/1960	0.80	0/2644
1	O	0.40	0/1960	0.85	2/2644 (0.1%)
1	P	0.37	0/1960	0.84	5/2644 (0.2%)
1	Q	0.43	0/1960	0.85	3/2644 (0.1%)
1	R	0.49	0/1960	0.86	3/2644 (0.1%)
1	S	0.40	0/1960	0.88	1/2644 (0.0%)
1	T	0.38	0/1960	0.86	5/2644 (0.2%)
All	All	0.56	19/39200 (0.0%)	0.87	71/52880 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	ALA	CA-CB	-7.45	1.42	1.52
1	H	94	VAL	C-O	-6.72	1.17	1.24
1	C	76	THR	CA-CB	-6.71	1.43	1.53
1	L	74	ALA	CA-CB	-5.95	1.44	1.52
1	B	75	TRP	C-O	-5.84	1.15	1.23
1	F	8	ILE	C-O	-5.66	1.18	1.24
1	C	75	TRP	C-O	-5.63	1.17	1.23
1	F	13	LYS	C-O	-5.57	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	165	VAL	C-O	-5.54	1.18	1.24
1	C	202	ALA	CA-CB	-5.46	1.44	1.53
1	H	171	PRO	C-O	-5.43	1.17	1.24
1	M	210	ARG	CA-C	-5.42	1.46	1.52
1	H	71	GLY	C-O	-5.40	1.18	1.23
1	G	71	GLY	C-O	-5.35	1.19	1.24
1	E	67	VAL	C-O	-5.30	1.17	1.23
1	C	165	VAL	C-O	-5.20	1.18	1.24
1	L	172	VAL	CA-CB	-5.17	1.48	1.54
1	L	75	TRP	CA-C	-5.06	1.46	1.53
1	J	203	ALA	CA-CB	-5.04	1.45	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	ILE	N-CA-C	9.86	119.89	110.42
1	L	137	ALA	N-CA-C	-9.71	100.54	112.38
1	T	221	ASN	N-CA-C	9.43	121.64	111.36
1	L	220	SER	N-CA-C	-8.74	100.41	112.12
1	C	216	SER	N-CA-C	-8.70	100.42	111.90
1	O	59	GLN	N-CA-C	8.46	120.59	111.36
1	L	178	GLY	N-CA-C	-8.36	104.34	115.21
1	F	219	GLY	N-CA-C	-8.18	103.53	113.99
1	T	222	ASP	N-CA-C	7.98	119.98	111.28
1	G	223	GLU	N-CA-C	-7.87	102.70	111.28
1	L	219	GLY	N-CA-C	-7.51	105.37	115.36
1	D	160	MET	N-CA-C	-7.37	104.42	113.19
1	K	161	LEU	N-CA-C	-7.29	103.41	111.36
1	C	77	GLY	CA-C-N	-7.24	111.22	122.59
1	C	77	GLY	C-N-CA	-7.24	111.22	122.59
1	R	216	SER	N-CA-C	-7.22	103.41	111.28
1	Q	5	ARG	CA-C-N	7.05	127.60	119.99
1	Q	5	ARG	C-N-CA	7.05	127.60	119.99
1	D	162	TRP	N-CA-C	-6.88	104.76	113.01
1	E	200	LYS	N-CA-C	6.82	121.68	112.88
1	A	175	ILE	N-CA-C	6.74	117.53	110.72
1	F	203	ALA	N-CA-C	6.51	118.17	111.14
1	Q	5	ARG	O-C-N	6.46	127.05	121.30
1	P	242	LYS	CA-C-N	6.38	127.82	119.84
1	P	242	LYS	C-N-CA	6.38	127.82	119.84
1	K	234	PHE	N-CA-C	6.32	119.32	109.52
1	G	220	SER	N-CA-C	6.31	118.16	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	228	CYS	N-CA-C	-6.29	100.43	109.48
1	R	162	TRP	N-CA-C	-6.10	105.55	112.87
1	L	174	SER	N-CA-C	5.93	118.28	108.49
1	T	201	VAL	N-CA-C	5.92	121.66	109.34
1	K	159	LYS	N-CA-C	-5.88	100.41	109.52
1	A	228	CYS	CA-C-N	5.86	125.24	118.85
1	A	228	CYS	C-N-CA	5.86	125.24	118.85
1	A	242	LYS	CA-C-N	5.81	125.43	119.56
1	A	242	LYS	C-N-CA	5.81	125.43	119.56
1	D	203	ALA	N-CA-C	5.69	117.56	111.36
1	G	203	ALA	N-CA-C	-5.61	105.16	111.28
1	F	13	LYS	CB-CA-C	-5.60	108.49	116.34
1	D	242	LYS	CA-C-N	5.59	125.30	119.82
1	D	242	LYS	C-N-CA	5.59	125.30	119.82
1	C	222	ASP	N-CA-C	5.54	118.08	111.71
1	H	152	GLY	N-CA-C	-5.51	105.71	112.77
1	G	228	CYS	CA-C-N	5.50	126.71	119.84
1	G	228	CYS	C-N-CA	5.50	126.71	119.84
1	D	219	GLY	N-CA-C	5.49	119.29	112.64
1	M	228	CYS	CA-C-N	5.47	125.13	119.05
1	M	228	CYS	C-N-CA	5.47	125.13	119.05
1	K	228	CYS	N-CA-C	-5.43	102.89	109.57
1	L	228	CYS	CA-C-N	5.38	125.02	119.05
1	L	228	CYS	C-N-CA	5.38	125.02	119.05
1	C	199	GLU	N-CA-C	5.36	117.20	111.36
1	L	217	ALA	N-CA-C	-5.27	102.24	110.10
1	E	228	CYS	CA-C-N	5.26	125.32	119.32
1	E	228	CYS	C-N-CA	5.26	125.32	119.32
1	L	45	ALA	N-CA-C	-5.20	105.62	111.28
1	L	233	GLY	N-CA-C	5.14	117.69	110.38
1	G	235	LEU	N-CA-C	-5.14	100.15	108.52
1	L	171	PRO	N-CA-C	-5.13	103.05	110.80
1	T	201	VAL	CB-CA-C	-5.12	102.88	111.29
1	P	228	CYS	CA-C-N	5.11	125.18	119.87
1	P	228	CYS	C-N-CA	5.11	125.18	119.87
1	T	3	ALA	N-CA-C	5.10	117.74	110.24
1	P	218	ASN	N-CA-C	5.10	116.05	108.60
1	A	137	ALA	N-CA-C	-5.09	106.90	113.01
1	G	37	VAL	N-CA-C	5.09	116.63	108.89
1	C	17	SER	N-CA-C	-5.08	101.58	109.72
1	G	204	GLU	N-CA-C	5.05	116.59	111.14
1	S	35	ASP	N-CA-C	-5.05	107.28	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	ASN	N-CA-C	-5.04	102.59	110.10
1	R	200	LYS	N-CA-C	5.04	119.58	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1928	0	1949	116	0
1	B	1928	0	1949	85	0
1	C	1928	0	1949	94	0
1	D	1928	0	1949	102	0
1	E	1928	0	1949	149	0
1	F	1928	0	1949	95	0
1	G	1928	0	1949	103	0
1	H	1928	0	1949	84	0
1	I	1928	0	1949	140	0
1	J	1928	0	1949	107	0
1	K	1928	0	1949	122	0
1	L	1928	0	1949	149	0
1	M	1928	0	1949	108	0
1	N	1928	0	1949	119	0
1	O	1928	0	1949	144	0
1	P	1928	0	1949	132	0
1	Q	1928	0	1949	207	0
1	R	1928	0	1949	194	0
1	S	1928	0	1949	195	0
1	T	1928	0	1949	137	0
All	All	38560	0	38980	2448	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 (2448) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:THR:CG2	1:D:98:GLU:OE1	1.67	1.42
1:T:115:LYS:HG2	1:T:155:LEU:CD2	1.47	1.41
1:B:66:ASN:HD22	1:B:67:VAL:N	1.25	1.31
1:L:177:THR:HG22	1:L:179:VAL:CG2	1.60	1.30
1:B:66:ASN:ND2	1:B:67:VAL:H	1.30	1.27
1:Q:75:TRP:CD1	1:R:14:CYS:HG	1.52	1.26
1:L:200:LYS:HD2	1:L:200:LYS:O	1.39	1.19
1:N:14:CYS:C	1:N:15:ASN:HD22	1.51	1.19
1:P:14:CYS:C	1:P:15:ASN:HD22	1.52	1.17
1:Q:183:PRO:HB3	1:Q:225:LEU:HD23	1.25	1.17
1:P:210:ARG:HH11	1:P:210:ARG:HG3	1.03	1.15
1:O:58:LYS:HG3	1:O:59:GLN:NE2	1.65	1.12
1:C:217:ALA:O	1:C:218:ASN:HB3	1.46	1.12
1:L:177:THR:HG22	1:L:179:VAL:HG23	1.13	1.12
1:T:115:LYS:CG	1:T:155:LEU:CD2	2.28	1.11
1:C:178:GLY:HA2	1:R:175:ILE:HD13	1.30	1.10
1:T:115:LYS:HG2	1:T:155:LEU:HD23	1.27	1.10
1:O:58:LYS:HE2	1:O:59:GLN:OE1	1.52	1.10
1:O:58:LYS:HG3	1:O:59:GLN:CD	1.77	1.10
1:T:115:LYS:CG	1:T:155:LEU:HD23	1.79	1.09
1:E:251:ILE:HA	1:E:254:LYS:HE3	1.32	1.09
1:E:171:PRO:HG2	1:E:215:GLY:HA3	1.16	1.08
1:L:177:THR:CG2	1:L:179:VAL:HG23	1.82	1.08
1:S:210:ARG:HG2	1:S:210:ARG:HH11	0.92	1.08
1:B:66:ASN:ND2	1:B:67:VAL:N	1.91	1.07
1:Q:183:PRO:CB	1:Q:225:LEU:HD23	1.83	1.07
1:G:213:TYR:HB3	1:G:234:PHE:CD1	1.89	1.07
1:E:171:PRO:CG	1:E:215:GLY:HA3	1.85	1.07
1:I:84:LEU:HD22	1:I:89:LEU:HD12	1.31	1.07
1:F:171:PRO:O	1:F:175:ILE:HD13	1.53	1.06
1:E:175:ILE:HA	1:I:176:GLY:HA3	1.33	1.06
1:E:217:ALA:HB3	1:I:178:GLY:CA	1.86	1.06
1:E:217:ALA:HB3	1:I:178:GLY:HA2	1.36	1.06
1:O:226:GLY:HA3	1:O:255:THR:HG21	1.36	1.06
1:Q:61:ARG:HH22	1:Q:90:LYS:HG2	1.19	1.06
1:L:222:ASP:OD2	1:L:248:MET:HE3	1.57	1.05
1:Q:210:ARG:HD3	1:Q:210:ARG:H	1.20	1.05
1:R:225:LEU:HB3	1:R:234:PHE:CE1	1.93	1.04
1:C:76:THR:HG23	1:D:98:GLU:CD	1.83	1.03
1:H:218:ASN:O	1:H:222:ASP:HB2	1.58	1.02
1:L:171:PRO:HG2	1:L:174:SER:OG	1.60	1.02
1:Q:197:PHE:O	1:Q:201:VAL:HB	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ILE:O	1:R:175:ILE:HG21	1.60	1.01
1:N:226:GLY:C	1:N:255:THR:HG21	1.83	1.01
1:O:218:ASN:HD22	1:O:220:SER:H	1.08	1.01
1:Q:75:TRP:CD1	1:R:14:CYS:SG	2.52	1.01
1:T:115:LYS:HG2	1:T:155:LEU:HD21	1.39	1.01
1:L:218:ASN:N	1:L:221:ASN:HD21	1.57	1.01
1:D:158:SER:OG	1:D:160:MET:HE2	1.60	1.01
1:S:158:SER:HB2	1:S:161:LEU:HD23	1.42	1.01
1:O:59:GLN:NE2	1:O:59:GLN:H	1.56	1.01
1:R:225:LEU:HB3	1:R:234:PHE:HE1	1.23	1.00
1:R:195:LYS:O	1:R:199:GLU:HB2	1.62	1.00
1:S:221:ASN:CB	1:S:224:LYS:HE2	1.92	1.00
1:L:177:THR:CG2	1:L:179:VAL:CG2	2.39	0.99
1:M:2:PRO:HG2	1:M:207:GLN:HB3	1.45	0.98
1:S:6:PRO:HG2	1:S:37:VAL:HA	1.46	0.98
1:P:173:TRP:O	1:P:177:THR:HG21	1.62	0.98
1:B:102:ILE:HG12	1:O:179:VAL:HG22	1.46	0.98
1:L:218:ASN:H	1:L:221:ASN:ND2	1.62	0.98
1:M:191:VAL:HG22	1:M:230:ASN:OD1	1.64	0.97
1:A:172:VAL:HA	1:A:175:ILE:CD1	1.95	0.97
1:O:171:PRO:HD2	1:O:214:GLY:O	1.63	0.96
1:S:210:ARG:HG2	1:S:210:ARG:NH1	1.72	0.96
1:R:251:ILE:O	1:R:255:THR:HB	1.66	0.96
1:K:159:LYS:O	1:K:160:MET:HG2	1.64	0.95
1:S:7:PHE:HE2	1:S:166:VAL:HG21	1.31	0.95
1:C:76:THR:HG23	1:D:98:GLU:OE1	0.77	0.95
1:H:160:MET:O	1:H:163:LYS:HG3	1.65	0.95
1:O:58:LYS:CG	1:O:59:GLN:NE2	2.30	0.94
1:S:173:TRP:CD1	1:S:173:TRP:H	1.76	0.94
1:E:190:HIS:HE2	1:E:213:TYR:HB2	1.28	0.94
1:G:97:SER:HB3	1:G:170:GLU:OE1	1.66	0.94
1:Q:61:ARG:NH2	1:Q:90:LYS:HG2	1.83	0.94
1:M:94:VAL:HG11	1:M:114:ALA:HB2	1.49	0.94
1:O:58:LYS:CG	1:O:59:GLN:HE22	1.80	0.94
1:H:217:ALA:HB1	1:H:248:MET:HE1	1.47	0.94
1:G:236:VAL:CG1	1:G:239:ALA:HB3	1.98	0.93
1:G:69:LEU:HD12	1:G:70:GLU:HG2	1.50	0.93
1:R:228:CYS:CB	1:R:231:ILE:HG13	1.99	0.92
1:G:195:LYS:O	1:G:199:GLU:HG3	1.69	0.92
1:E:169:TYR:CE1	1:E:189:VAL:HG11	2.04	0.92
1:Q:7:PHE:HD1	1:Q:38:ASP:HB2	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:89:LEU:HD12	1:Q:90:LYS:H	1.35	0.91
1:S:61:ARG:HH11	1:S:61:ARG:HG3	1.33	0.91
1:T:109:GLN:O	1:T:113:LYS:HG3	1.71	0.91
1:E:171:PRO:HD2	1:E:215:GLY:CA	1.99	0.91
1:E:190:HIS:NE2	1:E:213:TYR:HB2	1.85	0.90
1:H:126:PHE:CZ	1:H:151:LEU:HD11	2.06	0.90
1:E:171:PRO:HD2	1:E:215:GLY:HA2	1.52	0.90
1:L:221:ASN:HD22	1:L:222:ASP:N	1.69	0.89
1:P:210:ARG:HG3	1:P:210:ARG:NH1	1.82	0.89
1:D:4:ARG:HD3	1:D:207:GLN:O	1.72	0.89
1:E:4:ARG:HD3	1:E:207:GLN:O	1.72	0.89
1:K:172:VAL:HA	1:K:175:ILE:HD12	1.55	0.89
1:N:14:CYS:C	1:N:15:ASN:ND2	2.30	0.89
1:I:194:ARG:HH11	1:I:194:ARG:CG	1.86	0.89
1:S:210:ARG:HH11	1:S:210:ARG:CG	1.84	0.88
1:J:11:ASN:ND2	1:J:13:LYS:HG3	1.88	0.88
1:A:218:ASN:HD22	1:A:218:ASN:C	1.81	0.88
1:Q:89:LEU:HD12	1:Q:90:LYS:N	1.89	0.87
1:T:115:LYS:CD	1:T:155:LEU:HD23	2.04	0.87
1:M:99:ARG:HA	1:M:103:MET:HB2	1.54	0.87
1:Q:7:PHE:CD1	1:Q:38:ASP:HB2	2.09	0.87
1:E:135:ARG:HA	1:E:140:THR:HG22	1.54	0.87
1:R:66:ASN:OD1	1:R:67:VAL:N	2.07	0.87
1:A:217:ALA:HB1	1:A:248:MET:HE1	1.55	0.86
1:O:218:ASN:ND2	1:O:220:SER:H	1.73	0.86
1:S:141:MET:HE1	1:S:193:LEU:HD23	1.55	0.86
1:B:224:LYS:O	1:B:227:GLN:HG3	1.74	0.86
1:B:69:LEU:HD23	1:B:70:GLU:HG2	1.58	0.86
1:O:58:LYS:HG2	1:O:59:GLN:HE22	1.39	0.86
1:I:4:ARG:HG2	1:I:4:ARG:HH11	1.41	0.85
1:B:97:SER:HB3	1:B:170:GLU:OE1	1.76	0.85
1:O:59:GLN:H	1:O:59:GLN:HE21	1.19	0.85
1:Q:79:THR:HG21	1:Q:84:LEU:HD21	1.59	0.85
1:P:131:THR:HA	1:P:172:VAL:CG1	2.06	0.85
1:G:236:VAL:HG11	1:G:239:ALA:HB3	1.57	0.85
1:R:183:PRO:HG2	1:R:224:LYS:HD3	1.59	0.85
1:K:165:VAL:O	1:K:209:ILE:HD11	1.76	0.85
1:E:130:GLU:OE2	1:E:135:ARG:HB2	1.76	0.84
1:O:171:PRO:HG3	1:O:215:GLY:HA3	1.57	0.84
1:L:141:MET:HA	1:L:141:MET:HE3	1.57	0.84
1:B:222:ASP:OD2	1:B:248:MET:HE3	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:131:THR:HA	1:P:172:VAL:HG11	1.59	0.84
1:R:228:CYS:HB2	1:R:231:ILE:HG13	1.58	0.84
1:H:84:LEU:HD22	1:H:89:LEU:HD12	1.59	0.83
1:O:213:TYR:CZ	1:O:215:GLY:HA3	2.13	0.83
1:S:130:GLU:OE2	1:S:140:THR:HG23	1.77	0.83
1:C:69:LEU:HD23	1:C:70:GLU:HG2	1.58	0.83
1:T:155:LEU:HD22	1:T:161:LEU:HD12	1.59	0.83
1:Q:195:LYS:O	1:Q:199:GLU:HB2	1.78	0.83
1:Q:61:ARG:HH22	1:Q:90:LYS:CG	1.92	0.83
1:T:115:LYS:HD3	1:T:155:LEU:CD2	2.09	0.83
1:L:69:LEU:HD23	1:L:70:GLU:HG2	1.61	0.83
1:G:213:TYR:HB3	1:G:234:PHE:CE1	2.11	0.83
1:T:17:SER:O	1:T:21:ILE:HG12	1.78	0.83
1:F:218:ASN:HB2	1:F:220:SER:OG	1.78	0.83
1:C:175:ILE:O	1:R:175:ILE:CG2	2.26	0.82
1:E:141:MET:HA	1:E:141:MET:HE3	1.59	0.82
1:L:204:GLU:CD	1:L:204:GLU:H	1.86	0.82
1:O:171:PRO:HG3	1:O:215:GLY:CA	2.08	0.82
1:S:157:GLU:OE1	1:S:157:GLU:HA	1.78	0.82
1:F:171:PRO:HB3	1:F:173:TRP:NE1	1.93	0.82
1:Q:234:PHE:CD2	1:Q:248:MET:CE	2.61	0.82
1:R:217:ALA:O	1:R:218:ASN:C	2.22	0.82
1:A:172:VAL:HG13	1:A:175:ILE:HD12	1.59	0.82
1:E:218:ASN:OD1	1:E:219:GLY:N	2.13	0.82
1:D:218:ASN:HD22	1:D:219:GLY:N	1.77	0.82
1:S:8:ILE:HD11	1:S:245:PHE:CE1	2.15	0.82
1:Q:197:PHE:CD2	1:Q:206:ALA:HA	2.14	0.82
1:R:4:ARG:HD3	1:R:207:GLN:O	1.79	0.82
1:R:246:MET:HA	1:R:249:ILE:HD12	1.60	0.82
1:E:219:GLY:O	1:E:220:SER:HB3	1.79	0.81
1:I:194:ARG:HH11	1:I:194:ARG:HG2	1.45	0.81
1:K:218:ASN:HD22	1:K:219:GLY:N	1.78	0.81
1:S:183:PRO:HD2	1:S:184:GLU:OE1	1.81	0.81
1:P:173:TRP:O	1:P:177:THR:CG2	2.29	0.81
1:R:141:MET:HE1	1:R:193:LEU:HD23	1.63	0.81
1:R:2:PRO:HB3	1:R:207:GLN:HG2	1.62	0.81
1:R:63:ALA:HB2	1:R:91:HIS:HB2	1.60	0.81
1:S:7:PHE:CE2	1:S:166:VAL:HG21	2.15	0.81
1:J:242:LYS:HB3	1:J:244:GLU:OE1	1.80	0.80
1:N:15:ASN:HD22	1:N:15:ASN:N	1.78	0.80
1:I:13:LYS:HG3	1:J:76:THR:CG2	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:183:PRO:CB	1:Q:225:LEU:CD2	2.58	0.80
1:H:187:GLU:O	1:H:191:VAL:HG23	1.81	0.80
1:J:222:ASP:HA	1:J:225:LEU:HB2	1.63	0.80
1:K:223:GLU:HG3	1:K:254:LYS:HZ1	1.46	0.80
1:N:226:GLY:CA	1:N:255:THR:HG21	2.12	0.80
1:R:225:LEU:C	1:R:234:PHE:HZ	1.89	0.80
1:E:247:THR:O	1:E:251:ILE:HD13	1.81	0.80
1:T:115:LYS:HG2	1:T:155:LEU:CG	2.11	0.80
1:P:108:GLU:O	1:P:112:LYS:HG3	1.82	0.80
1:T:83:MET:O	1:T:86:ASP:HB3	1.82	0.80
1:O:226:GLY:CA	1:O:255:THR:HG21	2.12	0.79
1:T:115:LYS:CD	1:T:155:LEU:CD2	2.59	0.79
1:R:69:LEU:HD23	1:R:69:LEU:H	1.45	0.79
1:O:59:GLN:NE2	1:O:59:GLN:N	2.30	0.79
1:N:191:VAL:HG22	1:N:230:ASN:HD22	1.46	0.79
1:P:132:LEU:O	1:P:136:LYS:HG3	1.83	0.79
1:N:6:PRO:HB2	1:N:37:VAL:HG13	1.64	0.79
1:M:228:CYS:HB2	1:M:231:ILE:HD12	1.63	0.78
1:I:11:ASN:HD21	1:J:76:THR:HG21	1.47	0.78
1:I:109:GLN:O	1:I:113:LYS:HG3	1.82	0.78
1:K:159:LYS:O	1:K:160:MET:CG	2.30	0.78
1:S:221:ASN:HB2	1:S:224:LYS:HE2	1.65	0.78
1:H:160:MET:O	1:H:163:LYS:CG	2.31	0.78
1:J:240:SER:HA	1:J:245:PHE:HB2	1.65	0.78
1:L:108:GLU:O	1:L:112:LYS:HG3	1.83	0.78
1:P:5:ARG:O	1:P:210:ARG:HD3	1.82	0.78
1:Q:5:ARG:HH12	1:Q:36:SER:HA	1.48	0.78
1:R:225:LEU:HA	1:R:228:CYS:SG	2.23	0.78
1:G:69:LEU:CD1	1:G:70:GLU:HG2	2.13	0.78
1:G:225:LEU:HB3	1:G:234:PHE:HZ	1.48	0.78
1:M:225:LEU:O	1:M:231:ILE:HD12	1.83	0.78
1:S:177:THR:HG22	1:S:179:VAL:HG22	1.65	0.78
1:L:219:GLY:H	1:L:222:ASP:CG	1.91	0.78
1:S:61:ARG:HG3	1:S:61:ARG:NH1	1.96	0.78
1:O:61:ARG:HE	1:O:62:ILE:H	1.32	0.77
1:P:96:HIS:HD2	1:P:98:GLU:H	1.32	0.77
1:A:48:LEU:O	1:A:52:ILE:HG13	1.85	0.77
1:H:160:MET:O	1:H:163:LYS:CD	2.32	0.77
1:O:58:LYS:CE	1:O:59:GLN:OE1	2.30	0.77
1:K:171:PRO:HG3	1:K:213:TYR:CE1	2.19	0.77
1:R:14:CYS:SG	1:R:14:CYS:O	2.43	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ALA:CB	1:A:248:MET:HE1	2.14	0.77
1:L:171:PRO:HD2	1:L:214:GLY:O	1.85	0.77
1:R:225:LEU:CB	1:R:234:PHE:CE1	2.65	0.77
1:F:4:ARG:HD3	1:F:207:GLN:O	1.83	0.77
1:B:48:LEU:O	1:B:52:ILE:HG13	1.85	0.77
1:E:45:ALA:HA	1:E:48:LEU:CD2	2.15	0.77
1:E:217:ALA:HB3	1:I:178:GLY:HA3	1.66	0.77
1:H:160:MET:O	1:H:163:LYS:HD3	1.84	0.77
1:K:195:LYS:HG2	1:K:196:TRP:N	1.99	0.77
1:E:210:ARG:HA	1:E:232:ASP:OD2	1.85	0.77
1:K:171:PRO:HG3	1:K:213:TYR:HE1	1.50	0.77
1:A:172:VAL:HA	1:A:175:ILE:HD11	1.66	0.76
1:H:126:PHE:CD1	1:H:151:LEU:HD21	2.20	0.76
1:Q:7:PHE:CE2	1:Q:210:ARG:HG3	2.20	0.76
1:I:4:ARG:HH11	1:I:4:ARG:CG	1.97	0.76
1:D:52:ILE:HD11	1:D:89:LEU:HD21	1.67	0.76
1:N:223:GLU:HA	1:N:223:GLU:OE1	1.84	0.76
1:Q:248:MET:O	1:Q:251:ILE:HG22	1.86	0.76
1:I:11:ASN:HD21	1:J:76:THR:CG2	1.98	0.76
1:O:171:PRO:CG	1:O:215:GLY:HA2	2.15	0.76
1:Q:85:GLN:HE22	1:Q:120:LYS:HB3	1.48	0.76
1:N:45:ALA:HA	1:N:48:LEU:HD22	1.68	0.76
1:P:14:CYS:C	1:P:15:ASN:ND2	2.38	0.76
1:E:132:LEU:O	1:E:136:LYS:HG3	1.86	0.76
1:J:98:GLU:O	1:J:102:ILE:HB	1.86	0.76
1:N:226:GLY:O	1:N:255:THR:HG21	1.86	0.76
1:I:247:THR:O	1:I:251:ILE:HD13	1.86	0.75
1:J:182:THR:HG22	1:J:184:GLU:OE1	1.85	0.75
1:L:171:PRO:CG	1:L:174:SER:OG	2.33	0.75
1:N:217:ALA:HB1	1:N:248:MET:HE1	1.67	0.75
1:O:76:THR:HG23	1:P:65:GLN:HB3	1.67	0.75
1:N:191:VAL:HG22	1:N:230:ASN:ND2	2.02	0.75
1:G:224:LYS:O	1:G:227:GLN:HG3	1.85	0.75
1:J:177:THR:HG22	1:J:179:VAL:H	1.52	0.75
1:R:250:ASP:HA	1:R:253:THR:CG2	2.16	0.75
1:I:13:LYS:HG3	1:J:76:THR:HG22	1.68	0.75
1:K:218:ASN:O	1:K:222:ASP:HB2	1.87	0.75
1:L:109:GLN:O	1:L:113:LYS:HG3	1.86	0.75
1:Q:201:VAL:HG12	1:Q:202:ALA:N	2.01	0.75
1:M:2:PRO:HG2	1:M:207:GLN:CB	2.16	0.75
1:R:52:ILE:HD13	1:R:62:ILE:HD12	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:243:PRO:HA	1:T:246:MET:HE1	1.68	0.75
1:A:67:VAL:O	1:A:113:LYS:HD3	1.87	0.74
1:C:217:ALA:O	1:C:218:ASN:CB	2.31	0.74
1:T:236:VAL:HG13	1:T:239:ALA:HB3	1.69	0.74
1:B:189:VAL:O	1:B:193:LEU:HG	1.86	0.74
1:S:7:PHE:HD1	1:S:8:ILE:N	1.85	0.74
1:B:213:TYR:CZ	1:B:215:GLY:HA3	2.22	0.74
1:M:187:GLU:O	1:M:191:VAL:HG23	1.87	0.74
1:R:106:THR:OG1	1:R:109:GLN:HG3	1.87	0.74
1:I:222:ASP:OD2	1:I:248:MET:HE3	1.85	0.74
1:G:69:LEU:HD12	1:G:69:LEU:C	2.13	0.74
1:P:15:ASN:HD22	1:P:15:ASN:N	1.85	0.74
1:C:21:ILE:HG13	1:C:47:HIS:HB3	1.70	0.74
1:F:98:GLU:O	1:F:102:ILE:HB	1.86	0.74
1:J:69:LEU:HD23	1:J:69:LEU:H	1.51	0.74
1:L:98:GLU:HA	1:L:102:ILE:HD12	1.69	0.74
1:A:206:ALA:O	1:A:209:ILE:HG22	1.86	0.74
1:H:198:ALA:HA	1:H:202:ALA:O	1.88	0.74
1:J:24:HIS:O	1:J:28:ILE:HG13	1.87	0.74
1:N:69:LEU:HB3	1:N:113:LYS:HG2	1.70	0.74
1:P:177:THR:CG2	1:P:179:VAL:HG22	2.18	0.74
1:O:69:LEU:HD23	1:O:70:GLU:HG2	1.70	0.73
1:N:139:ARG:HB3	1:N:139:ARG:HH11	1.52	0.73
1:Q:123:THR:HA	1:Q:164:GLU:HG3	1.68	0.73
1:C:76:THR:HG22	1:D:13:LYS:HD3	1.69	0.73
1:C:218:ASN:C	1:C:218:ASN:OD1	2.29	0.73
1:F:175:ILE:HD12	1:F:175:ILE:N	2.02	0.73
1:Q:210:ARG:H	1:Q:210:ARG:CD	2.00	0.73
1:R:15:ASN:HD21	1:R:241:LEU:HD11	1.50	0.73
1:I:4:ARG:HD2	1:I:208:HIS:C	2.14	0.73
1:I:11:ASN:ND2	1:J:76:THR:HG21	2.03	0.73
1:N:226:GLY:O	1:N:255:THR:CG2	2.36	0.73
1:N:248:MET:O	1:N:251:ILE:HG22	1.89	0.73
1:O:58:LYS:HG3	1:O:59:GLN:OE1	1.88	0.73
1:R:190:HIS:CE1	1:R:231:ILE:HD13	2.24	0.73
1:S:130:GLU:OE2	1:S:135:ARG:NH2	2.21	0.73
1:N:90:LYS:HE3	1:N:91:HIS:CE1	2.24	0.73
1:M:95:GLY:O	1:M:127:CYS:HB2	1.87	0.73
1:O:220:SER:O	1:O:221:ASN:HB3	1.88	0.73
1:Q:4:ARG:HD2	1:Q:232:ASP:OD2	1.87	0.73
1:Q:62:ILE:O	1:Q:89:LEU:CD1	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ASN:ND2	1:D:220:SER:H	1.86	0.73
1:H:115:LYS:HE2	1:H:119:GLU:OE2	1.88	0.73
1:M:98:GLU:O	1:M:102:ILE:HB	1.88	0.73
1:P:170:GLU:OE2	1:P:235:LEU:HD23	1.89	0.72
1:I:194:ARG:CG	1:I:194:ARG:NH1	2.47	0.72
1:O:143:VAL:O	1:O:147:GLN:HG3	1.88	0.72
1:R:228:CYS:HB2	1:R:231:ILE:CG1	2.19	0.72
1:I:69:LEU:HD23	1:I:70:GLU:HG2	1.71	0.72
1:S:221:ASN:HB3	1:S:224:LYS:HE2	1.69	0.72
1:C:67:VAL:O	1:C:113:LYS:HD3	1.89	0.72
1:E:251:ILE:HA	1:E:254:LYS:CE	2.16	0.72
1:H:126:PHE:CE1	1:H:151:LEU:HD21	2.24	0.72
1:P:40:VAL:CG1	1:P:63:ALA:HB2	2.19	0.72
1:D:247:THR:O	1:D:251:ILE:HD13	1.88	0.72
1:M:2:PRO:CG	1:M:207:GLN:HB3	2.17	0.72
1:R:175:ILE:HG13	1:R:175:ILE:O	1.88	0.72
1:F:171:PRO:HB3	1:F:173:TRP:HE1	1.54	0.72
1:I:195:LYS:NZ	1:I:199:GLU:OE2	2.23	0.72
1:Q:234:PHE:CE2	1:Q:248:MET:HE1	2.25	0.72
1:R:175:ILE:HG23	1:R:177:THR:OG1	1.90	0.72
1:S:130:GLU:O	1:S:172:VAL:HB	1.90	0.72
1:T:98:GLU:HA	1:T:102:ILE:HD12	1.69	0.72
1:Q:210:ARG:HD3	1:Q:210:ARG:N	2.01	0.72
1:K:227:GLN:O	1:K:228:CYS:C	2.33	0.72
1:O:145:ILE:HG23	1:O:196:TRP:CD1	2.25	0.72
1:P:195:LYS:HG3	1:P:199:GLU:OE1	1.89	0.72
1:B:69:LEU:CD2	1:B:70:GLU:HG2	2.20	0.72
1:Q:61:ARG:HH11	1:Q:61:ARG:HG3	1.52	0.72
1:E:171:PRO:CD	1:E:215:GLY:CA	2.67	0.71
1:T:63:ALA:HB2	1:T:91:HIS:HB2	1.70	0.71
1:T:85:GLN:HE22	1:T:120:LYS:HB3	1.55	0.71
1:O:48:LEU:O	1:O:52:ILE:HG13	1.90	0.71
1:S:97:SER:O	1:S:101:ARG:HB2	1.90	0.71
1:T:46:VAL:HG23	1:T:47:HIS:CD2	2.25	0.71
1:T:195:LYS:O	1:T:199:GLU:HB2	1.90	0.71
1:T:242:LYS:HB2	1:T:243:PRO:HD2	1.72	0.71
1:G:213:TYR:HD2	1:G:234:PHE:CD1	2.09	0.71
1:J:24:HIS:NE2	1:J:240:SER:O	2.21	0.71
1:Q:183:PRO:HG3	1:Q:225:LEU:CD2	2.21	0.71
1:R:217:ALA:O	1:R:218:ASN:O	2.08	0.71
1:F:24:HIS:O	1:F:28:ILE:HG13	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:68:TYR:HB2	1:N:78:GLU:HB3	1.73	0.71
1:B:213:TYR:CE2	1:B:215:GLY:HA3	2.25	0.71
1:Q:230:ASN:HD22	1:Q:230:ASN:N	1.88	0.71
1:A:137:ALA:O	1:A:138:ASN:HB3	1.90	0.71
1:B:217:ALA:HB1	1:B:222:ASP:OD1	1.90	0.71
1:C:90:LYS:HD3	1:C:91:HIS:CE1	2.26	0.70
1:D:244:GLU:O	1:D:248:MET:HG3	1.91	0.70
1:G:213:TYR:CD2	1:G:234:PHE:CE1	2.79	0.70
1:L:242:LYS:HB3	1:L:243:PRO:HD2	1.72	0.70
1:P:177:THR:HG23	1:P:179:VAL:HG22	1.72	0.70
1:S:130:GLU:HG2	1:S:144:ASN:HD21	1.55	0.70
1:A:172:VAL:HA	1:A:175:ILE:CG1	2.20	0.70
1:S:155:LEU:HG	1:S:161:LEU:HD11	1.71	0.70
1:T:115:LYS:CG	1:T:155:LEU:HD21	2.07	0.70
1:L:200:LYS:O	1:L:200:LYS:CD	2.30	0.70
1:C:98:GLU:O	1:C:102:ILE:HB	1.91	0.70
1:I:145:ILE:HG12	1:I:196:TRP:CD1	2.26	0.70
1:Q:228:CYS:HB3	1:Q:231:ILE:HG13	1.73	0.70
1:C:69:LEU:H	1:C:69:LEU:HD22	1.54	0.70
1:C:115:LYS:O	1:C:119:GLU:HG3	1.90	0.70
1:K:83:MET:HE1	1:L:44:SER:OG	1.91	0.70
1:R:206:ALA:O	1:R:209:ILE:HG22	1.92	0.70
1:L:218:ASN:H	1:L:221:ASN:HD21	0.80	0.70
1:I:194:ARG:NH2	1:I:232:ASP:OD2	2.24	0.70
1:R:69:LEU:H	1:R:69:LEU:CD2	2.05	0.70
1:C:218:ASN:OD1	1:C:219:GLY:N	2.23	0.70
1:P:170:GLU:HG2	1:P:214:GLY:HA3	1.73	0.70
1:Q:234:PHE:CE2	1:Q:248:MET:CE	2.75	0.70
1:A:132:LEU:O	1:A:136:LYS:HG3	1.92	0.70
1:F:13:LYS:H	1:F:65:GLN:NE2	1.90	0.70
1:Q:46:VAL:HG23	1:Q:47:HIS:CD2	2.26	0.70
1:S:92:VAL:CG1	1:S:124:VAL:HG22	2.22	0.70
1:A:218:ASN:C	1:A:218:ASN:ND2	2.48	0.69
1:M:5:ARG:HG2	1:M:5:ARG:HH11	1.54	0.69
1:O:182:THR:H	1:O:185:GLN:HE21	1.37	0.69
1:Q:171:PRO:HB2	1:Q:174:SER:OG	1.92	0.69
1:M:5:ARG:HH11	1:M:5:ARG:CG	2.05	0.69
1:O:197:PHE:CD2	1:O:206:ALA:HA	2.27	0.69
1:Q:183:PRO:HA	1:Q:225:LEU:CD2	2.22	0.69
1:D:130:GLU:OE2	1:D:135:ARG:HB2	1.92	0.69
1:E:171:PRO:CG	1:E:215:GLY:CA	2.68	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:ASN:ND2	1:I:80:SER:OG	2.25	0.69
1:I:187:GLU:OE1	1:I:228:CYS:HB3	1.91	0.69
1:Q:197:PHE:HD2	1:Q:206:ALA:HA	1.54	0.69
1:Q:7:PHE:CE2	1:Q:210:ARG:NH1	2.61	0.69
1:F:171:PRO:O	1:F:175:ILE:CD1	2.34	0.69
1:G:225:LEU:HB3	1:G:234:PHE:CZ	2.26	0.69
1:H:100:ARG:NH2	1:H:126:PHE:CZ	2.60	0.69
1:I:37:VAL:HG21	1:I:253:THR:OG1	1.93	0.69
1:Q:17:SER:O	1:Q:21:ILE:HG12	1.92	0.69
1:Q:115:LYS:HE2	1:Q:119:GLU:OE2	1.92	0.69
1:G:18:LEU:O	1:G:22:LYS:HG3	1.92	0.69
1:I:194:ARG:NH1	1:I:194:ARG:HG3	2.07	0.69
1:Q:183:PRO:CG	1:Q:225:LEU:HD23	2.22	0.69
1:H:220:SER:O	1:H:221:ASN:HB3	1.90	0.69
1:A:158:SER:HB3	1:A:161:LEU:HG	1.73	0.69
1:F:182:THR:OG1	1:F:185:GLN:HB2	1.93	0.69
1:K:143:VAL:O	1:K:147:GLN:HG3	1.93	0.69
1:M:187:GLU:OE1	1:M:228:CYS:HB3	1.92	0.69
1:P:98:GLU:HA	1:P:102:ILE:HD12	1.74	0.69
1:Q:62:ILE:O	1:Q:89:LEU:HD13	1.92	0.69
1:Q:63:ALA:HA	1:Q:89:LEU:HD21	1.75	0.69
1:T:115:LYS:HD3	1:T:155:LEU:HD23	1.71	0.69
1:A:187:GLU:O	1:A:191:VAL:HG23	1.92	0.69
1:R:48:LEU:O	1:R:52:ILE:HG12	1.92	0.69
1:N:134:GLU:O	1:N:139:ARG:HB2	1.92	0.68
1:S:172:VAL:HA	1:S:175:ILE:HG12	1.75	0.68
1:S:197:PHE:CE2	1:S:209:ILE:HD13	2.27	0.68
1:J:216:SER:O	1:J:221:ASN:ND2	2.26	0.68
1:Q:61:ARG:HG3	1:Q:61:ARG:NH1	2.08	0.68
1:A:130:GLU:OE2	1:A:140:THR:HG23	1.94	0.68
1:C:77:GLY:HA3	1:D:99:ARG:HH11	1.59	0.68
1:E:98:GLU:OE2	1:F:74:ALA:HB1	1.93	0.68
1:E:195:LYS:O	1:E:199:GLU:HG2	1.93	0.68
1:F:69:LEU:HD23	1:F:70:GLU:HG2	1.74	0.68
1:S:63:ALA:HB2	1:S:91:HIS:HB2	1.75	0.68
1:A:145:ILE:O	1:A:149:GLU:HB2	1.93	0.68
1:L:43:PRO:HD2	1:L:48:LEU:CD1	2.23	0.68
1:S:118:LEU:HD13	1:S:161:LEU:HD12	1.74	0.68
1:H:48:LEU:O	1:H:52:ILE:HG13	1.92	0.68
1:K:187:GLU:OE1	1:K:228:CYS:HB3	1.93	0.68
1:I:83:MET:O	1:I:87:MET:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:198:ALA:HB2	1:O:206:ALA:CB	2.24	0.68
1:R:17:SER:O	1:R:21:ILE:HG12	1.93	0.68
1:K:106:THR:OG1	1:K:109:GLN:HG3	1.94	0.68
1:K:171:PRO:CG	1:K:213:TYR:CE1	2.77	0.68
1:L:177:THR:HG22	1:L:179:VAL:HG21	1.72	0.68
1:M:109:GLN:O	1:M:113:LYS:HG3	1.94	0.68
1:Q:44:SER:OG	1:R:83:MET:HE1	1.93	0.68
1:S:109:GLN:O	1:S:113:LYS:HG3	1.94	0.68
1:J:111:ALA:HB1	1:J:151:LEU:HA	1.76	0.68
1:K:247:THR:O	1:K:251:ILE:HD13	1.94	0.68
1:A:134:GLU:HG2	1:A:143:VAL:HG21	1.76	0.68
1:K:41:ILE:HG23	1:K:60:LEU:HD11	1.76	0.68
1:R:29:ALA:HA	1:R:57:SER:OG	1.93	0.68
1:S:177:THR:CG2	1:S:179:VAL:HG22	2.24	0.68
1:C:130:GLU:OE2	1:C:140:THR:HB	1.94	0.67
1:F:177:THR:O	1:F:177:THR:HG22	1.93	0.67
1:I:84:LEU:HD22	1:I:89:LEU:CD1	2.15	0.67
1:I:218:ASN:O	1:I:222:ASP:HB2	1.93	0.67
1:R:156:GLY:O	1:R:159:LYS:HG3	1.94	0.67
1:R:230:ASN:HD22	1:R:230:ASN:N	1.92	0.67
1:P:173:TRP:CD1	1:P:173:TRP:H	2.10	0.67
1:A:172:VAL:HA	1:A:175:ILE:HG13	1.74	0.67
1:I:4:ARG:HB2	1:I:4:ARG:CZ	2.25	0.67
1:K:159:LYS:O	1:K:160:MET:CB	2.41	0.67
1:O:221:ASN:HA	1:O:224:LYS:NZ	2.09	0.67
1:Q:197:PHE:O	1:Q:201:VAL:CB	2.39	0.67
1:R:194:ARG:HH11	1:R:209:ILE:HG23	1.60	0.67
1:T:69:LEU:HB3	1:T:113:LYS:HG2	1.76	0.67
1:A:24:HIS:O	1:A:28:ILE:HG13	1.95	0.67
1:D:109:GLN:O	1:D:113:LYS:HG3	1.95	0.67
1:K:81:VAL:HG13	1:K:122:MET:SD	2.33	0.67
1:O:171:PRO:CG	1:O:215:GLY:CA	2.73	0.67
1:R:194:ARG:HH11	1:R:209:ILE:CG2	2.06	0.67
1:S:65:GLN:O	1:S:93:ILE:HB	1.95	0.67
1:A:218:ASN:HD21	1:A:221:ASN:H	1.43	0.67
1:G:130:GLU:OE2	1:G:135:ARG:HB2	1.95	0.67
1:M:195:LYS:O	1:M:199:GLU:HG3	1.95	0.67
1:R:8:ILE:HG22	1:R:39:VAL:HA	1.75	0.67
1:S:160:MET:HE3	1:S:160:MET:H	1.58	0.67
1:S:171:PRO:HA	1:S:173:TRP:HE1	1.59	0.67
1:C:11:ASN:ND2	1:C:13:LYS:HG2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:MET:HE3	1:L:141:MET:CA	2.20	0.67
1:P:210:ARG:HH11	1:P:210:ARG:CG	1.95	0.67
1:D:159:LYS:C	1:D:161:LEU:H	2.03	0.67
1:O:18:LEU:O	1:O:22:LYS:HG3	1.94	0.67
1:R:34:PRO:HB2	1:R:36:SER:OG	1.94	0.67
1:R:71:GLY:CA	1:R:116:ARG:NH2	2.58	0.67
1:R:226:GLY:N	1:R:234:PHE:HZ	1.92	0.67
1:G:69:LEU:HD12	1:G:70:GLU:CG	2.25	0.67
1:I:218:ASN:HD21	1:I:220:SER:HB3	1.59	0.67
1:N:187:GLU:OE2	1:N:229:PRO:HG2	1.95	0.67
1:N:190:HIS:CE1	1:N:211:ILE:HG22	2.29	0.67
1:S:243:PRO:HA	1:S:246:MET:HE1	1.76	0.67
1:B:182:THR:OG1	1:B:185:GLN:HG3	1.96	0.66
1:E:115:LYS:HG2	1:E:155:LEU:HD23	1.75	0.66
1:Q:172:VAL:O	1:Q:175:ILE:HG22	1.95	0.66
1:Q:183:PRO:CA	1:Q:225:LEU:CD2	2.73	0.66
1:R:12:PHE:O	1:R:13:LYS:HB2	1.95	0.66
1:G:72:ASN:HA	1:H:14:CYS:O	1.95	0.66
1:H:21:ILE:O	1:H:25:VAL:HG23	1.94	0.66
1:Q:7:PHE:CD2	1:Q:210:ARG:HG3	2.30	0.66
1:Q:177:THR:O	1:Q:177:THR:CG2	2.43	0.66
1:R:114:ALA:O	1:R:118:LEU:HD13	1.95	0.66
1:R:118:LEU:HD23	1:R:161:LEU:HB3	1.76	0.66
1:H:218:ASN:OD1	1:H:219:GLY:N	2.29	0.66
1:S:67:VAL:O	1:S:113:LYS:HD3	1.94	0.66
1:T:213:TYR:HB2	1:T:231:ILE:HD13	1.76	0.66
1:H:155:LEU:HD12	1:H:162:TRP:NE1	2.10	0.66
1:L:97:SER:OG	1:L:175:ILE:CD1	2.43	0.66
1:N:226:GLY:C	1:N:255:THR:CG2	2.66	0.66
1:R:227:GLN:HA	1:R:227:GLN:HE21	1.59	0.66
1:N:145:ILE:HG23	1:N:196:TRP:CD1	2.30	0.66
1:E:254:LYS:C	1:E:255:THR:OG1	2.36	0.66
1:L:118:LEU:HD13	1:L:161:LEU:O	1.96	0.66
1:N:4:ARG:HD3	1:N:207:GLN:O	1.95	0.66
1:Q:13:LYS:HD3	1:R:74:ALA:HA	1.78	0.66
1:H:126:PHE:CG	1:H:151:LEU:HD21	2.30	0.66
1:K:4:ARG:HG2	1:K:208:HIS:HA	1.78	0.66
1:L:90:LYS:HE3	1:L:91:HIS:CE1	2.31	0.66
1:O:223:GLU:O	1:O:227:GLN:HG3	1.95	0.66
1:A:138:ASN:O	1:A:138:ASN:ND2	2.29	0.66
1:D:108:GLU:O	1:D:112:LYS:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:128:VAL:HG12	1:P:147:GLN:HB2	1.76	0.66
1:Q:225:LEU:O	1:Q:228:CYS:HB2	1.95	0.66
1:R:109:GLN:O	1:R:113:LYS:HG3	1.96	0.66
1:A:137:ALA:O	1:A:138:ASN:CB	2.41	0.66
1:M:170:GLU:HB2	1:M:175:ILE:HD11	1.78	0.66
1:B:18:LEU:O	1:B:22:LYS:HG3	1.96	0.66
1:I:244:GLU:O	1:I:248:MET:HG3	1.94	0.66
1:K:218:ASN:ND2	1:K:219:GLY:N	2.43	0.66
1:P:98:GLU:O	1:P:102:ILE:HB	1.95	0.66
1:F:116:ARG:O	1:F:120:LYS:HG3	1.96	0.65
1:G:64:ALA:O	1:G:93:ILE:HG23	1.96	0.65
1:R:174:SER:C	1:R:175:ILE:HG22	2.21	0.65
1:G:9:GLY:HA2	1:G:40:VAL:O	1.96	0.65
1:I:74:ALA:HB1	1:J:98:GLU:OE2	1.96	0.65
1:K:132:LEU:O	1:K:136:LYS:HG3	1.97	0.65
1:L:220:SER:OG	1:L:221:ASN:N	2.28	0.65
1:Q:165:VAL:O	1:Q:210:ARG:NE	2.28	0.65
1:D:158:SER:HG	1:D:160:MET:HE2	1.62	0.65
1:N:141:MET:HE3	1:N:145:ILE:HD11	1.77	0.65
1:T:236:VAL:CG1	1:T:239:ALA:HB3	2.26	0.65
1:K:109:GLN:O	1:K:113:LYS:HG3	1.97	0.65
1:L:177:THR:CG2	1:L:179:VAL:HG21	2.24	0.65
1:N:67:VAL:O	1:N:113:LYS:HD3	1.97	0.65
1:R:68:TYR:CD1	1:R:78:GLU:HG3	2.31	0.65
1:R:71:GLY:HA2	1:R:116:ARG:NH2	2.12	0.65
1:T:69:LEU:HD23	1:T:69:LEU:H	1.62	0.65
1:A:84:LEU:HD22	1:A:89:LEU:HD12	1.76	0.65
1:H:221:ASN:O	1:H:221:ASN:ND2	2.30	0.65
1:L:130:GLU:O	1:L:172:VAL:HB	1.97	0.65
1:S:115:LYS:O	1:S:119:GLU:HG3	1.97	0.65
1:G:17:SER:O	1:G:21:ILE:HG12	1.97	0.65
1:L:40:VAL:CG1	1:L:63:ALA:HB2	2.27	0.65
1:D:171:PRO:HD2	1:D:214:GLY:O	1.97	0.65
1:I:4:ARG:HD2	1:I:208:HIS:CA	2.27	0.65
1:I:83:MET:HG2	1:J:47:HIS:CE1	2.32	0.65
1:L:138:ASN:O	1:L:138:ASN:ND2	2.30	0.65
1:L:155:LEU:HD12	1:L:162:TRP:CE2	2.32	0.65
1:N:209:ILE:HG23	1:N:211:ILE:HD11	1.79	0.65
1:Q:222:ASP:HB2	1:Q:248:MET:HE1	1.79	0.65
1:P:14:CYS:O	1:P:15:ASN:ND2	2.30	0.65
1:P:48:LEU:O	1:P:52:ILE:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:OD2	1:A:248:MET:HE3	1.97	0.65
1:D:218:ASN:HD22	1:D:218:ASN:C	2.05	0.65
1:N:4:ARG:HE	1:N:232:ASP:CG	2.05	0.65
1:O:137:ALA:O	1:O:138:ASN:HB2	1.96	0.65
1:T:206:ALA:O	1:T:209:ILE:HG22	1.97	0.65
1:A:139:ARG:NH1	1:A:142:GLU:OE2	2.30	0.64
1:T:25:VAL:HA	1:T:28:ILE:HG13	1.78	0.64
1:E:155:LEU:HD12	1:E:162:TRP:CE2	2.32	0.64
1:L:134:GLU:O	1:L:139:ARG:N	2.30	0.64
1:A:217:ALA:HB1	1:A:248:MET:CE	2.27	0.64
1:H:99:ARG:HA	1:H:103:MET:HB2	1.80	0.64
1:Q:158:SER:HB2	1:Q:161:LEU:HD12	1.79	0.64
1:S:239:ALA:O	1:S:245:PHE:HB2	1.97	0.64
1:Q:143:VAL:O	1:Q:147:GLN:HG3	1.98	0.64
1:M:242:LYS:HB3	1:M:243:PRO:HD2	1.79	0.64
1:N:14:CYS:O	1:N:15:ASN:ND2	2.30	0.64
1:P:148:LEU:HB3	1:P:196:TRP:CH2	2.33	0.64
1:Q:7:PHE:CE1	1:Q:38:ASP:CG	2.76	0.64
1:I:233:GLY:HA2	1:I:252:LEU:CD1	2.28	0.64
1:J:137:ALA:O	1:J:138:ASN:CB	2.43	0.64
1:N:199:GLU:C	1:N:200:LYS:HD2	2.22	0.64
1:L:4:ARG:HD2	1:L:207:GLN:O	1.98	0.64
1:M:13:LYS:H	1:M:65:GLN:NE2	1.96	0.64
1:Q:132:LEU:HG	1:Q:136:LYS:HE2	1.80	0.64
1:Q:198:ALA:HB2	1:Q:206:ALA:CB	2.27	0.64
1:F:145:ILE:HG23	1:F:196:TRP:NE1	2.14	0.63
1:H:6:PRO:HB2	1:H:37:VAL:HG13	1.80	0.63
1:L:251:ILE:HD13	1:L:254:LYS:NZ	2.13	0.63
1:Q:239:ALA:O	1:Q:245:PHE:HB2	1.98	0.63
1:Q:244:GLU:O	1:Q:247:THR:HB	1.98	0.63
1:S:39:VAL:HG12	1:S:60:LEU:HD12	1.79	0.63
1:G:65:GLN:O	1:G:93:ILE:HG12	1.98	0.63
1:L:137:ALA:O	1:L:138:ASN:HB3	1.98	0.63
1:P:148:LEU:HB3	1:P:196:TRP:CZ3	2.34	0.63
1:R:82:GLU:H	1:R:82:GLU:CD	2.06	0.63
1:D:155:LEU:HD12	1:D:162:TRP:NE1	2.14	0.63
1:S:43:PRO:HG2	1:S:48:LEU:HD12	1.81	0.63
1:S:131:THR:OG1	1:S:134:GLU:HG3	1.98	0.63
1:B:244:GLU:O	1:B:248:MET:HG3	1.99	0.63
1:K:194:ARG:HD3	1:K:206:ALA:O	1.98	0.63
1:S:8:ILE:HD11	1:S:245:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:THR:CG2	1:D:98:GLU:CD	2.57	0.63
1:L:48:LEU:O	1:L:52:ILE:HG13	1.98	0.63
1:P:69:LEU:HD23	1:P:70:GLU:HG2	1.80	0.63
1:H:220:SER:O	1:H:221:ASN:CB	2.46	0.63
1:J:127:CYS:HB3	1:J:170:GLU:OE2	1.98	0.63
1:M:171:PRO:HG2	1:M:174:SER:HB2	1.80	0.63
1:N:137:ALA:HB3	1:N:139:ARG:HG3	1.80	0.63
1:S:173:TRP:CD1	1:S:173:TRP:N	2.56	0.63
1:T:34:PRO:HG2	1:T:253:THR:OG1	1.98	0.63
1:T:98:GLU:O	1:T:102:ILE:HB	1.99	0.63
1:B:175:ILE:O	1:O:176:GLY:N	2.32	0.63
1:D:18:LEU:O	1:D:22:LYS:HG3	1.98	0.63
1:G:67:VAL:O	1:G:113:LYS:HD3	1.99	0.63
1:L:182:THR:OG1	1:L:185:GLN:HG3	1.99	0.63
1:T:217:ALA:HB1	1:T:248:MET:HE1	1.81	0.63
1:D:57:SER:HB3	1:D:60:LEU:HB3	1.81	0.62
1:D:218:ASN:ND2	1:D:218:ASN:C	2.57	0.62
1:L:173:TRP:H	1:L:173:TRP:CD1	2.17	0.62
1:L:204:GLU:CD	1:L:204:GLU:N	2.55	0.62
1:E:97:SER:HB3	1:E:170:GLU:OE1	1.99	0.62
1:L:67:VAL:O	1:L:113:LYS:HD3	1.99	0.62
1:M:106:THR:OG1	1:M:109:GLN:HG3	1.99	0.62
1:N:171:PRO:HB2	1:N:174:SER:OG	1.98	0.62
1:O:109:GLN:O	1:O:113:LYS:HG3	1.99	0.62
1:P:149:GLU:OE1	1:P:200:LYS:HE3	1.98	0.62
1:E:190:HIS:CE1	1:E:213:TYR:HB2	2.32	0.62
1:F:175:ILE:HD12	1:F:175:ILE:H	1.61	0.62
1:I:141:MET:O	1:I:145:ILE:HB	1.99	0.62
1:K:204:GLU:HG2	1:K:205:GLY:N	2.14	0.62
1:Q:183:PRO:CG	1:Q:225:LEU:CD2	2.77	0.62
1:E:197:PHE:O	1:E:201:VAL:N	2.33	0.62
1:F:109:GLN:O	1:F:113:LYS:HG3	1.99	0.62
1:N:139:ARG:HH12	1:N:143:VAL:HG22	1.63	0.62
1:O:213:TYR:CE1	1:O:215:GLY:HA3	2.35	0.62
1:Q:8:ILE:CG2	1:Q:39:VAL:HG22	2.30	0.62
1:Q:222:ASP:OD1	1:Q:223:GLU:N	2.33	0.62
1:R:174:SER:O	1:R:175:ILE:CG2	2.48	0.62
1:S:130:GLU:CD	1:S:140:THR:HG23	2.25	0.62
1:N:48:LEU:O	1:N:52:ILE:HG13	1.98	0.62
1:Q:15:ASN:OD1	1:R:72:ASN:HB3	1.99	0.62
1:T:172:VAL:HA	1:T:175:ILE:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:ASP:O	1:E:226:GLY:N	2.27	0.62
1:G:9:GLY:O	1:G:235:LEU:HA	2.00	0.62
1:G:213:TYR:HD2	1:G:234:PHE:CE1	2.18	0.62
1:L:218:ASN:HB2	1:L:221:ASN:OD1	1.99	0.62
1:A:139:ARG:NH1	1:A:142:GLU:OE1	2.33	0.62
1:A:144:ASN:O	1:A:148:LEU:HB2	2.00	0.62
1:O:83:MET:O	1:O:87:MET:HG3	1.99	0.62
1:O:197:PHE:HD2	1:O:206:ALA:HA	1.64	0.62
1:R:228:CYS:CB	1:R:231:ILE:CG1	2.77	0.62
1:E:174:SER:O	1:I:176:GLY:HA3	2.00	0.62
1:G:69:LEU:O	1:G:116:ARG:HD2	2.00	0.61
1:M:40:VAL:CG1	1:M:63:ALA:HB2	2.29	0.61
1:M:118:LEU:HB3	1:M:161:LEU:HD22	1.82	0.61
1:S:6:PRO:CD	1:S:36:SER:O	2.48	0.61
1:G:109:GLN:O	1:G:113:LYS:HG3	2.00	0.61
1:G:218:ASN:O	1:G:220:SER:N	2.33	0.61
1:I:5:ARG:NH2	1:I:35:ASP:O	2.33	0.61
1:L:64:ALA:HB3	1:L:92:VAL:HG23	1.80	0.61
1:R:71:GLY:HA2	1:R:116:ARG:HH21	1.65	0.61
1:S:79:THR:HG21	1:S:84:LEU:HD21	1.82	0.61
1:C:178:GLY:CA	1:R:175:ILE:HD13	2.21	0.61
1:E:171:PRO:CD	1:E:215:GLY:HA3	2.30	0.61
1:E:175:ILE:HA	1:I:176:GLY:CA	2.20	0.61
1:G:21:ILE:O	1:G:25:VAL:HG23	2.01	0.61
1:J:95:GLY:HA2	1:J:110:SER:OG	2.00	0.61
1:K:98:GLU:O	1:K:102:ILE:HB	2.00	0.61
1:L:251:ILE:HD13	1:L:254:LYS:HZ3	1.65	0.61
1:O:171:PRO:CD	1:O:214:GLY:O	2.46	0.61
1:S:246:MET:O	1:S:249:ILE:HB	2.00	0.61
1:A:145:ILE:HG23	1:A:196:TRP:CD1	2.35	0.61
1:G:213:TYR:CD2	1:G:234:PHE:CD1	2.88	0.61
1:M:228:CYS:HB2	1:M:231:ILE:CD1	2.30	0.61
1:P:95:GLY:O	1:P:127:CYS:HB2	2.00	0.61
1:Q:7:PHE:HE1	1:Q:38:ASP:CG	2.07	0.61
1:S:83:MET:HE1	1:T:14:CYS:O	2.00	0.61
1:A:31:HIS:NE2	1:A:250:ASP:OD1	2.31	0.61
1:M:111:ALA:HB1	1:M:151:LEU:HA	1.81	0.61
1:N:109:GLN:O	1:N:113:LYS:HG3	2.00	0.61
1:Q:9:GLY:HA2	1:Q:40:VAL:HG13	1.83	0.61
1:A:177:THR:OG1	1:A:179:VAL:HG13	2.00	0.61
1:C:240:SER:HA	1:C:245:PHE:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:98:GLU:OE2	1:P:74:ALA:HB1	2.01	0.61
1:R:225:LEU:CB	1:R:234:PHE:HE1	2.03	0.61
1:R:251:ILE:HD13	1:R:251:ILE:N	2.15	0.61
1:C:72:ASN:ND2	1:C:80:SER:OG	2.33	0.61
1:H:197:PHE:O	1:H:201:VAL:HB	2.00	0.61
1:J:132:LEU:HD22	1:J:177:THR:HG21	1.83	0.61
1:Q:89:LEU:CD1	1:Q:91:HIS:H	2.13	0.61
1:Q:197:PHE:CE1	1:Q:209:ILE:HD13	2.35	0.61
1:Q:234:PHE:CD2	1:Q:248:MET:HE3	2.34	0.61
1:R:15:ASN:OD1	1:R:15:ASN:N	2.34	0.61
1:R:60:LEU:O	1:R:61:ARG:HD2	2.00	0.61
1:R:61:ARG:HH22	1:R:90:LYS:HD3	1.64	0.61
1:S:95:GLY:O	1:S:127:CYS:HB2	1.99	0.61
1:Q:243:PRO:HA	1:Q:246:MET:CE	2.31	0.61
1:A:21:ILE:O	1:A:25:VAL:HG23	2.01	0.61
1:A:123:THR:HA	1:A:164:GLU:HG3	1.81	0.61
1:E:95:GLY:C	1:E:127:CYS:HB2	2.26	0.61
1:E:195:LYS:O	1:E:199:GLU:CG	2.49	0.61
1:J:48:LEU:O	1:J:52:ILE:HG13	2.01	0.61
1:R:156:GLY:O	1:R:159:LYS:CG	2.49	0.61
1:C:6:PRO:HB2	1:C:37:VAL:HG13	1.83	0.60
1:C:195:LYS:O	1:C:199:GLU:HG3	2.01	0.60
1:E:191:VAL:HG22	1:E:230:ASN:ND2	2.16	0.60
1:F:175:ILE:CD1	1:F:175:ILE:H	2.14	0.60
1:N:143:VAL:O	1:N:147:GLN:HG3	2.01	0.60
1:Q:166:VAL:HG22	1:Q:210:ARG:CZ	2.31	0.60
1:S:83:MET:O	1:S:87:MET:HG3	2.01	0.60
1:B:4:ARG:HG2	1:B:208:HIS:O	2.02	0.60
1:C:215:GLY:O	1:C:216:SER:C	2.41	0.60
1:D:194:ARG:HD3	1:D:206:ALA:O	2.01	0.60
1:H:109:GLN:O	1:H:113:LYS:HG3	2.01	0.60
1:B:98:GLU:O	1:B:102:ILE:HB	2.00	0.60
1:E:98:GLU:HB2	1:F:76:THR:HG22	1.83	0.60
1:G:213:TYR:CD2	1:G:234:PHE:HE1	2.18	0.60
1:I:4:ARG:NH1	1:I:232:ASP:OD1	2.34	0.60
1:K:155:LEU:HD12	1:K:162:TRP:CE2	2.37	0.60
1:K:251:ILE:O	1:K:255:THR:HB	2.02	0.60
1:P:148:LEU:HG	1:P:196:TRP:CZ3	2.36	0.60
1:S:92:VAL:HG12	1:S:124:VAL:HG22	1.84	0.60
1:T:185:GLN:O	1:T:189:VAL:HG23	2.01	0.60
1:D:8:ILE:HB	1:D:252:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:O	1:D:85:GLN:HG3	2.02	0.60
1:O:160:MET:O	1:O:163:LYS:HB2	2.00	0.60
1:P:195:LYS:O	1:P:199:GLU:HB2	2.02	0.60
1:R:157:GLU:OE1	1:R:157:GLU:HA	2.01	0.60
1:C:76:THR:N	1:D:98:GLU:OE1	2.33	0.60
1:I:4:ARG:HD2	1:I:208:HIS:HA	1.83	0.60
1:I:4:ARG:NH1	1:I:4:ARG:CB	2.64	0.60
1:R:173:TRP:CD1	1:R:173:TRP:H	2.19	0.60
1:A:218:ASN:ND2	1:A:220:SER:N	2.50	0.60
1:J:130:GLU:OE2	1:J:173:TRP:CD1	2.54	0.60
1:Q:201:VAL:HG12	1:Q:202:ALA:H	1.65	0.60
1:P:184:GLU:CD	1:P:184:GLU:H	2.10	0.60
1:R:183:PRO:HB2	1:R:224:LYS:HE2	1.84	0.60
1:R:225:LEU:HB3	1:R:234:PHE:CZ	2.35	0.60
1:S:7:PHE:O	1:S:233:GLY:HA3	2.00	0.60
1:T:243:PRO:HA	1:T:246:MET:CE	2.32	0.60
1:B:155:LEU:HD12	1:B:162:TRP:NE1	2.16	0.60
1:J:123:THR:HG23	1:J:164:GLU:O	2.02	0.60
1:L:236:VAL:HG11	1:L:239:ALA:HB3	1.82	0.60
1:Q:92:VAL:HG12	1:Q:124:VAL:HG22	1.84	0.60
1:T:11:ASN:ND2	1:T:13:LYS:HG3	2.16	0.60
1:T:157:GLU:OE1	1:T:157:GLU:HA	2.00	0.60
1:A:83:MET:O	1:A:87:MET:HG3	2.02	0.60
1:I:215:GLY:O	1:I:216:SER:C	2.45	0.60
1:J:244:GLU:OE1	1:J:244:GLU:N	2.28	0.60
1:K:151:LEU:O	1:K:155:LEU:HG	2.01	0.60
1:R:227:GLN:HA	1:R:227:GLN:NE2	2.15	0.60
1:T:250:ASP:O	1:T:253:THR:HB	2.02	0.60
1:F:174:SER:HB2	1:F:179:VAL:HG12	1.82	0.59
1:G:97:SER:CB	1:G:170:GLU:OE1	2.45	0.59
1:K:197:PHE:CD1	1:K:206:ALA:HA	2.37	0.59
1:Q:248:MET:C	1:Q:251:ILE:HG22	2.27	0.59
1:C:111:ALA:HB1	1:C:151:LEU:HA	1.84	0.59
1:I:98:GLU:OE1	1:J:76:THR:HG23	2.02	0.59
1:S:21:ILE:O	1:S:25:VAL:HG23	2.02	0.59
1:L:203:ALA:HB3	1:L:204:GLU:OE2	2.03	0.59
1:O:137:ALA:O	1:O:138:ASN:CB	2.49	0.59
1:I:11:ASN:ND2	1:J:76:THR:CG2	2.63	0.59
1:O:162:TRP:CH2	1:O:196:TRP:HH2	2.21	0.59
1:E:171:PRO:HB2	1:E:174:SER:OG	2.01	0.59
1:E:219:GLY:O	1:E:220:SER:CB	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:TRP:CE3	1:H:197:PHE:HE2	2.20	0.59
1:J:21:ILE:O	1:J:25:VAL:HG23	2.01	0.59
1:Q:69:LEU:O	1:Q:116:ARG:HD2	2.02	0.59
1:C:215:GLY:C	1:C:217:ALA:N	2.56	0.59
1:F:155:LEU:HD12	1:F:162:TRP:NE1	2.16	0.59
1:H:141:MET:O	1:H:145:ILE:HG12	2.02	0.59
1:I:78:GLU:OE1	1:I:78:GLU:HA	2.02	0.59
1:M:5:ARG:HH12	1:M:36:SER:C	2.11	0.59
1:Q:39:VAL:HG12	1:Q:60:LEU:HD12	1.84	0.59
1:C:171:PRO:HD2	1:C:214:GLY:O	2.02	0.59
1:R:149:GLU:HG2	1:R:196:TRP:HZ2	1.68	0.59
1:S:151:LEU:O	1:S:155:LEU:HD13	2.03	0.59
1:B:95:GLY:C	1:B:127:CYS:HB2	2.28	0.59
1:B:97:SER:O	1:B:101:ARG:HB2	2.03	0.59
1:F:13:LYS:N	1:F:65:GLN:HE22	2.01	0.59
1:F:218:ASN:O	1:F:221:ASN:OD1	2.20	0.59
1:I:250:ASP:O	1:I:254:LYS:HD3	2.03	0.59
1:L:236:VAL:CG1	1:L:239:ALA:HB3	2.33	0.59
1:M:244:GLU:O	1:M:247:THR:HB	2.03	0.59
1:A:143:VAL:O	1:A:147:GLN:HG3	2.03	0.59
1:C:187:GLU:OE1	1:C:228:CYS:HB3	2.02	0.59
1:K:222:ASP:OD1	1:K:234:PHE:CZ	2.55	0.59
1:M:7:PHE:HB2	1:M:210:ARG:HH11	1.68	0.59
1:O:222:ASP:OD1	1:O:225:LEU:HD12	2.03	0.59
1:R:239:ALA:O	1:R:245:PHE:HB2	2.03	0.59
1:R:250:ASP:HA	1:R:253:THR:HG22	1.85	0.59
1:B:217:ALA:HB1	1:B:222:ASP:CG	2.28	0.59
1:O:218:ASN:HD22	1:O:220:SER:N	1.90	0.59
1:S:246:MET:H	1:S:246:MET:HE3	1.67	0.59
1:D:159:LYS:C	1:D:161:LEU:N	2.61	0.58
1:E:171:PRO:HG2	1:E:215:GLY:CA	2.10	0.58
1:K:218:ASN:ND2	1:K:219:GLY:H	2.00	0.58
1:L:177:THR:CB	1:L:179:VAL:HG23	2.33	0.58
1:L:200:LYS:HD2	1:L:200:LYS:C	2.11	0.58
1:M:81:VAL:HG13	1:M:122:MET:SD	2.43	0.58
1:O:14:CYS:SG	1:P:78:GLU:O	2.53	0.58
1:Q:173:TRP:CZ3	1:Q:174:SER:HB3	2.37	0.58
1:K:165:VAL:O	1:K:209:ILE:CD1	2.49	0.58
1:K:195:LYS:O	1:K:199:GLU:HG3	2.03	0.58
1:N:21:ILE:O	1:N:25:VAL:HG23	2.02	0.58
1:E:171:PRO:HD2	1:E:214:GLY:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:244:GLU:O	1:L:245:PHE:C	2.43	0.58
1:P:221:ASN:OD1	1:P:222:ASP:N	2.36	0.58
1:F:196:TRP:O	1:F:200:LYS:HB2	2.03	0.58
1:M:13:LYS:N	1:M:65:GLN:HE22	2.01	0.58
1:P:159:LYS:O	1:P:162:TRP:HD1	1.85	0.58
1:Q:173:TRP:CE3	1:Q:174:SER:HB3	2.38	0.58
1:R:228:CYS:SG	1:R:231:ILE:HG13	2.43	0.58
1:B:97:SER:CB	1:B:170:GLU:OE1	2.51	0.58
1:B:171:PRO:HG3	1:B:215:GLY:HA2	1.83	0.58
1:D:37:VAL:CG1	1:D:252:LEU:HD21	2.33	0.58
1:F:108:GLU:O	1:F:112:LYS:HG3	2.04	0.58
1:L:8:ILE:HB	1:L:252:LEU:HD22	1.85	0.58
1:M:13:LYS:N	1:M:65:GLN:NE2	2.51	0.58
1:R:174:SER:O	1:R:175:ILE:HG22	2.04	0.58
1:G:187:GLU:O	1:G:191:VAL:HG23	2.03	0.58
1:I:130:GLU:OE2	1:I:135:ARG:NE	2.31	0.58
1:K:69:LEU:HD23	1:K:70:GLU:HG2	1.86	0.58
1:S:221:ASN:O	1:S:224:LYS:HG3	2.02	0.58
1:F:18:LEU:O	1:F:22:LYS:HG3	2.04	0.58
1:K:221:ASN:ND2	1:K:221:ASN:H	2.01	0.58
1:O:164:GLU:OE1	1:O:164:GLU:HA	2.02	0.58
1:A:74:ALA:HB1	1:B:98:GLU:OE2	2.04	0.58
1:E:171:PRO:O	1:E:175:ILE:HG13	2.03	0.58
1:K:130:GLU:OE1	1:K:169:TYR:HE1	1.85	0.58
1:Q:7:PHE:HE2	1:Q:210:ARG:HG3	1.67	0.58
1:L:18:LEU:O	1:L:22:LYS:HG3	2.04	0.58
1:M:225:LEU:O	1:M:231:ILE:CD1	2.52	0.58
1:Q:91:HIS:CD2	1:Q:123:THR:HG21	2.39	0.58
1:Q:183:PRO:HG3	1:Q:225:LEU:HD21	1.86	0.58
1:Q:218:ASN:N	1:Q:221:ASN:OD1	2.36	0.58
1:T:82:GLU:CD	1:T:116:ARG:HH12	2.12	0.58
1:C:187:GLU:OE2	1:C:229:PRO:HG2	2.04	0.58
1:E:190:HIS:ND1	1:E:211:ILE:HG22	2.17	0.58
1:F:13:LYS:N	1:F:65:GLN:NE2	2.52	0.58
1:J:11:ASN:HD22	1:J:13:LYS:HG3	1.68	0.58
1:M:194:ARG:HD3	1:M:206:ALA:O	2.03	0.58
1:Q:243:PRO:HA	1:Q:246:MET:HE2	1.86	0.58
1:R:225:LEU:CB	1:R:234:PHE:CZ	2.85	0.58
1:S:34:PRO:HG2	1:S:253:THR:OG1	2.02	0.58
1:M:83:MET:O	1:M:87:MET:HG3	2.04	0.57
1:O:197:PHE:HE2	1:O:205:GLY:C	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:247:THR:O	1:O:251:ILE:HD13	2.04	0.57
1:R:66:ASN:ND2	1:R:99:ARG:NE	2.51	0.57
1:A:160:MET:H	1:A:160:MET:HE3	1.68	0.57
1:E:128:VAL:HG11	1:E:148:LEU:HD13	1.85	0.57
1:I:81:VAL:O	1:I:85:GLN:HG3	2.04	0.57
1:O:100:ARG:NH1	1:O:128:VAL:HA	2.19	0.57
1:P:64:ALA:HB3	1:P:92:VAL:HG23	1.84	0.57
1:Q:248:MET:HA	1:Q:251:ILE:HG22	1.85	0.57
1:T:246:MET:HA	1:T:249:ILE:CD1	2.34	0.57
1:I:57:SER:HB3	1:I:60:LEU:HB3	1.86	0.57
1:O:139:ARG:HD2	1:O:142:GLU:OE2	2.03	0.57
1:R:12:PHE:O	1:R:15:ASN:OD1	2.23	0.57
1:R:66:ASN:ND2	1:R:99:ARG:CD	2.67	0.57
1:R:186:ALA:O	1:R:189:VAL:HG22	2.04	0.57
1:S:75:TRP:HD1	1:T:14:CYS:SG	2.28	0.57
1:A:7:PHE:O	1:A:233:GLY:HA3	2.05	0.57
1:H:95:GLY:O	1:H:100:ARG:HG3	2.04	0.57
1:K:195:LYS:CG	1:K:196:TRP:N	2.68	0.57
1:L:251:ILE:HA	1:L:254:LYS:HD2	1.86	0.57
1:O:195:LYS:O	1:O:199:GLU:HG3	2.04	0.57
1:R:15:ASN:ND2	1:R:241:LEU:HD11	2.19	0.57
1:S:46:VAL:HG23	1:S:47:HIS:CD2	2.38	0.57
1:C:135:ARG:HA	1:C:140:THR:HG22	1.87	0.57
1:F:218:ASN:HB2	1:F:220:SER:HG	1.69	0.57
1:I:4:ARG:CG	1:I:4:ARG:NH1	2.63	0.57
1:I:155:LEU:HD12	1:I:162:TRP:CE2	2.39	0.57
1:J:222:ASP:N	1:J:222:ASP:OD1	2.36	0.57
1:K:251:ILE:HA	1:K:254:LYS:HE3	1.85	0.57
1:L:221:ASN:HD22	1:L:221:ASN:C	2.11	0.57
1:P:68:TYR:CE2	1:P:70:GLU:HB2	2.39	0.57
1:S:186:ALA:HB2	1:S:213:TYR:CE1	2.40	0.57
1:A:222:ASP:HA	1:A:225:LEU:HB2	1.87	0.57
1:B:5:ARG:NH1	1:B:35:ASP:O	2.32	0.57
1:J:182:THR:CG2	1:J:184:GLU:OE1	2.53	0.57
1:T:137:ALA:O	1:T:138:ASN:HB3	2.04	0.57
1:I:48:LEU:HD23	1:I:89:LEU:HD11	1.86	0.57
1:Q:177:THR:O	1:Q:177:THR:HG23	2.05	0.57
1:I:4:ARG:CD	1:I:208:HIS:HA	2.34	0.57
1:Q:61:ARG:HH11	1:Q:61:ARG:CG	2.18	0.57
1:Q:62:ILE:O	1:Q:89:LEU:HD11	2.04	0.57
1:R:169:TYR:CE2	1:R:189:VAL:HG21	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:6:PRO:HG2	1:S:37:VAL:CA	2.29	0.57
1:G:9:GLY:O	1:G:235:LEU:HD12	2.05	0.57
1:K:160:MET:HA	1:K:163:LYS:HG2	1.87	0.57
1:R:51:ALA:HB1	1:R:62:ILE:HD13	1.86	0.57
1:R:69:LEU:HD23	1:R:69:LEU:N	2.18	0.57
1:I:76:THR:HG23	1:J:65:GLN:HB3	1.87	0.56
1:M:83:MET:HE2	1:N:47:HIS:CE1	2.40	0.56
1:P:130:GLU:HG3	1:P:144:ASN:HD21	1.68	0.56
1:S:25:VAL:HA	1:S:28:ILE:HG13	1.87	0.56
1:S:151:LEU:HD23	1:S:162:TRP:CH2	2.40	0.56
1:B:5:ARG:O	1:B:210:ARG:HD2	2.05	0.56
1:E:72:ASN:ND2	1:E:80:SER:OG	2.38	0.56
1:H:126:PHE:CZ	1:H:151:LEU:HD21	2.40	0.56
1:H:141:MET:HE3	1:H:145:ILE:HD11	1.87	0.56
1:I:236:VAL:CG1	1:I:239:ALA:HB3	2.35	0.56
1:M:105:GLU:HG2	1:M:110:SER:OG	2.04	0.56
1:T:239:ALA:O	1:T:245:PHE:HB2	2.05	0.56
1:C:57:SER:HB3	1:C:60:LEU:HB3	1.88	0.56
1:D:221:ASN:O	1:D:224:LYS:HG2	2.04	0.56
1:E:143:VAL:O	1:E:147:GLN:HG3	2.05	0.56
1:F:90:LYS:HD3	1:F:91:HIS:CE1	2.39	0.56
1:F:174:SER:OG	1:F:175:ILE:HD12	2.06	0.56
1:G:69:LEU:CD1	1:G:69:LEU:C	2.77	0.56
1:I:194:ARG:HD2	1:I:230:ASN:OD1	2.05	0.56
1:J:223:GLU:OE2	1:J:254:LYS:HE3	2.05	0.56
1:M:98:GLU:HG2	1:N:74:ALA:O	2.05	0.56
1:M:210:ARG:HG3	1:M:232:ASP:CB	2.36	0.56
1:P:145:ILE:O	1:P:149:GLU:HG2	2.05	0.56
1:Q:18:LEU:O	1:Q:22:LYS:HG3	2.05	0.56
1:Q:114:ALA:O	1:Q:118:LEU:HG	2.05	0.56
1:R:66:ASN:ND2	1:R:99:ARG:HD2	2.20	0.56
1:R:116:ARG:O	1:R:119:GLU:OE1	2.22	0.56
1:A:138:ASN:HD22	1:A:138:ASN:C	2.11	0.56
1:C:64:ALA:HB3	1:C:92:VAL:HG23	1.88	0.56
1:E:90:LYS:HG3	1:E:90:LYS:O	2.05	0.56
1:I:155:LEU:HD12	1:I:162:TRP:NE1	2.20	0.56
1:J:180:VAL:HG22	1:J:181:ALA:N	2.19	0.56
1:P:198:ALA:HA	1:P:202:ALA:O	2.06	0.56
1:S:31:HIS:CB	1:S:246:MET:HG2	2.36	0.56
1:C:95:GLY:HA2	1:C:110:SER:OG	2.05	0.56
1:E:141:MET:HA	1:E:141:MET:CE	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:VAL:O	1:G:193:LEU:HG	2.05	0.56
1:M:222:ASP:OD1	1:M:223:GLU:N	2.38	0.56
1:N:131:THR:OG1	1:N:134:GLU:HG3	2.06	0.56
1:O:220:SER:O	1:O:221:ASN:CB	2.52	0.56
1:P:145:ILE:HG13	1:P:196:TRP:CD1	2.41	0.56
1:R:63:ALA:CB	1:R:91:HIS:HB2	2.31	0.56
1:S:172:VAL:HA	1:S:175:ILE:CG1	2.34	0.56
1:A:139:ARG:NH1	1:A:142:GLU:CD	2.63	0.56
1:J:114:ALA:O	1:J:118:LEU:HG	2.05	0.56
1:Q:183:PRO:HG3	1:Q:225:LEU:HD23	1.87	0.56
1:R:81:VAL:HG13	1:R:122:MET:SD	2.46	0.56
1:E:141:MET:HE2	1:E:145:ILE:HD12	1.87	0.56
1:N:139:ARG:HD2	1:N:142:GLU:OE1	2.03	0.56
1:O:69:LEU:HD22	1:O:69:LEU:H	1.69	0.56
1:Q:248:MET:O	1:Q:251:ILE:CG2	2.54	0.56
1:D:221:ASN:O	1:D:224:LYS:CG	2.54	0.56
1:I:4:ARG:NH1	1:I:194:ARG:NH2	2.53	0.56
1:J:191:VAL:HG22	1:J:230:ASN:ND2	2.21	0.56
1:O:108:GLU:O	1:O:112:LYS:HB2	2.06	0.56
1:O:148:LEU:HD23	1:O:193:LEU:HD22	1.88	0.56
1:D:67:VAL:O	1:D:113:LYS:HD3	2.06	0.56
1:K:213:TYR:HD2	1:K:234:PHE:HE1	1.53	0.56
1:O:139:ARG:HD2	1:O:142:GLU:CD	2.31	0.56
1:P:135:ARG:HE	1:P:173:TRP:HZ2	1.52	0.56
1:R:216:SER:O	1:R:217:ALA:HB3	2.06	0.56
1:C:128:VAL:HG11	1:C:148:LEU:HD13	1.86	0.56
1:D:24:HIS:O	1:D:28:ILE:HG13	2.06	0.56
1:K:42:ALA:HB1	1:K:65:GLN:HG3	1.88	0.56
1:Q:21:ILE:O	1:Q:25:VAL:HG23	2.05	0.56
1:T:222:ASP:HA	1:T:225:LEU:HD12	1.88	0.56
1:A:218:ASN:ND2	1:A:221:ASN:H	2.05	0.55
1:C:215:GLY:O	1:C:217:ALA:N	2.39	0.55
1:F:17:SER:O	1:F:21:ILE:HG12	2.06	0.55
1:K:41:ILE:HG12	1:K:62:ILE:HD12	1.87	0.55
1:L:169:TYR:CE2	1:L:189:VAL:HG21	2.41	0.55
1:P:62:ILE:HD12	1:P:62:ILE:N	2.21	0.55
1:R:127:CYS:HB3	1:R:170:GLU:OE2	2.07	0.55
1:T:99:ARG:HA	1:T:103:MET:HB2	1.88	0.55
1:T:242:LYS:CB	1:T:243:PRO:HD2	2.35	0.55
1:D:40:VAL:HG22	1:D:61:ARG:HB2	1.88	0.55
1:J:90:LYS:HG2	1:J:90:LYS:O	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:LEU:HD22	1:J:161:LEU:HB2	1.88	0.55
1:P:197:PHE:HD1	1:P:206:ALA:HB2	1.71	0.55
1:Q:166:VAL:HG22	1:Q:210:ARG:NE	2.21	0.55
1:S:5:ARG:HH22	1:S:35:ASP:C	2.14	0.55
1:S:91:HIS:HA	1:S:123:THR:O	2.06	0.55
1:D:37:VAL:HG11	1:D:252:LEU:CD2	2.37	0.55
1:F:240:SER:HA	1:F:245:PHE:CD1	2.41	0.55
1:J:81:VAL:HG13	1:J:122:MET:SD	2.46	0.55
1:J:187:GLU:OE1	1:J:228:CYS:HB3	2.05	0.55
1:M:74:ALA:HB1	1:N:98:GLU:OE2	2.05	0.55
1:M:218:ASN:O	1:M:222:ASP:HB3	2.07	0.55
1:O:65:GLN:HB3	1:P:76:THR:CG2	2.36	0.55
1:O:160:MET:HG2	1:O:161:LEU:N	2.21	0.55
1:O:184:GLU:CD	1:O:184:GLU:H	2.14	0.55
1:Q:175:ILE:O	1:Q:176:GLY:C	2.49	0.55
1:R:66:ASN:HD22	1:R:99:ARG:CZ	2.19	0.55
1:S:74:ALA:HB1	1:T:98:GLU:OE2	2.06	0.55
1:S:253:THR:HG22	1:S:254:LYS:N	2.20	0.55
1:C:4:ARG:CG	1:C:207:GLN:O	2.53	0.55
1:G:77:GLY:HA3	1:H:99:ARG:HH11	1.70	0.55
1:G:225:LEU:O	1:G:228:CYS:HB2	2.05	0.55
1:S:145:ILE:HG23	1:S:196:TRP:CD1	2.42	0.55
1:A:218:ASN:HD22	1:A:220:SER:N	2.05	0.55
1:L:251:ILE:HD13	1:L:254:LYS:HD2	1.89	0.55
1:R:251:ILE:N	1:R:251:ILE:CD1	2.69	0.55
1:A:218:ASN:ND2	1:A:220:SER:H	2.05	0.55
1:E:175:ILE:HG12	1:I:176:GLY:O	2.07	0.55
1:F:174:SER:O	1:F:179:VAL:HB	2.06	0.55
1:G:236:VAL:HG21	1:G:248:MET:SD	2.46	0.55
1:K:213:TYR:CE2	1:K:215:GLY:HA2	2.41	0.55
1:P:247:THR:O	1:P:251:ILE:HD13	2.07	0.55
1:S:204:GLU:OE1	1:S:208:HIS:HE1	1.89	0.55
1:N:222:ASP:O	1:N:223:GLU:C	2.48	0.55
1:O:58:LYS:CG	1:O:59:GLN:CD	2.66	0.55
1:S:197:PHE:CD1	1:S:206:ALA:HA	2.42	0.55
1:T:7:PHE:C	1:T:7:PHE:CD1	2.85	0.55
1:T:81:VAL:O	1:T:85:GLN:HG3	2.05	0.55
1:F:9:GLY:HA2	1:F:40:VAL:O	2.07	0.55
1:G:229:PRO:HB2	1:G:230:ASN:HD22	1.71	0.55
1:M:141:MET:O	1:M:145:ILE:HB	2.07	0.55
1:N:130:GLU:HG2	1:N:130:GLU:O	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:PRO:HD2	1:C:207:GLN:HG2	1.87	0.55
1:C:98:GLU:OE1	1:D:76:THR:N	2.34	0.55
1:E:198:ALA:HB2	1:E:206:ALA:CB	2.37	0.55
1:I:37:VAL:HG11	1:I:252:LEU:HD23	1.88	0.55
1:I:132:LEU:O	1:I:136:LYS:HG3	2.06	0.55
1:Q:84:LEU:CB	1:Q:122:MET:HE1	2.37	0.55
1:S:55:ASN:OD1	1:S:60:LEU:HD23	2.07	0.55
1:B:66:ASN:ND2	1:B:66:ASN:C	2.60	0.55
1:C:173:TRP:O	1:C:177:THR:HG21	2.07	0.55
1:C:244:GLU:O	1:C:247:THR:HB	2.07	0.55
1:H:158:SER:HB2	1:H:161:LEU:HG	1.88	0.55
1:P:114:ALA:O	1:P:118:LEU:HG	2.07	0.55
1:R:85:GLN:HE22	1:R:120:LYS:HB3	1.71	0.55
1:R:228:CYS:HB2	1:R:231:ILE:HB	1.89	0.55
1:C:33:ILE:HB	1:C:59:GLN:HE21	1.72	0.54
1:I:236:VAL:HG11	1:I:239:ALA:HB3	1.89	0.54
1:Q:236:VAL:HG12	1:Q:240:SER:HB3	1.89	0.54
1:T:24:HIS:O	1:T:27:ALA:HB3	2.07	0.54
1:H:197:PHE:CZ	1:H:201:VAL:HG11	2.42	0.54
1:L:37:VAL:CG1	1:L:252:LEU:HD23	2.38	0.54
1:L:218:ASN:HB2	1:L:221:ASN:CG	2.31	0.54
1:O:58:LYS:CG	1:O:59:GLN:OE1	2.55	0.54
1:P:31:HIS:CE1	1:P:246:MET:HB3	2.42	0.54
1:Q:27:ALA:O	1:Q:30:ALA:HB3	2.07	0.54
1:A:137:ALA:HB3	1:A:139:ARG:HG3	1.90	0.54
1:I:67:VAL:O	1:I:113:LYS:HD3	2.07	0.54
1:Q:139:ARG:O	1:Q:143:VAL:HG23	2.07	0.54
1:R:15:ASN:ND2	1:R:241:LEU:CD1	2.70	0.54
1:S:72:ASN:ND2	1:S:80:SER:OG	2.40	0.54
1:A:99:ARG:HD2	1:B:76:THR:O	2.08	0.54
1:E:187:GLU:O	1:E:191:VAL:HG23	2.06	0.54
1:L:244:GLU:O	1:L:247:THR:N	2.40	0.54
1:O:98:GLU:O	1:O:102:ILE:HB	2.07	0.54
1:A:4:ARG:HH22	1:A:230:ASN:HA	1.73	0.54
1:E:4:ARG:NH2	1:E:229:PRO:O	2.41	0.54
1:F:40:VAL:HG22	1:F:61:ARG:HB2	1.90	0.54
1:G:137:ALA:HB3	1:G:139:ARG:HG3	1.90	0.54
1:L:90:LYS:HE3	1:L:91:HIS:HE1	1.73	0.54
1:N:141:MET:O	1:N:145:ILE:CG1	2.56	0.54
1:Q:79:THR:CG2	1:Q:84:LEU:HD21	2.36	0.54
1:S:5:ARG:HG2	1:S:6:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:115:LYS:HD2	1:S:154:GLU:O	2.08	0.54
1:S:197:PHE:HE2	1:S:209:ILE:HD13	1.72	0.54
1:T:64:ALA:CB	1:T:84:LEU:HD11	2.38	0.54
1:A:131:THR:HG22	1:A:132:LEU:N	2.22	0.54
1:C:47:HIS:CE1	1:D:83:MET:HG2	2.42	0.54
1:D:102:ILE:HD11	1:N:179:VAL:HA	1.88	0.54
1:E:169:TYR:CZ	1:E:189:VAL:HG11	2.42	0.54
1:G:173:TRP:CD1	1:G:173:TRP:H	2.25	0.54
1:P:24:HIS:O	1:P:28:ILE:HG13	2.07	0.54
1:Q:83:MET:O	1:Q:87:MET:HG2	2.07	0.54
1:A:108:GLU:OE2	1:A:112:LYS:NZ	2.40	0.54
1:D:218:ASN:HD21	1:D:220:SER:H	1.53	0.54
1:G:93:ILE:HD11	1:G:96:HIS:HB2	1.89	0.54
1:H:144:ASN:HB3	1:H:193:LEU:HD21	1.90	0.54
1:N:226:GLY:HA3	1:N:255:THR:HG21	1.87	0.54
1:O:132:LEU:HD22	1:O:177:THR:HB	1.90	0.54
1:P:162:TRP:HA	1:P:165:VAL:CG2	2.38	0.54
1:Q:7:PHE:CD1	1:Q:38:ASP:CB	2.87	0.54
1:Q:175:ILE:O	1:Q:177:THR:HB	2.06	0.54
1:T:44:SER:O	1:T:48:LEU:HD13	2.08	0.54
1:O:6:PRO:HB2	1:O:37:VAL:HG13	1.90	0.54
1:P:21:ILE:O	1:P:25:VAL:HG23	2.08	0.54
1:P:180:VAL:HG22	1:P:181:ALA:N	2.22	0.54
1:Q:73:GLY:N	1:R:14:CYS:SG	2.81	0.54
1:A:162:TRP:CE3	1:A:197:PHE:HE2	2.26	0.54
1:C:253:THR:HG22	1:C:254:LYS:N	2.23	0.54
1:F:219:GLY:HA2	1:F:222:ASP:OD2	2.08	0.54
1:G:145:ILE:O	1:G:149:GLU:HG2	2.08	0.54
1:M:5:ARG:NH2	1:M:35:ASP:O	2.40	0.54
1:M:18:LEU:HD23	1:M:47:HIS:HD2	1.72	0.54
1:M:170:GLU:CB	1:M:175:ILE:HD11	2.38	0.54
1:N:223:GLU:OE1	1:N:251:ILE:HD11	2.08	0.54
1:O:103:MET:CE	1:P:78:GLU:HG3	2.38	0.54
1:P:162:TRP:HA	1:P:165:VAL:HG23	1.90	0.54
1:Q:218:ASN:O	1:Q:221:ASN:OD1	2.26	0.54
1:A:111:ALA:HB1	1:A:151:LEU:HA	1.89	0.53
1:D:6:PRO:HB3	1:D:252:LEU:HD11	1.90	0.53
1:D:218:ASN:O	1:D:222:ASP:HB3	2.07	0.53
1:G:123:THR:HA	1:G:164:GLU:HB3	1.89	0.53
1:Q:31:HIS:HE2	1:Q:250:ASP:CG	2.16	0.53
1:S:5:ARG:CG	1:S:6:PRO:HD2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:235:LEU:HD23	1:T:235:LEU:C	2.33	0.53
1:A:4:ARG:HD2	1:A:207:GLN:O	2.08	0.53
1:H:98:GLU:O	1:H:102:ILE:HB	2.08	0.53
1:L:233:GLY:HA2	1:L:252:LEU:HD11	1.91	0.53
1:Q:55:ASN:HD22	1:Q:62:ILE:HD13	1.73	0.53
1:T:48:LEU:O	1:T:52:ILE:HD12	2.09	0.53
1:H:24:HIS:O	1:H:28:ILE:HG13	2.09	0.53
1:K:115:LYS:HG3	1:K:155:LEU:HD23	1.90	0.53
1:O:66:ASN:ND2	1:O:67:VAL:H	2.07	0.53
1:Q:63:ALA:HB2	1:Q:91:HIS:HB2	1.90	0.53
1:S:6:PRO:CG	1:S:37:VAL:HG12	2.38	0.53
1:T:245:PHE:HA	1:T:248:MET:HG3	1.91	0.53
1:A:72:ASN:HD22	1:A:72:ASN:N	2.06	0.53
1:F:145:ILE:HG23	1:F:196:TRP:CD1	2.44	0.53
1:G:213:TYR:CB	1:G:234:PHE:CE1	2.88	0.53
1:I:12:PHE:O	1:I:13:LYS:HB2	2.07	0.53
1:J:203:ALA:HB3	1:M:200:LYS:HE3	1.91	0.53
1:J:217:ALA:O	1:J:248:MET:CE	2.57	0.53
1:O:46:VAL:HB	1:P:87:MET:SD	2.48	0.53
1:R:83:MET:O	1:R:86:ASP:HB3	2.07	0.53
1:S:224:LYS:HG3	1:S:225:LEU:H	1.73	0.53
1:B:144:ASN:HD22	1:B:193:LEU:CD2	2.21	0.53
1:D:158:SER:CB	1:D:160:MET:HE2	2.37	0.53
1:E:171:PRO:HG3	1:E:213:TYR:CE1	2.44	0.53
1:H:85:GLN:HE22	1:H:120:LYS:HB3	1.74	0.53
1:L:69:LEU:CD2	1:L:70:GLU:HG2	2.35	0.53
1:N:84:LEU:O	1:N:89:LEU:HB2	2.09	0.53
1:Q:31:HIS:O	1:Q:33:ILE:HG13	2.09	0.53
1:Q:92:VAL:CG1	1:Q:124:VAL:HG22	2.38	0.53
1:R:225:LEU:C	1:R:234:PHE:CZ	2.80	0.53
1:S:38:ASP:OD2	1:S:210:ARG:NH2	2.40	0.53
1:S:83:MET:HG2	1:T:46:VAL:HG21	1.91	0.53
1:S:151:LEU:HD23	1:S:162:TRP:CZ3	2.43	0.53
1:C:4:ARG:HG2	1:C:207:GLN:O	2.07	0.53
1:E:96:HIS:HB3	1:F:76:THR:HG21	1.89	0.53
1:E:116:ARG:NH2	1:E:120:LYS:HZ1	2.06	0.53
1:E:187:GLU:OE1	1:E:228:CYS:HB3	2.09	0.53
1:F:67:VAL:O	1:F:113:LYS:HD3	2.09	0.53
1:J:84:LEU:HD22	1:J:89:LEU:HD12	1.90	0.53
1:J:251:ILE:HD12	1:J:254:LYS:NZ	2.23	0.53
1:L:24:HIS:O	1:L:28:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:182:THR:H	1:O:185:GLN:NE2	2.05	0.53
1:S:158:SER:HB2	1:S:161:LEU:CD2	2.29	0.53
1:F:95:GLY:O	1:F:127:CYS:HB2	2.09	0.53
1:G:96:HIS:CE1	1:G:98:GLU:HG3	2.44	0.53
1:K:116:ARG:O	1:K:119:GLU:HB2	2.08	0.53
1:M:41:ILE:HG12	1:M:60:LEU:HD11	1.91	0.53
1:P:37:VAL:HG21	1:P:253:THR:OG1	2.09	0.53
1:Q:81:VAL:HG23	1:Q:116:ARG:HH11	1.74	0.53
1:C:4:ARG:HD3	1:C:207:GLN:O	2.09	0.53
1:E:194:ARG:NH1	1:E:211:ILE:HD12	2.24	0.53
1:I:148:LEU:HG	1:I:196:TRP:CZ3	2.43	0.53
1:L:155:LEU:HD22	1:L:161:LEU:HB2	1.91	0.53
1:M:18:LEU:O	1:M:22:LYS:HG3	2.07	0.53
1:O:66:ASN:ND2	1:O:67:VAL:N	2.56	0.53
1:P:8:ILE:HB	1:P:252:LEU:HD22	1.91	0.53
1:Q:12:PHE:HB2	1:Q:42:ALA:O	2.09	0.53
1:S:2:PRO:HD2	1:S:207:GLN:HB2	1.91	0.53
1:L:34:PRO:HG3	1:L:253:THR:OG1	2.08	0.53
1:O:139:ARG:CB	1:O:142:GLU:HB3	2.39	0.53
1:Q:242:LYS:O	1:Q:245:PHE:HB3	2.09	0.53
1:A:160:MET:H	1:A:160:MET:CE	2.22	0.53
1:E:130:GLU:OE2	1:E:140:THR:HB	2.09	0.53
1:F:236:VAL:CG1	1:F:239:ALA:HB3	2.39	0.53
1:G:5:ARG:HG3	1:G:36:SER:O	2.09	0.53
1:H:187:GLU:OE1	1:H:228:CYS:HB3	2.08	0.53
1:J:69:LEU:HB3	1:J:113:LYS:HG2	1.91	0.53
1:K:69:LEU:CD2	1:K:70:GLU:HG2	2.39	0.53
1:L:174:SER:O	1:L:215:GLY:HA3	2.09	0.53
1:N:255:THR:O	1:N:255:THR:HG22	2.09	0.53
1:Q:221:ASN:O	1:Q:225:LEU:HG	2.09	0.53
1:S:99:ARG:NH2	1:T:78:GLU:OE2	2.42	0.53
1:S:139:ARG:O	1:S:143:VAL:HG23	2.09	0.53
1:A:109:GLN:O	1:A:113:LYS:HG3	2.08	0.52
1:K:187:GLU:O	1:K:191:VAL:HG23	2.09	0.52
1:L:155:LEU:HD12	1:L:162:TRP:NE1	2.23	0.52
1:O:21:ILE:O	1:O:25:VAL:HG23	2.08	0.52
1:P:131:THR:HG22	1:P:172:VAL:HG11	1.91	0.52
1:Q:99:ARG:HD3	1:R:76:THR:O	2.09	0.52
1:R:242:LYS:HB3	1:R:243:PRO:HD2	1.91	0.52
1:T:127:CYS:HA	1:T:168:ALA:O	2.09	0.52
1:A:115:LYS:CE	1:A:119:GLU:OE2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:GLY:HA3	1:N:174:SER:O	2.09	0.52
1:N:139:ARG:HD2	1:N:142:GLU:CD	2.35	0.52
1:O:184:GLU:CD	1:O:184:GLU:N	2.67	0.52
1:Q:84:LEU:HB2	1:Q:122:MET:HE1	1.91	0.52
1:S:241:LEU:HD23	1:S:241:LEU:N	2.24	0.52
1:T:115:LYS:HG2	1:T:155:LEU:HG	1.90	0.52
1:B:213:TYR:HB2	1:B:231:ILE:HD13	1.91	0.52
1:C:76:THR:CG2	1:D:13:LYS:HD3	2.36	0.52
1:E:206:ALA:O	1:E:209:ILE:HG22	2.09	0.52
1:Q:75:TRP:NE1	1:R:14:CYS:SG	2.82	0.52
1:S:17:SER:O	1:S:21:ILE:HG12	2.09	0.52
1:T:37:VAL:HG11	1:T:252:LEU:HD23	1.91	0.52
1:D:180:VAL:HG13	1:D:181:ALA:N	2.24	0.52
1:E:69:LEU:HD23	1:E:70:GLU:HG2	1.91	0.52
1:E:178:GLY:HA3	1:I:172:VAL:CG1	2.39	0.52
1:I:13:LYS:HA	1:J:76:THR:HG22	1.90	0.52
1:K:44:SER:HB2	1:L:83:MET:HE1	1.92	0.52
1:O:217:ALA:HB1	1:O:222:ASP:OD1	2.09	0.52
1:E:236:VAL:CG1	1:E:239:ALA:HB3	2.39	0.52
1:J:56:THR:HG22	1:K:19:ASP:OD1	2.10	0.52
1:Q:183:PRO:HA	1:Q:225:LEU:HD22	1.91	0.52
1:R:11:ASN:OD1	1:R:13:LYS:N	2.42	0.52
1:S:6:PRO:CG	1:S:37:VAL:HA	2.31	0.52
1:S:185:GLN:HA	1:S:188:GLU:OE1	2.10	0.52
1:A:90:LYS:HE2	1:A:123:THR:OG1	2.09	0.52
1:A:115:LYS:HE3	1:A:119:GLU:OE2	2.10	0.52
1:A:131:THR:HG22	1:A:132:LEU:H	1.74	0.52
1:F:244:GLU:O	1:F:248:MET:HG3	2.09	0.52
1:P:171:PRO:HB2	1:P:174:SER:OG	2.09	0.52
1:R:81:VAL:HG21	1:R:116:ARG:HG2	1.92	0.52
1:A:68:TYR:HD1	1:A:78:GLU:OE1	1.93	0.52
1:F:236:VAL:HG11	1:F:239:ALA:HB3	1.91	0.52
1:I:4:ARG:HH12	1:I:232:ASP:CG	2.17	0.52
1:J:7:PHE:O	1:J:233:GLY:HA3	2.10	0.52
1:P:221:ASN:OD1	1:P:221:ASN:C	2.53	0.52
1:S:55:ASN:HB2	1:S:62:ILE:HD11	1.89	0.52
1:S:182:THR:OG1	1:S:185:GLN:HB2	2.10	0.52
1:T:213:TYR:CD2	1:T:225:LEU:HD13	2.45	0.52
1:B:4:ARG:HD3	1:B:207:GLN:O	2.10	0.52
1:C:84:LEU:HD22	1:C:89:LEU:HD12	1.90	0.52
1:E:217:ALA:CB	1:I:178:GLY:HA3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:VAL:HG11	1:I:252:LEU:CD2	2.40	0.52
1:L:12:PHE:HB2	1:L:42:ALA:O	2.08	0.52
1:P:194:ARG:HE	1:P:230:ASN:HD22	1.58	0.52
1:S:118:LEU:HD13	1:S:161:LEU:CD1	2.39	0.52
1:E:222:ASP:HB2	1:E:251:ILE:HG21	1.91	0.52
1:F:179:VAL:HG12	1:F:180:VAL:N	2.24	0.52
1:M:83:MET:HE1	1:N:44:SER:HB2	1.91	0.52
1:Q:7:PHE:HD1	1:Q:38:ASP:CB	2.13	0.52
1:C:68:TYR:HB2	1:C:78:GLU:HB3	1.92	0.52
1:G:69:LEU:HD12	1:G:70:GLU:N	2.24	0.52
1:I:13:LYS:HG2	1:J:74:ALA:HA	1.93	0.52
1:I:69:LEU:HB3	1:I:113:LYS:HG2	1.91	0.52
1:M:44:SER:OG	1:N:83:MET:HE1	2.10	0.52
1:S:171:PRO:HA	1:S:173:TRP:NE1	2.23	0.52
1:A:13:LYS:N	1:A:65:GLN:NE2	2.58	0.51
1:F:155:LEU:HD12	1:F:162:TRP:CE2	2.45	0.51
1:G:244:GLU:O	1:G:247:THR:HB	2.10	0.51
1:J:11:ASN:HD21	1:J:13:LYS:HG3	1.72	0.51
1:M:41:ILE:O	1:M:43:PRO:HD3	2.09	0.51
1:O:61:ARG:NE	1:O:62:ILE:H	2.03	0.51
1:O:103:MET:HE1	1:P:78:GLU:CG	2.40	0.51
1:R:161:LEU:C	1:R:163:LYS:N	2.68	0.51
1:B:139:ARG:HD2	1:B:142:GLU:OE1	2.10	0.51
1:C:134:GLU:O	1:C:139:ARG:HG3	2.09	0.51
1:F:69:LEU:HB3	1:F:113:LYS:HG2	1.91	0.51
1:G:83:MET:O	1:G:87:MET:HG3	2.10	0.51
1:H:130:GLU:OE2	1:H:140:THR:HG23	2.10	0.51
1:I:4:ARG:HB2	1:I:4:ARG:NH1	2.24	0.51
1:J:21:ILE:HG13	1:J:47:HIS:HB3	1.92	0.51
1:N:141:MET:O	1:N:145:ILE:HG13	2.10	0.51
1:R:174:SER:C	1:R:175:ILE:CG2	2.83	0.51
1:R:175:ILE:O	1:R:177:THR:HG23	2.10	0.51
1:T:13:LYS:H	1:T:65:GLN:NE2	2.08	0.51
1:A:6:PRO:HB2	1:A:37:VAL:HG22	1.92	0.51
1:E:46:VAL:HB	1:F:87:MET:SD	2.51	0.51
1:G:41:ILE:HG23	1:G:60:LEU:HD11	1.91	0.51
1:Q:165:VAL:C	1:Q:210:ARG:HE	2.18	0.51
1:R:128:VAL:HG11	1:R:148:LEU:HD13	1.92	0.51
1:R:175:ILE:CG2	1:R:177:THR:OG1	2.57	0.51
1:S:61:ARG:HH22	1:S:90:LYS:HB2	1.75	0.51
1:A:246:MET:HA	1:A:249:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:GLU:HG2	1:C:143:VAL:HG21	1.92	0.51
1:G:71:GLY:O	1:G:75:TRP:NE1	2.44	0.51
1:I:4:ARG:HH11	1:I:4:ARG:CB	2.22	0.51
1:I:194:ARG:HH12	1:I:211:ILE:HG13	1.74	0.51
1:L:222:ASP:OD2	1:L:248:MET:CE	2.46	0.51
1:R:15:ASN:HD21	1:R:241:LEU:CD1	2.21	0.51
1:S:210:ARG:NH1	1:S:210:ARG:CG	2.55	0.51
1:A:77:GLY:H	1:B:65:GLN:HE21	1.59	0.51
1:A:239:ALA:HA	1:A:242:LYS:HG2	1.91	0.51
1:C:24:HIS:NE2	1:C:240:SER:O	2.42	0.51
1:F:134:GLU:OE1	1:F:143:VAL:HG11	2.10	0.51
1:F:181:ALA:HB3	1:F:213:TYR:OH	2.11	0.51
1:M:174:SER:HA	1:M:179:VAL:O	2.10	0.51
1:M:228:CYS:CB	1:M:231:ILE:HD12	2.38	0.51
1:N:199:GLU:O	1:N:200:LYS:HD2	2.11	0.51
1:Q:95:GLY:C	1:Q:127:CYS:HB2	2.36	0.51
1:R:194:ARG:NH1	1:R:209:ILE:HG23	2.23	0.51
1:S:72:ASN:ND2	1:S:83:MET:HE3	2.26	0.51
1:S:160:MET:O	1:S:163:LYS:HB3	2.10	0.51
1:B:37:VAL:CG1	1:B:252:LEU:HD23	2.41	0.51
1:G:213:TYR:CB	1:G:234:PHE:CD1	2.80	0.51
1:H:145:ILE:HG23	1:H:196:TRP:CD1	2.45	0.51
1:J:221:ASN:OD1	1:J:222:ASP:N	2.43	0.51
1:P:81:VAL:O	1:P:85:GLN:HG3	2.11	0.51
1:S:112:LYS:O	1:S:116:ARG:HB2	2.11	0.51
1:S:202:ALA:O	1:S:206:ALA:HB2	2.11	0.51
1:T:106:THR:OG1	1:T:109:GLN:HG3	2.11	0.51
1:B:187:GLU:O	1:B:191:VAL:HG23	2.11	0.51
1:C:24:HIS:O	1:C:28:ILE:HG13	2.10	0.51
1:R:68:TYR:CG	1:R:78:GLU:HG3	2.46	0.51
1:S:108:GLU:O	1:S:112:LYS:HG3	2.10	0.51
1:A:159:LYS:O	1:A:162:TRP:HB2	2.11	0.51
1:E:141:MET:HE2	1:E:145:ILE:CD1	2.40	0.51
1:I:4:ARG:NH1	1:I:232:ASP:CG	2.69	0.51
1:K:173:TRP:CD1	1:K:173:TRP:H	2.28	0.51
1:P:135:ARG:NE	1:P:173:TRP:CZ2	2.78	0.51
1:Q:7:PHE:HE2	1:Q:210:ARG:HH11	1.59	0.51
1:A:155:LEU:HD12	1:A:162:TRP:NE1	2.26	0.51
1:B:171:PRO:HB2	1:B:174:SER:OG	2.10	0.51
1:D:139:ARG:O	1:D:143:VAL:HG23	2.10	0.51
1:E:4:ARG:CD	1:E:207:GLN:O	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:67:VAL:O	1:J:113:LYS:HD3	2.10	0.51
1:K:187:GLU:HB2	1:K:228:CYS:SG	2.51	0.51
1:K:209:ILE:HD12	1:K:210:ARG:H	1.75	0.51
1:L:135:ARG:O	1:L:138:ASN:HA	2.11	0.51
1:L:184:GLU:H	1:L:184:GLU:CD	2.19	0.51
1:T:158:SER:HB3	1:T:161:LEU:HG	1.93	0.51
1:C:58:LYS:HB2	1:C:59:GLN:OE1	2.11	0.51
1:D:161:LEU:C	1:D:163:LYS:H	2.19	0.51
1:M:213:TYR:CE2	1:M:214:GLY:O	2.64	0.51
1:O:76:THR:CG2	1:P:65:GLN:HB3	2.39	0.51
1:Q:197:PHE:HD2	1:Q:206:ALA:CA	2.22	0.51
1:S:31:HIS:HB2	1:S:246:MET:HG2	1.93	0.51
1:A:172:VAL:CA	1:A:175:ILE:HG13	2.41	0.50
1:E:190:HIS:CE1	1:E:211:ILE:HG22	2.46	0.50
1:F:128:VAL:HG11	1:F:148:LEU:HD13	1.92	0.50
1:G:150:ALA:O	1:G:154:GLU:HG2	2.11	0.50
1:Q:89:LEU:HD12	1:Q:91:HIS:H	1.74	0.50
1:R:187:GLU:OE2	1:R:230:ASN:N	2.44	0.50
1:T:187:GLU:OE2	1:T:229:PRO:HG2	2.10	0.50
1:A:172:VAL:CG1	1:A:175:ILE:HD12	2.37	0.50
1:D:69:LEU:O	1:D:116:ARG:HD2	2.10	0.50
1:B:2:PRO:HB3	1:B:207:GLN:HG2	1.93	0.50
1:B:244:GLU:O	1:B:247:THR:HB	2.11	0.50
1:G:82:GLU:OE1	1:G:82:GLU:N	2.44	0.50
1:L:137:ALA:O	1:L:138:ASN:CB	2.59	0.50
1:P:134:GLU:CD	1:P:143:VAL:HG21	2.37	0.50
1:T:108:GLU:OE2	1:T:112:LYS:HE3	2.10	0.50
1:A:218:ASN:H	1:A:222:ASP:CG	2.18	0.50
1:E:6:PRO:HB2	1:E:37:VAL:HG13	1.92	0.50
1:E:176:GLY:HA3	1:I:132:LEU:HB2	1.93	0.50
1:E:254:LYS:C	1:E:255:THR:HG1	2.15	0.50
1:F:218:ASN:C	1:F:220:SER:N	2.65	0.50
1:G:37:VAL:HG12	1:G:38:ASP:N	2.26	0.50
1:I:13:LYS:HG3	1:J:76:THR:HG23	1.92	0.50
1:N:70:GLU:OE1	1:N:70:GLU:HA	2.12	0.50
1:O:139:ARG:NH1	1:O:142:GLU:OE2	2.44	0.50
1:S:173:TRP:H	1:S:173:TRP:HD1	1.49	0.50
1:E:190:HIS:HE2	1:E:213:TYR:CB	2.14	0.50
1:L:180:VAL:HG22	1:L:181:ALA:N	2.26	0.50
1:L:206:ALA:O	1:L:209:ILE:HG22	2.12	0.50
1:N:196:TRP:O	1:N:200:LYS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:24:HIS:O	1:R:27:ALA:HB3	2.11	0.50
1:D:37:VAL:HG13	1:D:252:LEU:HD21	1.94	0.50
1:J:251:ILE:HD12	1:J:254:LYS:HZ1	1.76	0.50
1:O:224:LYS:O	1:O:227:GLN:HB2	2.11	0.50
1:I:4:ARG:NE	1:I:207:GLN:O	2.43	0.50
1:I:51:ALA:HB1	1:I:62:ILE:HD12	1.94	0.50
1:I:141:MET:CE	1:I:192:GLY:HA3	2.42	0.50
1:K:152:GLY:HA2	1:K:162:TRP:HZ2	1.77	0.50
1:K:174:SER:HA	1:K:179:VAL:O	2.11	0.50
1:K:221:ASN:C	1:K:221:ASN:HD22	2.20	0.50
1:M:18:LEU:HD23	1:M:47:HIS:CD2	2.47	0.50
1:P:137:ALA:O	1:P:138:ASN:HB3	2.11	0.50
1:Q:39:VAL:HG12	1:Q:60:LEU:CD1	2.41	0.50
1:R:91:HIS:CD2	1:R:123:THR:CG2	2.94	0.50
1:R:227:GLN:HE21	1:R:227:GLN:CA	2.21	0.50
1:S:7:PHE:CD1	1:S:7:PHE:C	2.87	0.50
1:T:7:PHE:CD1	1:T:8:ILE:N	2.80	0.50
1:T:64:ALA:HB2	1:T:84:LEU:HD11	1.94	0.50
1:E:194:ARG:CZ	1:E:211:ILE:HD12	2.42	0.50
1:F:21:ILE:HG13	1:F:47:HIS:HB3	1.93	0.50
1:M:37:VAL:HG12	1:M:38:ASP:N	2.25	0.50
1:H:147:GLN:O	1:H:151:LEU:HD13	2.12	0.50
1:K:218:ASN:H	1:K:221:ASN:HD21	1.59	0.50
1:M:9:GLY:HA2	1:M:40:VAL:O	2.12	0.50
1:M:17:SER:O	1:M:21:ILE:HG12	2.12	0.50
1:S:7:PHE:HD1	1:S:7:PHE:C	2.19	0.50
1:D:96:HIS:CE1	1:D:98:GLU:CD	2.90	0.49
1:E:134:GLU:HB3	1:E:143:VAL:HG21	1.94	0.49
1:E:198:ALA:HB2	1:E:206:ALA:HB2	1.93	0.49
1:F:99:ARG:HA	1:F:103:MET:HB2	1.93	0.49
1:F:184:GLU:H	1:F:184:GLU:CD	2.20	0.49
1:K:42:ALA:O	1:K:65:GLN:NE2	2.44	0.49
1:Q:166:VAL:HG23	1:Q:210:ARG:NH2	2.27	0.49
1:C:46:VAL:HB	1:D:87:MET:SD	2.53	0.49
1:H:100:ARG:NH2	1:H:126:PHE:CE2	2.80	0.49
1:H:156:GLY:O	1:H:159:LYS:HG2	2.12	0.49
1:I:40:VAL:HG22	1:I:61:ARG:HB2	1.94	0.49
1:J:250:ASP:O	1:J:254:LYS:HG2	2.12	0.49
1:K:209:ILE:HD12	1:K:210:ARG:N	2.27	0.49
1:L:251:ILE:HA	1:L:254:LYS:CD	2.42	0.49
1:O:58:LYS:CD	1:O:59:GLN:OE1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:106:THR:OG1	1:P:109:GLN:HG3	2.12	0.49
1:D:197:PHE:HD1	1:D:206:ALA:HB2	1.78	0.49
1:H:167:ILE:HB	1:H:211:ILE:HG23	1.94	0.49
1:I:149:GLU:O	1:I:153:LYS:N	2.42	0.49
1:K:40:VAL:CG1	1:K:63:ALA:HB2	2.42	0.49
1:K:213:TYR:O	1:K:215:GLY:N	2.36	0.49
1:M:5:ARG:O	1:M:210:ARG:NH1	2.45	0.49
1:N:190:HIS:ND1	1:N:211:ILE:HG22	2.28	0.49
1:O:67:VAL:HG22	1:O:68:TYR:H	1.77	0.49
1:P:42:ALA:HB1	1:P:65:GLN:HG2	1.93	0.49
1:Q:33:ILE:HB	1:Q:59:GLN:HE21	1.76	0.49
1:S:95:GLY:C	1:S:127:CYS:HB2	2.37	0.49
1:S:243:PRO:O	1:S:246:MET:HE3	2.13	0.49
1:A:251:ILE:O	1:A:255:THR:HB	2.12	0.49
1:H:126:PHE:CD2	1:H:151:LEU:HD21	2.47	0.49
1:K:150:ALA:O	1:K:154:GLU:HG2	2.12	0.49
1:L:169:TYR:CZ	1:L:189:VAL:HG21	2.47	0.49
1:N:184:GLU:H	1:N:184:GLU:CD	2.21	0.49
1:N:218:ASN:HD22	1:N:221:ASN:HD22	1.61	0.49
1:O:103:MET:HE1	1:P:78:GLU:HG3	1.94	0.49
1:P:141:MET:O	1:P:145:ILE:HB	2.12	0.49
1:Q:68:TYR:HB2	1:Q:78:GLU:HB3	1.94	0.49
1:Q:248:MET:CA	1:Q:251:ILE:HG22	2.41	0.49
1:S:75:TRP:HD1	1:T:14:CYS:CB	2.25	0.49
1:S:106:THR:HG23	1:S:109:GLN:CD	2.37	0.49
1:N:139:ARG:NH1	1:N:143:VAL:CG2	2.76	0.49
1:P:155:LEU:HD22	1:P:161:LEU:HB2	1.94	0.49
1:P:172:VAL:HG12	1:P:173:TRP:N	2.27	0.49
1:Q:4:ARG:HD2	1:Q:232:ASP:CG	2.37	0.49
1:R:24:HIS:O	1:R:28:ILE:HG13	2.12	0.49
1:S:195:LYS:HD3	1:S:199:GLU:OE2	2.13	0.49
1:H:64:ALA:HB3	1:H:92:VAL:HG23	1.93	0.49
1:J:109:GLN:O	1:J:113:LYS:HG3	2.13	0.49
1:J:180:VAL:CG2	1:J:181:ALA:N	2.75	0.49
1:K:84:LEU:CD1	1:K:122:MET:HE1	2.42	0.49
1:L:99:ARG:HA	1:L:103:MET:SD	2.53	0.49
1:L:149:GLU:HA	1:L:149:GLU:OE1	2.12	0.49
1:O:218:ASN:HB3	1:O:220:SER:O	2.12	0.49
1:R:36:SER:OG	1:R:37:VAL:HG23	2.12	0.49
1:R:246:MET:HA	1:R:249:ILE:CD1	2.35	0.49
1:S:6:PRO:CG	1:S:36:SER:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:7:PHE:CE1	1:S:40:VAL:CG2	2.95	0.49
1:T:118:LEU:HD13	1:T:155:LEU:HD11	1.94	0.49
1:B:66:ASN:HD22	1:B:67:VAL:H	0.58	0.49
1:B:128:VAL:HG11	1:B:148:LEU:HD13	1.95	0.49
1:F:171:PRO:HG2	1:F:213:TYR:OH	2.11	0.49
1:J:132:LEU:HD22	1:J:177:THR:CG2	2.41	0.49
1:N:98:GLU:O	1:N:102:ILE:HB	2.12	0.49
1:P:180:VAL:HG22	1:P:181:ALA:H	1.78	0.49
1:Q:236:VAL:CG1	1:Q:240:SER:N	2.76	0.49
1:S:2:PRO:HD2	1:S:207:GLN:CB	2.42	0.49
1:D:218:ASN:ND2	1:D:220:SER:N	2.56	0.49
1:D:222:ASP:HA	1:D:225:LEU:HD12	1.94	0.49
1:G:9:GLY:C	1:G:235:LEU:HD12	2.37	0.49
1:I:141:MET:HE1	1:I:192:GLY:HA3	1.94	0.49
1:O:221:ASN:OD1	1:O:221:ASN:O	2.31	0.49
1:T:182:THR:OG1	1:T:185:GLN:HG3	2.12	0.49
1:T:227:GLN:NE2	1:T:255:THR:HG22	2.28	0.49
1:A:132:LEU:HG	1:A:136:LYS:HE3	1.95	0.49
1:B:167:ILE:O	1:B:211:ILE:HA	2.13	0.49
1:M:79:THR:HG21	1:M:84:LEU:HD21	1.95	0.49
1:M:164:GLU:HA	1:M:164:GLU:OE1	2.13	0.49
1:P:55:ASN:HD22	1:P:62:ILE:CD1	2.25	0.49
1:Q:186:ALA:HB2	1:Q:213:TYR:CE1	2.48	0.49
1:S:221:ASN:CA	1:S:224:LYS:HE2	2.43	0.49
1:A:36:SER:HB3	1:G:160:MET:HE1	1.95	0.49
1:E:214:GLY:HA3	1:E:235:LEU:O	2.13	0.49
1:F:132:LEU:O	1:F:136:LYS:HB2	2.13	0.49
1:J:219:GLY:O	1:J:222:ASP:OD1	2.30	0.49
1:L:137:ALA:HB3	1:L:139:ARG:HG3	1.95	0.49
1:L:177:THR:C	1:L:179:VAL:H	2.20	0.49
1:L:218:ASN:CB	1:L:221:ASN:ND2	2.76	0.49
1:M:240:SER:HA	1:M:245:PHE:HB2	1.95	0.49
1:Q:198:ALA:HB2	1:Q:206:ALA:HB2	1.95	0.49
1:R:228:CYS:HB2	1:R:231:ILE:CB	2.43	0.49
1:S:228:CYS:CB	1:S:231:ILE:HG13	2.43	0.49
1:E:115:LYS:HE3	1:E:119:GLU:OE2	2.12	0.48
1:E:179:VAL:O	1:E:179:VAL:HG13	2.12	0.48
1:L:21:ILE:O	1:L:25:VAL:HG23	2.12	0.48
1:M:5:ARG:CG	1:M:5:ARG:NH1	2.69	0.48
1:O:59:GLN:HE21	1:O:59:GLN:N	1.98	0.48
1:P:190:HIS:CE1	1:P:231:ILE:HG12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:5:ARG:NH2	1:Q:35:ASP:O	2.44	0.48
1:Q:85:GLN:NE2	1:Q:120:LYS:HB3	2.20	0.48
1:E:81:VAL:HG11	1:E:120:LYS:HB2	1.94	0.48
1:E:99:ARG:HG3	1:F:76:THR:HG23	1.93	0.48
1:E:176:GLY:N	1:I:175:ILE:O	2.43	0.48
1:K:130:GLU:OE1	1:K:169:TYR:CE1	2.66	0.48
1:L:5:ARG:HE	1:L:38:ASP:CG	2.21	0.48
1:N:209:ILE:HG23	1:N:211:ILE:CD1	2.43	0.48
1:E:160:MET:HB2	1:E:160:MET:HE2	1.73	0.48
1:F:68:TYR:HB2	1:F:78:GLU:HB3	1.96	0.48
1:I:194:ARG:HH12	1:I:209:ILE:HG23	1.78	0.48
1:N:130:GLU:OE1	1:N:140:THR:HG23	2.14	0.48
1:O:123:THR:HG23	1:O:164:GLU:O	2.13	0.48
1:P:5:ARG:HE	1:P:38:ASP:CG	2.21	0.48
1:P:40:VAL:HG11	1:P:63:ALA:HB2	1.95	0.48
1:Q:31:HIS:NE2	1:Q:250:ASP:OD1	2.39	0.48
1:Q:80:SER:O	1:Q:83:MET:HB2	2.14	0.48
1:R:114:ALA:HB3	1:R:151:LEU:HD13	1.94	0.48
1:S:145:ILE:O	1:S:149:GLU:HG2	2.13	0.48
1:D:226:GLY:C	1:D:255:THR:HG21	2.38	0.48
1:E:139:ARG:O	1:E:143:VAL:HG23	2.13	0.48
1:E:141:MET:CE	1:E:145:ILE:HD12	2.43	0.48
1:H:229:PRO:HG2	1:H:230:ASN:HD22	1.78	0.48
1:K:81:VAL:O	1:K:85:GLN:HG3	2.13	0.48
1:M:187:GLU:OE2	1:M:230:ASN:OD1	2.31	0.48
1:N:139:ARG:HH12	1:N:143:VAL:CG2	2.26	0.48
1:R:236:VAL:CG1	1:R:239:ALA:HB3	2.44	0.48
1:T:198:ALA:HA	1:T:202:ALA:O	2.13	0.48
1:A:72:ASN:ND2	1:A:80:SER:OG	2.47	0.48
1:D:52:ILE:HA	1:D:62:ILE:HD13	1.95	0.48
1:E:84:LEU:HD13	1:E:122:MET:HE1	1.96	0.48
1:M:145:ILE:HG13	1:M:196:TRP:CD1	2.48	0.48
1:P:151:LEU:HD12	1:P:151:LEU:O	2.13	0.48
1:Q:145:ILE:O	1:Q:149:GLU:HG3	2.12	0.48
1:E:130:GLU:CD	1:E:140:THR:HB	2.39	0.48
1:L:5:ARG:NH1	1:L:35:ASP:O	2.46	0.48
1:L:79:THR:HG21	1:L:84:LEU:HD21	1.93	0.48
1:N:90:LYS:HE3	1:N:91:HIS:HE1	1.76	0.48
1:R:20:PHE:CE1	1:R:24:HIS:HB2	2.49	0.48
1:T:244:GLU:O	1:T:247:THR:HB	2.14	0.48
1:A:250:ASP:O	1:A:254:LYS:HE2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:GLU:OE1	1:D:228:CYS:HB3	2.14	0.48
1:G:236:VAL:HG13	1:G:239:ALA:HB3	1.91	0.48
1:J:57:SER:HB3	1:J:60:LEU:HB3	1.95	0.48
1:K:9:GLY:HA2	1:K:40:VAL:O	2.14	0.48
1:O:100:ARG:NH1	1:O:147:GLN:CD	2.72	0.48
1:Q:248:MET:HA	1:Q:251:ILE:CG2	2.44	0.48
1:R:226:GLY:N	1:R:234:PHE:CZ	2.78	0.48
1:G:24:HIS:O	1:G:28:ILE:HG13	2.14	0.48
1:K:14:CYS:SG	1:L:80:SER:HB3	2.54	0.48
1:K:48:LEU:O	1:K:52:ILE:HG13	2.14	0.48
1:K:246:MET:O	1:K:249:ILE:HB	2.14	0.48
1:O:132:LEU:O	1:O:136:LYS:HG3	2.14	0.48
1:S:196:TRP:CE3	1:S:197:PHE:HA	2.48	0.48
1:S:221:ASN:N	1:S:221:ASN:ND2	2.62	0.48
1:S:244:GLU:HG3	1:S:245:PHE:N	2.29	0.48
1:T:145:ILE:O	1:T:149:GLU:HG3	2.14	0.48
1:A:4:ARG:NH2	1:A:229:PRO:O	2.46	0.48
1:B:37:VAL:HG12	1:B:38:ASP:N	2.29	0.48
1:B:168:ALA:HA	1:B:212:ILE:O	2.14	0.48
1:D:219:GLY:O	1:D:222:ASP:OD1	2.31	0.48
1:E:171:PRO:CD	1:E:215:GLY:HA2	2.34	0.48
1:E:251:ILE:HD12	1:E:254:LYS:HE3	1.96	0.48
1:K:18:LEU:O	1:K:22:LYS:HG3	2.13	0.48
1:L:118:LEU:HD23	1:L:122:MET:O	2.14	0.48
1:N:32:LYS:O	1:N:32:LYS:HG3	2.14	0.48
1:R:64:ALA:CB	1:R:84:LEU:HD11	2.44	0.48
1:R:171:PRO:HD2	1:R:214:GLY:O	2.13	0.48
1:S:43:PRO:HG2	1:S:48:LEU:CD1	2.43	0.48
1:B:116:ARG:O	1:B:120:LYS:HG3	2.14	0.48
1:D:226:GLY:O	1:D:255:THR:HG21	2.14	0.48
1:F:179:VAL:CG1	1:F:180:VAL:N	2.76	0.48
1:I:72:ASN:HD21	1:I:82:GLU:HB2	1.79	0.48
1:K:24:HIS:O	1:K:28:ILE:HG13	2.14	0.48
1:K:171:PRO:HG2	1:K:213:TYR:CE1	2.48	0.48
1:M:2:PRO:HG2	1:M:207:GLN:CG	2.43	0.48
1:O:131:THR:HG23	1:O:134:GLU:OE1	2.13	0.48
1:Q:197:PHE:CD2	1:Q:206:ALA:CA	2.94	0.48
1:R:34:PRO:C	1:R:36:SER:H	2.22	0.48
1:R:39:VAL:O	1:R:60:LEU:HD12	2.14	0.48
1:S:7:PHE:CE1	1:S:40:VAL:HG21	2.49	0.48
1:S:247:THR:O	1:S:251:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:55:ASN:OD1	1:T:60:LEU:HD23	2.13	0.48
1:B:144:ASN:ND2	1:B:193:LEU:HD21	2.29	0.47
1:D:114:ALA:O	1:D:118:LEU:HG	2.14	0.47
1:I:4:ARG:HH12	1:I:194:ARG:NH2	2.12	0.47
1:M:2:PRO:CB	1:M:207:GLN:HB3	2.43	0.47
1:M:69:LEU:HD12	1:M:70:GLU:HG2	1.96	0.47
1:N:123:THR:HA	1:N:164:GLU:HB3	1.96	0.47
1:O:100:ARG:HH12	1:O:128:VAL:HA	1.78	0.47
1:S:12:PHE:HB2	1:S:43:PRO:HA	1.96	0.47
1:S:76:THR:O	1:T:99:ARG:HD2	2.14	0.47
1:S:188:GLU:HG2	1:S:189:VAL:N	2.28	0.47
1:A:68:TYR:CD1	1:A:78:GLU:HG3	2.49	0.47
1:C:68:TYR:HE2	1:C:70:GLU:HG3	1.79	0.47
1:E:190:HIS:CD2	1:E:231:ILE:HG12	2.49	0.47
1:F:40:VAL:CG1	1:F:63:ALA:HB2	2.44	0.47
1:G:97:SER:O	1:G:101:ARG:HG2	2.14	0.47
1:H:7:PHE:O	1:H:233:GLY:HA3	2.14	0.47
1:J:254:LYS:HG3	1:J:255:THR:H	1.79	0.47
1:L:187:GLU:OE1	1:L:228:CYS:HB3	2.13	0.47
1:M:99:ARG:CA	1:M:103:MET:HB2	2.37	0.47
1:O:66:ASN:HD22	1:O:67:VAL:H	1.60	0.47
1:B:99:ARG:HA	1:B:103:MET:HB2	1.97	0.47
1:D:190:HIS:CE1	1:D:211:ILE:O	2.67	0.47
1:E:196:TRP:O	1:E:200:LYS:N	2.38	0.47
1:R:161:LEU:C	1:R:163:LYS:H	2.22	0.47
1:R:248:MET:HE2	1:R:248:MET:HB3	1.69	0.47
1:R:250:ASP:HA	1:R:253:THR:HG23	1.96	0.47
1:E:183:PRO:HG2	1:E:224:LYS:CD	2.45	0.47
1:E:251:ILE:CA	1:E:254:LYS:HE3	2.24	0.47
1:G:80:SER:OG	1:G:83:MET:HG3	2.14	0.47
1:G:98:GLU:O	1:G:102:ILE:HB	2.14	0.47
1:G:164:GLU:OE1	1:G:164:GLU:HA	2.12	0.47
1:H:151:LEU:O	1:H:155:LEU:HG	2.15	0.47
1:K:7:PHE:CD1	1:K:7:PHE:C	2.93	0.47
1:L:43:PRO:HB2	1:L:47:HIS:HB2	1.97	0.47
1:M:236:VAL:CG1	1:M:239:ALA:HB3	2.45	0.47
1:O:41:ILE:HG23	1:O:60:LEU:HD11	1.96	0.47
1:Q:85:GLN:HE22	1:Q:120:LYS:CB	2.24	0.47
1:Q:183:PRO:HB3	1:Q:225:LEU:CD2	2.15	0.47
1:S:4:ARG:HD3	1:S:207:GLN:O	2.14	0.47
1:S:243:PRO:HA	1:S:246:MET:CE	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:LYS:HG3	1:D:255:THR:N	2.29	0.47
1:I:7:PHE:O	1:I:233:GLY:HA3	2.14	0.47
1:I:37:VAL:CG1	1:I:252:LEU:CD2	2.92	0.47
1:I:83:MET:HG2	1:J:47:HIS:HE1	1.79	0.47
1:M:90:LYS:HE3	1:M:123:THR:OG1	2.15	0.47
1:P:222:ASP:OD1	1:P:223:GLU:N	2.48	0.47
1:Q:73:GLY:O	1:R:14:CYS:SG	2.73	0.47
1:Q:234:PHE:CD2	1:Q:248:MET:HE2	2.49	0.47
1:R:123:THR:HA	1:R:164:GLU:HB3	1.96	0.47
1:S:6:PRO:HD2	1:S:36:SER:O	2.14	0.47
1:A:128:VAL:HG11	1:A:148:LEU:HD13	1.97	0.47
1:K:67:VAL:O	1:K:113:LYS:HD3	2.14	0.47
1:M:81:VAL:O	1:M:85:GLN:HG3	2.14	0.47
1:O:74:ALA:O	1:P:98:GLU:HG2	2.13	0.47
1:O:174:SER:HA	1:O:179:VAL:O	2.13	0.47
1:O:227:GLN:O	1:O:228:CYS:C	2.56	0.47
1:R:28:ILE:HG12	1:R:246:MET:HE3	1.96	0.47
1:R:71:GLY:HA3	1:R:116:ARG:NH2	2.29	0.47
1:R:141:MET:HE1	1:R:193:LEU:CD2	2.40	0.47
1:A:139:ARG:HH11	1:A:142:GLU:CD	2.22	0.47
1:A:173:TRP:CD1	1:A:173:TRP:H	2.32	0.47
1:A:239:ALA:O	1:A:242:LYS:HG3	2.14	0.47
1:C:145:ILE:O	1:C:149:GLU:HG2	2.15	0.47
1:D:132:LEU:O	1:D:136:LYS:HG3	2.15	0.47
1:E:109:GLN:O	1:E:113:LYS:HG3	2.14	0.47
1:F:219:GLY:HA2	1:F:222:ASP:CG	2.39	0.47
1:J:173:TRP:CD1	1:J:173:TRP:H	2.33	0.47
1:K:197:PHE:HD1	1:K:206:ALA:HB2	1.80	0.47
1:K:218:ASN:OD1	1:K:244:GLU:OE1	2.32	0.47
1:L:98:GLU:O	1:L:102:ILE:HB	2.15	0.47
1:N:190:HIS:NE2	1:N:213:TYR:HB2	2.30	0.47
1:O:100:ARG:CZ	1:O:127:CYS:O	2.62	0.47
1:P:145:ILE:O	1:P:149:GLU:N	2.42	0.47
1:Q:216:SER:O	1:Q:221:ASN:ND2	2.46	0.47
1:R:57:SER:HB2	1:R:60:LEU:HB3	1.97	0.47
1:R:85:GLN:HE22	1:R:120:LYS:CB	2.28	0.47
1:R:117:ALA:HB3	1:R:124:VAL:HG21	1.96	0.47
1:T:84:LEU:HD22	1:T:89:LEU:HD12	1.97	0.47
1:T:132:LEU:O	1:T:136:LYS:HG3	2.15	0.47
1:A:187:GLU:CD	1:A:229:PRO:HD2	2.40	0.47
1:F:175:ILE:N	1:F:175:ILE:CD1	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:197:PHE:HD2	1:I:206:ALA:HB2	1.80	0.47
1:N:4:ARG:NE	1:N:232:ASP:OD1	2.45	0.47
1:N:100:ARG:NH2	1:N:127:CYS:O	2.45	0.47
1:O:198:ALA:CA	1:O:206:ALA:HB2	2.45	0.47
1:Q:115:LYS:HG3	1:Q:155:LEU:HD23	1.96	0.47
1:R:213:TYR:O	1:R:234:PHE:HA	2.14	0.47
1:A:222:ASP:O	1:A:226:GLY:N	2.44	0.47
1:C:48:LEU:O	1:C:52:ILE:HG13	2.14	0.47
1:C:76:THR:O	1:D:99:ARG:HD2	2.15	0.47
1:E:116:ARG:CZ	1:E:120:LYS:NZ	2.78	0.47
1:E:173:TRP:O	1:E:177:THR:OG1	2.26	0.47
1:F:134:GLU:OE1	1:F:143:VAL:HG21	2.14	0.47
1:O:11:ASN:OD1	1:O:65:GLN:HG2	2.15	0.47
1:P:37:VAL:HG11	1:P:252:LEU:HD23	1.97	0.47
1:P:169:TYR:CE2	1:P:189:VAL:HG21	2.49	0.47
1:R:236:VAL:HG21	1:R:248:MET:SD	2.55	0.47
1:S:141:MET:HA	1:S:141:MET:HE3	1.95	0.47
1:S:186:ALA:CB	1:S:213:TYR:CE1	2.98	0.47
1:S:248:MET:HE2	1:S:248:MET:HB3	1.63	0.47
1:G:69:LEU:CD1	1:G:70:GLU:CG	2.88	0.47
1:H:126:PHE:CE2	1:H:151:LEU:HD21	2.50	0.47
1:J:17:SER:H	1:J:20:PHE:HB3	1.79	0.47
1:K:148:LEU:CD2	1:K:193:LEU:HD22	2.45	0.47
1:N:29:ALA:HB1	1:N:57:SER:HB2	1.97	0.47
1:N:167:ILE:O	1:N:212:ILE:N	2.41	0.47
1:N:191:VAL:CG2	1:N:230:ASN:HD22	2.22	0.47
1:O:187:GLU:OE1	1:O:228:CYS:HB3	2.15	0.47
1:A:2:PRO:HG2	1:A:207:GLN:HB3	1.96	0.46
1:D:148:LEU:O	1:D:151:LEU:HB3	2.15	0.46
1:D:151:LEU:O	1:D:155:LEU:HG	2.15	0.46
1:D:222:ASP:OD1	1:D:223:GLU:N	2.48	0.46
1:G:4:ARG:HD3	1:G:207:GLN:O	2.15	0.46
1:I:196:TRP:CD1	1:I:200:LYS:HG3	2.50	0.46
1:J:254:LYS:HG3	1:J:255:THR:N	2.31	0.46
1:K:80:SER:HB3	1:L:14:CYS:SG	2.55	0.46
1:L:240:SER:HA	1:L:245:PHE:HB2	1.97	0.46
1:N:222:ASP:O	1:N:225:LEU:N	2.48	0.46
1:S:61:ARG:HH11	1:S:61:ARG:CG	2.11	0.46
1:B:184:GLU:OE1	1:B:184:GLU:N	2.48	0.46
1:C:198:ALA:HA	1:C:203:ALA:HA	1.97	0.46
1:I:4:ARG:HH12	1:I:194:ARG:HH21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:251:ILE:HA	1:J:254:LYS:NZ	2.30	0.46
1:K:5:ARG:HE	1:K:38:ASP:CG	2.21	0.46
1:K:223:GLU:CG	1:K:254:LYS:HZ1	2.24	0.46
1:P:192:GLY:O	1:P:195:LYS:HB3	2.16	0.46
1:Q:223:GLU:HB2	1:Q:251:ILE:HD11	1.97	0.46
1:A:197:PHE:HD1	1:A:206:ALA:HB2	1.81	0.46
1:D:37:VAL:HG11	1:D:252:LEU:HD21	1.96	0.46
1:E:183:PRO:HG2	1:E:224:LYS:CE	2.45	0.46
1:Q:4:ARG:NH2	1:Q:229:PRO:O	2.47	0.46
1:Q:69:LEU:HD12	1:Q:113:LYS:HG3	1.98	0.46
1:Q:186:ALA:HB1	1:Q:213:TYR:CD1	2.51	0.46
1:R:34:PRO:C	1:R:36:SER:N	2.73	0.46
1:S:130:GLU:OE2	1:S:169:TYR:OH	2.30	0.46
1:S:196:TRP:O	1:S:200:LYS:HG2	2.15	0.46
1:T:218:ASN:N	1:T:218:ASN:HD22	2.13	0.46
1:B:128:VAL:HG21	1:B:144:ASN:ND2	2.31	0.46
1:C:18:LEU:HA	1:C:18:LEU:HD23	1.77	0.46
1:C:171:PRO:CD	1:C:214:GLY:O	2.63	0.46
1:F:197:PHE:CZ	1:F:201:VAL:HG11	2.50	0.46
1:K:41:ILE:O	1:K:43:PRO:HD3	2.15	0.46
1:L:155:LEU:HD23	1:L:155:LEU:HA	1.75	0.46
1:N:9:GLY:HA2	1:N:40:VAL:O	2.15	0.46
1:O:218:ASN:CG	1:O:219:GLY:N	2.74	0.46
1:O:221:ASN:HA	1:O:224:LYS:HZ1	1.80	0.46
1:Q:71:GLY:O	1:Q:75:TRP:NE1	2.35	0.46
1:S:5:ARG:HE	1:S:38:ASP:CG	2.23	0.46
1:T:248:MET:HE2	1:T:248:MET:HB3	1.59	0.46
1:A:145:ILE:O	1:A:149:GLU:N	2.42	0.46
1:C:177:THR:OG1	1:C:179:VAL:HG13	2.16	0.46
1:H:111:ALA:HB2	1:H:151:LEU:HD12	1.97	0.46
1:J:99:ARG:HA	1:J:103:MET:HB2	1.96	0.46
1:N:81:VAL:HG13	1:N:122:MET:SD	2.56	0.46
1:Q:201:VAL:CG1	1:Q:202:ALA:H	2.26	0.46
1:C:69:LEU:H	1:C:69:LEU:CD2	2.26	0.46
1:D:48:LEU:O	1:D:52:ILE:HG13	2.15	0.46
1:E:11:ASN:OD1	1:E:65:GLN:HG2	2.15	0.46
1:E:71:GLY:O	1:E:72:ASN:C	2.54	0.46
1:F:135:ARG:HE	1:F:135:ARG:HB2	1.58	0.46
1:F:171:PRO:HB2	1:F:174:SER:OG	2.14	0.46
1:G:114:ALA:HB3	1:G:151:LEU:HD13	1.97	0.46
1:G:135:ARG:HB2	1:G:135:ARG:HE	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:LYS:O	1:I:227:GLN:HB2	2.16	0.46
1:K:72:ASN:HA	1:L:14:CYS:O	2.16	0.46
1:M:98:GLU:HG3	1:M:102:ILE:HD12	1.97	0.46
1:O:173:TRP:CD1	1:O:173:TRP:H	2.34	0.46
1:O:222:ASP:HA	1:O:225:LEU:HB2	1.96	0.46
1:Q:186:ALA:CB	1:Q:213:TYR:CE1	2.99	0.46
1:Q:222:ASP:CB	1:Q:248:MET:HE1	2.44	0.46
1:R:2:PRO:HB3	1:R:207:GLN:CG	2.41	0.46
1:S:84:LEU:O	1:S:89:LEU:HB2	2.15	0.46
1:S:158:SER:CB	1:S:161:LEU:HD23	2.30	0.46
1:A:218:ASN:O	1:A:222:ASP:CG	2.59	0.46
1:E:141:MET:HE3	1:E:141:MET:CA	2.37	0.46
1:I:218:ASN:O	1:I:222:ASP:CB	2.61	0.46
1:K:76:THR:HG22	1:L:98:GLU:HB2	1.98	0.46
1:K:202:ALA:HB1	1:K:204:GLU:CD	2.41	0.46
1:L:251:ILE:O	1:L:254:LYS:HG2	2.16	0.46
1:N:29:ALA:CB	1:N:57:SER:HB2	2.46	0.46
1:Q:148:LEU:HD13	1:Q:148:LEU:HA	1.73	0.46
1:R:127:CYS:HA	1:R:168:ALA:O	2.16	0.46
1:T:180:VAL:CG2	1:T:181:ALA:N	2.78	0.46
1:A:72:ASN:HD22	1:A:72:ASN:H	1.63	0.46
1:E:90:LYS:HE2	1:E:91:HIS:CE1	2.51	0.46
1:H:248:MET:HE2	1:H:248:MET:HB3	1.77	0.46
1:K:43:PRO:C	1:K:65:GLN:NE2	2.74	0.46
1:M:137:ALA:HA	1:P:137:ALA:HA	1.97	0.46
1:O:40:VAL:HG11	1:O:63:ALA:HB2	1.97	0.46
1:O:213:TYR:CE2	1:O:215:GLY:O	2.69	0.46
1:Q:130:GLU:CD	1:Q:140:THR:HG23	2.41	0.46
1:Q:210:ARG:CD	1:Q:210:ARG:N	2.67	0.46
1:R:182:THR:OG1	1:R:185:GLN:HG3	2.15	0.46
1:S:164:GLU:OE1	1:S:164:GLU:HA	2.15	0.46
1:T:39:VAL:HG12	1:T:60:LEU:HD13	1.97	0.46
1:T:63:ALA:CB	1:T:91:HIS:HB2	2.41	0.46
1:T:155:LEU:HD13	1:T:161:LEU:HB2	1.96	0.46
1:T:213:TYR:O	1:T:234:PHE:HA	2.16	0.46
1:E:236:VAL:HG11	1:E:239:ALA:HB3	1.97	0.46
1:F:111:ALA:HB1	1:F:151:LEU:HA	1.96	0.46
1:H:111:ALA:HA	1:H:151:LEU:HG	1.97	0.46
1:N:244:GLU:O	1:N:248:MET:CG	2.64	0.46
1:O:21:ILE:HG13	1:O:47:HIS:HB3	1.98	0.46
1:O:198:ALA:HA	1:O:206:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:187:GLU:OE1	1:P:228:CYS:HB3	2.15	0.46
1:R:7:PHE:CD1	1:R:7:PHE:C	2.93	0.46
1:S:61:ARG:NH2	1:S:90:LYS:HB2	2.31	0.46
1:C:196:TRP:NE1	1:C:200:LYS:HG3	2.30	0.46
1:C:244:GLU:O	1:C:248:MET:HG3	2.16	0.46
1:G:224:LYS:HE3	1:G:224:LYS:HB3	1.33	0.46
1:J:218:ASN:N	1:J:218:ASN:OD1	2.49	0.46
1:L:244:GLU:OE1	1:L:244:GLU:HA	2.16	0.46
1:M:181:ALA:HB3	1:M:213:TYR:OH	2.16	0.46
1:N:140:THR:HG22	1:N:141:MET:N	2.29	0.46
1:R:250:ASP:O	1:R:253:THR:HG23	2.16	0.46
1:S:198:ALA:HB2	1:S:206:ALA:CB	2.46	0.46
1:S:213:TYR:HB2	1:S:231:ILE:HD13	1.98	0.46
1:T:187:GLU:OE2	1:T:191:VAL:HG23	2.16	0.46
1:B:9:GLY:HA2	1:B:40:VAL:O	2.16	0.45
1:B:109:GLN:O	1:B:113:LYS:HG3	2.16	0.45
1:E:136:LYS:HE2	1:E:136:LYS:HB3	1.79	0.45
1:G:76:THR:HG22	1:H:65:GLN:HB3	1.96	0.45
1:G:128:VAL:HG11	1:G:148:LEU:HD13	1.98	0.45
1:H:197:PHE:HB3	1:H:206:ALA:HB2	1.99	0.45
1:N:114:ALA:O	1:N:118:LEU:HG	2.17	0.45
1:O:196:TRP:CE3	1:O:197:PHE:N	2.84	0.45
1:P:204:GLU:O	1:P:208:HIS:CE1	2.69	0.45
1:S:15:ASN:OD1	1:T:72:ASN:HB3	2.15	0.45
1:T:197:PHE:CD1	1:T:201:VAL:HG21	2.50	0.45
1:A:81:VAL:O	1:A:85:GLN:HG3	2.16	0.45
1:B:114:ALA:HB2	1:B:126:PHE:CE1	2.51	0.45
1:G:221:ASN:O	1:G:224:LYS:HB2	2.17	0.45
1:J:137:ALA:O	1:J:138:ASN:HB2	2.17	0.45
1:K:159:LYS:O	1:K:160:MET:HB3	2.14	0.45
1:K:198:ALA:HB2	1:K:206:ALA:CB	2.46	0.45
1:M:34:PRO:HG3	1:M:253:THR:HG21	1.99	0.45
1:M:34:PRO:HB2	1:M:36:SER:OG	2.16	0.45
1:N:72:ASN:ND2	1:N:80:SER:OG	2.50	0.45
1:O:81:VAL:O	1:O:85:GLN:HG3	2.15	0.45
1:O:240:SER:HA	1:O:245:PHE:CD1	2.51	0.45
1:Q:251:ILE:HG23	1:Q:252:LEU:N	2.31	0.45
1:T:84:LEU:CD1	1:T:122:MET:HE1	2.46	0.45
1:T:118:LEU:CD1	1:T:155:LEU:HD11	2.46	0.45
1:A:13:LYS:HG2	1:B:76:THR:OG1	2.16	0.45
1:E:171:PRO:HG3	1:E:213:TYR:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:CYS:HA	1:F:229:PRO:HD3	1.83	0.45
1:G:190:HIS:ND1	1:G:231:ILE:HG12	2.31	0.45
1:J:158:SER:OG	1:J:161:LEU:HG	2.16	0.45
1:L:196:TRP:O	1:L:200:LYS:N	2.45	0.45
1:M:24:HIS:O	1:M:28:ILE:HG13	2.15	0.45
1:N:17:SER:O	1:N:21:ILE:HG12	2.17	0.45
1:O:210:ARG:HE	1:O:210:ARG:HB2	1.68	0.45
1:P:4:ARG:HD2	1:P:207:GLN:O	2.15	0.45
1:P:5:ARG:NH1	1:P:35:ASP:O	2.43	0.45
1:P:159:LYS:O	1:P:162:TRP:CD1	2.69	0.45
1:P:164:GLU:HA	1:P:164:GLU:OE1	2.15	0.45
1:Q:5:ARG:HA	1:Q:6:PRO:HD2	1.61	0.45
1:T:18:LEU:O	1:T:22:LYS:HG3	2.17	0.45
1:A:14:CYS:HA	1:B:83:MET:HE1	1.99	0.45
1:C:71:GLY:O	1:C:75:TRP:NE1	2.49	0.45
1:E:151:LEU:O	1:E:155:LEU:HG	2.17	0.45
1:E:184:GLU:CD	1:E:184:GLU:H	2.24	0.45
1:E:228:CYS:HB2	1:E:231:ILE:HD12	1.99	0.45
1:I:233:GLY:HA2	1:I:252:LEU:HD11	1.95	0.45
1:L:37:VAL:HG11	1:L:252:LEU:HD23	1.98	0.45
1:Q:218:ASN:N	1:Q:218:ASN:HD22	2.14	0.45
1:F:12:PHE:N	1:F:12:PHE:CD1	2.85	0.45
1:G:155:LEU:HD12	1:G:162:TRP:NE1	2.31	0.45
1:I:68:TYR:CE2	1:I:70:GLU:HG3	2.51	0.45
1:I:139:ARG:NH1	1:I:142:GLU:OE1	2.49	0.45
1:J:171:PRO:HB2	1:J:174:SER:OG	2.17	0.45
1:K:83:MET:O	1:K:87:MET:HG3	2.17	0.45
1:L:131:THR:HA	1:L:172:VAL:HB	1.99	0.45
1:R:190:HIS:NE2	1:R:231:ILE:HD13	2.31	0.45
1:S:171:PRO:HD3	1:S:214:GLY:O	2.17	0.45
1:T:45:ALA:HA	1:T:48:LEU:HD22	1.98	0.45
1:C:196:TRP:CD1	1:C:200:LYS:HG3	2.52	0.45
1:J:18:LEU:O	1:J:22:LYS:HG3	2.16	0.45
1:K:13:LYS:HD3	1:L:74:ALA:HA	1.99	0.45
1:M:228:CYS:HB2	1:M:231:ILE:CG1	2.46	0.45
1:O:226:GLY:C	1:O:255:THR:HG21	2.40	0.45
1:P:45:ALA:HA	1:P:48:LEU:HD22	1.98	0.45
1:P:194:ARG:NE	1:P:230:ASN:HD22	2.14	0.45
1:P:242:LYS:C	1:P:244:GLU:N	2.74	0.45
1:Q:12:PHE:HB2	1:Q:43:PRO:HA	1.99	0.45
1:Q:217:ALA:HA	1:Q:221:ASN:HD21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:221:ASN:OD1	1:R:221:ASN:N	2.50	0.45
1:S:2:PRO:CD	1:S:207:GLN:HB2	2.47	0.45
1:S:185:GLN:O	1:S:188:GLU:CD	2.60	0.45
1:S:194:ARG:HD3	1:S:206:ALA:O	2.16	0.45
1:B:5:ARG:NH2	1:B:38:ASP:OD1	2.48	0.45
1:E:97:SER:CB	1:E:170:GLU:OE1	2.64	0.45
1:G:160:MET:HE3	1:G:160:MET:HB2	1.76	0.45
1:L:136:LYS:C	1:L:138:ASN:N	2.69	0.45
1:L:171:PRO:CG	1:L:174:SER:HG	2.28	0.45
1:M:155:LEU:HD12	1:M:162:TRP:NE1	2.31	0.45
1:Q:46:VAL:CG2	1:Q:47:HIS:CD2	2.98	0.45
1:Q:74:ALA:HB1	1:R:98:GLU:OE2	2.17	0.45
1:Q:91:HIS:HA	1:Q:123:THR:O	2.16	0.45
1:S:171:PRO:CD	1:S:214:GLY:O	2.64	0.45
1:T:184:GLU:OE1	1:T:184:GLU:N	2.49	0.45
1:A:36:SER:HB3	1:G:160:MET:CE	2.47	0.45
1:D:251:ILE:HA	1:D:254:LYS:HG2	1.98	0.45
1:F:177:THR:O	1:F:177:THR:CG2	2.63	0.45
1:G:77:GLY:HA3	1:H:99:ARG:NH1	2.31	0.45
1:H:83:MET:O	1:H:87:MET:HG3	2.17	0.45
1:L:193:LEU:O	1:L:196:TRP:HB3	2.16	0.45
1:M:228:CYS:HA	1:M:229:PRO:HD3	1.82	0.45
1:O:97:SER:CB	1:O:170:GLU:OE1	2.64	0.45
1:Q:72:ASN:ND2	1:Q:80:SER:OG	2.50	0.45
1:Q:75:TRP:HD1	1:R:14:CYS:SG	2.29	0.45
1:T:128:VAL:HG11	1:T:148:LEU:HD13	1.99	0.45
1:A:91:HIS:CD2	1:A:123:THR:HB	2.52	0.45
1:G:166:VAL:HG13	1:G:210:ARG:HB3	1.98	0.45
1:H:173:TRP:CD1	1:H:173:TRP:H	2.33	0.45
1:R:68:TYR:CZ	1:R:69:LEU:HD21	2.52	0.45
1:S:8:ILE:HG22	1:S:252:LEU:CD2	2.47	0.45
1:S:101:ARG:HD3	1:S:101:ARG:N	2.31	0.45
1:S:141:MET:HE1	1:S:193:LEU:CD2	2.38	0.45
1:S:163:LYS:HG2	1:S:164:GLU:HG2	1.98	0.45
1:C:68:TYR:CE2	1:C:70:GLU:HG3	2.52	0.45
1:F:175:ILE:HG12	1:F:215:GLY:HA2	1.98	0.45
1:F:218:ASN:C	1:F:220:SER:H	2.24	0.45
1:G:90:LYS:HB3	1:G:91:HIS:CE1	2.52	0.45
1:I:6:PRO:HB2	1:I:37:VAL:HG13	1.98	0.45
1:I:9:GLY:HA2	1:I:40:VAL:O	2.16	0.45
1:I:180:VAL:HG23	1:I:181:ALA:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:243:PRO:HA	1:J:246:MET:CE	2.46	0.45
1:M:210:ARG:HG3	1:M:232:ASP:OD2	2.16	0.45
1:N:244:GLU:O	1:N:248:MET:HG3	2.17	0.45
1:P:67:VAL:HB	1:P:92:VAL:HG21	1.99	0.45
1:S:190:HIS:CE1	1:S:213:TYR:HB2	2.52	0.45
1:D:145:ILE:HG23	1:D:149:GLU:OE2	2.17	0.44
1:H:145:ILE:O	1:H:149:GLU:HG2	2.17	0.44
1:P:200:LYS:O	1:P:200:LYS:HG2	2.17	0.44
1:S:187:GLU:OE2	1:S:229:PRO:HG2	2.17	0.44
1:B:190:HIS:ND1	1:B:231:ILE:HG12	2.32	0.44
1:E:80:SER:HG	1:E:83:MET:H	1.65	0.44
1:H:111:ALA:HB1	1:H:151:LEU:HA	1.98	0.44
1:H:163:LYS:HG3	1:H:163:LYS:H	1.44	0.44
1:I:68:TYR:HB2	1:I:78:GLU:HB3	2.00	0.44
1:L:58:LYS:O	1:L:58:LYS:HD2	2.16	0.44
1:N:33:ILE:O	1:N:59:GLN:HG2	2.17	0.44
1:N:139:ARG:HB3	1:N:139:ARG:NH1	2.24	0.44
1:R:183:PRO:HG2	1:R:224:LYS:CD	2.40	0.44
1:T:227:GLN:OE1	1:T:227:GLN:N	2.50	0.44
1:A:187:GLU:HB2	1:A:228:CYS:SG	2.57	0.44
1:B:201:VAL:O	1:B:202:ALA:HB2	2.17	0.44
1:C:82:GLU:OE1	1:C:116:ARG:NH1	2.51	0.44
1:D:197:PHE:O	1:D:201:VAL:HB	2.17	0.44
1:G:11:ASN:OD1	1:G:65:GLN:HG2	2.18	0.44
1:H:247:THR:O	1:H:251:ILE:HG13	2.16	0.44
1:I:96:HIS:CE1	1:I:98:GLU:OE1	2.70	0.44
1:I:200:LYS:HE2	1:I:200:LYS:HB3	1.55	0.44
1:K:83:MET:CE	1:L:44:SER:OG	2.61	0.44
1:K:84:LEU:HD22	1:K:89:LEU:HD12	2.00	0.44
1:N:58:LYS:O	1:N:58:LYS:HG2	2.17	0.44
1:O:81:VAL:HG11	1:O:120:LYS:HD3	1.99	0.44
1:O:139:ARG:HB3	1:O:142:GLU:HB3	1.99	0.44
1:P:218:ASN:O	1:P:222:ASP:HB3	2.18	0.44
1:Q:96:HIS:HE1	1:Q:98:GLU:CD	2.25	0.44
1:R:187:GLU:OE1	1:R:187:GLU:HA	2.17	0.44
1:S:245:PHE:HA	1:S:248:MET:HG3	1.99	0.44
1:T:8:ILE:HB	1:T:252:LEU:HD22	1.98	0.44
1:D:161:LEU:C	1:D:163:LYS:N	2.72	0.44
1:G:4:ARG:HE	1:G:4:ARG:HB2	1.40	0.44
1:L:218:ASN:N	1:L:221:ASN:ND2	2.39	0.44
1:M:5:ARG:NH1	1:M:36:SER:C	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:67:VAL:O	1:O:113:LYS:HD3	2.17	0.44
1:R:195:LYS:HE3	1:R:195:LYS:HB3	1.82	0.44
1:R:229:PRO:C	1:R:230:ASN:HD22	2.24	0.44
1:T:57:SER:HB3	1:T:60:LEU:HB3	1.99	0.44
1:T:194:ARG:NH1	1:T:206:ALA:O	2.49	0.44
1:D:140:THR:HG22	1:D:141:MET:N	2.32	0.44
1:E:69:LEU:HD12	1:E:112:LYS:CB	2.47	0.44
1:I:194:ARG:NH1	1:I:211:ILE:HG13	2.33	0.44
1:M:145:ILE:CG1	1:M:196:TRP:CD1	3.01	0.44
1:M:166:VAL:HG22	1:M:210:ARG:HB3	2.00	0.44
1:O:65:GLN:HB3	1:P:76:THR:HG23	1.99	0.44
1:P:130:GLU:O	1:P:172:VAL:HB	2.17	0.44
1:A:140:THR:O	1:A:144:ASN:ND2	2.50	0.44
1:D:5:ARG:HA	1:D:6:PRO:HD3	1.86	0.44
1:G:145:ILE:HG23	1:G:196:TRP:NE1	2.32	0.44
1:G:160:MET:H	1:G:160:MET:HG3	1.33	0.44
1:I:87:MET:HE2	1:I:87:MET:HB3	1.90	0.44
1:K:213:TYR:C	1:K:215:GLY:N	2.76	0.44
1:L:140:THR:O	1:L:144:ASN:ND2	2.50	0.44
1:P:149:GLU:OE1	1:P:200:LYS:CE	2.65	0.44
1:P:171:PRO:HD2	1:P:214:GLY:O	2.18	0.44
1:R:222:ASP:OD1	1:R:223:GLU:N	2.50	0.44
1:S:149:GLU:CD	1:S:196:TRP:HE1	2.26	0.44
1:A:91:HIS:HA	1:A:123:THR:O	2.17	0.44
1:D:106:THR:OG1	1:D:109:GLN:HG3	2.18	0.44
1:E:24:HIS:O	1:E:27:ALA:HB3	2.17	0.44
1:E:174:SER:O	1:I:176:GLY:CA	2.65	0.44
1:I:190:HIS:CE1	1:I:211:ILE:HG22	2.52	0.44
1:J:173:TRP:HH2	1:J:185:GLN:OE1	2.00	0.44
1:K:242:LYS:HB3	1:K:242:LYS:HE2	1.68	0.44
1:N:160:MET:HE2	1:N:160:MET:HB2	1.72	0.44
1:O:41:ILE:O	1:O:43:PRO:HD3	2.18	0.44
1:P:95:GLY:C	1:P:127:CYS:HB2	2.43	0.44
1:P:251:ILE:N	1:P:251:ILE:HD12	2.33	0.44
1:D:172:VAL:HA	1:D:175:ILE:HG12	2.00	0.44
1:E:44:SER:O	1:E:48:LEU:HD22	2.18	0.44
1:G:28:ILE:HD13	1:G:245:PHE:CD2	2.52	0.44
1:G:74:ALA:HB1	1:H:98:GLU:OE2	2.17	0.44
1:J:91:HIS:CD2	1:J:123:THR:HB	2.53	0.44
1:J:246:MET:HA	1:J:249:ILE:HD12	1.99	0.44
1:N:184:GLU:CD	1:N:184:GLU:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:177:THR:HG21	1:P:179:VAL:HG22	1.98	0.44
1:R:138:ASN:CG	1:R:138:ASN:O	2.61	0.44
1:S:83:MET:HE1	1:T:14:CYS:C	2.43	0.44
1:A:13:LYS:H	1:A:65:GLN:NE2	2.16	0.44
1:A:167:ILE:HB	1:A:211:ILE:HG23	1.99	0.44
1:B:144:ASN:HD22	1:B:193:LEU:HD21	1.83	0.44
1:D:9:GLY:HA2	1:D:40:VAL:O	2.18	0.44
1:E:45:ALA:HA	1:E:48:LEU:HD21	1.95	0.44
1:E:184:GLU:OE1	1:E:184:GLU:N	2.51	0.44
1:H:94:VAL:HG11	1:H:114:ALA:HB2	2.00	0.44
1:H:148:LEU:HD12	1:H:148:LEU:HA	1.80	0.44
1:J:96:HIS:HA	1:J:127:CYS:HB2	2.00	0.44
1:L:37:VAL:HG13	1:L:252:LEU:HD23	2.00	0.44
1:O:63:ALA:HB2	1:O:91:HIS:HB2	1.99	0.44
1:S:196:TRP:CD2	1:S:196:TRP:C	2.96	0.44
1:B:82:GLU:OE2	1:B:116:ARG:NH2	2.45	0.43
1:C:221:ASN:N	1:C:221:ASN:HD22	2.14	0.43
1:C:222:ASP:OD1	1:C:223:GLU:N	2.51	0.43
1:F:52:ILE:HA	1:F:62:ILE:HD13	2.00	0.43
1:F:197:PHE:O	1:F:201:VAL:N	2.50	0.43
1:F:212:ILE:CD1	1:F:235:LEU:HB2	2.48	0.43
1:G:69:LEU:CD1	1:G:70:GLU:CD	2.91	0.43
1:G:80:SER:HG	1:G:83:MET:HG3	1.83	0.43
1:L:180:VAL:CG2	1:L:181:ALA:N	2.81	0.43
1:M:98:GLU:HA	1:M:102:ILE:HD12	2.00	0.43
1:N:45:ALA:HA	1:N:48:LEU:CD2	2.45	0.43
1:N:218:ASN:ND2	1:N:221:ASN:ND2	2.65	0.43
1:P:190:HIS:ND1	1:P:231:ILE:HG12	2.33	0.43
1:Q:70:GLU:HB2	1:Q:75:TRP:CE2	2.53	0.43
1:Q:229:PRO:HB2	1:Q:230:ASN:HD22	1.82	0.43
1:T:66:ASN:HD21	1:T:113:LYS:NZ	2.16	0.43
1:A:127:CYS:HB3	1:A:170:GLU:OE2	2.18	0.43
1:D:7:PHE:O	1:D:233:GLY:HA3	2.18	0.43
1:D:221:ASN:O	1:D:224:LYS:HG3	2.18	0.43
1:E:46:VAL:HG23	1:E:47:HIS:CD2	2.53	0.43
1:I:5:ARG:HA	1:I:6:PRO:HD3	1.86	0.43
1:M:21:ILE:HG13	1:M:47:HIS:HB3	2.00	0.43
1:N:218:ASN:HD22	1:N:221:ASN:ND2	2.16	0.43
1:N:221:ASN:O	1:N:222:ASP:C	2.61	0.43
1:P:81:VAL:HG21	1:P:117:ALA:HA	1.99	0.43
1:Q:4:ARG:NH1	1:Q:194:ARG:CZ	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:31:HIS:CE1	1:Q:246:MET:HB3	2.52	0.43
1:Q:72:ASN:HA	1:R:14:CYS:O	2.17	0.43
1:T:39:VAL:HG12	1:T:60:LEU:CD1	2.48	0.43
1:B:172:VAL:O	1:O:176:GLY:HA2	2.18	0.43
1:E:175:ILE:C	1:E:177:THR:H	2.24	0.43
1:E:239:ALA:HA	1:E:242:LYS:HE3	2.01	0.43
1:I:77:GLY:HA3	1:J:99:ARG:HH11	1.83	0.43
1:M:128:VAL:HG12	1:M:147:GLN:HB2	1.99	0.43
1:N:15:ASN:ND2	1:N:15:ASN:N	2.50	0.43
1:O:40:VAL:CG1	1:O:63:ALA:HB2	2.47	0.43
1:O:97:SER:HB3	1:O:170:GLU:OE1	2.18	0.43
1:P:81:VAL:HG13	1:P:122:MET:SD	2.58	0.43
1:Q:64:ALA:N	1:Q:89:LEU:HD21	2.33	0.43
1:Q:183:PRO:HG2	1:Q:224:LYS:HD3	2.00	0.43
1:S:67:VAL:HG23	1:S:79:THR:HG22	2.01	0.43
1:T:31:HIS:HE2	1:T:250:ASP:CG	2.25	0.43
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.78	0.43
1:D:151:LEU:HD23	1:D:162:TRP:CH2	2.53	0.43
1:I:48:LEU:CD2	1:I:89:LEU:HD11	2.48	0.43
1:I:228:CYS:HA	1:I:229:PRO:HD2	1.91	0.43
1:K:13:LYS:HG2	1:L:76:THR:OG1	2.18	0.43
1:L:40:VAL:HG11	1:L:63:ALA:HB2	1.99	0.43
1:O:182:THR:HG23	1:O:185:GLN:NE2	2.33	0.43
1:O:197:PHE:HE2	1:O:205:GLY:O	2.00	0.43
1:Q:226:GLY:C	1:Q:228:CYS:H	2.27	0.43
1:S:143:VAL:O	1:S:147:GLN:HG3	2.18	0.43
1:A:151:LEU:O	1:A:155:LEU:HG	2.19	0.43
1:E:116:ARG:CZ	1:E:120:LYS:HZ1	2.32	0.43
1:E:183:PRO:HG2	1:E:224:LYS:HE2	2.01	0.43
1:F:69:LEU:HD23	1:F:69:LEU:C	2.43	0.43
1:F:80:SER:OG	1:F:83:MET:HG3	2.19	0.43
1:F:118:LEU:HB3	1:F:161:LEU:HD22	2.00	0.43
1:I:182:THR:OG1	1:I:185:GLN:HG3	2.19	0.43
1:I:197:PHE:CD2	1:I:206:ALA:HA	2.53	0.43
1:J:69:LEU:HD22	1:J:113:LYS:HE2	2.00	0.43
1:J:166:VAL:HG13	1:J:210:ARG:HB3	1.99	0.43
1:K:40:VAL:HA	1:K:61:ARG:O	2.18	0.43
1:M:63:ALA:HB2	1:M:91:HIS:HB2	2.00	0.43
1:M:167:ILE:O	1:M:211:ILE:HA	2.18	0.43
1:N:248:MET:HE3	1:N:248:MET:HB3	1.75	0.43
1:O:181:ALA:HB3	1:O:213:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:7:PHE:HE1	1:Q:38:ASP:OD1	2.02	0.43
1:Q:166:VAL:CG2	1:Q:210:ARG:NH2	2.81	0.43
1:R:214:GLY:HA2	1:R:235:LEU:HB3	2.00	0.43
1:R:217:ALA:C	1:R:218:ASN:O	2.61	0.43
1:T:111:ALA:HB1	1:T:151:LEU:HA	2.01	0.43
1:T:180:VAL:HG22	1:T:181:ALA:N	2.34	0.43
1:B:21:ILE:O	1:B:25:VAL:HG23	2.19	0.43
1:B:144:ASN:HD22	1:B:193:LEU:HD22	1.83	0.43
1:B:217:ALA:HB1	1:B:222:ASP:OD2	2.17	0.43
1:E:155:LEU:HD12	1:E:162:TRP:NE1	2.33	0.43
1:E:251:ILE:O	1:E:254:LYS:HG2	2.18	0.43
1:H:94:VAL:HG12	1:H:126:PHE:CD1	2.54	0.43
1:L:117:ALA:O	1:L:122:MET:HB2	2.18	0.43
1:L:246:MET:HA	1:L:249:ILE:HD12	1.99	0.43
1:M:223:GLU:O	1:M:227:GLN:HG3	2.19	0.43
1:O:100:ARG:HH11	1:O:147:GLN:NE2	2.17	0.43
1:P:151:LEU:HD12	1:P:155:LEU:HG	2.01	0.43
1:Q:81:VAL:HG11	1:Q:117:ALA:HA	2.01	0.43
1:Q:189:VAL:O	1:Q:193:LEU:HG	2.19	0.43
1:S:24:HIS:NE2	1:S:241:LEU:HA	2.34	0.43
1:B:197:PHE:HD2	1:B:206:ALA:HB2	1.83	0.43
1:F:82:GLU:H	1:F:82:GLU:HG2	1.41	0.43
1:G:221:ASN:HA	1:G:224:LYS:HG3	2.00	0.43
1:I:115:LYS:HD2	1:I:154:GLU:O	2.18	0.43
1:J:69:LEU:H	1:J:69:LEU:CD2	2.27	0.43
1:L:189:VAL:O	1:L:193:LEU:HG	2.19	0.43
1:N:134:GLU:OE1	1:N:143:VAL:HG11	2.19	0.43
1:P:83:MET:O	1:P:87:MET:HG3	2.18	0.43
1:Q:85:GLN:NE2	1:Q:120:LYS:O	2.52	0.43
1:S:39:VAL:HG12	1:S:60:LEU:CD1	2.47	0.43
1:A:172:VAL:HA	1:A:175:ILE:HD12	1.95	0.43
1:C:78:GLU:OE1	1:C:78:GLU:HA	2.19	0.43
1:C:160:MET:O	1:C:163:LYS:HB2	2.19	0.43
1:K:42:ALA:C	1:K:65:GLN:HE21	2.26	0.43
1:K:135:ARG:HE	1:K:135:ARG:HB2	1.58	0.43
1:L:250:ASP:O	1:L:254:LYS:HE3	2.19	0.43
1:M:210:ARG:HE	1:M:210:ARG:HB2	1.19	0.43
1:Q:14:CYS:SG	1:R:80:SER:HB3	2.59	0.43
1:Q:16:GLY:O	1:Q:47:HIS:HE1	2.01	0.43
1:Q:77:GLY:H	1:R:65:GLN:NE2	2.17	0.43
1:T:99:ARG:HE	1:T:99:ARG:HB3	1.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:127:CYS:HB3	1:T:170:GLU:OE2	2.19	0.43
1:B:130:GLU:O	1:B:172:VAL:HB	2.19	0.43
1:C:195:LYS:HE3	1:C:195:LYS:HB2	1.76	0.43
1:F:151:LEU:HD23	1:F:162:TRP:CH2	2.54	0.43
1:J:132:LEU:HA	1:J:173:TRP:HB3	2.01	0.43
1:M:71:GLY:O	1:M:75:TRP:NE1	2.52	0.43
1:N:13:LYS:O	1:N:15:ASN:N	2.51	0.43
1:N:250:ASP:O	1:N:253:THR:HB	2.19	0.43
1:O:4:ARG:HD2	1:O:209:ILE:O	2.18	0.43
1:P:12:PHE:N	1:P:12:PHE:CD1	2.87	0.43
1:P:177:THR:C	1:P:179:VAL:H	2.27	0.43
1:Q:33:ILE:HB	1:Q:59:GLN:NE2	2.34	0.43
1:R:187:GLU:OE2	1:R:229:PRO:HB2	2.18	0.43
1:S:2:PRO:HG2	1:S:207:GLN:HB2	2.01	0.43
1:S:10:GLY:HA2	1:S:236:VAL:HB	2.00	0.43
1:T:157:GLU:OE1	1:T:157:GLU:CA	2.67	0.43
1:D:37:VAL:HG11	1:D:252:LEU:HD23	2.00	0.43
1:D:55:ASN:HD22	1:D:62:ILE:HD12	1.84	0.43
1:E:42:ALA:O	1:E:65:GLN:NE2	2.45	0.43
1:F:90:LYS:HE2	1:F:123:THR:OG1	2.19	0.43
1:F:198:ALA:HA	1:F:202:ALA:O	2.18	0.43
1:G:4:ARG:HD2	1:G:194:ARG:HH12	1.82	0.43
1:G:236:VAL:HG22	1:G:248:MET:HE1	2.00	0.43
1:J:71:GLY:O	1:J:75:TRP:NE1	2.49	0.43
1:K:93:ILE:HG12	1:K:125:ILE:HD12	2.01	0.43
1:K:154:GLU:HA	1:K:154:GLU:OE1	2.19	0.43
1:Q:69:LEU:HD12	1:Q:113:LYS:HE2	2.01	0.43
1:R:91:HIS:HA	1:R:123:THR:O	2.18	0.43
1:S:155:LEU:CG	1:S:161:LEU:HD11	2.46	0.43
1:T:115:LYS:CD	1:T:155:LEU:HD21	2.39	0.43
1:T:118:LEU:HD13	1:T:155:LEU:CD1	2.49	0.43
1:B:37:VAL:HG11	1:B:252:LEU:HD23	2.01	0.42
1:B:37:VAL:HG13	1:B:252:LEU:HD23	2.01	0.42
1:B:162:TRP:HA	1:B:165:VAL:HG23	2.00	0.42
1:D:148:LEU:HD12	1:D:148:LEU:HA	1.72	0.42
1:E:115:LYS:NZ	1:E:154:GLU:O	2.49	0.42
1:E:131:THR:HG23	1:E:134:GLU:CD	2.43	0.42
1:E:253:THR:C	1:E:255:THR:H	2.28	0.42
1:F:12:PHE:O	1:F:15:ASN:ND2	2.52	0.42
1:H:148:LEU:CD2	1:H:193:LEU:HD22	2.49	0.42
1:H:204:GLU:O	1:H:204:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:ARG:HG2	1:I:4:ARG:NH1	2.22	0.42
1:L:71:GLY:O	1:L:75:TRP:NE1	2.52	0.42
1:L:115:LYS:O	1:L:119:GLU:HG3	2.19	0.42
1:N:142:GLU:HG3	1:N:143:VAL:N	2.32	0.42
1:N:221:ASN:O	1:N:223:GLU:N	2.52	0.42
1:O:69:LEU:HD23	1:O:69:LEU:C	2.44	0.42
1:P:15:ASN:ND2	1:P:15:ASN:N	2.56	0.42
1:P:118:LEU:HD13	1:P:161:LEU:O	2.19	0.42
1:R:66:ASN:ND2	1:R:99:ARG:CZ	2.82	0.42
1:S:13:LYS:O	1:S:65:GLN:NE2	2.50	0.42
1:A:246:MET:O	1:A:249:ILE:HB	2.19	0.42
1:D:97:SER:O	1:D:101:ARG:HB2	2.18	0.42
1:E:84:LEU:HD22	1:E:89:LEU:HD12	2.00	0.42
1:I:114:ALA:O	1:I:118:LEU:HG	2.19	0.42
1:N:221:ASN:OD1	1:N:222:ASP:OD1	2.36	0.42
1:O:246:MET:O	1:O:249:ILE:HB	2.18	0.42
1:P:177:THR:O	1:P:179:VAL:N	2.46	0.42
1:Q:91:HIS:CD2	1:Q:123:THR:CG2	3.02	0.42
1:R:181:ALA:HA	1:R:185:GLN:OE1	2.19	0.42
1:R:197:PHE:CD2	1:R:206:ALA:HA	2.54	0.42
1:S:8:ILE:HG23	1:S:39:VAL:HG22	2.01	0.42
1:S:92:VAL:HG13	1:S:124:VAL:HG22	1.97	0.42
1:S:128:VAL:HG12	1:S:147:GLN:HB2	1.99	0.42
1:T:8:ILE:HG22	1:T:39:VAL:HG22	2.01	0.42
1:T:11:ASN:HD21	1:T:13:LYS:HG3	1.84	0.42
1:T:115:LYS:O	1:T:119:GLU:HG3	2.19	0.42
1:T:149:GLU:O	1:T:153:LYS:HB3	2.19	0.42
1:I:116:ARG:O	1:I:120:LYS:HG3	2.20	0.42
1:I:141:MET:HE1	1:I:192:GLY:C	2.44	0.42
1:K:76:THR:OG1	1:L:65:GLN:HB3	2.18	0.42
1:L:5:ARG:O	1:L:210:ARG:CD	2.67	0.42
1:L:196:TRP:O	1:L:200:LYS:HB3	2.19	0.42
1:R:6:PRO:HD2	1:R:36:SER:O	2.18	0.42
1:R:198:ALA:HB2	1:R:206:ALA:CB	2.50	0.42
1:R:236:VAL:HG11	1:R:239:ALA:HB3	2.00	0.42
1:S:58:LYS:N	1:S:58:LYS:HD2	2.34	0.42
1:S:73:GLY:O	1:T:14:CYS:HB3	2.19	0.42
1:T:148:LEU:HD12	1:T:148:LEU:HA	1.87	0.42
1:T:162:TRP:CD2	1:T:197:PHE:HE1	2.37	0.42
1:T:222:ASP:CG	1:T:223:GLU:N	2.77	0.42
1:D:190:HIS:CE1	1:D:231:ILE:HG12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:SER:HB3	1:E:60:LEU:HB3	2.02	0.42
1:H:4:ARG:HH22	1:H:230:ASN:HA	1.84	0.42
1:H:115:LYS:CE	1:H:119:GLU:OE2	2.64	0.42
1:K:251:ILE:N	1:K:251:ILE:CD1	2.83	0.42
1:O:97:SER:OG	1:O:170:GLU:OE1	2.35	0.42
1:O:141:MET:O	1:O:145:ILE:HG13	2.20	0.42
1:Q:183:PRO:CG	1:Q:225:LEU:HD21	2.48	0.42
1:Q:218:ASN:O	1:Q:219:GLY:C	2.61	0.42
1:R:28:ILE:HG12	1:R:246:MET:CE	2.49	0.42
1:S:85:GLN:NE2	1:S:120:LYS:O	2.52	0.42
1:C:5:ARG:HA	1:C:6:PRO:HD3	1.79	0.42
1:C:138:ASN:HD22	1:C:138:ASN:HA	1.68	0.42
1:D:141:MET:HA	1:D:141:MET:HE3	2.00	0.42
1:E:99:ARG:HH11	1:F:77:GLY:HA3	1.85	0.42
1:F:139:ARG:O	1:F:143:VAL:HG23	2.19	0.42
1:I:218:ASN:OD1	1:I:221:ASN:N	2.48	0.42
1:J:5:ARG:HA	1:J:6:PRO:HD3	1.80	0.42
1:J:118:LEU:HD13	1:J:161:LEU:O	2.20	0.42
1:J:242:LYS:CB	1:J:244:GLU:OE1	2.59	0.42
1:K:221:ASN:O	1:K:225:LEU:HD12	2.19	0.42
1:L:69:LEU:HB3	1:L:113:LYS:HG2	2.02	0.42
1:L:78:GLU:OE1	1:L:78:GLU:HA	2.20	0.42
1:L:141:MET:HE2	1:L:141:MET:HB3	1.84	0.42
1:L:218:ASN:HB3	1:L:220:SER:H	1.85	0.42
1:P:131:THR:CA	1:P:172:VAL:HG11	2.41	0.42
1:P:156:GLY:O	1:P:159:LYS:HG3	2.19	0.42
1:Q:132:LEU:O	1:Q:136:LYS:HG3	2.20	0.42
1:R:218:ASN:N	1:R:218:ASN:HD22	2.16	0.42
1:T:222:ASP:O	1:T:223:GLU:C	2.60	0.42
1:A:160:MET:HE3	1:A:160:MET:N	2.34	0.42
1:D:116:ARG:O	1:D:120:LYS:HG3	2.20	0.42
1:D:161:LEU:HD23	1:D:161:LEU:HA	1.83	0.42
1:D:221:ASN:HA	1:D:224:LYS:HG2	2.00	0.42
1:J:243:PRO:HA	1:J:246:MET:HE1	2.00	0.42
1:J:251:ILE:HA	1:J:254:LYS:HZ3	1.83	0.42
1:K:47:HIS:CE1	1:L:83:MET:HE2	2.54	0.42
1:L:21:ILE:HG13	1:L:47:HIS:HB3	2.01	0.42
1:N:4:ARG:NH2	1:N:232:ASP:OD1	2.52	0.42
1:O:255:THR:O	1:O:255:THR:HG22	2.19	0.42
1:Q:76:THR:N	1:R:98:GLU:OE1	2.47	0.42
1:Q:246:MET:HB2	1:Q:246:MET:HE3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:7:PHE:CE1	1:S:40:VAL:HG23	2.55	0.42
1:T:246:MET:HE2	1:T:246:MET:HB2	1.90	0.42
1:T:253:THR:HG22	1:T:254:LYS:N	2.33	0.42
1:A:106:THR:OG1	1:A:109:GLN:HG3	2.19	0.42
1:B:67:VAL:O	1:B:113:LYS:HD3	2.19	0.42
1:B:215:GLY:O	1:B:217:ALA:N	2.53	0.42
1:D:171:PRO:CD	1:D:214:GLY:O	2.66	0.42
1:D:183:PRO:CG	1:D:224:LYS:HD3	2.50	0.42
1:E:139:ARG:HH11	1:E:142:GLU:CD	2.28	0.42
1:I:83:MET:HE1	1:J:14:CYS:SG	2.60	0.42
1:J:173:TRP:CH2	1:J:185:GLN:OE1	2.73	0.42
1:J:244:GLU:O	1:J:248:MET:HG3	2.19	0.42
1:M:87:MET:HE2	1:M:87:MET:HB3	1.79	0.42
1:P:62:ILE:N	1:P:62:ILE:CD1	2.82	0.42
1:Q:48:LEU:HD12	1:Q:48:LEU:HA	1.70	0.42
1:R:43:PRO:HG2	1:R:51:ALA:CB	2.50	0.42
1:S:5:ARG:O	1:S:210:ARG:NH1	2.52	0.42
1:T:139:ARG:HG2	1:T:142:GLU:OE1	2.20	0.42
1:T:197:PHE:CE1	1:T:201:VAL:HG21	2.55	0.42
1:C:90:LYS:O	1:C:90:LYS:HG2	2.18	0.42
1:E:245:PHE:HA	1:E:248:MET:HG3	2.02	0.42
1:F:212:ILE:HD11	1:F:235:LEU:HB2	2.01	0.42
1:H:8:ILE:HB	1:H:252:LEU:HD23	2.01	0.42
1:H:43:PRO:HG2	1:H:48:LEU:CD1	2.49	0.42
1:L:34:PRO:C	1:L:36:SER:H	2.28	0.42
1:N:95:GLY:O	1:N:127:CYS:HB2	2.18	0.42
1:O:116:ARG:O	1:O:120:LYS:HG3	2.19	0.42
1:P:242:LYS:C	1:P:244:GLU:H	2.26	0.42
1:R:12:PHE:N	1:R:12:PHE:CD1	2.88	0.42
1:R:25:VAL:HA	1:R:28:ILE:HG13	2.01	0.42
1:S:145:ILE:O	1:S:149:GLU:CG	2.68	0.42
1:B:4:ARG:HE	1:B:4:ARG:HB2	1.43	0.42
1:D:218:ASN:OD1	1:D:221:ASN:OD1	2.38	0.42
1:D:221:ASN:HA	1:D:224:LYS:HE3	2.02	0.42
1:I:144:ASN:O	1:I:148:LEU:HB2	2.19	0.42
1:I:212:ILE:CD1	1:I:235:LEU:HB2	2.50	0.42
1:L:97:SER:OG	1:L:175:ILE:HD11	2.18	0.42
1:P:134:GLU:HG2	1:P:143:VAL:HG21	2.00	0.42
1:Q:34:PRO:HG2	1:Q:37:VAL:HG23	2.02	0.42
1:K:213:TYR:C	1:K:215:GLY:H	2.21	0.42
1:M:177:THR:C	1:M:179:VAL:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:236:VAL:HG11	1:Q:240:SER:N	2.35	0.42
1:R:187:GLU:CD	1:R:230:ASN:H	2.27	0.42
1:D:68:TYR:HB2	1:D:78:GLU:HB3	2.01	0.41
1:G:37:VAL:CG1	1:G:38:ASP:N	2.83	0.41
1:G:196:TRP:O	1:G:200:LYS:HB2	2.20	0.41
1:K:197:PHE:CD1	1:K:206:ALA:CA	3.02	0.41
1:L:177:THR:HG21	1:L:179:VAL:HG21	2.00	0.41
1:M:151:LEU:HD23	1:M:162:TRP:CH2	2.55	0.41
1:N:32:LYS:O	1:N:32:LYS:CG	2.67	0.41
1:P:87:MET:HE2	1:P:87:MET:HB3	1.85	0.41
1:R:116:ARG:NH1	1:R:116:ARG:HG3	2.35	0.41
1:T:66:ASN:ND2	1:T:67:VAL:H	2.18	0.41
1:T:242:LYS:HB2	1:T:243:PRO:CD	2.43	0.41
1:B:83:MET:O	1:B:87:MET:HG3	2.20	0.41
1:D:101:ARG:CZ	1:D:131:THR:HG23	2.50	0.41
1:F:21:ILE:O	1:F:25:VAL:HG23	2.20	0.41
1:F:145:ILE:HD13	1:F:196:TRP:CD1	2.55	0.41
1:F:148:LEU:HB3	1:F:196:TRP:CH2	2.54	0.41
1:I:76:THR:CG2	1:J:65:GLN:HB3	2.49	0.41
1:L:141:MET:HA	1:L:141:MET:CE	2.41	0.41
1:L:219:GLY:HA2	1:L:222:ASP:HB2	2.02	0.41
1:M:83:MET:HE1	1:N:44:SER:CB	2.50	0.41
1:M:145:ILE:O	1:M:149:GLU:HG2	2.20	0.41
1:M:148:LEU:HD12	1:M:148:LEU:HA	1.82	0.41
1:N:141:MET:O	1:N:145:ILE:HG12	2.20	0.41
1:Q:65:GLN:O	1:Q:93:ILE:HG22	2.20	0.41
1:Q:138:ASN:O	1:Q:138:ASN:ND2	2.53	0.41
1:R:33:ILE:O	1:R:59:GLN:NE2	2.53	0.41
1:T:40:VAL:HG12	1:T:41:ILE:N	2.34	0.41
1:J:164:GLU:OE1	1:J:164:GLU:HA	2.20	0.41
1:J:217:ALA:O	1:J:248:MET:HE1	2.20	0.41
1:J:228:CYS:HA	1:J:229:PRO:HD2	1.80	0.41
1:N:11:ASN:OD1	1:N:65:GLN:HG2	2.20	0.41
1:N:61:ARG:HD2	1:N:61:ARG:HA	1.87	0.41
1:O:116:ARG:HG2	1:O:116:ARG:HH11	1.84	0.41
1:R:82:GLU:CD	1:R:82:GLU:N	2.76	0.41
1:R:151:LEU:HD12	1:R:151:LEU:O	2.21	0.41
1:S:6:PRO:HG3	1:S:37:VAL:HG12	2.02	0.41
1:S:74:ALA:HA	1:T:13:LYS:HD3	2.02	0.41
1:T:7:PHE:O	1:T:233:GLY:HA3	2.20	0.41
1:T:242:LYS:CB	1:T:243:PRO:CD	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:PHE:N	1:A:12:PHE:CD1	2.88	0.41
1:B:115:LYS:O	1:B:119:GLU:HB2	2.20	0.41
1:B:128:VAL:CG2	1:B:144:ASN:HD21	2.33	0.41
1:B:145:ILE:HG12	1:B:196:TRP:CD1	2.55	0.41
1:E:131:THR:OG1	1:E:134:GLU:HG3	2.21	0.41
1:G:12:PHE:CD1	1:G:12:PHE:N	2.88	0.41
1:J:5:ARG:O	1:J:210:ARG:HD2	2.21	0.41
1:K:193:LEU:HD23	1:K:193:LEU:HA	1.89	0.41
1:M:69:LEU:H	1:M:69:LEU:HG	1.71	0.41
1:N:107:ASP:OD1	1:N:107:ASP:N	2.53	0.41
1:S:7:PHE:HE1	1:S:40:VAL:CG2	2.32	0.41
1:S:180:VAL:HG23	1:S:216:SER:HB3	2.01	0.41
1:A:167:ILE:HG13	1:A:211:ILE:HG12	2.02	0.41
1:A:190:HIS:HB3	1:A:230:ASN:O	2.20	0.41
1:B:95:GLY:O	1:B:127:CYS:HB2	2.21	0.41
1:B:247:THR:O	1:B:251:ILE:HD13	2.21	0.41
1:D:34:PRO:HB2	1:D:36:SER:OG	2.21	0.41
1:H:221:ASN:HD22	1:H:224:LYS:HB2	1.85	0.41
1:J:217:ALA:O	1:J:248:MET:HE3	2.20	0.41
1:J:217:ALA:HB1	1:J:234:PHE:CD1	2.56	0.41
1:J:243:PRO:HD2	1:J:244:GLU:OE1	2.21	0.41
1:K:197:PHE:HE1	1:K:206:ALA:N	2.18	0.41
1:L:218:ASN:HB3	1:L:220:SER:OG	2.21	0.41
1:R:82:GLU:CD	1:R:116:ARG:HH21	2.28	0.41
1:R:229:PRO:HB2	1:R:230:ASN:HD22	1.85	0.41
1:S:33:ILE:HA	1:S:34:PRO:HD3	1.91	0.41
1:S:182:THR:HB	1:S:184:GLU:OE1	2.21	0.41
1:A:137:ALA:HB3	1:A:139:ARG:CG	2.49	0.41
1:C:72:ASN:N	1:C:72:ASN:HD22	2.17	0.41
1:C:174:SER:HB2	1:C:180:VAL:HA	2.02	0.41
1:C:228:CYS:HA	1:C:229:PRO:HD2	1.90	0.41
1:K:67:VAL:HG22	1:K:68:TYR:H	1.85	0.41
1:K:142:GLU:HG2	1:K:143:VAL:N	2.36	0.41
1:K:229:PRO:HB2	1:K:230:ASN:HD22	1.86	0.41
1:N:87:MET:HE2	1:N:87:MET:HB3	1.96	0.41
1:N:142:GLU:CG	1:N:143:VAL:N	2.82	0.41
1:N:171:PRO:O	1:N:174:SER:OG	2.38	0.41
1:O:67:VAL:HG22	1:O:68:TYR:N	2.36	0.41
1:Q:253:THR:C	1:Q:255:THR:N	2.77	0.41
1:A:218:ASN:HD22	1:A:220:SER:H	1.64	0.41
1:B:128:VAL:HB	1:B:147:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:HG2	1:B:160:MET:N	2.35	0.41
1:C:169:TYR:CE1	1:C:189:VAL:HG11	2.56	0.41
1:G:7:PHE:CZ	1:G:40:VAL:HG11	2.56	0.41
1:G:95:GLY:C	1:G:127:CYS:HB2	2.46	0.41
1:G:213:TYR:CD2	1:G:234:PHE:HD1	2.36	0.41
1:I:143:VAL:O	1:I:147:GLN:HG3	2.20	0.41
1:I:189:VAL:O	1:I:193:LEU:HG	2.21	0.41
1:I:253:THR:HG22	1:I:254:LYS:HD2	2.02	0.41
1:J:8:ILE:HD13	1:J:245:PHE:CE1	2.55	0.41
1:J:145:ILE:HG22	1:J:149:GLU:HG2	2.01	0.41
1:K:8:ILE:HG13	1:K:9:GLY:N	2.36	0.41
1:K:190:HIS:CE1	1:K:211:ILE:HG22	2.56	0.41
1:K:195:LYS:HE3	1:K:195:LYS:HB2	1.70	0.41
1:L:218:ASN:CB	1:L:221:ASN:CG	2.92	0.41
1:L:221:ASN:HD22	1:L:222:ASP:H	1.61	0.41
1:N:221:ASN:C	1:N:223:GLU:N	2.78	0.41
1:R:4:ARG:NH2	1:R:194:ARG:NH2	2.68	0.41
1:F:171:PRO:HG2	1:F:213:TYR:CZ	2.54	0.41
1:K:204:GLU:HG2	1:K:205:GLY:H	1.83	0.41
1:N:134:GLU:HB3	1:N:143:VAL:HG21	2.01	0.41
1:O:221:ASN:O	1:O:225:LEU:HG	2.21	0.41
1:P:189:VAL:O	1:P:193:LEU:HG	2.20	0.41
1:Q:44:SER:O	1:Q:45:ALA:C	2.64	0.41
1:Q:166:VAL:CG2	1:Q:210:ARG:CZ	2.99	0.41
1:S:34:PRO:C	1:S:36:SER:H	2.28	0.41
1:T:197:PHE:O	1:T:201:VAL:HB	2.21	0.41
1:B:128:VAL:HG21	1:B:144:ASN:HD21	1.86	0.41
1:C:166:VAL:CG1	1:C:212:ILE:HD13	2.51	0.41
1:C:169:TYR:CZ	1:C:189:VAL:HG11	2.56	0.41
1:C:236:VAL:CG1	1:C:239:ALA:HB3	2.51	0.41
1:C:250:ASP:O	1:C:253:THR:HB	2.21	0.41
1:E:96:HIS:CG	1:F:76:THR:HG21	2.56	0.41
1:E:171:PRO:HD2	1:E:214:GLY:C	2.45	0.41
1:E:173:TRP:CD1	1:E:173:TRP:H	2.39	0.41
1:E:178:GLY:HA3	1:I:172:VAL:HG13	2.03	0.41
1:E:250:ASP:O	1:E:254:LYS:HG2	2.20	0.41
1:G:74:ALA:HA	1:H:13:LYS:HD3	2.03	0.41
1:H:163:LYS:HB2	1:H:163:LYS:HE2	1.89	0.41
1:H:223:GLU:O	1:H:227:GLN:HG3	2.21	0.41
1:I:72:ASN:N	1:I:72:ASN:HD22	2.18	0.41
1:I:137:ALA:HB3	1:I:139:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:194:ARG:NH1	1:I:209:ILE:HG23	2.36	0.41
1:I:218:ASN:OD1	1:I:221:ASN:ND2	2.53	0.41
1:K:76:THR:HG1	1:L:65:GLN:HB3	1.86	0.41
1:K:130:GLU:OE2	1:K:169:TYR:OH	2.34	0.41
1:K:160:MET:HA	1:K:163:LYS:HZ2	1.86	0.41
1:M:95:GLY:O	1:M:100:ARG:NE	2.50	0.41
1:M:180:VAL:HG23	1:M:215:GLY:O	2.21	0.41
1:O:31:HIS:HB2	1:O:246:MET:HG2	2.03	0.41
1:P:128:VAL:HG12	1:P:147:GLN:OE1	2.20	0.41
1:Q:96:HIS:CE1	1:Q:98:GLU:CD	2.99	0.41
1:Q:222:ASP:O	1:Q:226:GLY:N	2.49	0.41
1:R:48:LEU:HD12	1:R:48:LEU:HA	1.75	0.41
1:R:67:VAL:HG23	1:R:79:THR:HG22	2.02	0.41
1:R:116:ARG:HG3	1:R:116:ARG:HH11	1.86	0.41
1:R:118:LEU:HD21	1:R:165:VAL:HG23	2.02	0.41
1:S:195:LYS:O	1:S:199:GLU:HG3	2.21	0.41
1:A:130:GLU:O	1:A:173:TRP:HD1	2.04	0.41
1:C:13:LYS:HA	1:C:65:GLN:OE1	2.21	0.41
1:D:160:MET:O	1:D:163:LYS:HB2	2.21	0.41
1:D:224:LYS:HG3	1:D:225:LEU:N	2.36	0.41
1:G:96:HIS:ND1	1:G:98:GLU:HG3	2.36	0.41
1:H:66:ASN:HD21	1:H:113:LYS:NZ	2.19	0.41
1:H:155:LEU:HD12	1:H:162:TRP:CE2	2.55	0.41
1:I:63:ALA:HB2	1:I:91:HIS:HB2	2.03	0.41
1:J:247:THR:O	1:J:251:ILE:HD13	2.21	0.41
1:K:202:ALA:HB1	1:K:204:GLU:OE1	2.20	0.41
1:M:183:PRO:HA	1:M:225:LEU:HD23	2.03	0.41
1:P:57:SER:HB3	1:P:60:LEU:HB3	2.03	0.41
1:Q:61:ARG:HD2	1:Q:61:ARG:HA	1.50	0.41
1:R:184:GLU:OE1	1:R:224:LYS:NZ	2.48	0.41
1:S:5:ARG:NH1	1:S:35:ASP:O	2.47	0.41
1:S:224:LYS:O	1:S:227:GLN:HB2	2.21	0.41
1:S:246:MET:H	1:S:246:MET:CE	2.34	0.41
1:T:84:LEU:HD12	1:T:122:MET:HE1	2.01	0.41
1:A:218:ASN:ND2	1:A:218:ASN:O	2.53	0.40
1:A:218:ASN:N	1:A:222:ASP:CG	2.79	0.40
1:B:66:ASN:ND2	1:B:67:VAL:O	2.53	0.40
1:B:118:LEU:HD12	1:B:155:LEU:HD21	2.03	0.40
1:C:116:ARG:O	1:C:120:LYS:HG3	2.20	0.40
1:D:68:TYR:CE2	1:D:75:TRP:HB3	2.55	0.40
1:E:161:LEU:C	1:E:163:LYS:N	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:ILE:HG23	1:I:176:GLY:O	2.21	0.40
1:G:65:GLN:HB3	1:H:76:THR:HG23	2.03	0.40
1:G:111:ALA:HB1	1:G:154:GLU:CG	2.51	0.40
1:H:55:ASN:OD1	1:H:55:ASN:C	2.64	0.40
1:L:59:GLN:HE21	1:L:59:GLN:HB2	1.71	0.40
1:L:204:GLU:O	1:L:207:GLN:HB2	2.22	0.40
1:L:218:ASN:C	1:L:220:SER:H	2.29	0.40
1:N:187:GLU:O	1:N:191:VAL:HG23	2.21	0.40
1:O:125:ILE:HG21	1:O:235:LEU:HD13	2.02	0.40
1:O:194:ARG:CG	1:O:206:ALA:O	2.69	0.40
1:P:69:LEU:CD2	1:P:70:GLU:HG2	2.50	0.40
1:S:55:ASN:CG	1:S:60:LEU:HD23	2.46	0.40
1:S:160:MET:HE2	1:S:160:MET:HB3	1.77	0.40
1:T:217:ALA:CB	1:T:248:MET:HE1	2.49	0.40
1:A:251:ILE:HD12	1:A:251:ILE:HA	1.80	0.40
1:F:68:TYR:CE1	1:F:69:LEU:HD22	2.57	0.40
1:I:130:GLU:O	1:I:130:GLU:HG2	2.18	0.40
1:M:83:MET:HG2	1:N:47:HIS:HE1	1.86	0.40
1:P:186:ALA:HB1	1:P:231:ILE:HD11	2.03	0.40
1:Q:195:LYS:O	1:Q:199:GLU:CB	2.60	0.40
1:R:68:TYR:CE1	1:R:69:LEU:CD2	3.04	0.40
1:B:87:MET:HE2	1:B:87:MET:HB3	1.87	0.40
1:E:61:ARG:HA	1:E:61:ARG:HD2	1.85	0.40
1:F:5:ARG:O	1:F:210:ARG:HD2	2.21	0.40
1:F:90:LYS:O	1:F:90:LYS:HG2	2.21	0.40
1:H:222:ASP:OD1	1:H:234:PHE:CZ	2.74	0.40
1:L:112:LYS:HE3	1:L:154:GLU:OE2	2.22	0.40
1:L:190:HIS:CE1	1:L:211:ILE:HG22	2.57	0.40
1:L:218:ASN:N	1:L:222:ASP:OD1	2.55	0.40
1:M:5:ARG:HH12	1:M:37:VAL:N	2.19	0.40
1:M:33:ILE:O	1:M:59:GLN:HG2	2.20	0.40
1:M:52:ILE:HD11	1:M:89:LEU:HD21	2.04	0.40
1:M:240:SER:HA	1:M:245:PHE:CD1	2.57	0.40
1:N:150:ALA:O	1:N:154:GLU:HG2	2.22	0.40
1:N:168:ALA:HA	1:N:212:ILE:O	2.21	0.40
1:O:218:ASN:ND2	1:O:219:GLY:N	2.70	0.40
1:Q:24:HIS:NE2	1:Q:28:ILE:HD11	2.36	0.40
1:T:12:PHE:O	1:T:13:LYS:HB2	2.20	0.40
1:T:117:ALA:O	1:T:122:MET:HB2	2.21	0.40
1:C:5:ARG:HE	1:C:38:ASP:CG	2.28	0.40
1:D:37:VAL:HG12	1:D:38:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:GLU:OE1	1:E:113:LYS:NZ	2.46	0.40
1:E:187:GLU:O	1:E:187:GLU:HG3	2.21	0.40
1:G:75:TRP:HD1	1:H:14:CYS:HB3	1.86	0.40
1:I:97:SER:N	1:I:170:GLU:OE1	2.54	0.40
1:K:196:TRP:CE3	1:K:197:PHE:N	2.89	0.40
1:L:68:TYR:CE2	1:L:70:GLU:HB2	2.56	0.40
1:P:12:PHE:HA	1:P:241:LEU:HD21	2.02	0.40
1:P:149:GLU:OE1	1:P:149:GLU:HA	2.21	0.40
1:R:65:GLN:O	1:R:93:ILE:O	2.40	0.40
1:S:21:ILE:HD13	1:S:21:ILE:N	2.37	0.40
1:S:158:SER:O	1:S:161:LEU:HD23	2.22	0.40
1:S:225:LEU:O	1:S:228:CYS:HB2	2.21	0.40
1:T:249:ILE:O	1:T:252:LEU:HB3	2.21	0.40
1:C:114:ALA:O	1:C:118:LEU:HG	2.21	0.40
1:E:95:GLY:O	1:E:96:HIS:C	2.64	0.40
1:E:252:LEU:O	1:E:255:THR:C	2.65	0.40
1:G:93:ILE:HA	1:G:125:ILE:HB	2.04	0.40
1:J:33:ILE:HB	1:J:59:GLN:HE21	1.86	0.40
1:J:132:LEU:O	1:J:136:LYS:HB2	2.22	0.40
1:K:46:VAL:HG13	1:L:45:ALA:HB1	2.04	0.40
1:K:72:ASN:ND2	1:K:80:SER:OG	2.55	0.40
1:L:12:PHE:N	1:L:12:PHE:CD1	2.90	0.40
1:O:228:CYS:HA	1:O:229:PRO:HD3	1.79	0.40
1:Q:226:GLY:C	1:Q:228:CYS:N	2.80	0.40
1:S:8:ILE:CG2	1:S:39:VAL:HG22	2.52	0.40
1:S:128:VAL:HG11	1:S:148:LEU:HD13	2.03	0.40
1:S:186:ALA:HB1	1:S:213:TYR:CD1	2.57	0.40
1:T:84:LEU:HD23	1:T:84:LEU:HA	1.67	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	252/255 (99%)	241 (96%)	10 (4%)	1 (0%)	30	54
1	B	252/255 (99%)	247 (98%)	5 (2%)	0	100	100
1	C	252/255 (99%)	240 (95%)	11 (4%)	1 (0%)	30	54
1	D	252/255 (99%)	244 (97%)	7 (3%)	1 (0%)	30	54
1	E	252/255 (99%)	240 (95%)	11 (4%)	1 (0%)	30	54
1	F	252/255 (99%)	244 (97%)	7 (3%)	1 (0%)	30	54
1	G	252/255 (99%)	243 (96%)	8 (3%)	1 (0%)	30	54
1	H	252/255 (99%)	240 (95%)	12 (5%)	0	100	100
1	I	252/255 (99%)	243 (96%)	9 (4%)	0	100	100
1	J	252/255 (99%)	244 (97%)	8 (3%)	0	100	100
1	K	252/255 (99%)	240 (95%)	11 (4%)	1 (0%)	30	54
1	L	252/255 (99%)	239 (95%)	13 (5%)	0	100	100
1	M	252/255 (99%)	244 (97%)	8 (3%)	0	100	100
1	N	252/255 (99%)	239 (95%)	11 (4%)	2 (1%)	16	37
1	O	252/255 (99%)	237 (94%)	14 (6%)	1 (0%)	30	54
1	P	252/255 (99%)	233 (92%)	18 (7%)	1 (0%)	30	54
1	Q	252/255 (99%)	237 (94%)	14 (6%)	1 (0%)	30	54
1	R	252/255 (99%)	242 (96%)	7 (3%)	3 (1%)	10	27
1	S	252/255 (99%)	238 (94%)	14 (6%)	0	100	100
1	T	252/255 (99%)	246 (98%)	6 (2%)	0	100	100
All	All	5040/5100 (99%)	4821 (96%)	204 (4%)	15 (0%)	36	60

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	ASN
1	E	220	SER
1	G	219	GLY
1	R	218	ASN
1	Q	201	VAL
1	R	13	LYS
1	K	214	GLY
1	N	13	LYS
1	O	138	ASN
1	R	156	GLY
1	A	156	GLY

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Mol	Chain	Res	Type
1	P	243	PRO
1	D	201	VAL
1	N	156	GLY
1	F	201	VAL

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	202/203 (100%)	179 (89%)	23 (11%)	5	14
1	B	202/203 (100%)	183 (91%)	19 (9%)	8	21
1	C	202/203 (100%)	180 (89%)	22 (11%)	6	16
1	D	202/203 (100%)	174 (86%)	28 (14%)	3	9
1	E	202/203 (100%)	174 (86%)	28 (14%)	3	9
1	F	202/203 (100%)	182 (90%)	20 (10%)	7	19
1	G	202/203 (100%)	177 (88%)	25 (12%)	4	11
1	H	202/203 (100%)	178 (88%)	24 (12%)	5	13
1	I	202/203 (100%)	171 (85%)	31 (15%)	3	7
1	J	202/203 (100%)	181 (90%)	21 (10%)	7	17
1	K	202/203 (100%)	178 (88%)	24 (12%)	5	13
1	L	202/203 (100%)	183 (91%)	19 (9%)	8	21
1	M	202/203 (100%)	175 (87%)	27 (13%)	4	9
1	N	202/203 (100%)	175 (87%)	27 (13%)	4	9
1	O	202/203 (100%)	171 (85%)	31 (15%)	3	7
1	P	202/203 (100%)	178 (88%)	24 (12%)	5	13
1	Q	202/203 (100%)	167 (83%)	35 (17%)	2	5
1	R	202/203 (100%)	180 (89%)	22 (11%)	6	16
1	S	202/203 (100%)	157 (78%)	45 (22%)	1	3
1	T	202/203 (100%)	162 (80%)	40 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4040/4060 (100%)	3505 (87%)	535 (13%)	4 10

All (535) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	32	LYS
1	A	40	VAL
1	A	48	LEU
1	A	49	SER
1	A	57	SER
1	A	72	ASN
1	A	99	ARG
1	A	134	GLU
1	A	139	ARG
1	A	142	GLU
1	A	145	ILE
1	A	149	GLU
1	A	157	GLU
1	A	167	ILE
1	A	179	VAL
1	A	191	VAL
1	A	195	LYS
1	A	218	ASN
1	A	221	ASN
1	A	251	ILE
1	A	252	LEU
1	A	255	THR
1	B	4	ARG
1	B	35	ASP
1	B	52	ILE
1	B	69	LEU
1	B	101	ARG
1	B	138	ASN
1	B	144	ASN
1	B	145	ILE
1	B	148	LEU
1	B	159	LYS
1	B	160	MET
1	B	166	VAL
1	B	177	THR
1	B	179	VAL

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Mol	Chain	Res	Type
1	B	184	GLU
1	B	210	ARG
1	B	221	ASN
1	B	223	GLU
1	B	247	THR
1	C	8	ILE
1	C	44	SER
1	C	48	LEU
1	C	49	SER
1	C	61	ARG
1	C	62	ILE
1	C	69	LEU
1	C	110	SER
1	C	112	LYS
1	C	116	ARG
1	C	138	ASN
1	C	139	ARG
1	C	140	THR
1	C	148	LEU
1	C	158	SER
1	C	159	LYS
1	C	160	MET
1	C	179	VAL
1	C	207	GLN
1	C	218	ASN
1	C	251	ILE
1	C	253	THR
1	D	4	ARG
1	D	8	ILE
1	D	32	LYS
1	D	36	SER
1	D	44	SER
1	D	48	LEU
1	D	58	LYS
1	D	62	ILE
1	D	67	VAL
1	D	69	LEU
1	D	83	MET
1	D	99	ARG
1	D	116	ARG
1	D	135	ARG
1	D	138	ASN

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Mol	Chain	Res	Type
1	D	140	THR
1	D	145	ILE
1	D	148	LEU
1	D	160	MET
1	D	172	VAL
1	D	179	VAL
1	D	180	VAL
1	D	188	GLU
1	D	194	ARG
1	D	195	LYS
1	D	218	ASN
1	D	244	GLU
1	D	252	LEU
1	E	48	LEU
1	E	49	SER
1	E	62	ILE
1	E	69	LEU
1	E	89	LEU
1	E	115	LYS
1	E	116	ARG
1	E	119	GLU
1	E	130	GLU
1	E	131	THR
1	E	138	ASN
1	E	140	THR
1	E	141	MET
1	E	145	ILE
1	E	148	LEU
1	E	149	GLU
1	E	157	GLU
1	E	158	SER
1	E	160	MET
1	E	184	GLU
1	E	195	LYS
1	E	199	GLU
1	E	220	SER
1	E	222	ASP
1	E	225	LEU
1	E	247	THR
1	E	248	MET
1	E	255	THR
1	F	15	ASN

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Mol	Chain	Res	Type
1	F	44	SER
1	F	48	LEU
1	F	58	LYS
1	F	61	ARG
1	F	62	ILE
1	F	69	LEU
1	F	82	GLU
1	F	89	LEU
1	F	112	LYS
1	F	135	ARG
1	F	148	LEU
1	F	159	LYS
1	F	160	MET
1	F	175	ILE
1	F	180	VAL
1	F	209	ILE
1	F	211	ILE
1	F	221	ASN
1	F	236	VAL
1	G	4	ARG
1	G	8	ILE
1	G	23	SER
1	G	36	SER
1	G	40	VAL
1	G	62	ILE
1	G	93	ILE
1	G	116	ARG
1	G	130	GLU
1	G	135	ARG
1	G	138	ASN
1	G	139	ARG
1	G	148	LEU
1	G	159	LYS
1	G	160	MET
1	G	179	VAL
1	G	180	VAL
1	G	207	GLN
1	G	211	ILE
1	G	224	LYS
1	G	225	LEU
1	G	242	LYS
1	G	247	THR

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Mol	Chain	Res	Type
1	G	252	LEU
1	G	254	LYS
1	H	40	VAL
1	H	48	LEU
1	H	49	SER
1	H	58	LYS
1	H	69	LEU
1	H	86	ASP
1	H	94	VAL
1	H	109	GLN
1	H	112	LYS
1	H	115	LYS
1	H	138	ASN
1	H	142	GLU
1	H	148	LEU
1	H	154	GLU
1	H	158	SER
1	H	159	LYS
1	H	160	MET
1	H	163	LYS
1	H	164	GLU
1	H	180	VAL
1	H	195	LYS
1	H	211	ILE
1	H	248	MET
1	H	252	LEU
1	I	4	ARG
1	I	8	ILE
1	I	13	LYS
1	I	32	LYS
1	I	36	SER
1	I	44	SER
1	I	46	VAL
1	I	48	LEU
1	I	69	LEU
1	I	90	LYS
1	I	130	GLU
1	I	134	GLU
1	I	138	ASN
1	I	142	GLU
1	I	145	ILE
1	I	148	LEU

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Mol	Chain	Res	Type
1	I	157	GLU
1	I	163	LYS
1	I	167	ILE
1	I	179	VAL
1	I	180	VAL
1	I	191	VAL
1	I	194	ARG
1	I	200	LYS
1	I	209	ILE
1	I	218	ASN
1	I	227	GLN
1	I	240	SER
1	I	251	ILE
1	I	252	LEU
1	I	253	THR
1	J	8	ILE
1	J	17	SER
1	J	23	SER
1	J	48	LEU
1	J	49	SER
1	J	58	LYS
1	J	61	ARG
1	J	110	SER
1	J	112	LYS
1	J	115	LYS
1	J	135	ARG
1	J	148	LEU
1	J	153	LYS
1	J	159	LYS
1	J	160	MET
1	J	163	LYS
1	J	177	THR
1	J	218	ASN
1	J	224	LYS
1	J	240	SER
1	J	255	THR
1	K	8	ILE
1	K	28	ILE
1	K	46	VAL
1	K	48	LEU
1	K	60	LEU
1	K	62	ILE

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Mol	Chain	Res	Type
1	K	69	LEU
1	K	98	GLU
1	K	135	ARG
1	K	142	GLU
1	K	143	VAL
1	K	148	LEU
1	K	157	GLU
1	K	195	LYS
1	K	209	ILE
1	K	210	ARG
1	K	218	ASN
1	K	220	SER
1	K	221	ASN
1	K	242	LYS
1	K	248	MET
1	K	251	ILE
1	K	254	LYS
1	K	255	THR
1	L	48	LEU
1	L	49	SER
1	L	59	GLN
1	L	69	LEU
1	L	99	ARG
1	L	100	ARG
1	L	141	MET
1	L	148	LEU
1	L	173	TRP
1	L	179	VAL
1	L	189	VAL
1	L	199	GLU
1	L	204	GLU
1	L	218	ASN
1	L	221	ASN
1	L	232	ASP
1	L	236	VAL
1	L	240	SER
1	L	254	LYS
1	M	5	ARG
1	M	32	LYS
1	M	35	ASP
1	M	44	SER
1	M	48	LEU

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Mol	Chain	Res	Type
1	M	49	SER
1	M	58	LYS
1	M	62	ILE
1	M	69	LEU
1	M	75	TRP
1	M	97	SER
1	M	98	GLU
1	M	103	MET
1	M	106	THR
1	M	112	LYS
1	M	145	ILE
1	M	148	LEU
1	M	159	LYS
1	M	160	MET
1	M	170	GLU
1	M	179	VAL
1	M	209	ILE
1	M	210	ARG
1	M	224	LYS
1	M	251	ILE
1	M	253	THR
1	M	255	THR
1	N	15	ASN
1	N	32	LYS
1	N	36	SER
1	N	44	SER
1	N	48	LEU
1	N	49	SER
1	N	62	ILE
1	N	69	LEU
1	N	89	LEU
1	N	120	LYS
1	N	130	GLU
1	N	139	ARG
1	N	140	THR
1	N	142	GLU
1	N	145	ILE
1	N	148	LEU
1	N	160	MET
1	N	175	ILE
1	N	179	VAL
1	N	180	VAL

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Mol	Chain	Res	Type
1	N	184	GLU
1	N	224	LYS
1	N	225	LEU
1	N	240	SER
1	N	244	GLU
1	N	247	THR
1	N	248	MET
1	O	8	ILE
1	O	13	LYS
1	O	36	SER
1	O	37	VAL
1	O	48	LEU
1	O	49	SER
1	O	59	GLN
1	O	69	LEU
1	O	86	ASP
1	O	90	LYS
1	O	112	LYS
1	O	120	LYS
1	O	131	THR
1	O	138	ASN
1	O	139	ARG
1	O	140	THR
1	O	145	ILE
1	O	148	LEU
1	O	160	MET
1	O	163	LYS
1	O	166	VAL
1	O	167	ILE
1	O	180	VAL
1	O	204	GLU
1	O	210	ARG
1	O	231	ILE
1	O	236	VAL
1	O	244	GLU
1	O	247	THR
1	O	248	MET
1	O	251	ILE
1	P	15	ASN
1	P	35	ASP
1	P	48	LEU
1	P	50	THR

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Mol	Chain	Res	Type
1	P	59	GLN
1	P	61	ARG
1	P	69	LEU
1	P	89	LEU
1	P	108	GLU
1	P	115	LYS
1	P	128	VAL
1	P	130	GLU
1	P	145	ILE
1	P	148	LEU
1	P	159	LYS
1	P	160	MET
1	P	172	VAL
1	P	173	TRP
1	P	199	GLU
1	P	209	ILE
1	P	210	ARG
1	P	221	ASN
1	P	223	GLU
1	P	236	VAL
1	Q	8	ILE
1	Q	23	SER
1	Q	28	ILE
1	Q	37	VAL
1	Q	46	VAL
1	Q	48	LEU
1	Q	50	THR
1	Q	58	LYS
1	Q	59	GLN
1	Q	61	ARG
1	Q	75	TRP
1	Q	81	VAL
1	Q	93	ILE
1	Q	103	MET
1	Q	106	THR
1	Q	115	LYS
1	Q	116	ARG
1	Q	139	ARG
1	Q	148	LEU
1	Q	153	LYS
1	Q	158	SER
1	Q	159	LYS

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Mol	Chain	Res	Type
1	Q	160	MET
1	Q	177	THR
1	Q	179	VAL
1	Q	189	VAL
1	Q	195	LYS
1	Q	209	ILE
1	Q	210	ARG
1	Q	220	SER
1	Q	230	ASN
1	Q	231	ILE
1	Q	236	VAL
1	Q	252	LEU
1	Q	255	THR
1	R	8	ILE
1	R	15	ASN
1	R	28	ILE
1	R	33	ILE
1	R	48	LEU
1	R	49	SER
1	R	69	LEU
1	R	80	SER
1	R	87	MET
1	R	89	LEU
1	R	119	GLU
1	R	120	LYS
1	R	148	LEU
1	R	153	LYS
1	R	210	ARG
1	R	230	ASN
1	R	231	ILE
1	R	244	GLU
1	R	248	MET
1	R	251	ILE
1	R	253	THR
1	R	255	THR
1	S	8	ILE
1	S	23	SER
1	S	28	ILE
1	S	32	LYS
1	S	40	VAL
1	S	44	SER
1	S	48	LEU

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Mol	Chain	Res	Type
1	S	49	SER
1	S	52	ILE
1	S	61	ARG
1	S	69	LEU
1	S	87	MET
1	S	89	LEU
1	S	99	ARG
1	S	101	ARG
1	S	102	ILE
1	S	106	THR
1	S	108	GLU
1	S	116	ARG
1	S	128	VAL
1	S	130	GLU
1	S	138	ASN
1	S	148	LEU
1	S	157	GLU
1	S	158	SER
1	S	159	LYS
1	S	160	MET
1	S	163	LYS
1	S	180	VAL
1	S	185	GLN
1	S	188	GLU
1	S	195	LYS
1	S	207	GLN
1	S	210	ARG
1	S	220	SER
1	S	221	ASN
1	S	231	ILE
1	S	241	LEU
1	S	244	GLU
1	S	246	MET
1	S	247	THR
1	S	248	MET
1	S	250	ASP
1	S	253	THR
1	S	254	LYS
1	T	7	PHE
1	T	8	ILE
1	T	22	LYS
1	T	23	SER

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Mol	Chain	Res	Type
1	T	28	ILE
1	T	32	LYS
1	T	33	ILE
1	T	48	LEU
1	T	49	SER
1	T	67	VAL
1	T	84	LEU
1	T	87	MET
1	T	89	LEU
1	T	93	ILE
1	T	99	ARG
1	T	112	LYS
1	T	115	LYS
1	T	148	LEU
1	T	153	LYS
1	T	158	SER
1	T	159	LYS
1	T	160	MET
1	T	163	LYS
1	T	164	GLU
1	T	170	GLU
1	T	174	SER
1	T	180	VAL
1	T	199	GLU
1	T	209	ILE
1	T	210	ARG
1	T	211	ILE
1	T	216	SER
1	T	220	SER
1	T	223	GLU
1	T	231	ILE
1	T	240	SER
1	T	242	LYS
1	T	244	GLU
1	T	248	MET
1	T	253	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	72	ASN

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Mol	Chain	Res	Type
1	A	91	HIS
1	A	109	GLN
1	A	138	ASN
1	A	144	ASN
1	A	218	ASN
1	B	11	ASN
1	B	65	GLN
1	B	66	ASN
1	B	72	ASN
1	B	144	ASN
1	B	221	ASN
1	C	47	HIS
1	C	59	GLN
1	C	66	ASN
1	C	72	ASN
1	C	91	HIS
1	C	138	ASN
1	C	221	ASN
1	D	31	HIS
1	D	47	HIS
1	D	59	GLN
1	D	72	ASN
1	D	138	ASN
1	D	144	ASN
1	D	207	GLN
1	D	218	ASN
1	E	72	ASN
1	E	91	HIS
1	F	65	GLN
1	F	91	HIS
1	F	144	ASN
1	G	15	ASN
1	G	66	ASN
1	G	72	ASN
1	G	144	ASN
1	G	230	ASN
1	H	47	HIS
1	H	66	ASN
1	H	85	GLN
1	H	221	ASN
1	H	230	ASN
1	I	11	ASN

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Mol	Chain	Res	Type
1	I	59	GLN
1	I	72	ASN
1	I	91	HIS
1	I	138	ASN
1	I	221	ASN
1	J	11	ASN
1	J	47	HIS
1	J	72	ASN
1	J	91	HIS
1	J	207	GLN
1	K	59	GLN
1	K	66	ASN
1	K	72	ASN
1	K	218	ASN
1	K	221	ASN
1	K	230	ASN
1	L	59	GLN
1	L	72	ASN
1	L	91	HIS
1	L	138	ASN
1	L	144	ASN
1	L	208	HIS
1	L	221	ASN
1	M	47	HIS
1	M	59	GLN
1	M	66	ASN
1	M	72	ASN
1	M	190	HIS
1	N	15	ASN
1	N	47	HIS
1	N	72	ASN
1	N	91	HIS
1	N	109	GLN
1	N	218	ASN
1	O	59	GLN
1	O	66	ASN
1	O	72	ASN
1	O	185	GLN
1	O	190	HIS
1	O	208	HIS
1	O	218	ASN
1	P	15	ASN

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Mol	Chain	Res	Type
1	P	59	GLN
1	P	66	ASN
1	P	72	ASN
1	P	91	HIS
1	P	96	HIS
1	P	138	ASN
1	P	144	ASN
1	P	230	ASN
1	Q	47	HIS
1	Q	59	GLN
1	Q	66	ASN
1	Q	72	ASN
1	Q	85	GLN
1	Q	91	HIS
1	Q	190	HIS
1	Q	218	ASN
1	Q	230	ASN
1	R	47	HIS
1	R	85	GLN
1	R	96	HIS
1	R	138	ASN
1	R	147	GLN
1	R	208	HIS
1	R	218	ASN
1	R	230	ASN
1	S	47	HIS
1	S	66	ASN
1	S	72	ASN
1	S	144	ASN
1	S	190	HIS
1	S	221	ASN
1	S	230	ASN
1	T	15	ASN
1	T	47	HIS
1	T	65	GLN
1	T	66	ASN
1	T	72	ASN
1	T	85	GLN
1	T	109	GLN
1	T	144	ASN
1	T	190	HIS
1	T	218	ASN

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Mol	Chain	Res	Type
1	T	221	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	254/255 (99%)	-0.98	2 (0%) 82 81	26, 40, 72, 88	0
1	B	254/255 (99%)	-0.98	0 100 100	21, 37, 70, 89	0
1	C	254/255 (99%)	-1.01	1 (0%) 88 87	22, 39, 72, 93	0
1	D	254/255 (99%)	-1.05	0 100 100	25, 40, 71, 84	0
1	E	254/255 (99%)	-0.95	1 (0%) 88 87	24, 44, 75, 90	0
1	F	254/255 (99%)	-1.02	0 100 100	23, 39, 71, 88	0
1	G	254/255 (99%)	-1.00	0 100 100	24, 38, 70, 92	0
1	H	254/255 (99%)	-0.99	1 (0%) 88 87	24, 39, 73, 91	0
1	I	254/255 (99%)	-1.08	0 100 100	25, 40, 70, 85	0
1	J	254/255 (99%)	-1.04	1 (0%) 88 87	24, 38, 72, 93	0
1	K	254/255 (99%)	-0.96	1 (0%) 88 87	25, 48, 76, 93	0
1	L	254/255 (99%)	-0.92	0 100 100	27, 52, 79, 90	0
1	M	254/255 (99%)	-0.99	0 100 100	24, 42, 75, 87	0
1	N	254/255 (99%)	-0.98	0 100 100	23, 43, 76, 92	0
1	O	254/255 (99%)	-0.99	1 (0%) 88 87	24, 45, 77, 93	0
1	P	254/255 (99%)	-0.92	1 (0%) 88 87	27, 51, 80, 95	0
1	Q	254/255 (99%)	-0.70	3 (1%) 76 75	40, 65, 86, 96	0
1	R	254/255 (99%)	-0.81	2 (0%) 82 81	35, 64, 87, 95	0
1	S	254/255 (99%)	-0.83	0 100 100	41, 64, 85, 96	0
1	T	254/255 (99%)	-0.78	3 (1%) 76 75	36, 62, 87, 96	0
All	All	5080/5100 (99%)	-0.95	17 (0%) 90 89	21, 46, 79, 96	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	214	GLY	2.6
1	A	217	ALA	2.6
1	Q	178	GLY	2.5
1	T	40	VAL	2.4
1	T	168	ALA	2.3
1	P	110	SER	2.3
1	H	11	ASN	2.2
1	C	2	PRO	2.2
1	Q	40	VAL	2.2
1	A	222	ASP	2.2
1	E	63	ALA	2.2
1	Q	168	ALA	2.2
1	R	2	PRO	2.1
1	J	111	ALA	2.1
1	T	63	ALA	2.1
1	K	216	SER	2.0
1	R	176	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.