Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:52 AM GMT

PDB ID	:	2BTV
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

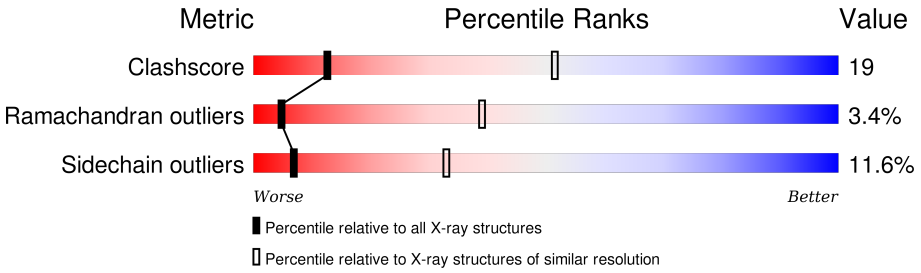
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	901	37% 42% 13% • 6%
1	B	901	45% 41% 12% ••
2	C	349	69% 29% •
2	D	349	74% 23% •
2	E	349	67% 28% 5%
2	F	349	64% 30% 5%
2	G	349	66% 29% •

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Mol	Chain	Length	Quality of chain
2	H	349	69% 27%
2	I	349	64% 31% 5%
2	J	349	66% 30%
2	P	349	69% 27%
2	Q	349	65% 30% 5%
2	R	349	64% 30% 5%
2	S	349	61% 35% 5%
2	T	349	68% 27% 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

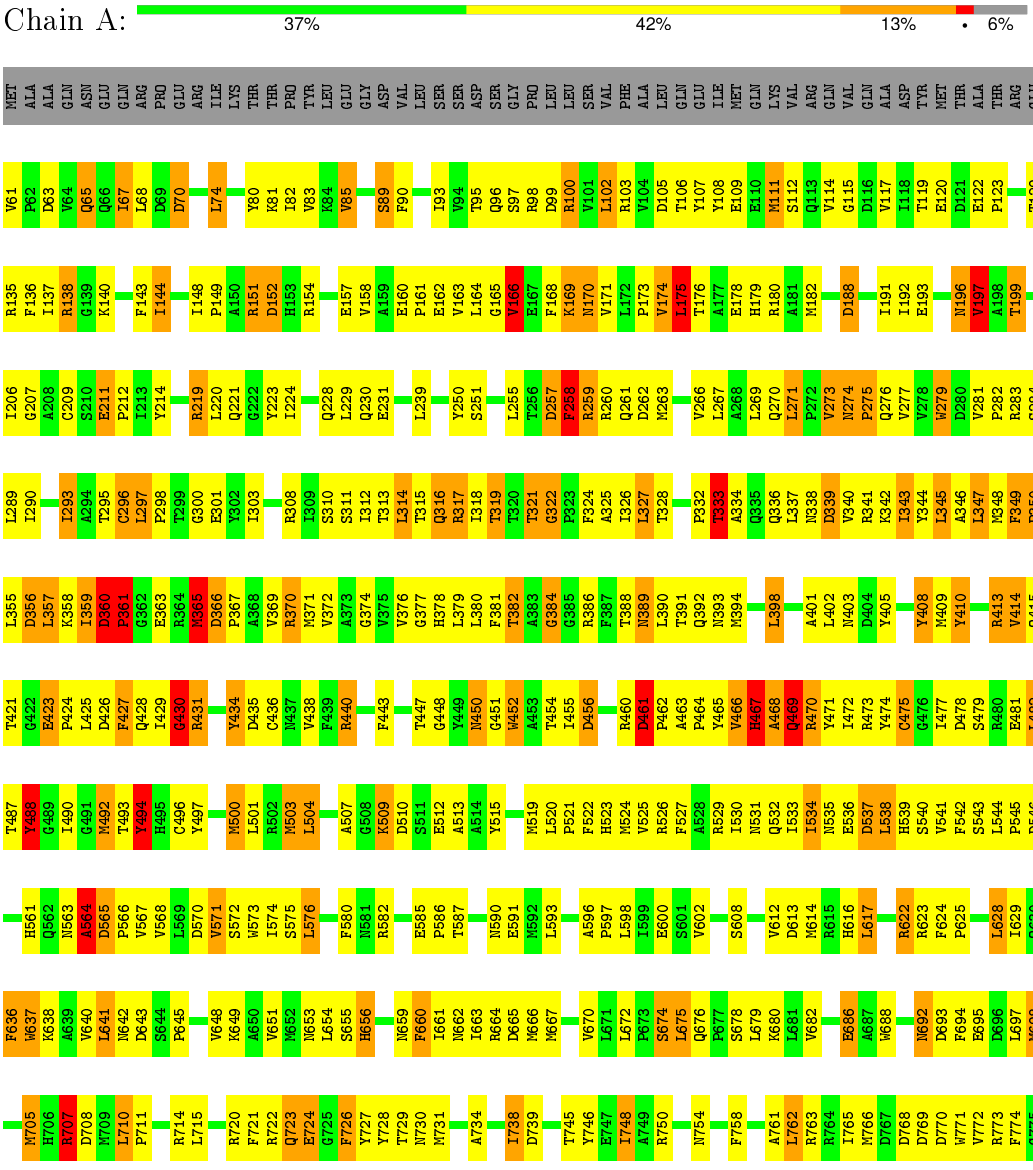
3 Residue-property plots (i)

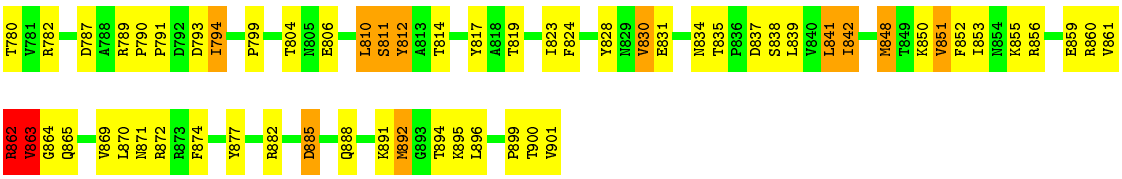
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

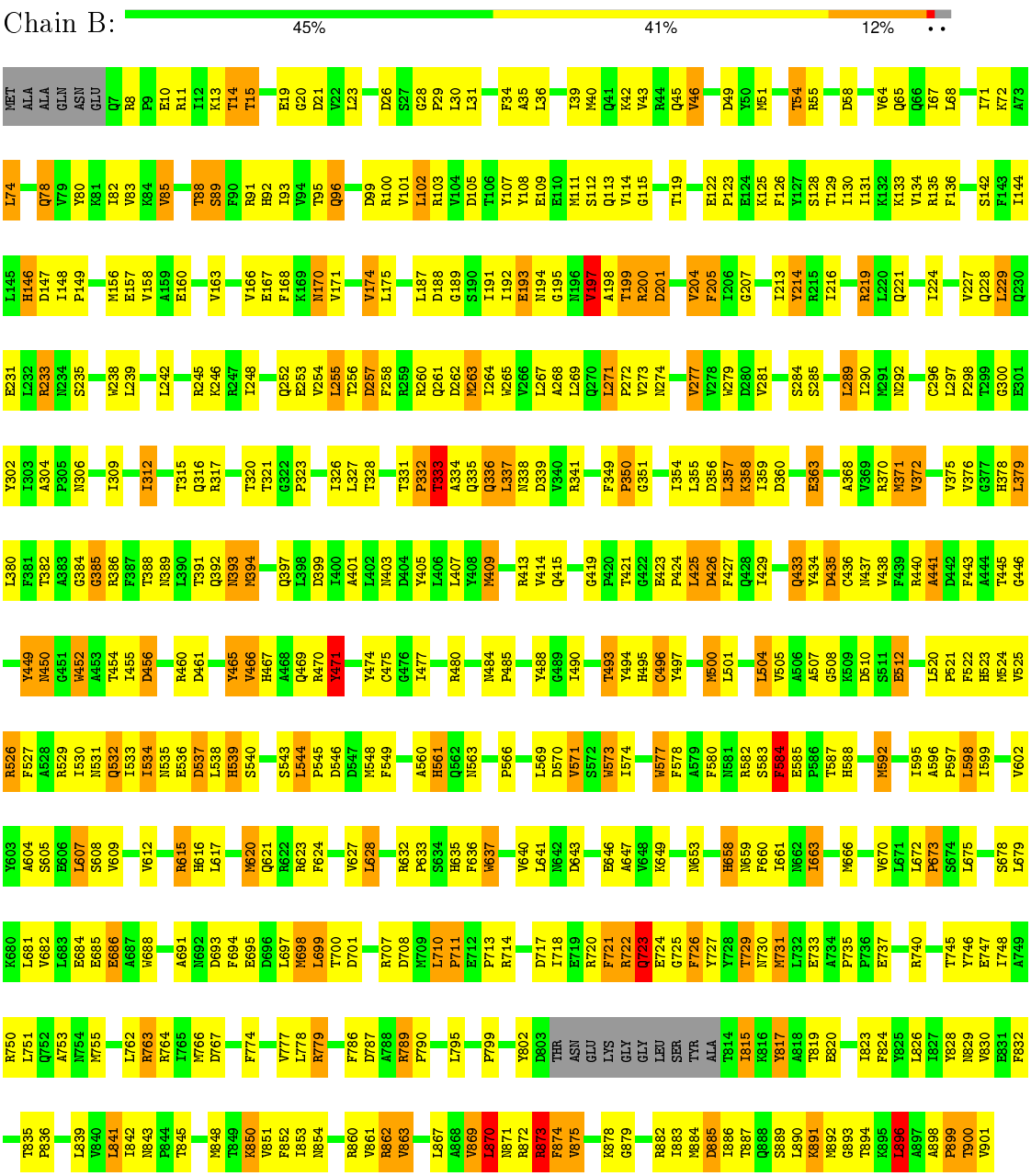
Note EDS failed to run properly.

- Molecule 1: PROTEIN (VP3 CORE PROTEIN)

Chain A:





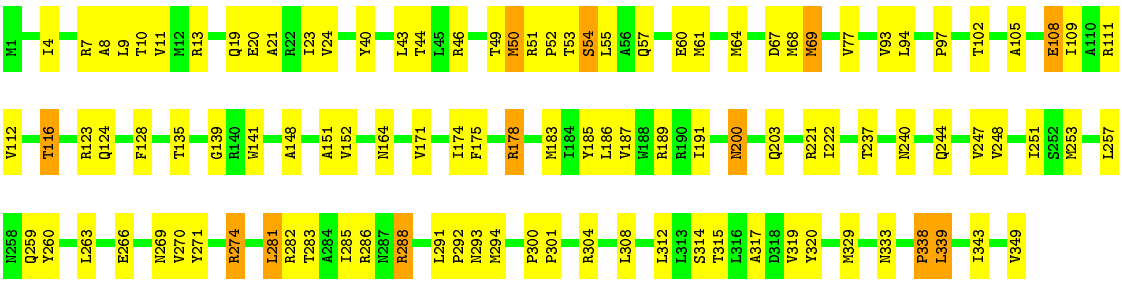


• Molecule 1: PROTEIN (VP3 CORE PROTEIN)

Chain B:

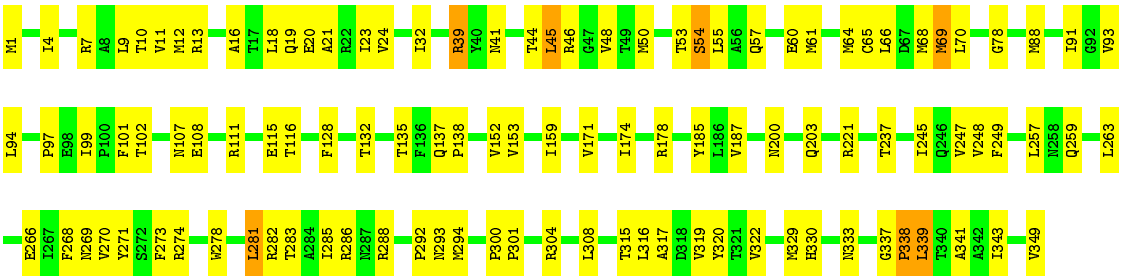
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain P:



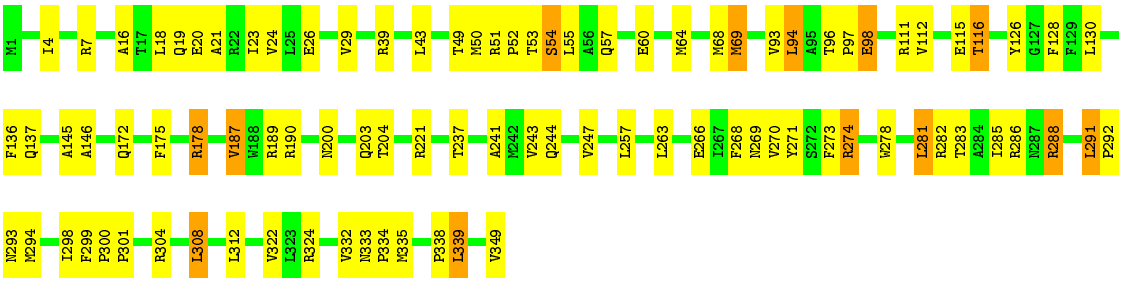
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain C:



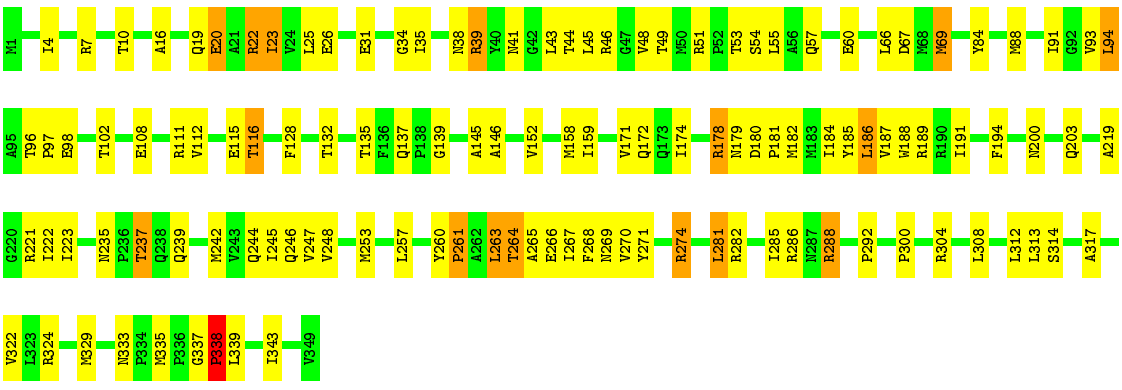
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain D:



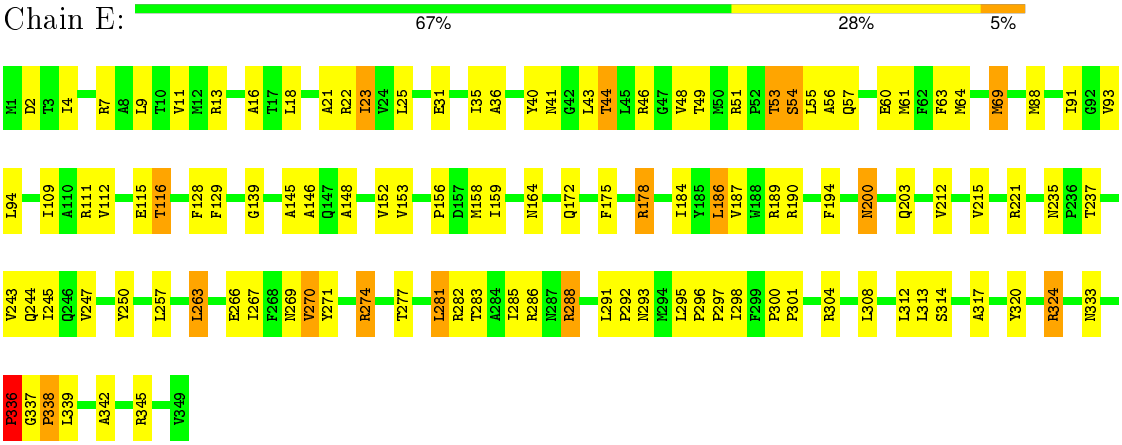
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain Q:



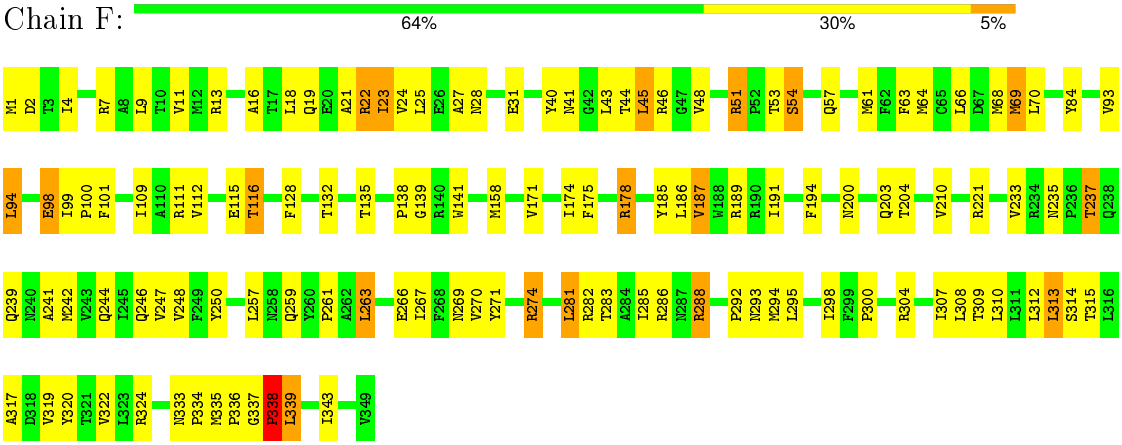
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain E:



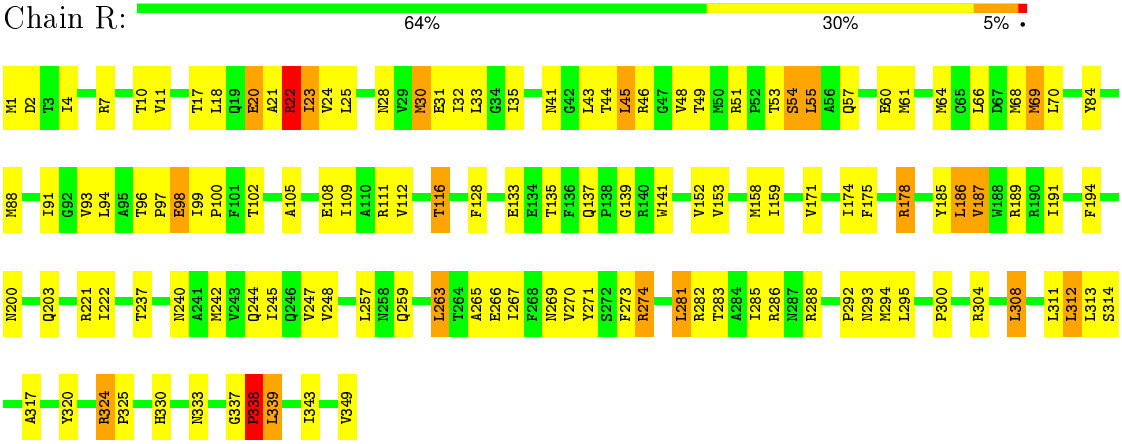
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain F:



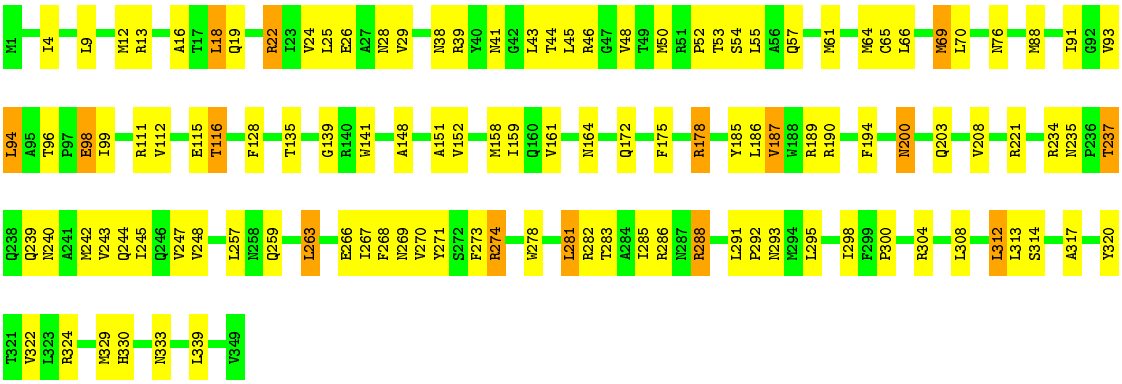
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain R:



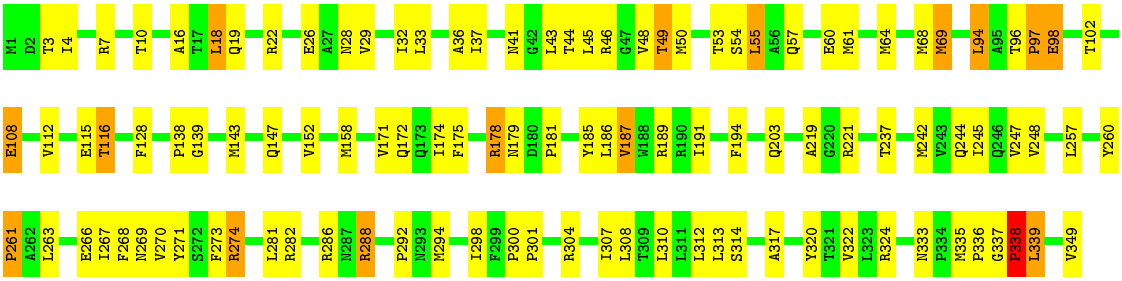
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain G:



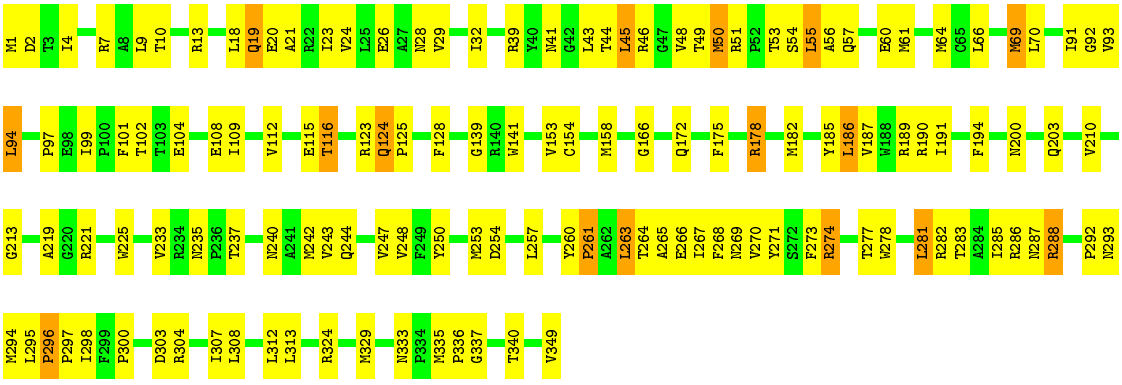
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain H:



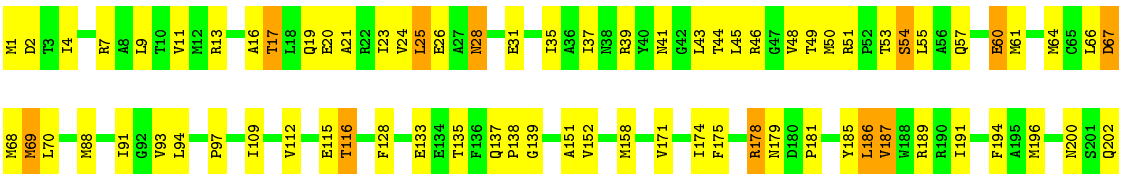
• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

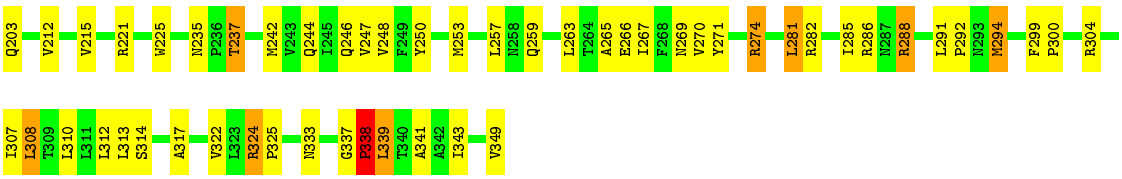
Chain S:



• Molecule 2: PROTEIN (VP7 CORE PROTEIN)

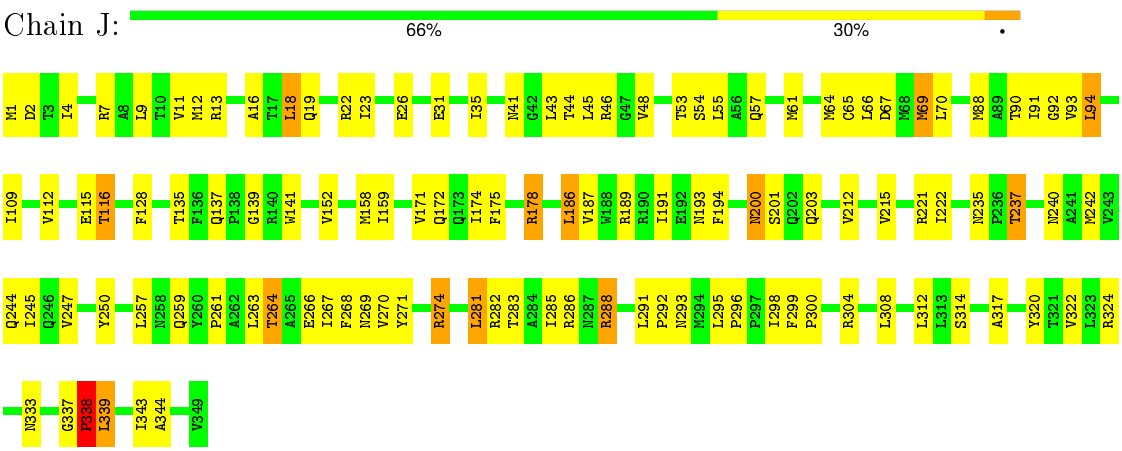
Chain I:





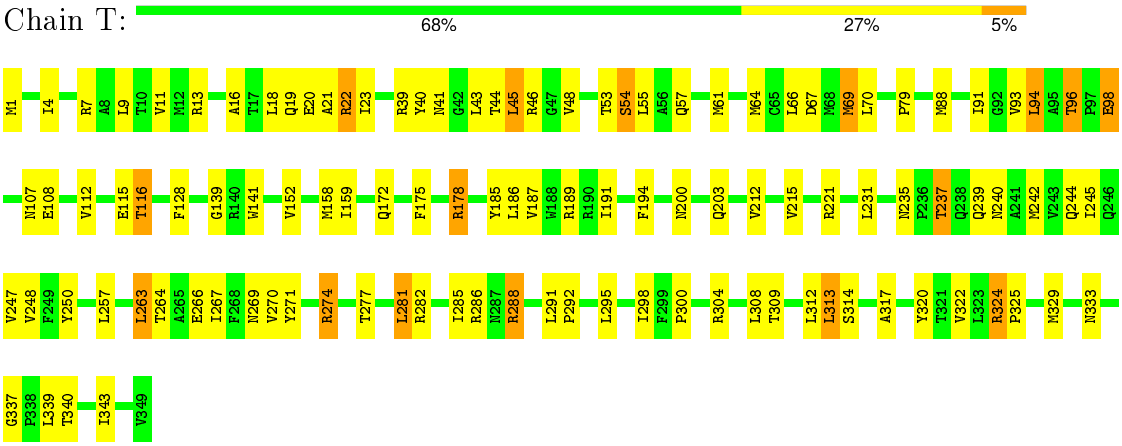
- Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain J:



- Molecule 2: PROTEIN (VP7 CORE PROTEIN)

Chain T:



4 Data and refinement statistics (i)

EDS failed to run properly - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	54.0 (100.00-3.50)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.83 (at 3.49Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.266 , (Not available)	Depositor
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.015	Xtriage
Estimated twinning fraction	0.078 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 3524397 reflections	Xtriage
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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.46	0/6978	0.80	7/9479 (0.1%)
1	B	0.46	0/7308	0.78	3/9925 (0.0%)
2	C	0.33	0/2757	0.59	0/3756
2	D	0.32	0/2757	0.58	0/3756
2	E	0.35	0/2757	0.63	0/3756
2	F	0.36	0/2757	0.64	0/3756
2	G	0.38	0/2757	0.64	0/3756
2	H	0.37	0/2757	0.64	0/3756
2	I	0.37	0/2757	0.64	0/3756
2	J	0.36	0/2757	0.64	0/3756
2	P	0.33	0/2757	0.59	0/3756
2	Q	0.37	0/2757	0.67	0/3756
2	R	0.37	0/2757	0.65	1/3756 (0.0%)
2	S	0.39	0/2757	0.66	0/3756
2	T	0.37	0/2757	0.64	0/3756
All	All	0.39	0/50127	0.68	11/68232 (0.0%)

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	467	HIS	N-CA-C	-6.11	94.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	564	ALA	N-CA-C	-5.88	95.12	111.00
1	A	271	LEU	N-CA-C	5.82	126.71	111.00
1	A	360	ASP	N-CA-C	5.41	125.61	111.00
2	R	20	GLU	N-CA-C	-5.38	96.48	111.00
1	B	896	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	197	VAL	N-CA-C	5.17	124.97	111.00
1	A	494	TYR	N-CA-CB	-5.12	101.38	110.60
1	B	471	TYR	CA-CB-CG	5.08	123.06	113.40
1	B	360	ASP	N-CA-C	-5.05	97.37	111.00
1	A	430	GLY	N-CA-C	5.02	125.64	113.10

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	484	0
1	B	7150	0	7137	456	0
2	C	2699	0	2697	66	0
2	D	2699	0	2697	58	0
2	E	2699	0	2697	82	0
2	F	2699	0	2697	89	0
2	G	2699	0	2697	90	0
2	H	2699	0	2697	77	0
2	I	2699	0	2697	104	0
2	J	2699	0	2697	89	0
2	P	2699	0	2697	66	0
2	Q	2699	0	2697	95	0
2	R	2699	0	2697	94	0
2	S	2699	0	2697	102	0
2	T	2699	0	2697	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49061	0	49002	1904	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 19.

All (1904) 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: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: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
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: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
2:F:158:MET:HE2	2:F:244:GLN:HB2	1.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ARG:NH1	1:B:869:VAL:HG22	1.92	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:509:LYS:HB3	1:A:512:GLU:HG3	1.57	0.84
1:A:339:ASP:O	1:A:343:ILE:HG22	1.77	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
2:D:282:ARG:HD3	2:D:286:ARG:NH1	1.94	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:E:282:ARG:HD3	2:E:286:ARG:NH1	1.93	0.82
1:B:854:ASN:HD22	2:H:49:THR:HG21	1.43	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
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
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:H:158:MET:HE2	2:H:244:GLN:HB2	1.63	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: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:B:748:ILE:HD13	2:S:53:THR:HG21	1.65	0.78
1:A:463:ALA:HB3	1:A:469:GLN:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:PRO:HG3	1:B:663:ILE:HG23	1.66	0.78
2:J:4:ILE:HG23	2:J:94:LEU:HB3	1.66	0.77
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
1:B:379:LEU:HD12	1:B:500:MET:HG3	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:H:263:LEU:HD22	2:H:267:ILE:HD11	1.66	0.77
2:C:269:ASN:HD21	2:C:274:ARG:HH22	1.33	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
2:Q:263:LEU:HD22	2:Q:267:ILE:HD11	1.65	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
1:B:523:HIS:O	1:B:526:ARG:HD2	1.84	0.77
2:G:269:ASN:HD21	2:G:274:ARG:HH22	1.33	0.77
2:I:257:LEU:HD12	2:I:300:PRO:HB3	1.65	0.76
2:J:269:ASN:HD21	2:J:274:ARG:HH22	1.32	0.76
1:A:114:VAL:HB	1:A:133:LYS:HE2	1.66	0.76
2:H:96:THR:HG22	2:H:98:GLU:HB2	1.66	0.76
2:R:28:ASN:HD21	2:G:28:ASN:H	1.30	0.76
2:G:158:MET:HE2	2:G:244:GLN:HB2	1.66	0.76
2:I:54:SER:H	2:I:57:GLN:HE21	1.31	0.76
1:B:72:LYS:HZ1	1:B:595:ILE:HB	1.50	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
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:S:158:MET:HE2	2:S:244:GLN:HB2	1.66	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: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:353:ILE:HG23	1:A:567:VAL:HB	1.69	0.75
2:Q:158:MET:HE2	2:Q:244:GLN:HB2	1.69	0.75
1:B:596:ALA:HA	1:B:599:ILE:HD12	1.69	0.74
1:A:386:ARG:CZ	1:A:456:ASP:HB2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:724:GLU:HB2	1:A:860:ARG:HH21	1.52	0.73
1:A:267:LEU:HD21	1:A:270:GLN:H	1.53	0.73
1:B:592:MET:HE2	1:B:592:MET:HA	1.70	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
2:E:2:ASP:HB3	2:E:109:ILE:HG21	1.71	0.73
1:B:707:ARG:HB2	1:B:766:MET:HG3	1.68	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
2:S:53:THR:H	2:S:57:GLN:HE21	1.37	0.72
1:B:900:THR:HG22	2:G:22:ARG:HH11	1.53	0.72
2:I:294:MET:SD	2:I:349:VAL:HG23	2.28	0.72
1:A:206:ILE:HG22	1:A:870:LEU:O	1.88	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:109:GLU:O	1:B:112:SER:HB3	1.89	0.72
1:B:371:MET:HB2	1:B:405:TYR:CG	2.24	0.72
1:B:85:VAL:HG12	1:B:163:VAL:HA	1.71	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:B:722:ARG:O	1:B:722:ARG:HG2	1.89	0.72
1:A:666:MET:O	1:A:670:VAL:HG23	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:B:774:PHE:HB3	1:B:817:TYR:HE1	1.54	0.72
1:B:338:ASN:HA	1:B:341:ARG:HD3	1.72	0.72
1:A:862:ARG:HB2	1:A:865:GLN:HB2	1.72	0.72
1:B:724:GLU:CD	1:B:860:ARG:HB2	2.09	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:873:ARG:HG2	1:B:874:PHE:N	2.05	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: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:HD12	2:T:298:ILE:H	1.53	0.71
2:Q:20:GLU:HB3	2:Q:22:ARG:HH22	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:MET:HB3	1:A:405:TYR:HB2	1.72	0.71
2:H:257:LEU:HD12	2:H:300:PRO:HB3	1.72	0.71
1:B:403:ASN:HB2	1:B:425:LEU:HD22	1.70	0.71
1:A:300:GLY:HA2	1:A:587:THR:H	1.56	0.71
1:B:623:ARG:HH21	1:B:694:PHE:HE2	1.37	0.71
1:A:633:PRO:O	1:A:636:PHE:HD1	1.74	0.71
1:B:471:TYR:HB2	1:B:535:ASN:HB2	1.71	0.71
2:S:266:GLU:O	2:S:270:VAL:HG23	1.90	0.71
1:B:71:ILE:HA	1:B:74:LEU:HD12	1.72	0.71
1:A:591:GLU:HA	1:A:895:LYS:HE3	1.72	0.71
2:T:158:MET:HE2	2:T:244:GLN:HB2	1.72	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
1:A:429:ILE:HG21	1:A:507:ALA:HA	1.72	0.71
2:T:269:ASN:HD21	2:T:274:ARG:HH22	1.39	0.71
1:A:468:ALA:HB3	1:A:546:ASP:HB2	1.71	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
2:G:112:VAL:O	2:G:116:THR:HB	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
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: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:T:116:THR:HG21	2:T:304:ARG:HB2	1.73	0.69
2:H:112:VAL:O	2:H:116:THR:HB	1.92	0.69
1:A:380:LEU:HD13	1:A:580:PHE:HD1	1.57	0.69
1:A:344:TYR:HA	1:A:347:LEU:HD23	1.73	0.69
2:T:189:ARG:HD2	2:T:244:GLN:HE21	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:263:LEU:HD22	2:F:267:ILE:HD11	1.75	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: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
1:A:275:PRO:HB3	1:A:467:HIS:ND1	2.07	0.68
2:R:269:ASN:HD21	2:R:274:ARG:HH22	1.41	0.68
2:D:298:ILE:H	2:D:298:ILE:HD12	1.58	0.68
2:H:269:ASN:HD21	2:H:274:ARG:HH22	1.38	0.68
1:A:707:ARG:HD3	1:A:766:MET:HB3	1.75	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
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:526:ARG:HB2	1:B:583:SER:HB2	1.76	0.68
1:B:403:ASN:ND2	1:B:425:LEU:H	1.92	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: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
2:R:271:TYR:OH	2:R:292:PRO:HG2	1.93	0.67
1:B:901:VAL:HG22	2:Q:43:LEU:HG	1.74	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
2:T:53:THR:H	2:T:57:GLN:NE2	1.92	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
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:HH11	2:I:288:ARG:HG3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:GLU:HB2	1:A:860:ARG:NH2	2.10	0.66
1:A:207:GLY:O	1:A:872:ARG:HB2	1.94	0.66
2:Q:128:PHE:HB2	2:Q:247:VAL:HG11	1.77	0.66
2:P:69:MET:HG2	2:P:312:LEU:HB3	1.76	0.66
2:J:69:MET:HG2	2:J:312:LEU:HB3	1.77	0.66
2:Q:4:ILE:HG23	2:Q:94:LEU:HB3	1.77	0.66
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:H:96:THR:HG23	2:H:98:GLU:OE2	1.95	0.66
2:Q:16:ALA:HA	2:Q:322:VAL:HG21	1.78	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:Q:282:ARG:HD3	2:Q:286:ARG:CZ	2.26	0.66
2:C:16:ALA:HA	2:C:322:VAL:HG21	1.77	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:B:624:PHE:CD2	1:B:778:LEU:HD21	2.32	0.65
1:A:414:VAL:HG21	1:A:507:ALA:O	1.97	0.65
1:B:520:LEU:HB3	1:B:521:PRO:HD3	1.79	0.65
1:B:403:ASN:HD22	1:B:425:LEU:H	1.41	0.65
1:A:279:TRP:HZ3	1:A:541:VAL:O	1.79	0.65
2:D:69:MET:HG2	2:D:312:LEU:HB3	1.79	0.65
1:B:465:TYR:O	1:B:466:VAL:HB	1.95	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
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:151:ARG:HG3	1:A:152:ASP:N	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:53:THR:H	2:J:57:GLN:NE2	1.95	0.65
2:T:266:GLU:O	2:T:270:VAL:HG23	1.97	0.64
1:A:715:LEU:HD21	1:A:830:VAL:HG11	1.78	0.64
2:H:54:SER:H	2:H:57:GLN:NE2	1.95	0.64
1:A:273:VAL:HG12	1:A:274:ASN:H	1.62	0.64
1:B:336:GLN:HA	1:B:339:ASP:HB2	1.78	0.64
1:A:413:ARG:HD2	1:A:413:ARG:C	2.17	0.64
2:G:266:GLU:O	2:G:270:VAL:HG23	1.97	0.64
2:Q:288:ARG:HH11	2:Q:288:ARG:HG3	1.62	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
2:Q:43:LEU:CD1	2:Q:93:VAL:HG22	2.27	0.64
1:B:465:TYR:HD2	1:B:539:HIS:HD2	1.46	0.64
2:I:54:SER:H	2:I:57:GLN:NE2	1.95	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:H:189:ARG:HD2	2:H:244:GLN:HE21	1.63	0.64
1:B:598:LEU:O	1:B:602:VAL:HG23	1.98	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
2:I:97:PRO:HD3	2:J:22:ARG:NH2	2.07	0.63
1:A:266:VAL:O	1:A:885:ASP:HB2	1.98	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
1:A:622:ARG:NH2	2:Q:26:GLU:HG3	2.12	0.63
2:Q:39:ARG:NH2	2:Q:96:THR:HG21	2.13	0.63
2:S:112:VAL:O	2:S:116:THR:HB	1.98	0.63
1:B:337:LEU:HD23	1:B:582:ARG:HH12	1.64	0.63
1:B:95:THR:CG2	1:B:725:GLY:HA3	2.29	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:A:287:ALA:HA	1:A:290:ILE:HD12	1.80	0.63
2:G:66:LEU:O	2:G:70:LEU:HG	1.98	0.63
1:A:376:VAL:HG13	1:A:580:PHE:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:VAL:HG23	2:G:22:ARG:HD3	1.79	0.63
1:A:705:MET:HG2	1:A:772:VAL:HG22	1.81	0.63
2:S:277:THR:HA	2:S:329:MET:HE1	1.81	0.63
1:A:357:LEU:HD12	1:A:357:LEU:H	1.64	0.63
2:J:282:ARG:HD3	2:J:286:ARG:CZ	2.28	0.63
2:Q:53:THR:H	2:Q:57:GLN:HE21	1.47	0.63
2:C:20:GLU:HG2	2:C:21:ALA:H	1.63	0.63
2:H:44:THR:HG22	2:H:46:ARG:HG3	1.79	0.63
1:A:340:VAL:HA	1:A:343:ILE:CG2	2.29	0.63
2:I:4:ILE:HG23	2:I:94:LEU:HB3	1.81	0.63
1:A:622:ARG:NH1	2:F:100:PRO:HB2	2.14	0.63
2:T:235:ASN:OD1	2:T:237:THR:HG22	1.98	0.63
2:R:338:PRO:O	2:R:339:LEU:HB2	1.99	0.63
2:D:53:THR:H	2:D:57:GLN:NE2	1.97	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:B:407:LEU:HA	1:B:413:ARG:NH2	2.09	0.62
1:A:812:TYR:N	1:A:812:TYR:HD1	1.98	0.62
2:I:69:MET:HG2	2:I:312:LEU:HB3	1.81	0.62
2:C:266:GLU:O	2:C:270:VAL:HG23	1.99	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
2:S:139:GLY:O	2:S:194:PHE:HB2	1.99	0.62
1:B:64:VAL:O	1:B:67:ILE:HG22	1.99	0.62
2:C:294:MET:SD	2:C:349:VAL:HG23	2.39	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:B:263:MET:HE2	1:B:884:MET:SD	2.40	0.62
1:A:533:ILE:HG22	1:A:538:LEU:HD21	1.82	0.62
1:B:873:ARG:O	1:B:874:PHE:HB2	2.00	0.62
1:A:434:TYR:CD2	1:A:503:MET:HB2	2.35	0.62
2:R:44:THR:HG22	2:R:46:ARG:HG3	1.81	0.62
1:B:617:LEU:O	1:B:620:MET:HB2	1.99	0.62
2:I:28:ASN:HD22	2:I:28:ASN:N	1.98	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
2:C:257:LEU:CD1	2:C:300:PRO:HB3	2.29	0.61
2:T:263:LEU:HD22	2:T:267:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:819:THR:HG22	1:B:820:GLU:H	1.65	0.61
2:T:44:THR:O	2:T:45:LEU:HB2	2.00	0.61
1:A:842:ILE:HD12	1:A:842:ILE:H	1.65	0.61
1:B:357:LEU:HD22	1:B:357:LEU:H	1.65	0.61
1:B:302:TYR:HE1	1:B:584:PHE:CD2	2.18	0.61
1:B:842:ILE:H	1:B:842:ILE:HD12	1.65	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:A:138:ARG:NH2	1:A:680:LYS:HG2	2.15	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:763:ARG:HD3	1:B:767:ASP:OD1	2.00	0.61
1:A:430:GLY:O	1:A:431:ARG:HB2	2.00	0.61
2:G:9:LEU:O	2:G:13:ARG:HG3	2.00	0.61
1:B:332:PRO:HG2	1:B:574:ILE:HG21	1.82	0.61
2:G:41:ASN:HD21	2:G:48:VAL:H	1.47	0.61
1:B:460:ARG:HE	2:E:51:ARG:NH2	1.99	0.61
1:A:70:ASP:O	1:A:74:LEU:HD23	2.00	0.61
2:F:112:VAL:O	2:F:116:THR:HB	2.01	0.61
1:B:409:MET:HB3	1:B:413:ARG:NH1	2.16	0.61
1:B:248:ILE:HD11	1:B:892:MET:SD	2.41	0.61
1:B:356:ASP:O	1:B:570:ASP:HA	2.01	0.61
2:E:21:ALA:O	2:E:51:ARG:HD2	2.01	0.61
1:B:684:GLU:O	1:B:688:TRP:HB2	2.00	0.61
2:H:128:PHE:HB2	2:H:247:VAL:HG11	1.82	0.61
2:G:53:THR:H	2:G:57:GLN:NE2	1.98	0.61
2:D:266:GLU:O	2:D:270:VAL:HG23	2.01	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:H:175:PHE:O	2:H:178:ARG:HG3	2.01	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:661:ILE:HG23	1:A:665:ASP:HB2	1.82	0.61
1:A:470:ARG:HB3	1:A:546:ASP:OD2	2.01	0.60
2:R:189:ARG:HD2	2:R:244:GLN:HE21	1.66	0.60
2:D:257:LEU:HD12	2:D:300:PRO:HB3	1.81	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:H	1:A:427:PHE:HD1	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:381:PHE:CG	1:A:390:LEU:HD21	2.36	0.60
1:A:105:ASP:O	1:A:107:TYR:N	2.35	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:B:627:VAL:HG21	1:B:778:LEU:HD23	1.84	0.60
1:A:391:THR:HB	1:A:394:MET:H	1.67	0.60
2:S:54:SER:H	2:S:57:GLN:NE2	1.99	0.60
1:B:729:THR:HG22	1:B:731:MET:N	2.17	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:P:112:VAL:O	2:P:116:THR:HB	2.01	0.60
1:A:774:PHE:HB3	1:A:817:TYR:CE2	2.37	0.59
2:P:200:ASN:HD22	2:P:200:ASN:H	1.49	0.59
2:H:266:GLU:O	2:H:270:VAL:HG23	2.01	0.59
1:B:100:ARG:HD3	1:B:724:GLU:HG2	1.82	0.59
1:A:497:TYR:O	1:A:501:LEU:HG	2.02	0.59
1:A:359:ILE:HG22	1:A:361:PRO:CD	2.31	0.59
1:A:57:VAL:HG21	1:A:301:GLU:HG2	1.84	0.59
1:B:460:ARG:HB2	2:E:51:ARG:HG2	1.84	0.59
2:H:4:ILE:HG23	2:H:94:LEU:HB3	1.84	0.59
2:R:2:ASP:HB3	2:R:109:ILE:HG21	1.83	0.59
2:R:128:PHE:HB2	2:R:247:VAL:HG11	1.82	0.59
1:B:403:ASN:ND2	1:B:427:PHE:HE1	1.99	0.59
1:A:57:VAL:HG23	1:A:300:GLY:O	2.03	0.59
2:P:7:ARG:O	2:P:11:VAL:HG23	2.03	0.59
1:B:129:THR:O	1:B:133:LYS:HG3	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:E:269:ASN:HD21	2:E:274:ARG:HH22	1.48	0.59
2:G:200:ASN:ND2	2:G:200:ASN:H	2.00	0.59
1:A:58:ASP:H	1:B:317:ARG:HH12	1.49	0.59
1:B:331:THR:HA	1:B:578:PHE:CE2	2.38	0.59
1:A:617:LEU:HB3	1:A:636:PHE:HD2	1.68	0.59
2:E:112:VAL:O	2:E:116:THR:HB	2.02	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
1:A:608:SER:O	1:A:612:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:MET:HG2	1:B:413:ARG:HD3	1.85	0.59
1:A:474:TYR:HB2	1:A:531:ASN:HD21	1.66	0.59
2:R:10:THR:CG2	2:R:102:THR:HG23	2.32	0.59
1:A:830:VAL:HG12	1:A:834:ASN:HD22	1.67	0.59
2:T:54:SER:H	2:T:57:GLN:NE2	2.01	0.59
1:B:336:GLN:HA	1:B:339:ASP:CB	2.33	0.59
2:C:53:THR:H	2:C:57:GLN:NE2	2.01	0.59
2:H:10:THR:HG23	2:H:102:THR:HG23	1.85	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:C:7:ARG:O	2:C:11:VAL:HG23	2.03	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:B:854:ASN:ND2	2:H:49:THR:HG21	2.16	0.58
1:A:151:ARG:HH12	1:A:188:ASP:HB3	1.68	0.58
2:J:54:SER:H	2:J:57:GLN:HE21	1.50	0.58
2:Q:185:TYR:O	2:Q:248:VAL:HG12	2.03	0.58
1:B:779:ARG:HH12	1:B:799:PRO:CB	2.14	0.58
1:B:108:TYR:HB3	1:B:698:MET:CE	2.33	0.58
2:P:315:THR:O	2:P:319:VAL:HG23	2.02	0.58
2:F:4:ILE:HG23	2:F:94:LEU:HB3	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
1:A:98:ARG:HG2	1:A:174:VAL:HG12	1.85	0.58
2:P:175:PHE:O	2:P:178:ARG:HG3	2.03	0.58
1:A:349:PHE:H	1:A:350:PRO:HA	1.69	0.58
2:E:9:LEU:HG	2:E:13:ARG:HD2	1.85	0.58
2:T:175:PHE:O	2:T:178:ARG:HG3	2.03	0.58
1:A:388:THR:HG22	1:A:389:ASN:N	2.17	0.58
2:E:337:GLY:N	2:E:338:PRO:HD3	2.18	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: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:Q:288:ARG:NH1	2:Q:288:ARG:HG3	2.18	0.58
1:A:169:LYS:O	1:A:173:PRO:HD3	2.02	0.58
2:P:266:GLU:O	2:P:270:VAL:HG23	2.04	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:T:4:ILE:HG23	2:T:94:LEU:HB3	1.86	0.58
2:S:277:THR:HG23	2:S:329:MET:HE1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:244:GLN:CD	2:C:135:THR:HG21	2.24	0.58
2:T:41:ASN:HD21	2:T:48:VAL:H	1.51	0.58
1:B:470:ARG:NH1	1:B:549:PHE:CG	2.72	0.58
1:A:273:VAL:HG12	1:A:274:ASN:N	2.19	0.58
2:Q:44:THR:HG22	2:Q:46:ARG:HG3	1.86	0.58
1:A:482:LEU:HD12	1:A:899:PRO:HD3	1.85	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
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
1:A:645:PRO:HB2	1:A:648:VAL:HG23	1.85	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
2:I:2:ASP:HB3	2:I:109:ILE:HG21	1.86	0.57
1:B:192:ILE:O	1:B:192:ILE:HG22	2.03	0.57
1:A:483:ILE:HG23	1:A:488:TYR:HD2	1.69	0.57
2:E:200:ASN:H	2:E:200:ASN:ND2	2.01	0.57
1:B:753:ALA:CB	1:B:815:ILE:HB	2.35	0.57
1:A:109:GLU:O	1:A:112:SER:HB3	2.04	0.57
2:R:25:LEU:HD21	2:H:32:ILE:HD11	1.85	0.57
1:B:356:ASP:HA	1:B:394:MET:CG	2.33	0.57
1:A:509:LYS:CD	1:A:509:LYS:H	2.14	0.57
1:A:729:THR:HG22	1:A:730:ASN:N	2.20	0.57
2:G:53:THR:H	2:G:57:GLN:HE21	1.51	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: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:A:468:ALA:HB3	1:A:546:ASP:CG	2.24	0.57
2:G:116:THR:HG21	2:G:304:ARG:HB2	1.87	0.57
2:I:288:ARG:NH1	2:I:288:ARG:HG3	2.17	0.57
1:B:200:ARG:O	1:B:201:ASP:HB2	2.04	0.57
2:D:112:VAL:O	2:D:116:THR:HB	2.05	0.57
2:R:96:THR:HG22	2:R:98:GLU:HB2	1.87	0.57
2:F:283:THR:HG23	2:F:293:ASN:HB2	1.87	0.57
2:Q:339:LEU:HA	2:Q:343:ILE:HD12	1.86	0.57
2:R:54:SER:H	2:R:57:GLN:NE2	2.00	0.57
1:B:774:PHE:HB3	1:B:817:TYR:CE1	2.37	0.57
1:B:134:VAL:HG11	1:B:688:TRP:CE3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:GLN:HB3	1:B:80:TYR:CE1	2.39	0.57
1:A:251:SER:HB3	1:A:892:MET:HB3	1.86	0.57
2:F:64:MET:O	2:F:68:MET:HG3	2.05	0.57
2:H:282:ARG:HD3	2:H:286:ARG:CZ	2.33	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:B:101:VAL:HG12	1:B:102:LEU:H	1.70	0.57
1:A:711:PRO:HG2	1:A:828:TYR:OH	2.05	0.57
2:I:271:TYR:OH	2:I:292:PRO:HG2	2.05	0.56
2:I:53:THR:H	2:I:57:GLN:NE2	2.03	0.56
2:Q:53:THR:H	2:Q:57:GLN:NE2	2.03	0.56
2:R:158:MET:HE2	2:R:244:GLN:HB2	1.85	0.56
1:A:148:ILE:HD13	1:A:163:VAL:HG21	1.87	0.56
2:J:53:THR:H	2:J:57:GLN:HE21	1.51	0.56
1:B:532:GLN:O	1:B:536:GLU:HB3	2.06	0.56
2:G:271:TYR:OH	2:G:292:PRO:HG2	2.05	0.56
2:R:324:ARG:N	2:R:325:PRO:HD3	2.20	0.56
2:R:49:THR:HG22	2:R:51:ARG:H	1.70	0.56
2:S:2:ASP:HB3	2:S:109:ILE:HG21	1.87	0.56
2:J:200:ASN:ND2	2:J:200:ASN:H	2.03	0.56
2:S:97:PRO:O	2:I:24:VAL:HG22	2.05	0.56
1:B:95:THR:HG22	1:B:96:GLN:H	1.70	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
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
2:H:288:ARG:HG3	2:H:288:ARG:NH1	2.20	0.56
1:A:293:ILE:O	1:A:297:LEU:HB2	2.04	0.56
1:B:721:PHE:C	1:B:723:GLN:H	2.08	0.56
2:E:40:TYR:CE2	2:E:44:THR:HG21	2.40	0.56
2:Q:116:THR:HG21	2:Q:304:ARG:HB2	1.86	0.56
1:A:168:PHE:O	1:A:170:ASN:N	2.39	0.56
1:A:487:THR:O	1:A:488:TYR:HB2	2.06	0.56
1:B:255:LEU:H	1:B:896:LEU:HA	1.70	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
2:Q:178:ARG:N	2:Q:178:ARG:HD2	2.21	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:T:185:TYR:O	2:T:248:VAL:HG12	2.05	0.56
2:Q:268:PHE:CD2	2:F:259:GLN:HA	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLY:H	1:B:133:LYS:HE3	1.70	0.56
2:R:69:MET:HG2	2:R:312:LEU:HB3	1.87	0.56
1:A:356:ASP:CG	1:A:568:VAL:HA	2.25	0.56
1:B:693:ASP:O	1:B:694:PHE:HB2	2.06	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
2:S:10:THR:HG23	2:S:102:THR:HG23	1.88	0.56
1:B:326:ILE:HG13	1:B:327:LEU:N	2.20	0.56
2:S:20:GLU:HG2	2:S:21:ALA:H	1.70	0.56
1:B:13:LYS:HD2	1:B:19:GLU:HG3	1.88	0.56
2:G:69:MET:HG2	2:G:312:LEU:HB3	1.87	0.56
2:C:330:HIS:HB3	2:F:336:PRO:HB3	1.87	0.56
2:S:282:ARG:HD3	2:S:286:ARG:CZ	2.36	0.56
1:A:339:ASP:OD1	1:A:571:VAL:HA	2.06	0.56
2:I:44:THR:CG2	2:I:46:ARG:HB2	2.35	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
1:B:718:ILE:HD13	1:B:832:PHE:HA	1.88	0.56
2:I:259:GLN:HA	2:J:268:PHE:CD2	2.41	0.56
1:A:425:LEU:HB3	1:A:436:CYS:O	2.06	0.55
1:B:471:TYR:HB2	1:B:535:ASN:CB	2.36	0.55
1:B:336:GLN:O	1:B:339:ASP:HB3	2.06	0.55
2:G:330:HIS:HB3	2:T:337:GLY:HA3	1.88	0.55
1:A:178:GLU:HG2	1:A:179:HIS:H	1.71	0.55
2:F:41:ASN:HD21	2:F:48:VAL:HG23	1.71	0.55
1:B:384:GLY:HA2	1:B:446:GLY:HA3	1.87	0.55
2:R:314:SER:O	2:R:317:ALA:HB3	2.05	0.55
1:B:103:ARG:HE	1:B:861:VAL:HG21	1.71	0.55
2:E:43:LEU:HD12	2:E:93:VAL:HG22	1.86	0.55
2:E:4:ILE:HG23	2:E:94:LEU:HB3	1.88	0.55
2:R:88:MET:O	2:R:91:ILE:HG22	2.05	0.55
2:R:282:ARG:HD3	2:R:286:ARG:CZ	2.36	0.55
1:A:465:TYR:HE1	1:A:541:VAL:HG13	1.68	0.55
2:R:339:LEU:HA	2:R:343:ILE:HD12	1.87	0.55
2:P:189:ARG:HH11	2:P:244:GLN:HE21	1.55	0.55
1:A:863:VAL:HG23	1:A:864:GLY:H	1.70	0.55
1:A:428:GLN:HG2	1:A:435:ASP:HB3	1.88	0.55
2:H:108:GLU:HG3	2:H:260:TYR:OH	2.06	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:I:189:ARG:HD2	2:I:244:GLN:HE21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:314:SER:O	2:T:317:ALA:HB3	2.05	0.55
2:D:269:ASN:HD21	2:D:274:ARG:HH22	1.53	0.55
2:R:116:THR:HG21	2:R:304:ARG:HB2	1.87	0.55
1:B:628:LEU:N	1:B:628:LEU:HD23	2.21	0.55
2:T:257:LEU:CD1	2:T:300:PRO:HB3	2.31	0.55
2:J:116:THR:HG21	2:J:304:ARG:CB	2.29	0.55
1:B:331:THR:O	1:B:333:THR:N	2.39	0.55
2:E:266:GLU:O	2:E:270:VAL:HG23	2.07	0.55
1:A:57:VAL:HG22	1:A:57:VAL:O	2.05	0.55
2:D:43:LEU:HD12	2:D:93:VAL:HG22	1.88	0.55
2:T:191:ILE:HD12	2:T:242:MET: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:286:ILE:HG23	1:A:655:SER:HB3	1.89	0.55
1:A:379:LEU:HD22	1:A:497:TYR:HD1	1.70	0.55
2:E:270:VAL:HB	2:E:286:ARG:NH2	2.22	0.55
1:B:214:TYR:CD2	1:B:872:ARG:HD2	2.41	0.55
1:A:403:ASN:HB2	1:A:425:LEU:HD22	1.89	0.55
1:B:901:VAL:CG2	2:G:22:ARG:HD3	2.37	0.55
1:A:541:VAL:HG22	1:A:600:GLU:CD	2.27	0.55
2:T:112:VAL:O	2:T:116:THR:HB	2.07	0.55
2:I:28:ASN:H	2:I:28:ASN:ND2	2.05	0.55
1:B:666:MET:O	1:B:670:VAL:HG23	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:B:636:PHE:O	1:B:640:VAL:HG23	2.07	0.55
1:B:370:ARG:HG2	1:B:573:TRP:CE2	2.41	0.55
1:A:655:SER:O	1:A:659:ASN:HB2	2.07	0.55
1:A:693:ASP:OD2	1:A:695:GLU:HB2	2.07	0.55
2:I:324:ARG:N	2:I:325:PRO:HD3	2.22	0.55
1:A:664:ARG:HG3	1:B:485:PRO:CG	2.37	0.55
2:C:39:ARG:HG3	2:C:39:ARG:HH11	1.72	0.55
1:A:314:LEU:CD1	1:A:512:GLU:HA	2.36	0.54
1:B:108:TYR:HB3	1:B:698:MET:HE2	1.88	0.54
2:R:7:ARG:O	2:R:11:VAL:HG23	2.07	0.54
2:P:294:MET:SD	2:P:349:VAL:HG23	2.47	0.54
1:A:529:ARG:O	1:A:533:ILE:HG13	2.06	0.54
2:G:237:THR:HG23	2:G:239:GLN:H	1.73	0.54
1:B:227:VAL:HG13	1:B:231:GLU:HG3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:337:GLY:O	2:H:339:LEU:HD13	2.08	0.54
2:F:51:ARG:O	2:F:51:ARG:HD3	2.08	0.54
2:Q:263:LEU:HD22	2:Q:267:ILE:CD1	2.37	0.54
2:P:200:ASN:ND2	2:P:200:ASN:H	2.06	0.54
2:H:288:ARG:HG3	2:H:288:ARG:HH11	1.71	0.54
2:C:88:MET:O	2:C:91:ILE:HG22	2.08	0.54
2:J:314:SER:O	2:J:317:ALA:HB3	2.07	0.54
2:S:210:VAL:HG22	2:S:233:VAL:HG13	1.90	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
2:J:257:LEU:HD23	2:J:264:THR:HG23	1.90	0.54
2:Q:31:GLU:O	2:Q:35:ILE:HG13	2.08	0.54
1:B:265:TRP:CD1	1:B:886:ILE:HD11	2.42	0.54
2:R:294:MET:SD	2:R:349:VAL:HG23	2.47	0.54
2:C:128:PHE:HB2	2:C:247:VAL:HG11	1.88	0.54
2:G:282:ARG:HD3	2:G:286:ARG:CZ	2.37	0.54
2:Q:43:LEU:HD12	2:Q:93:VAL:HG22	1.88	0.54
2:T:281:LEU:O	2:T:285:ILE:HG13	2.07	0.54
1:A:341:ARG:NH1	1:B:317:ARG:HD3	2.22	0.54
2:T:282:ARG:HD3	2:T:286:ARG:CZ	2.38	0.54
1:A:165:GLY:O	1:A:166:VAL:HB	2.07	0.54
2:T:324:ARG:N	2:T:325:PRO:HD3	2.23	0.54
2:H:69:MET:HG2	2:H:312:LEU:HB3	1.90	0.54
1:B:267:LEU:HD21	1:B:269:LEU:O	2.08	0.54
1:A:746:TYR:O	1:A:750:ARG:HG2	2.07	0.54
2:E:244:GLN:CD	2:F:135:THR:HG21	2.27	0.54
1:A:379:LEU:HD22	1:A:497:TYR:CD1	2.43	0.54
2:T:53:THR:H	2:T:57:GLN:HE21	1.56	0.54
2:F:116:THR:HG21	2:F:304:ARG:HB2	1.89	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
2:F:204:THR:HG23	2:F:241:ALA:HB1	1.90	0.54
2:E:40:TYR:O	2:E:44:THR:HB	2.08	0.54
2:J:54:SER:H	2:J:57:GLN:NE2	2.06	0.54
2:S:116:THR:HG21	2:S:304:ARG:HB2	1.89	0.54
2:J:158:MET:HE2	2:J:244:GLN:HB2	1.90	0.54
1:A:283:ARG:HH21	1:B:490:ILE:HA	1.73	0.54
2:Q:108:GLU:HG3	2:Q:260:TYR:OH	2.07	0.53
1:A:748:ILE:CD1	2:Q:49:THR:HG23	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLU:HG3	1:A:587:THR:CG2	2.38	0.53
2:C:339:LEU:HA	2:C:343:ILE:HD12	1.90	0.53
2:I:17:THR:HG21	2:I:25:LEU:HD11	1.90	0.53
2:S:128:PHE:HB2	2:S:247:VAL:HG11	1.90	0.53
2:P:54:SER:H	2:P:57:GLN:NE2	2.06	0.53
1:A:532:GLN:O	1:A:536:GLU:HB3	2.08	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
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:523:HIS:O	1:A:526:ARG:HG2	2.09	0.53
1:A:377:GLY:HA3	1:A:398:LEU:HD21	1.91	0.53
2:I:97:PRO:HB3	2:J:22:ARG:HE	1.74	0.53
2:R:270:VAL:HG13	2:R:313:LEU:HB3	1.90	0.53
1:A:413:ARG:O	1:A:413:ARG:HD2	2.08	0.53
2:Q:338:PRO:O	2:Q:339:LEU:HB2	2.07	0.53
2:I:185:TYR:O	2:I:248:VAL:HG12	2.08	0.53
2:F:25:LEU:H	2:F:25:LEU:HD22	1.73	0.53
1:B:724:GLU:OE2	1:B:860:ARG:HB2	2.09	0.53
1:B:354:ILE:CD1	1:B:566:PRO:HB2	2.38	0.53
2:I:337:GLY:O	2:I:339:LEU:N	2.41	0.53
2:R:133:GLU:HG2	2:H:219:ALA:O	2.09	0.53
2:G:96:THR:CG2	2:G:98:GLU:HB2	2.38	0.53
1:A:96:GLN:HE22	1:A:830:VAL:HG23	1.74	0.53
2:Q:43:LEU:HD13	2:Q:93:VAL:HG22	1.90	0.53
1:B:424:PRO:O	1:B:425:LEU:HB2	2.09	0.53
1:A:419:GLY:HA3	1:A:426:ASP:OD1	2.07	0.53
2:R:283:THR:HG23	2:R:293:ASN:HB2	1.90	0.53
1:A:529:ARG:HG3	1:A:529:ARG:HH11	1.73	0.53
1:A:296:CYS:HG	1:A:538:LEU:HA	1.73	0.53
2:Q:271:TYR:OH	2:Q:292:PRO:HG2	2.09	0.53
1:B:616:HIS:CG	1:B:688:TRP:NE1	2.76	0.53
1:B:80:TYR:HA	1:B:142:SER:HB3	1.89	0.53
2:Q:191:ILE:HD12	2:Q:242:MET:HB3	1.91	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:95:THR:HG22	1:B:96:GLN:N	2.24	0.53
1:B:80:TYR:OH	1:B:885:ASP:HB3	2.09	0.53
2:S:287:ASN:OD1	2:S:293:ASN:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:257:LEU:CD1	2:J:300:PRO:HB3	2.34	0.52
2:S:273:PHE:O	2:S:278:TRP:HD1	1.92	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
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
1:A:263:MET:CE	1:A:882:ARG:HD2	2.38	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: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
1:A:806:GLU:OE2	1:B:263:MET:HE1	2.10	0.52
2:R:337:GLY:O	2:R:339:LEU:N	2.43	0.52
2:P:7:ARG:NH2	2:C:23:ILE:HG22	2.25	0.52
2:G:200:ASN:HD22	2:G:200:ASN:H	1.57	0.52
1:A:196:ASN:ND2	1:A:197:VAL:HG23	2.24	0.52
1:A:144:ILE:HG13	1:A:220:LEU:HD21	1.92	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:B:23:LEU:HG	1:B:582:ARG:HG2	1.90	0.52
1:A:494:TYR:HB3	1:A:497:TYR:CB	2.38	0.52
2:F:257:LEU:CD1	2:F:300:PRO:HB3	2.35	0.52
1:B:302:TYR:CE1	1:B:584:PHE:CD2	2.98	0.52
2:Q:41:ASN:ND2	2:Q:46:ARG:O	2.42	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
2:C:41:ASN:HD21	2:C:48:VAL:HG23	1.75	0.52
1:A:381:PHE:HE2	1:A:576:LEU:HD11	1.74	0.52
2:I:28:ASN:N	2:I:28:ASN:ND2	2.57	0.52
2:F:171:VAL:O	2:F:174:ILE:HG22	2.10	0.52
2:Q:10:THR:HG23	2:Q:102:THR:HG23	1.91	0.52
2:R:185:TYR:O	2:R:248:VAL:HG12	2.10	0.52
2:F:16:ALA:HA	2:F:322:VAL:HG21	1.90	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:F:315:THR:O	2:F:319:VAL:HG23	2.10	0.52
1:B:745:THR:HG22	1:B:746:TYR:N	2.25	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:A:382:THR:HG22	1:A:384:GLY:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ILE:O	1:A:228:GLN:HG2	2.10	0.52
1:A:359:ILE:HG22	1:A:360:ASP:N	2.25	0.52
1:A:96:GLN:HE22	1:A:830:VAL:H	1.58	0.52
2:H:257:LEU:CD1	2:H:300:PRO:HB3	2.39	0.52
2:H:53:THR:H	2:H:57:GLN:HE21	1.56	0.52
2:Q:186:LEU:O	2:Q:222:ILE:HA	2.09	0.52
1:B:465:TYR:CD2	1:B:539:HIS:HD2	2.27	0.52
1:B:105:ASP:HB3	1:B:108:TYR:HD2	1.74	0.52
1:B:698:MET:C	1:B:699:LEU:HD23	2.30	0.52
2:C:185:TYR:O	2:C:248:VAL:HG12	2.10	0.52
1:A:259:ARG:HD2	1:A:263:MET:HE2	1.92	0.52
1:B:235:SER:HB3	1:B:271:LEU:H	1.75	0.52
1:A:724:GLU:OE2	1:A:860:ARG:HA	2.10	0.52
1:A:465:TYR:HB3	1:A:467:HIS:HB2	1.92	0.52
2:C:283:THR:HG23	2:C:293:ASN:HB2	1.91	0.52
2:R:41:ASN:HD21	2:R:48:VAL:H	1.57	0.52
2:F:2:ASP:HB3	2:F:109:ILE:HG21	1.92	0.52
1:B:171:VAL:O	1:B:174:VAL:HG23	2.09	0.52
2:C:200:ASN:ND2	2:C:200:ASN:H	2.08	0.52
2:I:269:ASN:ND2	2:I:274:ARG:HH22	2.07	0.52
2:F:54:SER:H	2:F:57:GLN:NE2	2.08	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:J:66:LEU:O	2:J:70:LEU:HG	2.09	0.52
2:C:315:THR:O	2:C:319:VAL:HG23	2.10	0.52
1:B:605:SER:O	1:B:609:VAL:HG23	2.10	0.52
2:P:135:THR:HG21	2:D:244:GLN:CD	2.31	0.52
1:A:221:GLN:NE2	1:A:877:TYR:OH	2.43	0.52
2:I:44:THR:HG22	2:I:46:ARG:HB2	1.93	0.51
1:A:637:TRP:CE3	1:A:666:MET:HG2	2.45	0.51
1:A:613:ASP:O	1:A:617:LEU:HD22	2.10	0.51
1:A:82:ILE:HG12	1:A:144:ILE:HD13	1.92	0.51
1:A:424:PRO:O	1:A:425:LEU:HB2	2.11	0.51
2:J:2:ASP:HB3	2:J:109:ILE:CG2	2.40	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:271:TYR:CE1	2:G:286:ARG:NH1	2.78	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
1:A:526:ARG:HG3	1:A:527:PHE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:159:ILE:HD11	2:C:245:ILE:HD12	1.93	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: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:289:LEU:O	1:A:293:ILE:HG23	2.10	0.51
2:R:135:THR:HG21	2:H:244:GLN:CD	2.30	0.51
2:P:8:ALA:HB2	2:P:94:LEU:HD21	1.92	0.51
2:S:23:ILE:HD13	2:J:7:ARG:HH21	1.74	0.51
1:A:705:MET:HA	1:A:848:MET:O	2.11	0.51
2:I:270:VAL:HG13	2:I:313:LEU:HB3	1.92	0.51
2:G:54:SER:H	2:G:57:GLN:HE21	1.57	0.51
2:I:25:LEU:HD12	2:I:26:GLU:H	1.75	0.51
1:A:144:ILE:H	1:A:144:ILE:HD12	1.75	0.51
1:B:323:PRO:HG3	1:B:512:GLU:HA	1.93	0.51
2:C:44:THR:O	2:C:45:LEU:HB2	2.11	0.51
2:F:337:GLY:O	2:F:339:LEU:N	2.43	0.51
1:A:540:SER:HB2	1:A:600:GLU:OE2	2.11	0.51
2:Q:54:SER:H	2:Q:57:GLN:NE2	2.07	0.51
2:D:257:LEU:CD1	2:D:300:PRO:HB3	2.39	0.51
2:D:175:PHE:O	2:D:178:ARG:HG3	2.10	0.51
2:I:31:GLU:O	2:I:35:ILE:HG13	2.09	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:245:ARG:HH22	1:B:471:TYR:HD2	1.59	0.51
2:C:20:GLU:HG2	2:C:21:ALA:N	2.24	0.51
1:B:753:ALA:HB1	1:B:815:ILE:HD13	1.91	0.51
1:A:130:ILE:O	1:A:134:VAL:HG23	2.11	0.51
2:F:263:LEU:O	2:F:267:ILE:HG13	2.11	0.51
2:Q:237:THR:HG23	2:Q:239:GLN:H	1.76	0.51
2:Q:96:THR:HG22	2:Q:98:GLU:HB2	1.91	0.51
1:B:248:ILE:CD1	1:B:892:MET:SD	2.99	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:B:577:TRP:HE3	1:B:577:TRP:HA	1.75	0.51
1:A:311:SER:HA	1:A:315:THR:HB	1.92	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:170:ASN:O	1:A:173:PRO:HD2	2.11	0.51
2:F:271:TYR:OH	2:F:292:PRO:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:O	1:A:376:VAL:HG23	2.11	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:S:270:VAL:HG13	2:S:313:LEU:HB3	1.93	0.51
2:G:44:THR:HG22	2:G:46:ARG:HB2	1.92	0.51
1:B:577:TRP:CE3	1:B:577:TRP:HA	2.46	0.51
1:A:370:ARG:O	1:A:401:ALA:HB1	2.11	0.51
1:A:148:ILE:HG23	1:A:149:PRO:HD2	1.92	0.50
1:B:425:LEU:HD12	1:B:436:CYS:HB3	1.92	0.50
1:A:175:LEU:HD13	1:A:180:ARG:HB2	1.93	0.50
2:P:20:GLU:HG2	2:P:21:ALA:H	1.75	0.50
1:B:54:THR:HG23	1:B:55:ARG:N	2.26	0.50
2:E:288:ARG:HG3	2:E:288:ARG:HH11	1.76	0.50
2:Q:34:GLY:O	2:Q:38:ASN:HB2	2.11	0.50
2:P:314:SER:O	2:P:317:ALA:HB3	2.11	0.50
2:J:339:LEU:HA	2:J:343:ILE:HD12	1.93	0.50
1:B:378:HIS:HA	1:B:449:TYR:CD2	2.46	0.50
2:I:191:ILE:HD12	2:I:242:MET:HB3	1.93	0.50
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
1:B:584:PHE:CD1	1:B:584:PHE:C	2.85	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
2:I:253:MET:HE1	2:J:344:ALA:HB3	1.92	0.50
1:B:653:ASN:CG	1:B:658:HIS:HD2	2.14	0.50
2:I:257:LEU:CD1	2:I:300:PRO:HB3	2.40	0.50
2:H:338:PRO:O	2:H:339:LEU:HB2	2.11	0.50
2:C:61:MET:O	2:C:64:MET:HB3	2.12	0.50
1:A:448:GLY:O	1:A:496:CYS:SG	2.66	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
2:R:257:LEU:CD1	2:R:300:PRO:HB3	2.38	0.50
2:G:273:PHE:O	2:G:278:TRP:HD1	1.95	0.50
1:B:693:ASP:OD2	1:B:695:GLU:HB2	2.12	0.50
1:A:622:ARG:HG3	2:F:31:GLU:OE1	2.12	0.50
2:G:257:LEU:HD12	2:G:300:PRO:HB3	1.92	0.50
2:C:259:GLN:HA	2:D:268:PHE:CD2	2.46	0.50
2:J:283:THR:HG23	2:J:293:ASN:HB2	1.93	0.50
2:Q:66:LEU:HD23	2:Q:84:TYR:CE2	2.46	0.50
2:I:16:ALA:HA	2:I:322:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:LEU:HD12	2:F:93:VAL:HG22	1.93	0.50
1:B:264:ILE:N	1:B:264:ILE:HD12	2.27	0.50
1:B:170:ASN:OD1	1:B:170:ASN:N	2.43	0.50
2:G:159:ILE:HD11	2:G:245:ILE:HB	1.94	0.50
2:G:43:LEU:HD12	2:G:93:VAL:HG22	1.93	0.50
1:A:388:THR:OG1	1:A:553:LEU:HD13	2.10	0.50
2:E:288:ARG:NH1	2:E:288:ARG:HG3	2.26	0.50
1:B:454:THR:HG22	1:B:455:ILE:N	2.27	0.50
1:A:193:GLU:HB3	1:A:204:VAL:HG23	1.94	0.50
2:I:281:LEU:O	2:I:285:ILE:HG13	2.12	0.50
1:B:357:LEU:HD21	1:B:397:GLN:HG3	1.92	0.50
1:A:454:THR:HG22	1:A:455:ILE:N	2.27	0.50
2:R:4:ILE:HG23	2:R:94:LEU:HB3	1.92	0.50
2:P:317:ALA:O	2:P:320:TYR:HB3	2.12	0.50
1:B:82:ILE:HA	1:B:144:ILE:HB	1.94	0.50
2:E:88:MET:O	2:E:91:ILE:HG22	2.12	0.50
2:P:282:ARG:HD3	2:P:286:ARG:CZ	2.42	0.50
1:B:497:TYR:CD1	1:B:520:LEU:HD23	2.47	0.50
1:B:526:ARG:CG	1:B:526:ARG:HH11	2.25	0.50
2:G:54:SER:H	2:G:57:GLN:NE2	2.09	0.50
1:A:487:THR:O	1:A:488:TYR:CB	2.60	0.50
2:R:317:ALA:O	2:R:320:TYR:HB3	2.12	0.50
1:B:265:TRP:CE2	1:B:886:ILE:HD11	2.46	0.50
2:D:64:MET:O	2:D:68:MET:HG3	2.11	0.50
2:G:50:MET:O	2:G:52:PRO:HD3	2.11	0.50
1:A:806:GLU:HA	1:A:811:SER:HA	1.93	0.50
1:A:300:GLY:HA3	1:A:586:PRO:HA	1.94	0.50
2:S:277:THR:HG23	2:S:329:MET:CE	2.42	0.50
2:E:158:MET:CE	2:E:244:GLN:HB2	2.41	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
1:A:340:VAL:O	1:A:343:ILE:HG23	2.12	0.49
2:J:269:ASN:ND2	2:J:274:ARG:HH22	2.06	0.49
1:A:303:ILE:HD11	1:A:585:GLU:CB	2.38	0.49
2:F:9:LEU:O	2:F:13:ARG:HG3	2.11	0.49
2:T:44:THR:HG22	2:T:46:ARG:HG3	1.93	0.49
2:F:40:TYR:CE1	2:F:64:MET:HG3	2.46	0.49
2:H:143:MET:SD	2:H:147:GLN:O	2.70	0.49
2:R:31:GLU:O	2:R:35:ILE:HG13	2.10	0.49
2:P:186:LEU:O	2:P:222:ILE:HA	2.12	0.49
1:A:281:VAL:HB	1:A:284:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLN:HA	1:A:443:PHE:CE2	2.47	0.49
2:E:148:ALA:HA	2:E:164:ASN:ND2	2.27	0.49
1:B:724:GLU:OE1	1:B:860:ARG:HB2	2.13	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:900:THR:HG22	1:A:901:VAL:H	1.77	0.49
1:A:485:PRO:HD2	1:A:901:VAL:HG13	1.95	0.49
2:Q:268:PHE:CE2	2:F:259:GLN:HA	2.48	0.49
2:P:64:MET:O	2:P:68:MET:HG3	2.12	0.49
1:A:614:MET:HG3	1:A:640:VAL:HG21	1.94	0.49
2:T:61:MET:O	2:T:64:MET:HB3	2.12	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
1:A:336:GLN:HE22	1:A:574:ILE:HD13	1.76	0.49
2:I:307:ILE:HA	2:I:310:LEU:HD12	1.93	0.49
2:S:288:ARG:NH1	2:S:288:ARG:HG3	2.27	0.49
2:T:69:MET:HG2	2:T:312:LEU:HB3	1.93	0.49
1:A:675:LEU:HD22	1:A:675:LEU:N	2.27	0.49
1:B:371:MET:HB2	1:B:405:TYR:CD1	2.46	0.49
1:A:408:TYR:CZ	1:A:410:TYR:HB3	2.47	0.49
2:G:288:ARG:HG3	2:G:288:ARG:HH11	1.77	0.49
2:P:281:LEU:HB2	2:P:329:MET:HE1	1.94	0.49
2:J:141:TRP:CZ3	2:J:240:ASN:HB3	2.48	0.49
2:P:253:MET:HE1	2:C:341:ALA:O	2.13	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
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:B:730:ASN:HB2	1:B:850:LYS:HA	1.95	0.49
1:A:303:ILE:O	1:A:582:ARG:HA	2.12	0.49
2:I:41:ASN:HD21	2:I:48:VAL:H	1.61	0.49
2:F:339:LEU:HA	2:F:343:ILE:HD12	1.95	0.49
1:A:721:PHE:C	1:A:723:GLN:H	2.13	0.49
2:F:210:VAL:HG22	2:F:233:VAL:HG13	1.94	0.49
1:A:382:THR:HG21	1:A:386:ARG:HH21	1.78	0.49
1:A:206:ILE:N	1:A:206:ILE:HD12	2.26	0.49
1:B:623:ARG:NH2	1:B:694:PHE:HE2	2.05	0.49
1:A:526:ARG:O	1:A:530:ILE:HG13	2.13	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
2:I:44:THR:O	2:I:45:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:7:ARG:NH2	2:Q:97:PRO:HA	2.28	0.49
1:B:197:VAL:HG21	1:B:200:ARG:HG3	1.93	0.49
2:T:40:TYR:CE2	2:T:64:MET:HG3	2.48	0.49
2:Q:182:MET:SD	2:Q:253:MET:HG3	2.53	0.49
1:B:873:ARG:NH2	2:G:38:ASN:ND2	2.61	0.49
1:B:497:TYR:O	1:B:501:LEU:HG	2.12	0.49
2:I:244:GLN:NE2	2:J:135:THR:HG21	2.28	0.49
2:D:53:THR:H	2:D:57:GLN:HE21	1.61	0.49
1:A:484:ASN:ND2	1:A:486:THR:OG1	2.46	0.49
1:B:802:TYR:CD2	1:B:815:ILE:HD11	2.48	0.49
2:S:7:ARG:NH2	2:I:23:ILE:HG22	2.28	0.49
1:B:54:THR:CG2	1:B:55:ARG:N	2.75	0.49
2:I:138:PRO:O	2:J:137:GLN:HG3	2.13	0.49
2:F:237:THR:HG23	2:F:239:GLN:H	1.78	0.49
2:H:33:LEU:HB2	2:H:50:MET:HE3	1.95	0.49
2:S:268:PHE:CD2	2:J:259:GLN:HA	2.48	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:A:57:VAL:CG2	1:A:301:GLU:HG2	2.42	0.49
1:B:718:ILE:CD1	1:B:832:PHE:HA	2.43	0.49
2:S:101:PHE:HE1	2:I:17:THR:HG22	1.77	0.49
2:F:93:VAL:O	2:F:99:ILE:HD12	2.13	0.49
2:H:41:ASN:HD21	2:H:48:VAL:HG23	1.77	0.49
1:B:717:ASP:HB3	1:B:720:ARG:HB2	1.95	0.49
1:B:461:ASP:HA	2:E:22:ARG:O	2.13	0.49
2:G:314:SER:O	2:G:317:ALA:HB3	2.12	0.49
2:T:288:ARG:HG3	2:T:288:ARG:NH1	2.28	0.49
1:A:314:LEU:HD13	1:A:515:TYR:HB2	1.95	0.48
1:B:205:PHE:N	1:B:205:PHE:CD1	2.80	0.48
2:I:4:ILE:HG23	2:I:94:LEU:CB	2.43	0.48
1:A:429:ILE:N	1:A:429:ILE:HD12	2.28	0.48
1:A:205:PHE:CE1	1:A:874:PHE:HB3	2.47	0.48
2:P:148:ALA:HA	2:P:164:ASN:ND2	2.28	0.48
1:B:890:LEU:HD22	1:B:890:LEU:N	2.28	0.48
2:R:135:THR:HG21	2:H:244:GLN:NE2	2.28	0.48
1:A:95:THR:OG1	1:A:102:LEU:HD21	2.13	0.48
2:I:41:ASN:ND2	2:I:46:ARG:O	2.46	0.48
2:F:53:THR:H	2:F:57:GLN:HE22	1.58	0.48
2:Q:41:ASN:HD21	2:Q:48:VAL:H	1.61	0.48
2:S:41:ASN:HD21	2:S:48:VAL:H	1.62	0.48
1:B:627:VAL:CG2	1:B:777:VAL:HA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:LEU:O	1:B:523:HIS:HB3	2.13	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
2:Q:39:ARG:HB3	2:Q:39:ARG:HH11	1.79	0.48
2:T:7:ARG:O	2:T:11:VAL:HG23	2.14	0.48
1:A:316:GLN:HG2	1:A:317:ARG:N	2.29	0.48
2:T:271:TYR:OH	2:T:292:PRO:HG2	2.13	0.48
1:B:873:ARG:CZ	2:G:39:ARG:HB2	2.43	0.48
2:J:271:TYR:CE1	2:J:286:ARG:NH1	2.82	0.48
1:A:402:LEU:CD1	1:A:425:LEU:HD11	2.42	0.48
2:D:54:SER:H	2:D:57:GLN:HE21	1.60	0.48
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:E:54:SER:H	2:E:57:GLN:NE2	2.12	0.48
1:A:624:PHE:HE2	1:A:694:PHE:CZ	2.32	0.48
2:R:96:THR:CG2	2:R:98:GLU:HB2	2.44	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
2:Q:188:TRP:CZ2	2:Q:219:ALA:HB2	2.48	0.48
2:S:43:LEU:HD12	2:S:93:VAL:HG22	1.96	0.48
1:A:410:TYR:HD1	1:A:410:TYR:H	1.61	0.48
2:H:158:MET:HE3	2:H:245:ILE:O	2.12	0.48
2:I:308:LEU:O	2:I:312:LEU:HD13	2.13	0.48
2:Q:178:ARG:H	2:Q:178:ARG:HD2	1.77	0.48
1:A:283:ARG:HA	1:A:563:ASN:HD21	1.79	0.48
2:F:338:PRO:O	2:F:339:LEU:HB2	2.14	0.48
1:B:646:GLU:HA	1:B:649:LYS:HD3	1.96	0.48
2:R:271:TYR:CD1	2:R:286:ARG:NH1	2.82	0.48
1:B:100:ARG:CD	1:B:724:GLU:HG2	2.43	0.48
2:R:53:THR:H	2:R:57:GLN:NE2	2.11	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:584:PHE:HD1	1:B:584:PHE:C	2.17	0.48
2:H:171:VAL:O	2:H:174:ILE:HG22	2.13	0.48
2:F:61:MET:O	2:F:64:MET:HB3	2.14	0.48
1:B:386:ARG:HG3	1:B:456:ASP:OD1	2.14	0.48
2:S:288:ARG:HH11	2:S:288:ARG:HG3	1.79	0.48
2:G:141:TRP:CZ3	2:G:240:ASN:HB3	2.47	0.48
2:E:7:ARG:O	2:E:11:VAL:HG23	2.14	0.48
2:G:26:GLU:HG2	2:G:29:VAL:HG23	1.96	0.48
1:B:281:VAL:HB	1:B:284:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:200:ASN:H	2:R:200:ASN:ND2	2.11	0.48
1:B:385:GLY:HA2	1:B:443:PHE:O	2.13	0.48
1:B:315:THR:HG22	1:B:317:ARG:H	1.79	0.48
1:B:875:VAL:HG21	2:G:38:ASN:ND2	2.27	0.48
1:A:275:PRO:HB3	1:A:467:HIS:CE1	2.49	0.48
2:J:44:THR:O	2:J:45:LEU:HB2	2.14	0.48
1:A:484:ASN:HB3	1:A:487:THR:H	1.78	0.48
2:S:44:THR:HG22	2:S:46:ARG:HB2	1.95	0.48
1:B:219:ARG:HG3	1:B:686:GLU:HG3	1.94	0.48
2:T:88:MET:O	2:T:91:ILE:HG22	2.13	0.48
2:H:317:ALA:O	2:H:320:TYR:HB3	2.13	0.48
2:G:281:LEU:O	2:G:285:ILE:HG13	2.14	0.48
2:I:200:ASN:H	2:I:200:ASN:ND2	2.11	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:B:526:ARG:HH11	1:B:526:ARG:HG3	1.79	0.48
1:A:301:GLU:HG3	1:A:587:THR:HG23	1.95	0.48
2:G:317:ALA:O	2:G:320:TYR:HB3	2.14	0.48
2:D:281:LEU:O	2:D:285:ILE:HG13	2.14	0.48
1:A:345:LEU:HA	1:A:348:MET:HG2	1.96	0.48
2:S:53:THR:N	2:S:57:GLN:NE2	2.59	0.47
1:A:279:TRP:CZ3	1:A:541:VAL:O	2.62	0.47
1:B:92:HIS:HD2	1:B:167:GLU:O	1.96	0.47
1:A:761:ALA:O	1:A:765:ILE:HG13	2.14	0.47
1:A:283:ARG:NH2	1:B:490:ILE:HA	2.29	0.47
2:R:66:LEU:O	2:R:70:LEU:HG	2.13	0.47
1:A:771:TRP:N	1:A:771:TRP:CD1	2.82	0.47
2:C:107:ASN:HD22	2:C:107:ASN:H	1.60	0.47
1:B:882:ARG:HB3	1:B:884:MET:HE2	1.96	0.47
1:A:705:MET:HE3	1:A:799:PRO:HD2	1.95	0.47
1:A:653:ASN:HA	1:A:656:HIS:HB2	1.95	0.47
2:J:337:GLY:O	2:J:339:LEU:HD12	2.15	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:G:16:ALA:HA	2:G:322:VAL:HG21	1.95	0.47
2:F:281:LEU:O	2:F:285:ILE:HG13	2.14	0.47
2:J:88:MET:O	2:J:91:ILE:HG22	2.14	0.47
2:T:212:VAL:O	2:T:215:VAL:HG12	2.14	0.47
1:B:790:PRO:HG2	1:B:795:LEU:CD2	2.33	0.47
2:H:271:TYR:OH	2:H:292:PRO:HG2	2.13	0.47
2:P:23:ILE:HG22	2:D:7:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:270:VAL:HG13	2:E:313:LEU:HB3	1.96	0.47
2:Q:189:ARG:HD2	2:Q:244:GLN:HE21	1.78	0.47
2:I:338:PRO:O	2:I:339:LEU:HB2	2.14	0.47
1:A:900:THR:HG22	1:A:901:VAL:N	2.29	0.47
2:S:7:ARG:NH2	2:S:97:PRO:HA	2.30	0.47
1:B:446:GLY:O	1:B:452:TRP:HB2	2.14	0.47
2:S:39:ARG:HB3	2:S:93:VAL:HG13	1.95	0.47
2:E:212:VAL:O	2:E:215:VAL:HG12	2.14	0.47
1:A:810:LEU:O	1:A:811:SER:HB3	2.13	0.47
1:A:314:LEU:HD11	1:A:512:GLU:HA	1.94	0.47
1:B:873:ARG:HH21	2:G:38:ASN:ND2	2.12	0.47
1:B:663:ILE:H	1:B:663:ILE:HD12	1.78	0.47
2:H:68:MET:CE	2:H:94:LEU:HD11	2.44	0.47
1:B:126:PHE:CZ	1:B:130:ILE:HD11	2.50	0.47
2:T:1:MET:HA	2:T:4:ILE:HD12	1.97	0.47
2:Q:178:ARG:HG2	2:Q:178:ARG:HH11	1.79	0.47
2:D:189:ARG:HD2	2:D:244:GLN:HE21	1.79	0.47
1:A:321:THR:O	1:A:325:ALA:HB2	2.14	0.47
2:H:61:MET:O	2:H:64:MET:HB3	2.15	0.47
1:B:233:ARG:NH1	1:B:233:ARG:HG2	2.28	0.47
1:B:393:ASN:O	1:B:397:GLN:HG2	2.14	0.47
1:A:324:PHE:CE1	1:A:372:VAL:HG22	2.50	0.47
1:A:494:TYR:CG	1:A:497:TYR:HB2	2.49	0.47
2:Q:271:TYR:CE1	2:Q:286:ARG:NH1	2.82	0.47
1:B:530:ILE:O	1:B:534:ILE:HG13	2.13	0.47
2:E:337:GLY:H	2:E:338:PRO:HD3	1.78	0.47
2:I:23:ILE:HD12	2:I:23:ILE:O	2.14	0.47
1:B:228:GLN:O	1:B:231:GLU:HG2	2.14	0.47
2:P:281:LEU:O	2:P:285:ILE:HG13	2.14	0.47
1:A:81:LYS:O	1:A:143:PHE:HA	2.14	0.47
2:D:50:MET:C	2:D:52:PRO:HD3	2.35	0.47
1:A:598:LEU:O	1:A:602:VAL:HG23	2.15	0.47
2:C:138:PRO:O	2:D:137:GLN:HG3	2.15	0.47
1:A:349:PHE:N	1:A:350:PRO:HA	2.30	0.47
1:B:526:ARG:NH1	1:B:526:ARG:HG3	2.29	0.47
2:F:54:SER:H	2:F:57:GLN:HE21	1.62	0.47
2:J:7:ARG:O	2:J:11:VAL:HG23	2.15	0.47
2:R:25:LEU:HG	2:H:28:ASN:HD21	1.80	0.47
2:C:66:LEU:O	2:C:70:LEU:HG	2.14	0.47
1:B:790:PRO:CG	1:B:795:LEU:HD21	2.35	0.47
1:A:332:PRO:HB2	1:A:336:GLN:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:MET:HE2	1:B:853:ILE:H	1.80	0.47
1:B:71:ILE:HG13	1:B:647:ALA:HB1	1.97	0.47
1:A:842:ILE:N	1:A:842:ILE:HD12	2.30	0.47
1:B:421:THR:HB	1:B:426:ASP:OD2	2.15	0.47
2:G:44:THR:O	2:G:45:LEU:HB2	2.15	0.47
1:A:175:LEU:O	1:A:175:LEU:HD12	2.14	0.47
1:B:755:MET:HG3	2:S:50:MET:HG3	1.95	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:623:ARG:HE	2:F:98:GLU:HG2	1.79	0.47
2:R:186:LEU:O	2:R:222:ILE:HA	2.14	0.47
1:A:471:TYR:CB	1:A:535:ASN:HD21	2.20	0.47
1:A:356:ASP:O	1:A:394:MET:SD	2.73	0.47
2:D:271:TYR:OH	2:D:292:PRO:HG2	2.15	0.47
1:A:160:GLU:O	1:A:163:VAL:HG12	2.15	0.47
1:A:466:VAL:O	1:A:466:VAL:HG12	2.14	0.47
1:A:179:HIS:HA	1:A:182:MET:HE2	1.96	0.47
1:A:659:ASN:O	1:A:660:PHE:HB3	2.14	0.47
2:P:40:TYR:CE1	2:P:64:MET:HG3	2.49	0.47
2:J:61:MET:O	2:J:64:MET:HB3	2.15	0.47
2:S:69:MET:HG2	2:S:312:LEU:HB3	1.95	0.47
2:G:208:VAL:HG13	2:G:234:ARG:O	2.15	0.47
2:D:98:GLU:HG3	2:D:98:GLU:H	1.52	0.47
1:A:354:ILE:HG22	1:A:355:LEU:N	2.29	0.47
1:A:729:THR:HG21	1:A:731:MET:HB2	1.97	0.47
1:A:591:GLU:HA	1:A:895:LYS:CE	2.43	0.47
2:J:200:ASN:HD22	2:J:200:ASN:H	1.61	0.47
2:G:141:TRP:HA	2:G:242:MET:SD	2.55	0.47
2:S:271:TYR:CD1	2:S:286:ARG:NH1	2.82	0.47
1:B:20:GLY:HA3	1:B:304:ALA:O	2.15	0.47
2:J:189:ARG:HD2	2:J:244:GLN:HE21	1.81	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:D:128:PHE:HB2	2:D:247:VAL:HG11	1.97	0.47
1:A:65:GLN:C	1:A:67:ILE:H	2.18	0.47
1:A:65:GLN:C	1:A:67:ILE:N	2.67	0.47
1:B:777:VAL:HG23	1:B:779:ARG:HE	1.80	0.46
2:G:96:THR:HG22	2:G:98:GLU:CB	2.41	0.46
2:C:269:ASN:ND2	2:C:274:ARG:HH22	2.08	0.46
1:A:274:ASN:O	1:A:277:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:22:ARG:C	2:F:23:ILE:HG13	2.35	0.46
2:T:41:ASN:ND2	2:T:48:VAL:H	2.12	0.46
1:A:90:PHE:HB2	1:A:166:VAL:HG23	1.96	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:C:12:MET:HG2	2:C:65:CYS:HB3	1.97	0.46
1:B:242:LEU:HD23	1:B:242:LEU:O	2.15	0.46
2:E:129:PHE:CE2	2:E:159:ILE:HG23	2.50	0.46
2:Q:88:MET:O	2:Q:91:ILE:HG22	2.15	0.46
2:E:317:ALA:O	2:E:320:TYR:HB3	2.15	0.46
1:B:724:GLU:C	1:B:726:PHE:N	2.69	0.46
1:B:368:ALA:O	1:B:372:VAL:HG23	2.15	0.46
2:E:44:THR:CG2	2:E:46:ARG:HB2	2.45	0.46
1:B:533:ILE:HG22	1:B:538:LEU:HD23	1.97	0.46
2:S:26:GLU:HB3	2:S:29:VAL:CG2	2.45	0.46
1:A:165:GLY:O	1:A:166:VAL:CB	2.63	0.46
2:T:277:THR:O	2:T:329:MET:HE1	2.14	0.46
1:B:315:THR:HG22	1:B:316:GLN:N	2.30	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: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:H:44:THR:CG2	2:H:46:ARG:HG3	2.43	0.46
2:T:317:ALA:O	2:T:320:TYR:HB3	2.15	0.46
1:B:213:ILE:HD12	1:B:213:ILE:N	2.30	0.46
2:R:4:ILE:HG23	2:R:94:LEU:CB	2.46	0.46
2:J:67:ASP:HB3	2:J:90:THR:HG21	1.97	0.46
2:Q:314:SER:O	2:Q:317:ALA:HB3	2.14	0.46
2:S:61:MET:O	2:S:64:MET:HB3	2.15	0.46
1:A:454:THR:HG21	1:A:475:CYS:HA	1.96	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:B:678:SER:OG	1:B:681:LEU:HB2	2.15	0.46
1:A:223:TYR:CD2	1:A:679:LEU:HD12	2.49	0.46
1:A:754:ASN:HD22	1:B:256:THR:HA	1.79	0.46
1:B:900:THR:HG22	1:B:901:VAL:H	1.80	0.46
1:B:584:PHE:HD1	1:B:585:GLU:N	2.14	0.46
1:A:662:ASN:OD1	1:B:485:PRO:HB3	2.16	0.46
1:A:877:TYR:N	1:A:877:TYR:CD1	2.83	0.46
2:I:64:MET:O	2:I:68:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:190:ARG:HA	2:S:243:VAL:HG12	1.97	0.46
2:C:10:THR:HG22	2:C:32:ILE:HD13	1.97	0.46
1:B:216:ILE:HD12	1:B:216:ILE:N	2.30	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
1:A:672:LEU:HD23	1:A:672:LEU:HA	1.67	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
2:F:24:VAL:HG23	2:F:24:VAL:O	2.15	0.46
2:Q:41:ASN:HD21	2:Q:48:VAL:HG23	1.81	0.46
2:J:128:PHE:HB2	2:J:247:VAL:HG11	1.97	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
1:A:178:GLU:HG2	1:A:179:HIS:N	2.29	0.46
2:I:9:LEU:O	2:I:13:ARG:HG3	2.16	0.46
2:E:189:ARG:HG2	2:F:132:THR:O	2.15	0.46
1:B:851:VAL:HG12	1:B:852:PHE:N	2.30	0.46
2:R:191:ILE:HA	2:G:135:THR:O	2.16	0.46
2:T:271:TYR:CD1	2:T:286:ARG:NH1	2.84	0.46
1:A:403:ASN:ND2	1:A:425:LEU:N	2.63	0.46
1:A:239:LEU:HG	1:A:271:LEU:HD13	1.98	0.46
2:Q:269:ASN:ND2	2:Q:274:ARG:HH22	2.09	0.46
1:A:705:MET:CE	1:A:799:PRO:HD2	2.46	0.46
1:A:321:THR:O	1:A:322:GLY:O	2.34	0.46
1:A:651:VAL:O	1:A:654:LEU:HG	2.16	0.46
1:B:835:THR:HG22	1:B:836:PRO:HD2	1.97	0.46
1:B:312:ILE:H	1:B:312:ILE:HD12	1.80	0.46
2:F:141:TRP:HA	2:F:242:MET:SD	2.56	0.46
1:A:319:THR:O	1:A:319:THR:HG22	2.16	0.46
2:S:271:TYR:OH	2:S:292:PRO:HG2	2.15	0.46
2:T:271:TYR:CE1	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
1:B:522:PHE:CZ	1:B:583:SER:HB3	2.51	0.45
2:S:124:GLN:OE1	2:S:254:ASP:HB2	2.15	0.45
1:A:596:ALA:O	1:A:600:GLU:HG3	2.16	0.45
2:C:135:THR:HA	2:C:153:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:THR:HG21	2:C:101:PHE:HA	1.97	0.45
2:R:187:VAL:O	2:R:187:VAL:HG13	2.16	0.45
1:B:126:PHE:O	1:B:129:THR:HB	2.16	0.45
2:E:56:ALA:O	2:E:60:GLU:HB2	2.16	0.45
1:B:882:ARG:HB3	1:B:884:MET:CE	2.46	0.45
1:B:331:THR:CG2	1:B:337:LEU:HB2	2.46	0.45
1:A:469:GLN:CD	1:A:469:GLN:H	2.18	0.45
2:E:49:THR:HG22	2:E:51:ARG:H	1.81	0.45
2:R:23:ILE:O	2:R:23:ILE:HD12	2.16	0.45
1:A:483:ILE:HD11	1:A:532:GLN:HG3	1.98	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:782:ARG:HD3	1:A:782:ARG:HA	1.71	0.45
2:H:187:VAL:HG13	2:H:187:VAL:O	2.17	0.45
2:S:271:TYR:CE1	2:S:286:ARG:NH1	2.85	0.45
1:A:754:ASN:HD21	1:B:257:ASP:H	1.62	0.45
2:R:99:ILE:HA	2:R:100:PRO:HD3	1.73	0.45
2:J:41:ASN:HD21	2:J:48:VAL:HG23	1.80	0.45
2:I:28:ASN:H	2:I:28:ASN:HD22	1.62	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
2:P:257:LEU:HD12	2:P:300:PRO:HB3	1.98	0.45
2:R:17:THR:HG22	2:R:17:THR:O	2.17	0.45
2:G:329:MET:HE3	2:G:329:MET:HB2	1.89	0.45
1:A:460:ARG:HG3	1:A:471:TYR:CZ	2.51	0.45
1:B:337:LEU:CD2	1:B:582:ARG:HH12	2.29	0.45
1:B:873:ARG:HG3	2:G:39:ARG:HD3	1.99	0.45
1:B:271:LEU:HD23	1:B:890:LEU:HD12	1.98	0.45
1:B:746:TYR:HA	1:B:817:TYR:CD2	2.52	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:460:ARG:NH2	1:B:480:ARG:HH12	2.15	0.45
2:R:22:ARG:C	2:R:23:ILE:HG13	2.36	0.45
2:J:263:LEU:O	2:J:267:ILE:HG13	2.17	0.45
1:B:612:VAL:O	1:B:616:HIS:HD2	1.98	0.45
1:B:115:GLY:HA3	1:B:129:THR:HG23	1.99	0.45
1:B:470:ARG:HD3	1:B:546:ASP:OD1	2.16	0.45
2:J:244:GLN:O	2:J:244:GLN:HG3	2.16	0.45
2:D:20:GLU:HG2	2:D:21:ALA:H	1.82	0.45
1:A:161:PRO:HG2	1:A:162:GLU:OE2	2.16	0.45
1:B:409:MET:CG	1:B:413:ARG:HD3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:54:SER:OG	2:J:57:GLN:HG3	2.16	0.45
1:A:282:PRO:O	1:A:656:HIS:HE1	1.99	0.45
1:B:255:LEU:HD22	1:B:255:LEU:HA	1.81	0.45
2:H:139:GLY:O	2:H:194:PHE:HB2	2.17	0.45
1:A:738:ILE:HG13	1:A:739:ASP:N	2.31	0.45
2:S:303:ASP:O	2:S:307:ILE:HG12	2.17	0.45
2:E:271:TYR:CE1	2:E:286:ARG:NH1	2.84	0.45
1:A:425:LEU:HD12	1:A:436:CYS:CB	2.44	0.45
2:Q:44:THR:O	2:Q:45:LEU:HB2	2.17	0.45
1:B:268:ALA:O	1:B:269:LEU:HD23	2.16	0.45
2:T:288:ARG:HG3	2:T:288:ARG:HH11	1.82	0.45
1:A:421:THR:HG22	1:A:423:GLU:HB2	1.99	0.45
1:B:826:LEU:HD12	1:B:828:TYR:CE1	2.51	0.45
2:F:200:ASN:H	2:F:200:ASN:ND2	2.15	0.45
2:F:189:ARG:HD2	2:F:244:GLN:HE21	1.80	0.45
1:A:662:ASN:ND2	1:B:485:PRO:HB3	2.32	0.45
1:A:526:ARG:CG	1:A:527:PHE:N	2.79	0.45
1:A:284:SER:HB2	1:A:288:ASN:ND2	2.32	0.45
1:B:414:VAL:HG12	1:B:415:GLN:N	2.32	0.45
1:A:365:MET:O	1:A:366:ASP:C	2.55	0.45
2:S:269:ASN:ND2	2:S:274:ARG:HH22	2.08	0.45
2:R:273:PHE:O	2:R:274:ARG:HB2	2.17	0.45
2:P:191:ILE:HA	2:C:135:THR:O	2.17	0.45
2:I:186:LEU:HA	2:I:246:GLN:O	2.17	0.45
2:C:69:MET:HG3	2:C:316:LEU:HD22	1.98	0.45
1:A:814:THR:OG1	1:B:253:GLU:HG2	2.17	0.45
2:J:186:LEU:O	2:J:222:ILE:HA	2.16	0.45
2:Q:200:ASN:ND2	2:Q:200:ASN:H	2.14	0.45
1:B:869:VAL:O	1:B:870:LEU:C	2.55	0.45
1:A:367:PRO:O	1:A:371:MET:HG3	2.17	0.45
1:A:332:PRO:HB2	1:A:336:GLN:CG	2.46	0.45
1:A:129:THR:O	1:A:133:LYS:HG3	2.17	0.45
2:I:46:ARG:NH2	2:I:67:ASP:OD2	2.50	0.45
1:B:14:THR:HG22	1:B:15:THR:N	2.32	0.45
1:B:842:ILE:N	1:B:842:ILE:HD12	2.29	0.45
1:B:628:LEU:H	1:B:628:LEU:HD23	1.82	0.45
2:C:337:GLY:O	2:C:339:LEU:N	2.50	0.45
1:B:454:THR:HG22	1:B:455:ILE:H	1.82	0.45
2:H:37:ILE:HG23	2:H:48:VAL:HB	1.99	0.45
1:A:623:ARG:NH2	1:A:692:ASN:O	2.49	0.45
2:Q:281:LEU:O	2:Q:285:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ASP:HA	1:A:566:PRO:HD2	1.75	0.45
2:C:171:VAL:O	2:C:174:ILE:HG22	2.17	0.45
1:A:710:LEU:HD22	1:A:710:LEU:HA	1.72	0.45
2:R:271:TYR:CE1	2:R:286:ARG:NH1	2.86	0.44
1:A:424:PRO:O	1:A:440:ARG:HD2	2.17	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:G:54:SER:OG	2:G:57:GLN:HG3	2.17	0.44
2:C:41:ASN:ND2	2:C:46:ARG:O	2.50	0.44
2:P:61:MET:O	2:P:64:MET:HB3	2.17	0.44
1:B:494:TYR:HD1	1:B:524:MET:CE	2.30	0.44
2:G:4:ILE:HG23	2:G:94:LEU:HB3	1.98	0.44
1:B:193:GLU:HG3	1:B:204:VAL:HB	1.99	0.44
2:Q:159:ILE:HD11	2:Q:245:ILE:HB	1.98	0.44
2:J:112:VAL:O	2:J:116:THR:HB	2.17	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
2:E:158:MET:HE1	2:E:244:GLN:HB2	1.98	0.44
1:B:221:GLN:O	1:B:224:ILE:HG12	2.16	0.44
1:A:616:HIS:CE1	1:A:688:TRP:HB3	2.52	0.44
2:E:61:MET:O	2:E:64:MET:HB3	2.17	0.44
2:I:151:ALA:CB	2:I:171:VAL:HG13	2.47	0.44
1:B:659:ASN:C	1:B:660:PHE:CD1	2.90	0.44
1:A:343:ILE:O	1:A:347:LEU:HB3	2.17	0.44
2:D:270:VAL:HB	2:D:286:ARG:NH2	2.32	0.44
2:G:235:ASN:OD1	2:G:237:THR:HG22	2.18	0.44
1:A:90:PHE:O	1:A:166:VAL:HA	2.17	0.44
2:R:66:LEU:HD23	2:R:84:TYR:CE1	2.53	0.44
2:J:193:ASN:HD21	2:J:201:SER:HB3	1.83	0.44
2:P:105:ALA:O	2:P:109:ILE:HG12	2.17	0.44
2:S:253:MET:HE1	2:I:341:ALA:O	2.17	0.44
1:B:349:PHE:HA	1:B:350:PRO:HD2	1.63	0.44
1:B:279:TRP:CZ2	1:B:544:LEU:HA	2.53	0.44
2:S:104:GLU:O	2:S:108:GLU:HG3	2.17	0.44
2:S:263:LEU:O	2:S:267:ILE:HG13	2.18	0.44
2:Q:189:ARG:HH11	2:Q:244:GLN:HE21	1.65	0.44
1:B:729:THR:HA	1:B:824:PHE:O	2.17	0.44
1:A:274:ASN:HA	1:A:275:PRO:HD2	1.67	0.44
2:R:313:LEU:HA	2:R:313:LEU:HD23	1.85	0.44
1:A:250:TYR:HD1	1:A:892:MET:O	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:308:LEU:HD22	2:R:312:LEU:HD22	1.99	0.44
2:S:191:ILE:HA	2:I:135:THR:O	2.18	0.44
1:B:312:ILE:HD12	1:B:312:ILE:N	2.33	0.44
2:I:43:LEU:HD12	2:I:93:VAL:HG22	1.99	0.44
2:S:166:GLY:HA2	2:S:235:ASN:O	2.17	0.44
2:R:259:GLN:HA	2:G:268:PHE:CD2	2.53	0.44
2:J:235:ASN:OD1	2:J:237:THR:HG22	2.17	0.44
1:A:117:VAL:HG12	1:A:819:THR:CG2	2.47	0.44
2:I:271:TYR:CD1	2:I:286:ARG:NH1	2.85	0.44
1:B:337:LEU:HD22	1:B:337:LEU:O	2.18	0.44
1:A:85:VAL:CG1	1:A:163:VAL:HA	2.44	0.44
1:B:427:PHE:HD2	1:B:429:ILE:HG13	1.82	0.44
1:B:425:LEU:HB3	1:B:436:CYS:O	2.18	0.44
1:B:71:ILE:CG1	1:B:647:ALA:HB1	2.47	0.44
1:A:596:ALA:N	1:A:597:PRO:HD2	2.33	0.44
2:C:10:THR:HG23	2:C:102:THR:HG23	1.99	0.44
2:H:185:TYR:O	2:H:248:VAL:HG12	2.18	0.44
2:R:141:TRP:CZ3	2:R:240:ASN:HB3	2.53	0.44
1:B:149:PRO:HB2	1:B:160:GLU:HG3	2.00	0.44
2:S:91:ILE:HG23	2:S:92:GLY:N	2.33	0.44
2:J:23:ILE:O	2:J:23:ILE:HD12	2.17	0.44
1:B:358:LYS:HB3	1:B:571:VAL:O	2.17	0.44
1:B:873:ARG:HG2	1:B:874:PHE:H	1.80	0.44
1:A:332:PRO:HG2	1:A:336:GLN:HE21	1.82	0.44
2:S:189:ARG:HD2	2:S:244:GLN:HE21	1.81	0.44
2:S:124:GLN:HB3	2:S:125:PRO:HD2	1.98	0.44
1:B:435:ASP:OD1	1:B:437:ASN:HB2	2.18	0.44
1:B:289:LEU:HD13	1:B:290:ILE:N	2.32	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
1:B:146:HIS:CE1	1:B:879:GLY:HA2	2.53	0.44
1:A:572:SER:HB2	1:A:575:SER:HB3	1.99	0.44
1:B:333:THR:HB	1:B:335:GLN:H	1.82	0.44
1:A:522:PHE:O	1:A:525:VAL:HG22	2.17	0.44
2:J:338:PRO:O	2:J:339:LEU:HB2	2.18	0.44
2:R:61:MET:O	2:R:64:MET:HB3	2.17	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:T:200:ASN:ND2	2:T:200:ASN:H	2.16	0.44
1:A:355:LEU:HA	1:A:355:LEU:HD23	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:271:TYR:HH	2:J:292:PRO:HG2	1.82	0.44
1:A:111:MET:HA	1:A:114:VAL:CG2	2.47	0.44
1:A:465:TYR:HD2	1:A:539:HIS:CD2	2.35	0.44
1:A:277:VAL:HG12	1:A:674:SER:O	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:J:281:LEU:O	2:J:285:ILE:HG13	2.18	0.44
1:A:888:GLN:O	1:A:891:LYS:HG2	2.17	0.44
2:D:26:GLU:HB3	2:D:29:VAL:HG23	1.99	0.44
2:S:9:LEU:O	2:S:13:ARG:HG3	2.18	0.44
2:F:295:LEU:HD23	2:F:295:LEU:HA	1.82	0.44
2:R:265:ALA:HB1	2:H:261:PRO:HD3	2.00	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
1:A:388:THR:CG2	1:A:389:ASN:N	2.81	0.44
2:G:12:MET:HG2	2:G:65:CYS:HB3	2.00	0.44
1:A:678:SER:O	1:A:682:VAL:HG22	2.18	0.44
2:I:7:ARG:HH21	2:J:23:ILE:HG22	1.82	0.43
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:I:7:ARG:O	2:I:11:VAL:HG23	2.18	0.43
1:A:390:LEU:HD13	1:A:394:MET:HG2	2.00	0.43
2:I:116:THR:HG21	2:I:304:ARG:CB	2.40	0.43
1:A:111:MET:HE2	1:A:137:ILE:HD11	2.00	0.43
1:A:472:ILE:N	1:A:472:ILE:HD12	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
1:A:82:ILE:HG12	1:A:144:ILE:CD1	2.48	0.43
1:A:312:ILE:O	1:A:316:GLN:HB2	2.18	0.43
2:S:182:MET:SD	2:S:253:MET:HG3	2.57	0.43
2:Q:187:VAL:HG13	2:Q:246:GLN:HB3	1.99	0.43
2:J:12:MET:HG2	2:J:65:CYS:HB3	2.00	0.43
1:A:119:THR:HG22	1:A:120:GLU:O	2.18	0.43
2:Q:264:THR:HA	2:Q:267:ILE:HD12	1.99	0.43
1:A:405:TYR:O	1:A:408:TYR:HB3	2.18	0.43
1:A:451:GLY:O	1:A:452:TRP:HB3	2.17	0.43
1:A:450:ASN:HB2	1:A:494:TYR:OH	2.19	0.43
1:A:133:LYS:O	1:A:136:PHE:HB3	2.17	0.43
2:G:158:MET:HE3	2:G:245:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:TRP:HZ2	1:B:14:THR:CG2	2.30	0.43
1:B:36:LEU:HG	1:B:290:ILE:CD1	2.45	0.43
1:A:563:ASN:O	1:A:564:ALA:HB2	2.18	0.43
1:B:455:ILE:HD12	1:B:455:ILE:N	2.33	0.43
2:E:53:THR:H	2:E:57:GLN:NE2	2.16	0.43
2:D:204:THR:HG23	2:D:241:ALA:HB1	2.01	0.43
1:A:122:GLU:N	1:A:123:PRO:HD3	2.33	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
2:R:105:ALA:O	2:R:109:ILE:HG12	2.17	0.43
2:D:50:MET:O	2:D:52:PRO:HD3	2.18	0.43
2:I:61:MET:O	2:I:64:MET:HB3	2.18	0.43
1:B:187:LEU:C	1:B:189:GLY:H	2.21	0.43
1:B:475:CYS:HB2	1:B:477:ILE:CD1	2.48	0.43
1:A:841:LEU:N	1:A:841:LEU:HD23	2.33	0.43
1:A:494:TYR:CD1	1:A:497:TYR:HB2	2.54	0.43
2:D:271:TYR:CE1	2:D:286:ARG:NH1	2.86	0.43
1:A:102:LEU:HD23	1:A:102:LEU:N	2.34	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
1:B:538:LEU:O	1:B:538:LEU:HD12	2.18	0.43
1:B:192:ILE:O	1:B:194:ASN:N	2.51	0.43
2:J:288:ARG:HG3	2:J:288:ARG:HH11	1.83	0.43
1:B:543:SER:O	1:B:544:LEU:HB3	2.18	0.43
2:R:281:LEU:O	2:R:285:ILE:HG13	2.19	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
2:Q:23:ILE:HG22	2:F:101:PHE:CE2	2.54	0.43
2:R:24:VAL:HG11	2:R:30:MET:HE2	2.00	0.43
2:I:271:TYR:CE1	2:I:286:ARG:NH1	2.86	0.43
2:Q:260:TYR:O	2:Q:263:LEU:HB2	2.18	0.43
1:A:540:SER:C	1:A:542:PHE:H	2.22	0.43
2:C:249:PHE:HZ	2:D:298:ILE:HG23	1.82	0.43
1:A:521:PRO:O	1:A:525:VAL:HG13	2.19	0.43
1:B:200:ARG:O	1:B:201:ASP:CB	2.67	0.43
1:A:622:ARG:HH11	2:F:100:PRO:CB	2.31	0.43
1:B:300:GLY:HA3	1:B:584:PHE:CE1	2.53	0.43
1:B:384:GLY:C	1:B:386:ARG:H	2.22	0.43
2:I:179:ASN:HB2	2:I:181:PRO:HD3	1.99	0.43
2:F:128:PHE:HB2	2:F:247:VAL:HG11	2.00	0.43
2:C:329:MET:HB2	2:C:329:MET:HE3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:309:THR:O	2:T:313:LEU:HB2	2.19	0.43
2:C:300:PRO:HA	2:C:301:PRO:HD3	1.91	0.43
2:H:96:THR:CG2	2:H:98:GLU:HB2	2.40	0.43
1:B:721:PHE:C	1:B:723:GLN:N	2.71	0.43
2:T:116:THR:HG21	2:T:304:ARG:CB	2.44	0.43
2:T:44:THR:CG2	2:T:46:ARG:HG3	2.47	0.43
2:H:174:ILE:HG23	2:H:175:PHE:CD1	2.54	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
1:A:694:PHE:HA	1:A:697:LEU:HG	2.01	0.43
2:I:171:VAL:O	2:I:174:ILE:HG22	2.18	0.43
1:A:338:ASN:O	1:A:342:LYS:HG3	2.18	0.43
1:A:58:ASP:N	1:B:317:ARG:HH12	2.13	0.43
2:H:271:TYR:CD1	2:H:286:ARG:NH1	2.87	0.43
1:A:343:ILE:HG13	1:A:381:PHE:HE1	1.84	0.43
1:B:375:VAL:HG13	1:B:500:MET:SD	2.59	0.43
1:A:346:ALA:HA	1:A:353:ILE:HB	2.00	0.43
2:E:46:ARG:NH2	2:E:63:PHE:HB3	2.34	0.43
2:H:68:MET:HE3	2:H:94:LEU:HD11	2.00	0.43
2:D:304:ARG:O	2:D:308:LEU:HB2	2.19	0.43
2:C:200:ASN:H	2:C:200:ASN:HD22	1.65	0.43
1:A:348:MET:HA	1:A:534:ILE:HD11	2.00	0.43
2:F:191:ILE:HD12	2:F:242:MET:HB3	2.00	0.43
1:B:587:THR:HG22	1:B:588:HIS:CD2	2.53	0.43
2:R:171:VAL:O	2:R:174:ILE:HG22	2.19	0.43
1:B:399:ASP:OD2	1:B:441:ALA:HB2	2.19	0.43
2:D:200:ASN:HD22	2:D:200:ASN:H	1.67	0.43
2:H:18:LEU:N	2:H:18:LEU:CD1	2.82	0.43
2:G:269:ASN:ND2	2:G:274:ARG:HH22	2.10	0.43
1:A:425:LEU:HD13	1:A:427:PHE:HE1	1.84	0.43
1:A:427:PHE:N	1:A:427:PHE:CD1	2.79	0.43
1:A:465:TYR:O	1:A:466:VAL:HB	2.19	0.43
1:A:467:HIS:O	1:A:468:ALA:C	2.57	0.43
2:J:41:ASN:ND2	2:J:46:ARG:O	2.51	0.43
2:D:54:SER:H	2:D:57:GLN:NE2	2.16	0.43
1:B:88:THR:O	1:B:89:SER:HB2	2.18	0.43
2:T:22:ARG:HG3	2:T:22:ARG:H	1.61	0.43
2:J:18:LEU:CD1	2:J:18:LEU:N	2.82	0.43
1:B:357:LEU:O	1:B:358:LYS:HB3	2.19	0.43
2:H:260:TYR:HA	2:H:261:PRO:HD2	1.77	0.43
2:R:28:ASN:OD1	2:G:28:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:ND2	1:A:276:GLN:HB2	2.33	0.43
2:Q:116:THR:HG21	2:Q:304:ARG:CB	2.49	0.43
1:A:138:ARG:HH21	1:A:680:LYS:HG2	1.84	0.43
2:D:299:PHE:HA	2:D:300:PRO:HD2	1.84	0.43
2:E:148:ALA:HA	2:E:164:ASN:HD22	1.83	0.43
2:P:148:ALA:HA	2:P:164:ASN:HD22	1.84	0.43
1:A:308:ARG:O	1:A:312:ILE:HG22	2.18	0.43
1:B:475:CYS:HB2	1:B:477:ILE:HD11	2.01	0.43
2:I:196:MET:HG2	2:I:202:GLN:HB2	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:T:270:VAL:HB	2:T:286:ARG:NH2	2.33	0.42
1:A:111:MET:HE1	1:A:133:LYS:HB3	2.01	0.42
2:H:3:THR:O	2:H:7:ARG:HG3	2.19	0.42
1:A:425:LEU:HD13	1:A:427:PHE:CE1	2.55	0.42
1:A:279:TRP:CE2	1:A:545:PRO:HD3	2.54	0.42
2:Q:96:THR:CG2	2:Q:98:GLU:HB2	2.49	0.42
1:A:774:PHE:HB3	1:A:817:TYR:CD2	2.53	0.42
2:D:116:THR:HG21	2:D:304:ARG:HB2	2.01	0.42
1:B:82:ILE:HG12	1:B:144:ILE:HG13	2.01	0.42
2:J:295:LEU:HA	2:J:296:PRO:HD3	1.95	0.42
1:B:128:SER:HA	1:B:131:ILE:HD12	2.00	0.42
2:G:190:ARG:HA	2:G:243:VAL:HG12	2.01	0.42
1:A:191:ILE:HG12	1:A:192:ILE:N	2.34	0.42
1:A:474:TYR:C	1:A:475:CYS:SG	2.98	0.42
1:B:778:LEU:O	1:B:779:ARG:HB2	2.19	0.42
1:B:748:ILE:HD13	2:S:53:THR:CG2	2.44	0.42
1:B:616:HIS:CG	1:B:688:TRP:HE1	2.37	0.42
2:E:158:MET:HE3	2:E:245:ILE:O	2.19	0.42
2:H:37:ILE:HD12	2:H:50:MET:HG2	2.00	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:S:219:ALA:O	2:I:133:GLU:HG2	2.19	0.42
2:Q:145:ALA:O	2:Q:146:ALA:HB3	2.19	0.42
2:P:259:GLN:HA	2:C:268:PHE:CD2	2.55	0.42
2:P:9:LEU:O	2:P:13:ARG:HG3	2.18	0.42
2:H:294:MET:SD	2:H:349:VAL:HG23	2.60	0.42
2:T:39:ARG:HD3	2:T:39:ARG:HA	1.80	0.42
1:A:58:ASP:OD1	1:A:58:ASP:N	2.52	0.42
1:B:722:ARG:C	1:B:723:GLN:O	2.55	0.42
2:I:244:GLN:O	2:I:244:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:ALA:O	2:F:23:ILE:N	2.52	0.42
1:B:327:LEU:HD13	1:B:327:LEU:O	2.20	0.42
1:A:663:ILE:HD12	1:B:485:PRO:HD3	2.01	0.42
1:B:786:PHE:HB2	1:B:826:LEU:HD23	2.00	0.42
2:R:259:GLN:HA	2:G:268:PHE:CE2	2.53	0.42
2:T:16:ALA:HA	2:T:322:VAL:HG21	1.99	0.42
2:P:43:LEU:HD12	2:P:93:VAL:HG22	2.02	0.42
1:A:856:ARG:HD3	1:A:859:GLU:OE2	2.19	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
2:G:273:PHE:O	2:G:274:ARG:HB2	2.19	0.42
1:B:599:ILE:HG13	1:B:599:ILE:H	1.60	0.42
1:B:427:PHE:CD2	1:B:429:ILE:HG13	2.55	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
2:I:187:VAL:O	2:I:187:VAL:HG13	2.19	0.42
1:B:357:LEU:CD2	1:B:357:LEU:H	2.32	0.42
2:C:271:TYR:OH	2:C:292:PRO:HG2	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:B:238:TRP:HE3	1:B:239:LEU:CD2	2.26	0.42
1:A:388:THR:HG22	1:A:389:ASN:H	1.83	0.42
1:A:662:ASN:CG	1:B:485:PRO:HB3	2.40	0.42
2:D:291:LEU:HD11	2:D:301:PRO:HG2	2.00	0.42
2:C:78:GLY:HA2	2:F:324:ARG:NH1	2.34	0.42
2:D:136:PHE:CD1	2:D:136:PHE:N	2.87	0.42
1:A:297:LEU:HD13	1:A:298:PRO:HD2	2.01	0.42
1:A:296:CYS:SG	1:A:537:ASP:O	2.77	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:B:745:THR:CG2	1:B:746:TYR:N	2.82	0.42
1:B:258:PHE:CD1	1:B:258:PHE:C	2.92	0.42
1:A:429:ILE:HD12	1:A:429:ILE:H	1.85	0.42
2:I:44:THR:HG22	2:I:46:ARG:H	1.85	0.42
2:H:300:PRO:HA	2:H:301:PRO:HD3	1.86	0.42
1:A:482:LEU:N	1:A:482:LEU:HD22	2.34	0.42
1:B:265:TRP:NE1	1:B:886:ILE:HD11	2.34	0.42
2:P:257:LEU:CD1	2:P:300:PRO:HB3	2.49	0.42
1:A:117:VAL:HG12	1:A:819:THR:HG21	2.00	0.42
2:T:340:THR:OG1	2:T:343:ILE:HG13	2.19	0.42
1:A:374:GLY:O	1:A:378:HIS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:HG3	1:A:473:ARG:O	2.20	0.42
1:A:263:MET:HE2	1:A:882:ARG:HD2	2.00	0.42
1:A:861:VAL:HA	1:A:865:GLN:OE1	2.20	0.42
1:A:465:TYR:CE2	1:A:540:SER:HA	2.55	0.42
2:Q:7:ARG:HD2	2:Q:94:LEU:O	2.20	0.42
1:B:533:ILE:HA	1:B:537:ASP:HB2	2.02	0.42
1:B:452:TRP:CE2	1:B:495:HIS:HE1	2.38	0.42
1:B:615:ARG:HA	1:B:670:VAL:CG1	2.49	0.42
2:J:189:ARG:HH11	2:J:244:GLN:HE21	1.68	0.42
2:D:200:ASN:ND2	2:D:200:ASN:H	2.18	0.42
1:B:679:LEU:O	1:B:682:VAL:HG22	2.20	0.42
2:C:281:LEU:O	2:C:285:ILE:HG13	2.19	0.42
2:J:159:ILE:HD11	2:J:245:ILE:HB	2.02	0.42
2:R:159:ILE:HD11	2:R:245:ILE:HB	2.02	0.42
1:A:343:ILE:HA	1:A:355:LEU:HD21	2.02	0.42
2:H:96:THR:HA	2:H:97:PRO:HD2	1.83	0.42
1:A:637:TRP:HZ3	1:A:666:MET:HE1	1.85	0.42
2:T:159:ILE:CD1	2:T:245:ILE:HB	2.49	0.42
1:B:43:VAL:HA	1:B:46:VAL:HG23	2.01	0.42
2:R:41:ASN:ND2	2:R:48:VAL:H	2.17	0.42
2:S:186:LEU:HD21	2:S:225:TRP:HE3	1.84	0.42
2:F:288:ARG:HH11	2:F:288:ARG:HG3	1.83	0.42
2:S:260:TYR:HA	2:S:261:PRO:HD2	1.78	0.42
2:H:307:ILE:HA	2:H:310:LEU:HD12	2.02	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
1:A:810:LEU:HB2	1:A:812:TYR:CE1	2.55	0.42
1:A:474:TYR:H	1:A:531:ASN:ND2	2.17	0.42
2:C:271:TYR:CE1	2:C:286:ARG:NH1	2.88	0.42
1:A:376:VAL:HG12	1:A:380:LEU:HD22	2.02	0.42
1:B:466:VAL:HA	1:B:469:GLN:NE2	2.35	0.42
2:S:296:PRO:HA	2:S:297:PRO:HD2	1.87	0.42
2:E:145:ALA:O	2:E:146:ALA:HB3	2.20	0.42
2:P:24:VAL:HG22	2:D:97:PRO:O	2.20	0.42
2:D:23:ILE:HD12	2:D:23:ILE:O	2.20	0.42
2:R:295:LEU:HA	2:R:295:LEU:HD23	1.81	0.42
1:A:350:PRO:CD	1:A:351:GLY:H	2.32	0.42
1:A:310:SER:HB2	1:A:327:LEU:HD11	2.02	0.42
1:A:282:PRO:HB2	1:A:661:ILE:HD12	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:HIS:O	1:B:496:CYS:CB	2.68	0.42
2:T:96:THR:HG22	2:T:98:GLU:OE2	2.20	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
1:A:768:ASP:C	1:A:770:ASP:H	2.23	0.42
1:B:746:TYR:CA	1:B:817:TYR:HE2	2.27	0.41
2:S:124:GLN:HE21	2:S:125:PRO:CD	2.34	0.41
1:B:403:ASN:HB2	1:B:425:LEU:CD2	2.44	0.41
1:A:151:ARG:HG2	1:A:158:VAL:HB	2.02	0.41
1:B:819:THR:HG22	1:B:820:GLU:N	2.33	0.41
2:T:7:ARG:HD2	2:T:94:LEU:O	2.20	0.41
1:A:664:ARG:HG3	1:B:485:PRO:HG3	2.02	0.41
1:B:727:TYR:HA	1:B:826:LEU:O	2.20	0.41
1:A:89:SER:OG	1:A:209:CYS:HA	2.20	0.41
1:B:883:ILE:N	1:B:883:ILE:HD12	2.34	0.41
1:A:259:ARG:HB3	1:A:263:MET:HE3	2.02	0.41
1:B:710:LEU:HB2	1:B:845:THR:HB	2.02	0.41
1:A:403:ASN:HD22	1:A:425:LEU:HD22	1.86	0.41
2:H:273:PHE:O	2:H:274:ARG:HB2	2.21	0.41
1:B:35:ALA:O	1:B:39:ILE:HG13	2.20	0.41
2:R:200:ASN:HD22	2:R:200:ASN:H	1.67	0.41
2:E:129:PHE:O	2:E:156:PRO:HA	2.20	0.41
1:A:790:PRO:HB3	1:A:791:PRO:HD2	2.02	0.41
2:T:107:ASN:HD22	2:T:107:ASN:H	1.68	0.41
1:B:569:LEU:HD13	1:B:569:LEU:HA	1.90	0.41
1:A:297:LEU:O	1:A:590:ASN:HB3	2.20	0.41
1:B:333:THR:HG22	1:B:334:ALA:H	1.86	0.41
1:B:873:ARG:HE	1:B:875:VAL:HG22	1.85	0.41
1:B:376:VAL:O	1:B:379:LEU:HD22	2.20	0.41
2:J:271:TYR:CD1	2:J:286:ARG:NH1	2.88	0.41
1:B:460:ARG:NE	2:E:51:ARG:NH2	2.65	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
1:B:264:ILE:H	1:B:264:ILE:HD12	1.85	0.41
2:S:104:GLU:CD	2:S:104:GLU:H	2.24	0.41
2:P:139:GLY:HA3	2:C:137:GLN:HG3	2.03	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
1:B:214:TYR:HD2	1:B:872:ARG:HD2	1.84	0.41
1:A:336:GLN:NE2	1:A:574:ILE:HD13	2.35	0.41
1:B:636:PHE:CD1	1:B:637:TRP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:96:THR:C	2:H:98:GLU:H	2.24	0.41
2:I:44:THR:HG21	2:I:46:ARG:HB2	2.01	0.41
1:B:296:CYS:HB3	1:B:538:LEU:HA	2.03	0.41
1:A:409:MET:SD	1:A:413:ARG:HA	2.61	0.41
2:S:139:GLY:HA3	2:I:137:GLN:HG3	2.03	0.41
2:T:45:LEU:HA	2:T:45:LEU:HD12	1.79	0.41
1:A:284:SER:O	1:A:285:SER:C	2.59	0.41
2:S:49:THR:HG22	2:S:51:ARG:H	1.86	0.41
1:A:492:MET:O	1:A:520:LEU:HD21	2.20	0.41
2:J:212:VAL:O	2:J:215:VAL:HG12	2.21	0.41
2:C:317:ALA:O	2:C:320:TYR:HB3	2.20	0.41
2:J:191:ILE:HD12	2:J:242:MET:HB3	2.02	0.41
2:F:309:THR:O	2:F:313:LEU:HB2	2.19	0.41
2:F:63:PHE:CE1	2:F:84:TYR:HB2	2.55	0.41
2:E:336:PRO:HB3	2:R:330:HIS:HB3	2.02	0.41
2:D:288:ARG:NH1	2:D:288:ARG:HG3	2.34	0.41
2:S:18:LEU:HD12	2:S:18:LEU:N	2.36	0.41
2:Q:313:LEU:HD23	2:Q:313:LEU:HA	1.88	0.41
2:I:7:ARG:NH2	2:I:97:PRO:HA	2.36	0.41
1:A:219:ARG:CG	1:A:686:GLU:HG3	2.33	0.41
2:F:271:TYR:CD1	2:F:286:ARG:NH1	2.89	0.41
2:P:271:TYR:CE1	2:P:286:ARG:NH1	2.89	0.41
1:B:100:ARG:HA	1:B:862:ARG:O	2.20	0.41
1:A:358:LYS:HE2	1:A:358:LYS:HB3	1.75	0.41
2:H:260:TYR:O	2:H:263:LEU:HB2	2.20	0.41
1:A:133:LYS:O	1:A:137:ILE:HG12	2.21	0.41
2:S:28:ASN:ND2	2:I:26:GLU:HG3	2.36	0.41
2:Q:265:ALA:HB1	2:F:261:PRO:HD3	2.02	0.41
1:B:320:THR:HG22	1:B:321:THR:N	2.36	0.41
1:A:211:GLU:HB3	1:A:212:PRO:CD	2.49	0.41
1:B:898:ALA:HA	1:B:899:PRO:HD2	1.67	0.41
1:A:641:LEU:O	1:A:649:LYS:HE2	2.19	0.41
2:C:273:PHE:O	2:C:278:TRP:HD1	2.04	0.41
1:B:391:THR:HG22	1:B:392:GLN:N	2.36	0.41
1:B:205:PHE:O	1:B:873:ARG:O	2.38	0.41
1:A:95:THR:HG22	1:A:96:GLN:N	2.36	0.41
1:A:273:VAL:HA	1:A:676:GLN:HG3	2.03	0.41
2:C:54:SER:H	2:C:57:GLN:HE21	1.67	0.41
1:B:157:GLU:HG2	1:B:192:ILE:HD12	2.02	0.41
2:I:151:ALA:HB2	2:I:171:VAL:HG13	2.03	0.41
1:A:120:GLU:H	1:A:120:GLU:HG2	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:158:VAL:HG12	1:B:191:ILE:HG22	2.03	0.41
2:J:16:ALA:HA	2:J:322:VAL:HG21	2.02	0.41
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.85	0.41
2:S:200:ASN:H	2:S:200:ASN:ND2	2.19	0.41
1:A:61:VAL:HG12	1:B:315:THR:HA	2.02	0.41
1:B:331:THR:HA	1:B:578:PHE:HE2	1.81	0.41
1:B:578:PHE:O	1:B:582:ARG:HD2	2.21	0.41
1:A:754:ASN:ND2	1:B:257:ASP:H	2.18	0.41
1:A:500:MET:SD	1:A:504:LEU:HD23	2.61	0.41
2:G:41:ASN:ND2	2:G:48:VAL:H	2.17	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
2:E:184:ILE:HG22	2:E:186:LEU:CD1	2.51	0.41
2:T:9:LEU:O	2:T:13:ARG:HG3	2.21	0.41
2:S:185:TYR:O	2:S:248:VAL:HG12	2.19	0.41
1:A:734:ALA:HA	1:A:852:PHE:CE1	2.55	0.41
2:P:185:TYR:O	2:P:248:VAL:HG12	2.20	0.41
1:B:168:PHE:CD1	1:B:168:PHE:N	2.89	0.41
2:S:295:LEU:HD23	2:S:295:LEU:HA	1.87	0.41
1:A:405:TYR:OH	1:A:509:LYS:HD3	2.21	0.41
1:B:96:GLN:HG3	1:B:829:ASN:ND2	2.35	0.41
2:R:54:SER:OG	2:R:55:LEU:N	2.53	0.41
1:B:521:PRO:O	1:B:525:VAL:HG23	2.21	0.41
2:I:299:PHE:HA	2:I:300:PRO:HD2	1.90	0.41
2:E:2:ASP:HB3	2:E:109:ILE:CG2	2.45	0.41
1:A:622:ARG:NH2	2:F:28:ASN:HD21	2.19	0.41
1:B:67:ILE:HG23	1:B:68:LEU:N	2.36	0.41
1:B:470:ARG:NH1	1:B:549:PHE:HB2	2.35	0.41
2:P:50:MET:C	2:P:52:PRO:HD3	2.40	0.41
2:F:235:ASN:OD1	2:F:237:THR:HG22	2.20	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:P:283:THR:HG23	2:P:293:ASN:HB2	2.01	0.41
2:P:77:VAL:HA	2:P:288:ARG:HD3	2.03	0.41
1:B:28:GLY:N	1:B:29:PRO:HD2	2.35	0.41
2:Q:25:LEU:N	2:Q:25:LEU:HD22	2.36	0.41
2:G:18:LEU:N	2:G:18:LEU:HD13	2.36	0.41
2:R:311:LEU:HD23	2:R:311:LEU:HA	1.92	0.41
1:A:477:ILE:HG22	1:A:479:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:VAL:HG23	1:B:777:VAL:HA	2.01	0.41
2:P:271:TYR:OH	2:P:292:PRO:HG2	2.21	0.41
2:Q:260:TYR:HA	2:Q:261:PRO:HD2	1.77	0.41
1:B:371:MET:HG3	1:B:372:VAL:N	2.36	0.41
2:J:299:PHE:HA	2:J:300:PRO:HD2	1.86	0.41
2:S:54:SER:OG	2:S:55:LEU:N	2.54	0.41
1:A:103:ARG:HB3	1:A:861:VAL:HG21	2.03	0.41
2:Q:186:LEU:HD12	2:Q:247:VAL:HA	2.02	0.41
1:B:123:PRO:HG2	1:B:635:HIS:ND1	2.36	0.41
2:E:13:ARG:O	2:E:16:ALA:HB3	2.21	0.41
1:A:664:ARG:HG3	1:B:485:PRO:HG2	2.02	0.41
1:B:219:ARG:CG	1:B:686:GLU:HG3	2.51	0.41
2:J:91:ILE:HG23	2:J:92:GLY:N	2.35	0.41
2:R:191:ILE:HD12	2:R:242:MET:HB3	2.02	0.41
2:F:200:ASN:H	2:F:200:ASN:HD22	1.69	0.41
1:A:768:ASP:O	1:A:769:ASP:HB3	2.20	0.41
2:T:141:TRP:CZ3	2:T:240:ASN:HB3	2.56	0.41
2:C:93:VAL:O	2:C:99:ILE:HD12	2.21	0.41
1:B:608:SER:HB2	1:B:675:LEU:HD12	2.03	0.41
2:E:295:LEU:HA	2:E:296:PRO:HD3	1.94	0.41
2:D:126:TYR:HB3	2:D:130:LEU:HD22	2.01	0.41
2:P:97:PRO:O	2:C:24:VAL:HG22	2.20	0.41
1:B:65:GLN:OE1	1:B:65:GLN:HA	2.20	0.41
2:D:187:VAL:HG13	2:D:187:VAL:O	2.21	0.41
2:T:231:LEU:HA	2:T:231:LEU:HD12	1.82	0.41
2:E:271:TYR:CD1	2:E:286:ARG:NH1	2.89	0.41
1:A:730:ASN:HB3	1:A:850:LYS:HA	2.03	0.41
1:A:637:TRP:HZ3	1:A:666:MET:CE	2.34	0.41
2:Q:222:ILE:C	2:Q:223:ILE:HG13	2.41	0.41
1:B:382:THR:HA	1:B:450:ASN:HB2	2.03	0.41
1:A:434:TYR:CE2	1:A:503:MET:HB2	2.55	0.41
1:B:114:VAL:HG11	1:B:133:LYS:HA	2.02	0.41
1:A:318:ILE:O	1:A:319:THR:CB	2.69	0.41
1:A:791:PRO:HG2	1:A:794:ILE:HB	2.03	0.41
2:T:107:ASN:HD22	2:T:107:ASN:N	2.18	0.41
2:E:31:GLU:O	2:E:35:ILE:HG13	2.21	0.41
1:A:410:TYR:N	1:A:410:TYR:CD1	2.89	0.40
1:B:256:THR:C	1:B:258:PHE:H	2.25	0.40
1:A:464:PRO:O	1:A:465:TYR:HB2	2.21	0.40
1:A:622:ARG:HH12	2:F:100:PRO:HB2	1.85	0.40
1:A:842:ILE:CD1	1:A:842:ILE:H	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PRO:O	1:B:126:PHE:HB3	2.21	0.40
2:E:337:GLY:N	2:E:338:PRO:CD	2.83	0.40
1:B:452:TRP:C	1:B:452:TRP:CD1	2.94	0.40
1:A:614:MET:CG	1:A:640:VAL:HG21	2.50	0.40
2:P:151:ALA:HB2	2:P:171:VAL:HG13	2.03	0.40
2:E:324:ARG:HH11	2:E:324:ARG:HB3	1.86	0.40
1:B:392:GLN:HA	1:B:443:PHE:HE2	1.85	0.40
1:A:355:LEU:HB2	1:A:390:LEU:CD2	2.51	0.40
2:P:269:ASN:ND2	2:P:274:ARG:HH22	2.10	0.40
2:S:274:ARG:HB2	2:S:278:TRP:CD1	2.57	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
2:D:96:THR:HA	2:D:97:PRO:HD2	1.87	0.40
1:A:625:PRO:O	1:A:629:ILE:HG13	2.21	0.40
2:H:179:ASN:HB2	2:H:181:PRO:HD3	2.02	0.40
2:G:187:VAL:O	2:G:187:VAL:HG13	2.21	0.40
2:T:23:ILE:O	2:T:23:ILE:HD12	2.21	0.40
2:T:295:LEU:HA	2:T:295:LEU:HD23	1.95	0.40
1:A:59:PHE:CB	1:B:317:ARG:HD2	2.36	0.40
1:B:375:VAL:HG12	1:B:379:LEU:HD11	2.03	0.40
1:B:72:LYS:NZ	1:B:595:ILE:HB	2.30	0.40
1:B:14:THR:CG2	1:B:15:THR:N	2.84	0.40
1:B:429:ILE:O	1:B:433:GLN:O	2.40	0.40
2:H:54:SER:OG	2:H:55:LEU:N	2.54	0.40
2:Q:184:ILE:HG22	2:Q:186:LEU:HD13	2.03	0.40
2:S:7:ARG:HD3	2:S:99:ILE:HB	2.04	0.40
1:B:39:ILE:O	1:B:42:LYS:HB3	2.20	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
1:B:848:MET:O	1:B:850:LYS:HD2	2.22	0.40
1:B:306:ASN:HB2	1:B:309:ILE:HG13	2.02	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
1:B:545:PRO:HG2	1:B:548:MET:HG3	2.04	0.40
2:G:295:LEU:HD23	2:G:295:LEU:HA	1.91	0.40
2:T:257:LEU:HD23	2:T:264:THR:HG23	2.03	0.40
2:D:271:TYR:CD1	2:D:286:ARG:NH1	2.90	0.40
1:B:271:LEU:O	1:B:273:VAL:N	2.54	0.40
1:A:637:TRP:CZ2	1:B:14:THR:HG23	2.57	0.40
1:B:122:GLU:HB3	1:B:125:LYS:HB2	2.03	0.40
2:I:2:ASP:HB3	2:I:109:ILE:CG2	2.50	0.40

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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	843/901 (94%)	674 (80%)	109 (13%)	60 (7%)	1 17
1	B	881/901 (98%)	715 (81%)	110 (12%)	56 (6%)	2 20
2	C	347/349 (99%)	313 (90%)	29 (8%)	5 (1%)	14 58
2	D	347/349 (99%)	316 (91%)	25 (7%)	6 (2%)	11 54
2	E	347/349 (99%)	296 (85%)	40 (12%)	11 (3%)	5 40
2	F	347/349 (99%)	305 (88%)	34 (10%)	8 (2%)	8 48
2	G	347/349 (99%)	303 (87%)	39 (11%)	5 (1%)	14 58
2	H	347/349 (99%)	302 (87%)	37 (11%)	8 (2%)	8 48
2	I	347/349 (99%)	300 (86%)	40 (12%)	7 (2%)	9 51
2	J	347/349 (99%)	296 (85%)	45 (13%)	6 (2%)	11 54
2	P	347/349 (99%)	312 (90%)	28 (8%)	7 (2%)	9 51
2	Q	347/349 (99%)	300 (86%)	39 (11%)	8 (2%)	8 48
2	R	347/349 (99%)	299 (86%)	39 (11%)	9 (3%)	7 45
2	S	347/349 (99%)	296 (85%)	40 (12%)	11 (3%)	5 40
2	T	347/349 (99%)	306 (88%)	35 (10%)	6 (2%)	11 54
All	All	6235/6339 (98%)	5333 (86%)	689 (11%)	213 (3%)	5 39

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	744/793 (94%)	592 (80%)	152 (20%)	1 8
1	B	782/793 (99%)	644 (82%)	138 (18%)	2 13
2	C	284/284 (100%)	263 (93%)	21 (7%)	17 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	284/284 (100%)	262 (92%)	22 (8%)	16 54
2	E	284/284 (100%)	259 (91%)	25 (9%)	12 48
2	F	284/284 (100%)	260 (92%)	24 (8%)	13 49
2	G	284/284 (100%)	258 (91%)	26 (9%)	11 45
2	H	284/284 (100%)	258 (91%)	26 (9%)	11 45
2	I	284/284 (100%)	260 (92%)	24 (8%)	13 49
2	J	284/284 (100%)	261 (92%)	23 (8%)	15 52
2	P	284/284 (100%)	262 (92%)	22 (8%)	16 54
2	Q	284/284 (100%)	258 (91%)	26 (9%)	11 45
2	R	284/284 (100%)	259 (91%)	25 (9%)	12 48
2	S	284/284 (100%)	260 (92%)	24 (8%)	13 49
2	T	284/284 (100%)	256 (90%)	28 (10%)	10 41
All	All	5218/5278 (99%)	4612 (88%)	606 (12%)	7 33

All (606) 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	100	ARG
1	A	102	LEU
1	A	111	MET
1	A	135	ARG
1	A	138	ARG
1	A	140	LYS
1	A	144	ILE
1	A	151	ARG
1	A	152	ASP
1	A	154	ARG
1	A	157	GLU

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Mol	Chain	Res	Type
1	A	164	LEU
1	A	166	VAL
1	A	170	ASN
1	A	174	VAL
1	A	175	LEU
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	229	LEU
1	A	231	GLU
1	A	255	LEU
1	A	258	PHE
1	A	259	ARG
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	317	ARG
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	356	ASP
1	A	361	PRO
1	A	363	GLU
1	A	365	MET
1	A	370	ARG
1	A	382	THR
1	A	389	ASN

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Mol	Chain	Res	Type
1	A	393	ASN
1	A	398	LEU
1	A	408	TYR
1	A	410	TYR
1	A	413	ARG
1	A	423	GLU
1	A	427	PHE
1	A	434	TYR
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	475	CYS
1	A	478	ASP
1	A	481	GLU
1	A	482	LEU
1	A	488	TYR
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	573	TRP
1	A	576	LEU
1	A	593	LEU
1	A	617	LEU
1	A	622	ARG

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Mol	Chain	Res	Type
1	A	628	LEU
1	A	632	ARG
1	A	636	PHE
1	A	637	TRP
1	A	641	LEU
1	A	643	ASP
1	A	656	HIS
1	A	667	MET
1	A	675	LEU
1	A	686	GLU
1	A	692	ASN
1	A	699	LEU
1	A	705	MET
1	A	707	ARG
1	A	708	ASP
1	A	710	LEU
1	A	714	ARG
1	A	720	ARG
1	A	723	GLN
1	A	724	GLU
1	A	726	PHE
1	A	727	TYR
1	A	738	ILE
1	A	745	THR
1	A	748	ILE
1	A	762	LEU
1	A	763	ARG
1	A	773	ARG
1	A	780	THR
1	A	787	ASP
1	A	789	ARG
1	A	793	ASP
1	A	794	ILE
1	A	804	THR
1	A	811	SER
1	A	812	TYR
1	A	830	VAL
1	A	831	GLU
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	885	ASP
1	A	892	MET
1	A	894	THR
1	B	10	GLU
1	B	14	THR
1	B	15	THR
1	B	21	ASP
1	B	30	LEU
1	B	40	MET
1	B	46	VAL
1	B	51	MET
1	B	54	THR
1	B	58	ASP
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	102	LEU
1	B	111	MET
1	B	113	GLN
1	B	119	THR
1	B	135	ARG
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	204	VAL
1	B	205	PHE
1	B	214	TYR
1	B	219	ARG
1	B	233	ARG
1	B	252	GLN

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Mol	Chain	Res	Type
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	277	VAL
1	B	289	LEU
1	B	292	ASN
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	409	MET
1	B	426	ASP
1	B	435	ASP
1	B	438	VAL
1	B	445	THR
1	B	449	TYR
1	B	452	TRP
1	B	456	ASP
1	B	465	TYR
1	B	467	HIS
1	B	471	TYR
1	B	484	ASN
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	527	PHE
1	B	529	ARG
1	B	532	GLN

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Mol	Chain	Res	Type
1	B	537	ASP
1	B	539	HIS
1	B	561	HIS
1	B	563	ASN
1	B	573	TRP
1	B	577	TRP
1	B	584	PHE
1	B	592	MET
1	B	598	LEU
1	B	607	LEU
1	B	615	ARG
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	672	LEU
1	B	673	PRO
1	B	685	GLU
1	B	686	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	726	PHE
1	B	731	MET
1	B	733	GLU
1	B	737	GLU
1	B	740	ARG
1	B	750	ARG
1	B	751	LEU
1	B	762	LEU
1	B	763	ARG
1	B	764	ARG
1	B	787	ASP
1	B	789	ARG

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Mol	Chain	Res	Type
1	B	815	ILE
1	B	817	TYR
1	B	830	VAL
1	B	841	LEU
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
2	P	19	GLN
2	P	50	MET
2	P	60	GLU
2	P	67	ASP
2	P	69	MET
2	P	108	GLU
2	P	111	ARG
2	P	116	THR
2	P	123	ARG
2	P	152	VAL
2	P	178	ARG
2	P	200	ASN
2	P	203	GLN
2	P	221	ARG
2	P	237	THR
2	P	263	LEU
2	P	281	LEU
2	P	288	ARG
2	P	291	LEU
2	P	308	LEU
2	P	333	ASN
2	P	338	PRO
2	C	18	LEU
2	C	19	GLN
2	C	39	ARG

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Mol	Chain	Res	Type
2	C	45	LEU
2	C	50	MET
2	C	60	GLU
2	C	69	MET
2	C	108	GLU
2	C	111	ARG
2	C	115	GLU
2	C	152	VAL
2	C	178	ARG
2	C	203	GLN
2	C	221	ARG
2	C	237	THR
2	C	263	LEU
2	C	281	LEU
2	C	288	ARG
2	C	308	LEU
2	C	333	ASN
2	C	338	PRO
2	D	18	LEU
2	D	19	GLN
2	D	39	ARG
2	D	60	GLU
2	D	69	MET
2	D	94	LEU
2	D	98	GLU
2	D	111	ARG
2	D	115	GLU
2	D	116	THR
2	D	178	ARG
2	D	203	GLN
2	D	221	ARG
2	D	237	THR
2	D	263	LEU
2	D	281	LEU
2	D	288	ARG
2	D	291	LEU
2	D	308	LEU
2	D	324	ARG
2	D	333	ASN
2	D	335	MET
2	Q	20	GLU
2	Q	23	ILE

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Mol	Chain	Res	Type
2	Q	39	ARG
2	Q	60	GLU
2	Q	67	ASP
2	Q	69	MET
2	Q	94	LEU
2	Q	111	ARG
2	Q	115	GLU
2	Q	116	THR
2	Q	152	VAL
2	Q	178	ARG
2	Q	186	LEU
2	Q	203	GLN
2	Q	221	ARG
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	69	MET
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	250	TYR
2	E	263	LEU
2	E	270	VAL
2	E	277	THR

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Mol	Chain	Res	Type
2	E	281	LEU
2	E	288	ARG
2	E	291	LEU
2	E	308	LEU
2	E	324	ARG
2	E	333	ASN
2	E	336	PRO
2	F	18	LEU
2	F	19	GLN
2	F	45	LEU
2	F	51	ARG
2	F	69	MET
2	F	94	LEU
2	F	98	GLU
2	F	111	ARG
2	F	115	GLU
2	F	116	THR
2	F	178	ARG
2	F	186	LEU
2	F	203	GLN
2	F	221	ARG
2	F	237	THR
2	F	250	TYR
2	F	263	LEU
2	F	281	LEU
2	F	288	ARG
2	F	308	LEU
2	F	313	LEU
2	F	333	ASN
2	F	335	MET
2	F	338	PRO
2	R	22	ARG
2	R	30	MET
2	R	33	LEU
2	R	45	LEU
2	R	60	GLU
2	R	69	MET
2	R	98	GLU
2	R	108	GLU
2	R	111	ARG
2	R	116	THR
2	R	152	VAL

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Mol	Chain	Res	Type
2	R	153	VAL
2	R	178	ARG
2	R	186	LEU
2	R	203	GLN
2	R	221	ARG
2	R	237	THR
2	R	263	LEU
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	69	MET
2	G	76	ASN
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	178	ARG
2	G	186	LEU
2	G	200	ASN
2	G	203	GLN
2	G	221	ARG
2	G	237	THR
2	G	263	LEU
2	G	281	LEU
2	G	288	ARG
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

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Mol	Chain	Res	Type
2	H	22	ARG
2	H	43	LEU
2	H	49	THR
2	H	60	GLU
2	H	69	MET
2	H	94	LEU
2	H	98	GLU
2	H	108	GLU
2	H	115	GLU
2	H	116	THR
2	H	152	VAL
2	H	178	ARG
2	H	186	LEU
2	H	203	GLN
2	H	221	ARG
2	H	237	THR
2	H	281	LEU
2	H	288	ARG
2	H	308	LEU
2	H	313	LEU
2	H	324	ARG
2	H	333	ASN
2	H	338	PRO
2	H	339	LEU
2	S	19	GLN
2	S	45	LEU
2	S	50	MET
2	S	69	MET
2	S	94	LEU
2	S	115	GLU
2	S	116	THR
2	S	123	ARG
2	S	124	GLN
2	S	153	VAL
2	S	178	ARG
2	S	186	LEU
2	S	203	GLN
2	S	221	ARG
2	S	237	THR
2	S	250	TYR
2	S	263	LEU
2	S	264	THR

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Mol	Chain	Res	Type
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	69	MET
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	221	ARG
2	I	237	THR
2	I	250	TYR
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
2	J	19	GLN
2	J	26	GLU
2	J	69	MET
2	J	94	LEU
2	J	115	GLU
2	J	116	THR
2	J	152	VAL
2	J	178	ARG
2	J	186	LEU
2	J	200	ASN
2	J	203	GLN

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Mol	Chain	Res	Type
2	J	221	ARG
2	J	237	THR
2	J	250	TYR
2	J	264	THR
2	J	281	LEU
2	J	288	ARG
2	J	291	LEU
2	J	308	LEU
2	J	324	ARG
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	69	MET
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	178	ARG
2	T	186	LEU
2	T	203	GLN
2	T	221	ARG
2	T	237	THR
2	T	250	TYR
2	T	263	LEU
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	339	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	179	HIS
1	A	221	GLN
1	A	261	GLN
1	A	274	ASN
1	A	292	ASN
1	A	378	HIS
1	A	389	ASN
1	A	393	ASN
1	A	403	ASN
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	B	92	HIS
1	B	179	HIS
1	B	228	GLN
1	B	292	ASN
1	B	316	GLN
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	539	HIS
1	B	588	HIS
1	B	616	HIS
1	B	656	HIS
1	B	658	HIS
1	B	692	ASN
1	B	854	ASN
2	P	41	ASN
2	P	57	GLN
2	P	76	ASN
2	P	200	ASN

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Mol	Chain	Res	Type
2	P	244	GLN
2	P	269	ASN
2	C	41	ASN
2	C	57	GLN
2	C	76	ASN
2	C	124	GLN
2	C	147	GLN
2	C	200	ASN
2	C	244	GLN
2	C	269	ASN
2	D	41	ASN
2	D	57	GLN
2	D	76	ASN
2	D	200	ASN
2	D	244	GLN
2	D	259	GLN
2	D	269	ASN
2	Q	28	ASN
2	Q	41	ASN
2	Q	57	GLN
2	Q	76	ASN
2	Q	124	GLN
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	76	ASN
2	E	200	ASN
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	76	ASN
2	F	200	ASN
2	F	244	GLN
2	F	269	ASN

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Mol	Chain	Res	Type
2	R	28	ASN
2	R	38	ASN
2	R	41	ASN
2	R	57	GLN
2	R	76	ASN
2	R	124	GLN
2	R	200	ASN
2	R	244	GLN
2	R	269	ASN
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	244	GLN
2	G	269	ASN
2	H	28	ASN
2	H	38	ASN
2	H	41	ASN
2	H	57	GLN
2	H	124	GLN
2	H	193	ASN
2	H	240	ASN
2	H	244	GLN
2	H	269	ASN
2	S	41	ASN
2	S	57	GLN
2	S	76	ASN
2	S	124	GLN
2	S	244	GLN
2	S	269	ASN
2	I	28	ASN
2	I	41	ASN
2	I	57	GLN
2	I	76	ASN
2	I	124	GLN
2	I	164	ASN
2	I	193	ASN
2	I	200	ASN

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Mol	Chain	Res	Type
2	I	240	ASN
2	I	244	GLN
2	I	269	ASN
2	J	38	ASN
2	J	41	ASN
2	J	57	GLN
2	J	76	ASN
2	J	193	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	76	ASN
2	T	107	ASN
2	T	193	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers

EDS failed to run properly - this section will therefore be empty.