



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:49 AM UTC

PDB ID : 2BTV / pdb_00002btv
Title : ATOMIC MODEL FOR BLUETONGUE VIRUS (BTV) CORE
Authors : Grimes, J.M.; Burroughs, J.N.; Gouet, P.; Diprose, J.M.; Malby, R.; Zientras, S.; Mertens, P.P.C.; Stuart, D.I.
Deposited on : 1998-09-05
Resolution : 3.50 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

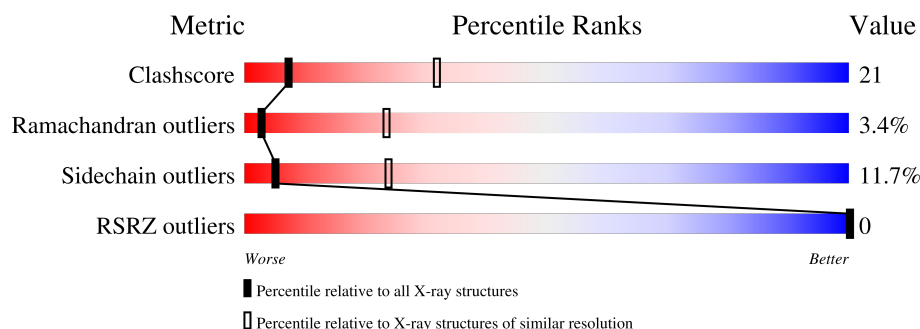
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	901	34% 40% 16% • 6%
1	B	901	40% 41% 15% • •
2	C	349	66% 29% •
2	D	349	71% 25% •
2	E	349	63% 31% 6%
2	F	349	60% 32% 7% •
2	G	349	63% 31% 5%

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Mol	Chain	Length	Quality of chain
2	H	349	 64% 29% 6% •
2	I	349	 62% 31% 7%
2	J	349	 64% 30% 6%
2	P	349	 66% 30% •
2	Q	349	 61% 32% 6% •
2	R	349	 61% 30% 8% •
2	S	349	 58% 35% 5% •
2	T	349	 65% 30% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 49061 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 PROTEIN (VP3 CORE PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	845	Total	C	N	O	S	0	0	0
			6824	4357	1181	1248	38			
1	B	885	Total	C	N	O	S	0	0	0
			7150	4561	1238	1311	40			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLU	ALA	conflict	UNP P56582
A	213	ILE	PHE	conflict	UNP P56582
A	220	LEU	PHE	conflict	UNP P56582
A	772	VAL	ILE	conflict	UNP P56582
A	773	ARG	GLY	conflict	UNP P56582
B	77	GLU	ALA	conflict	UNP P56582
B	213	ILE	PHE	conflict	UNP P56582
B	220	LEU	PHE	conflict	UNP P56582
B	772	VAL	ILE	conflict	UNP P56582
B	773	ARG	GLY	conflict	UNP P56582

- Molecule 2 is a protein called PROTEIN (VP7 CORE PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	C	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	D	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	Q	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	E	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	R	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	G	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	H	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	S	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	I	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	J	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			
2	T	349	Total	C	N	O	S	0	0	0
			2699	1706	478	492	23			

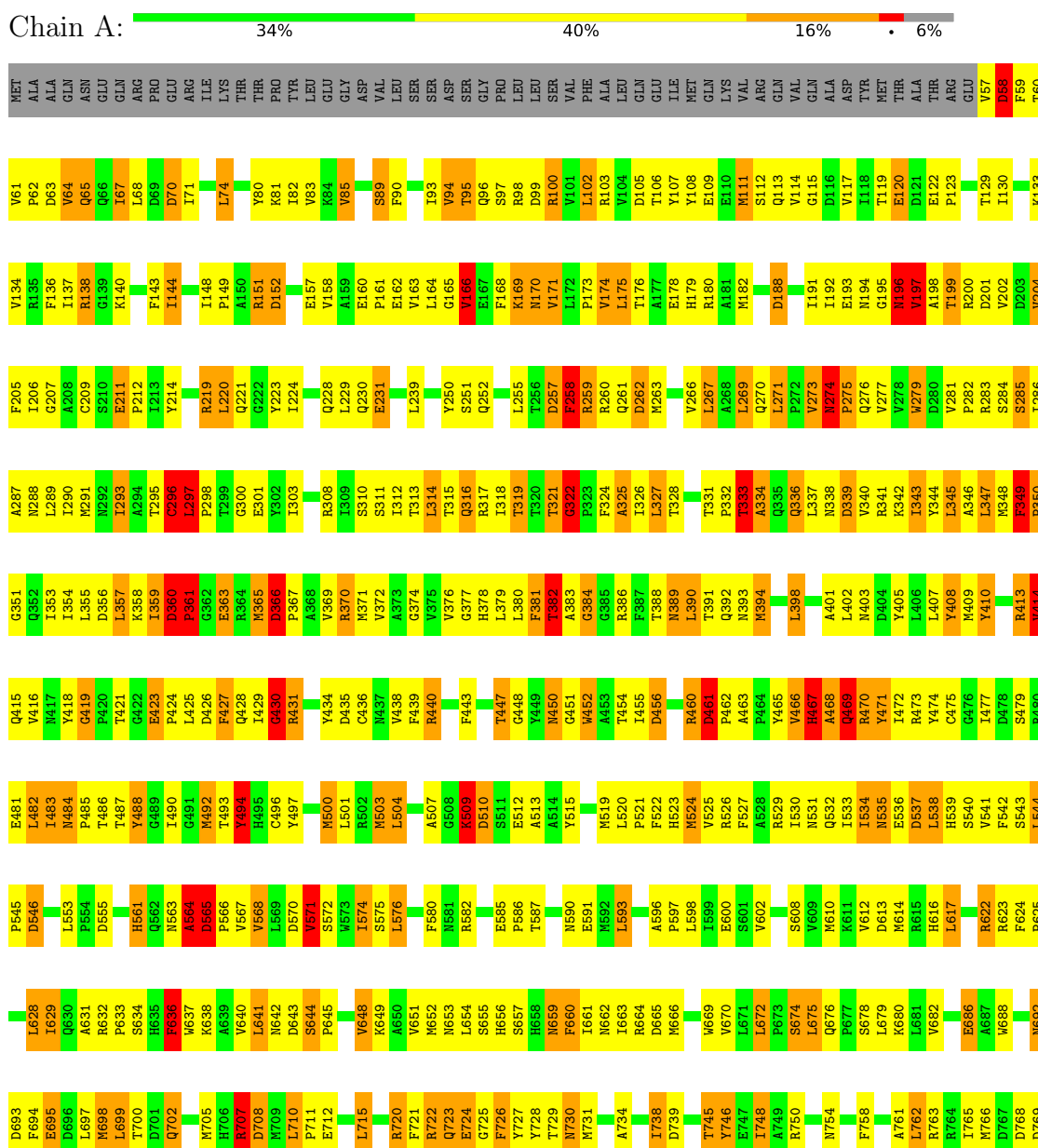
There are 13 discrepancies between the modelled and reference sequences:

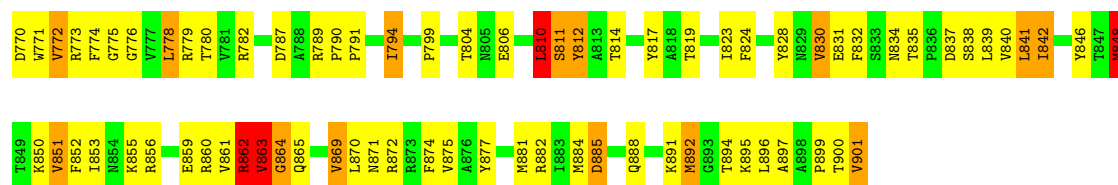
Chain	Residue	Modelled	Actual	Comment	Reference
P	278	TRP	GLY	conflict	UNP P18259
C	278	TRP	GLY	conflict	UNP P18259
D	278	TRP	GLY	conflict	UNP P18259
Q	278	TRP	GLY	conflict	UNP P18259
E	278	TRP	GLY	conflict	UNP P18259
F	278	TRP	GLY	conflict	UNP P18259
R	278	TRP	GLY	conflict	UNP P18259
G	278	TRP	GLY	conflict	UNP P18259
H	278	TRP	GLY	conflict	UNP P18259
S	278	TRP	GLY	conflict	UNP P18259
I	278	TRP	GLY	conflict	UNP P18259
J	278	TRP	GLY	conflict	UNP P18259
T	278	TRP	GLY	conflict	UNP P18259

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

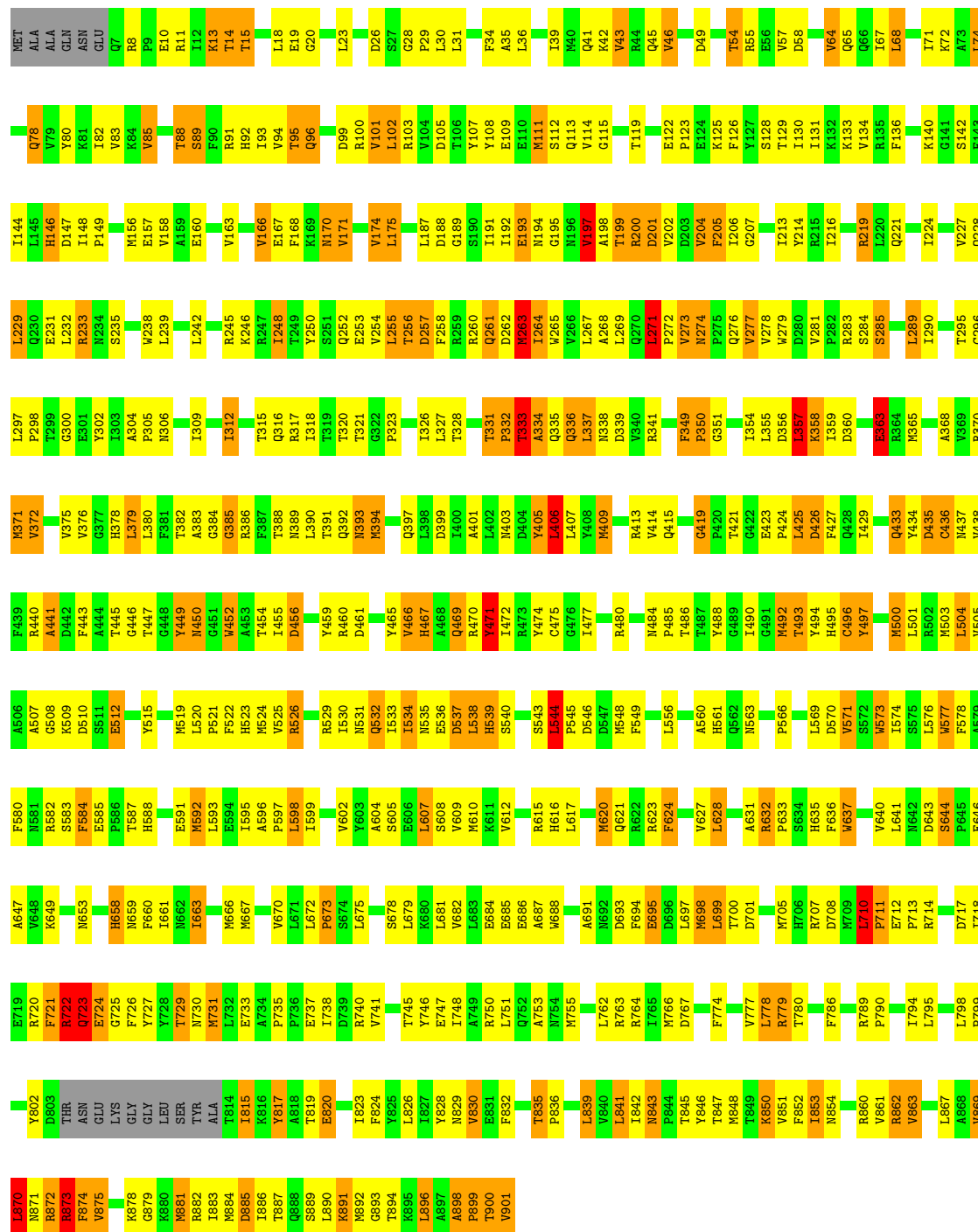
• Molecule 1: PROTEIN (VP3 CORE PROTEIN)





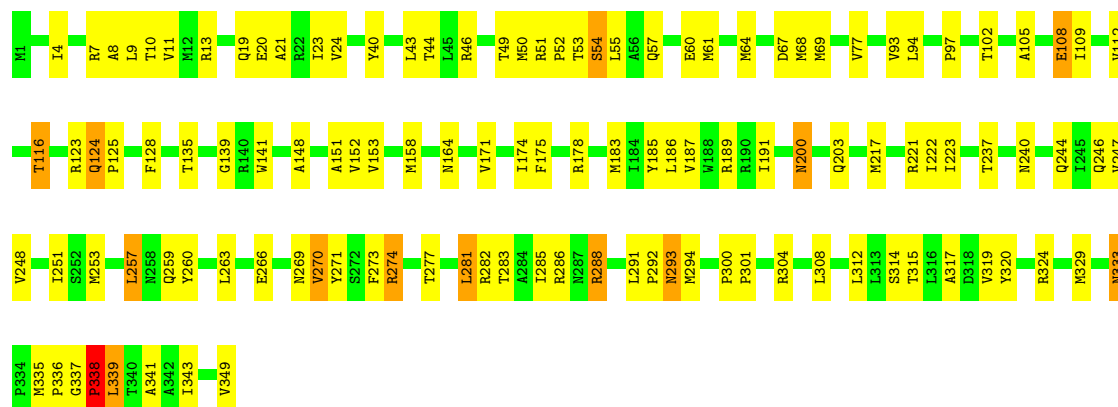
• Molecule 1: PROTEIN (VP3 CORE PROTEIN)

Chain B: 40% 41% 15% . .



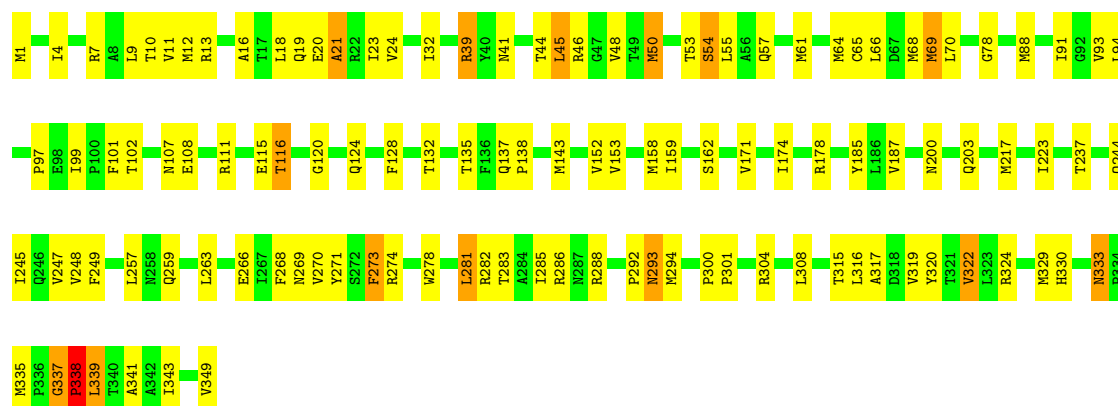
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain P:  66% 30%



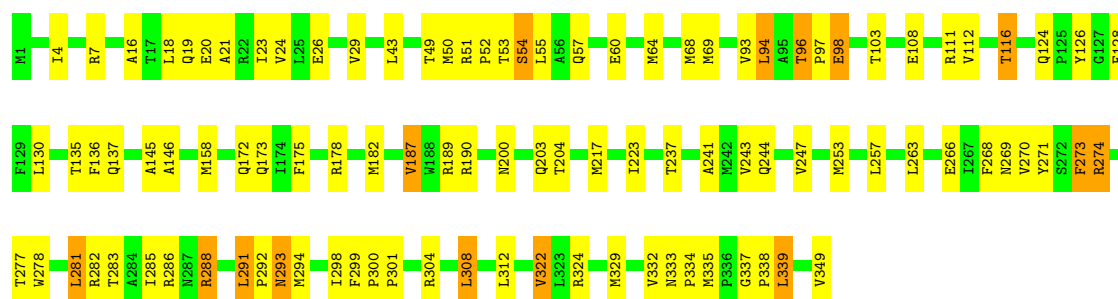
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain C:  66% 29%



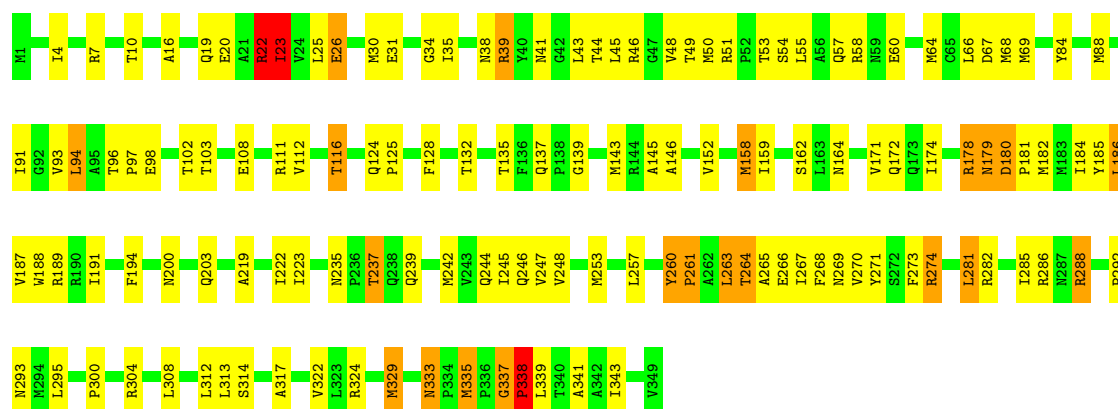
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain D:  71% 25%



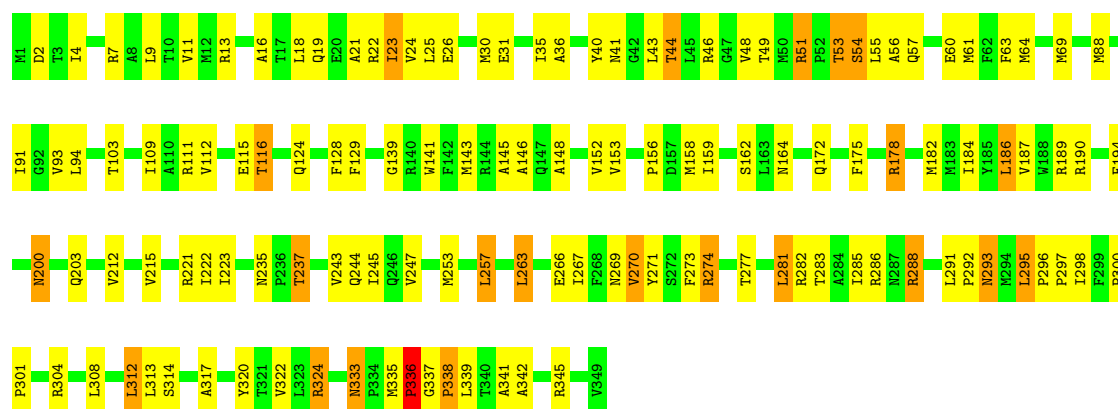
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain Q:  61% 32% 6%



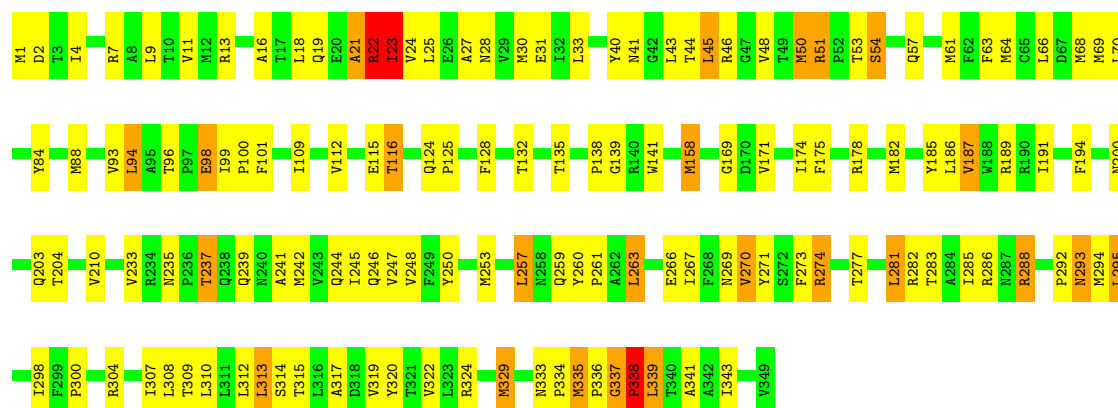
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain E: 63% 31% 6%



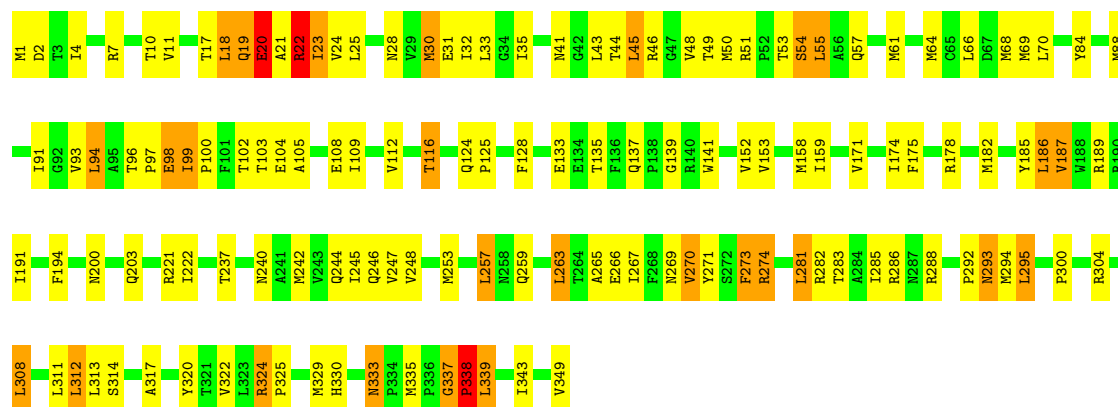
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain F: 60% 32% 7%



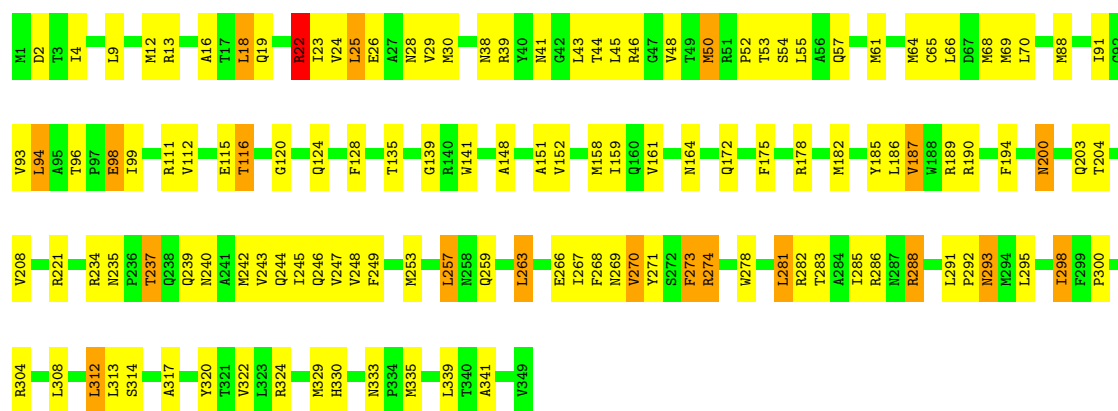
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain R: 61% 30% 8%



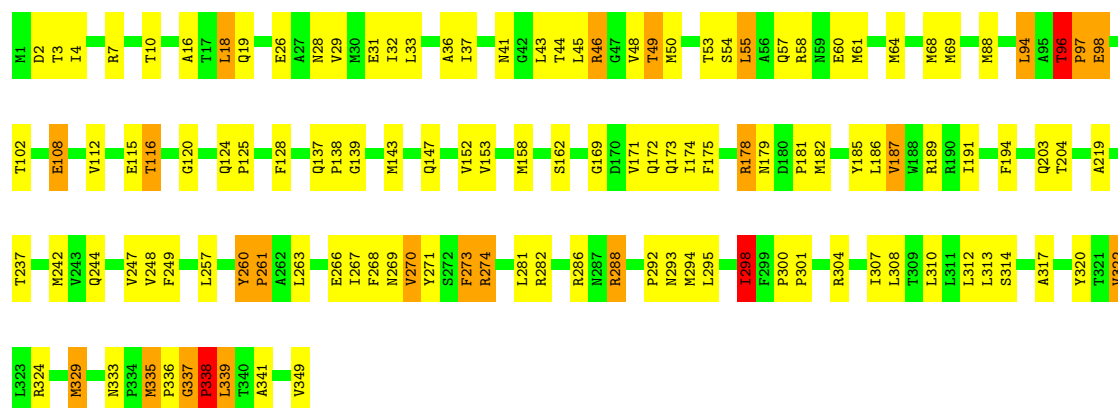
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain G: 63% 31% 5%



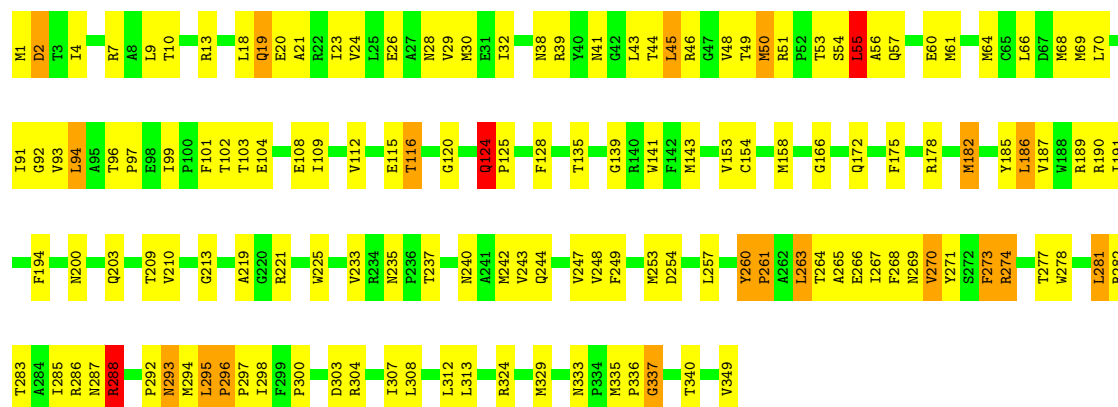
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain H: 64% 29% 6%



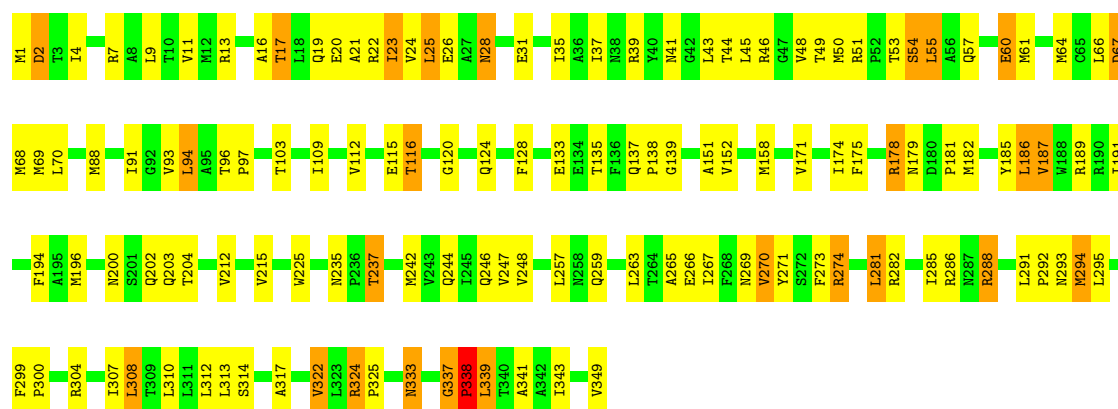
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain S: 58% 35% 5%



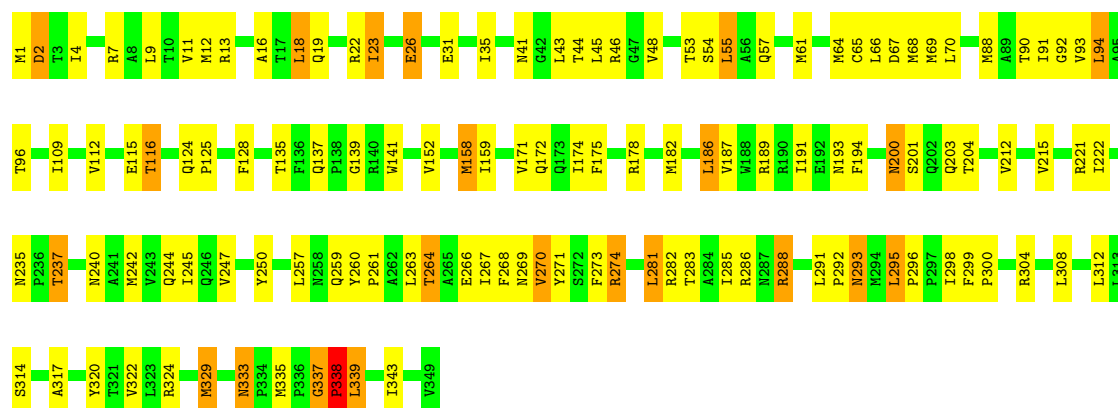
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain I: 62% 31% 7%



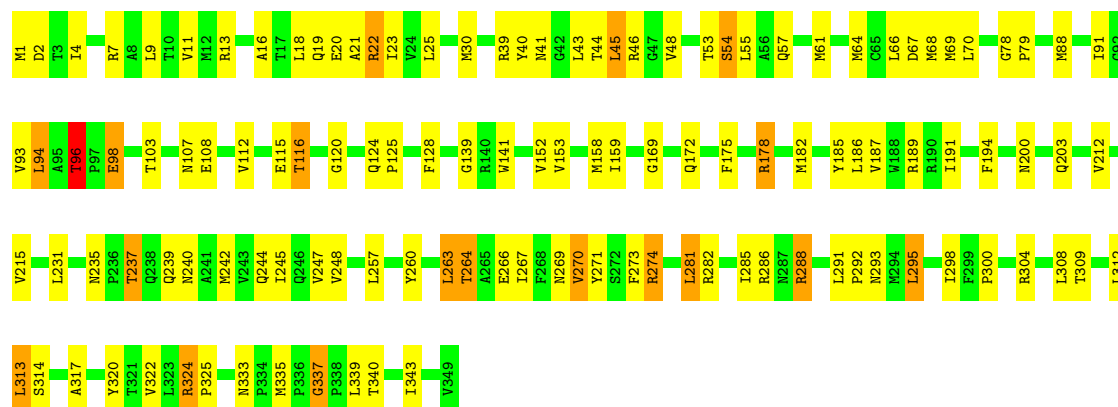
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain J: 64% 30% 6%



• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain T: 65% 30% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	795.60Å 821.80Å 753.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.50 100.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	54.0 (100.00-3.50) 48.2 (100.00-3.50)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 3.49Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.266 , (Not available) 0.408 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.078 for k,h,-l	Xtriage
F_o, F_c correlation	0.26	EDS
Total number of atoms	49061	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.55	1/6978 (0.0%)	1.25	90/9479 (0.9%)
1	B	0.56	1/7308 (0.0%)	1.21	74/9925 (0.7%)
2	C	0.42	0/2757	1.03	15/3756 (0.4%)
2	D	0.41	0/2757	0.96	11/3756 (0.3%)
2	E	0.43	0/2757	1.04	17/3756 (0.5%)
2	F	0.44	0/2757	1.07	21/3756 (0.6%)
2	G	0.45	0/2757	1.04	14/3756 (0.4%)
2	H	0.46	0/2757	1.06	25/3756 (0.7%)
2	I	0.44	0/2757	1.06	21/3756 (0.6%)
2	J	0.43	0/2757	1.07	23/3756 (0.6%)
2	P	0.42	0/2757	1.03	13/3756 (0.3%)
2	Q	0.45	0/2757	1.08	22/3756 (0.6%)
2	R	0.46	0/2757	1.08	20/3756 (0.5%)
2	S	0.46	0/2757	1.03	17/3756 (0.5%)
2	T	0.45	0/2757	1.05	21/3756 (0.6%)
All	All	0.47	2/50127 (0.0%)	1.10	404/68232 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	THR	CA-CB	5.26	1.61	1.53
1	A	95	THR	CA-CB	5.18	1.61	1.53

All (404) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	722	ARG	N-CA-C	-12.17	98.42	113.02
2	P	337	GLY	CA-C-N	11.39	134.08	119.84
2	P	337	GLY	C-N-CA	11.39	134.08	119.84
1	B	406	LEU	N-CA-C	-11.12	99.24	111.36
1	A	695	GLU	N-CA-C	-11.00	98.37	112.23
2	C	337	GLY	CA-C-N	10.62	133.11	119.84
2	C	337	GLY	C-N-CA	10.62	133.11	119.84
1	B	467	HIS	N-CA-C	-10.35	99.55	111.03
2	I	337	GLY	CA-C-N	10.29	132.71	119.84
2	I	337	GLY	C-N-CA	10.29	132.71	119.84
1	B	472	ILE	N-CA-C	10.18	123.12	109.37
1	A	546	ASP	N-CA-C	10.14	122.41	111.36
1	A	325	ALA	N-CA-C	-10.00	101.08	113.18
1	A	722	ARG	N-CA-C	-9.98	101.04	113.02
1	B	166	VAL	N-CA-C	9.89	122.56	108.42
2	R	337	GLY	CA-C-N	9.55	131.78	119.84
2	R	337	GLY	C-N-CA	9.55	131.78	119.84
1	B	898	ALA	CA-C-N	9.46	131.66	119.84
1	B	898	ALA	C-N-CA	9.46	131.66	119.84
2	S	273	PHE	N-CA-C	9.15	121.19	111.03
2	T	124	GLN	CA-C-N	9.14	129.20	119.05
2	T	124	GLN	C-N-CA	9.14	129.20	119.05
2	F	337	GLY	CA-C-N	9.09	131.20	119.84
2	F	337	GLY	C-N-CA	9.09	131.20	119.84
2	H	124	GLN	CA-C-N	8.89	128.22	118.97
2	H	124	GLN	C-N-CA	8.89	128.22	118.97
2	F	21	ALA	N-CA-C	-8.51	101.95	111.14
1	B	334	ALA	N-CA-C	-8.45	102.23	112.54
1	A	383	ALA	N-CA-C	-8.39	102.60	113.17
2	J	124	GLN	CA-C-N	8.39	127.69	118.97
2	J	124	GLN	C-N-CA	8.39	127.69	118.97
1	A	64	VAL	N-CA-C	-8.36	102.94	113.22
2	I	273	PHE	N-CA-C	8.35	120.30	111.03
2	E	273	PHE	N-CA-C	8.25	120.18	111.03
1	A	727	TYR	N-CA-C	8.23	121.29	111.33
2	P	124	GLN	CA-C-N	8.21	128.16	119.05
2	P	124	GLN	C-N-CA	8.21	128.16	119.05
2	J	273	PHE	N-CA-C	8.17	120.10	111.03
1	A	544	LEU	CA-C-N	8.01	127.96	120.03
1	A	544	LEU	C-N-CA	8.01	127.96	120.03
1	B	881	MET	N-CA-C	7.89	122.16	110.48
1	B	872	ARG	N-CA-C	7.86	121.36	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	124	GLN	CA-C-N	7.85	127.13	118.97
2	D	124	GLN	C-N-CA	7.85	127.13	118.97
1	A	864	GLY	N-CA-C	-7.85	106.04	114.67
2	R	273	PHE	N-CA-C	7.78	119.66	111.03
1	B	263	MET	N-CA-C	7.75	121.37	108.73
1	A	467	HIS	N-CA-C	-7.73	94.52	108.58
1	B	436	CYS	N-CA-C	-7.72	102.02	113.61
1	A	544	LEU	N-CA-C	7.71	120.56	109.84
1	B	360	ASP	N-CA-C	-7.68	97.37	109.04
1	A	271	LEU	N-CA-C	7.65	126.71	109.81
1	B	695	GLU	N-CA-C	-7.64	102.96	111.82
1	A	419	GLY	CA-C-N	7.61	127.50	119.05
1	A	419	GLY	C-N-CA	7.61	127.50	119.05
1	A	95	THR	N-CA-C	-7.61	100.72	110.53
2	H	273	PHE	N-CA-C	7.58	119.45	111.03
1	A	274	ASN	CA-C-N	7.58	129.32	119.84
1	A	274	ASN	C-N-CA	7.58	129.32	119.84
2	Q	273	PHE	N-CA-C	7.58	119.44	111.03
1	A	561	HIS	N-CA-C	7.57	121.74	109.40
2	P	293	ASN	N-CA-C	7.54	121.58	112.38
1	A	197	VAL	N-CA-C	7.51	124.97	109.34
1	B	644	SER	CA-C-N	7.50	129.22	119.84
1	B	644	SER	C-N-CA	7.50	129.22	119.84
2	Q	124	GLN	CA-C-N	7.46	126.98	118.85
2	Q	124	GLN	C-N-CA	7.46	126.98	118.85
2	C	293	ASN	N-CA-C	7.45	120.28	111.71
1	A	702	GLN	N-CA-C	7.39	121.38	108.52
1	A	194	ASN	N-CA-C	7.39	120.33	109.69
1	A	564	ALA	N-CA-C	-7.36	95.12	110.80
1	B	349	PHE	CA-C-N	7.36	129.03	119.84
1	B	349	PHE	C-N-CA	7.36	129.03	119.84
1	A	636	PHE	N-CA-C	7.33	119.27	111.28
1	A	408	TYR	N-CA-C	-7.25	101.89	111.24
1	A	778	LEU	N-CA-C	7.23	119.06	111.03
1	A	360	ASP	N-CA-C	7.15	125.61	109.81
1	B	383	ALA	N-CA-C	-7.10	104.62	112.72
2	F	124	GLN	CA-C-N	7.01	126.49	118.85
2	F	124	GLN	C-N-CA	7.01	126.49	118.85
2	E	335	MET	CA-C-N	7.00	128.59	119.84
2	E	335	MET	C-N-CA	7.00	128.59	119.84
1	A	568	VAL	N-CA-C	6.97	116.65	106.55
1	A	259	ARG	N-CA-C	-6.93	104.81	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	ASN	CA-C-N	6.92	128.49	119.84
1	B	274	ASN	C-N-CA	6.92	128.49	119.84
2	R	124	GLN	CA-C-N	6.89	126.36	118.85
2	R	124	GLN	C-N-CA	6.89	126.36	118.85
1	B	94	VAL	N-CA-C	6.88	117.98	108.89
1	A	571	VAL	N-CA-C	6.88	119.44	108.85
2	J	337	GLY	CA-C-N	6.87	128.43	119.84
2	J	337	GLY	C-N-CA	6.87	128.43	119.84
1	A	94	VAL	N-CA-C	6.84	118.41	107.73
1	A	509	LYS	N-CA-C	6.84	120.30	110.24
1	B	471	TYR	CB-CA-C	6.84	119.69	110.94
2	R	19	GLN	N-CA-C	-6.78	104.27	112.54
2	R	20	GLU	N-CA-C	-6.72	96.48	110.80
2	I	22	ARG	N-CA-C	6.72	120.46	112.93
2	D	293	ASN	N-CA-C	6.72	120.58	112.38
1	A	201	ASP	N-CA-C	6.71	120.44	109.76
2	F	273	PHE	N-CA-C	6.71	119.90	111.24
2	H	2	ASP	N-CA-C	-6.70	103.91	111.14
2	F	182	MET	N-CA-C	-6.66	105.78	114.04
1	A	363	GLU	N-CA-C	-6.66	105.12	113.18
1	B	171	VAL	N-CA-C	6.65	116.78	110.53
1	A	712	GLU	CA-C-N	6.63	126.55	119.85
1	A	712	GLU	C-N-CA	6.63	126.55	119.85
2	G	2	ASP	N-CA-C	-6.63	103.97	111.07
1	A	336	GLN	N-CA-C	6.62	119.09	111.02
1	B	624	PHE	CA-C-N	6.59	126.28	119.56
1	B	624	PHE	C-N-CA	6.59	126.28	119.56
2	Q	180	ASP	N-CA-C	6.56	122.95	108.64
2	I	124	GLN	CA-C-N	6.53	128.00	119.84
2	I	124	GLN	C-N-CA	6.53	128.00	119.84
1	B	271	LEU	N-CA-C	6.53	124.23	109.81
2	D	273	PHE	N-CA-C	6.52	119.66	111.24
1	B	43	VAL	N-CA-C	6.52	116.68	110.42
2	G	273	PHE	N-CA-C	6.51	119.64	111.24
2	I	2	ASP	N-CA-C	-6.49	104.28	111.36
1	A	297	LEU	N-CA-C	6.48	118.90	109.04
2	E	293	ASN	N-CA-C	6.48	120.76	112.34
2	T	273	PHE	N-CA-C	6.47	119.58	111.24
2	C	124	GLN	CA-C-N	6.46	126.04	119.19
2	C	124	GLN	C-N-CA	6.46	126.04	119.19
1	A	331	THR	CA-C-N	6.45	127.90	119.84
1	A	331	THR	C-N-CA	6.45	127.90	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	THR	N-CA-C	6.45	119.92	109.15
2	F	22	ARG	N-CA-C	6.42	124.47	110.80
2	F	88	MET	N-CA-C	6.41	118.35	111.36
2	F	293	ASN	N-CA-C	6.40	120.55	112.87
2	E	124	GLN	CA-C-N	6.38	127.81	119.84
2	E	124	GLN	C-N-CA	6.38	127.81	119.84
2	R	293	ASN	N-CA-C	6.38	120.16	112.38
1	B	830	VAL	N-CA-C	6.37	117.87	108.45
2	G	22	ARG	N-CA-C	6.36	119.20	111.82
2	S	182	MET	N-CA-C	-6.35	106.17	114.04
1	B	175	LEU	N-CA-C	6.34	120.21	110.20
1	B	820	GLU	N-CA-C	-6.32	101.16	110.52
2	R	103	THR	N-CA-C	-6.30	104.49	111.36
1	A	252	GLN	N-CA-C	-6.29	105.64	113.38
1	B	331	THR	CA-C-N	6.26	127.66	119.84
1	B	331	THR	C-N-CA	6.26	127.66	119.84
1	A	745	THR	N-CA-C	-6.24	100.47	110.14
2	Q	337	GLY	CA-C-N	6.20	127.59	119.84
2	Q	337	GLY	C-N-CA	6.20	127.59	119.84
1	A	644	SER	CA-C-N	6.20	126.56	119.93
1	A	644	SER	C-N-CA	6.20	126.56	119.93
1	B	459	TYR	N-CA-C	-6.19	100.42	110.20
2	J	333	ASN	CA-C-N	6.19	125.95	119.76
2	J	333	ASN	C-N-CA	6.19	125.95	119.76
2	T	125	PRO	N-CA-C	6.19	122.13	113.53
1	B	509	LYS	N-CA-C	6.18	118.47	109.07
1	A	195	GLY	N-CA-C	6.17	122.50	111.02
1	A	390	LEU	N-CA-C	6.17	119.25	109.81
2	F	96	THR	CA-C-N	6.16	126.34	119.32
2	F	96	THR	C-N-CA	6.16	126.34	119.32
2	D	322	VAL	N-CA-C	6.15	116.93	110.72
2	R	99	ILE	N-CA-C	6.13	113.96	107.76
2	G	124	GLN	CA-C-N	6.13	127.51	119.84
2	G	124	GLN	C-N-CA	6.13	127.51	119.84
2	D	96	THR	CA-C-N	6.13	126.31	119.32
2	D	96	THR	C-N-CA	6.13	126.31	119.32
1	B	278	VAL	CB-CA-C	-6.12	104.00	112.02
2	H	335	MET	CA-C-N	6.12	125.52	118.85
2	H	335	MET	C-N-CA	6.12	125.52	118.85
1	B	469	GLN	N-CA-C	-6.11	105.78	113.72
2	S	2	ASP	N-CA-C	-6.11	104.70	111.36
2	I	322	VAL	N-CA-C	6.10	117.58	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	778	LEU	N-CA-C	6.10	120.89	111.56
1	A	494	TYR	N-CA-CB	-6.09	101.38	111.06
1	A	810	LEU	N-CA-C	6.09	123.77	110.80
1	A	708	ASP	N-CA-C	6.08	118.82	108.90
2	Q	103	THR	N-CA-C	-6.06	104.67	111.28
2	J	182	MET	N-CA-C	-6.06	106.52	114.04
2	E	26	GLU	N-CA-C	-6.04	100.45	109.15
1	B	538	LEU	N-CA-C	6.04	121.66	112.54
1	A	171	VAL	N-CA-C	6.04	116.22	110.42
2	P	335	MET	CA-C-N	6.02	125.70	119.56
2	P	335	MET	C-N-CA	6.02	125.70	119.56
2	P	338	PRO	N-CA-C	6.01	124.85	112.47
2	H	337	GLY	CA-C-N	6.00	127.34	119.84
2	H	337	GLY	C-N-CA	6.00	127.34	119.84
1	B	405	TYR	N-CA-C	5.99	120.87	113.50
2	H	293	ASN	N-CA-C	5.99	119.41	111.75
2	P	273	PHE	N-CA-C	5.99	118.70	111.40
2	G	293	ASN	N-CA-C	5.98	120.12	112.34
1	A	447	THR	N-CA-C	5.98	123.54	110.80
2	I	23	ILE	N-CA-C	5.97	117.75	109.80
1	A	196	ASN	N-CA-C	5.97	123.52	110.80
2	J	26	GLU	N-CA-C	-5.97	100.81	109.59
2	R	335	MET	CA-C-N	5.96	125.64	119.56
2	R	335	MET	C-N-CA	5.96	125.64	119.56
2	I	333	ASN	CA-C-N	5.96	126.26	119.83
2	I	333	ASN	C-N-CA	5.96	126.26	119.83
2	G	298	ILE	N-CA-C	-5.94	104.72	110.72
1	A	297	LEU	CA-C-N	5.93	126.43	120.14
1	A	297	LEU	C-N-CA	5.93	126.43	120.14
1	B	357	LEU	N-CA-C	5.93	123.43	110.80
1	A	846	TYR	N-CA-C	5.93	119.71	110.17
1	B	631	ALA	N-CA-C	5.91	117.52	108.12
1	B	276	GLN	N-CA-C	5.90	117.38	111.07
1	B	632	ARG	CA-C-N	5.89	126.04	119.32
1	B	632	ARG	C-N-CA	5.89	126.04	119.32
2	T	2	ASP	N-CA-C	-5.89	104.77	111.07
1	A	366	ASP	CA-C-N	5.89	127.20	119.84
1	A	366	ASP	C-N-CA	5.89	127.20	119.84
2	I	182	MET	N-CA-C	-5.87	106.66	113.88
2	T	103	THR	N-CA-C	-5.87	104.96	111.36
2	J	2	ASP	N-CA-C	-5.86	104.97	111.36
2	J	96	THR	CA-C-N	5.86	125.72	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	96	THR	C-N-CA	5.86	125.72	119.28
1	B	712	GLU	CA-C-N	5.84	126.30	120.52
1	B	712	GLU	C-N-CA	5.84	126.30	120.52
2	I	103	THR	N-CA-C	-5.83	104.92	111.28
2	F	169	GLY	N-CA-C	5.82	118.99	110.38
2	J	295	LEU	CA-C-N	5.80	126.35	120.38
2	J	295	LEU	C-N-CA	5.80	126.35	120.38
1	A	565	ASP	CA-C-N	5.79	125.72	119.76
1	A	565	ASP	C-N-CA	5.79	125.72	119.76
1	A	659	ASN	N-CA-C	5.79	120.47	113.41
1	A	269	LEU	N-CA-C	5.77	121.19	114.04
2	H	120	GLY	CA-C-N	5.77	125.53	119.76
2	H	120	GLY	C-N-CA	5.77	125.53	119.76
2	S	288	ARG	N-CA-C	-5.75	106.30	113.38
2	I	295	LEU	CA-C-N	5.75	126.31	120.38
2	I	295	LEU	C-N-CA	5.75	126.31	120.38
2	I	293	ASN	N-CA-C	5.75	119.77	112.87
2	T	96	THR	CA-C-N	5.74	126.13	119.47
2	T	96	THR	C-N-CA	5.74	126.13	119.47
2	F	295	LEU	CA-C-N	5.74	126.29	120.38
2	F	295	LEU	C-N-CA	5.74	126.29	120.38
2	S	295	LEU	CA-C-N	5.73	126.28	120.38
2	S	295	LEU	C-N-CA	5.73	126.28	120.38
2	R	246	GLN	N-CA-C	5.69	118.18	108.90
1	A	869	VAL	N-CA-C	5.68	121.16	109.34
2	F	335	MET	CA-C-N	5.68	125.35	119.56
2	F	335	MET	C-N-CA	5.68	125.35	119.56
1	A	460	ARG	N-CA-C	-5.66	98.49	108.23
1	B	206	ILE	N-CA-C	5.66	119.08	113.53
1	A	231	GLU	N-CA-C	5.65	122.84	110.80
2	D	182	MET	N-CA-C	-5.65	106.74	113.97
2	R	333	ASN	CA-C-N	5.64	125.92	119.83
2	R	333	ASN	C-N-CA	5.64	125.92	119.83
1	B	390	LEU	N-CA-C	5.63	118.87	110.14
2	R	322	VAL	N-CA-C	5.63	116.36	110.62
1	A	296	CYS	N-CA-C	5.60	122.73	110.80
2	C	333	ASN	CA-C-N	5.59	125.87	119.83
2	C	333	ASN	C-N-CA	5.59	125.87	119.83
2	H	88	MET	N-CA-C	5.59	117.18	111.14
2	Q	293	ASN	N-CA-C	5.59	119.60	112.34
2	S	124	GLN	CA-C-N	5.58	126.82	119.84
2	S	124	GLN	C-N-CA	5.58	126.82	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	23	ILE	N-CA-C	5.57	117.01	108.71
2	J	293	ASN	N-CA-C	5.57	119.58	112.34
2	E	103	THR	N-CA-C	-5.56	105.22	111.28
2	T	120	GLY	CA-C-N	5.56	125.74	119.90
2	T	120	GLY	C-N-CA	5.56	125.74	119.90
1	B	497	TYR	N-CA-C	-5.55	105.32	111.71
2	R	125	PRO	N-CA-C	5.55	120.83	113.40
2	E	295	LEU	CA-C-N	5.54	126.09	120.38
2	E	295	LEU	C-N-CA	5.54	126.09	120.38
2	T	260	TYR	CA-C-N	5.54	126.77	119.84
2	T	260	TYR	C-N-CA	5.54	126.77	119.84
1	A	510	ASP	N-CA-C	-5.53	104.08	112.04
1	A	565	ASP	N-CA-C	5.53	118.27	109.64
2	T	78	GLY	CA-C-N	5.48	126.69	119.84
2	T	78	GLY	C-N-CA	5.48	126.69	119.84
2	Q	179	ASN	N-CA-C	5.47	122.46	110.80
1	B	250	TYR	N-CA-C	5.47	118.90	110.42
1	B	687	ALA	N-CA-C	-5.47	105.32	111.28
2	J	158	MET	N-CA-C	5.47	118.37	109.24
2	G	246	GLN	N-CA-C	5.46	117.87	109.07
1	A	775	GLY	N-CA-C	5.46	121.18	111.02
2	G	335	MET	CA-C-N	5.46	125.13	119.56
2	G	335	MET	C-N-CA	5.46	125.13	119.56
1	A	730	ASN	N-CA-C	-5.46	104.98	111.69
2	Q	125	PRO	N-CA-C	5.45	120.71	113.40
2	H	137	GLN	CA-C-N	5.44	125.61	119.90
2	H	137	GLN	C-N-CA	5.44	125.61	119.90
1	B	710	LEU	CA-C-N	5.44	126.64	119.84
1	B	710	LEU	C-N-CA	5.44	126.64	119.84
2	J	260	TYR	CA-C-N	5.42	126.62	119.84
2	J	260	TYR	C-N-CA	5.42	126.62	119.84
1	B	419	GLY	CA-C-N	5.42	125.24	119.28
1	B	419	GLY	C-N-CA	5.42	125.24	119.28
2	R	182	MET	N-CA-C	-5.42	107.22	113.88
2	C	120	GLY	CA-C-N	5.41	125.17	119.76
2	C	120	GLY	C-N-CA	5.41	125.17	119.76
2	H	260	TYR	CA-C-N	5.40	126.59	119.84
2	H	260	TYR	C-N-CA	5.40	126.59	119.84
2	P	333	ASN	CA-C-N	5.39	125.56	119.90
2	P	333	ASN	C-N-CA	5.39	125.56	119.90
2	H	169	GLY	N-CA-C	5.39	118.32	111.37
2	J	335	MET	CA-C-N	5.39	125.72	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	335	MET	C-N-CA	5.39	125.72	119.47
2	F	260	TYR	CA-C-N	5.39	126.57	119.84
2	F	260	TYR	C-N-CA	5.39	126.57	119.84
2	H	125	PRO	N-CA-C	5.39	121.17	113.47
2	H	295	LEU	CA-C-N	5.38	125.92	120.38
2	H	295	LEU	C-N-CA	5.38	125.92	120.38
2	Q	260	TYR	CA-C-N	5.38	126.57	119.84
2	Q	260	TYR	C-N-CA	5.38	126.57	119.84
1	B	486	THR	N-CA-C	-5.38	105.83	112.72
2	D	103	THR	N-CA-C	-5.38	105.50	111.36
2	P	125	PRO	N-CA-C	5.38	121.00	113.53
2	Q	22	ARG	N-CA-C	-5.38	99.35	110.80
2	Q	335	MET	CA-C-N	5.37	125.04	119.56
2	Q	335	MET	C-N-CA	5.37	125.04	119.56
1	A	535	ASN	N-CA-C	5.37	117.57	111.02
2	Q	333	ASN	CA-C-N	5.37	126.20	119.98
2	Q	333	ASN	C-N-CA	5.37	126.20	119.98
1	B	593	LEU	N-CA-C	5.36	120.22	111.37
2	C	335	MET	CA-C-N	5.36	124.97	119.56
2	C	335	MET	C-N-CA	5.36	124.97	119.56
1	A	267	LEU	N-CA-C	-5.36	101.72	109.59
2	E	322	VAL	N-CA-C	5.36	116.72	110.62
2	S	120	GLY	CA-C-N	5.35	125.52	119.90
2	S	120	GLY	C-N-CA	5.35	125.52	119.90
1	B	846	TYR	N-CA-C	5.34	118.77	110.17
2	E	182	MET	N-CA-C	-5.34	107.31	113.88
2	C	273	PHE	N-CA-C	5.34	118.12	111.24
1	A	746	TYR	N-CA-C	-5.33	104.71	111.11
2	S	337	GLY	N-CA-C	5.32	123.20	112.34
1	A	382	THR	N-CA-C	5.32	117.30	108.20
2	I	96	THR	CA-C-N	5.32	125.13	119.28
2	I	96	THR	C-N-CA	5.32	125.13	119.28
1	A	494	TYR	N-CA-C	-5.32	106.56	114.64
1	A	629	ILE	N-CA-C	-5.32	105.94	111.58
2	T	293	ASN	N-CA-C	5.32	118.87	112.38
2	G	50	MET	N-CA-C	-5.31	105.39	111.07
1	A	349	PHE	N-CA-C	5.29	121.51	109.81
1	A	322	GLY	N-CA-C	5.29	123.14	112.34
2	Q	26	GLU	N-CA-C	-5.29	101.82	109.59
2	T	337	GLY	CA-C-N	5.28	126.45	119.84
2	T	337	GLY	C-N-CA	5.28	126.45	119.84
2	T	182	MET	N-CA-C	-5.28	107.50	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	125	PRO	N-CA-C	5.28	120.47	113.40
1	B	843	ASN	CA-C-N	5.27	125.56	119.92
1	B	843	ASN	C-N-CA	5.27	125.56	119.92
1	A	897	ALA	N-CA-C	5.26	117.12	110.33
1	A	430	GLY	N-CA-C	5.26	125.64	113.18
1	A	471	TYR	N-CA-C	5.26	116.99	108.26
2	Q	158	MET	N-CA-C	5.26	118.02	109.24
2	I	55	LEU	N-CA-C	-5.25	99.62	110.80
2	F	158	MET	N-CA-C	5.24	117.72	108.75
1	A	832	PHE	N-CA-C	5.24	117.90	111.82
2	R	295	LEU	CA-C-N	5.24	125.78	120.38
2	R	295	LEU	C-N-CA	5.24	125.78	120.38
2	S	260	TYR	CA-C-N	5.23	126.38	119.84
2	S	260	TYR	C-N-CA	5.23	126.38	119.84
2	E	19	GLN	N-CA-C	-5.22	104.51	111.24
2	J	125	PRO	N-CA-C	5.21	120.92	113.47
2	Q	295	LEU	CA-C-N	5.20	125.74	120.38
2	Q	295	LEU	C-N-CA	5.20	125.74	120.38
1	B	41	GLN	N-CA-C	-5.20	105.50	111.07
1	A	71	ILE	N-CA-C	-5.20	104.48	111.44
2	E	333	ASN	CA-C-N	5.19	126.32	119.84
2	E	333	ASN	C-N-CA	5.19	126.32	119.84
1	B	544	LEU	CA-C-N	5.18	125.19	119.90
1	B	544	LEU	C-N-CA	5.18	125.19	119.90
2	P	336	PRO	N-CA-C	5.17	120.57	113.84
2	S	55	LEU	N-CA-C	-5.17	99.78	110.80
1	B	318	ILE	N-CA-C	5.16	115.53	107.99
1	A	848	MET	N-CA-C	5.15	119.56	113.12
2	C	21	ALA	N-CA-C	5.15	117.68	111.40
2	D	337	GLY	CA-C-N	5.15	124.76	119.56
2	D	337	GLY	C-N-CA	5.15	124.76	119.56
1	B	741	VAL	N-CA-C	5.14	115.36	108.17
1	B	853	ILE	N-CA-C	5.13	118.56	113.53
1	A	593	LEU	N-CA-C	5.13	119.78	111.37
2	E	51	ARG	CA-C-N	5.13	125.34	120.31
2	E	51	ARG	C-N-CA	5.13	125.34	120.31
1	A	672	LEU	CA-C-N	5.12	126.25	119.84
1	A	672	LEU	C-N-CA	5.12	126.25	119.84
1	A	120	GLU	N-CA-C	-5.12	103.84	110.19
1	B	264	ILE	N-CA-C	-5.12	100.51	107.99
2	S	209	THR	N-CA-C	5.12	117.78	109.24
2	H	298	ILE	N-CA-C	-5.11	105.51	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	THR	N-CA-C	-5.11	101.64	109.76
2	T	295	LEU	CA-C-N	5.10	125.63	120.38
2	T	295	LEU	C-N-CA	5.10	125.63	120.38
1	B	248	ILE	N-CA-C	5.09	116.97	109.63
2	G	120	GLY	CA-C-N	5.09	125.25	119.90
2	G	120	GLY	C-N-CA	5.09	125.25	119.90
1	A	657	SER	N-CA-C	-5.09	107.04	113.20
1	B	471	TYR	CA-CB-CG	5.09	123.06	113.90
2	S	293	ASN	N-CA-C	5.08	118.95	112.34
2	I	120	GLY	CA-C-N	5.08	124.99	119.76
2	I	120	GLY	C-N-CA	5.08	124.99	119.76
2	S	103	THR	N-CA-C	-5.07	105.64	111.07
2	J	23	ILE	N-CA-C	5.06	119.86	109.34
2	C	322	VAL	N-CA-C	5.06	115.83	110.72
2	C	338	PRO	N-CA-C	5.04	122.86	112.47
2	H	322	VAL	N-CA-C	5.04	115.76	110.62
2	H	96	THR	CA-C-N	5.04	126.14	119.84
2	H	96	THR	C-N-CA	5.04	126.14	119.84
2	H	182	MET	N-CA-C	-5.03	107.53	113.97
1	B	13	LYS	CA-C-N	5.03	126.98	120.44
1	B	13	LYS	C-N-CA	5.03	126.98	120.44
2	J	55	LEU	N-CA-C	-5.03	100.09	110.80
2	T	169	GLY	N-CA-C	5.03	117.85	111.37
1	B	738	ILE	N-CA-C	5.01	118.09	111.17
1	A	381	PHE	N-CA-C	5.01	117.77	109.85
2	G	182	MET	N-CA-C	-5.01	107.72	113.88

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	494	TYR	Sidechain
1	B	471	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6824	0	6804	510	0
1	B	7150	0	7137	483	0
2	C	2699	0	2697	72	0
2	D	2699	0	2697	65	0
2	E	2699	0	2697	88	0
2	F	2699	0	2697	97	0
2	G	2699	0	2697	97	0
2	H	2699	0	2697	83	0
2	I	2699	0	2697	106	0
2	J	2699	0	2697	92	0
2	P	2699	0	2697	71	0
2	Q	2699	0	2697	103	0
2	R	2699	0	2697	101	0
2	S	2699	0	2697	108	0
2	T	2699	0	2697	73	0
All	All	49061	0	49002	2020	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 21.

All (2020) 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)
2:I:97:PRO:HD3	2:J:22:ARG:HH21	1.27	0.99
1:A:263:MET:HE2	1:A:882:ARG:HD2	1.46	0.97
2:E:158:MET:HE2	2:E:244:GLN:HB2	1.48	0.94
1:B:358:LYS:HB2	1:B:570:ASP:HB3	1.49	0.94
2:S:282:ARG:HD3	2:S:286:ARG:NH1	1.83	0.94
2:T:257:LEU:HD12	2:T:300:PRO:HB3	1.47	0.94
1:A:219:ARG:HG3	1:A:686:GLU:HG3	1.46	0.94
1:A:59:PHE:HB3	1:B:317:ARG:HD2	1.50	0.93
1:B:494:TYR:HD1	1:B:524:MET:HE3	1.34	0.93
1:B:407:LEU:HA	1:B:413:ARG:HH22	1.32	0.92
2:J:116:THR:HG21	2:J:304:ARG:HB2	1.49	0.92
1:B:790:PRO:HG2	1:B:795:LEU:HD21	1.51	0.91
2:R:24:VAL:HG21	2:R:30:MET:HG2	1.51	0.91
2:T:282:ARG:HD3	2:T:286:ARG:NH1	1.86	0.90
2:C:257:LEU:HD12	2:C:300:PRO:HB3	1.53	0.90
1:B:260:ARG:HD2	1:B:263:MET:SD	2.11	0.90
2:Q:20:GLU:HB3	2:Q:22:ARG:NH2	1.87	0.89
2:S:257:LEU:HD12	2:S:300:PRO:HB3	1.54	0.89
2:H:282:ARG:HD3	2:H:286:ARG:NH1	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:TYR:HB2	1:A:535:ASN:HD21	1.39	0.88
2:R:282:ARG:HD3	2:R:286:ARG:NH1	1.88	0.88
2:I:282:ARG:HD3	2:I:286:ARG:NH1	1.86	0.88
2:F:158:MET:HE2	2:F:244:GLN:HB2	1.56	0.88
2:G:282:ARG:HD3	2:G:286:ARG:NH1	1.89	0.88
1:A:296:CYS:SG	1:A:538:LEU:HA	2.14	0.88
2:C:282:ARG:HD3	2:C:286:ARG:NH1	1.89	0.87
1:B:23:LEU:HD21	1:B:304:ALA:HB2	1.55	0.87
1:A:415:GLN:HB2	1:A:430:GLY:HA3	1.57	0.87
1:B:779:ARG:HH12	1:B:799:PRO:HB2	1.40	0.87
1:A:111:MET:HE1	1:A:133:LYS:HB3	1.56	0.86
2:R:43:LEU:HD12	2:R:93:VAL:HG22	1.56	0.85
2:F:282:ARG:HD3	2:F:286:ARG:NH1	1.91	0.85
1:B:413:ARG:HD2	1:B:414:VAL:H	1.39	0.85
1:B:260:ARG:HD3	1:B:262:ASP:HB2	1.58	0.85
2:P:282:ARG:HD3	2:P:286:ARG:NH1	1.91	0.85
1:A:263:MET:HG2	1:A:882:ARG:HB3	1.57	0.85
2:R:10:THR:HG23	2:R:102:THR:HG23	1.58	0.85
1:B:103:ARG:NH1	1:B:869:VAL:HG22	1.92	0.84
2:H:158:MET:HE2	2:H:244:GLN:HB2	1.59	0.84
1:B:72:LYS:HZ1	1:B:595:ILE:HB	1.42	0.84
1:A:509:LYS:HB3	1:A:512:GLU:HG3	1.57	0.84
1:B:371:MET:SD	1:B:405:TYR:HB3	2.18	0.84
2:Q:257:LEU:HD12	2:Q:300:PRO:HB3	1.57	0.84
1:A:339:ASP:O	1:A:343:ILE:HG22	1.77	0.84
1:B:111:MET:HE1	1:B:133:LYS:HB3	1.60	0.84
1:A:428:GLN:HA	1:A:435:ASP:HA	1.60	0.83
1:B:297:LEU:HD22	1:B:298:PRO:HD2	1.59	0.83
2:Q:282:ARG:HD3	2:Q:286:ARG:NH1	1.92	0.83
1:B:713:PRO:HD2	1:B:839:LEU:HD13	1.61	0.83
1:B:95:THR:HG21	1:B:725:GLY:HA3	1.60	0.82
1:A:748:ILE:HD11	2:Q:49:THR:HG23	1.59	0.82
2:D:4:ILE:HG23	2:D:94:LEU:HB3	1.61	0.82
2:D:282:ARG:HD3	2:D:286:ARG:NH1	1.94	0.82
1:A:637:TRP:HZ3	1:A:666:MET:HE2	1.42	0.82
1:B:854:ASN:HD22	2:H:49:THR:HG21	1.43	0.82
2:E:282:ARG:HD3	2:E:286:ARG:NH1	1.93	0.82
1:A:324:PHE:HA	1:A:326:ILE:HG22	1.60	0.82
2:G:96:THR:HG22	2:G:98:GLU:HB2	1.61	0.81
1:A:359:ILE:HG22	1:A:361:PRO:HD2	1.62	0.81
2:I:116:THR:HG21	2:I:304:ARG:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:LEU:HD13	1:B:711:PRO:HD2	1.63	0.81
2:F:269:ASN:HD21	2:F:274:ARG:HH22	1.28	0.80
1:A:461:ASP:HB3	1:A:462:PRO:HD3	1.62	0.80
1:B:45:GLN:O	1:B:49:ASP:HB2	1.81	0.80
2:J:257:LEU:HD12	2:J:300:PRO:HB3	1.62	0.80
2:S:158:MET:HE2	2:S:244:GLN:HB2	1.64	0.80
1:B:235:SER:HB2	1:B:271:LEU:HB2	1.64	0.80
1:A:332:PRO:HD2	1:A:336:GLN:HG3	1.65	0.79
2:R:54:SER:H	2:R:57:GLN:HE21	1.29	0.79
2:I:1:MET:HA	2:I:4:ILE:HD12	1.62	0.79
1:A:93:ILE:HG23	1:A:102:LEU:HG	1.65	0.79
2:Q:158:MET:HE2	2:Q:244:GLN:HB2	1.65	0.79
2:F:257:LEU:HD12	2:F:300:PRO:HB3	1.62	0.79
2:P:269:ASN:HD21	2:P:274:ARG:HH22	1.31	0.79
1:A:356:ASP:HA	1:A:391:THR:OG1	1.81	0.79
2:S:53:THR:H	2:S:57:GLN:NE2	1.81	0.78
1:B:474:TYR:HB2	1:B:531:ASN:HD21	1.48	0.78
1:A:700:THR:HG22	1:A:702:GLN:H	1.49	0.78
2:S:269:ASN:HD21	2:S:274:ARG:HH22	1.32	0.78
1:A:729:THR:HG22	1:A:731:MET:H	1.47	0.78
2:R:257:LEU:HD12	2:R:300:PRO:HB3	1.64	0.78
1:A:463:ALA:HB3	1:A:469:GLN:HB3	1.64	0.78
1:B:633:PRO:HG3	1:B:663:ILE:HG23	1.66	0.78
1:B:748:ILE:HD13	2:S:53:THR:HG21	1.65	0.78
1:B:229:LEU:HD11	1:B:257:ASP:HB2	1.66	0.77
2:R:32:ILE:HG23	2:R:100:PRO:HD2	1.65	0.77
2:J:4:ILE:HG23	2:J:94:LEU:HB3	1.66	0.77
1:B:379:LEU:HD12	1:B:500:MET:HG3	1.66	0.77
2:D:158:MET:HE2	2:D:244:GLN:HB2	1.66	0.77
1:B:356:ASP:HA	1:B:394:MET:HG2	1.66	0.77
1:B:746:TYR:HA	1:B:817:TYR:CE2	2.20	0.77
2:C:269:ASN:HD21	2:C:274:ARG:HH22	1.33	0.77
2:H:263:LEU:HD22	2:H:267:ILE:HD11	1.66	0.77
1:B:887:THR:O	1:B:890:LEU:HD23	1.85	0.77
1:B:214:TYR:OH	1:B:873:ARG:HB3	1.83	0.77
2:J:282:ARG:HD3	2:J:286:ARG:NH1	1.99	0.77
1:B:523:HIS:O	1:B:526:ARG:HD2	1.84	0.77
2:Q:263:LEU:HD22	2:Q:267:ILE:HD11	1.65	0.77
2:G:269:ASN:HD21	2:G:274:ARG:HH22	1.33	0.77
2:S:263:LEU:HD22	2:S:267:ILE:HD11	1.67	0.77
2:I:139:GLY:O	2:I:194:PHE:HB2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:GLU:CD	1:B:860:ARG:HB2	2.09	0.77
2:I:257:LEU:HD12	2:I:300:PRO:HB3	1.65	0.76
1:A:114:VAL:HB	1:A:133:LYS:HE2	1.66	0.76
2:J:269:ASN:HD21	2:J:274:ARG:HH22	1.32	0.76
2:H:96:THR:HG22	2:H:98:GLU:HB2	1.66	0.76
2:R:24:VAL:HG11	2:R:30:MET:HE2	1.67	0.76
2:R:28:ASN:HD21	2:G:28:ASN:H	1.30	0.76
2:I:54:SER:H	2:I:57:GLN:HE21	1.31	0.76
1:A:303:ILE:HD11	1:A:585:GLU:HB2	1.66	0.75
2:F:282:ARG:HD3	2:F:286:ARG:CZ	2.16	0.75
2:G:158:MET:HE2	2:G:244:GLN:HB2	1.66	0.75
1:A:509:LYS:H	1:A:509:LYS:HD2	1.50	0.75
1:B:526:ARG:HH22	1:B:580:PHE:HA	1.52	0.75
1:B:238:TRP:HE3	1:B:239:LEU:HD23	1.52	0.75
2:I:269:ASN:HD21	2:I:274:ARG:HH22	1.34	0.75
1:B:334:ALA:HA	1:B:337:LEU:HB3	1.69	0.75
1:A:353:ILE:HG23	1:A:567:VAL:HB	1.69	0.75
1:A:425:LEU:HA	1:A:427:PHE:CE1	2.21	0.75
2:R:139:GLY:O	2:R:194:PHE:HB2	1.86	0.75
1:A:386:ARG:CZ	1:A:456:ASP:HB2	2.17	0.74
1:B:596:ALA:HA	1:B:599:ILE:HD12	1.69	0.74
2:C:158:MET:HE2	2:C:244:GLN:HB2	1.68	0.74
1:B:494:TYR:CD1	1:B:524:MET:HE3	2.22	0.74
1:A:99:ASP:HB2	1:A:722:ARG:HE	1.50	0.74
2:F:9:LEU:HG	2:F:13:ARG:HD2	1.69	0.74
1:B:746:TYR:HA	1:B:817:TYR:HE2	1.53	0.74
2:P:4:ILE:HG23	2:P:94:LEU:HB3	1.70	0.74
1:A:267:LEU:HD21	1:A:270:GLN:H	1.53	0.73
1:A:724:GLU:HB2	1:A:860:ARG:HH21	1.52	0.73
2:F:298:ILE:H	2:F:298:ILE:HD12	1.51	0.73
1:B:239:LEU:HD21	1:B:271:LEU:HG	1.71	0.73
2:S:124:GLN:HE21	2:S:124:GLN:HA	1.51	0.73
1:B:707:ARG:HB2	1:B:766:MET:HG3	1.68	0.73
2:E:2:ASP:HB3	2:E:109:ILE:HG21	1.71	0.73
1:B:724:GLU:HG3	1:B:860:ARG:NH1	2.04	0.73
1:A:85:VAL:HG12	1:A:163:VAL:HA	1.69	0.73
2:I:46:ARG:HD2	2:I:60:GLU:HG3	1.71	0.73
1:A:206:ILE:HG22	1:A:870:LEU:O	1.88	0.72
1:B:900:THR:HG22	2:G:22:ARG:HH11	1.53	0.72
2:S:53:THR:H	2:S:57:GLN:HE21	1.37	0.72
2:I:294:MET:SD	2:I:349:VAL:HG23	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:O	1:B:112:SER:HB3	1.89	0.72
1:B:409:MET:HB3	1:B:413:ARG:HH11	1.51	0.72
1:B:729:THR:HG22	1:B:731:MET:H	1.52	0.72
1:B:85:VAL:HG12	1:B:163:VAL:HA	1.71	0.72
1:B:371:MET:HB2	1:B:405:TYR:CG	2.24	0.72
2:I:37:ILE:HD12	2:I:50:MET:HG2	1.71	0.72
2:D:294:MET:SD	2:D:349:VAL:HG23	2.30	0.72
1:A:666:MET:O	1:A:670:VAL:HG23	1.89	0.72
1:B:722:ARG:O	1:B:722:ARG:HG2	1.89	0.72
1:A:509:LYS:CB	1:A:512:GLU:HG3	2.19	0.72
1:B:274:ASN:O	1:B:277:VAL:HG23	1.90	0.72
1:A:862:ARG:HB2	1:A:865:GLN:HB2	1.72	0.72
1:B:338:ASN:HA	1:B:341:ARG:HD3	1.72	0.72
1:B:774:PHE:HB3	1:B:817:TYR:HE1	1.54	0.72
2:R:158:MET:HE2	2:R:244:GLN:HB2	1.70	0.72
2:G:9:LEU:HG	2:G:13:ARG:HD2	1.72	0.72
2:H:298:ILE:H	2:H:298:ILE:HD12	1.53	0.72
1:B:148:ILE:HG23	1:B:163:VAL:HG11	1.72	0.72
2:G:298:ILE:HD12	2:G:298:ILE:H	1.55	0.72
1:B:731:MET:HE3	1:B:853:ILE:H	1.55	0.71
1:B:501:LEU:O	1:B:505:VAL:HG23	1.90	0.71
2:Q:266:GLU:O	2:Q:270:VAL:HG23	1.89	0.71
2:T:298:ILE:H	2:T:298:ILE:HD12	1.53	0.71
1:B:882:ARG:HB3	1:B:884:MET:HE3	1.71	0.71
2:Q:20:GLU:HB3	2:Q:22:ARG:HH22	1.54	0.71
1:A:371:MET:HB3	1:A:405:TYR:HB2	1.72	0.71
1:B:403:ASN:HB2	1:B:425:LEU:HD22	1.70	0.71
2:H:257:LEU:HD12	2:H:300:PRO:HB3	1.72	0.71
2:T:158:MET:HE2	2:T:244:GLN:HB2	1.72	0.71
1:A:300:GLY:HA2	1:A:587:THR:H	1.56	0.71
1:A:637:TRP:CZ3	1:A:666:MET:HE2	2.24	0.71
1:A:633:PRO:O	1:A:636:PHE:HD1	1.74	0.71
1:B:71:ILE:HA	1:B:74:LEU:HD12	1.72	0.71
1:B:471:TYR:HB2	1:B:535:ASN:HB2	1.71	0.71
1:B:623:ARG:HH21	1:B:694:PHE:HE2	1.37	0.71
2:S:266:GLU:O	2:S:270:VAL:HG23	1.90	0.71
1:A:591:GLU:HA	1:A:895:LYS:HE3	1.72	0.71
1:B:261:GLN:O	1:B:881:MET:HE3	1.91	0.71
1:B:873:ARG:HG2	1:B:874:PHE:N	2.05	0.71
2:H:53:THR:H	2:H:57:GLN:NE2	1.89	0.71
1:A:425:LEU:HA	1:A:427:PHE:HE1	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ILE:HG21	1:A:507:ALA:HA	1.72	0.71
1:A:468:ALA:HB3	1:A:546:ASP:HB2	1.71	0.71
2:T:269:ASN:HD21	2:T:274:ARG:HH22	1.39	0.71
2:Q:269:ASN:HD21	2:Q:274:ARG:HH22	1.38	0.70
1:A:381:PHE:O	1:A:450:ASN:HB3	1.91	0.70
1:A:504:LEU:HD12	1:A:513:ALA:HB2	1.73	0.70
2:G:139:GLY:O	2:G:194:PHE:HB2	1.90	0.70
2:G:93:VAL:HG12	2:G:99:ILE:HD11	1.72	0.70
2:P:339:LEU:HA	2:P:343:ILE:HD12	1.73	0.70
2:R:22:ARG:O	2:R:23:ILE:HG13	1.92	0.70
1:A:333:THR:HG23	1:A:337:LEU:HD12	1.74	0.70
1:A:465:TYR:CE1	1:A:541:VAL:HG13	2.27	0.70
1:B:205:PHE:CE1	1:B:874:PHE:HB3	2.26	0.70
1:B:633:PRO:CG	1:B:663:ILE:HG23	2.22	0.70
2:T:139:GLY:O	2:T:194:PHE:HB2	1.92	0.70
2:E:235:ASN:OD1	2:E:237:THR:HG22	1.92	0.69
1:A:257:ASP:O	1:A:258:PHE:HB3	1.92	0.69
1:B:354:ILE:HD11	1:B:566:PRO:HB2	1.74	0.69
2:G:112:VAL:O	2:G:116:THR:HB	1.92	0.69
2:H:68:MET:HE2	2:H:94:LEU:HD11	1.74	0.69
2:S:30:MET:HG2	2:S:50:MET:HE1	1.73	0.69
1:A:293:ILE:HG22	1:A:349:PHE:CZ	2.26	0.69
2:E:175:PHE:O	2:E:178:ARG:HG3	1.92	0.69
1:A:413:ARG:HD2	1:A:413:ARG:C	2.17	0.69
1:B:103:ARG:HH12	1:B:869:VAL:HG22	1.55	0.69
2:E:128:PHE:HB2	2:E:247:VAL:HG11	1.74	0.69
2:H:112:VAL:O	2:H:116:THR:HB	1.92	0.69
2:T:116:THR:HG21	2:T:304:ARG:HB2	1.73	0.69
1:A:344:TYR:HA	1:A:347:LEU:HD23	1.73	0.69
1:A:380:LEU:HD13	1:A:580:PHE:HD1	1.57	0.69
1:A:731:MET:HE1	1:A:853:ILE:O	1.92	0.69
1:B:406:LEU:HD11	1:B:503:MET:HE3	1.75	0.69
2:F:263:LEU:HD22	2:F:267:ILE:HD11	1.75	0.69
2:T:189:ARG:HD2	2:T:244:GLN:HE21	1.58	0.69
2:R:18:LEU:HD12	2:R:21:ALA:HB2	1.75	0.69
1:B:724:GLU:HG3	1:B:860:ARG:CZ	2.23	0.68
1:A:275:PRO:HB3	1:A:467:HIS:ND1	2.07	0.68
1:A:471:TYR:HB2	1:A:535:ASN:ND2	2.08	0.68
1:B:873:ARG:HD2	2:G:98:GLU:HG2	1.74	0.68
2:D:298:ILE:H	2:D:298:ILE:HD12	1.58	0.68
2:R:269:ASN:HD21	2:R:274:ARG:HH22	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ARG:HD3	1:A:766:MET:HB3	1.75	0.68
2:H:269:ASN:HD21	2:H:274:ARG:HH22	1.38	0.68
1:A:460:ARG:HG3	1:A:471:TYR:CE1	2.28	0.68
1:B:779:ARG:NH1	1:B:799:PRO:HB2	2.09	0.68
2:R:263:LEU:HD22	2:R:267:ILE:HD11	1.76	0.68
2:I:158:MET:HE2	2:I:244:GLN:HB2	1.75	0.68
2:E:298:ILE:H	2:E:298:ILE:HD12	1.59	0.68
1:B:403:ASN:ND2	1:B:425:LEU:H	1.92	0.68
1:B:526:ARG:HB2	1:B:583:SER:HB2	1.76	0.68
2:R:24:VAL:HG21	2:R:30:MET:CG	2.23	0.68
2:S:54:SER:H	2:S:57:GLN:HE21	1.40	0.68
1:B:403:ASN:HD22	1:B:425:LEU:N	1.92	0.68
2:J:2:ASP:HB3	2:J:109:ILE:HG21	1.75	0.68
2:T:54:SER:H	2:T:57:GLN:HE21	1.41	0.68
1:A:259:ARG:HB3	1:A:263:MET:HE3	1.76	0.68
1:A:729:THR:HG23	1:A:824:PHE:O	1.94	0.68
2:E:116:THR:HG21	2:E:304:ARG:HB2	1.74	0.68
1:B:332:PRO:HB2	1:B:336:GLN:HB3	1.76	0.68
1:B:8:ARG:HB3	1:B:11:ARG:HB2	1.75	0.67
2:I:339:LEU:HA	2:I:343:ILE:HD12	1.76	0.67
2:F:53:THR:H	2:F:57:GLN:NE2	1.90	0.67
1:B:391:THR:HB	1:B:394:MET:HB2	1.74	0.67
2:J:271:TYR:OH	2:J:292:PRO:HG2	1.95	0.67
1:B:901:VAL:HG22	2:Q:43:LEU:HG	1.74	0.67
2:R:271:TYR:OH	2:R:292:PRO:HG2	1.93	0.67
2:E:44:THR:HG22	2:E:46:ARG:H	1.59	0.67
2:Q:235:ASN:OD1	2:Q:237:THR:HG22	1.94	0.67
1:A:699:LEU:HD12	1:A:778:LEU:HD13	1.76	0.67
2:G:128:PHE:HB2	2:G:247:VAL:HG11	1.76	0.67
2:G:263:LEU:HD22	2:G:267:ILE:HD11	1.77	0.67
2:T:53:THR:H	2:T:57:GLN:NE2	1.92	0.67
1:A:485:PRO:HB2	1:A:525:VAL:HG11	1.76	0.66
2:R:266:GLU:O	2:R:270:VAL:HG23	1.94	0.66
2:I:288:ARG:HG3	2:I:288:ARG:HH11	1.60	0.66
1:A:207:GLY:O	1:A:872:ARG:HB2	1.94	0.66
1:A:439:PHE:CD1	1:A:503:MET:HE3	2.30	0.66
1:A:724:GLU:HB2	1:A:860:ARG:NH2	2.10	0.66
2:P:69:MET:HG2	2:P:312:LEU:HB3	1.76	0.66
2:Q:4:ILE:HG23	2:Q:94:LEU:HB3	1.77	0.66
2:Q:128:PHE:HB2	2:Q:247:VAL:HG11	1.77	0.66
2:J:69:MET:HG2	2:J:312:LEU:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:298:ILE:HD12	2:J:298:ILE:H	1.60	0.66
2:T:128:PHE:HB2	2:T:247:VAL:HG11	1.77	0.66
2:Q:16:ALA:HA	2:Q:322:VAL:HG21	1.78	0.66
2:H:96:THR:HG23	2:H:98:GLU:OE2	1.95	0.66
1:A:425:LEU:HD12	1:A:436:CYS:HB3	1.78	0.66
2:C:116:THR:HG21	2:C:304:ARG:HB2	1.77	0.66
2:J:266:GLU:O	2:J:270:VAL:HG23	1.96	0.66
1:A:214:TYR:CD2	1:A:872:ARG:HD2	2.30	0.66
2:C:16:ALA:HA	2:C:322:VAL:HG21	1.77	0.66
2:Q:282:ARG:HD3	2:Q:286:ARG:CZ	2.26	0.66
1:A:291:MET:HE3	1:A:651:VAL:HG13	1.78	0.66
1:B:620:MET:HE3	1:B:694:PHE:HZ	1.59	0.66
1:B:873:ARG:NH1	2:G:39:ARG:HB2	2.10	0.66
1:A:359:ILE:HG22	1:A:360:ASP:H	1.61	0.66
1:B:198:ALA:O	1:B:200:ARG:N	2.29	0.66
1:B:382:THR:H	1:B:389:ASN:HD22	1.44	0.66
1:A:115:GLY:HA3	1:A:129:THR:HG23	1.77	0.65
1:A:414:VAL:HG21	1:A:507:ALA:O	1.97	0.65
1:B:624:PHE:CD2	1:B:778:LEU:HD21	2.32	0.65
1:B:520:LEU:HB3	1:B:521:PRO:HD3	1.79	0.65
1:A:279:TRP:HZ3	1:A:541:VAL:O	1.79	0.65
1:B:403:ASN:HD22	1:B:425:LEU:H	1.41	0.65
1:B:465:TYR:O	1:B:466:VAL:HB	1.95	0.65
2:D:69:MET:HG2	2:D:312:LEU:HB3	1.79	0.65
2:S:23:ILE:HD12	2:S:24:VAL:H	1.62	0.65
2:J:139:GLY:O	2:J:194:PHE:HB2	1.96	0.65
1:B:413:ARG:HD2	1:B:414:VAL:N	2.10	0.65
2:I:175:PHE:O	2:I:178:ARG:HG3	1.96	0.65
1:B:355:LEU:O	1:B:394:MET:HG3	1.97	0.65
1:B:633:PRO:HA	1:B:636:PHE:CE2	2.32	0.65
2:I:235:ASN:OD1	2:I:237:THR:HG22	1.97	0.65
1:A:151:ARG:HG3	1:A:152:ASP:N	2.12	0.65
2:I:7:ARG:NH2	2:J:23:ILE:HG22	2.12	0.65
2:I:282:ARG:HD3	2:I:286:ARG:CZ	2.27	0.65
1:A:830:VAL:HG12	1:A:834:ASN:ND2	2.11	0.65
1:B:500:MET:O	1:B:504:LEU:HD12	1.97	0.65
2:J:44:THR:HG22	2:J:46:ARG:HG3	1.78	0.65
2:J:53:THR:H	2:J:57:GLN:NE2	1.95	0.65
1:A:273:VAL:HG12	1:A:274:ASN:H	1.62	0.64
1:A:715:LEU:HD21	1:A:830:VAL:HG11	1.78	0.64
1:B:336:GLN:HA	1:B:339:ASP:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:288:ARG:HG3	2:Q:288:ARG:HH11	1.62	0.64
2:G:266:GLU:O	2:G:270:VAL:HG23	1.97	0.64
2:H:54:SER:H	2:H:57:GLN:NE2	1.95	0.64
2:T:266:GLU:O	2:T:270:VAL:HG23	1.97	0.64
1:A:314:LEU:HD23	1:A:327:LEU:HD12	1.80	0.64
2:J:263:LEU:HD22	2:J:267:ILE:HD11	1.79	0.64
1:A:468:ALA:HB3	1:A:546:ASP:CB	2.27	0.64
2:G:88:MET:O	2:G:91:ILE:HG22	1.98	0.64
1:B:235:SER:CB	1:B:271:LEU:HB2	2.27	0.64
1:B:296:CYS:SG	1:B:540:SER:HB3	2.36	0.64
2:S:26:GLU:HB3	2:S:29:VAL:HG23	1.79	0.64
2:J:9:LEU:HG	2:J:13:ARG:HD2	1.79	0.64
1:A:263:MET:SD	1:A:884:MET:HE3	2.36	0.64
1:B:465:TYR:HD2	1:B:539:HIS:HD2	1.46	0.64
2:Q:43:LEU:CD1	2:Q:93:VAL:HG22	2.27	0.64
1:A:429:ILE:CD1	1:A:436:CYS:SG	2.86	0.64
2:Q:112:VAL:O	2:Q:116:THR:HB	1.97	0.64
2:I:54:SER:H	2:I:57:GLN:NE2	1.95	0.64
1:B:598:LEU:O	1:B:602:VAL:HG23	1.98	0.64
2:H:189:ARG:HD2	2:H:244:GLN:HE21	1.63	0.64
2:T:20:GLU:HG2	2:T:21:ALA:H	1.63	0.64
1:B:891:LYS:HE3	1:B:893:GLY:H	1.63	0.64
2:F:1:MET:HA	2:F:4:ILE:HD12	1.79	0.63
1:A:266:VAL:O	1:A:885:ASP:HB2	1.98	0.63
1:A:622:ARG:NH2	2:Q:26:GLU:HG3	2.12	0.63
2:Q:96:THR:HG22	2:Q:98:GLU:H	1.63	0.63
2:I:20:GLU:HG2	2:I:21:ALA:H	1.63	0.63
2:I:97:PRO:HD3	2:J:22:ARG:NH2	2.07	0.63
2:Q:39:ARG:NH2	2:Q:96:THR:HG21	2.13	0.63
2:S:64:MET:HG2	2:S:68:MET:HE3	1.79	0.63
2:S:112:VAL:O	2:S:116:THR:HB	1.98	0.63
1:A:287:ALA:HA	1:A:290:ILE:HD12	1.80	0.63
1:A:715:LEU:HD11	1:A:839:LEU:HD12	1.79	0.63
1:B:91:ARG:HG2	1:B:92:HIS:N	2.14	0.63
1:B:95:THR:CG2	1:B:725:GLY:HA3	2.29	0.63
1:B:337:LEU:HD23	1:B:582:ARG:HH12	1.64	0.63
2:G:66:LEU:O	2:G:70:LEU:HG	1.98	0.63
1:A:357:LEU:H	1:A:357:LEU:HD12	1.64	0.63
1:A:376:VAL:HG13	1:A:580:PHE:HB2	1.81	0.63
1:A:705:MET:HG2	1:A:772:VAL:HG22	1.81	0.63
1:B:901:VAL:HG23	2:G:22:ARG:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:20:GLU:HG2	2:C:21:ALA:H	1.63	0.63
2:Q:53:THR:H	2:Q:57:GLN:HE21	1.47	0.63
2:H:44:THR:HG22	2:H:46:ARG:HG3	1.79	0.63
2:J:282:ARG:HD3	2:J:286:ARG:CZ	2.28	0.63
1:A:340:VAL:HA	1:A:343:ILE:CG2	2.29	0.63
1:A:622:ARG:NH1	2:F:100:PRO:HB2	2.14	0.63
2:R:338:PRO:O	2:R:339:LEU:HB2	1.99	0.63
2:I:4:ILE:HG23	2:I:94:LEU:HB3	1.81	0.63
2:T:235:ASN:OD1	2:T:237:THR:HG22	1.98	0.63
2:D:53:THR:H	2:D:57:GLN:NE2	1.97	0.62
2:S:277:THR:HA	2:S:329:MET:HE1	1.82	0.62
1:B:610:MET:HE2	1:B:644:SER:HB2	1.81	0.62
2:P:244:GLN:CD	2:C:135:THR:HG21	2.24	0.62
2:G:259:GLN:HA	2:H:268:PHE:CD2	2.33	0.62
1:B:875:VAL:HG21	2:G:38:ASN:HD21	1.65	0.62
1:A:812:TYR:N	1:A:812:TYR:HD1	1.98	0.62
1:B:407:LEU:HA	1:B:413:ARG:NH2	2.09	0.62
2:C:266:GLU:O	2:C:270:VAL:HG23	1.99	0.62
2:I:69:MET:HG2	2:I:312:LEU:HB3	1.81	0.62
2:J:175:PHE:O	2:J:178:ARG:HG3	1.99	0.62
1:A:468:ALA:CB	1:A:546:ASP:HB2	2.29	0.62
1:B:370:ARG:HH21	1:B:401:ALA:HA	1.62	0.62
1:B:64:VAL:O	1:B:67:ILE:HG22	1.99	0.62
1:B:263:MET:HE3	1:B:884:MET:HE1	1.80	0.62
2:C:294:MET:SD	2:C:349:VAL:HG23	2.39	0.62
2:S:139:GLY:O	2:S:194:PHE:HB2	1.99	0.62
1:A:80:TYR:OH	1:A:885:ASP:HB3	1.99	0.62
1:B:688:TRP:O	1:B:691:ALA:HB3	1.99	0.62
1:A:434:TYR:CD2	1:A:503:MET:HB2	2.35	0.62
1:A:533:ILE:HG22	1:A:538:LEU:HD21	1.82	0.62
1:B:617:LEU:O	1:B:620:MET:HB2	1.99	0.62
2:R:44:THR:HG22	2:R:46:ARG:HG3	1.81	0.62
2:I:28:ASN:HD22	2:I:28:ASN:N	1.98	0.62
2:P:158:MET:HE2	2:P:244:GLN:HB2	1.80	0.62
2:E:271:TYR:OH	2:E:292:PRO:HG2	2.00	0.62
1:A:812:TYR:N	1:A:812:TYR:CD1	2.67	0.62
2:I:112:VAL:O	2:I:116:THR:HB	2.00	0.62
2:I:266:GLU:O	2:I:270:VAL:HG23	1.99	0.62
1:A:842:ILE:H	1:A:842:ILE:HD12	1.65	0.61
1:B:819:THR:HG22	1:B:820:GLU:H	1.65	0.61
2:C:257:LEU:CD1	2:C:300:PRO:HB3	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:44:THR:O	2:T:45:LEU:HB2	2.00	0.61
2:T:263:LEU:HD22	2:T:267:ILE:HD11	1.82	0.61
1:A:468:ALA:HB3	1:A:546:ASP:CG	2.24	0.61
1:B:302:TYR:HE1	1:B:584:PHE:CD2	2.18	0.61
1:B:357:LEU:HD22	1:B:357:LEU:H	1.65	0.61
1:B:842:ILE:H	1:B:842:ILE:HD12	1.65	0.61
1:A:138:ARG:NH2	1:A:680:LYS:HG2	2.15	0.61
1:A:332:PRO:CD	1:A:336:GLN:HG3	2.28	0.61
1:A:765:ILE:HG21	1:A:772:VAL:HG12	1.81	0.61
2:G:175:PHE:O	2:G:178:ARG:HG3	1.99	0.61
1:B:763:ARG:HD3	1:B:767:ASP:OD1	2.00	0.61
2:Q:49:THR:HG22	2:Q:51:ARG:H	1.65	0.61
2:F:27:ALA:O	2:F:31:GLU:HG3	2.01	0.61
2:S:1:MET:HA	2:S:4:ILE:HD12	1.83	0.61
1:B:332:PRO:HG2	1:B:574:ILE:HG21	1.82	0.61
2:G:9:LEU:O	2:G:13:ARG:HG3	2.00	0.61
2:G:41:ASN:HD21	2:G:48:VAL:H	1.47	0.61
1:A:70:ASP:O	1:A:74:LEU:HD23	2.00	0.61
1:B:460:ARG:HE	2:E:51:ARG:NH2	1.99	0.61
2:F:112:VAL:O	2:F:116:THR:HB	2.01	0.61
1:A:436:CYS:SG	1:A:503:MET:HE2	2.40	0.61
1:B:248:ILE:HD11	1:B:892:MET:SD	2.41	0.61
1:B:409:MET:HB3	1:B:413:ARG:NH1	2.16	0.61
1:B:873:ARG:O	1:B:874:PHE:HB2	2.00	0.61
1:B:263:MET:HE2	1:B:884:MET:SD	2.41	0.61
1:B:356:ASP:O	1:B:570:ASP:HA	2.01	0.61
1:B:684:GLU:O	1:B:688:TRP:HB2	2.00	0.61
2:E:21:ALA:O	2:E:51:ARG:HD2	2.01	0.61
2:G:53:THR:H	2:G:57:GLN:NE2	1.98	0.61
2:H:128:PHE:HB2	2:H:247:VAL:HG11	1.82	0.61
1:A:456:ASP:O	1:A:472:ILE:HA	2.00	0.61
1:B:421:THR:HG22	1:B:423:GLU:H	1.66	0.61
2:D:266:GLU:O	2:D:270:VAL:HG23	2.01	0.61
2:H:175:PHE:O	2:H:178:ARG:HG3	2.01	0.61
1:A:661:ILE:HG23	1:A:665:ASP:HB2	1.82	0.61
2:S:4:ILE:HG23	2:S:94:LEU:HB3	1.82	0.61
2:T:159:ILE:HD11	2:T:245:ILE:HB	1.83	0.61
1:A:430:GLY:O	1:A:431:ARG:HB2	2.00	0.60
1:B:721:PHE:C	1:B:723:GLN:H	2.08	0.60
1:A:356:ASP:CG	1:A:568:VAL:HA	2.25	0.60
1:A:470:ARG:HB3	1:A:546:ASP:OD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:LEU:HD12	2:D:300:PRO:HB3	1.81	0.60
2:R:189:ARG:HD2	2:R:244:GLN:HE21	1.66	0.60
2:H:7:ARG:NH2	2:H:97:PRO:HA	2.16	0.60
2:T:237:THR:HG23	2:T:239:GLN:H	1.67	0.60
1:A:427:PHE:HD1	1:A:427:PHE:H	1.49	0.60
2:Q:54:SER:H	2:Q:57:GLN:HE21	1.48	0.60
2:F:44:THR:HG22	2:F:46:ARG:HG3	1.83	0.60
1:B:93:ILE:HG23	1:B:102:LEU:HG	1.84	0.60
2:I:128:PHE:HB2	2:I:247:VAL:HG11	1.83	0.60
1:A:105:ASP:O	1:A:107:TYR:N	2.35	0.60
1:A:381:PHE:CG	1:A:390:LEU:HD21	2.36	0.60
1:B:36:LEU:HG	1:B:290:ILE:HD13	1.82	0.60
2:P:44:THR:HG22	2:P:46:ARG:HG3	1.84	0.60
1:A:391:THR:HB	1:A:394:MET:H	1.67	0.60
1:B:627:VAL:HG21	1:B:778:LEU:HD23	1.84	0.60
1:B:729:THR:HG22	1:B:731:MET:N	2.17	0.60
2:P:112:VAL:O	2:P:116:THR:HB	2.01	0.60
2:D:283:THR:HG23	2:D:293:ASN:HB2	1.82	0.60
2:Q:139:GLY:O	2:Q:194:PHE:HB2	2.02	0.60
2:S:54:SER:H	2:S:57:GLN:NE2	1.99	0.60
1:A:774:PHE:HB3	1:A:817:TYR:CE2	2.37	0.59
2:P:200:ASN:H	2:P:200:ASN:HD22	1.49	0.59
1:A:541:VAL:HG22	1:A:600:GLU:CD	2.27	0.59
2:H:266:GLU:O	2:H:270:VAL:HG23	2.01	0.59
1:A:57:VAL:HG21	1:A:301:GLU:HG2	1.84	0.59
1:A:359:ILE:HG22	1:A:361:PRO:CD	2.31	0.59
1:A:497:TYR:O	1:A:501:LEU:HG	2.02	0.59
1:B:100:ARG:HD3	1:B:724:GLU:HG2	1.82	0.59
1:B:460:ARG:HB2	2:E:51:ARG:HG2	1.84	0.59
2:R:2:ASP:HB3	2:R:109:ILE:HG21	1.83	0.59
2:H:4:ILE:HG23	2:H:94:LEU:HB3	1.84	0.59
2:R:128:PHE:HB2	2:R:247:VAL:HG11	1.82	0.59
1:A:57:VAL:HG23	1:A:300:GLY:O	2.03	0.59
1:B:129:THR:O	1:B:133:LYS:HG3	2.03	0.59
1:B:403:ASN:ND2	1:B:427:PHE:HE1	1.99	0.59
2:P:7:ARG:O	2:P:11:VAL:HG23	2.03	0.59
1:B:460:ARG:HG3	2:E:51:ARG:NH1	2.18	0.59
2:F:314:SER:O	2:F:317:ALA:HB3	2.01	0.59
2:S:277:THR:HG23	2:S:329:MET:HE1	1.83	0.59
2:E:269:ASN:HD21	2:E:274:ARG:HH22	1.48	0.59
1:A:58:ASP:H	1:B:317:ARG:HH12	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:SER:O	1:A:612:VAL:HG23	2.03	0.59
1:A:617:LEU:HB3	1:A:636:PHE:HD2	1.68	0.59
1:B:331:THR:HA	1:B:578:PHE:CE2	2.38	0.59
1:B:465:TYR:HD2	1:B:539:HIS:CD2	2.20	0.59
2:C:97:PRO:O	2:D:24:VAL:HG22	2.02	0.59
2:E:112:VAL:O	2:E:116:THR:HB	2.02	0.59
1:A:474:TYR:HB2	1:A:531:ASN:HD21	1.66	0.59
1:A:830:VAL:HG12	1:A:834:ASN:HD22	1.67	0.59
1:B:336:GLN:HA	1:B:339:ASP:CB	2.33	0.59
1:B:409:MET:HG2	1:B:413:ARG:HD3	1.85	0.59
2:C:7:ARG:O	2:C:11:VAL:HG23	2.03	0.59
2:C:53:THR:H	2:C:57:GLN:NE2	2.01	0.59
2:D:16:ALA:HA	2:D:322:VAL:HG21	1.84	0.59
2:E:9:LEU:O	2:E:13:ARG:HG3	2.03	0.59
2:R:10:THR:CG2	2:R:102:THR:HG23	2.32	0.59
2:H:10:THR:HG23	2:H:102:THR:HG23	1.85	0.59
2:T:54:SER:H	2:T:57:GLN:NE2	2.01	0.59
2:E:25:LEU:HD23	2:E:51:ARG:NH2	2.18	0.59
2:F:23:ILE:O	2:F:24:VAL:HG22	2.03	0.59
1:A:151:ARG:HH12	1:A:188:ASP:HB3	1.68	0.58
1:B:854:ASN:ND2	2:H:49:THR:HG21	2.16	0.58
2:Q:185:TYR:O	2:Q:248:VAL:HG12	2.03	0.58
2:J:54:SER:H	2:J:57:GLN:HE21	1.50	0.58
1:B:108:TYR:HB3	1:B:698:MET:CE	2.33	0.58
1:B:779:ARG:HH12	1:B:799:PRO:CB	2.14	0.58
2:P:315:THR:O	2:P:319:VAL:HG23	2.02	0.58
2:E:244:GLN:CD	2:F:135:THR:HG21	2.27	0.58
1:A:98:ARG:HG2	1:A:174:VAL:HG12	1.85	0.58
1:B:370:ARG:NH2	1:B:401:ALA:HA	2.18	0.58
2:P:53:THR:H	2:P:57:GLN:NE2	2.00	0.58
2:P:175:PHE:O	2:P:178:ARG:HG3	2.03	0.58
2:F:4:ILE:HG23	2:F:94:LEU:HB3	1.85	0.58
1:A:349:PHE:H	1:A:350:PRO:HA	1.69	0.58
1:A:388:THR:HG22	1:A:389:ASN:N	2.17	0.58
2:E:9:LEU:HG	2:E:13:ARG:HD2	1.85	0.58
2:E:337:GLY:N	2:E:338:PRO:HD3	2.18	0.58
2:T:175:PHE:O	2:T:178:ARG:HG3	2.03	0.58
1:B:305:PRO:HG3	1:B:519:MET:HE1	1.83	0.58
1:B:465:TYR:CE2	1:B:540:SER:HA	2.39	0.58
2:Q:69:MET:HG2	2:Q:312:LEU:HB3	1.85	0.58
1:A:169:LYS:O	1:A:173:PRO:HD3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ILE:CG2	1:A:507:ALA:HA	2.32	0.58
1:A:637:TRP:CZ3	1:A:666:MET:HG2	2.39	0.58
2:P:266:GLU:O	2:P:270:VAL:HG23	2.04	0.58
2:Q:288:ARG:HG3	2:Q:288:ARG:NH1	2.18	0.58
2:G:200:ASN:H	2:G:200:ASN:ND2	2.00	0.58
1:A:314:LEU:HD13	1:A:515:TYR:CB	2.33	0.58
1:A:386:ARG:NH1	1:A:456:ASP:HB2	2.18	0.58
2:E:158:MET:HE3	2:E:245:ILE:O	2.03	0.58
2:T:4:ILE:HG23	2:T:94:LEU:HB3	1.86	0.58
1:B:470:ARG:NH1	1:B:549:PHE:CG	2.72	0.58
2:T:41:ASN:HD21	2:T:48:VAL:H	1.51	0.58
1:A:273:VAL:HG12	1:A:274:ASN:N	2.19	0.58
1:A:482:LEU:HD12	1:A:899:PRO:HD3	1.85	0.58
2:Q:44:THR:HG22	2:Q:46:ARG:HG3	1.86	0.58
1:A:293:ILE:HG22	1:A:349:PHE:HZ	1.68	0.57
2:G:257:LEU:CD1	2:G:300:PRO:HB3	2.32	0.57
1:A:474:TYR:O	1:A:477:ILE:HG12	2.03	0.57
1:A:645:PRO:HB2	1:A:648:VAL:HG23	1.85	0.57
2:C:1:MET:HA	2:C:4:ILE:HD12	1.85	0.57
2:F:266:GLU:O	2:F:270:VAL:HG23	2.04	0.57
2:G:25:LEU:HD22	2:G:25:LEU:N	2.19	0.57
2:H:44:THR:O	2:H:45:LEU:HB2	2.04	0.57
2:I:263:LEU:HD22	2:I:267:ILE:HD11	1.85	0.57
1:A:483:ILE:HG23	1:A:488:TYR:HD2	1.69	0.57
1:B:192:ILE:HG22	1:B:192:ILE:O	2.03	0.57
2:E:200:ASN:H	2:E:200:ASN:ND2	2.01	0.57
2:I:2:ASP:HB3	2:I:109:ILE:HG21	1.86	0.57
1:A:109:GLU:O	1:A:112:SER:HB3	2.04	0.57
1:B:753:ALA:CB	1:B:815:ILE:HB	2.35	0.57
2:R:25:LEU:HD21	2:H:32:ILE:HD11	1.85	0.57
1:A:509:LYS:H	1:A:509:LYS:CD	2.14	0.57
1:A:729:THR:HG22	1:A:730:ASN:N	2.20	0.57
1:B:356:ASP:HA	1:B:394:MET:CG	2.33	0.57
1:B:620:MET:HE3	1:B:694:PHE:CZ	2.40	0.57
2:P:116:THR:HG21	2:P:304:ARG:HB2	1.87	0.57
2:R:112:VAL:O	2:R:116:THR:HB	2.04	0.57
2:G:53:THR:H	2:G:57:GLN:HE21	1.51	0.57
2:S:64:MET:CG	2:S:68:MET:HE3	2.34	0.57
2:T:66:LEU:O	2:T:70:LEU:HG	2.05	0.57
1:A:403:ASN:ND2	1:A:425:LEU:H	2.03	0.57
1:B:200:ARG:O	1:B:201:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:VAL:O	2:D:116:THR:HB	2.05	0.57
2:Q:339:LEU:HA	2:Q:343:ILE:HD12	1.86	0.57
2:F:283:THR:HG23	2:F:293:ASN:HB2	1.87	0.57
2:R:96:THR:HG22	2:R:98:GLU:HB2	1.87	0.57
2:G:116:THR:HG21	2:G:304:ARG:HB2	1.87	0.57
2:I:288:ARG:HG3	2:I:288:ARG:NH1	2.17	0.57
1:A:251:SER:HB3	1:A:892:MET:HB3	1.86	0.57
1:B:78:GLN:HB3	1:B:80:TYR:CE1	2.39	0.57
1:B:134:VAL:HG11	1:B:688:TRP:CE3	2.39	0.57
1:B:774:PHE:HB3	1:B:817:TYR:CE1	2.37	0.57
2:F:64:MET:O	2:F:68:MET:HG3	2.05	0.57
2:R:54:SER:H	2:R:57:GLN:NE2	2.00	0.57
1:A:474:TYR:O	1:A:475:CYS:SG	2.60	0.57
1:A:494:TYR:HB3	1:A:497:TYR:HB3	1.87	0.57
1:A:711:PRO:HG2	1:A:828:TYR:OH	2.05	0.57
1:B:101:VAL:HG12	1:B:102:LEU:H	1.70	0.57
2:H:282:ARG:HD3	2:H:286:ARG:CZ	2.33	0.57
2:Q:53:THR:H	2:Q:57:GLN:NE2	2.03	0.56
2:I:53:THR:H	2:I:57:GLN:NE2	2.03	0.56
2:I:271:TYR:OH	2:I:292:PRO:HG2	2.05	0.56
1:A:148:ILE:HD13	1:A:163:VAL:HG21	1.87	0.56
1:B:532:GLN:O	1:B:536:GLU:HB3	2.06	0.56
1:B:698:MET:C	1:B:699:LEU:HD23	2.30	0.56
2:J:53:THR:H	2:J:57:GLN:HE21	1.51	0.56
2:P:135:THR:HG21	2:D:244:GLN:CD	2.31	0.56
2:R:49:THR:HG22	2:R:51:ARG:H	1.70	0.56
2:R:324:ARG:N	2:R:325:PRO:HD3	2.20	0.56
2:G:271:TYR:OH	2:G:292:PRO:HG2	2.05	0.56
2:S:2:ASP:HB3	2:S:109:ILE:HG21	1.87	0.56
2:S:97:PRO:O	2:I:24:VAL:HG22	2.05	0.56
1:A:196:ASN:HD22	1:A:197:VAL:HG23	1.70	0.56
1:B:42:LYS:O	1:B:46:VAL:HG22	2.05	0.56
1:B:95:THR:HG22	1:B:96:GLN:H	1.70	0.56
2:H:288:ARG:HG3	2:H:288:ARG:NH1	2.20	0.56
2:I:186:LEU:HD21	2:I:225:TRP:HE3	1.70	0.56
2:I:186:LEU:HD21	2:I:225:TRP:CE3	2.40	0.56
1:A:168:PHE:O	1:A:170:ASN:N	2.39	0.56
1:A:293:ILE:O	1:A:297:LEU:HB2	2.04	0.56
1:A:487:THR:O	1:A:488:TYR:HB2	2.06	0.56
1:B:72:LYS:NZ	1:B:592:MET:HE2	2.20	0.56
1:B:255:LEU:H	1:B:896:LEU:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:116:THR:HG21	2:Q:304:ARG:HB2	1.86	0.56
2:Q:178:ARG:N	2:Q:178:ARG:HD2	2.21	0.56
2:E:40:TYR:CE2	2:E:44:THR:HG21	2.40	0.56
2:F:7:ARG:O	2:F:11:VAL:HG23	2.05	0.56
2:S:41:ASN:ND2	2:S:46:ARG:O	2.38	0.56
1:B:331:THR:HG21	1:B:337:LEU:HB2	1.88	0.56
1:B:745:THR:HB	1:B:748:ILE:HG13	1.87	0.56
2:Q:268:PHE:CD2	2:F:259:GLN:HA	2.40	0.56
2:J:200:ASN:H	2:J:200:ASN:ND2	2.03	0.56
2:T:185:TYR:O	2:T:248:VAL:HG12	2.05	0.56
1:B:115:GLY:H	1:B:133:LYS:HE3	1.70	0.56
2:F:30:MET:HA	2:F:50:MET:HE1	1.88	0.56
2:R:69:MET:HG2	2:R:312:LEU:HB3	1.87	0.56
1:A:467:HIS:CD2	1:A:543:SER:O	2.59	0.56
1:B:419:GLY:HA3	1:B:426:ASP:OD1	2.05	0.56
1:B:693:ASP:O	1:B:694:PHE:HB2	2.06	0.56
2:R:135:THR:HG21	2:H:244:GLN:CD	2.30	0.56
2:S:10:THR:HG23	2:S:102:THR:HG23	1.88	0.56
1:B:13:LYS:HD2	1:B:19:GLU:HG3	1.88	0.56
1:B:326:ILE:HG13	1:B:327:LEU:N	2.20	0.56
2:C:330:HIS:HB3	2:F:336:PRO:HB3	1.87	0.56
2:G:69:MET:HG2	2:G:312:LEU:HB3	1.87	0.56
2:S:20:GLU:HG2	2:S:21:ALA:H	1.70	0.56
1:A:339:ASP:OD1	1:A:571:VAL:HA	2.06	0.56
1:B:718:ILE:HD13	1:B:832:PHE:HA	1.88	0.56
2:R:175:PHE:O	2:R:178:ARG:HG3	2.05	0.56
2:H:26:GLU:HB3	2:H:29:VAL:HG23	1.87	0.56
2:S:282:ARG:HD3	2:S:286:ARG:CZ	2.36	0.56
2:I:44:THR:CG2	2:I:46:ARG:HB2	2.35	0.56
2:I:259:GLN:HA	2:J:268:PHE:CD2	2.41	0.56
1:A:178:GLU:HG2	1:A:179:HIS:H	1.71	0.55
1:A:425:LEU:HB3	1:A:436:CYS:O	2.06	0.55
1:B:336:GLN:O	1:B:339:ASP:HB3	2.06	0.55
1:B:384:GLY:HA2	1:B:446:GLY:HA3	1.87	0.55
1:B:471:TYR:HB2	1:B:535:ASN:CB	2.36	0.55
2:F:41:ASN:HD21	2:F:48:VAL:HG23	1.71	0.55
2:R:314:SER:O	2:R:317:ALA:HB3	2.05	0.55
2:G:330:HIS:HB3	2:T:337:GLY:HA3	1.88	0.55
1:B:103:ARG:HE	1:B:861:VAL:HG21	1.71	0.55
2:E:4:ILE:HG23	2:E:94:LEU:HB3	1.88	0.55
2:E:43:LEU:HD12	2:E:93:VAL:HG22	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:88:MET:O	2:R:91:ILE:HG22	2.05	0.55
1:A:465:TYR:HE1	1:A:541:VAL:HG13	1.68	0.55
1:A:863:VAL:HG23	1:A:864:GLY:H	1.70	0.55
2:P:189:ARG:HH11	2:P:244:GLN:HE21	1.55	0.55
2:R:282:ARG:HD3	2:R:286:ARG:CZ	2.36	0.55
2:R:339:LEU:HA	2:R:343:ILE:HD12	1.87	0.55
1:A:281:VAL:HG13	1:A:652:MET:HE2	1.86	0.55
1:A:428:GLN:HG2	1:A:435:ASP:HB3	1.88	0.55
1:B:526:ARG:NH2	1:B:580:PHE:HA	2.21	0.55
1:B:731:MET:HG3	1:B:823:ILE:HD13	1.88	0.55
2:D:269:ASN:HD21	2:D:274:ARG:HH22	1.53	0.55
2:H:108:GLU:HG3	2:H:260:TYR:OH	2.06	0.55
2:I:189:ARG:HD2	2:I:244:GLN:HE21	1.71	0.55
2:T:314:SER:O	2:T:317:ALA:HB3	2.05	0.55
1:B:628:LEU:HD23	1:B:628:LEU:N	2.21	0.55
2:R:116:THR:HG21	2:R:304:ARG:HB2	1.87	0.55
1:A:57:VAL:HG22	1:A:57:VAL:O	2.05	0.55
1:B:331:THR:O	1:B:333:THR:N	2.39	0.55
1:B:653:ASN:CG	1:B:658:HIS:HD2	2.14	0.55
2:D:43:LEU:HD12	2:D:93:VAL:HG22	1.88	0.55
2:E:266:GLU:O	2:E:270:VAL:HG23	2.07	0.55
2:J:116:THR:HG21	2:J:304:ARG:CB	2.29	0.55
2:T:191:ILE:HD12	2:T:242:MET:HB3	1.89	0.55
2:T:257:LEU:CD1	2:T:300:PRO:HB3	2.31	0.55
1:A:286:ILE:HG23	1:A:655:SER:HB3	1.89	0.55
2:E:25:LEU:HD23	2:E:51:ARG:HH22	1.72	0.55
2:R:44:THR:O	2:R:45:LEU:HB2	2.07	0.55
1:A:379:LEU:HD22	1:A:497:TYR:HD1	1.70	0.55
1:A:403:ASN:HB2	1:A:425:LEU:HD22	1.89	0.55
1:B:214:TYR:CD2	1:B:872:ARG:HD2	2.41	0.55
1:B:584:PHE:C	1:B:584:PHE:CD1	2.85	0.55
1:B:666:MET:O	1:B:670:VAL:HG23	2.07	0.55
1:B:901:VAL:CG2	2:G:22:ARG:HD3	2.37	0.55
2:E:270:VAL:HB	2:E:286:ARG:NH2	2.22	0.55
2:I:28:ASN:ND2	2:I:28:ASN:H	2.05	0.55
2:T:112:VAL:O	2:T:116:THR:HB	2.07	0.55
2:F:334:PRO:O	2:F:336:PRO:HD3	2.07	0.55
1:A:358:LYS:HG2	1:A:394:MET:SD	2.47	0.55
1:A:655:SER:O	1:A:659:ASN:HB2	2.07	0.55
1:A:664:ARG:HG3	1:B:485:PRO:CG	2.37	0.55
1:A:693:ASP:OD2	1:A:695:GLU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:GLU:HB3	1:B:365:MET:HE2	1.89	0.55
1:B:370:ARG:HG2	1:B:573:TRP:CE2	2.41	0.55
1:B:636:PHE:O	1:B:640:VAL:HG23	2.07	0.55
2:C:39:ARG:HH11	2:C:39:ARG:HG3	1.72	0.55
2:I:324:ARG:N	2:I:325:PRO:HD3	2.22	0.55
1:A:314:LEU:CD1	1:A:512:GLU:HA	2.36	0.54
2:P:294:MET:SD	2:P:349:VAL:HG23	2.47	0.54
2:R:7:ARG:O	2:R:11:VAL:HG23	2.07	0.54
1:A:529:ARG:O	1:A:533:ILE:HG13	2.06	0.54
1:B:227:VAL:HG13	1:B:231:GLU:HG3	1.89	0.54
2:G:237:THR:HG23	2:G:239:GLN:H	1.73	0.54
2:H:191:ILE:HD12	2:H:242:MET:HB3	1.89	0.54
2:S:265:ALA:HB1	2:J:261:PRO:HD3	1.89	0.54
1:A:295:THR:O	1:A:590:ASN:ND2	2.39	0.54
1:B:861:VAL:HG12	1:B:862:ARG:N	2.21	0.54
2:P:253:MET:HE1	2:C:341:ALA:O	2.07	0.54
2:F:51:ARG:O	2:F:51:ARG:HD3	2.08	0.54
2:H:337:GLY:O	2:H:339:LEU:HD13	2.08	0.54
1:B:731:MET:HE3	1:B:853:ILE:N	2.23	0.54
2:P:200:ASN:H	2:P:200:ASN:ND2	2.06	0.54
2:C:88:MET:O	2:C:91:ILE:HG22	2.08	0.54
2:Q:263:LEU:HD22	2:Q:267:ILE:CD1	2.37	0.54
2:H:288:ARG:HG3	2:H:288:ARG:HH11	1.71	0.54
2:S:210:VAL:HG22	2:S:233:VAL:HG13	1.90	0.54
2:J:314:SER:O	2:J:317:ALA:HB3	2.07	0.54
1:A:326:ILE:HG21	1:A:372:VAL:HG21	1.88	0.54
1:A:715:LEU:CD1	1:A:839:LEU:HD12	2.37	0.54
1:B:265:TRP:CD1	1:B:886:ILE:HD11	2.42	0.54
2:P:217:MET:HE2	2:P:223:ILE:HG12	1.88	0.54
2:C:128:PHE:HB2	2:C:247:VAL:HG11	1.88	0.54
2:Q:31:GLU:O	2:Q:35:ILE:HG13	2.08	0.54
2:R:294:MET:SD	2:R:349:VAL:HG23	2.47	0.54
2:J:257:LEU:HD23	2:J:264:THR:HG23	1.90	0.54
2:Q:43:LEU:HD12	2:Q:93:VAL:HG22	1.88	0.54
2:G:282:ARG:HD3	2:G:286:ARG:CZ	2.37	0.54
2:T:281:LEU:O	2:T:285:ILE:HG13	2.07	0.54
1:A:165:GLY:O	1:A:166:VAL:HB	2.07	0.54
1:A:341:ARG:NH1	1:B:317:ARG:HD3	2.22	0.54
1:A:746:TYR:O	1:A:750:ARG:HG2	2.07	0.54
1:B:267:LEU:HD21	1:B:269:LEU:O	2.08	0.54
2:H:69:MET:HG2	2:H:312:LEU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:282:ARG:HD3	2:T:286:ARG:CZ	2.38	0.54
2:T:324:ARG:N	2:T:325:PRO:HD3	2.23	0.54
1:A:379:LEU:HD22	1:A:497:TYR:CD1	2.43	0.54
1:A:483:ILE:HG23	1:A:488:TYR:CD2	2.43	0.54
1:A:758:PHE:O	1:A:762:LEU:HD23	2.07	0.54
1:B:130:ILE:HD13	1:B:620:MET:HE2	1.89	0.54
2:F:116:THR:HG21	2:F:304:ARG:HB2	1.89	0.54
2:F:204:THR:HG23	2:F:241:ALA:HB1	1.90	0.54
2:T:53:THR:H	2:T:57:GLN:HE21	1.56	0.54
1:A:283:ARG:HH21	1:B:490:ILE:HA	1.73	0.54
1:B:108:TYR:CD1	1:B:698:MET:HE2	2.43	0.54
2:E:40:TYR:O	2:E:44:THR:HB	2.08	0.54
2:S:116:THR:HG21	2:S:304:ARG:HB2	1.89	0.54
2:J:54:SER:H	2:J:57:GLN:NE2	2.06	0.54
1:A:301:GLU:HG3	1:A:587:THR:CG2	2.38	0.53
1:A:748:ILE:CD1	2:Q:49:THR:HG23	2.37	0.53
2:C:339:LEU:HA	2:C:343:ILE:HD12	1.90	0.53
2:Q:108:GLU:HG3	2:Q:260:TYR:OH	2.07	0.53
2:S:128:PHE:HB2	2:S:247:VAL:HG11	1.90	0.53
2:I:17:THR:HG21	2:I:25:LEU:HD11	1.90	0.53
1:A:532:GLN:O	1:A:536:GLU:HB3	2.08	0.53
1:A:721:PHE:C	1:A:723:GLN:H	2.13	0.53
2:P:54:SER:H	2:P:57:GLN:NE2	2.06	0.53
2:E:257:LEU:HD12	2:E:300:PRO:HB3	1.90	0.53
2:F:139:GLY:O	2:F:194:PHE:HB2	2.07	0.53
1:A:377:GLY:HA3	1:A:398:LEU:HD21	1.91	0.53
1:A:523:HIS:O	1:A:526:ARG:HG2	2.09	0.53
2:Q:257:LEU:CD1	2:Q:300:PRO:HB3	2.34	0.53
2:F:175:PHE:O	2:F:178:ARG:HG3	2.08	0.53
1:A:413:ARG:HD2	1:A:413:ARG:O	2.08	0.53
2:Q:338:PRO:O	2:Q:339:LEU:HB2	2.07	0.53
2:F:25:LEU:H	2:F:25:LEU:HD22	1.73	0.53
2:R:270:VAL:HG13	2:R:313:LEU:HB3	1.90	0.53
2:I:97:PRO:HB3	2:J:22:ARG:HE	1.74	0.53
2:I:185:TYR:O	2:I:248:VAL:HG12	2.08	0.53
1:B:354:ILE:CD1	1:B:566:PRO:HB2	2.38	0.53
1:B:724:GLU:OE2	1:B:860:ARG:HB2	2.09	0.53
2:T:25:LEU:HB2	2:T:30:MET:HE3	1.90	0.53
1:B:72:LYS:HZ3	1:B:592:MET:HE2	1.74	0.53
2:R:133:GLU:HG2	2:H:219:ALA:O	2.09	0.53
2:I:337:GLY:O	2:I:339:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLN:HE22	1:A:830:VAL:HG23	1.74	0.53
1:A:419:GLY:HA3	1:A:426:ASP:OD1	2.07	0.53
2:Q:43:LEU:HD13	2:Q:93:VAL:HG22	1.90	0.53
2:R:283:THR:HG23	2:R:293:ASN:HB2	1.90	0.53
2:G:96:THR:CG2	2:G:98:GLU:HB2	2.38	0.53
1:A:529:ARG:HH11	1:A:529:ARG:HG3	1.73	0.53
1:B:80:TYR:HA	1:B:142:SER:HB3	1.89	0.53
1:B:616:HIS:CG	1:B:688:TRP:NE1	2.76	0.53
2:Q:191:ILE:HD12	2:Q:242:MET:HB3	1.91	0.53
2:Q:271:TYR:OH	2:Q:292:PRO:HG2	2.09	0.53
2:E:139:GLY:O	2:E:194:PHE:HB2	2.08	0.53
1:A:283:ARG:HA	1:A:563:ASN:ND2	2.24	0.53
2:F:66:LEU:O	2:F:70:LEU:HG	2.08	0.53
2:S:66:LEU:O	2:S:70:LEU:HG	2.09	0.53
1:B:80:TYR:OH	1:B:885:ASP:HB3	2.09	0.53
1:B:95:THR:HG22	1:B:96:GLN:N	2.24	0.53
1:B:584:PHE:C	1:B:584:PHE:HD1	2.17	0.53
2:S:287:ASN:OD1	2:S:293:ASN:HB3	2.09	0.53
1:A:806:GLU:OE2	1:B:263:MET:HE1	2.10	0.52
1:B:107:TYR:CD1	1:B:213:ILE:HD11	2.44	0.52
2:P:183:MET:HB3	2:P:251:ILE:HD11	1.91	0.52
2:C:4:ILE:HG23	2:C:94:LEU:HB3	1.91	0.52
2:E:263:LEU:HD22	2:E:267:ILE:HD11	1.91	0.52
2:S:273:PHE:O	2:S:278:TRP:HD1	1.92	0.52
2:J:257:LEU:CD1	2:J:300:PRO:HB3	2.34	0.52
1:B:219:ARG:CD	1:B:686:GLU:HG3	2.38	0.52
2:D:338:PRO:O	2:D:339:LEU:HB2	2.09	0.52
2:E:200:ASN:H	2:E:200:ASN:HD22	1.55	0.52
2:J:43:LEU:HD12	2:J:93:VAL:HG22	1.91	0.52
1:A:144:ILE:HG13	1:A:220:LEU:HD21	1.92	0.52
1:A:196:ASN:ND2	1:A:197:VAL:HG23	2.24	0.52
2:P:7:ARG:NH2	2:C:23:ILE:HG22	2.25	0.52
2:R:337:GLY:O	2:R:339:LEU:N	2.43	0.52
2:G:200:ASN:H	2:G:200:ASN:HD22	1.57	0.52
1:A:99:ASP:HB3	1:A:100:ARG:HG2	1.92	0.52
1:A:105:ASP:HB3	1:A:108:TYR:HD2	1.75	0.52
2:G:44:THR:CG2	2:G:46:ARG:HB2	2.39	0.52
1:A:494:TYR:HB3	1:A:497:TYR:CB	2.38	0.52
1:B:23:LEU:HG	1:B:582:ARG:HG2	1.90	0.52
1:B:302:TYR:CE1	1:B:584:PHE:CD2	2.98	0.52
2:C:41:ASN:HD21	2:C:48:VAL:HG23	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:41:ASN:ND2	2:Q:46:ARG:O	2.42	0.52
2:F:257:LEU:CD1	2:F:300:PRO:HB3	2.35	0.52
2:G:185:TYR:O	2:G:248:VAL:HG12	2.10	0.52
2:S:175:PHE:O	2:S:178:ARG:HG3	2.10	0.52
1:A:381:PHE:HE2	1:A:576:LEU:HD11	1.74	0.52
1:B:26:ASP:OD2	1:B:31:LEU:HD21	2.10	0.52
2:C:9:LEU:O	2:C:13:ARG:HG3	2.10	0.52
2:D:50:MET:C	2:D:52:PRO:HD3	2.35	0.52
2:Q:10:THR:HG23	2:Q:102:THR:HG23	1.91	0.52
2:F:16:ALA:HA	2:F:322:VAL:HG21	1.90	0.52
2:F:171:VAL:O	2:F:174:ILE:HG22	2.10	0.52
2:F:315:THR:O	2:F:319:VAL:HG23	2.10	0.52
2:R:185:TYR:O	2:R:248:VAL:HG12	2.10	0.52
2:I:28:ASN:N	2:I:28:ASN:ND2	2.57	0.52
1:A:224:ILE:O	1:A:228:GLN:HG2	2.10	0.52
1:A:382:THR:HG22	1:A:384:GLY:H	1.74	0.52
1:B:526:ARG:O	1:B:530:ILE:HG13	2.09	0.52
1:B:596:ALA:N	1:B:597:PRO:HD2	2.25	0.52
1:B:745:THR:HG22	1:B:746:TYR:N	2.25	0.52
1:A:96:GLN:HE22	1:A:830:VAL:H	1.58	0.52
1:A:359:ILE:HG22	1:A:360:ASP:N	2.25	0.52
1:B:105:ASP:HB3	1:B:108:TYR:HD2	1.74	0.52
1:B:465:TYR:CD2	1:B:539:HIS:HD2	2.27	0.52
2:C:185:TYR:O	2:C:248:VAL:HG12	2.10	0.52
2:Q:186:LEU:O	2:Q:222:ILE:HA	2.09	0.52
2:H:53:THR:H	2:H:57:GLN:HE21	1.56	0.52
2:H:257:LEU:CD1	2:H:300:PRO:HB3	2.39	0.52
1:A:465:TYR:HB3	1:A:467:HIS:HB2	1.92	0.52
1:A:724:GLU:OE2	1:A:860:ARG:HA	2.10	0.52
1:B:171:VAL:O	1:B:174:VAL:HG23	2.09	0.52
1:B:235:SER:HB3	1:B:271:LEU:H	1.75	0.52
2:C:283:THR:HG23	2:C:293:ASN:HB2	1.91	0.52
2:F:2:ASP:HB3	2:F:109:ILE:HG21	1.92	0.52
2:R:41:ASN:HD21	2:R:48:VAL:H	1.57	0.52
1:A:221:GLN:NE2	1:A:877:TYR:OH	2.43	0.52
1:B:605:SER:O	1:B:609:VAL:HG23	2.10	0.52
1:B:697:LEU:O	1:B:698:MET:HB2	2.10	0.52
2:P:49:THR:HG22	2:P:51:ARG:H	1.75	0.52
2:P:50:MET:O	2:P:52:PRO:HD3	2.09	0.52
2:C:200:ASN:ND2	2:C:200:ASN:H	2.08	0.52
2:C:315:THR:O	2:C:319:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:SER:H	2:F:57:GLN:NE2	2.08	0.52
2:G:64:MET:CG	2:G:68:MET:HE3	2.40	0.52
2:I:269:ASN:ND2	2:I:274:ARG:HH22	2.07	0.52
2:J:66:LEU:O	2:J:70:LEU:HG	2.09	0.52
1:A:82:ILE:HG12	1:A:144:ILE:HD13	1.92	0.51
1:A:613:ASP:O	1:A:617:LEU:HD22	2.10	0.51
1:A:637:TRP:CE3	1:A:666:MET:HG2	2.45	0.51
2:I:44:THR:HG22	2:I:46:ARG:HB2	1.93	0.51
1:A:610:MET:HE3	1:A:644:SER:OG	2.10	0.51
1:A:705:MET:CG	1:A:772:VAL:HG22	2.40	0.51
2:R:1:MET:HA	2:R:4:ILE:HD12	1.92	0.51
2:G:253:MET:HE1	2:H:341:ALA:O	2.10	0.51
2:J:2:ASP:HB3	2:J:109:ILE:CG2	2.40	0.51
1:A:65:GLN:C	1:A:67:ILE:H	2.18	0.51
1:A:65:GLN:C	1:A:67:ILE:N	2.67	0.51
1:A:526:ARG:HG3	1:A:527:PHE:N	2.25	0.51
1:B:745:THR:HG22	1:B:747:GLU:H	1.76	0.51
1:B:900:THR:HG22	2:G:22:ARG:NH1	2.21	0.51
2:C:159:ILE:HD11	2:C:245:ILE:HD12	1.93	0.51
2:E:25:LEU:HB2	2:E:30:MET:HE3	1.91	0.51
2:G:271:TYR:CE1	2:G:286:ARG:NH1	2.78	0.51
1:A:96:GLN:NE2	1:A:830:VAL:H	2.08	0.51
1:A:273:VAL:O	1:A:274:ASN:HB2	2.10	0.51
1:A:469:GLN:H	1:A:469:GLN:CD	2.18	0.51
1:B:616:HIS:HB2	1:B:688:TRP:CZ2	2.46	0.51
2:P:10:THR:HG23	2:P:102:THR:HG23	1.91	0.51
2:G:288:ARG:HG3	2:G:288:ARG:NH1	2.25	0.51
1:A:144:ILE:H	1:A:144:ILE:HD12	1.75	0.51
1:A:289:LEU:O	1:A:293:ILE:HG23	2.10	0.51
1:A:705:MET:HA	1:A:848:MET:O	2.11	0.51
1:B:323:PRO:HG3	1:B:512:GLU:HA	1.93	0.51
2:P:8:ALA:HB2	2:P:94:LEU:HD21	1.92	0.51
2:F:337:GLY:O	2:F:339:LEU:N	2.43	0.51
2:G:54:SER:H	2:G:57:GLN:HE21	1.57	0.51
2:S:23:ILE:HD13	2:J:7:ARG:HH21	1.74	0.51
2:I:25:LEU:HD12	2:I:26:GLU:H	1.75	0.51
2:I:270:VAL:HG13	2:I:313:LEU:HB3	1.92	0.51
1:A:540:SER:HB2	1:A:600:GLU:OE2	2.11	0.51
2:D:175:PHE:O	2:D:178:ARG:HG3	2.10	0.51
2:D:257:LEU:CD1	2:D:300:PRO:HB3	2.39	0.51
2:Q:54:SER:H	2:Q:57:GLN:NE2	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:31:GLU:O	2:I:35:ILE:HG13	2.09	0.51
1:A:130:ILE:O	1:A:134:VAL:HG23	2.11	0.51
1:A:424:PRO:O	1:A:425:LEU:HB2	2.11	0.51
1:B:245:ARG:HH22	1:B:471:TYR:HD2	1.59	0.51
1:B:297:LEU:HD13	1:B:298:PRO:O	2.11	0.51
1:B:729:THR:CG2	1:B:731:MET:H	2.23	0.51
1:B:753:ALA:HB1	1:B:815:ILE:HD13	1.91	0.51
2:C:20:GLU:HG2	2:C:21:ALA:N	2.24	0.51
1:A:311:SER:HA	1:A:315:THR:HB	1.92	0.51
1:B:248:ILE:CD1	1:B:892:MET:SD	2.99	0.51
1:B:424:PRO:O	1:B:425:LEU:HB2	2.09	0.51
1:B:577:TRP:HE3	1:B:577:TRP:HA	1.75	0.51
2:C:44:THR:O	2:C:45:LEU:HB2	2.11	0.51
2:Q:96:THR:HG22	2:Q:98:GLU:HB2	1.91	0.51
2:Q:237:THR:HG23	2:Q:239:GLN:H	1.76	0.51
2:F:263:LEU:O	2:F:267:ILE:HG13	2.11	0.51
2:S:28:ASN:O	2:S:32:ILE:HD12	2.11	0.51
2:S:191:ILE:HD12	2:S:242:MET:HB3	1.92	0.51
1:A:170:ASN:O	1:A:173:PRO:HD2	2.11	0.51
1:B:460:ARG:HG3	2:E:51:ARG:CZ	2.41	0.51
2:H:116:THR:HG21	2:H:304:ARG:HB2	1.91	0.51
1:A:370:ARG:O	1:A:401:ALA:HB1	2.11	0.51
1:A:372:VAL:O	1:A:376:VAL:HG23	2.11	0.51
1:B:577:TRP:HA	1:B:577:TRP:CE3	2.46	0.51
2:D:7:ARG:HD2	2:D:94:LEU:O	2.11	0.51
2:E:25:LEU:HD22	2:E:25:LEU:N	2.25	0.51
2:F:22:ARG:C	2:F:23:ILE:HG13	2.35	0.51
2:F:271:TYR:OH	2:F:292:PRO:HG2	2.11	0.51
2:G:44:THR:HG22	2:G:46:ARG:HB2	1.92	0.51
2:S:270:VAL:HG13	2:S:313:LEU:HB3	1.93	0.51
1:A:148:ILE:HG23	1:A:149:PRO:HD2	1.92	0.50
1:A:175:LEU:HD13	1:A:180:ARG:HB2	1.93	0.50
1:B:54:THR:HG23	1:B:55:ARG:N	2.26	0.50
1:B:425:LEU:HD12	1:B:436:CYS:HB3	1.92	0.50
2:P:20:GLU:HG2	2:P:21:ALA:H	1.75	0.50
2:E:288:ARG:HH11	2:E:288:ARG:HG3	1.76	0.50
1:B:378:HIS:HA	1:B:449:TYR:CD2	2.46	0.50
2:P:314:SER:O	2:P:317:ALA:HB3	2.11	0.50
2:Q:34:GLY:O	2:Q:38:ASN:HB2	2.11	0.50
2:I:191:ILE:HD12	2:I:242:MET:HB3	1.93	0.50
2:J:339:LEU:HA	2:J:343:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ASN:O	1:A:535:ASN:HB2	2.12	0.50
1:A:633:PRO:O	1:A:636:PHE:CD1	2.59	0.50
1:B:370:ARG:HH21	1:B:401:ALA:CA	2.23	0.50
2:S:44:THR:O	2:S:45:LEU:HB2	2.10	0.50
2:I:314:SER:O	2:I:317:ALA:HB3	2.10	0.50
1:A:448:GLY:O	1:A:496:CYS:SG	2.66	0.50
2:C:61:MET:O	2:C:64:MET:HB3	2.12	0.50
2:H:338:PRO:O	2:H:339:LEU:HB2	2.11	0.50
2:I:257:LEU:CD1	2:I:300:PRO:HB3	2.40	0.50
2:J:64:MET:CG	2:J:68:MET:HE3	2.41	0.50
1:A:310:SER:HB2	1:A:327:LEU:CD1	2.42	0.50
1:A:461:ASP:HB3	1:A:462:PRO:CD	2.38	0.50
1:A:622:ARG:HG3	2:F:31:GLU:OE1	2.12	0.50
1:B:170:ASN:N	1:B:170:ASN:OD1	2.43	0.50
1:B:264:ILE:N	1:B:264:ILE:HD12	2.27	0.50
1:B:693:ASP:OD2	1:B:695:GLU:HB2	2.12	0.50
2:C:259:GLN:HA	2:D:268:PHE:CD2	2.46	0.50
2:Q:66:LEU:HD23	2:Q:84:TYR:CE2	2.46	0.50
2:F:43:LEU:HD12	2:F:93:VAL:HG22	1.93	0.50
2:R:257:LEU:CD1	2:R:300:PRO:HB3	2.38	0.50
2:G:257:LEU:HD12	2:G:300:PRO:HB3	1.92	0.50
2:G:273:PHE:O	2:G:278:TRP:HD1	1.95	0.50
2:I:16:ALA:HA	2:I:322:VAL:HG21	1.92	0.50
2:J:283:THR:HG23	2:J:293:ASN:HB2	1.93	0.50
1:A:193:GLU:HB3	1:A:204:VAL:HG23	1.94	0.50
1:A:388:THR:OG1	1:A:553:LEU:HD13	2.10	0.50
1:B:454:THR:HG22	1:B:455:ILE:N	2.27	0.50
2:E:288:ARG:HG3	2:E:288:ARG:NH1	2.26	0.50
2:G:43:LEU:HD12	2:G:93:VAL:HG22	1.93	0.50
2:G:159:ILE:HD11	2:G:245:ILE:HB	1.94	0.50
2:I:281:LEU:O	2:I:285:ILE:HG13	2.12	0.50
1:A:454:THR:HG22	1:A:455:ILE:N	2.27	0.50
1:B:82:ILE:HA	1:B:144:ILE:HB	1.94	0.50
1:B:108:TYR:HD1	1:B:698:MET:HE2	1.76	0.50
1:B:357:LEU:HD21	1:B:397:GLN:HG3	1.92	0.50
2:P:317:ALA:O	2:P:320:TYR:HB3	2.12	0.50
2:E:88:MET:O	2:E:91:ILE:HG22	2.12	0.50
2:R:4:ILE:HG23	2:R:94:LEU:HB3	1.92	0.50
1:A:487:THR:O	1:A:488:TYR:CB	2.60	0.50
1:B:265:TRP:CE2	1:B:886:ILE:HD11	2.46	0.50
1:B:497:TYR:CD1	1:B:520:LEU:HD23	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:ARG:CG	1:B:526:ARG:HH11	2.25	0.50
2:P:282:ARG:HD3	2:P:286:ARG:CZ	2.42	0.50
2:D:64:MET:O	2:D:68:MET:HG3	2.11	0.50
2:R:22:ARG:C	2:R:23:ILE:HG13	2.36	0.50
2:R:317:ALA:O	2:R:320:TYR:HB3	2.12	0.50
2:G:50:MET:O	2:G:52:PRO:HD3	2.11	0.50
2:G:54:SER:H	2:G:57:GLN:NE2	2.09	0.50
1:A:300:GLY:HA3	1:A:586:PRO:HA	1.94	0.50
1:A:806:GLU:HA	1:A:811:SER:HA	1.93	0.50
1:B:449:TYR:CD1	1:B:449:TYR:N	2.80	0.50
2:F:69:MET:HG2	2:F:312:LEU:HB3	1.92	0.50
2:S:253:MET:HE1	2:I:341:ALA:O	2.12	0.50
2:S:277:THR:HG23	2:S:329:MET:CE	2.42	0.50
1:A:281:VAL:HB	1:A:284:SER:HB3	1.94	0.49
1:A:303:ILE:HD11	1:A:585:GLU:CB	2.38	0.49
1:A:340:VAL:O	1:A:343:ILE:HG23	2.12	0.49
1:A:392:GLN:HA	1:A:443:PHE:CE2	2.47	0.49
2:P:186:LEU:O	2:P:222:ILE:HA	2.12	0.49
2:E:148:ALA:HA	2:E:164:ASN:ND2	2.27	0.49
2:F:9:LEU:O	2:F:13:ARG:HG3	2.11	0.49
2:F:40:TYR:CE1	2:F:64:MET:HG3	2.46	0.49
2:R:31:GLU:O	2:R:35:ILE:HG13	2.10	0.49
2:H:143:MET:SD	2:H:147:GLN:O	2.70	0.49
2:J:269:ASN:ND2	2:J:274:ARG:HH22	2.06	0.49
2:T:44:THR:HG22	2:T:46:ARG:HG3	1.93	0.49
1:A:96:GLN:NE2	1:A:830:VAL:HG23	2.26	0.49
1:A:271:LEU:O	1:A:273:VAL:HG23	2.11	0.49
1:A:485:PRO:HD2	1:A:901:VAL:HG13	1.95	0.49
1:A:614:MET:HG3	1:A:640:VAL:HG21	1.94	0.49
1:A:900:THR:HG22	1:A:901:VAL:H	1.77	0.49
1:B:724:GLU:OE1	1:B:860:ARG:HB2	2.13	0.49
1:B:882:ARG:CB	1:B:884:MET:HE3	2.38	0.49
2:P:64:MET:O	2:P:68:MET:HG3	2.12	0.49
2:Q:268:PHE:CE2	2:F:259:GLN:HA	2.48	0.49
2:F:307:ILE:HA	2:F:310:LEU:HD12	1.95	0.49
2:G:61:MET:O	2:G:64:MET:HB3	2.11	0.49
2:J:194:PHE:HE1	2:J:204:THR:HG1	1.60	0.49
2:T:61:MET:O	2:T:64:MET:HB3	2.12	0.49
1:A:336:GLN:HE22	1:A:574:ILE:HD13	1.76	0.49
1:A:365:MET:O	1:A:366:ASP:C	2.55	0.49
1:A:614:MET:HE1	1:A:669:TRP:HZ3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:LEU:HD22	1:A:675:LEU:N	2.27	0.49
2:S:288:ARG:HG3	2:S:288:ARG:NH1	2.27	0.49
2:I:307:ILE:HA	2:I:310:LEU:HD12	1.93	0.49
2:T:64:MET:CG	2:T:68:MET:HE3	2.43	0.49
2:T:69:MET:HG2	2:T:312:LEU:HB3	1.93	0.49
1:A:408:TYR:CZ	1:A:410:TYR:HB3	2.47	0.49
1:B:371:MET:HB2	1:B:405:TYR:CD1	2.46	0.49
1:B:869:VAL:O	1:B:870:LEU:C	2.55	0.49
2:G:288:ARG:HG3	2:G:288:ARG:HH11	1.77	0.49
2:J:141:TRP:CZ3	2:J:240:ASN:HB3	2.48	0.49
2:J:288:ARG:HG3	2:J:288:ARG:NH1	2.28	0.49
1:A:343:ILE:HG13	1:A:355:LEU:HD11	1.95	0.49
1:B:730:ASN:HB2	1:B:850:LYS:HA	1.95	0.49
2:J:4:ILE:HG23	2:J:94:LEU:CB	2.41	0.49
2:T:43:LEU:HD12	2:T:93:VAL:HG22	1.92	0.49
1:A:303:ILE:O	1:A:582:ARG:HA	2.12	0.49
1:B:659:ASN:C	1:B:660:PHE:CD1	2.90	0.49
2:F:210:VAL:HG22	2:F:233:VAL:HG13	1.94	0.49
2:F:339:LEU:HA	2:F:343:ILE:HD12	1.95	0.49
2:I:41:ASN:HD21	2:I:48:VAL:H	1.61	0.49
1:A:206:ILE:HD12	1:A:206:ILE:N	2.26	0.49
1:A:382:THR:HG21	1:A:386:ARG:HH21	1.78	0.49
1:A:526:ARG:O	1:A:530:ILE:HG13	2.13	0.49
1:B:623:ARG:NH2	1:B:694:PHE:HE2	2.05	0.49
2:E:69:MET:HG2	2:E:312:LEU:HB3	1.94	0.49
2:R:64:MET:O	2:R:68:MET:HG3	2.12	0.49
1:A:179:HIS:HA	1:A:182:MET:HE2	1.94	0.49
1:B:197:VAL:HG21	1:B:200:ARG:HG3	1.93	0.49
2:Q:7:ARG:NH2	2:Q:97:PRO:HA	2.28	0.49
2:Q:182:MET:SD	2:Q:253:MET:HG3	2.53	0.49
2:I:44:THR:O	2:I:45:LEU:HB2	2.12	0.49
2:T:40:TYR:CE2	2:T:64:MET:HG3	2.48	0.49
1:A:484:ASN:ND2	1:A:486:THR:OG1	2.46	0.49
1:B:54:THR:CG2	1:B:55:ARG:N	2.75	0.49
1:B:497:TYR:O	1:B:501:LEU:HG	2.12	0.49
1:B:802:TYR:CD2	1:B:815:ILE:HD11	2.48	0.49
1:B:873:ARG:NH2	2:G:38:ASN:ND2	2.61	0.49
2:D:53:THR:H	2:D:57:GLN:HE21	1.61	0.49
2:F:237:THR:HG23	2:F:239:GLN:H	1.78	0.49
2:S:7:ARG:NH2	2:I:23:ILE:HG22	2.28	0.49
2:S:268:PHE:CD2	2:J:259:GLN:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:138:PRO:O	2:J:137:GLN:HG3	2.13	0.49
2:I:244:GLN:NE2	2:J:135:THR:HG21	2.28	0.49
1:A:57:VAL:CG2	1:A:301:GLU:HG2	2.42	0.49
1:A:267:LEU:CD2	1:A:270:GLN:H	2.24	0.49
1:B:34:PHE:CE1	1:B:338:ASN:HB3	2.48	0.49
1:B:461:ASP:HA	2:E:22:ARG:O	2.13	0.49
1:B:717:ASP:HB3	1:B:720:ARG:HB2	1.95	0.49
1:B:718:ILE:CD1	1:B:832:PHE:HA	2.43	0.49
2:F:93:VAL:O	2:F:99:ILE:HD12	2.13	0.49
2:G:314:SER:O	2:G:317:ALA:HB3	2.12	0.49
2:H:41:ASN:HD21	2:H:48:VAL:HG23	1.77	0.49
2:H:329:MET:HB2	2:H:329:MET:HE3	1.66	0.49
2:S:101:PHE:HE1	2:I:17:THR:HG22	1.77	0.49
2:T:288:ARG:HG3	2:T:288:ARG:NH1	2.28	0.49
1:A:205:PHE:CE1	1:A:874:PHE:HB3	2.47	0.48
1:A:314:LEU:HD13	1:A:515:TYR:HB2	1.95	0.48
1:A:429:ILE:HD12	1:A:429:ILE:N	2.28	0.48
1:B:205:PHE:N	1:B:205:PHE:CD1	2.80	0.48
2:P:148:ALA:HA	2:P:164:ASN:ND2	2.28	0.48
2:I:4:ILE:HG23	2:I:94:LEU:CB	2.43	0.48
1:A:95:THR:OG1	1:A:102:LEU:HD21	2.13	0.48
1:B:890:LEU:HD22	1:B:890:LEU:N	2.28	0.48
2:Q:41:ASN:HD21	2:Q:48:VAL:H	1.61	0.48
2:F:53:THR:H	2:F:57:GLN:HE22	1.58	0.48
2:R:135:THR:HG21	2:H:244:GLN:NE2	2.28	0.48
2:S:41:ASN:HD21	2:S:48:VAL:H	1.62	0.48
2:I:41:ASN:ND2	2:I:46:ARG:O	2.46	0.48
1:B:520:LEU:O	1:B:523:HIS:HB3	2.13	0.48
1:B:627:VAL:CG2	1:B:777:VAL:HA	2.43	0.48
2:E:53:THR:H	2:E:57:GLN:HE21	1.61	0.48
2:G:283:THR:HG23	2:G:293:ASN:HB2	1.95	0.48
1:A:316:GLN:HG2	1:A:317:ARG:N	2.29	0.48
1:B:264:ILE:HD11	1:B:881:MET:HE2	1.96	0.48
2:Q:39:ARG:HB3	2:Q:39:ARG:HH11	1.79	0.48
2:G:25:LEU:HD23	2:G:30:MET:HE3	1.95	0.48
2:T:7:ARG:O	2:T:11:VAL:HG23	2.14	0.48
1:A:402:LEU:CD1	1:A:425:LEU:HD11	2.42	0.48
1:A:624:PHE:HE2	1:A:694:PHE:CZ	2.32	0.48
1:B:873:ARG:CZ	2:G:39:ARG:HB2	2.43	0.48
2:D:54:SER:H	2:D:57:GLN:HE21	1.60	0.48
2:E:54:SER:H	2:E:57:GLN:NE2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:317:ALA:O	2:F:320:TYR:HB3	2.13	0.48
2:S:2:ASP:HB3	2:S:109:ILE:CG2	2.44	0.48
2:J:271:TYR:CE1	2:J:286:ARG:NH1	2.82	0.48
2:T:271:TYR:OH	2:T:292:PRO:HG2	2.13	0.48
2:Q:188:TRP:CZ2	2:Q:219:ALA:HB2	2.48	0.48
2:R:96:THR:CG2	2:R:98:GLU:HB2	2.44	0.48
2:S:43:LEU:HD12	2:S:93:VAL:HG22	1.96	0.48
2:S:49:THR:HG22	2:S:50:MET:N	2.28	0.48
2:S:281:LEU:O	2:S:285:ILE:HG13	2.13	0.48
1:A:283:ARG:HA	1:A:563:ASN:HD21	1.79	0.48
1:A:410:TYR:HD1	1:A:410:TYR:H	1.61	0.48
1:A:477:ILE:HD11	1:A:524:MET:HE3	1.95	0.48
1:B:646:GLU:HA	1:B:649:LYS:HD3	1.96	0.48
2:Q:178:ARG:HD2	2:Q:178:ARG:H	1.77	0.48
2:F:338:PRO:O	2:F:339:LEU:HB2	2.14	0.48
2:G:194:PHE:HE1	2:G:204:THR:HG1	1.61	0.48
2:I:308:LEU:O	2:I:312:LEU:HD13	2.13	0.48
1:A:93:ILE:CG2	1:A:102:LEU:HG	2.40	0.48
1:A:500:MET:O	1:A:504:LEU:HB2	2.13	0.48
1:B:100:ARG:CD	1:B:724:GLU:HG2	2.43	0.48
1:B:187:LEU:C	1:B:189:GLY:H	2.21	0.48
1:B:281:VAL:HB	1:B:284:SER:HB3	1.95	0.48
1:B:386:ARG:HG3	1:B:456:ASP:OD1	2.14	0.48
2:E:7:ARG:O	2:E:11:VAL:HG23	2.14	0.48
2:F:61:MET:O	2:F:64:MET:HB3	2.14	0.48
2:R:53:THR:H	2:R:57:GLN:NE2	2.11	0.48
2:R:200:ASN:H	2:R:200:ASN:ND2	2.11	0.48
2:R:271:TYR:CD1	2:R:286:ARG:NH1	2.82	0.48
2:G:26:GLU:HG2	2:G:29:VAL:HG23	1.96	0.48
2:G:141:TRP:CZ3	2:G:240:ASN:HB3	2.47	0.48
2:H:171:VAL:O	2:H:174:ILE:HG22	2.13	0.48
2:S:288:ARG:HG3	2:S:288:ARG:HH11	1.79	0.48
1:A:275:PRO:HB3	1:A:467:HIS:CE1	2.49	0.48
1:A:484:ASN:HB3	1:A:487:THR:H	1.78	0.48
1:A:540:SER:C	1:A:542:PHE:H	2.22	0.48
1:B:219:ARG:HG3	1:B:686:GLU:HG3	1.94	0.48
1:B:315:THR:HG22	1:B:317:ARG:H	1.79	0.48
1:B:384:GLY:C	1:B:386:ARG:H	2.22	0.48
1:B:385:GLY:HA2	1:B:443:PHE:O	2.13	0.48
1:B:875:VAL:HG21	2:G:38:ASN:ND2	2.27	0.48
2:Q:30:MET:HE2	2:Q:50:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:281:LEU:O	2:G:285:ILE:HG13	2.14	0.48
2:H:317:ALA:O	2:H:320:TYR:HB3	2.13	0.48
2:S:44:THR:HG22	2:S:46:ARG:HB2	1.95	0.48
2:J:44:THR:O	2:J:45:LEU:HB2	2.14	0.48
2:T:88:MET:O	2:T:91:ILE:HG22	2.13	0.48
1:A:301:GLU:HG3	1:A:587:THR:HG23	1.95	0.48
1:A:345:LEU:HA	1:A:348:MET:HG2	1.96	0.48
1:B:500:MET:HE1	1:B:503:MET:HE2	1.96	0.48
1:B:526:ARG:HH11	1:B:526:ARG:HG3	1.79	0.48
2:D:281:LEU:O	2:D:285:ILE:HG13	2.14	0.48
2:G:317:ALA:O	2:G:320:TYR:HB3	2.14	0.48
2:H:271:TYR:CE1	2:H:286:ARG:NH1	2.82	0.48
2:J:1:MET:SD	2:J:4:ILE:HD12	2.54	0.48
1:A:279:TRP:CZ3	1:A:541:VAL:O	2.62	0.47
1:A:283:ARG:NH2	1:B:490:ILE:HA	2.29	0.47
1:A:761:ALA:O	1:A:765:ILE:HG13	2.14	0.47
1:A:771:TRP:N	1:A:771:TRP:CD1	2.82	0.47
1:B:92:HIS:HD2	1:B:167:GLU:O	1.96	0.47
1:B:721:PHE:C	1:B:723:GLN:N	2.71	0.47
2:C:107:ASN:HD22	2:C:107:ASN:H	1.60	0.47
2:C:217:MET:HE2	2:C:223:ILE:HG23	1.94	0.47
2:R:66:LEU:O	2:R:70:LEU:HG	2.13	0.47
2:S:53:THR:N	2:S:57:GLN:NE2	2.59	0.47
1:A:467:HIS:O	1:A:468:ALA:C	2.57	0.47
1:A:653:ASN:HA	1:A:656:HIS:HB2	1.95	0.47
1:B:492:MET:O	1:B:524:MET:HE1	2.14	0.47
1:B:705:MET:HE3	1:B:798:LEU:HD22	1.97	0.47
2:F:281:LEU:O	2:F:285:ILE:HG13	2.14	0.47
2:G:16:ALA:HA	2:G:322:VAL:HG21	1.95	0.47
2:I:49:THR:HG22	2:I:51:ARG:H	1.78	0.47
2:I:88:MET:O	2:I:91:ILE:HG22	2.13	0.47
2:J:88:MET:O	2:J:91:ILE:HG22	2.14	0.47
2:J:337:GLY:O	2:J:339:LEU:HD12	2.15	0.47
2:T:212:VAL:O	2:T:215:VAL:HG12	2.14	0.47
1:A:900:THR:HG22	1:A:901:VAL:N	2.29	0.47
1:B:446:GLY:O	1:B:452:TRP:HB2	2.14	0.47
1:B:790:PRO:HG2	1:B:795:LEU:CD2	2.33	0.47
2:P:23:ILE:HG22	2:D:7:ARG:NH2	2.29	0.47
2:Q:189:ARG:HD2	2:Q:244:GLN:HE21	1.78	0.47
2:E:212:VAL:O	2:E:215:VAL:HG12	2.14	0.47
2:E:270:VAL:HG13	2:E:313:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:271:TYR:OH	2:H:292:PRO:HG2	2.13	0.47
2:S:7:ARG:NH2	2:S:97:PRO:HA	2.30	0.47
2:S:39:ARG:HB3	2:S:93:VAL:HG13	1.95	0.47
2:I:338:PRO:O	2:I:339:LEU:HB2	2.14	0.47
1:A:314:LEU:HD11	1:A:512:GLU:HA	1.94	0.47
1:A:321:THR:O	1:A:325:ALA:HB2	2.14	0.47
1:A:810:LEU:O	1:A:811:SER:HB3	2.13	0.47
1:B:126:PHE:CZ	1:B:130:ILE:HD11	2.50	0.47
1:B:233:ARG:HG2	1:B:233:ARG:NH1	2.28	0.47
1:B:663:ILE:H	1:B:663:ILE:HD12	1.78	0.47
1:B:873:ARG:HH21	2:G:38:ASN:ND2	2.12	0.47
2:D:189:ARG:HD2	2:D:244:GLN:HE21	1.79	0.47
2:Q:178:ARG:HG2	2:Q:178:ARG:HH11	1.79	0.47
2:H:61:MET:O	2:H:64:MET:HB3	2.15	0.47
2:T:1:MET:HA	2:T:4:ILE:HD12	1.97	0.47
1:A:81:LYS:O	1:A:143:PHE:HA	2.14	0.47
1:A:324:PHE:CE1	1:A:372:VAL:HG22	2.50	0.47
1:A:474:TYR:C	1:A:475:CYS:SG	2.98	0.47
1:A:494:TYR:CG	1:A:497:TYR:HB2	2.49	0.47
1:A:598:LEU:O	1:A:602:VAL:HG23	2.15	0.47
1:B:228:GLN:O	1:B:231:GLU:HG2	2.14	0.47
1:B:393:ASN:O	1:B:397:GLN:HG2	2.14	0.47
1:B:530:ILE:O	1:B:534:ILE:HG13	2.13	0.47
2:P:281:LEU:O	2:P:285:ILE:HG13	2.14	0.47
2:C:138:PRO:O	2:D:137:GLN:HG3	2.15	0.47
2:Q:271:TYR:CE1	2:Q:286:ARG:NH1	2.82	0.47
2:E:337:GLY:H	2:E:338:PRO:HD3	1.78	0.47
2:H:68:MET:CE	2:H:94:LEU:HD11	2.44	0.47
2:I:23:ILE:HD12	2:I:23:ILE:O	2.14	0.47
1:A:349:PHE:N	1:A:350:PRO:HA	2.30	0.47
1:B:526:ARG:HG3	1:B:526:ARG:NH1	2.29	0.47
2:C:66:LEU:O	2:C:70:LEU:HG	2.14	0.47
2:F:54:SER:H	2:F:57:GLN:HE21	1.62	0.47
2:R:25:LEU:HG	2:H:28:ASN:HD21	1.80	0.47
2:I:200:ASN:ND2	2:I:200:ASN:H	2.11	0.47
2:J:7:ARG:O	2:J:11:VAL:HG23	2.15	0.47
1:A:175:LEU:HD12	1:A:175:LEU:O	2.14	0.47
1:A:296:CYS:HG	1:A:538:LEU:HA	1.78	0.47
1:A:332:PRO:HB2	1:A:336:GLN:HG3	1.95	0.47
1:A:623:ARG:HE	2:F:98:GLU:HG2	1.79	0.47
1:A:662:ASN:CG	1:B:485:PRO:HB3	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:ILE:HD12	1:A:842:ILE:N	2.30	0.47
1:B:71:ILE:HG13	1:B:647:ALA:HB1	1.97	0.47
1:B:258:PHE:CD1	1:B:258:PHE:C	2.92	0.47
1:B:421:THR:HB	1:B:426:ASP:OD2	2.15	0.47
1:B:722:ARG:C	1:B:723:GLN:O	2.55	0.47
1:B:755:MET:HG3	2:S:50:MET:HG3	1.95	0.47
1:B:790:PRO:CG	1:B:795:LEU:HD21	2.35	0.47
2:Q:253:MET:HE1	2:E:341:ALA:O	2.13	0.47
2:F:277:THR:HG22	2:F:329:MET:HE1	1.97	0.47
2:R:186:LEU:O	2:R:222:ILE:HA	2.14	0.47
2:G:44:THR:O	2:G:45:LEU:HB2	2.15	0.47
2:H:16:ALA:HA	2:H:322:VAL:HG21	1.97	0.47
2:S:186:LEU:HD21	2:S:225:TRP:CE3	2.49	0.47
2:S:294:MET:SD	2:S:349:VAL:HG23	2.54	0.47
1:A:160:GLU:O	1:A:163:VAL:HG12	2.15	0.47
1:A:356:ASP:O	1:A:394:MET:SD	2.73	0.47
1:A:466:VAL:O	1:A:466:VAL:HG12	2.14	0.47
1:A:471:TYR:CB	1:A:535:ASN:HD21	2.20	0.47
2:P:40:TYR:CE1	2:P:64:MET:HG3	2.49	0.47
2:D:98:GLU:H	2:D:98:GLU:HG3	1.52	0.47
2:D:271:TYR:OH	2:D:292:PRO:HG2	2.15	0.47
2:G:208:VAL:HG13	2:G:234:ARG:O	2.15	0.47
2:S:69:MET:HG2	2:S:312:LEU:HB3	1.95	0.47
2:J:61:MET:O	2:J:64:MET:HB3	2.15	0.47
1:A:354:ILE:HG22	1:A:355:LEU:N	2.29	0.47
1:A:591:GLU:HA	1:A:895:LYS:CE	2.43	0.47
1:A:729:THR:HG21	1:A:731:MET:HB2	1.97	0.47
2:G:141:TRP:HA	2:G:242:MET:SD	2.55	0.47
2:J:200:ASN:H	2:J:200:ASN:HD22	1.61	0.47
1:B:20:GLY:HA3	1:B:304:ALA:O	2.15	0.47
2:D:128:PHE:HB2	2:D:247:VAL:HG11	1.97	0.47
2:E:257:LEU:CD1	2:E:300:PRO:HB3	2.46	0.47
2:S:141:TRP:CZ3	2:S:240:ASN:HB3	2.49	0.47
2:S:271:TYR:CD1	2:S:286:ARG:NH1	2.82	0.47
2:J:189:ARG:HD2	2:J:244:GLN:HE21	1.81	0.47
1:A:90:PHE:HB2	1:A:166:VAL:HG23	1.96	0.46
1:A:274:ASN:O	1:A:277:VAL:HG22	2.15	0.46
1:B:242:LEU:O	1:B:242:LEU:HD23	2.15	0.46
1:B:777:VAL:HG23	1:B:779:ARG:HE	1.80	0.46
2:C:12:MET:HG2	2:C:65:CYS:HB3	1.97	0.46
2:C:269:ASN:ND2	2:C:274:ARG:HH22	2.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:88:MET:O	2:Q:91:ILE:HG22	2.15	0.46
2:E:129:PHE:CE2	2:E:159:ILE:HG23	2.50	0.46
2:E:317:ALA:O	2:E:320:TYR:HB3	2.15	0.46
2:G:96:THR:HG22	2:G:98:GLU:CB	2.41	0.46
2:H:314:SER:O	2:H:317:ALA:HB3	2.16	0.46
2:I:66:LEU:O	2:I:70:LEU:HG	2.16	0.46
2:J:158:MET:HE2	2:J:244:GLN:HB2	1.98	0.46
2:T:41:ASN:ND2	2:T:48:VAL:H	2.12	0.46
1:A:165:GLY:O	1:A:166:VAL:CB	2.63	0.46
1:A:768:ASP:C	1:A:770:ASP:H	2.23	0.46
1:B:368:ALA:O	1:B:372:VAL:HG23	2.15	0.46
1:B:533:ILE:HG22	1:B:538:LEU:HD23	1.97	0.46
2:E:44:THR:CG2	2:E:46:ARG:HB2	2.45	0.46
2:S:26:GLU:HB3	2:S:29:VAL:CG2	2.45	0.46
1:A:314:LEU:HD13	1:A:515:TYR:HB3	1.97	0.46
1:A:724:GLU:HG3	1:A:860:ARG:NE	2.29	0.46
1:B:213:ILE:HD12	1:B:213:ILE:N	2.30	0.46
1:B:425:LEU:O	1:B:437:ASN:HA	2.15	0.46
1:B:460:ARG:HD3	1:B:471:TYR:OH	2.16	0.46
2:C:143:MET:HE1	2:C:162:SER:O	2.15	0.46
2:Q:314:SER:O	2:Q:317:ALA:HB3	2.14	0.46
2:R:4:ILE:HG23	2:R:94:LEU:CB	2.46	0.46
2:H:44:THR:CG2	2:H:46:ARG:HG3	2.43	0.46
2:S:61:MET:O	2:S:64:MET:HB3	2.15	0.46
2:J:67:ASP:HB3	2:J:90:THR:HG21	1.97	0.46
2:T:317:ALA:O	2:T:320:TYR:HB3	2.15	0.46
1:A:223:TYR:CD2	1:A:679:LEU:HD12	2.49	0.46
1:A:454:THR:HG21	1:A:475:CYS:HA	1.96	0.46
1:B:678:SER:OG	1:B:681:LEU:HB2	2.15	0.46
1:B:711:PRO:O	1:B:713:PRO:HD3	2.16	0.46
2:J:44:THR:CG2	2:J:46:ARG:HG3	2.43	0.46
2:J:317:ALA:O	2:J:320:TYR:HB3	2.16	0.46
1:A:662:ASN:OD1	1:B:485:PRO:HB3	2.16	0.46
1:A:754:ASN:HD22	1:B:256:THR:HA	1.79	0.46
1:A:877:TYR:N	1:A:877:TYR:CD1	2.83	0.46
1:B:216:ILE:N	1:B:216:ILE:HD12	2.30	0.46
1:B:315:THR:HG22	1:B:316:GLN:N	2.30	0.46
1:B:584:PHE:HD1	1:B:585:GLU:N	2.14	0.46
1:B:900:THR:HG22	1:B:901:VAL:H	1.80	0.46
2:C:10:THR:HG22	2:C:32:ILE:HD13	1.97	0.46
2:D:277:THR:O	2:D:329:MET:HE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:104:GLU:H	2:S:104:GLU:CD	2.24	0.46
2:S:190:ARG:HA	2:S:243:VAL:HG12	1.97	0.46
2:I:64:MET:O	2:I:68:MET:HG3	2.15	0.46
1:A:284:SER:O	1:A:285:SER:C	2.59	0.46
1:A:672:LEU:HA	1:A:672:LEU:HD23	1.67	0.46
2:C:282:ARG:HD3	2:C:286:ARG:HH11	1.75	0.46
2:Q:180:ASP:HA	2:Q:181:PRO:HD2	1.93	0.46
2:E:190:ARG:HA	2:E:243:VAL:HG12	1.97	0.46
2:F:288:ARG:HG3	2:F:288:ARG:NH1	2.29	0.46
2:H:96:THR:C	2:H:98:GLU:H	2.24	0.46
1:A:297:LEU:HD22	1:A:538:LEU:HD22	1.97	0.46
1:A:418:TYR:HD1	1:A:427:PHE:HB3	1.81	0.46
1:A:823:ILE:HG12	1:A:851:VAL:HG21	1.98	0.46
1:A:853:ILE:HG22	1:A:855:LYS:HB2	1.98	0.46
2:Q:41:ASN:HD21	2:Q:48:VAL:HG23	1.81	0.46
2:H:33:LEU:HB2	2:H:50:MET:HE3	1.98	0.46
2:J:128:PHE:HB2	2:J:247:VAL:HG11	1.97	0.46
1:A:178:GLU:HG2	1:A:179:HIS:N	2.29	0.46
1:B:851:VAL:HG12	1:B:852:PHE:N	2.30	0.46
2:P:50:MET:C	2:P:52:PRO:HD3	2.40	0.46
2:P:277:THR:O	2:P:329:MET:HE1	2.15	0.46
2:E:189:ARG:HG2	2:F:132:THR:O	2.15	0.46
2:R:191:ILE:HA	2:G:135:THR:O	2.16	0.46
2:I:9:LEU:O	2:I:13:ARG:HG3	2.16	0.46
1:A:239:LEU:HG	1:A:271:LEU:HD13	1.98	0.46
1:A:319:THR:HG22	1:A:319:THR:O	2.16	0.46
1:A:321:THR:O	1:A:322:GLY:O	2.34	0.46
1:A:403:ASN:ND2	1:A:425:LEU:N	2.63	0.46
1:A:651:VAL:O	1:A:654:LEU:HG	2.16	0.46
1:A:705:MET:CE	1:A:799:PRO:HD2	2.46	0.46
1:B:312:ILE:H	1:B:312:ILE:HD12	1.80	0.46
1:B:835:THR:HG22	1:B:836:PRO:HD2	1.97	0.46
2:Q:269:ASN:ND2	2:Q:274:ARG:HH22	2.09	0.46
2:F:141:TRP:HA	2:F:242:MET:SD	2.56	0.46
2:H:162:SER:OG	2:H:242:MET:HE3	2.16	0.46
2:T:271:TYR:CD1	2:T:286:ARG:NH1	2.84	0.46
1:A:376:VAL:HG11	1:A:576:LEU:O	2.16	0.46
1:B:95:THR:OG1	1:B:102:LEU:HD21	2.16	0.46
2:Q:135:THR:O	2:F:191:ILE:HA	2.15	0.46
2:G:148:ALA:HA	2:G:164:ASN:HD22	1.81	0.46
2:S:271:TYR:OH	2:S:292:PRO:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:194:PHE:HE1	2:I:204:THR:HG1	1.63	0.46
2:T:271:TYR:CE1	2:T:286:ARG:NH1	2.84	0.46
1:A:596:ALA:O	1:A:600:GLU:HG3	2.16	0.45
1:B:522:PHE:CZ	1:B:583:SER:HB3	2.51	0.45
2:C:10:THR:HG21	2:C:101:PHE:HA	1.97	0.45
2:C:135:THR:HA	2:C:153:VAL:HG23	1.98	0.45
2:R:187:VAL:HG13	2:R:187:VAL:O	2.16	0.45
2:S:124:GLN:OE1	2:S:254:ASP:HB2	2.15	0.45
1:A:659:ASN:O	1:A:660:PHE:HB3	2.14	0.45
1:B:126:PHE:O	1:B:129:THR:HB	2.16	0.45
2:Q:143:MET:HE1	2:Q:162:SER:O	2.17	0.45
2:E:56:ALA:O	2:E:60:GLU:HB2	2.16	0.45
2:E:253:MET:HE1	2:F:341:ALA:O	2.16	0.45
1:A:483:ILE:HD11	1:A:532:GLN:HG3	1.98	0.45
1:A:782:ARG:HD3	1:A:782:ARG:HA	1.71	0.45
1:B:331:THR:CG2	1:B:337:LEU:HB2	2.46	0.45
1:B:724:GLU:C	1:B:726:PHE:N	2.69	0.45
2:Q:222:ILE:C	2:Q:223:ILE:HG13	2.41	0.45
2:E:49:THR:HG22	2:E:51:ARG:H	1.81	0.45
2:R:23:ILE:HD12	2:R:23:ILE:O	2.16	0.45
2:H:187:VAL:HG13	2:H:187:VAL:O	2.17	0.45
2:S:261:PRO:HD3	2:I:265:ALA:HB1	1.99	0.45
2:J:171:VAL:O	2:J:174:ILE:HG22	2.16	0.45
1:A:171:VAL:O	1:A:174:VAL:HG23	2.16	0.45
1:A:697:LEU:O	1:A:698:MET:HB2	2.16	0.45
1:A:754:ASN:HD21	1:B:257:ASP:H	1.62	0.45
1:B:256:THR:C	1:B:258:PHE:H	2.25	0.45
1:B:452:TRP:C	1:B:452:TRP:CD1	2.94	0.45
2:P:257:LEU:HD12	2:P:300:PRO:HB3	1.98	0.45
2:R:17:THR:O	2:R:17:THR:HG22	2.17	0.45
2:R:24:VAL:CG1	2:R:30:MET:HE2	2.41	0.45
2:R:99:ILE:HA	2:R:100:PRO:HD3	1.73	0.45
2:H:194:PHE:HE1	2:H:204:THR:HG1	1.63	0.45
2:S:271:TYR:CE1	2:S:286:ARG:NH1	2.85	0.45
2:I:28:ASN:HD22	2:I:28:ASN:H	1.62	0.45
2:J:41:ASN:HD21	2:J:48:VAL:HG23	1.80	0.45
1:A:161:PRO:HG2	1:A:162:GLU:OE2	2.16	0.45
1:A:460:ARG:HG3	1:A:471:TYR:CZ	2.51	0.45
1:A:700:THR:HG22	1:A:702:GLN:N	2.23	0.45
1:A:729:THR:HG22	1:A:731:MET:N	2.26	0.45
1:B:115:GLY:HA3	1:B:129:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LEU:HD23	1:B:890:LEU:HD12	1.98	0.45
1:B:337:LEU:CD2	1:B:582:ARG:HH12	2.29	0.45
1:B:460:ARG:NH2	1:B:480:ARG:HH12	2.15	0.45
1:B:470:ARG:HD3	1:B:546:ASP:OD1	2.16	0.45
1:B:612:VAL:O	1:B:616:HIS:HD2	1.98	0.45
1:B:746:TYR:HA	1:B:817:TYR:CD2	2.52	0.45
1:B:873:ARG:HG3	2:G:39:ARG:HD3	1.99	0.45
2:D:20:GLU:HG2	2:D:21:ALA:H	1.82	0.45
2:J:244:GLN:O	2:J:244:GLN:HG3	2.16	0.45
2:J:263:LEU:O	2:J:267:ILE:HG13	2.17	0.45
1:A:282:PRO:O	1:A:656:HIS:HE1	1.99	0.45
1:A:738:ILE:HG13	1:A:739:ASP:N	2.31	0.45
1:B:255:LEU:HD22	1:B:255:LEU:HA	1.81	0.45
1:B:409:MET:CG	1:B:413:ARG:HD3	2.45	0.45
2:H:139:GLY:O	2:H:194:PHE:HB2	2.17	0.45
2:S:303:ASP:O	2:S:307:ILE:HG12	2.17	0.45
2:J:54:SER:OG	2:J:57:GLN:HG3	2.16	0.45
1:A:421:THR:HG22	1:A:423:GLU:HB2	1.99	0.45
1:A:425:LEU:HD12	1:A:436:CYS:CB	2.44	0.45
1:B:268:ALA:O	1:B:269:LEU:HD23	2.16	0.45
1:B:826:LEU:HD12	1:B:828:TYR:CE1	2.51	0.45
2:Q:44:THR:O	2:Q:45:LEU:HB2	2.17	0.45
2:E:271:TYR:CE1	2:E:286:ARG:NH1	2.84	0.45
2:F:24:VAL:O	2:F:24:VAL:HG23	2.15	0.45
2:F:200:ASN:ND2	2:F:200:ASN:H	2.15	0.45
2:T:288:ARG:HG3	2:T:288:ARG:HH11	1.82	0.45
1:A:284:SER:HB2	1:A:288:ASN:ND2	2.32	0.45
1:A:526:ARG:CG	1:A:527:PHE:N	2.79	0.45
1:A:662:ASN:ND2	1:B:485:PRO:HB3	2.32	0.45
2:F:189:ARG:HD2	2:F:244:GLN:HE21	1.80	0.45
2:G:96:THR:C	2:G:98:GLU:H	2.25	0.45
1:A:814:THR:OG1	1:B:253:GLU:HG2	2.17	0.45
1:B:414:VAL:HG12	1:B:415:GLN:N	2.32	0.45
2:P:191:ILE:HA	2:C:135:THR:O	2.17	0.45
2:C:69:MET:HG3	2:C:316:LEU:HD22	1.98	0.45
2:Q:200:ASN:ND2	2:Q:200:ASN:H	2.14	0.45
2:R:273:PHE:O	2:R:274:ARG:HB2	2.17	0.45
2:S:269:ASN:ND2	2:S:274:ARG:HH22	2.08	0.45
2:I:186:LEU:HA	2:I:246:GLN:O	2.17	0.45
2:J:186:LEU:O	2:J:222:ILE:HA	2.16	0.45
1:A:129:THR:O	1:A:133:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:PRO:HB2	1:A:336:GLN:CG	2.46	0.45
1:A:367:PRO:O	1:A:371:MET:HG3	2.17	0.45
1:A:565:ASP:HA	1:A:566:PRO:HD2	1.75	0.45
1:A:623:ARG:NH2	1:A:692:ASN:O	2.49	0.45
1:A:710:LEU:HD22	1:A:710:LEU:HA	1.72	0.45
1:B:14:THR:HG22	1:B:15:THR:N	2.32	0.45
1:B:454:THR:HG22	1:B:455:ILE:H	1.82	0.45
1:B:628:LEU:HD23	1:B:628:LEU:H	1.82	0.45
1:B:842:ILE:HD12	1:B:842:ILE:N	2.29	0.45
2:C:171:VAL:O	2:C:174:ILE:HG22	2.17	0.45
2:C:337:GLY:O	2:C:339:LEU:N	2.50	0.45
2:Q:281:LEU:O	2:Q:285:ILE:HG13	2.17	0.45
2:H:37:ILE:HG23	2:H:48:VAL:HB	1.99	0.45
2:I:46:ARG:NH2	2:I:67:ASP:OD2	2.50	0.45
1:A:424:PRO:O	1:A:440:ARG:HD2	2.17	0.44
1:B:193:GLU:HG3	1:B:204:VAL:HB	1.99	0.44
1:B:197:VAL:HG23	1:B:200:ARG:HE	1.81	0.44
1:B:302:TYR:HA	1:B:584:PHE:HA	1.99	0.44
1:B:842:ILE:H	1:B:842:ILE:CD1	2.30	0.44
2:P:61:MET:O	2:P:64:MET:HB3	2.17	0.44
2:C:41:ASN:ND2	2:C:46:ARG:O	2.50	0.44
2:Q:159:ILE:HD11	2:Q:245:ILE:HB	1.98	0.44
2:E:141:TRP:CZ2	2:E:143:MET:HE2	2.52	0.44
2:R:271:TYR:CE1	2:R:286:ARG:NH1	2.86	0.44
2:G:4:ILE:HG23	2:G:94:LEU:HB3	1.98	0.44
2:G:54:SER:OG	2:G:57:GLN:HG3	2.17	0.44
2:G:329:MET:HB2	2:G:329:MET:HE3	1.63	0.44
1:A:376:VAL:CG1	1:A:580:PHE:HB2	2.47	0.44
1:A:403:ASN:HB2	1:A:425:LEU:CD2	2.47	0.44
1:A:616:HIS:CE1	1:A:688:TRP:HB3	2.52	0.44
1:A:724:GLU:CD	1:A:860:ARG:HG3	2.41	0.44
1:B:221:GLN:O	1:B:224:ILE:HG12	2.16	0.44
2:E:61:MET:O	2:E:64:MET:HB3	2.17	0.44
2:F:158:MET:HE3	2:F:245:ILE:O	2.17	0.44
2:R:329:MET:HE3	2:R:329:MET:HB2	1.72	0.44
2:I:151:ALA:CB	2:I:171:VAL:HG13	2.47	0.44
2:J:112:VAL:O	2:J:116:THR:HB	2.17	0.44
1:A:90:PHE:O	1:A:166:VAL:HA	2.17	0.44
1:A:198:ALA:C	1:A:200:ARG:H	2.26	0.44
1:A:343:ILE:O	1:A:347:LEU:HB3	2.17	0.44
1:B:279:TRP:CZ2	1:B:544:LEU:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:PHE:HA	1:B:350:PRO:HD2	1.63	0.44
1:B:724:GLU:C	1:B:726:PHE:H	2.26	0.44
2:P:105:ALA:O	2:P:109:ILE:HG12	2.17	0.44
2:D:217:MET:HE2	2:D:223:ILE:HG23	1.99	0.44
2:D:270:VAL:HB	2:D:286:ARG:NH2	2.32	0.44
2:R:66:LEU:HD23	2:R:84:TYR:CE1	2.53	0.44
2:G:235:ASN:OD1	2:G:237:THR:HG22	2.18	0.44
2:S:104:GLU:O	2:S:108:GLU:HG3	2.17	0.44
2:J:193:ASN:HD21	2:J:201:SER:HB3	1.83	0.44
1:A:117:VAL:HG12	1:A:819:THR:CG2	2.47	0.44
1:A:250:TYR:HD1	1:A:892:MET:O	1.99	0.44
1:A:274:ASN:HA	1:A:275:PRO:HD2	1.67	0.44
1:B:312:ILE:HD12	1:B:312:ILE:N	2.33	0.44
1:B:729:THR:HA	1:B:824:PHE:O	2.17	0.44
2:Q:189:ARG:HH11	2:Q:244:GLN:HE21	1.65	0.44
2:R:259:GLN:HA	2:G:268:PHE:CD2	2.53	0.44
2:R:308:LEU:HD22	2:R:312:LEU:HD22	1.99	0.44
2:R:313:LEU:HD23	2:R:313:LEU:HA	1.85	0.44
2:S:166:GLY:HA2	2:S:235:ASN:O	2.17	0.44
2:S:191:ILE:HA	2:I:135:THR:O	2.18	0.44
2:S:263:LEU:O	2:S:267:ILE:HG13	2.18	0.44
2:I:43:LEU:HD12	2:I:93:VAL:HG22	1.99	0.44
2:J:235:ASN:OD1	2:J:237:THR:HG22	2.17	0.44
1:A:85:VAL:CG1	1:A:163:VAL:HA	2.44	0.44
1:A:596:ALA:N	1:A:597:PRO:HD2	2.33	0.44
1:B:71:ILE:CG1	1:B:647:ALA:HB1	2.47	0.44
1:B:149:PRO:HB2	1:B:160:GLU:HG3	2.00	0.44
1:B:337:LEU:O	1:B:337:LEU:HD22	2.18	0.44
1:B:425:LEU:HB3	1:B:436:CYS:O	2.18	0.44
1:B:427:PHE:HD2	1:B:429:ILE:HG13	1.82	0.44
2:C:10:THR:HG23	2:C:102:THR:HG23	1.99	0.44
2:R:141:TRP:CZ3	2:R:240:ASN:HB3	2.53	0.44
2:H:185:TYR:O	2:H:248:VAL:HG12	2.18	0.44
2:S:91:ILE:HG23	2:S:92:GLY:N	2.33	0.44
2:S:135:THR:HG21	2:J:244:GLN:CD	2.43	0.44
2:I:271:TYR:CD1	2:I:286:ARG:NH1	2.85	0.44
1:A:332:PRO:HG2	1:A:336:GLN:HE21	1.82	0.44
1:A:572:SER:HB2	1:A:575:SER:HB3	1.99	0.44
1:B:146:HIS:CE1	1:B:879:GLY:HA2	2.53	0.44
1:B:289:LEU:HD13	1:B:290:ILE:N	2.32	0.44
1:B:358:LYS:HB3	1:B:571:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ASP:OD1	1:B:437:ASN:HB2	2.18	0.44
1:B:873:ARG:HG2	1:B:874:PHE:H	1.80	0.44
2:S:124:GLN:HB3	2:S:125:PRO:HD2	1.98	0.44
2:S:189:ARG:HD2	2:S:244:GLN:HE21	1.81	0.44
2:I:17:THR:CG2	2:I:25:LEU:HD11	2.47	0.44
2:I:212:VAL:O	2:I:215:VAL:HG12	2.18	0.44
2:J:23:ILE:HD12	2:J:23:ILE:O	2.17	0.44
1:A:522:PHE:O	1:A:525:VAL:HG22	2.17	0.44
1:B:333:THR:HB	1:B:335:GLN:H	1.82	0.44
1:B:723:GLN:C	1:B:725:GLY:H	2.26	0.44
1:B:841:LEU:HD12	1:B:843:ASN:O	2.17	0.44
2:P:171:VAL:O	2:P:174:ILE:HG22	2.18	0.44
2:D:273:PHE:O	2:D:278:TRP:HD1	2.00	0.44
2:F:33:LEU:HB2	2:F:50:MET:HE3	1.99	0.44
2:R:61:MET:O	2:R:64:MET:HB3	2.17	0.44
2:I:50:MET:HE2	2:I:50:MET:HB3	1.82	0.44
2:J:338:PRO:O	2:J:339:LEU:HB2	2.18	0.44
2:T:200:ASN:ND2	2:T:200:ASN:H	2.16	0.44
1:A:111:MET:HA	1:A:114:VAL:CG2	2.47	0.44
1:A:277:VAL:HG12	1:A:674:SER:O	2.17	0.44
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.50	0.44
1:A:465:TYR:HD2	1:A:539:HIS:CD2	2.35	0.44
1:A:888:GLN:O	1:A:891:LYS:HG2	2.17	0.44
1:B:91:ARG:HA	1:B:167:GLU:HB3	2.00	0.44
2:C:53:THR:H	2:C:57:GLN:HE21	1.64	0.44
2:D:26:GLU:HB3	2:D:29:VAL:HG23	1.99	0.44
2:F:295:LEU:HA	2:F:295:LEU:HD23	1.82	0.44
2:S:9:LEU:O	2:S:13:ARG:HG3	2.18	0.44
2:J:281:LEU:O	2:J:285:ILE:HG13	2.18	0.44
1:A:388:THR:CG2	1:A:389:ASN:N	2.81	0.44
1:A:678:SER:O	1:A:682:VAL:HG22	2.18	0.44
1:B:133:LYS:O	1:B:136:PHE:HB3	2.18	0.44
2:P:53:THR:H	2:P:57:GLN:HE21	1.65	0.44
2:R:265:ALA:HB1	2:H:261:PRO:HD3	2.00	0.44
2:G:12:MET:HG2	2:G:65:CYS:HB3	2.00	0.44
1:A:729:THR:CG2	1:A:731:MET:HB2	2.48	0.43
1:B:382:THR:O	1:B:388:THR:HA	2.18	0.43
1:B:466:VAL:HA	1:B:469:GLN:HE21	1.82	0.43
2:P:108:GLU:HG2	2:P:260:TYR:OH	2.18	0.43
2:D:173:GLN:CD	2:D:173:GLN:H	2.26	0.43
2:Q:64:MET:CG	2:Q:68:MET:HE3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:7:ARG:HH21	2:J:23:ILE:HG22	1.82	0.43
1:A:82:ILE:HG12	1:A:144:ILE:CD1	2.48	0.43
1:A:119:THR:HG22	1:A:120:GLU:O	2.18	0.43
1:A:312:ILE:O	1:A:316:GLN:HB2	2.18	0.43
1:A:390:LEU:HD13	1:A:394:MET:HG2	2.00	0.43
1:A:472:ILE:HD12	1:A:472:ILE:N	2.33	0.43
1:A:722:ARG:HG2	1:A:722:ARG:O	2.18	0.43
1:B:465:TYR:O	1:B:466:VAL:CB	2.65	0.43
2:Q:187:VAL:HG13	2:Q:246:GLN:HB3	1.99	0.43
2:H:320:TYR:CD1	2:H:320:TYR:C	2.96	0.43
2:S:182:MET:SD	2:S:253:MET:HG3	2.57	0.43
2:I:7:ARG:O	2:I:11:VAL:HG23	2.18	0.43
2:I:116:THR:HG21	2:I:304:ARG:CB	2.40	0.43
2:J:12:MET:HG2	2:J:65:CYS:HB3	2.00	0.43
1:A:122:GLU:N	1:A:123:PRO:HD3	2.33	0.43
1:A:133:LYS:O	1:A:136:PHE:HB3	2.17	0.43
1:A:405:TYR:O	1:A:408:TYR:HB3	2.18	0.43
1:A:450:ASN:HB2	1:A:494:TYR:OH	2.19	0.43
1:A:451:GLY:O	1:A:452:TRP:HB3	2.17	0.43
1:A:563:ASN:O	1:A:564:ALA:HB2	2.18	0.43
1:A:637:TRP:HZ2	1:B:14:THR:CG2	2.30	0.43
1:A:638:LYS:O	1:A:642:ASN:HB2	2.18	0.43
1:A:835:THR:HG22	1:A:837:ASP:H	1.83	0.43
1:B:36:LEU:HG	1:B:290:ILE:CD1	2.45	0.43
1:B:455:ILE:N	1:B:455:ILE:HD12	2.33	0.43
2:D:204:THR:HG23	2:D:241:ALA:HB1	2.01	0.43
2:Q:264:THR:HA	2:Q:267:ILE:HD12	1.99	0.43
2:E:24:VAL:C	2:E:25:LEU:HD22	2.44	0.43
2:E:53:THR:H	2:E:57:GLN:NE2	2.16	0.43
1:A:725:GLY:O	1:A:726:PHE:C	2.61	0.43
1:A:841:LEU:N	1:A:841:LEU:HD23	2.33	0.43
1:B:475:CYS:HB2	1:B:477:ILE:CD1	2.48	0.43
2:D:50:MET:O	2:D:52:PRO:HD3	2.18	0.43
2:R:105:ALA:O	2:R:109:ILE:HG12	2.17	0.43
2:I:61:MET:O	2:I:64:MET:HB3	2.18	0.43
1:A:102:LEU:N	1:A:102:LEU:HD23	2.34	0.43
1:A:356:ASP:O	1:A:357:LEU:C	2.60	0.43
1:A:494:TYR:CD1	1:A:497:TYR:HB2	2.54	0.43
1:A:628:LEU:HB3	1:A:631:ALA:HB2	2.00	0.43
1:A:631:ALA:O	1:A:632:ARG:HD2	2.18	0.43
1:B:192:ILE:O	1:B:194:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:LEU:O	1:B:538:LEU:HD12	2.18	0.43
1:B:543:SER:O	1:B:544:LEU:HB3	2.18	0.43
2:D:271:TYR:CE1	2:D:286:ARG:NH1	2.86	0.43
2:Q:23:ILE:HG22	2:F:101:PHE:CE2	2.54	0.43
2:R:281:LEU:O	2:R:285:ILE:HG13	2.19	0.43
2:G:189:ARG:HD2	2:G:244:GLN:HE21	1.82	0.43
2:S:154:CYS:SG	2:S:158:MET:HG3	2.58	0.43
2:J:288:ARG:HG3	2:J:288:ARG:HH11	1.83	0.43
1:A:258:PHE:CD1	1:A:258:PHE:C	2.96	0.43
1:A:521:PRO:O	1:A:525:VAL:HG13	2.19	0.43
1:A:622:ARG:HH11	2:F:100:PRO:CB	2.31	0.43
1:B:200:ARG:O	1:B:201:ASP:CB	2.67	0.43
1:B:300:GLY:HA3	1:B:584:PHE:CE1	2.53	0.43
2:C:249:PHE:HZ	2:D:298:ILE:HG23	1.82	0.43
2:Q:260:TYR:O	2:Q:263:LEU:HB2	2.18	0.43
2:F:128:PHE:HB2	2:F:247:VAL:HG11	2.00	0.43
2:I:179:ASN:HB2	2:I:181:PRO:HD3	1.99	0.43
2:I:271:TYR:CE1	2:I:286:ARG:NH1	2.86	0.43
2:T:309:THR:O	2:T:313:LEU:HB2	2.19	0.43
1:A:338:ASN:O	1:A:342:LYS:HG3	2.18	0.43
1:A:474:TYR:C	1:A:475:CYS:HG	2.23	0.43
1:A:694:PHE:HA	1:A:697:LEU:HG	2.01	0.43
2:P:329:MET:HE3	2:P:329:MET:HB2	1.81	0.43
2:C:300:PRO:HA	2:C:301:PRO:HD3	1.91	0.43
2:F:44:THR:O	2:F:45:LEU:HB2	2.17	0.43
2:R:97:PRO:O	2:G:24:VAL:HG22	2.17	0.43
2:H:96:THR:CG2	2:H:98:GLU:HB2	2.40	0.43
2:H:174:ILE:HG23	2:H:175:PHE:CD1	2.54	0.43
2:I:171:VAL:O	2:I:174:ILE:HG22	2.18	0.43
2:J:329:MET:HE3	2:J:329:MET:HB2	1.58	0.43
2:T:44:THR:CG2	2:T:46:ARG:HG3	2.47	0.43
2:T:116:THR:HG21	2:T:304:ARG:CB	2.44	0.43
1:A:58:ASP:N	1:B:317:ARG:HH12	2.13	0.43
1:A:168:PHE:O	1:A:169:LYS:C	2.61	0.43
1:A:343:ILE:HG13	1:A:381:PHE:HE1	1.84	0.43
1:A:346:ALA:HA	1:A:353:ILE:HB	2.00	0.43
1:A:348:MET:HA	1:A:534:ILE:HD11	2.00	0.43
1:B:375:VAL:HG13	1:B:500:MET:SD	2.59	0.43
1:B:399:ASP:OD2	1:B:441:ALA:HB2	2.19	0.43
1:B:587:THR:HG22	1:B:588:HIS:CD2	2.53	0.43
1:B:882:ARG:HB3	1:B:884:MET:CE	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:ASN:H	2:C:200:ASN:HD22	1.65	0.43
2:D:200:ASN:HD22	2:D:200:ASN:H	1.67	0.43
2:D:304:ARG:O	2:D:308:LEU:HB2	2.19	0.43
2:E:46:ARG:NH2	2:E:63:PHE:HB3	2.34	0.43
2:F:191:ILE:HD12	2:F:242:MET:HB3	2.00	0.43
2:R:171:VAL:O	2:R:174:ILE:HG22	2.19	0.43
2:H:18:LEU:N	2:H:18:LEU:CD1	2.82	0.43
2:H:271:TYR:CD1	2:H:286:ARG:NH1	2.87	0.43
1:A:62:PRO:C	1:A:64:VAL:H	2.27	0.43
1:A:425:LEU:HD13	1:A:427:PHE:HE1	1.84	0.43
1:A:427:PHE:CD1	1:A:427:PHE:N	2.79	0.43
1:A:465:TYR:O	1:A:466:VAL:HB	2.19	0.43
1:A:540:SER:C	1:A:542:PHE:N	2.77	0.43
1:A:720:ARG:C	1:A:722:ARG:H	2.25	0.43
1:B:88:THR:O	1:B:89:SER:HB2	2.18	0.43
2:C:50:MET:HE2	2:C:50:MET:HB3	1.82	0.43
2:D:54:SER:H	2:D:57:GLN:NE2	2.16	0.43
2:Q:329:MET:HB2	2:Q:329:MET:HE3	1.53	0.43
2:G:269:ASN:ND2	2:G:274:ARG:HH22	2.10	0.43
2:J:18:LEU:N	2:J:18:LEU:CD1	2.82	0.43
2:J:41:ASN:ND2	2:J:46:ARG:O	2.51	0.43
2:T:22:ARG:H	2:T:22:ARG:HG3	1.61	0.43
1:A:138:ARG:HH21	1:A:680:LYS:HG2	1.84	0.43
1:A:274:ASN:ND2	1:A:276:GLN:HB2	2.33	0.43
1:A:308:ARG:O	1:A:312:ILE:HG22	2.18	0.43
1:B:357:LEU:O	1:B:358:LYS:HB3	2.19	0.43
1:B:475:CYS:HB2	1:B:477:ILE:HD11	2.01	0.43
1:B:604:ALA:O	1:B:607:LEU:HB2	2.19	0.43
2:P:141:TRP:CZ3	2:P:240:ASN:HB3	2.54	0.43
2:P:148:ALA:HA	2:P:164:ASN:HD22	1.84	0.43
2:D:299:PHE:HA	2:D:300:PRO:HD2	1.84	0.43
2:Q:116:THR:HG21	2:Q:304:ARG:CB	2.49	0.43
2:E:148:ALA:HA	2:E:164:ASN:HD22	1.83	0.43
2:R:28:ASN:OD1	2:G:28:ASN:HB2	2.19	0.43
2:H:260:TYR:HA	2:H:261:PRO:HD2	1.77	0.43
2:I:196:MET:HG2	2:I:202:GLN:HB2	2.01	0.43
1:A:279:TRP:CE2	1:A:545:PRO:HD3	2.54	0.42
1:A:425:LEU:HD13	1:A:427:PHE:CE1	2.55	0.42
1:A:774:PHE:HB3	1:A:817:TYR:CD2	2.53	0.42
1:B:82:ILE:HG12	1:B:144:ILE:HG13	2.01	0.42
1:B:128:SER:HA	1:B:131:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:THR:HG21	2:D:304:ARG:HB2	2.01	0.42
2:Q:96:THR:CG2	2:Q:98:GLU:HB2	2.49	0.42
2:E:222:ILE:C	2:E:223:ILE:HG13	2.43	0.42
2:R:244:GLN:CD	2:G:135:THR:HG21	2.43	0.42
2:G:190:ARG:HA	2:G:243:VAL:HG12	2.01	0.42
2:H:3:THR:O	2:H:7:ARG:HG3	2.19	0.42
2:J:295:LEU:HA	2:J:296:PRO:HD3	1.95	0.42
2:T:270:VAL:HB	2:T:286:ARG:NH2	2.33	0.42
1:B:556:LEU:HD13	1:B:556:LEU:C	2.44	0.42
1:B:616:HIS:CG	1:B:688:TRP:HE1	2.37	0.42
1:B:748:ILE:HD13	2:S:53:THR:CG2	2.44	0.42
1:B:778:LEU:O	1:B:779:ARG:HB2	2.19	0.42
2:P:9:LEU:O	2:P:13:ARG:HG3	2.18	0.42
2:P:259:GLN:HA	2:C:268:PHE:CD2	2.55	0.42
2:Q:145:ALA:O	2:Q:146:ALA:HB3	2.19	0.42
2:R:30:MET:SD	2:R:50:MET:HE1	2.59	0.42
2:R:137:GLN:HG3	2:H:138:PRO:O	2.19	0.42
2:G:151:ALA:HA	2:G:161:VAL:HA	2.00	0.42
2:H:37:ILE:HD12	2:H:50:MET:HG2	2.00	0.42
2:H:294:MET:SD	2:H:349:VAL:HG23	2.60	0.42
2:S:219:ALA:O	2:I:133:GLU:HG2	2.19	0.42
2:T:39:ARG:HD3	2:T:39:ARG:HA	1.80	0.42
1:A:58:ASP:N	1:A:58:ASP:OD1	2.52	0.42
1:A:663:ILE:HD12	1:B:485:PRO:HD3	2.01	0.42
1:A:856:ARG:HD3	1:A:859:GLU:OE2	2.19	0.42
1:B:327:LEU:O	1:B:327:LEU:HD13	2.20	0.42
1:B:786:PHE:HB2	1:B:826:LEU:HD23	2.00	0.42
2:P:43:LEU:HD12	2:P:93:VAL:HG22	2.02	0.42
2:Q:341:ALA:O	2:F:253:MET:HE1	2.19	0.42
2:F:21:ALA:O	2:F:23:ILE:N	2.52	0.42
2:R:259:GLN:HA	2:G:268:PHE:CE2	2.53	0.42
2:I:244:GLN:O	2:I:244:GLN:HG3	2.19	0.42
2:T:16:ALA:HA	2:T:322:VAL:HG21	1.99	0.42
2:T:39:ARG:HH12	2:T:98:GLU:CD	2.27	0.42
1:A:326:ILE:HD12	1:A:369:VAL:HA	2.01	0.42
1:A:450:ASN:OD1	1:A:451:GLY:N	2.52	0.42
1:A:705:MET:HE3	1:A:799:PRO:HD2	2.01	0.42
1:B:427:PHE:CD2	1:B:429:ILE:HG13	2.55	0.42
1:B:599:ILE:H	1:B:599:ILE:HG13	1.60	0.42
1:B:735:PRO:HD3	1:B:852:PHE:CZ	2.55	0.42
2:P:300:PRO:HA	2:P:301:PRO:HD3	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:273:PHE:O	2:G:274:ARG:HB2	2.19	0.42
2:I:64:MET:CG	2:I:68:MET:HE3	2.49	0.42
2:I:187:VAL:O	2:I:187:VAL:HG13	2.19	0.42
1:A:313:THR:OG1	1:A:515:TYR:HB2	2.20	0.42
1:A:366:ASP:HA	1:A:367:PRO:HD2	1.84	0.42
1:A:388:THR:HG22	1:A:389:ASN:H	1.83	0.42
1:B:238:TRP:HE3	1:B:239:LEU:CD2	2.26	0.42
1:B:357:LEU:H	1:B:357:LEU:CD2	2.32	0.42
2:C:78:GLY:HA2	2:F:324:ARG:NH1	2.34	0.42
2:C:271:TYR:OH	2:C:292:PRO:HG2	2.19	0.42
2:D:136:PHE:N	2:D:136:PHE:CD1	2.87	0.42
2:D:291:LEU:HD11	2:D:301:PRO:HG2	2.00	0.42
1:A:117:VAL:HG12	1:A:819:THR:HG21	2.00	0.42
1:A:296:CYS:SG	1:A:537:ASP:O	2.77	0.42
1:A:297:LEU:HD13	1:A:298:PRO:HD2	2.01	0.42
1:A:343:ILE:HA	1:A:355:LEU:HD11	2.02	0.42
1:A:355:LEU:HB2	1:A:390:LEU:HD23	2.00	0.42
1:A:374:GLY:O	1:A:378:HIS:HD2	2.02	0.42
1:A:429:ILE:HD12	1:A:429:ILE:H	1.85	0.42
1:A:473:ARG:HG3	1:A:473:ARG:O	2.20	0.42
1:A:482:LEU:HD22	1:A:482:LEU:N	2.34	0.42
1:B:265:TRP:NE1	1:B:886:ILE:HD11	2.34	0.42
1:B:745:THR:CG2	1:B:746:TYR:N	2.82	0.42
1:B:824:PHE:CD1	1:B:824:PHE:C	2.97	0.42
2:P:257:LEU:CD1	2:P:300:PRO:HB3	2.49	0.42
2:R:158:MET:HE3	2:R:245:ILE:O	2.19	0.42
2:H:300:PRO:HA	2:H:301:PRO:HD3	1.86	0.42
2:I:44:THR:HG22	2:I:46:ARG:H	1.85	0.42
2:T:340:THR:OG1	2:T:343:ILE:HG13	2.19	0.42
1:A:465:TYR:CE2	1:A:540:SER:HA	2.55	0.42
1:A:861:VAL:HA	1:A:865:GLN:OE1	2.20	0.42
1:B:452:TRP:CE2	1:B:495:HIS:HE1	2.38	0.42
1:B:533:ILE:HA	1:B:537:ASP:HB2	2.02	0.42
1:B:615:ARG:HA	1:B:670:VAL:CG1	2.49	0.42
1:B:679:LEU:O	1:B:682:VAL:HG22	2.20	0.42
2:C:244:GLN:CD	2:D:135:THR:HG21	2.45	0.42
2:C:281:LEU:O	2:C:285:ILE:HG13	2.19	0.42
2:D:200:ASN:H	2:D:200:ASN:ND2	2.18	0.42
2:Q:7:ARG:HD2	2:Q:94:LEU:O	2.20	0.42
2:R:159:ILE:HD11	2:R:245:ILE:HB	2.02	0.42
2:J:159:ILE:HD11	2:J:245:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:189:ARG:HH11	2:J:244:GLN:HE21	1.68	0.42
1:A:343:ILE:HA	1:A:355:LEU:HD21	2.02	0.42
1:B:43:VAL:HA	1:B:46:VAL:HG23	2.01	0.42
2:P:128:PHE:HB2	2:P:247:VAL:HG11	2.02	0.42
2:D:332:VAL:O	2:D:334:PRO:HD3	2.18	0.42
2:F:288:ARG:HG3	2:F:288:ARG:HH11	1.83	0.42
2:R:41:ASN:ND2	2:R:48:VAL:H	2.17	0.42
2:H:96:THR:HA	2:H:97:PRO:HD2	1.83	0.42
2:H:249:PHE:CD1	2:H:249:PHE:C	2.98	0.42
2:H:307:ILE:HA	2:H:310:LEU:HD12	2.02	0.42
2:S:186:LEU:HD21	2:S:225:TRP:HE3	1.84	0.42
2:S:260:TYR:HA	2:S:261:PRO:HD2	1.78	0.42
2:T:159:ILE:CD1	2:T:245:ILE:HB	2.49	0.42
1:A:376:VAL:HG12	1:A:380:LEU:HD22	2.02	0.42
1:A:474:TYR:H	1:A:531:ASN:ND2	2.17	0.42
1:A:810:LEU:HB2	1:A:812:TYR:CE1	2.55	0.42
1:B:466:VAL:HA	1:B:469:GLN:NE2	2.35	0.42
2:P:24:VAL:HG22	2:D:97:PRO:O	2.20	0.42
2:C:271:TYR:CE1	2:C:286:ARG:NH1	2.88	0.42
2:D:23:ILE:HD12	2:D:23:ILE:O	2.20	0.42
2:E:145:ALA:O	2:E:146:ALA:HB3	2.20	0.42
2:R:253:MET:HE1	2:G:341:ALA:O	2.20	0.42
2:R:295:LEU:HD23	2:R:295:LEU:HA	1.81	0.42
2:S:296:PRO:HA	2:S:297:PRO:HD2	1.87	0.42
2:J:64:MET:HG3	2:J:68:MET:HE3	2.01	0.42
1:A:282:PRO:HB2	1:A:661:ILE:HD12	2.01	0.42
1:A:310:SER:HB2	1:A:327:LEU:HD11	2.02	0.42
1:A:333:THR:O	1:A:334:ALA:C	2.62	0.42
1:A:350:PRO:CD	1:A:351:GLY:H	2.32	0.42
1:B:495:HIS:O	1:B:496:CYS:CB	2.68	0.42
2:P:189:ARG:HG2	2:C:132:THR:O	2.20	0.42
2:Q:337:GLY:O	2:Q:339:LEU:N	2.53	0.42
2:E:283:THR:HG23	2:E:293:ASN:HB2	2.00	0.42
2:S:56:ALA:O	2:S:60:GLU:HB2	2.20	0.42
2:S:249:PHE:CD1	2:S:249:PHE:C	2.98	0.42
2:T:96:THR:HG22	2:T:98:GLU:OE2	2.20	0.42
1:A:89:SER:OG	1:A:209:CYS:HA	2.20	0.41
1:A:151:ARG:HG2	1:A:158:VAL:HB	2.02	0.41
1:A:191:ILE:HG12	1:A:192:ILE:N	2.34	0.41
1:A:664:ARG:HG3	1:B:485:PRO:HG3	2.02	0.41
1:B:403:ASN:HB2	1:B:425:LEU:CD2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:TYR:HA	1:B:826:LEU:O	2.20	0.41
1:B:746:TYR:CA	1:B:817:TYR:HE2	2.27	0.41
1:B:819:THR:HG22	1:B:820:GLU:N	2.33	0.41
1:B:883:ILE:HD12	1:B:883:ILE:N	2.34	0.41
2:H:173:GLN:H	2:H:173:GLN:CD	2.28	0.41
2:S:124:GLN:HE21	2:S:125:PRO:CD	2.34	0.41
2:T:7:ARG:HD2	2:T:94:LEU:O	2.20	0.41
1:A:403:ASN:HD22	1:A:425:LEU:HD22	1.86	0.41
1:A:790:PRO:HB3	1:A:791:PRO:HD2	2.02	0.41
1:B:35:ALA:O	1:B:39:ILE:HG13	2.20	0.41
1:B:569:LEU:HD13	1:B:569:LEU:HA	1.90	0.41
1:B:710:LEU:HB2	1:B:845:THR:HB	2.02	0.41
2:E:129:PHE:O	2:E:156:PRO:HA	2.20	0.41
2:F:329:MET:HB2	2:F:329:MET:HE3	1.76	0.41
2:R:200:ASN:H	2:R:200:ASN:HD22	1.67	0.41
2:H:273:PHE:O	2:H:274:ARG:HB2	2.21	0.41
2:T:107:ASN:HD22	2:T:107:ASN:H	1.68	0.41
1:A:297:LEU:O	1:A:590:ASN:HB3	2.20	0.41
1:B:264:ILE:HD12	1:B:264:ILE:H	1.85	0.41
1:B:333:THR:HG22	1:B:334:ALA:H	1.86	0.41
1:B:376:VAL:O	1:B:379:LEU:HD22	2.20	0.41
1:B:460:ARG:NE	2:E:51:ARG:NH2	2.65	0.41
1:B:873:ARG:HE	1:B:875:VAL:HG22	1.85	0.41
2:P:139:GLY:HA3	2:C:137:GLN:HG3	2.03	0.41
2:Q:7:ARG:NH2	2:E:23:ILE:HG22	2.35	0.41
2:S:44:THR:CG2	2:S:46:ARG:HB2	2.50	0.41
2:J:271:TYR:CD1	2:J:286:ARG:NH1	2.88	0.41
1:A:336:GLN:NE2	1:A:574:ILE:HD13	2.35	0.41
1:A:390:LEU:HD22	1:A:394:MET:HE2	2.02	0.41
1:A:409:MET:SD	1:A:413:ARG:HA	2.61	0.41
1:A:492:MET:O	1:A:520:LEU:HD21	2.20	0.41
1:B:214:TYR:HD2	1:B:872:ARG:HD2	1.84	0.41
1:B:296:CYS:HB3	1:B:538:LEU:HA	2.03	0.41
1:B:636:PHE:CD1	1:B:637:TRP:N	2.88	0.41
2:C:317:ALA:O	2:C:320:TYR:HB3	2.20	0.41
2:C:329:MET:HE3	2:C:329:MET:HB2	1.59	0.41
2:D:288:ARG:NH1	2:D:288:ARG:HG3	2.34	0.41
2:Q:132:THR:O	2:F:189:ARG:HG2	2.21	0.41
2:Q:271:TYR:CD1	2:Q:286:ARG:NH1	2.88	0.41
2:Q:313:LEU:HD23	2:Q:313:LEU:HA	1.88	0.41
2:E:336:PRO:HB3	2:R:330:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:PHE:CE1	2:F:84:TYR:HB2	2.55	0.41
2:F:309:THR:O	2:F:313:LEU:HB2	2.19	0.41
2:S:18:LEU:HD12	2:S:18:LEU:N	2.36	0.41
2:S:49:THR:HG22	2:S:51:ARG:H	1.86	0.41
2:S:139:GLY:HA3	2:I:137:GLN:HG3	2.03	0.41
2:I:44:THR:HG21	2:I:46:ARG:HB2	2.01	0.41
2:J:191:ILE:HD12	2:J:242:MET:HB3	2.02	0.41
2:J:212:VAL:O	2:J:215:VAL:HG12	2.21	0.41
2:T:45:LEU:HD12	2:T:45:LEU:HA	1.79	0.41
1:A:133:LYS:O	1:A:137:ILE:HG12	2.21	0.41
1:A:211:GLU:HB3	1:A:212:PRO:CD	2.49	0.41
1:A:219:ARG:CG	1:A:686:GLU:HG3	2.33	0.41
1:A:358:LYS:HE2	1:A:358:LYS:HB3	1.75	0.41
1:A:641:LEU:O	1:A:649:LYS:HE2	2.19	0.41
1:A:852:PHE:C	1:A:853:ILE:HG13	2.46	0.41
1:B:100:ARG:HA	1:B:862:ARG:O	2.20	0.41
1:B:284:SER:O	1:B:285:SER:C	2.63	0.41
1:B:320:THR:HG22	1:B:321:THR:N	2.36	0.41
1:B:898:ALA:HA	1:B:899:PRO:HD2	1.67	0.41
2:P:271:TYR:CE1	2:P:286:ARG:NH1	2.89	0.41
2:C:273:PHE:O	2:C:278:TRP:HD1	2.04	0.41
2:Q:135:THR:HG21	2:F:244:GLN:CD	2.45	0.41
2:Q:265:ALA:HB1	2:F:261:PRO:HD3	2.02	0.41
2:F:271:TYR:CD1	2:F:286:ARG:NH1	2.89	0.41
2:H:260:TYR:O	2:H:263:LEU:HB2	2.20	0.41
2:S:28:ASN:ND2	2:I:26:GLU:HG3	2.36	0.41
2:I:7:ARG:NH2	2:I:97:PRO:HA	2.36	0.41
1:A:95:THR:HG22	1:A:96:GLN:N	2.36	0.41
1:A:120:GLU:H	1:A:120:GLU:HG2	1.72	0.41
1:A:262:ASP:HB3	1:A:881:MET:HE2	2.02	0.41
1:A:273:VAL:HA	1:A:676:GLN:HG3	2.03	0.41
1:B:157:GLU:HG2	1:B:192:ILE:HD12	2.02	0.41
1:B:158:VAL:HG12	1:B:191:ILE:HG22	2.03	0.41
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.85	0.41
1:B:205:PHE:O	1:B:873:ARG:O	2.38	0.41
1:B:391:THR:HG22	1:B:392:GLN:N	2.36	0.41
2:P:341:ALA:O	2:D:253:MET:HE1	2.19	0.41
2:C:54:SER:H	2:C:57:GLN:HE21	1.67	0.41
2:D:49:THR:HG22	2:D:51:ARG:H	1.84	0.41
2:F:185:TYR:O	2:F:248:VAL:HG12	2.20	0.41
2:R:104:GLU:CD	2:R:104:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:141:TRP:CZ2	2:S:143:MET:HE2	2.56	0.41
2:I:151:ALA:HB2	2:I:171:VAL:HG13	2.03	0.41
2:J:16:ALA:HA	2:J:322:VAL:HG21	2.02	0.41
1:A:61:VAL:HG12	1:B:315:THR:HA	2.02	0.41
1:A:279:TRP:HH2	1:A:542:PHE:C	2.28	0.41
1:A:500:MET:SD	1:A:504:LEU:HD23	2.61	0.41
1:A:734:ALA:HA	1:A:852:PHE:CE1	2.55	0.41
1:A:754:ASN:ND2	1:B:257:ASP:H	2.18	0.41
1:B:168:PHE:CD1	1:B:168:PHE:N	2.89	0.41
1:B:331:THR:HA	1:B:578:PHE:HE2	1.81	0.41
1:B:350:PRO:HB2	1:B:351:GLY:H	1.61	0.41
1:B:543:SER:O	1:B:544:LEU:CB	2.68	0.41
1:B:578:PHE:O	1:B:582:ARG:HD2	2.21	0.41
1:B:592:MET:HA	1:B:592:MET:CE	2.51	0.41
2:P:185:TYR:O	2:P:248:VAL:HG12	2.20	0.41
2:E:143:MET:HE1	2:E:162:SER:O	2.20	0.41
2:E:184:ILE:HG22	2:E:186:LEU:CD1	2.51	0.41
2:G:41:ASN:ND2	2:G:48:VAL:H	2.17	0.41
2:S:185:TYR:O	2:S:248:VAL:HG12	2.19	0.41
2:S:295:LEU:HD23	2:S:295:LEU:HA	1.87	0.41
2:T:9:LEU:O	2:T:13:ARG:HG3	2.21	0.41
1:A:405:TYR:OH	1:A:509:LYS:HD3	2.21	0.41
1:A:622:ARG:NH2	2:F:28:ASN:HD21	2.19	0.41
1:B:28:GLY:N	1:B:29:PRO:HD2	2.35	0.41
1:B:67:ILE:HG23	1:B:68:LEU:N	2.36	0.41
1:B:96:GLN:HG3	1:B:829:ASN:ND2	2.35	0.41
1:B:470:ARG:NH1	1:B:549:PHE:HB2	2.35	0.41
1:B:515:TYR:OH	1:B:519:MET:HE2	2.21	0.41
1:B:521:PRO:O	1:B:525:VAL:HG23	2.21	0.41
2:P:77:VAL:HA	2:P:288:ARG:HD3	2.03	0.41
2:P:283:THR:HG23	2:P:293:ASN:HB2	2.01	0.41
2:Q:25:LEU:HD22	2:Q:25:LEU:N	2.36	0.41
2:E:2:ASP:HB3	2:E:109:ILE:CG2	2.45	0.41
2:E:54:SER:H	2:E:57:GLN:HE21	1.68	0.41
2:E:314:SER:O	2:E:317:ALA:HB3	2.21	0.41
2:F:235:ASN:OD1	2:F:237:THR:HG22	2.20	0.41
2:R:54:SER:OG	2:R:55:LEU:N	2.53	0.41
2:R:311:LEU:HD23	2:R:311:LEU:HA	1.92	0.41
2:G:18:LEU:HD13	2:G:18:LEU:N	2.36	0.41
2:G:249:PHE:CD1	2:G:249:PHE:C	2.99	0.41
2:I:299:PHE:HA	2:I:300:PRO:HD2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HB3	1:A:861:VAL:HG21	2.03	0.41
1:A:348:MET:HE1	1:A:533:ILE:CG2	2.51	0.41
1:A:348:MET:HE2	1:A:538:LEU:HD11	2.03	0.41
1:A:477:ILE:HG22	1:A:479:SER:HB2	2.02	0.41
1:A:664:ARG:HG3	1:B:485:PRO:HG2	2.02	0.41
1:A:723:GLN:C	1:A:725:GLY:H	2.28	0.41
1:A:768:ASP:O	1:A:769:ASP:HB3	2.20	0.41
1:B:65:GLN:OE1	1:B:65:GLN:HA	2.20	0.41
1:B:123:PRO:HG2	1:B:635:HIS:ND1	2.36	0.41
1:B:219:ARG:CG	1:B:686:GLU:HG3	2.51	0.41
1:B:332:PRO:HD2	1:B:336:GLN:CD	2.46	0.41
1:B:371:MET:HG3	1:B:372:VAL:N	2.36	0.41
1:B:608:SER:HB2	1:B:675:LEU:HD12	2.03	0.41
1:B:627:VAL:HG23	1:B:777:VAL:HA	2.01	0.41
2:P:97:PRO:O	2:C:24:VAL:HG22	2.20	0.41
2:P:271:TYR:OH	2:P:292:PRO:HG2	2.21	0.41
2:C:93:VAL:O	2:C:99:ILE:HD12	2.21	0.41
2:D:126:TYR:HB3	2:D:130:LEU:HD22	2.01	0.41
2:D:187:VAL:O	2:D:187:VAL:HG13	2.21	0.41
2:Q:186:LEU:HD12	2:Q:247:VAL:HA	2.02	0.41
2:Q:260:TYR:HA	2:Q:261:PRO:HD2	1.77	0.41
2:E:13:ARG:O	2:E:16:ALA:HB3	2.21	0.41
2:E:295:LEU:HA	2:E:296:PRO:HD3	1.94	0.41
2:F:200:ASN:H	2:F:200:ASN:HD22	1.69	0.41
2:R:191:ILE:HD12	2:R:242:MET:HB3	2.02	0.41
2:S:54:SER:OG	2:S:55:LEU:N	2.54	0.41
2:J:91:ILE:HG23	2:J:92:GLY:N	2.35	0.41
2:J:299:PHE:HA	2:J:300:PRO:HD2	1.86	0.41
2:T:141:TRP:CZ3	2:T:240:ASN:HB3	2.56	0.41
2:T:231:LEU:HA	2:T:231:LEU:HD12	1.82	0.41
1:A:318:ILE:O	1:A:319:THR:CB	2.69	0.41
1:A:434:TYR:CE2	1:A:503:MET:HB2	2.55	0.41
1:A:730:ASN:HB3	1:A:850:LYS:HA	2.03	0.41
1:A:791:PRO:HG2	1:A:794:ILE:HB	2.03	0.41
1:B:114:VAL:HG11	1:B:133:LYS:HA	2.02	0.41
1:B:382:THR:HA	1:B:450:ASN:HB2	2.03	0.41
2:D:329:MET:HE3	2:D:329:MET:HB2	1.82	0.41
2:E:31:GLU:O	2:E:35:ILE:HG13	2.21	0.41
2:E:271:TYR:CD1	2:E:286:ARG:NH1	2.89	0.41
2:T:107:ASN:HD22	2:T:107:ASN:N	2.18	0.41
1:A:314:LEU:C	1:A:316:GLN:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TYR:CD1	1:A:410:TYR:N	2.89	0.40
1:A:614:MET:CG	1:A:640:VAL:HG21	2.50	0.40
1:A:622:ARG:HH12	2:F:100:PRO:HB2	1.85	0.40
1:A:842:ILE:H	1:A:842:ILE:CD1	2.27	0.40
1:B:123:PRO:O	1:B:126:PHE:HB3	2.21	0.40
2:P:151:ALA:HB2	2:P:171:VAL:HG13	2.03	0.40
2:P:158:MET:HE1	2:P:246:GLN:HB2	2.02	0.40
2:E:324:ARG:HH11	2:E:324:ARG:HB3	1.86	0.40
2:E:337:GLY:N	2:E:338:PRO:CD	2.83	0.40
2:S:200:ASN:ND2	2:S:200:ASN:H	2.19	0.40
1:A:355:LEU:HB2	1:A:390:LEU:CD2	2.51	0.40
1:A:625:PRO:O	1:A:629:ILE:HG13	2.21	0.40
1:A:861:VAL:HG12	1:A:862:ARG:N	2.36	0.40
1:B:233:ARG:HG2	1:B:233:ARG:HH11	1.85	0.40
1:B:392:GLN:HA	1:B:443:PHE:HE2	1.85	0.40
2:P:269:ASN:ND2	2:P:274:ARG:HH22	2.10	0.40
2:C:158:MET:HE3	2:C:245:ILE:O	2.20	0.40
2:D:96:THR:HA	2:D:97:PRO:HD2	1.87	0.40
2:G:187:VAL:O	2:G:187:VAL:HG13	2.21	0.40
2:H:179:ASN:HB2	2:H:181:PRO:HD3	2.02	0.40
2:S:274:ARG:HB2	2:S:278:TRP:CD1	2.57	0.40
2:T:23:ILE:HD12	2:T:23:ILE:O	2.21	0.40
2:T:295:LEU:HD23	2:T:295:LEU:HA	1.95	0.40
1:A:58:ASP:CG	1:B:317:ARG:HH22	2.30	0.40
1:A:59:PHE:CB	1:B:317:ARG:HD2	2.36	0.40
1:B:14:THR:CG2	1:B:15:THR:N	2.84	0.40
1:B:39:ILE:O	1:B:42:LYS:HB3	2.20	0.40
1:B:306:ASN:HB2	1:B:309:ILE:HG13	2.02	0.40
1:B:375:VAL:HG12	1:B:379:LEU:HD11	2.03	0.40
1:B:429:ILE:O	1:B:433:GLN:O	2.40	0.40
1:B:545:PRO:HG2	1:B:548:MET:HG3	2.04	0.40
1:B:848:MET:O	1:B:850:LYS:HD2	2.22	0.40
2:D:145:ALA:O	2:D:146:ALA:HB3	2.21	0.40
2:Q:137:GLN:HG3	2:F:138:PRO:O	2.21	0.40
2:Q:143:MET:HE3	2:Q:164:ASN:ND2	2.37	0.40
2:Q:184:ILE:HG22	2:Q:186:LEU:HD13	2.03	0.40
2:G:295:LEU:HD23	2:G:295:LEU:HA	1.91	0.40
2:H:54:SER:OG	2:H:55:LEU:N	2.54	0.40
2:S:7:ARG:HD3	2:S:99:ILE:HB	2.04	0.40
2:S:283:THR:HG23	2:S:293:ASN:HB2	2.02	0.40
2:J:337:GLY:O	2:J:339:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD23	1:A:267:LEU:C	2.46	0.40
1:A:637:TRP:CZ2	1:B:14:THR:HG23	2.57	0.40
1:A:896:LEU:HD23	1:A:896:LEU:HA	1.83	0.40
1:B:122:GLU:HB3	1:B:125:LYS:HB2	2.03	0.40
1:B:271:LEU:O	1:B:273:VAL:N	2.54	0.40
2:C:64:MET:O	2:C:68:MET:HG3	2.21	0.40
2:D:190:ARG:HA	2:D:243:VAL:HG12	2.03	0.40
2:D:271:TYR:CD1	2:D:286:ARG:NH1	2.90	0.40
2:E:41:ASN:HD21	2:E:48:VAL:H	1.69	0.40
2:E:296:PRO:HA	2:E:297:PRO:HD2	1.98	0.40
2:S:298:ILE:H	2:S:298:ILE:HG13	1.65	0.40
2:I:2:ASP:HB3	2:I:109:ILE:CG2	2.50	0.40
2:T:257:LEU:HD23	2:T:264:THR:HG23	2.03	0.40
1:A:148:ILE:HG23	1:A:163:VAL:HG21	2.03	0.40
1:A:337:LEU:HA	1:A:337:LEU:HD23	1.72	0.40
1:A:379:LEU:HD13	1:A:497:TYR:CE1	2.57	0.40
1:A:380:LEU:HD12	1:A:380:LEU:HA	1.89	0.40
1:B:122:GLU:HA	1:B:123:PRO:HD2	1.98	0.40
1:B:242:LEU:CD2	1:B:246:LYS:HD2	2.52	0.40
1:B:531:ASN:N	1:B:531:ASN:HD22	2.20	0.40
1:B:900:THR:HG22	1:B:901:VAL:N	2.36	0.40
2:P:54:SER:H	2:P:57:GLN:HE21	1.70	0.40
2:Q:171:VAL:O	2:Q:174:ILE:HG22	2.22	0.40
2:Q:257:LEU:HD23	2:Q:264:THR:HG23	2.04	0.40
2:E:281:LEU:O	2:E:285:ILE:HG13	2.22	0.40
2:E:342:ALA:O	2:E:345:ARG:HB3	2.22	0.40
2:F:187:VAL:HG13	2:F:246:GLN:HB3	2.04	0.40
2:R:96:THR:HA	2:R:97:PRO:HD3	1.94	0.40
2:R:271:TYR:CD2	2:R:286:ARG:NH2	2.89	0.40
2:H:335:MET:HA	2:H:336:PRO:HD3	1.83	0.40
2:S:116:THR:HG21	2:S:304:ARG:CB	2.51	0.40
2:J:31:GLU:O	2:J:35:ILE:HG13	2.21	0.40
2:J:53:THR:N	2:J:57:GLN:NE2	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	843/901 (94%)	674 (80%)	109 (13%)	60 (7%)	1	10
1	B	881/901 (98%)	715 (81%)	110 (12%)	56 (6%)	1	11
2	C	347/349 (99%)	313 (90%)	29 (8%)	5 (1%)	9	38
2	D	347/349 (99%)	316 (91%)	25 (7%)	6 (2%)	7	35
2	E	347/349 (99%)	296 (85%)	40 (12%)	11 (3%)	3	24
2	F	347/349 (99%)	305 (88%)	34 (10%)	8 (2%)	5	30
2	G	347/349 (99%)	303 (87%)	39 (11%)	5 (1%)	9	38
2	H	347/349 (99%)	302 (87%)	37 (11%)	8 (2%)	5	30
2	I	347/349 (99%)	300 (86%)	40 (12%)	7 (2%)	6	32
2	J	347/349 (99%)	296 (85%)	45 (13%)	6 (2%)	7	35
2	P	347/349 (99%)	312 (90%)	28 (8%)	7 (2%)	6	32
2	Q	347/349 (99%)	300 (86%)	39 (11%)	8 (2%)	5	30
2	R	347/349 (99%)	299 (86%)	39 (11%)	9 (3%)	4	27
2	S	347/349 (99%)	296 (85%)	40 (12%)	11 (3%)	3	24
2	T	347/349 (99%)	306 (88%)	35 (10%)	6 (2%)	7	35
All	All	6235/6339 (98%)	5333 (86%)	689 (11%)	213 (3%)	3	23

All (213) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	THR
1	A	166	VAL
1	A	169	LYS
1	A	175	LEU
1	A	197	VAL
1	A	257	ASP
1	A	274	ASN
1	A	319	THR

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Mol	Chain	Res	Type
1	A	322	GLY
1	A	333	THR
1	A	350	PRO
1	A	357	LEU
1	A	359	ILE
1	A	361	PRO
1	A	430	GLY
1	A	447	THR
1	A	450	ASN
1	A	469	GLN
1	A	490	ILE
1	A	564	ALA
1	A	728	TYR
1	A	863	VAL
1	B	193	GLU
1	B	199	THR
1	B	200	ARG
1	B	207	GLY
1	B	285	SER
1	B	350	PRO
1	B	450	ASN
1	B	466	VAL
1	B	488	TYR
1	B	496	CYS
1	B	508	GLY
1	B	544	LEU
1	B	561	HIS
1	B	673	PRO
1	B	870	LEU
1	B	873	ARG
2	P	54	SER
2	P	338	PRO
2	C	54	SER
2	C	338	PRO
2	C	339	LEU
2	D	54	SER
2	Q	19	GLN
2	Q	22	ARG
2	Q	55	LEU
2	Q	179	ASN
2	E	23	ILE
2	E	336	PRO

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Mol	Chain	Res	Type
2	F	22	ARG
2	F	23	ILE
2	F	54	SER
2	F	338	PRO
2	R	20	GLU
2	R	55	LEU
2	R	338	PRO
2	G	55	LEU
2	H	55	LEU
2	S	55	LEU
2	S	336	PRO
2	S	337	GLY
2	I	338	PRO
2	J	55	LEU
2	T	55	LEU
1	A	63	ASP
1	A	258	PHE
1	A	285	SER
1	A	431	ARG
1	A	466	VAL
1	A	468	ALA
1	A	488	TYR
1	A	707	ARG
1	A	838	SER
1	A	869	VAL
1	A	871	ASN
1	B	328	THR
1	B	441	ALA
1	B	534	ILE
1	B	560	ALA
1	B	584	PHE
1	B	723	GLN
1	B	863	VAL
1	B	899	PRO
2	P	55	LEU
2	P	187	VAL
2	D	172	GLN
2	Q	172	GLN
2	Q	338	PRO
2	E	54	SER
2	E	55	LEU
2	R	187	VAL

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Mol	Chain	Res	Type
2	H	187	VAL
2	I	54	SER
2	I	55	LEU
2	J	187	VAL
2	J	338	PRO
2	T	172	GLN
1	A	58	ASP
1	A	196	ASN
1	A	776	GLY
1	B	201	ASP
1	B	229	LEU
1	B	332	PRO
1	B	357	LEU
1	B	363	GLU
1	B	698	MET
1	B	711	PRO
1	B	862	ARG
1	B	871	ASN
2	P	124	GLN
2	C	55	LEU
2	D	55	LEU
2	E	36	ALA
2	E	339	LEU
2	R	22	ARG
2	H	338	PRO
2	S	19	GLN
2	S	172	GLN
2	S	340	THR
2	I	187	VAL
1	A	211	GLU
1	A	230	GLN
1	A	273	VAL
1	A	365	MET
1	A	452	TRP
1	A	779	ARG
1	A	810	LEU
1	A	862	ARG
1	B	147	ASP
1	B	195	GLY
1	B	333	THR
1	B	433	GLN
1	B	440	ARG

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Mol	Chain	Res	Type
1	B	507	ALA
1	B	632	ARG
1	B	658	HIS
1	B	729	THR
1	B	779	ARG
1	B	900	THR
2	D	274	ARG
2	Q	274	ARG
2	E	172	GLN
2	F	274	ARG
2	R	23	ILE
2	R	339	LEU
2	G	172	GLN
2	G	274	ARG
2	G	339	LEU
2	H	36	ALA
2	H	172	GLN
2	S	187	VAL
2	J	274	ARG
2	T	54	SER
1	A	199	THR
1	A	275	PRO
1	A	334	ALA
1	A	360	ASP
1	A	366	ASP
1	A	414	VAL
1	A	726	PHE
1	B	425	LEU
1	B	434	TYR
1	B	493	THR
1	B	789	ARG
1	B	874	PHE
2	P	274	ARG
2	P	339	LEU
2	E	274	ARG
2	E	338	PRO
2	F	294	MET
2	F	339	LEU
2	R	274	ARG
2	G	187	VAL
2	H	274	ARG
2	S	213	GLY

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Mol	Chain	Res	Type
2	S	274	ARG
2	I	274	ARG
2	I	339	LEU
2	J	172	GLN
2	J	339	LEU
1	A	97	SER
1	A	534	ILE
1	A	660	PHE
1	A	674	SER
1	A	698	MET
1	B	358	LYS
1	B	385	GLY
1	B	663	ILE
2	C	187	VAL
2	D	339	LEU
2	R	54	SER
2	I	294	MET
2	T	187	VAL
2	T	274	ARG
1	B	571	VAL
2	H	261	PRO
2	S	261	PRO
2	S	296	PRO
1	A	349	PHE
1	A	384	GLY
1	B	197	VAL
1	B	661	ILE
2	T	79	PRO
1	A	484	ASN
2	D	187	VAL
2	Q	261	PRO
2	E	301	PRO
2	E	187	VAL
2	F	187	VAL
2	H	97	PRO
1	A	461	ASP
1	B	272	PRO

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	744/793 (94%)	597 (80%)	147 (20%)	1	7
1	B	782/793 (99%)	636 (81%)	146 (19%)	1	9
2	C	284/284 (100%)	263 (93%)	21 (7%)	13	37
2	D	284/284 (100%)	266 (94%)	18 (6%)	16	42
2	E	284/284 (100%)	258 (91%)	26 (9%)	8	32
2	F	284/284 (100%)	259 (91%)	25 (9%)	9	32
2	G	284/284 (100%)	257 (90%)	27 (10%)	8	31
2	H	284/284 (100%)	253 (89%)	31 (11%)	6	26
2	I	284/284 (100%)	261 (92%)	23 (8%)	11	35
2	J	284/284 (100%)	261 (92%)	23 (8%)	11	35
2	P	284/284 (100%)	262 (92%)	22 (8%)	12	37
2	Q	284/284 (100%)	261 (92%)	23 (8%)	11	35
2	R	284/284 (100%)	257 (90%)	27 (10%)	8	31
2	S	284/284 (100%)	261 (92%)	23 (8%)	11	35
2	T	284/284 (100%)	255 (90%)	29 (10%)	7	28
All	All	5218/5278 (99%)	4607 (88%)	611 (12%)	5	24

All (611) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASP
1	A	60	THR
1	A	65	GLN
1	A	67	ILE
1	A	68	LEU
1	A	70	ASP
1	A	74	LEU
1	A	83	VAL
1	A	85	VAL
1	A	89	SER
1	A	94	VAL
1	A	100	ARG
1	A	102	LEU
1	A	111	MET

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Mol	Chain	Res	Type
1	A	113	GLN
1	A	138	ARG
1	A	140	LYS
1	A	144	ILE
1	A	151	ARG
1	A	152	ASP
1	A	157	GLU
1	A	164	LEU
1	A	166	VAL
1	A	170	ASN
1	A	174	VAL
1	A	176	THR
1	A	188	ASP
1	A	199	THR
1	A	202	VAL
1	A	204	VAL
1	A	219	ARG
1	A	220	LEU
1	A	229	LEU
1	A	231	GLU
1	A	255	LEU
1	A	258	PHE
1	A	260	ARG
1	A	261	GLN
1	A	262	ASP
1	A	269	LEU
1	A	279	TRP
1	A	293	ILE
1	A	296	CYS
1	A	297	LEU
1	A	314	LEU
1	A	316	GLN
1	A	321	THR
1	A	327	LEU
1	A	328	THR
1	A	333	THR
1	A	339	ASP
1	A	343	ILE
1	A	345	LEU
1	A	347	LEU
1	A	361	PRO
1	A	363	GLU

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Mol	Chain	Res	Type
1	A	370	ARG
1	A	382	THR
1	A	389	ASN
1	A	393	ASN
1	A	394	MET
1	A	398	LEU
1	A	407	LEU
1	A	410	TYR
1	A	413	ARG
1	A	414	VAL
1	A	416	VAL
1	A	423	GLU
1	A	427	PHE
1	A	438	VAL
1	A	440	ARG
1	A	456	ASP
1	A	461	ASP
1	A	467	HIS
1	A	469	GLN
1	A	470	ARG
1	A	481	GLU
1	A	482	LEU
1	A	483	ILE
1	A	492	MET
1	A	493	THR
1	A	500	MET
1	A	503	MET
1	A	504	LEU
1	A	509	LYS
1	A	510	ASP
1	A	519	MET
1	A	524	MET
1	A	537	ASP
1	A	538	LEU
1	A	544	LEU
1	A	555	ASP
1	A	561	HIS
1	A	565	ASP
1	A	570	ASP
1	A	571	VAL
1	A	574	ILE
1	A	576	LEU

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Mol	Chain	Res	Type
1	A	593	LEU
1	A	617	LEU
1	A	622	ARG
1	A	628	LEU
1	A	634	SER
1	A	636	PHE
1	A	641	LEU
1	A	643	ASP
1	A	648	VAL
1	A	675	LEU
1	A	686	GLU
1	A	692	ASN
1	A	699	LEU
1	A	707	ARG
1	A	708	ASP
1	A	710	LEU
1	A	715	LEU
1	A	720	ARG
1	A	723	GLN
1	A	724	GLU
1	A	738	ILE
1	A	745	THR
1	A	748	ILE
1	A	762	LEU
1	A	763	ARG
1	A	772	VAL
1	A	773	ARG
1	A	780	THR
1	A	787	ASP
1	A	789	ARG
1	A	794	ILE
1	A	804	THR
1	A	810	LEU
1	A	811	SER
1	A	812	TYR
1	A	830	VAL
1	A	831	GLU
1	A	840	VAL
1	A	841	LEU
1	A	842	ILE
1	A	848	MET
1	A	851	VAL

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Mol	Chain	Res	Type
1	A	862	ARG
1	A	863	VAL
1	A	875	VAL
1	A	885	ASP
1	A	892	MET
1	A	894	THR
1	A	901	VAL
1	B	10	GLU
1	B	14	THR
1	B	15	THR
1	B	18	LEU
1	B	30	LEU
1	B	46	VAL
1	B	54	THR
1	B	57	VAL
1	B	58	ASP
1	B	64	VAL
1	B	68	LEU
1	B	74	LEU
1	B	78	GLN
1	B	83	VAL
1	B	85	VAL
1	B	88	THR
1	B	89	SER
1	B	96	GLN
1	B	99	ASP
1	B	101	VAL
1	B	102	LEU
1	B	111	MET
1	B	113	GLN
1	B	119	THR
1	B	140	LYS
1	B	146	HIS
1	B	156	MET
1	B	166	VAL
1	B	170	ASN
1	B	174	VAL
1	B	188	ASP
1	B	197	VAL
1	B	199	THR
1	B	202	VAL
1	B	204	VAL

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Mol	Chain	Res	Type
1	B	205	PHE
1	B	219	ARG
1	B	232	LEU
1	B	233	ARG
1	B	252	GLN
1	B	254	VAL
1	B	255	LEU
1	B	257	ASP
1	B	261	GLN
1	B	263	MET
1	B	271	LEU
1	B	273	VAL
1	B	277	VAL
1	B	283	ARG
1	B	289	LEU
1	B	295	THR
1	B	312	ILE
1	B	333	THR
1	B	336	GLN
1	B	337	LEU
1	B	359	ILE
1	B	363	GLU
1	B	371	MET
1	B	372	VAL
1	B	379	LEU
1	B	380	LEU
1	B	393	ASN
1	B	394	MET
1	B	406	LEU
1	B	409	MET
1	B	426	ASP
1	B	435	ASP
1	B	438	VAL
1	B	445	THR
1	B	447	THR
1	B	449	TYR
1	B	452	TRP
1	B	456	ASP
1	B	467	HIS
1	B	471	TYR
1	B	484	ASN
1	B	492	MET

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Mol	Chain	Res	Type
1	B	493	THR
1	B	500	MET
1	B	504	LEU
1	B	510	ASP
1	B	512	GLU
1	B	526	ARG
1	B	529	ARG
1	B	532	GLN
1	B	537	ASP
1	B	539	HIS
1	B	563	ASN
1	B	573	TRP
1	B	576	LEU
1	B	577	TRP
1	B	591	GLU
1	B	592	MET
1	B	598	LEU
1	B	607	LEU
1	B	620	MET
1	B	621	GLN
1	B	628	LEU
1	B	637	TRP
1	B	641	LEU
1	B	643	ASP
1	B	667	MET
1	B	672	LEU
1	B	673	PRO
1	B	685	GLU
1	B	699	LEU
1	B	700	THR
1	B	701	ASP
1	B	708	ASP
1	B	710	LEU
1	B	714	ARG
1	B	721	PHE
1	B	722	ARG
1	B	723	GLN
1	B	724	GLU
1	B	731	MET
1	B	733	GLU
1	B	737	GLU
1	B	740	ARG

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Mol	Chain	Res	Type
1	B	750	ARG
1	B	751	LEU
1	B	762	LEU
1	B	764	ARG
1	B	780	THR
1	B	794	ILE
1	B	815	ILE
1	B	817	TYR
1	B	830	VAL
1	B	835	THR
1	B	839	LEU
1	B	841	LEU
1	B	847	THR
1	B	850	LYS
1	B	863	VAL
1	B	867	LEU
1	B	869	VAL
1	B	870	LEU
1	B	873	ARG
1	B	875	VAL
1	B	878	LYS
1	B	885	ASP
1	B	889	SER
1	B	891	LYS
1	B	894	THR
1	B	896	LEU
1	B	901	VAL
2	P	19	GLN
2	P	60	GLU
2	P	67	ASP
2	P	108	GLU
2	P	116	THR
2	P	123	ARG
2	P	152	VAL
2	P	153	VAL
2	P	200	ASN
2	P	203	GLN
2	P	221	ARG
2	P	237	THR
2	P	257	LEU
2	P	263	LEU
2	P	270	VAL

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Mol	Chain	Res	Type
2	P	281	LEU
2	P	288	ARG
2	P	291	LEU
2	P	308	LEU
2	P	324	ARG
2	P	333	ASN
2	P	338	PRO
2	C	18	LEU
2	C	19	GLN
2	C	39	ARG
2	C	45	LEU
2	C	50	MET
2	C	69	MET
2	C	108	GLU
2	C	111	ARG
2	C	115	GLU
2	C	116	THR
2	C	152	VAL
2	C	178	ARG
2	C	203	GLN
2	C	237	THR
2	C	263	LEU
2	C	281	LEU
2	C	288	ARG
2	C	308	LEU
2	C	324	ARG
2	C	333	ASN
2	C	338	PRO
2	D	18	LEU
2	D	19	GLN
2	D	60	GLU
2	D	94	LEU
2	D	98	GLU
2	D	108	GLU
2	D	111	ARG
2	D	116	THR
2	D	203	GLN
2	D	237	THR
2	D	263	LEU
2	D	281	LEU
2	D	288	ARG
2	D	291	LEU

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Mol	Chain	Res	Type
2	D	308	LEU
2	D	324	ARG
2	D	333	ASN
2	D	335	MET
2	Q	23	ILE
2	Q	39	ARG
2	Q	58	ARG
2	Q	60	GLU
2	Q	67	ASP
2	Q	94	LEU
2	Q	111	ARG
2	Q	116	THR
2	Q	152	VAL
2	Q	178	ARG
2	Q	186	LEU
2	Q	203	GLN
2	Q	237	THR
2	Q	263	LEU
2	Q	264	THR
2	Q	281	LEU
2	Q	288	ARG
2	Q	308	LEU
2	Q	324	ARG
2	Q	329	MET
2	Q	333	ASN
2	Q	335	MET
2	Q	338	PRO
2	E	18	LEU
2	E	44	THR
2	E	53	THR
2	E	111	ARG
2	E	115	GLU
2	E	116	THR
2	E	152	VAL
2	E	153	VAL
2	E	178	ARG
2	E	186	LEU
2	E	200	ASN
2	E	203	GLN
2	E	221	ARG
2	E	237	THR
2	E	257	LEU

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Mol	Chain	Res	Type
2	E	263	LEU
2	E	270	VAL
2	E	277	THR
2	E	281	LEU
2	E	288	ARG
2	E	291	LEU
2	E	308	LEU
2	E	312	LEU
2	E	324	ARG
2	E	333	ASN
2	E	336	PRO
2	F	18	LEU
2	F	19	GLN
2	F	23	ILE
2	F	45	LEU
2	F	50	MET
2	F	51	ARG
2	F	94	LEU
2	F	98	GLU
2	F	115	GLU
2	F	116	THR
2	F	186	LEU
2	F	203	GLN
2	F	237	THR
2	F	250	TYR
2	F	257	LEU
2	F	263	LEU
2	F	270	VAL
2	F	281	LEU
2	F	288	ARG
2	F	308	LEU
2	F	313	LEU
2	F	329	MET
2	F	333	ASN
2	F	335	MET
2	F	338	PRO
2	R	18	LEU
2	R	19	GLN
2	R	20	GLU
2	R	22	ARG
2	R	30	MET
2	R	33	LEU

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Mol	Chain	Res	Type
2	R	45	LEU
2	R	94	LEU
2	R	98	GLU
2	R	108	GLU
2	R	116	THR
2	R	152	VAL
2	R	153	VAL
2	R	186	LEU
2	R	203	GLN
2	R	221	ARG
2	R	237	THR
2	R	257	LEU
2	R	263	LEU
2	R	270	VAL
2	R	281	LEU
2	R	288	ARG
2	R	308	LEU
2	R	312	LEU
2	R	324	ARG
2	R	333	ASN
2	R	338	PRO
2	G	18	LEU
2	G	19	GLN
2	G	22	ARG
2	G	23	ILE
2	G	25	LEU
2	G	94	LEU
2	G	98	GLU
2	G	111	ARG
2	G	115	GLU
2	G	116	THR
2	G	152	VAL
2	G	186	LEU
2	G	200	ASN
2	G	203	GLN
2	G	221	ARG
2	G	237	THR
2	G	257	LEU
2	G	263	LEU
2	G	270	VAL
2	G	281	LEU
2	G	288	ARG

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Mol	Chain	Res	Type
2	G	291	LEU
2	G	308	LEU
2	G	312	LEU
2	G	313	LEU
2	G	324	ARG
2	G	333	ASN
2	H	18	LEU
2	H	19	GLN
2	H	31	GLU
2	H	43	LEU
2	H	46	ARG
2	H	49	THR
2	H	58	ARG
2	H	60	GLU
2	H	94	LEU
2	H	96	THR
2	H	98	GLU
2	H	108	GLU
2	H	115	GLU
2	H	116	THR
2	H	152	VAL
2	H	153	VAL
2	H	178	ARG
2	H	186	LEU
2	H	203	GLN
2	H	237	THR
2	H	270	VAL
2	H	281	LEU
2	H	288	ARG
2	H	298	ILE
2	H	308	LEU
2	H	313	LEU
2	H	324	ARG
2	H	329	MET
2	H	333	ASN
2	H	338	PRO
2	H	339	LEU
2	S	19	GLN
2	S	38	ASN
2	S	45	LEU
2	S	50	MET
2	S	94	LEU

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Mol	Chain	Res	Type
2	S	96	THR
2	S	115	GLU
2	S	116	THR
2	S	124	GLN
2	S	153	VAL
2	S	186	LEU
2	S	203	GLN
2	S	221	ARG
2	S	237	THR
2	S	263	LEU
2	S	264	THR
2	S	270	VAL
2	S	281	LEU
2	S	288	ARG
2	S	308	LEU
2	S	324	ARG
2	S	333	ASN
2	S	335	MET
2	I	17	THR
2	I	19	GLN
2	I	25	LEU
2	I	28	ASN
2	I	39	ARG
2	I	60	GLU
2	I	67	ASP
2	I	94	LEU
2	I	115	GLU
2	I	116	THR
2	I	152	VAL
2	I	178	ARG
2	I	186	LEU
2	I	203	GLN
2	I	237	THR
2	I	270	VAL
2	I	281	LEU
2	I	288	ARG
2	I	291	LEU
2	I	308	LEU
2	I	324	ARG
2	I	333	ASN
2	I	338	PRO
2	J	18	LEU

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Mol	Chain	Res	Type
2	J	19	GLN
2	J	26	GLU
2	J	94	LEU
2	J	115	GLU
2	J	116	THR
2	J	152	VAL
2	J	186	LEU
2	J	200	ASN
2	J	203	GLN
2	J	221	ARG
2	J	237	THR
2	J	250	TYR
2	J	264	THR
2	J	270	VAL
2	J	281	LEU
2	J	288	ARG
2	J	291	LEU
2	J	308	LEU
2	J	324	ARG
2	J	329	MET
2	J	333	ASN
2	J	338	PRO
2	T	18	LEU
2	T	19	GLN
2	T	22	ARG
2	T	45	LEU
2	T	67	ASP
2	T	94	LEU
2	T	96	THR
2	T	98	GLU
2	T	108	GLU
2	T	115	GLU
2	T	116	THR
2	T	152	VAL
2	T	153	VAL
2	T	178	ARG
2	T	186	LEU
2	T	203	GLN
2	T	237	THR
2	T	263	LEU
2	T	264	THR
2	T	270	VAL

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Mol	Chain	Res	Type
2	T	281	LEU
2	T	288	ARG
2	T	291	LEU
2	T	308	LEU
2	T	313	LEU
2	T	324	ARG
2	T	333	ASN
2	T	335	MET
2	T	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (182) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	78	GLN
1	A	96	GLN
1	A	179	HIS
1	A	221	GLN
1	A	261	GLN
1	A	292	ASN
1	A	336	GLN
1	A	378	HIS
1	A	389	ASN
1	A	393	ASN
1	A	403	ASN
1	A	415	GLN
1	A	432	ASN
1	A	469	GLN
1	A	484	ASN
1	A	495	HIS
1	A	531	ASN
1	A	561	HIS
1	A	563	ASN
1	A	616	HIS
1	A	621	GLN
1	A	656	HIS
1	A	754	ASN
1	A	757	GLN
1	A	829	ASN
1	B	78	GLN
1	B	153	HIS
1	B	316	GLN

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Mol	Chain	Res	Type
1	B	389	ASN
1	B	403	ASN
1	B	411	ASN
1	B	484	ASN
1	B	495	HIS
1	B	531	ASN
1	B	532	GLN
1	B	539	HIS
1	B	562	GLN
1	B	588	HIS
1	B	616	HIS
1	B	656	HIS
1	B	658	HIS
1	B	692	ASN
1	B	829	ASN
1	B	834	ASN
1	B	854	ASN
2	P	41	ASN
2	P	57	GLN
2	P	59	ASN
2	P	124	GLN
2	P	147	GLN
2	P	164	ASN
2	P	193	ASN
2	P	200	ASN
2	P	203	GLN
2	P	244	GLN
2	P	269	ASN
2	C	19	GLN
2	C	28	ASN
2	C	41	ASN
2	C	57	GLN
2	C	76	ASN
2	C	124	GLN
2	C	164	ASN
2	C	193	ASN
2	C	200	ASN
2	C	203	GLN
2	C	205	GLN
2	C	244	GLN
2	C	269	ASN
2	D	41	ASN

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Mol	Chain	Res	Type
2	D	57	GLN
2	D	147	GLN
2	D	164	ASN
2	D	179	ASN
2	D	200	ASN
2	D	203	GLN
2	D	205	GLN
2	D	244	GLN
2	D	269	ASN
2	D	276	HIS
2	Q	19	GLN
2	Q	28	ASN
2	Q	41	ASN
2	Q	57	GLN
2	Q	164	ASN
2	Q	179	ASN
2	Q	193	ASN
2	Q	200	ASN
2	Q	244	GLN
2	Q	269	ASN
2	E	41	ASN
2	E	57	GLN
2	E	86	GLN
2	E	164	ASN
2	E	200	ASN
2	E	205	GLN
2	E	244	GLN
2	E	269	ASN
2	E	330	HIS
2	F	28	ASN
2	F	38	ASN
2	F	41	ASN
2	F	57	GLN
2	F	164	ASN
2	F	193	ASN
2	F	200	ASN
2	F	203	GLN
2	F	244	GLN
2	F	269	ASN
2	R	28	ASN
2	R	38	ASN
2	R	41	ASN

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Mol	Chain	Res	Type
2	R	57	GLN
2	R	147	GLN
2	R	200	ASN
2	R	244	GLN
2	R	269	ASN
2	R	330	HIS
2	G	19	GLN
2	G	28	ASN
2	G	38	ASN
2	G	41	ASN
2	G	57	GLN
2	G	76	ASN
2	G	164	ASN
2	G	193	ASN
2	G	200	ASN
2	G	205	GLN
2	G	244	GLN
2	G	269	ASN
2	H	19	GLN
2	H	28	ASN
2	H	38	ASN
2	H	41	ASN
2	H	57	GLN
2	H	147	GLN
2	H	164	ASN
2	H	179	ASN
2	H	193	ASN
2	H	203	GLN
2	H	205	GLN
2	H	240	ASN
2	H	244	GLN
2	H	269	ASN
2	S	41	ASN
2	S	57	GLN
2	S	124	GLN
2	S	205	GLN
2	S	244	GLN
2	S	269	ASN
2	I	19	GLN
2	I	28	ASN
2	I	41	ASN
2	I	57	GLN

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Mol	Chain	Res	Type
2	I	76	ASN
2	I	147	GLN
2	I	164	ASN
2	I	193	ASN
2	I	200	ASN
2	I	203	GLN
2	I	240	ASN
2	I	244	GLN
2	I	269	ASN
2	J	28	ASN
2	J	38	ASN
2	J	41	ASN
2	J	57	GLN
2	J	76	ASN
2	J	147	GLN
2	J	164	ASN
2	J	200	ASN
2	J	244	GLN
2	J	269	ASN
2	J	330	HIS
2	T	41	ASN
2	T	57	GLN
2	T	107	ASN
2	T	164	ASN
2	T	200	ASN
2	T	244	GLN
2	T	269	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	845/901 (93%)	-1.26	0 100 100	0, 31, 86, 139	0
1	B	885/901 (98%)	-1.29	0 100 100	0, 24, 72, 141	0
2	C	349/349 (100%)	-0.95	0 100 100	18, 90, 152, 172	0
2	D	349/349 (100%)	-0.96	0 100 100	32, 102, 161, 182	0
2	E	349/349 (100%)	-1.08	0 100 100	1, 64, 122, 151	0
2	F	349/349 (100%)	-1.13	0 100 100	2, 61, 123, 151	0
2	G	349/349 (100%)	-1.15	0 100 100	0, 52, 107, 140	0
2	H	349/349 (100%)	-1.16	0 100 100	1, 51, 113, 148	0
2	I	349/349 (100%)	-1.16	0 100 100	0, 54, 120, 147	0
2	J	349/349 (100%)	-1.15	0 100 100	1, 56, 119, 142	0
2	P	349/349 (100%)	-0.86	0 100 100	35, 108, 162, 181	0
2	Q	349/349 (100%)	-1.11	0 100 100	1, 60, 125, 151	0
2	R	349/349 (100%)	-1.10	0 100 100	1, 57, 118, 146	0
2	S	349/349 (100%)	-1.19	0 100 100	0, 47, 116, 143	0
2	T	349/349 (100%)	-1.23	0 100 100	1, 48, 99, 134	0
All	All	6267/6339 (98%)	-1.14	0 100 100	0, 52, 135, 182	0

There are no RSRZ outliers to report.

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.