



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:30 am BST

PDB ID : 1UF2
Title : The Atomic Structure of Rice dwarf Virus (RDV)
Authors : Nakagawa, A.; Miyazaki, N.; Taka, J.; Naitow, H.; Ogawa, A.; Fujimoto, Z.; Mizuno, H.; Higashi, T.; Watanabe, Y.; Omura, T.; Cheng, R.H.; Tsukihara, T.
Deposited on : 2003-05-23
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

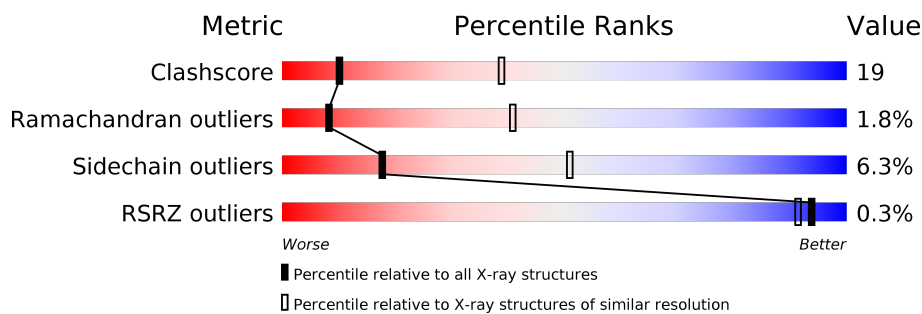
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION







The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1019	
1	B	1019	
2	C	421	
2	D	421	
2	E	421	
2	F	421	
2	G	421	

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Mol	Chain	Length	Quality of chain
2	H	421	<div><div></div><div>65%33%</div><div></div></div>
2	I	421	<div><div></div><div>59%36%5%</div><div></div></div>
2	J	421	<div><div></div><div>56%38%</div><div></div></div>
2	P	421	<div><div></div><div>%62%33%</div><div></div></div>
2	Q	421	<div><div></div><div>59%37%</div><div></div></div>
2	R	421	<div><div></div><div>69%28%</div><div></div></div>
2	S	421	<div><div></div><div>62%33%5%</div><div></div></div>
2	T	421	<div><div></div><div>65%32%</div><div></div></div>
3	K	506	<div><div></div><div>98%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 58130 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 Core protein P3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	967	Total	C	N	O	S	0	0	0
			7653	4885	1309	1427	32			
1	B	1019	Total	C	N	O	S	0	0	0
			8053	5138	1370	1512	33			

- Molecule 2 is a protein called Outer capsid protein P8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	414	Total	C	N	O	S	0	0	0
			3227	2060	542	608	17			
2	C	415	Total	C	N	O	S	0	0	0
			3234	2065	543	609	17			
2	D	417	Total	C	N	O	S	0	0	0
			3247	2073	545	612	17			
2	Q	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			
2	E	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			
2	F	415	Total	C	N	O	S	0	0	0
			3234	2065	543	609	17			
2	R	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			
2	G	417	Total	C	N	O	S	0	0	0
			3253	2079	545	612	17			
2	H	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			
2	S	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			
2	I	419	Total	C	N	O	S	0	0	0
			3265	2085	547	616	17			
2	J	413	Total	C	N	O	S	0	0	0
			3221	2057	541	606	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	421	Total	C	N	O	S	0	0	0
			3274	2090	549	618	17			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	178	ALA	-	SEE REMARK 999	UNP P17379
C	178	ALA	-	SEE REMARK 999	UNP P17379
D	178	ALA	-	SEE REMARK 999	UNP P17379
Q	178	ALA	-	SEE REMARK 999	UNP P17379
E	178	ALA	-	SEE REMARK 999	UNP P17379
F	178	ALA	-	SEE REMARK 999	UNP P17379
R	178	ALA	-	SEE REMARK 999	UNP P17379
G	178	ALA	-	SEE REMARK 999	UNP P17379
H	178	ALA	-	SEE REMARK 999	UNP P17379
S	178	ALA	-	SEE REMARK 999	UNP P17379
I	178	ALA	-	SEE REMARK 999	UNP P17379
J	178	ALA	-	SEE REMARK 999	UNP P17379
T	178	ALA	-	SEE REMARK 999	UNP P17379

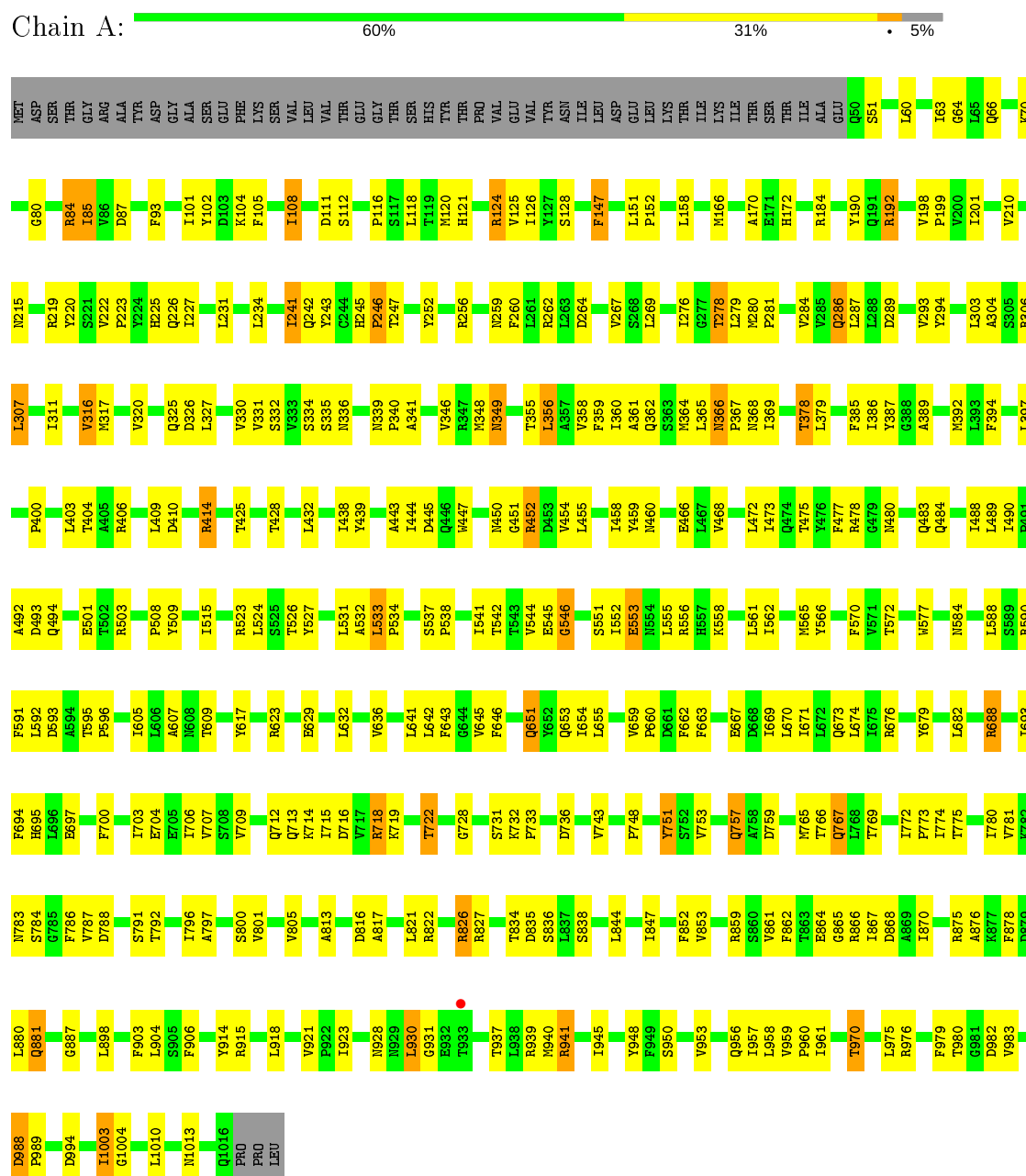
- Molecule 3 is a protein called Structural protein P7.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	12	Total	C	N	O	0	0	0
			99	60	16	23			

3 Residue-property plots

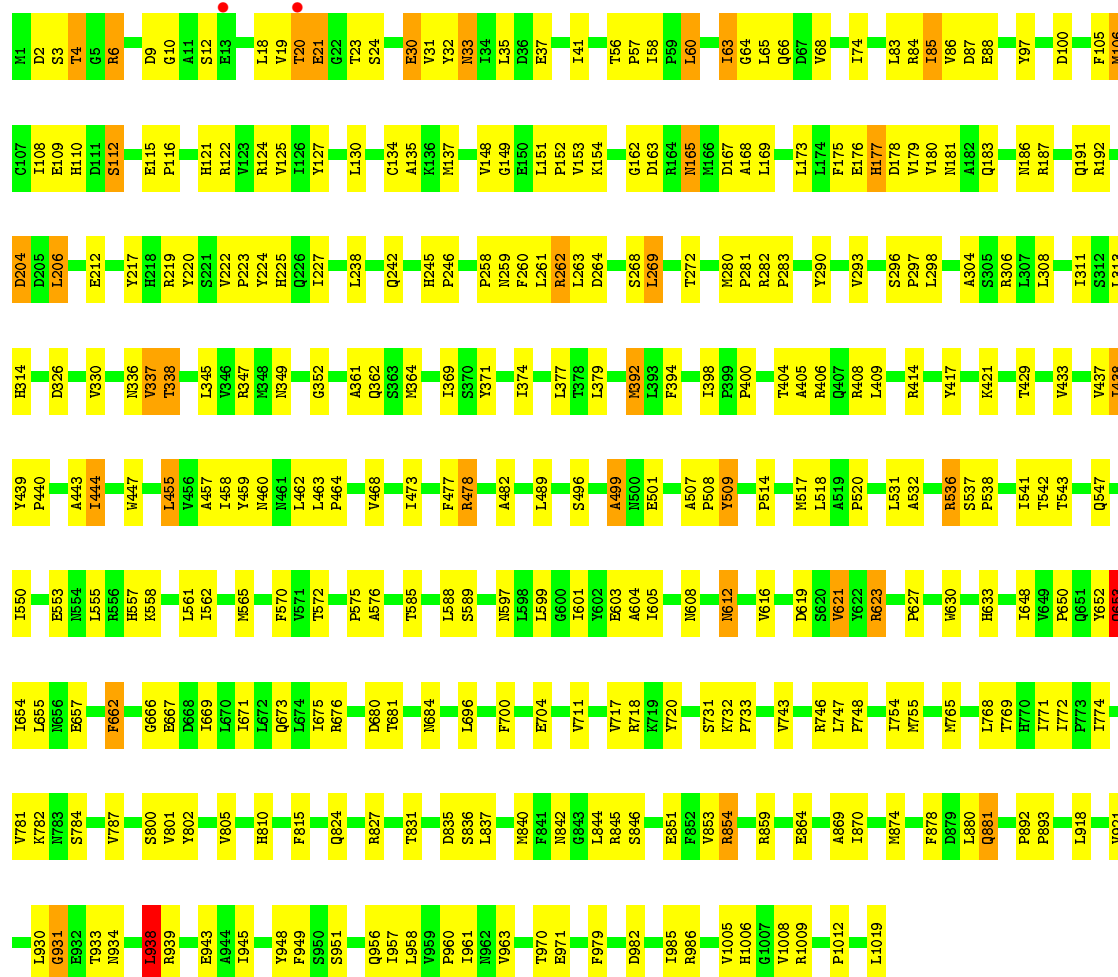
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Core protein P3



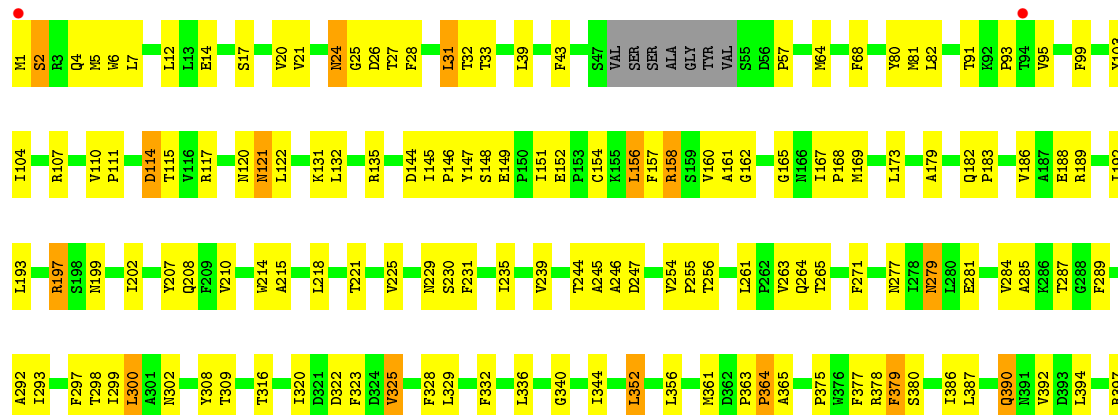
- Molecule 1: Core protein P3

Chain B:



- Molecule 2: Outer capsid protein P8

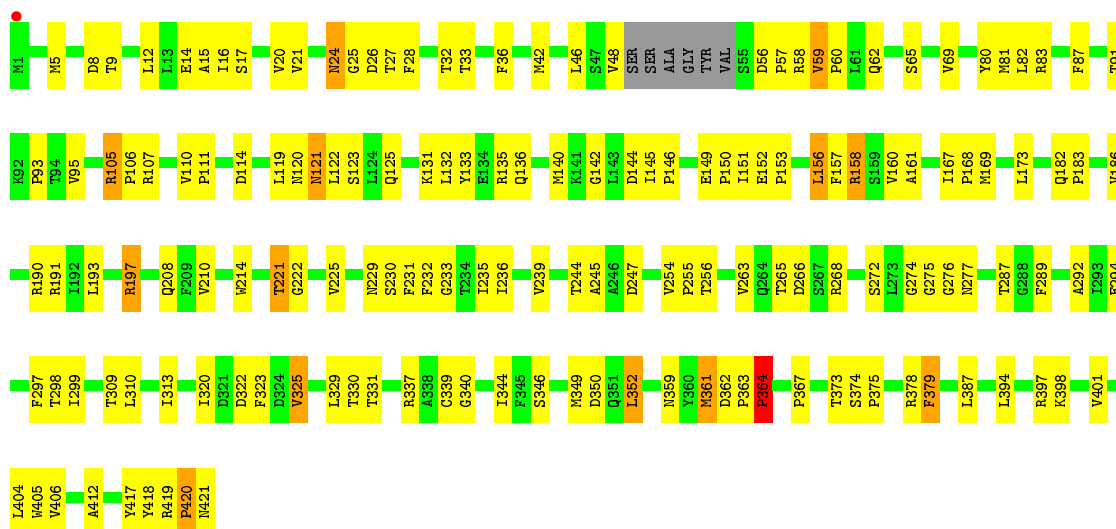
Chain P:





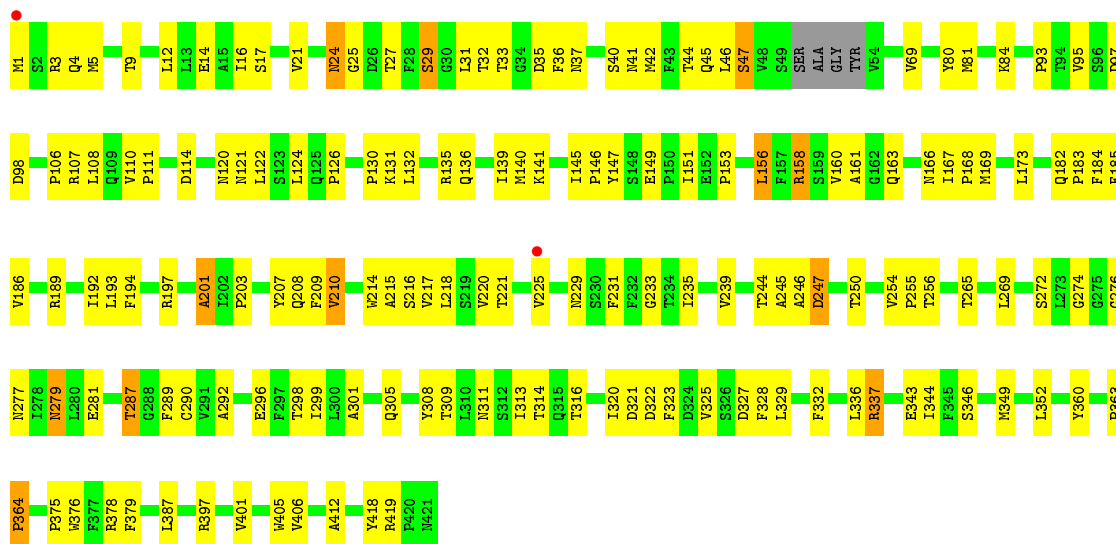
• Molecule 2: Outer capsid protein P8

Chain C: 61% 34% . .



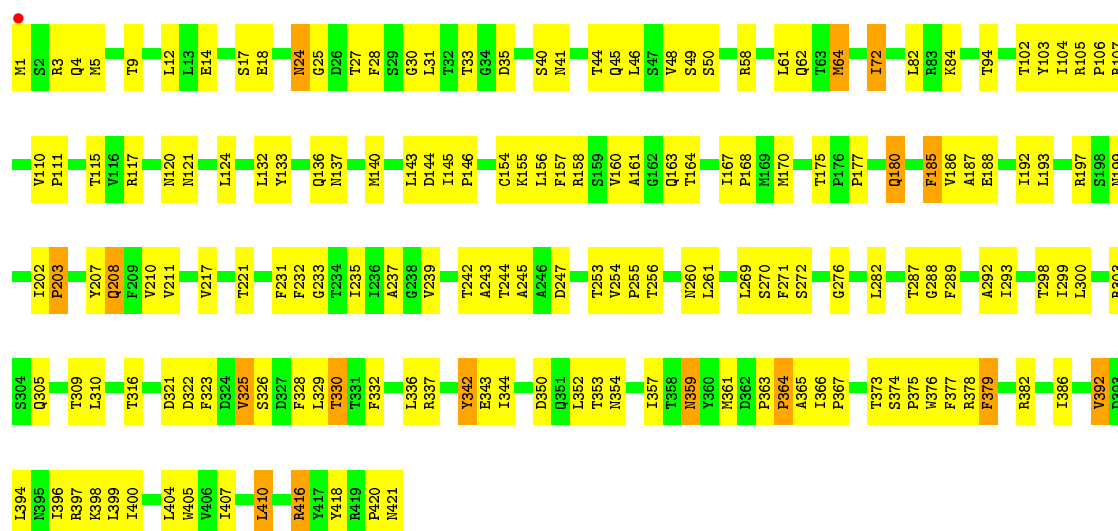
• Molecule 2: Outer capsid protein P8

Chain D: 61% 35% . .



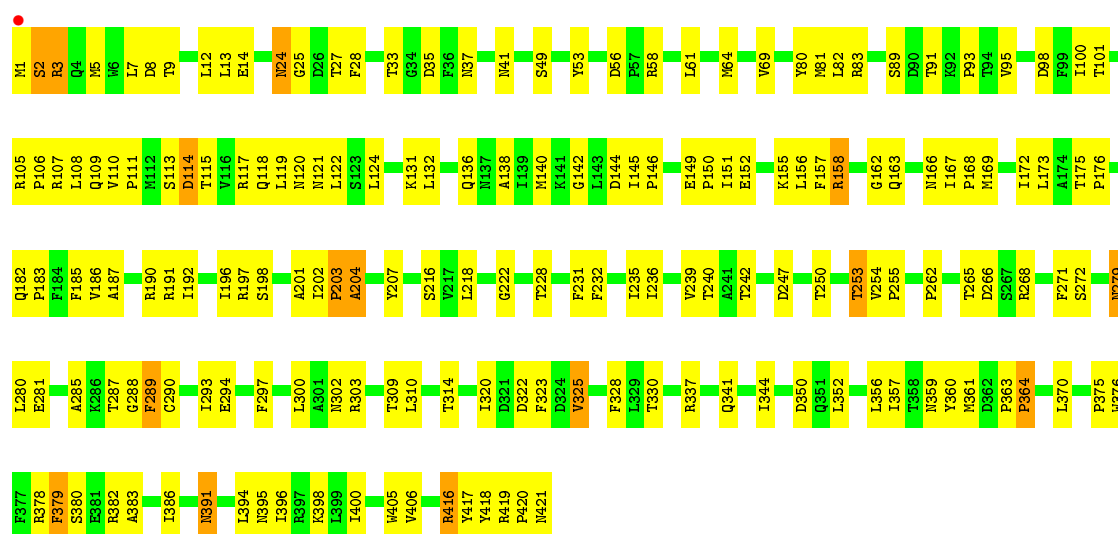
• Molecule 2: Outer capsid protein P8

Chain Q: 59% 37% .



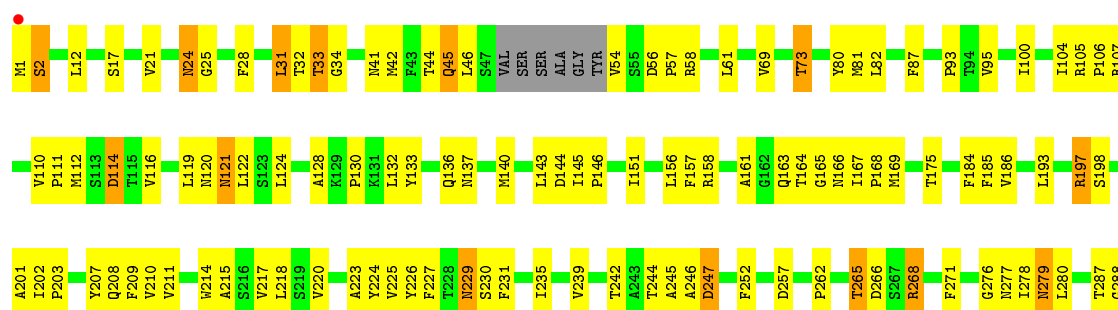
• Molecule 2: Outer capsid protein P8

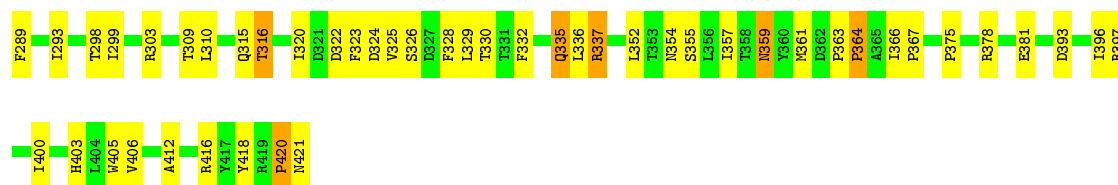
Chain E: 58% 38%



• Molecule 2: Outer capsid protein P8

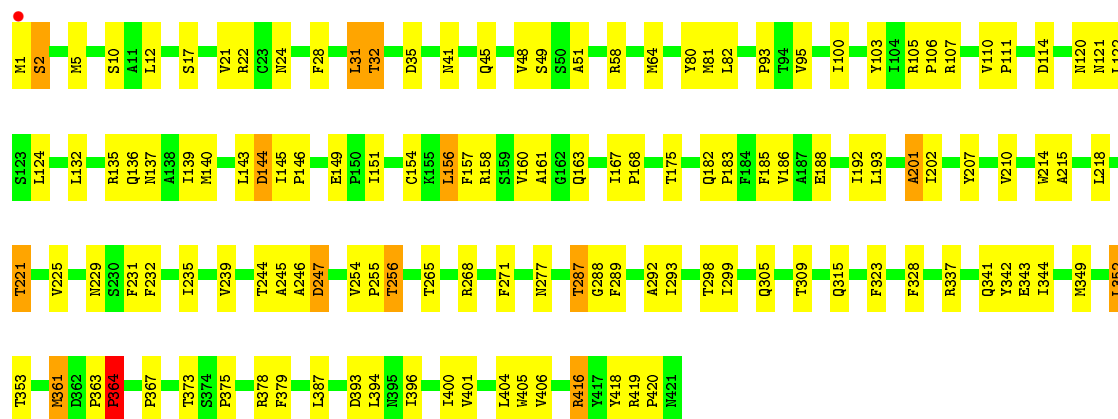
Chain F: 60% 34% 5%





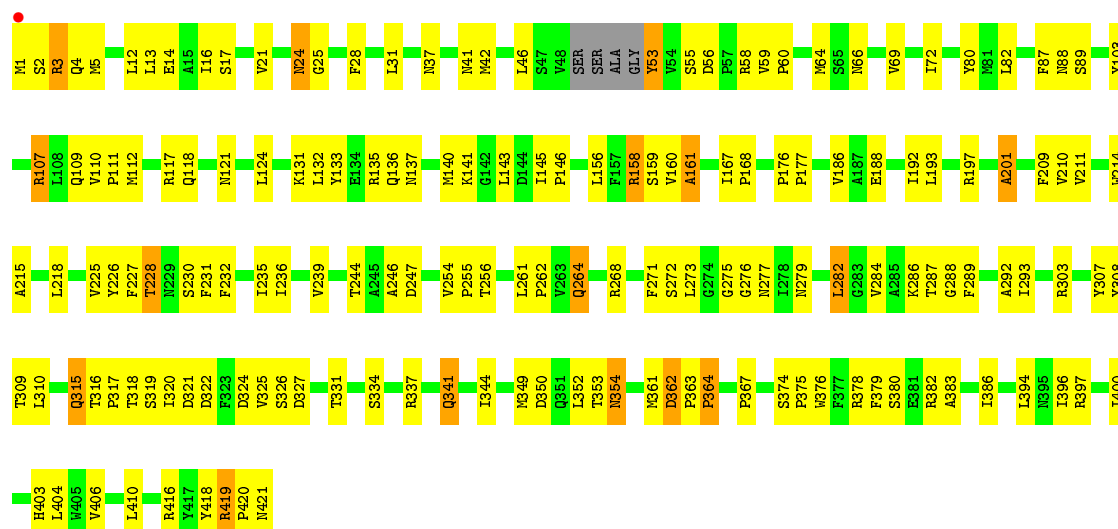
• Molecule 2: Outer capsid protein P8

Chain R: 69% 28%



• Molecule 2: Outer capsid protein P8

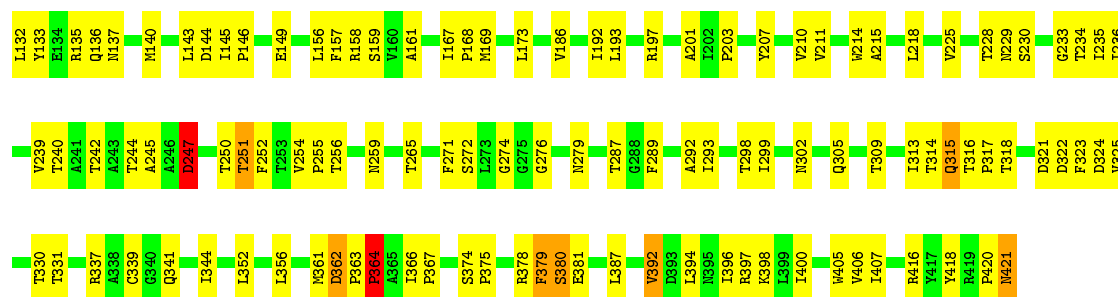
Chain G: 60% 35%



• Molecule 2: Outer capsid protein P8

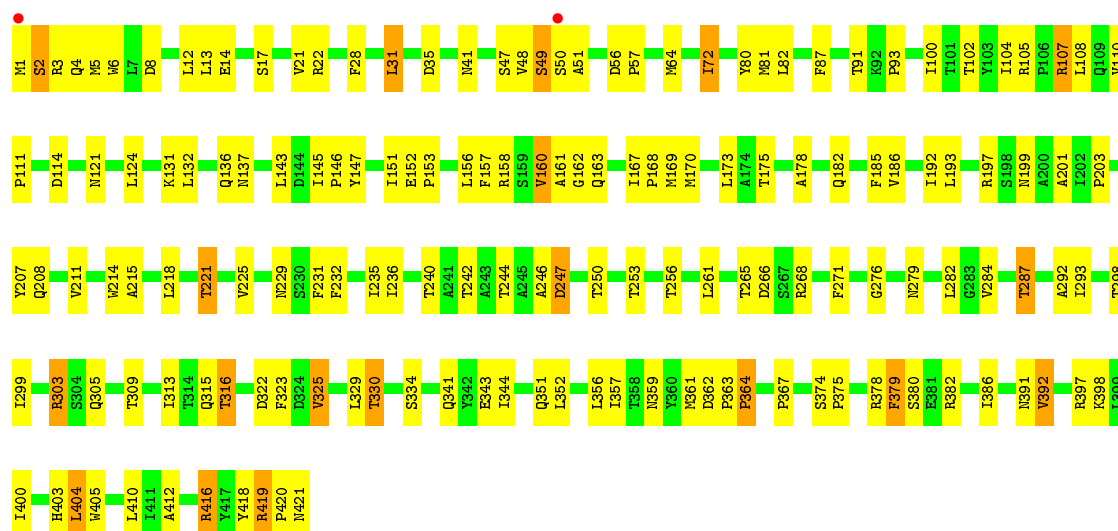
Chain H: 65% 33%





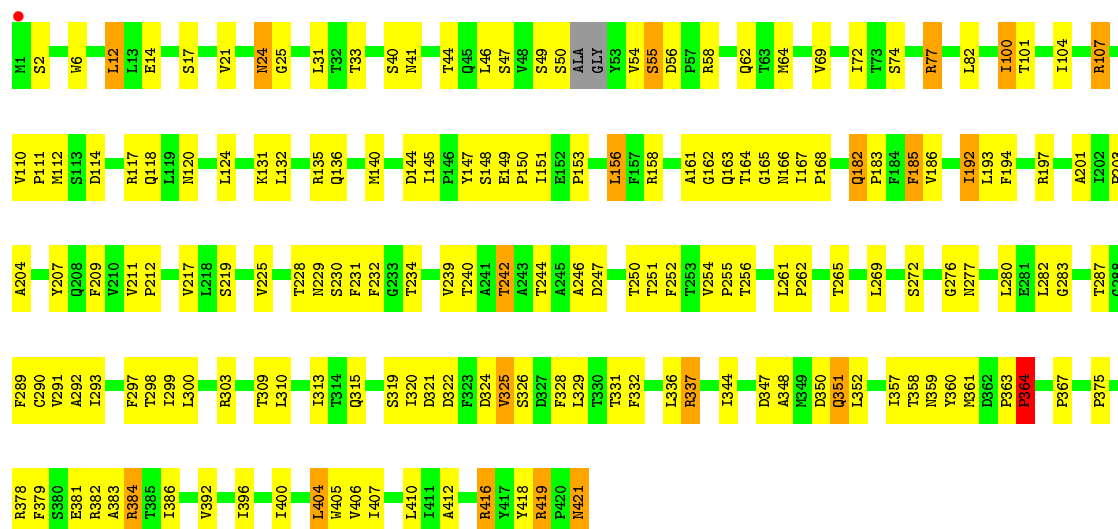
• Molecule 2: Outer capsid protein P8

Chain S: 62% 33% 5%



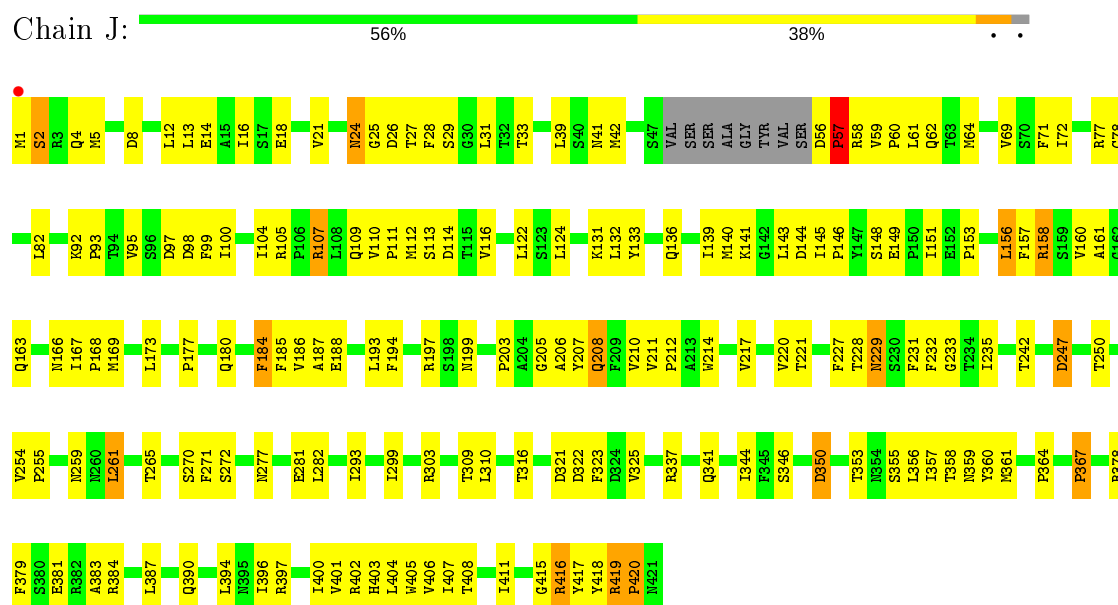
• Molecule 2: Outer capsid protein P8

Chain I: 59% 36% 5%



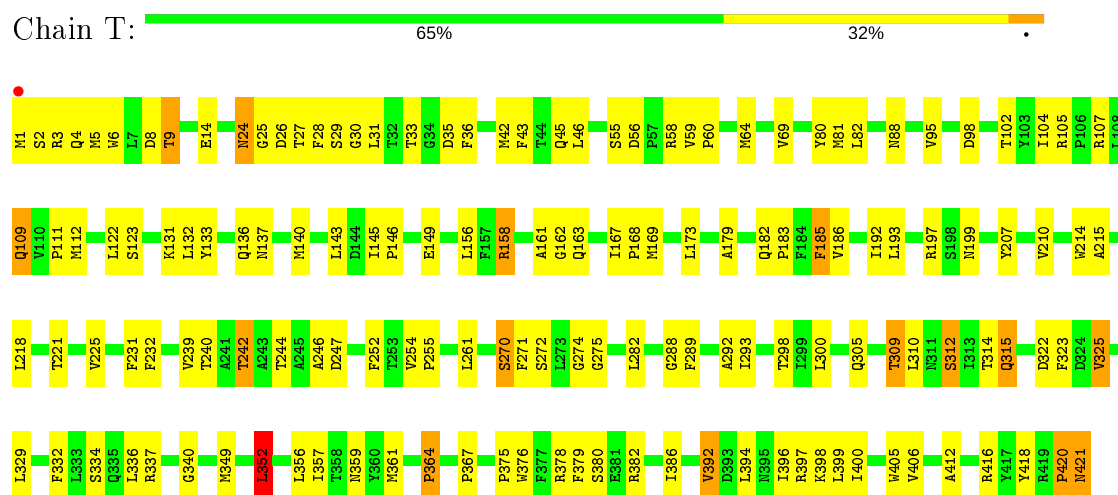
• Molecule 2: Outer capsid protein P8

Chain J:

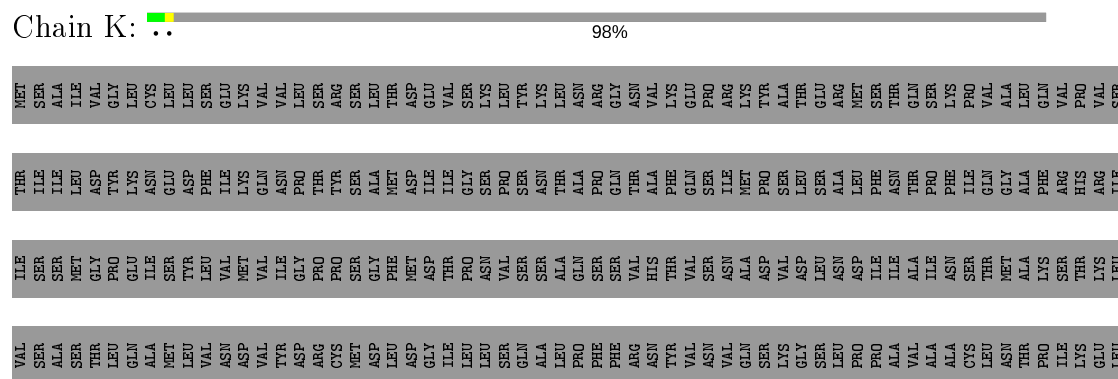


- Molecule 2: Outer capsid protein P8

Chain T:



- Molecule 3: Structural protein P7

Chain K: ..

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	770.00Å 795.00Å 814.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	228.74 – 3.50 327.81 – 3.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (228.74-3.50) 90.2 (327.81-3.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.49Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.303 , 0.306 0.308 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	58130	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/7816	0.72	1/10641 (0.0%)
1	B	0.52	0/8224	0.74	6/11197 (0.1%)
2	C	0.41	0/3308	0.65	0/4508
2	D	0.42	0/3321	0.69	1/4526 (0.0%)
2	E	0.45	0/3350	0.69	0/4567
2	F	0.44	0/3308	0.70	0/4508
2	G	0.48	0/3328	0.70	0/4536
2	H	0.52	3/3350 (0.1%)	0.72	0/4567
2	I	0.47	0/3340	0.70	0/4552
2	J	0.43	0/3295	0.68	0/4490
2	P	0.41	0/3301	0.65	0/4498
2	Q	0.45	0/3350	0.69	0/4567
2	R	0.46	0/3350	0.69	0/4567
2	S	0.43	0/3350	0.68	0/4567
2	T	0.51	1/3350 (0.0%)	0.73	1/4567 (0.0%)
3	K	1.00	0/100	1.28	0/132
All	All	0.47	4/59441 (0.0%)	0.70	9/80990 (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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	421	ASN	C-O	6.87	1.36	1.23
2	H	421	ASN	CB-CG	6.18	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	421	ASN	C-O	5.30	1.33	1.23
2	H	421	ASN	CA-CB	5.19	1.66	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1019	LEU	CA-C-O	-8.56	102.13	120.10
1	B	1019	LEU	CB-CG-CD1	-8.01	97.38	111.00
1	A	651	GLN	N-CA-C	-7.82	89.89	111.00
1	B	149	GLY	N-CA-C	-5.66	98.96	113.10
1	B	1019	LEU	CB-CG-CD2	5.58	120.48	111.00
1	B	499	ALA	N-CA-C	5.32	125.35	111.00
1	B	938	LEU	CA-CB-CG	5.21	127.29	115.30
2	T	352	LEU	CA-CB-CG	5.06	126.94	115.30
2	D	29	SER	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	751	TYR	Sidechain
1	B	509	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	7653	0	7664	275	0
1	B	8053	0	8062	248	0
2	C	3234	0	3208	145	0
2	D	3247	0	3222	140	0
2	E	3274	0	3245	147	0
2	F	3234	0	3208	172	0
2	G	3253	0	3226	157	0
2	H	3274	0	3245	132	0
2	I	3265	0	3236	152	0
2	J	3221	0	3194	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	3227	0	3199	123	0
2	Q	3274	0	3245	158	0
2	R	3274	0	3245	131	0
2	S	3274	0	3245	147	0
2	T	3274	0	3245	107	0
3	K	99	0	89	2	0
All	All	58130	0	57778	2194	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 (2194) 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:S:235:ILE:HD11	2:J:235:ILE:HD12	1.19	1.14
2:S:361:MET:HE1	2:S:367:PRO:HD3	1.24	1.12
2:P:235:ILE:HD13	2:D:229:ASN:HD21	1.06	1.09
2:S:344:ILE:HD12	2:S:344:ILE:H	1.20	1.07
1:B:225:HIS:ND1	1:B:227:ILE:HG22	1.71	1.05
2:J:361:MET:HE1	2:J:367:PRO:HD3	1.07	1.05
2:Q:353:THR:HG22	2:Q:404:LEU:HD21	1.37	1.04
1:B:106:MET:HG2	1:B:772:ILE:HG21	1.40	1.03
2:E:344:ILE:H	2:E:344:ILE:HD12	1.22	1.01
2:H:366:ILE:H	2:H:366:ILE:HD12	1.22	1.01
2:F:197:ARG:HG2	2:F:197:ARG:HH11	1.19	1.00
2:H:361:MET:HE1	2:H:367:PRO:HD3	1.44	1.00
2:C:229:ASN:HD21	2:D:235:ILE:HD13	1.26	0.99
2:S:107:ARG:HG3	2:S:107:ARG:HH11	1.27	0.97
2:E:163:GLN:HE22	2:E:185:PHE:H	1.06	0.97
2:S:82:LEU:HD11	2:S:352:LEU:HD12	1.47	0.96
2:E:122:LEU:HD21	2:F:335:GLN:HE22	1.26	0.96
2:S:361:MET:CE	2:S:367:PRO:HD3	1.95	0.95
2:E:5:MET:HE2	2:E:105:ARG:HA	1.47	0.94
1:A:51:SER:HA	1:A:713:GLN:HE22	1.32	0.93
2:D:5:MET:HE3	2:D:106:PRO:HD3	1.46	0.93
2:F:337:ARG:HH11	2:F:337:ARG:HG3	1.31	0.92
2:R:31:LEU:CD2	2:H:41:ASN:HB3	1.99	0.92
2:S:235:ILE:HD11	2:J:235:ILE:CD1	1.99	0.92
2:P:229:ASN:HD21	2:C:235:ILE:HD13	1.32	0.91
2:R:31:LEU:HD22	2:H:41:ASN:HB3	1.49	0.91
1:A:693:ILE:HG23	1:B:31:VAL:HG13	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:296:GLU:O	3:K:297:ARG:HB2	1.71	0.91
1:B:669:ILE:HD12	1:B:669:ILE:H	1.36	0.90
2:G:362:ASP:OD1	2:G:362:ASP:O	1.90	0.90
2:J:361:MET:CE	2:J:367:PRO:HD3	2.00	0.89
2:C:142:GLY:HA3	2:Q:344:ILE:HD11	1.54	0.89
2:C:255:PRO:HG2	2:C:275:GLY:HA3	1.51	0.89
2:I:244:THR:HG22	2:I:246:ALA:H	1.37	0.88
2:H:344:ILE:H	2:H:344:ILE:HD12	1.37	0.88
2:J:62:GLN:HE21	2:J:419:ARG:HB3	1.39	0.87
2:S:240:THR:HG22	2:S:242:THR:H	1.40	0.87
2:R:344:ILE:H	2:R:344:ILE:HD12	1.39	0.87
2:E:253:THR:HG22	2:E:279:ASN:HB2	1.56	0.86
2:P:182:GLN:HG3	2:P:183:PRO:HD2	1.57	0.86
2:C:344:ILE:HD12	2:C:344:ILE:H	1.41	0.86
2:C:208:GLN:OE1	2:F:210:VAL:HG21	1.75	0.86
2:F:361:MET:HE2	2:F:367:PRO:HD3	1.58	0.86
1:B:616:VAL:HG23	1:B:662:PHE:O	1.75	0.86
2:T:244:THR:HG22	2:T:246:ALA:H	1.41	0.85
2:F:197:ARG:CG	2:F:197:ARG:HH11	1.90	0.85
2:S:161:ALA:HA	2:S:315:GLN:HE22	1.41	0.85
1:A:349:ASN:H	1:A:349:ASN:HD22	1.24	0.85
2:E:391:ASN:ND2	2:E:391:ASN:H	1.71	0.85
1:B:60:LEU:HD12	1:B:60:LEU:H	1.41	0.84
1:B:684:ASN:HB3	2:R:32:THR:HG21	1.59	0.84
2:E:41:ASN:HB3	2:F:31:LEU:HD22	1.57	0.84
2:P:235:ILE:HD13	2:D:229:ASN:ND2	1.91	0.84
2:Q:3:ARG:HD2	2:Q:140:MET:HE3	1.60	0.84
2:P:344:ILE:H	2:P:344:ILE:HD12	1.42	0.83
2:S:375:PRO:HD2	2:S:378:ARG:HE	1.41	0.83
2:R:145:ILE:HG12	2:R:146:PRO:HD2	1.60	0.83
2:E:391:ASN:H	2:E:391:ASN:HD22	1.24	0.83
2:G:66:ASN:HD21	2:G:419:ARG:H	1.27	0.82
2:H:82:LEU:HD11	2:H:352:LEU:HD22	1.62	0.82
1:A:226:GLN:HE22	1:A:982:ASP:H	1.28	0.82
2:H:228:THR:HG22	2:H:229:ASN:H	1.43	0.82
2:P:20:VAL:HG23	2:P:39:LEU:HD11	1.60	0.81
1:B:696:LEU:HD23	1:B:700:PHE:HE1	1.43	0.81
2:G:227:PHE:H	2:G:264:GLN:HE22	1.26	0.81
1:A:438:ILE:HD11	1:A:447:TRP:CZ2	2.16	0.80
2:J:62:GLN:NE2	2:J:419:ARG:HB3	1.94	0.80
2:G:361:MET:SD	2:G:367:PRO:HG3	2.21	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:HIS:HA	1:B:180:VAL:HG12	1.63	0.80
1:A:226:GLN:NE2	1:A:982:ASP:H	1.79	0.80
2:F:316:THR:HG21	2:F:397:ARG:HH12	1.46	0.80
2:J:344:ILE:HD12	2:J:344:ILE:H	1.47	0.79
2:J:361:MET:HE1	2:J:367:PRO:CD	2.03	0.79
2:S:341:GLN:HA	2:S:344:ILE:HD13	1.64	0.79
2:C:323:PHE:HB2	2:C:405:TRP:HE1	1.47	0.79
2:J:378:ARG:HD2	2:J:381:GLU:OE1	1.82	0.79
2:F:322:ASP:HB2	2:F:325:VAL:HG12	1.63	0.79
2:H:107:ARG:HG3	2:H:107:ARG:HH11	1.48	0.79
2:E:118:GLN:HG2	2:G:421:ASN:O	1.81	0.79
2:F:337:ARG:HH11	2:F:337:ARG:CG	1.96	0.79
2:I:329:LEU:HD23	2:I:412:ALA:HB2	1.65	0.79
2:J:177:PRO:HG2	2:J:199:ASN:HB3	1.64	0.79
1:A:544:VAL:H	1:A:1013:ASN:ND2	1.81	0.79
2:S:2:SER:HB2	2:S:5:MET:HG3	1.64	0.78
1:A:286:GLN:HE21	1:A:287:LEU:N	1.81	0.78
2:H:159:SER:HB2	2:H:318:THR:HG22	1.63	0.78
2:H:192:ILE:HG22	2:H:293:ILE:HB	1.65	0.77
2:J:323:PHE:HB2	2:J:405:TRP:HE1	1.49	0.77
2:I:124:LEU:CD2	2:J:416:ARG:HD3	2.14	0.77
1:B:258:PRO:HG2	1:B:261:LEU:HD12	1.66	0.77
2:H:366:ILE:CD1	2:H:366:ILE:H	1.96	0.77
1:B:405:ALA:HA	1:B:408:ARG:NH1	1.99	0.76
2:H:173:LEU:HB3	2:H:236:ILE:HG23	1.65	0.76
2:D:255:PRO:HG3	2:D:276:GLY:H	1.49	0.76
2:D:344:ILE:H	2:D:344:ILE:HD12	1.51	0.76
2:F:229:ASN:HD22	2:F:229:ASN:C	1.89	0.76
2:Q:217:VAL:HG12	2:Q:299:ILE:HG23	1.68	0.76
2:G:228:THR:HG22	2:H:234:THR:OG1	1.84	0.75
2:I:229:ASN:HD21	2:J:235:ILE:HG12	1.51	0.75
2:Q:322:ASP:O	2:Q:325:VAL:HG22	1.86	0.75
2:T:6:TRP:CZ2	2:T:81:MET:HE1	2.22	0.75
1:B:165:ASN:C	1:B:165:ASN:HD22	1.88	0.75
2:E:122:LEU:CD2	2:F:335:GLN:HE22	1.98	0.75
2:J:163:GLN:NE2	2:J:169:MET:HG3	2.02	0.75
2:I:256:THR:HB	2:J:337:ARG:HH12	1.51	0.75
2:S:235:ILE:HG13	2:J:229:ASN:HD21	1.51	0.75
2:E:182:GLN:HE21	2:E:183:PRO:HD2	1.50	0.74
2:P:151:ILE:O	2:P:151:ILE:HD12	1.87	0.74
2:T:349:MET:HE1	2:T:352:LEU:HG	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:349:MET:CE	2:G:352:LEU:HD23	2.18	0.74
2:H:322:ASP:O	2:H:325:VAL:HG23	1.87	0.74
2:S:261:LEU:HD23	2:I:378:ARG:NH2	2.02	0.74
2:J:14:GLU:OE1	2:J:131:LYS:HB3	1.88	0.74
2:S:192:ILE:HG22	2:S:293:ILE:HB	1.70	0.74
2:C:375:PRO:HD2	2:C:378:ARG:HD3	1.69	0.73
2:Q:210:VAL:HG21	2:J:208:GLN:HG2	1.68	0.73
2:H:240:THR:HG22	2:H:242:THR:H	1.53	0.73
2:Q:145:ILE:HG12	2:Q:146:PRO:HD2	1.70	0.73
2:I:12:LEU:HD12	2:I:107:ARG:HG2	1.71	0.73
2:S:416:ARG:HD3	2:J:124:LEU:CD2	2.18	0.72
1:A:241:ILE:HG21	1:A:753:VAL:HG21	1.70	0.72
2:F:41:ASN:O	2:F:44:THR:HG22	1.89	0.72
2:S:124:LEU:CD2	2:I:416:ARG:HD3	2.19	0.72
2:H:361:MET:HE1	2:H:367:PRO:CD	2.20	0.72
2:I:361:MET:HE2	2:I:367:PRO:HD3	1.70	0.72
2:Q:192:ILE:HG22	2:Q:293:ILE:HB	1.72	0.72
2:H:339:CYS:HB3	2:H:421:ASN:HD21	1.54	0.72
2:I:250:THR:HG23	2:I:282:LEU:HA	1.71	0.72
2:H:418:TYR:CE1	2:H:420:PRO:HG3	2.25	0.72
2:T:357:ILE:HD13	2:T:400:ILE:HG21	1.69	0.72
2:F:209:PHE:HB2	2:F:278:ILE:HG23	1.71	0.72
2:H:145:ILE:HG12	2:H:146:PRO:HD2	1.70	0.72
2:Q:361:MET:HG2	2:Q:392:VAL:HG11	1.72	0.72
2:T:361:MET:CE	2:T:367:PRO:HD3	2.20	0.72
2:F:151:ILE:HD13	2:F:156:LEU:HD13	1.72	0.72
2:H:228:THR:HG22	2:H:229:ASN:N	2.04	0.72
2:J:2:SER:HB3	2:J:5:MET:HB2	1.72	0.72
2:R:31:LEU:HD22	2:H:41:ASN:CB	2.20	0.72
1:B:985:ILE:HD12	1:B:985:ILE:O	1.90	0.71
2:E:391:ASN:N	2:E:391:ASN:HD22	1.86	0.71
2:F:361:MET:CE	2:F:367:PRO:HD3	2.19	0.71
2:P:31:LEU:HD22	2:D:41:ASN:HB3	1.71	0.71
2:P:80:TYR:CE2	2:P:81:MET:HG3	2.25	0.71
2:S:344:ILE:HD12	2:S:344:ILE:N	2.02	0.71
2:S:82:LEU:HD11	2:S:352:LEU:CD1	2.18	0.71
2:I:361:MET:CE	2:I:367:PRO:HD3	2.20	0.71
1:B:187:ARG:HG2	1:B:187:ARG:HH11	1.56	0.71
1:B:222:VAL:HG13	1:B:223:PRO:HD2	1.71	0.71
2:G:159:SER:H	2:G:318:THR:HG23	1.55	0.71
2:J:18:GLU:O	2:J:21:VAL:HG12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:HG23	1:A:276:ILE:HA	1.73	0.71
1:B:408:ARG:NH2	1:B:501:GLU:OE2	2.24	0.71
2:C:208:GLN:CD	2:F:210:VAL:HG21	2.11	0.70
1:A:304:ALA:HB2	1:A:369:ILE:HG13	1.73	0.70
2:C:231:PHE:O	2:C:232:PHE:HB2	1.92	0.70
2:G:41:ASN:HB3	2:H:31:LEU:CD2	2.22	0.70
2:S:357:ILE:HD11	2:S:386:ILE:HD12	1.74	0.70
2:S:416:ARG:HD3	2:J:124:LEU:HD21	1.74	0.70
2:J:205:GLY:O	2:J:281:GLU:HB2	1.91	0.70
2:J:396:ILE:O	2:J:400:ILE:HG13	1.91	0.70
2:P:375:PRO:HD2	2:P:378:ARG:HD3	1.74	0.70
1:A:316:VAL:HG21	1:A:651:GLN:NE2	2.07	0.70
1:B:2:ASP:OD2	1:B:4:THR:HG22	1.91	0.70
1:B:308:LEU:HD22	1:B:362:GLN:HB2	1.73	0.70
2:C:5:MET:HE3	2:C:106:PRO:HD3	1.74	0.70
2:I:54:VAL:HG12	2:I:55:SER:N	2.06	0.70
1:A:286:GLN:HE21	1:A:287:LEU:H	1.39	0.70
2:C:142:GLY:CA	2:Q:344:ILE:HD11	2.22	0.70
2:I:344:ILE:HD12	2:I:344:ILE:H	1.56	0.70
2:T:361:MET:HE2	2:T:367:PRO:HD3	1.74	0.70
2:H:362:ASP:OD1	2:H:362:ASP:C	2.30	0.70
2:R:157:PHE:O	2:R:158:ARG:HD2	1.91	0.70
2:R:361:MET:HE1	2:R:367:PRO:HD3	1.73	0.70
1:A:289:ASP:H	1:A:673:GLN:NE2	1.90	0.70
2:P:229:ASN:ND2	2:C:235:ILE:HD13	2.06	0.70
2:T:59:VAL:HG13	2:T:60:PRO:HD3	1.73	0.70
2:F:110:VAL:CG2	2:F:111:PRO:HA	2.22	0.70
1:A:970:THR:HG21	2:J:41:ASN:OD1	1.91	0.69
1:B:787:VAL:HG21	1:B:853:VAL:HG12	1.73	0.69
2:J:59:VAL:HB	2:J:60:PRO:HD3	1.74	0.69
1:A:234:LEU:HD22	1:A:757:GLN:HE21	1.57	0.69
2:R:146:PRO:HG2	2:R:149:GLU:HB2	1.74	0.69
2:S:344:ILE:CD1	2:S:344:ILE:H	1.99	0.69
1:A:623:ARG:HG3	1:A:623:ARG:HH11	1.58	0.69
1:B:212:GLU:OE1	1:B:986:ARG:NH1	2.26	0.69
2:Q:366:ILE:HD12	2:Q:366:ILE:H	1.58	0.69
2:D:80:TYR:CE2	2:D:81:MET:HG3	2.28	0.69
2:H:344:ILE:HD12	2:H:344:ILE:N	2.07	0.69
2:P:158:ARG:NH2	2:P:320:ILE:HG13	2.07	0.69
1:A:788:ASP:OD2	1:A:791:SER:HB2	1.92	0.69
2:R:235:ILE:HD13	2:H:229:ASN:HD21	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:124:LEU:HD21	2:J:416:ARG:HD3	1.73	0.69
2:R:254:VAL:HG13	2:R:255:PRO:HD2	1.74	0.69
2:Q:208:GLN:HG2	2:J:210:VAL:HG21	1.73	0.69
2:H:94:THR:O	2:H:94:THR:HG23	1.91	0.68
2:Q:137:ASN:HB3	2:Q:143:LEU:HD12	1.74	0.68
1:A:120:MET:HG3	1:A:682:LEU:HD11	1.76	0.68
2:D:140:MET:CE	2:D:406:VAL:HG11	2.23	0.68
2:S:6:TRP:CZ2	2:S:81:MET:HE1	2.27	0.68
2:I:24:ASN:HD22	2:I:25:GLY:N	1.90	0.68
2:H:254:VAL:HG12	2:H:256:THR:H	1.58	0.68
1:B:655:LEU:HG	1:B:657:GLU:HG3	1.74	0.68
2:G:41:ASN:HB3	2:H:31:LEU:HD21	1.75	0.68
2:G:210:VAL:HA	2:G:277:ASN:HB3	1.75	0.68
2:E:344:ILE:HD12	2:E:344:ILE:N	2.04	0.68
2:F:82:LEU:HD11	2:F:352:LEU:HD22	1.75	0.68
1:B:844:LEU:HD11	1:B:870:ILE:HG13	1.75	0.68
2:E:163:GLN:NE2	2:E:185:PHE:H	1.86	0.68
2:G:69:VAL:HG21	2:G:418:TYR:CE1	2.29	0.68
2:J:12:LEU:O	2:J:16:ILE:HG12	1.94	0.68
1:A:219:ARG:HH11	1:A:219:ARG:HG3	1.59	0.67
2:J:156:LEU:HD21	2:J:299:ILE:HD11	1.76	0.67
1:A:280:MET:HG2	1:A:281:PRO:HD2	1.75	0.67
1:A:438:ILE:HD11	1:A:447:TRP:CH2	2.29	0.67
2:E:173:LEU:HB3	2:E:236:ILE:HG23	1.75	0.67
2:G:320:ILE:HD11	2:G:383:ALA:HB1	1.75	0.67
2:F:197:ARG:HG2	2:F:197:ARG:NH1	2.01	0.67
2:H:186:VAL:HG23	2:H:193:LEU:HB2	1.74	0.67
2:Q:394:LEU:HG	2:Q:398:LYS:HE3	1.77	0.67
2:R:239:VAL:HG13	2:R:289:PHE:HA	1.77	0.67
2:E:344:ILE:H	2:E:344:ILE:CD1	2.00	0.67
2:I:322:ASP:O	2:I:325:VAL:HG22	1.95	0.67
2:D:69:VAL:HG21	2:D:418:TYR:CD1	2.30	0.67
2:Q:261:LEU:HD23	2:E:378:ARG:NH2	2.10	0.67
2:P:323:PHE:HB2	2:P:405:TRP:NE1	2.09	0.67
2:S:266:ASP:HB2	2:I:319:SER:HB3	1.76	0.67
1:A:108:ILE:HG22	1:A:774:ILE:HD11	1.76	0.67
2:C:361:MET:CE	2:C:367:PRO:HD3	2.25	0.67
2:D:309:THR:O	2:D:309:THR:HG22	1.95	0.67
2:E:204:ALA:HB2	2:E:285:ALA:N	2.09	0.67
2:G:344:ILE:H	2:G:344:ILE:HD12	1.59	0.67
2:H:344:ILE:H	2:H:344:ILE:CD1	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:419:ARG:HE	2:I:421:ASN:HD21	1.43	0.67
1:B:732:LYS:N	1:B:733:PRO:HD2	2.10	0.67
2:C:374:SER:HB2	2:C:375:PRO:HD2	1.76	0.67
2:F:186:VAL:HG23	2:F:193:LEU:HB2	1.77	0.67
2:C:26:ASP:HA	2:C:28:PHE:HE1	1.60	0.66
2:S:378:ARG:HH12	2:J:261:LEU:HD22	1.59	0.66
1:A:561:LEU:HG	1:A:565:MET:CE	2.25	0.66
2:E:5:MET:HE2	2:E:106:PRO:HD3	1.76	0.66
2:F:54:VAL:HG12	2:F:54:VAL:O	1.94	0.66
2:G:3:ARG:HG2	2:G:4:GLN:N	2.11	0.66
2:Q:180:GLN:HE21	2:Q:202:ILE:HG22	1.61	0.66
1:A:1003:ILE:H	1:A:1003:ILE:HD13	1.61	0.66
1:B:444:ILE:H	1:B:444:ILE:CD1	2.07	0.66
2:D:158:ARG:NH2	2:D:320:ILE:HG13	2.10	0.66
2:G:353:THR:HG22	2:G:404:LEU:HD11	1.77	0.66
2:G:418:TYR:CZ	2:G:420:PRO:HG3	2.30	0.66
2:H:378:ARG:HD2	2:H:381:GLU:OE2	1.95	0.66
2:I:320:ILE:HD11	2:I:383:ALA:HB1	1.77	0.66
2:I:49:SER:O	2:I:50:SER:HB3	1.93	0.66
2:S:49:SER:C	2:S:51:ALA:H	1.98	0.66
2:T:33:THR:HG22	2:T:35:ASP:H	1.59	0.66
1:A:349:ASN:N	1:A:349:ASN:HD22	1.92	0.66
2:I:261:LEU:HD23	2:J:378:ARG:CZ	2.26	0.66
1:A:781:VAL:HG23	1:A:868:ASP:O	1.96	0.66
2:D:272:SER:C	2:D:274:GLY:H	1.98	0.66
2:J:353:THR:O	2:J:357:ILE:HG13	1.96	0.66
2:S:107:ARG:HH11	2:S:107:ARG:CG	2.03	0.66
2:S:12:LEU:HD22	2:S:107:ARG:HD2	1.76	0.66
2:I:230:SER:HB3	2:J:233:GLY:O	1.96	0.66
1:B:616:VAL:HG22	1:B:662:PHE:CE2	2.31	0.66
2:C:323:PHE:HB2	2:C:405:TRP:NE1	2.10	0.66
1:B:669:ILE:CD1	1:B:669:ILE:H	2.09	0.65
2:I:24:ASN:HD22	2:I:24:ASN:C	1.99	0.65
2:Q:210:VAL:HG21	2:J:208:GLN:CG	2.26	0.65
2:T:255:PRO:HB2	2:T:275:GLY:HA3	1.78	0.65
1:A:976:ARG:O	1:A:980:THR:HG23	1.96	0.65
2:E:7:LEU:CD2	2:E:136:GLN:HE21	2.09	0.65
2:F:120:ASN:O	2:F:122:LEU:N	2.30	0.65
2:F:239:VAL:HA	2:F:288:GLY:HA3	1.78	0.65
2:Q:366:ILE:HD12	2:Q:366:ILE:N	2.11	0.65
2:J:24:ASN:HD22	2:J:25:GLY:N	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ILE:HD11	1:B:458:ILE:HG12	1.78	0.65
2:H:239:VAL:HG13	2:H:289:PHE:HA	1.78	0.65
2:T:375:PRO:HD2	2:T:378:ARG:HD3	1.79	0.65
2:G:110:VAL:HG22	2:G:111:PRO:HA	1.79	0.65
2:G:244:THR:HG22	2:G:246:ALA:H	1.60	0.65
2:P:239:VAL:HG13	2:P:289:PHE:HA	1.77	0.65
2:R:309:THR:O	2:R:309:THR:HG22	1.95	0.65
2:T:349:MET:CE	2:T:352:LEU:HG	2.27	0.65
1:B:930:LEU:O	1:B:931:GLY:O	2.14	0.65
2:J:254:VAL:HG11	2:J:272:SER:O	1.97	0.65
2:P:12:LEU:HD22	2:P:107:ARG:HD2	1.78	0.65
2:G:244:THR:HB	2:G:247:ASP:OD1	1.95	0.65
2:P:82:LEU:HD11	2:P:352:LEU:HD22	1.77	0.65
2:Q:357:ILE:HG23	2:Q:400:ILE:HD13	1.78	0.65
2:I:329:LEU:CD2	2:I:412:ALA:HB2	2.27	0.65
1:B:60:LEU:HD12	1:B:60:LEU:N	2.12	0.64
1:B:669:ILE:HD12	1:B:669:ILE:N	2.10	0.64
2:C:309:THR:O	2:C:309:THR:HG22	1.96	0.64
2:P:165:GLY:O	2:P:169:MET:HG2	1.96	0.64
2:E:115:THR:HG21	2:F:57:PRO:HD2	1.80	0.64
2:E:391:ASN:ND2	2:E:391:ASN:N	2.42	0.64
2:G:137:ASN:HB3	2:G:143:LEU:HD12	1.79	0.64
2:G:211:VAL:HG22	2:G:276:GLY:O	1.98	0.64
2:J:140:MET:CE	2:J:406:VAL:HG11	2.27	0.64
2:P:254:VAL:HG13	2:P:255:PRO:HD2	1.79	0.64
2:T:158:ARG:HD2	2:T:312:SER:HB3	1.79	0.64
2:C:59:VAL:HB	2:C:60:PRO:CD	2.27	0.64
1:A:844:LEU:HD11	1:A:870:ILE:HG13	1.79	0.64
2:E:132:LEU:O	2:E:136:GLN:HG3	1.96	0.64
2:F:209:PHE:HB2	2:F:278:ILE:CG2	2.26	0.64
2:C:337:ARG:HH11	2:C:337:ARG:HG3	1.61	0.64
2:Q:115:THR:HG23	2:E:58:ARG:HG2	1.79	0.64
2:G:110:VAL:CG2	2:G:111:PRO:HA	2.27	0.64
2:P:309:THR:HG22	2:P:309:THR:O	1.98	0.64
2:Q:5:MET:HE3	2:Q:106:PRO:HD3	1.79	0.64
1:A:544:VAL:H	1:A:1013:ASN:HD22	1.45	0.64
2:D:110:VAL:CG2	2:D:111:PRO:HA	2.27	0.64
2:D:201:ALA:HA	2:D:287:THR:HA	1.79	0.64
2:Q:133:TYR:HA	2:Q:136:GLN:OE1	1.97	0.64
1:A:124:ARG:HD3	1:A:124:ARG:C	2.18	0.64
1:B:392:MET:HG2	1:B:565:MET:HE1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:24:ASN:HD22	2:P:25:GLY:N	1.96	0.64
1:B:85:ILE:HG12	1:B:933:THR:OG1	1.98	0.63
2:S:124:LEU:HD23	2:I:416:ARG:HD3	1.79	0.63
1:A:915:ARG:HA	1:B:1005:VAL:HG23	1.80	0.63
1:B:151:LEU:HD12	1:B:152:PRO:HD2	1.80	0.63
1:B:19:VAL:O	1:B:21:GLU:N	2.31	0.63
2:E:95:VAL:CG2	2:E:100:ILE:HG21	2.28	0.63
2:G:192:ILE:HD11	2:G:218:LEU:CD1	2.29	0.63
2:F:316:THR:HG21	2:F:397:ARG:NH1	2.13	0.63
2:G:107:ARG:HG3	2:G:107:ARG:HH11	1.61	0.63
2:P:323:PHE:HB2	2:P:405:TRP:HE1	1.64	0.63
2:S:382:ARG:O	2:S:386:ILE:HG12	1.98	0.63
2:F:167:ILE:N	2:F:168:PRO:HD2	2.13	0.63
2:Q:163:GLN:HE22	2:Q:185:PHE:H	1.47	0.63
2:Q:58:ARG:HG2	2:F:119:LEU:HD13	1.80	0.63
2:T:24:ASN:HD22	2:T:25:GLY:N	1.97	0.63
1:B:377:LEU:O	1:B:414:ARG:NH1	2.32	0.63
2:G:239:VAL:HG13	2:G:289:PHE:HA	1.81	0.63
2:T:163:GLN:NE2	2:T:185:PHE:O	2.27	0.63
2:G:315:GLN:HE21	2:G:315:GLN:CA	2.12	0.63
2:Q:353:THR:O	2:Q:357:ILE:HG13	1.98	0.63
2:Q:33:THR:HG22	2:Q:35:ASP:H	1.63	0.63
1:A:432:LEU:HB3	1:A:438:ILE:HG22	1.81	0.63
2:C:12:LEU:HD22	2:C:107:ARG:HD3	1.81	0.63
2:C:33:THR:HG23	2:C:36:PHE:HB3	1.80	0.63
2:F:69:VAL:O	2:F:73:THR:HB	1.99	0.63
1:B:304:ALA:HB2	1:B:369:ILE:HB	1.79	0.63
2:C:210:VAL:HG21	2:F:208:GLN:NE2	2.14	0.63
2:H:361:MET:CE	2:H:367:PRO:HD3	2.24	0.63
2:R:5:MET:HE2	2:R:105:ARG:HA	1.80	0.63
2:D:349:MET:HE2	2:D:349:MET:HA	1.81	0.62
2:Q:379:PHE:CE1	2:Q:404:LEU:HD12	2.34	0.62
1:B:269:LEU:HA	1:B:272:THR:HG22	1.80	0.62
2:Q:342:TYR:O	2:Q:342:TYR:HD2	1.83	0.62
1:A:531:LEU:O	1:A:532:ALA:HB3	2.00	0.62
2:H:214:TRP:CZ3	2:H:215:ALA:HB2	2.34	0.62
2:I:217:VAL:HG13	2:I:303:ARG:HB3	1.79	0.62
1:B:115:GLU:HB3	1:B:116:PRO:HD3	1.81	0.62
1:B:619:ASP:OD1	1:B:621:VAL:HG23	1.98	0.62
2:F:208:GLN:HG2	2:F:279:ASN:HD21	1.64	0.62
2:E:124:LEU:CD2	2:F:416:ARG:HD3	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:24:ASN:HD22	2:G:25:GLY:N	1.97	0.62
2:G:361:MET:HE1	2:G:367:PRO:HG3	1.81	0.62
2:S:186:VAL:HG23	2:S:193:LEU:HB2	1.82	0.62
2:S:303:ARG:HH11	2:S:303:ARG:HB3	1.62	0.62
2:C:160:VAL:HG12	2:C:161:ALA:H	1.64	0.62
2:T:357:ILE:HD11	2:T:386:ILE:HD12	1.81	0.62
1:A:480:ASN:ND2	1:A:503:ARG:HD3	2.14	0.62
2:C:420:PRO:O	2:C:421:ASN:OXT	2.17	0.62
2:D:140:MET:HE3	2:D:406:VAL:HG11	1.81	0.62
2:Q:197:ARG:HG2	2:Q:239:VAL:HG23	1.81	0.62
1:B:553:GLU:HG2	2:Q:30:GLY:HA2	1.82	0.62
2:Q:379:PHE:HE1	2:Q:404:LEU:HD12	1.62	0.62
1:A:769:THR:O	1:A:772:ILE:HG12	2.00	0.62
1:A:835:ASP:OD1	1:A:838:SER:HB2	2.00	0.62
1:B:782:LYS:HG2	1:B:846:SER:HB2	1.79	0.62
2:Q:235:ILE:HD11	2:E:235:ILE:HD11	1.82	0.62
1:B:313:LEU:HD22	1:B:604:ALA:HB1	1.81	0.62
2:C:140:MET:CE	2:C:406:VAL:HG11	2.29	0.62
2:D:24:ASN:HD22	2:D:25:GLY:N	1.96	0.62
2:G:255:PRO:HB2	2:G:275:GLY:HA3	1.80	0.62
1:A:286:GLN:NE2	1:A:287:LEU:H	1.98	0.62
1:B:268:SER:O	1:B:272:THR:HG22	1.99	0.62
2:F:110:VAL:HG22	2:F:111:PRO:HA	1.80	0.62
2:Q:167:ILE:N	2:Q:168:PRO:HD2	2.15	0.62
2:Q:271:PHE:HZ	2:Q:293:ILE:HD13	1.63	0.62
1:B:31:VAL:HG12	1:B:32:TYR:N	2.14	0.61
1:B:33:ASN:H	1:B:33:ASN:HD22	1.47	0.61
2:J:323:PHE:HB2	2:J:405:TRP:NE1	2.14	0.61
2:R:375:PRO:HD3	2:H:259:ASN:HD22	1.65	0.61
2:S:329:LEU:HD23	2:S:412:ALA:HB2	1.81	0.61
1:A:355:THR:O	1:A:358:VAL:HG12	2.00	0.61
1:A:660:PRO:HG2	1:A:662:PHE:CE1	2.35	0.61
2:C:151:ILE:O	2:C:151:ILE:HD12	2.00	0.61
2:C:255:PRO:CG	2:C:275:GLY:HA3	2.27	0.61
1:A:366:ASN:HD22	1:A:368:ASN:H	1.46	0.61
2:D:329:LEU:HD23	2:D:412:ALA:HB2	1.82	0.61
2:S:107:ARG:HG3	2:S:107:ARG:NH1	2.07	0.61
2:J:160:VAL:HG22	2:J:161:ALA:H	1.64	0.61
1:A:669:ILE:N	1:A:669:ILE:HD12	2.14	0.61
2:F:1:MET:HG3	2:F:100:ILE:HG21	1.81	0.61
2:Q:271:PHE:CZ	2:Q:293:ILE:HD13	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:ILE:HD12	2:D:151:ILE:O	1.99	0.61
2:J:167:ILE:N	2:J:168:PRO:HD2	2.15	0.61
1:A:595:THR:HA	1:A:645:VAL:HG13	1.83	0.61
2:C:230:SER:HB3	2:D:233:GLY:O	2.00	0.61
2:G:309:THR:HG22	2:G:309:THR:O	2.00	0.61
2:R:145:ILE:CG1	2:R:146:PRO:HD2	2.30	0.61
1:B:153:VAL:HG21	1:B:191:GLN:CD	2.19	0.61
1:B:746:ARG:HD3	2:G:37:ASN:HD21	1.64	0.61
2:D:24:ASN:C	2:D:24:ASN:HD22	2.03	0.61
2:I:298:THR:HG22	2:I:299:ILE:N	2.14	0.61
2:P:344:ILE:H	2:P:344:ILE:CD1	2.12	0.61
1:A:80:GLY:HA3	1:A:930:LEU:O	2.01	0.60
1:B:361:ALA:HA	1:B:605:ILE:HD12	1.83	0.60
2:F:329:LEU:HD13	2:F:412:ALA:HB2	1.82	0.60
1:B:227:ILE:HD11	1:B:768:LEU:HD21	1.83	0.60
2:J:383:ALA:O	2:J:387:LEU:HD23	2.01	0.60
2:S:145:ILE:HG12	2:S:146:PRO:HD2	1.82	0.60
1:A:60:LEU:HD22	1:A:60:LEU:N	2.16	0.60
1:B:696:LEU:HD23	1:B:700:PHE:CE1	2.31	0.60
2:H:140:MET:HE3	2:H:406:VAL:HG11	1.82	0.60
2:Q:48:VAL:HG23	2:Q:102:THR:O	2.01	0.60
2:C:42:MET:HG2	2:D:31:LEU:HD21	1.82	0.60
2:Q:167:ILE:HB	2:F:266:ASP:OD1	2.01	0.60
2:S:48:VAL:HG22	2:S:102:THR:HG23	1.82	0.60
1:B:63:ILE:HG22	1:B:137:MET:O	2.01	0.60
1:B:958:LEU:C	1:B:958:LEU:HD12	2.22	0.60
2:C:362:ASP:OD2	2:Q:366:ILE:HD13	2.02	0.60
1:A:533:LEU:HB3	1:A:534:PRO:HD2	1.83	0.60
2:F:24:ASN:HD22	2:F:25:GLY:N	2.00	0.60
2:S:41:ASN:HB3	2:I:31:LEU:CD1	2.30	0.60
1:A:108:ILE:N	1:A:108:ILE:HD12	2.17	0.60
2:E:235:ILE:HD11	2:F:235:ILE:HD11	1.83	0.60
2:G:209:PHE:O	2:G:277:ASN:HB2	2.02	0.60
2:G:254:VAL:HG13	2:G:255:PRO:HD2	1.84	0.60
2:S:378:ARG:NH1	2:J:261:LEU:HD22	2.17	0.60
1:A:85:ILE:HD12	1:A:85:ILE:H	1.67	0.60
2:P:145:ILE:HG12	2:P:146:PRO:HD2	1.84	0.60
1:B:438:ILE:HD11	1:B:458:ILE:CG1	2.30	0.60
2:I:186:VAL:CG2	2:I:193:LEU:HB2	2.32	0.60
1:B:165:ASN:C	1:B:165:ASN:ND2	2.56	0.60
1:B:30:GLU:HB3	1:B:35:LEU:HG	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:ILE:HD11	2:C:149:GLU:OE2	2.01	0.60
2:G:362:ASP:C	2:G:362:ASP:OD1	2.40	0.60
2:C:167:ILE:HB	2:C:168:PRO:HD3	1.83	0.59
2:G:4:GLN:HE22	2:G:141:LYS:HE3	1.67	0.59
2:Q:115:THR:CG2	2:E:58:ARG:HG2	2.32	0.59
1:B:468:VAL:HG23	2:D:98:ASP:OD1	2.02	0.59
1:B:65:LEU:O	1:B:68:VAL:HG23	2.02	0.59
2:E:202:ILE:HD13	2:E:288:GLY:H	1.66	0.59
2:E:203:PRO:HG2	2:E:207:TYR:OH	2.01	0.59
2:P:43:PHE:CE1	2:P:57:PRO:HB3	2.37	0.59
2:Q:361:MET:SD	2:Q:367:PRO:HG3	2.43	0.59
1:B:337:VAL:O	1:B:338:THR:C	2.41	0.59
2:F:193:LEU:HD12	2:F:231:PHE:HD1	1.66	0.59
2:Q:110:VAL:CG2	2:Q:111:PRO:HA	2.32	0.59
1:A:438:ILE:HD12	1:A:439:TYR:H	1.68	0.59
2:D:145:ILE:HG12	2:D:146:PRO:HD2	1.84	0.59
2:G:344:ILE:N	2:G:344:ILE:HD12	2.17	0.59
2:G:361:MET:CE	2:G:367:PRO:HG3	2.32	0.59
2:S:157:PHE:O	2:S:158:ARG:HD2	2.02	0.59
2:T:244:THR:HB	2:T:247:ASP:OD1	2.02	0.59
2:J:61:LEU:HD12	2:J:417:TYR:CE1	2.37	0.59
2:Q:217:VAL:CG1	2:Q:299:ILE:HG23	2.33	0.59
1:A:392:MET:O	1:A:558:LYS:HD2	2.03	0.59
1:A:813:ALA:HB2	2:E:101:THR:HB	1.85	0.59
2:F:214:TRP:CZ3	2:F:215:ALA:HB2	2.37	0.59
2:R:256:THR:CG2	2:G:337:ARG:NH1	2.65	0.59
2:T:69:VAL:HG21	2:T:418:TYR:CD1	2.38	0.59
2:P:31:LEU:HD21	2:D:45:GLN:CG	2.33	0.59
2:G:349:MET:HE1	2:G:352:LEU:HD23	1.84	0.59
2:C:140:MET:HE3	2:C:406:VAL:HG11	1.84	0.59
2:J:1:MET:HG2	2:J:93:PRO:HD2	1.85	0.59
1:A:366:ASN:ND2	1:A:368:ASN:H	2.00	0.59
2:Q:124:LEU:CD2	2:E:416:ARG:HD3	2.33	0.59
2:T:56:ASP:C	2:T:58:ARG:H	2.05	0.59
1:B:371:TYR:CE2	1:B:633:HIS:HB3	2.38	0.59
2:C:344:ILE:N	2:C:344:ILE:HD12	2.15	0.59
2:S:235:ILE:CD1	2:J:235:ILE:HD12	2.12	0.59
1:B:414:ARG:HD3	1:B:414:ARG:N	2.18	0.58
2:H:145:ILE:HG12	2:H:146:PRO:CD	2.33	0.58
2:H:396:ILE:O	2:H:400:ILE:HG13	2.03	0.58
2:J:77:ARG:NE	2:J:97:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:235:ILE:HD13	2:H:229:ASN:ND2	2.18	0.58
2:R:337:ARG:NH1	2:H:256:THR:HG22	2.18	0.58
2:T:122:LEU:HD12	2:T:122:LEU:N	2.18	0.58
1:A:475:THR:CG2	1:A:561:LEU:HD13	2.33	0.58
1:B:835:ASP:O	1:B:837:LEU:N	2.36	0.58
2:F:145:ILE:HG12	2:F:146:PRO:HD2	1.84	0.58
2:T:14:GLU:OE2	2:T:131:LYS:HB3	2.03	0.58
2:C:160:VAL:HG12	2:C:161:ALA:N	2.18	0.58
2:G:145:ILE:HG12	2:G:146:PRO:HD2	1.85	0.58
1:A:262:ARG:HD3	1:A:1003:ILE:HG22	1.85	0.58
2:E:7:LEU:HD22	2:E:136:GLN:HE21	1.67	0.58
1:A:688:ARG:NH2	2:E:37:ASN:OD1	2.36	0.58
2:I:167:ILE:N	2:I:168:PRO:CD	2.66	0.58
2:I:182:GLN:CG	2:I:183:PRO:HD2	2.32	0.58
2:I:54:VAL:O	2:I:55:SER:CB	2.51	0.58
2:T:221:THR:HA	2:T:270:SER:HB3	1.83	0.58
2:E:254:VAL:CG1	2:E:255:PRO:HD2	2.34	0.58
2:F:224:TYR:CE2	2:F:268:ARG:HD3	2.39	0.58
2:Q:14:GLU:OE2	2:Q:132:LEU:N	2.25	0.58
2:R:80:TYR:CE2	2:R:100:ILE:HD11	2.38	0.58
2:S:169:MET:O	2:S:173:LEU:HG	2.03	0.58
2:S:163:GLN:NE2	2:S:185:PHE:O	2.36	0.58
2:S:244:THR:N	2:S:247:ASP:OD2	2.25	0.58
1:A:366:ASN:HD22	1:A:366:ASN:C	2.07	0.58
1:B:206:LEU:H	1:B:206:LEU:HD12	1.67	0.58
1:B:945:ILE:O	1:B:948:TYR:HB3	2.04	0.58
2:E:157:PHE:C	2:E:158:ARG:HD2	2.23	0.58
2:G:4:GLN:HE22	2:G:141:LYS:CE	2.15	0.58
2:H:254:VAL:HG13	2:H:255:PRO:HD2	1.84	0.58
2:I:396:ILE:N	2:I:396:ILE:HD12	2.18	0.58
2:P:192:ILE:HD11	2:P:218:LEU:CD1	2.34	0.58
2:T:98:ASP:O	2:T:102:THR:HG23	2.02	0.58
1:B:165:ASN:HD21	1:B:167:ASP:HB2	1.69	0.58
1:B:290:TYR:O	1:B:293:VAL:HG23	2.03	0.58
1:B:438:ILE:HG23	1:B:447:TRP:HZ2	1.69	0.58
1:B:400:PRO:HG3	1:B:509:TYR:HB2	1.86	0.58
2:G:349:MET:HE1	2:G:352:LEU:CD2	2.34	0.58
2:Q:180:GLN:HE21	2:Q:202:ILE:CG2	2.16	0.58
2:R:41:ASN:ND2	2:G:31:LEU:HB2	2.18	0.58
2:T:309:THR:O	2:T:310:LEU:HB2	2.04	0.58
1:A:475:THR:HG22	1:A:561:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:349:MET:HE3	2:G:352:LEU:HD23	1.86	0.58
2:T:161:ALA:HA	2:T:315:GLN:NE2	2.19	0.58
1:B:33:ASN:H	1:B:33:ASN:ND2	2.02	0.58
2:E:254:VAL:HG13	2:E:255:PRO:HD2	1.86	0.58
2:E:337:ARG:HH11	2:E:337:ARG:HG3	1.66	0.58
2:J:140:MET:HE3	2:J:406:VAL:HG11	1.85	0.58
2:R:151:ILE:O	2:R:151:ILE:HD12	2.03	0.58
2:T:161:ALA:HA	2:T:315:GLN:HE22	1.67	0.58
1:A:527:TYR:CZ	1:A:531:LEU:HD11	2.39	0.58
2:C:65:SER:OG	2:C:417:TYR:HB2	2.04	0.58
2:E:228:THR:O	2:E:290:CYS:HB3	2.04	0.58
2:F:355:SER:O	2:F:359:ASN:ND2	2.36	0.58
2:I:261:LEU:HD23	2:J:378:ARG:NH1	2.18	0.58
2:J:110:VAL:HG23	2:J:111:PRO:HA	1.85	0.58
2:P:322:ASP:O	2:P:325:VAL:HG22	2.03	0.58
2:E:382:ARG:O	2:E:386:ILE:HG12	2.04	0.57
2:D:239:VAL:HG13	2:D:289:PHE:HA	1.86	0.57
2:E:360:TYR:HB2	2:E:400:ILE:HD11	1.87	0.57
2:H:12:LEU:HD22	2:H:107:ARG:HD2	1.86	0.57
1:B:781:VAL:HG12	1:B:869:ALA:HB2	1.85	0.57
2:C:254:VAL:HG11	2:C:272:SER:O	2.04	0.57
2:C:344:ILE:H	2:C:344:ILE:CD1	2.13	0.57
2:F:326:SER:HA	2:F:329:LEU:HD23	1.85	0.57
2:I:12:LEU:HD13	2:I:46:LEU:HD11	1.85	0.57
2:H:394:LEU:HG	2:H:398:LYS:HE3	1.87	0.57
1:A:632:LEU:HD12	1:A:632:LEU:N	2.19	0.57
2:E:145:ILE:HD11	2:E:149:GLU:OE2	2.05	0.57
2:R:182:GLN:HB3	2:R:183:PRO:HD2	1.86	0.57
2:R:22:ARG:HD3	2:R:35:ASP:OD2	2.04	0.57
2:S:316:THR:HG21	2:S:397:ARG:NH1	2.18	0.57
1:A:307:LEU:HD13	1:A:307:LEU:O	2.03	0.57
1:A:406:ARG:O	1:A:409:LEU:HB3	2.04	0.57
2:Q:155:LYS:HE2	2:F:268:ARG:HH21	1.70	0.57
1:A:286:GLN:CA	1:A:286:GLN:HE21	2.18	0.57
2:C:5:MET:HG2	2:C:106:PRO:HG3	1.85	0.57
2:G:349:MET:CE	2:G:352:LEU:CD2	2.83	0.57
2:R:175:THR:OG1	2:H:242:THR:HG23	2.05	0.57
2:S:110:VAL:CG2	2:S:111:PRO:HA	2.34	0.57
1:B:187:ARG:HH11	1:B:187:ARG:CG	2.17	0.57
1:B:192:ARG:HG3	1:B:220:TYR:CE2	2.40	0.57
2:F:197:ARG:CG	2:F:197:ARG:NH1	2.59	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:350:ASP:OD1	2:I:382:ARG:NH2	2.34	0.57
2:P:229:ASN:O	2:P:229:ASN:ND2	2.38	0.57
2:T:394:LEU:HG	2:T:398:LYS:HE3	1.86	0.57
1:B:731:SER:OG	1:B:733:PRO:HG2	2.05	0.57
2:C:110:VAL:CG2	2:C:111:PRO:HA	2.34	0.57
2:F:375:PRO:HD2	2:F:378:ARG:HG3	1.86	0.57
2:G:239:VAL:HA	2:G:288:GLY:O	2.05	0.57
2:J:316:THR:HG21	2:J:397:ARG:HH12	1.70	0.57
1:A:508:PRO:HG2	1:A:509:TYR:CE1	2.40	0.57
1:B:204:ASP:OD1	1:B:282:ARG:NH1	2.38	0.57
2:E:124:LEU:HD21	2:F:416:ARG:HD3	1.86	0.57
2:G:419:ARG:HD2	2:G:421:ASN:ND2	2.20	0.57
2:I:41:ASN:HB3	2:J:31:LEU:CD1	2.35	0.57
2:P:239:VAL:HG13	2:P:289:PHE:CA	2.35	0.57
2:S:225:VAL:HA	2:S:292:ALA:O	2.05	0.57
2:D:145:ILE:CG1	2:D:146:PRO:HD2	2.34	0.56
2:Q:124:LEU:HD21	2:E:416:ARG:HD3	1.86	0.56
2:G:82:LEU:HD11	2:G:352:LEU:HD12	1.87	0.56
2:G:13:LEU:HD21	2:G:64:MET:HE2	1.87	0.56
2:H:145:ILE:HD11	2:H:149:GLU:OE2	2.04	0.56
2:H:24:ASN:HD22	2:H:25:GLY:N	2.03	0.56
2:J:403:HIS:CD2	2:J:407:ILE:HD11	2.39	0.56
2:J:16:ILE:CD1	2:J:42:MET:HB3	2.35	0.56
2:Q:254:VAL:HG13	2:Q:255:PRO:HD2	1.87	0.56
2:S:132:LEU:O	2:S:136:GLN:HG3	2.05	0.56
2:S:231:PHE:O	2:S:232:PHE:HB2	2.05	0.56
2:T:305:GLN:O	2:T:309:THR:HB	2.04	0.56
1:A:151:LEU:HD12	1:A:152:PRO:HD2	1.85	0.56
1:A:219:ARG:NH1	1:A:219:ARG:HG3	2.20	0.56
1:B:60:LEU:CD1	1:B:60:LEU:H	2.08	0.56
2:E:95:VAL:HG21	2:E:100:ILE:HG21	1.87	0.56
2:G:344:ILE:H	2:G:344:ILE:CD1	2.18	0.56
1:B:654:ILE:HD12	1:B:654:ILE:N	2.20	0.56
2:P:344:ILE:HD12	2:P:344:ILE:N	2.17	0.56
1:A:331:VAL:O	1:A:332:SER:HB3	2.05	0.56
1:B:1012:PRO:HB3	2:F:32:THR:O	2.05	0.56
2:D:46:LEU:O	2:D:47:SER:HB3	2.03	0.56
2:T:145:ILE:HG12	2:T:146:PRO:HD2	1.87	0.56
1:A:112:SER:HB3	1:A:118:LEU:HD23	1.85	0.56
1:A:105:PHE:CE2	1:A:765:MET:HB3	2.41	0.56
1:B:2:ASP:O	1:B:4:THR:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:ILE:C	1:B:985:ILE:HD12	2.26	0.56
2:Q:31:LEU:HD11	2:F:42:MET:HG2	1.86	0.56
2:Q:305:GLN:O	2:Q:309:THR:HB	2.05	0.56
2:R:156:LEU:HD21	2:R:299:ILE:HD11	1.86	0.56
1:B:112:SER:HB3	1:B:918:LEU:CB	2.36	0.56
2:G:109:GLN:HE21	2:G:112:MET:HB3	1.71	0.56
2:J:344:ILE:H	2:J:344:ILE:CD1	2.18	0.56
2:P:64:MET:HG3	2:P:103:TYR:CD2	2.41	0.56
2:Q:309:THR:O	2:Q:310:LEU:HB2	2.05	0.56
1:B:815:PHE:HA	1:B:874:MET:CE	2.36	0.56
2:H:325:VAL:CG2	2:H:405:TRP:NE1	2.69	0.56
2:I:110:VAL:HG23	2:I:111:PRO:HA	1.87	0.56
2:I:269:LEU:HD22	2:I:269:LEU:N	2.21	0.56
2:Q:359:ASN:N	2:Q:359:ASN:HD22	2.03	0.56
2:R:256:THR:HG21	2:G:337:ARG:NH1	2.21	0.56
1:A:124:ARG:HD3	1:A:124:ARG:O	2.06	0.56
2:I:375:PRO:HD2	2:I:378:ARG:HD3	1.87	0.56
2:Q:361:MET:HG2	2:Q:392:VAL:CG1	2.35	0.56
1:B:444:ILE:H	1:B:444:ILE:HD12	1.70	0.56
1:B:361:ALA:CA	1:B:605:ILE:HD12	2.36	0.56
2:T:322:ASP:O	2:T:325:VAL:HG22	2.04	0.56
1:A:210:VAL:HG21	1:A:245:HIS:NE2	2.21	0.56
1:B:537:SER:HB3	1:B:538:PRO:HD2	1.88	0.56
2:E:2:SER:HB2	2:E:5:MET:H	1.71	0.56
2:F:166:ASN:C	2:F:168:PRO:HD2	2.26	0.56
2:R:122:LEU:O	2:G:331:THR:HG21	2.06	0.56
2:Q:211:VAL:HG12	2:Q:276:GLY:C	2.26	0.56
2:T:252:PHE:CE1	2:T:261:LEU:HD12	2.41	0.56
1:B:815:PHE:HA	1:B:874:MET:HE2	1.87	0.56
2:C:17:SER:O	2:C:21:VAL:HG23	2.06	0.56
2:D:17:SER:O	2:D:21:VAL:HG23	2.06	0.56
2:E:5:MET:CE	2:E:106:PRO:HD3	2.36	0.56
2:E:309:THR:HG22	2:E:309:THR:O	2.06	0.56
2:E:33:THR:HG22	2:E:35:ASP:H	1.69	0.56
2:J:407:ILE:HD12	2:J:407:ILE:N	2.21	0.55
2:T:323:PHE:HB2	2:T:405:TRP:NE1	2.21	0.55
1:A:930:LEU:HD22	1:A:930:LEU:N	2.21	0.55
2:D:209:PHE:O	2:D:277:ASN:HB3	2.05	0.55
2:E:152:GLU:OE1	2:E:155:LYS:HE3	2.05	0.55
2:E:231:PHE:O	2:E:232:PHE:HB2	2.06	0.55
2:F:244:THR:HG22	2:F:246:ALA:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:109:GLN:HE21	2:G:112:MET:CB	2.20	0.55
2:H:137:ASN:HB3	2:H:143:LEU:HD12	1.87	0.55
2:I:124:LEU:HD23	2:J:416:ARG:HD3	1.87	0.55
2:I:337:ARG:HG3	2:I:337:ARG:HH11	1.70	0.55
2:J:344:ILE:N	2:J:344:ILE:HD12	2.20	0.55
2:P:361:MET:HE1	2:P:392:VAL:HG22	1.87	0.55
2:Q:24:ASN:HD22	2:Q:25:GLY:N	2.04	0.55
2:Q:239:VAL:HG13	2:Q:289:PHE:HA	1.88	0.55
2:Q:5:MET:HB3	2:Q:104:ILE:HG22	1.88	0.55
2:E:201:ALA:HA	2:E:287:THR:HA	1.86	0.55
2:I:337:ARG:NH1	2:I:337:ARG:HG3	2.21	0.55
2:Q:5:MET:HE3	2:Q:105:ARG:HA	1.88	0.55
2:R:361:MET:HE1	2:R:367:PRO:CD	2.35	0.55
1:A:796:ILE:HG23	1:A:928:ASN:HB2	1.89	0.55
2:E:192:ILE:HG22	2:E:293:ILE:HB	1.87	0.55
2:H:225:VAL:HA	2:H:292:ALA:O	2.07	0.55
1:A:108:ILE:H	1:A:108:ILE:HD12	1.70	0.55
1:A:243:TYR:HB3	1:A:279:LEU:HB3	1.88	0.55
1:B:304:ALA:CB	1:B:369:ILE:HB	2.36	0.55
1:B:112:SER:HB3	1:B:918:LEU:HB2	1.88	0.55
2:D:337:ARG:HB3	2:D:337:ARG:HH11	1.71	0.55
2:I:192:ILE:HG22	2:I:293:ILE:HB	1.88	0.55
2:Q:416:ARG:HD3	2:F:124:LEU:HD21	1.89	0.55
2:R:244:THR:HG22	2:R:245:ALA:N	2.22	0.55
2:R:361:MET:CE	2:R:367:PRO:HD3	2.35	0.55
1:B:206:LEU:HD12	1:B:206:LEU:N	2.21	0.55
1:B:666:GLY:HA2	1:B:669:ILE:HD13	1.88	0.55
2:C:191:ARG:HB3	2:C:294:GLU:HG3	1.87	0.55
2:D:12:LEU:CD2	2:D:107:ARG:HD3	2.36	0.55
2:G:124:LEU:CD2	2:H:416:ARG:HD3	2.37	0.55
2:P:186:VAL:HG23	2:P:193:LEU:HB2	1.88	0.55
1:A:339:ASN:HD21	1:A:341:ALA:HB3	1.71	0.55
2:G:394:LEU:O	2:G:397:ARG:HB2	2.07	0.55
2:Q:5:MET:CE	2:Q:105:ARG:HA	2.36	0.55
2:S:329:LEU:CD2	2:S:412:ALA:HB2	2.37	0.55
1:A:800:SER:OG	1:A:801:VAL:N	2.40	0.55
2:H:110:VAL:CG2	2:H:111:PRO:HA	2.36	0.55
2:P:120:ASN:O	2:P:122:LEU:N	2.40	0.55
2:R:64:MET:HG3	2:R:103:TYR:CD2	2.42	0.55
2:C:244:THR:HB	2:C:247:ASP:OD1	2.07	0.55
2:D:244:THR:HB	2:D:247:ASP:OD1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:MET:CE	2:F:406:VAL:HG21	2.37	0.55
2:I:69:VAL:HG21	2:I:418:TYR:CD1	2.42	0.55
1:A:866:ARG:NH1	2:J:92:LYS:HD2	2.22	0.55
2:P:329:LEU:HD23	2:P:412:ALA:HB2	1.88	0.55
2:R:254:VAL:HG12	2:R:256:THR:H	1.71	0.55
1:A:801:VAL:O	1:A:961:ILE:HG13	2.07	0.55
1:B:121:HIS:O	1:B:125:VAL:HG23	2.07	0.55
2:C:26:ASP:HA	2:C:28:PHE:CE1	2.42	0.55
2:Q:350:ASP:OD1	2:Q:382:ARG:NH2	2.39	0.55
1:A:303:LEU:C	1:A:303:LEU:HD23	2.27	0.54
1:A:700:PHE:O	1:A:704:GLU:HG3	2.07	0.54
1:A:791:SER:HB2	1:A:859:ARG:HH12	1.71	0.54
1:B:105:PHE:CE2	1:B:765:MET:HB3	2.42	0.54
1:B:153:VAL:HG22	1:B:154:LYS:N	2.22	0.54
2:G:318:THR:HG22	2:G:319:SER:N	2.21	0.54
2:J:403:HIS:HD2	2:J:407:ILE:HD11	1.72	0.54
2:R:344:ILE:H	2:R:344:ILE:CD1	2.16	0.54
2:R:416:ARG:HD3	2:H:124:LEU:CD2	2.37	0.54
2:D:158:ARG:NH2	2:D:321:ASP:OD2	2.41	0.54
2:D:225:VAL:HA	2:D:292:ALA:O	2.07	0.54
2:Q:155:LYS:HE2	2:F:268:ARG:NH2	2.22	0.54
2:J:141:LYS:HB2	2:J:143:LEU:CD2	2.37	0.54
2:J:145:ILE:HG12	2:J:146:PRO:HD2	1.89	0.54
1:B:392:MET:HG2	1:B:565:MET:CE	2.37	0.54
2:C:361:MET:HE1	2:C:367:PRO:HD3	1.90	0.54
2:Q:233:GLY:O	2:F:230:SER:HB2	2.06	0.54
2:J:69:VAL:HG21	2:J:418:TYR:CD1	2.43	0.54
2:R:225:VAL:HA	2:R:292:ALA:O	2.07	0.54
2:R:416:ARG:HD3	2:H:124:LEU:HD21	1.88	0.54
2:T:382:ARG:O	2:T:386:ILE:HG12	2.07	0.54
1:A:158:LEU:HD13	1:A:166:MET:HB2	1.89	0.54
1:A:286:GLN:HG3	1:A:748:PRO:HA	1.90	0.54
1:A:346:VAL:C	1:A:348:MET:H	2.10	0.54
1:B:374:ILE:HD11	1:B:394:PHE:HE2	1.72	0.54
2:G:16:ILE:HD13	2:G:42:MET:HB3	1.90	0.54
2:H:418:TYR:CZ	2:H:420:PRO:HG3	2.41	0.54
1:A:225:HIS:ND1	1:A:227:ILE:HG12	2.23	0.54
1:A:339:ASN:HB2	1:A:340:PRO:HD2	1.90	0.54
1:B:960:PRO:O	1:B:963:VAL:HG12	2.06	0.54
2:D:146:PRO:HG2	2:D:149:GLU:HB2	1.89	0.54
2:F:337:ARG:NH1	2:F:337:ARG:CG	2.63	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:31:LEU:HD23	2:H:41:ASN:HB3	1.86	0.54
2:J:110:VAL:CG2	2:J:111:PRO:HA	2.38	0.54
2:J:217:VAL:HG12	2:J:303:ARG:HD2	1.89	0.54
2:Q:186:VAL:HB	2:Q:231:PHE:CE1	2.43	0.54
2:C:24:ASN:C	2:C:24:ASN:HD22	2.11	0.54
2:C:322:ASP:O	2:C:325:VAL:HG22	2.08	0.54
2:D:145:ILE:HD11	2:D:149:GLU:OE2	2.07	0.54
2:F:80:TYR:HB3	2:F:95:VAL:HG21	1.89	0.54
2:G:375:PRO:HD2	2:G:378:ARG:HD3	1.89	0.54
2:Q:110:VAL:HG23	2:Q:111:PRO:HA	1.89	0.54
2:Q:158:ARG:NH2	2:Q:321:ASP:OD1	2.41	0.54
2:R:2:SER:HB3	2:R:5:MET:HG3	1.90	0.54
2:G:227:PHE:H	2:G:264:GLN:NE2	2.02	0.54
2:I:14:GLU:OE1	2:I:131:LYS:HB3	2.07	0.54
2:Q:323:PHE:HB2	2:Q:405:TRP:HE1	1.72	0.54
2:T:182:GLN:HG3	2:T:183:PRO:HD2	1.89	0.54
2:T:214:TRP:CZ3	2:T:215:ALA:HB2	2.42	0.54
1:A:245:HIS:CE1	1:A:247:THR:HG1	2.26	0.54
1:B:536:ARG:NH1	1:B:616:VAL:O	2.40	0.54
2:C:244:THR:HG22	2:C:245:ALA:N	2.22	0.54
2:E:13:LEU:HD21	2:E:64:MET:HE2	1.89	0.54
2:G:382:ARG:O	2:G:386:ILE:HG12	2.08	0.54
2:I:228:THR:O	2:I:290:CYS:HB3	2.07	0.54
2:S:156:LEU:HD22	2:S:218:LEU:HD21	1.89	0.54
2:T:145:ILE:CG1	2:T:146:PRO:HD2	2.38	0.54
2:T:156:LEU:HD12	2:T:218:LEU:HD21	1.90	0.54
1:A:796:ILE:CG2	1:A:928:ASN:HB2	2.38	0.54
2:F:121:ASN:HA	2:F:146:PRO:HA	1.90	0.54
2:H:107:ARG:HH11	2:H:107:ARG:CG	2.17	0.54
2:H:133:TYR:HA	2:H:136:GLN:NE2	2.23	0.54
2:H:374:SER:HB2	2:H:375:PRO:HD2	1.90	0.54
2:I:229:ASN:ND2	2:J:235:ILE:HG12	2.21	0.54
2:P:329:LEU:CD2	2:P:412:ALA:HB2	2.37	0.54
2:R:110:VAL:CG2	2:R:111:PRO:HA	2.38	0.54
1:A:428:THR:HG23	1:A:466:GLU:OE2	2.08	0.54
1:A:923:ILE:O	1:A:923:ILE:HG23	2.07	0.54
2:I:82:LEU:HD11	2:I:352:LEU:HD12	1.89	0.54
2:I:82:LEU:HD21	2:I:352:LEU:HD11	1.89	0.54
2:J:61:LEU:HD12	2:J:417:TYR:CD1	2.42	0.54
2:Q:160:VAL:HG12	2:Q:161:ALA:N	2.23	0.54
2:T:282:LEU:HD11	2:T:289:PHE:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PHE:CE1	1:B:122:ARG:HB3	2.43	0.53
1:B:311:ILE:HD11	1:B:362:GLN:HA	1.90	0.53
1:B:349:ASN:OD1	1:B:352:GLY:N	2.38	0.53
2:D:147:TYR:CE1	2:D:301:ALA:HB1	2.43	0.53
2:D:156:LEU:HD21	2:D:299:ILE:HD11	1.89	0.53
2:F:262:PRO:HB2	2:F:265:THR:OG1	2.08	0.53
2:G:225:VAL:HA	2:G:292:ALA:O	2.09	0.53
2:H:69:VAL:HG21	2:H:418:TYR:CD1	2.43	0.53
1:A:958:LEU:HD12	1:A:958:LEU:C	2.27	0.53
1:B:827:ARG:HB3	1:B:827:ARG:NH1	2.24	0.53
2:E:167:ILE:N	2:E:168:PRO:CD	2.71	0.53
2:E:156:LEU:HD12	2:E:218:LEU:HD21	1.89	0.53
2:T:239:VAL:HG13	2:T:289:PHE:HA	1.91	0.53
1:A:293:VAL:HG23	1:A:294:TYR:N	2.24	0.53
2:C:132:LEU:O	2:C:136:GLN:HG3	2.08	0.53
2:G:228:THR:CG2	2:H:234:THR:OG1	2.56	0.53
2:H:105:ARG:O	2:H:107:ARG:HG2	2.08	0.53
2:H:211:VAL:HG22	2:H:276:GLY:O	2.08	0.53
2:J:16:ILE:HD13	2:J:42:MET:HB3	1.91	0.53
2:T:254:VAL:HG11	2:T:272:SER:O	2.08	0.53
2:C:157:PHE:C	2:C:158:ARG:HD2	2.29	0.53
2:H:161:ALA:HA	2:H:315:GLN:NE2	2.22	0.53
2:H:313:ILE:HD13	2:H:387:LEU:HD13	1.90	0.53
2:I:382:ARG:O	2:I:386:ILE:HG13	2.08	0.53
2:R:163:GLN:NE2	2:R:185:PHE:H	2.07	0.53
2:R:214:TRP:CZ3	2:R:215:ALA:HB2	2.42	0.53
2:R:80:TYR:CE2	2:R:81:MET:HG3	2.43	0.53
1:B:374:ILE:HD11	1:B:394:PHE:CE2	2.43	0.53
2:C:197:ARG:HH11	2:C:197:ARG:HG3	1.74	0.53
2:E:222:GLY:HA3	2:E:268:ARG:NH1	2.23	0.53
2:I:231:PHE:O	2:I:232:PHE:HB2	2.07	0.53
2:Q:366:ILE:CD1	2:Q:366:ILE:H	2.20	0.53
2:R:161:ALA:HA	2:R:315:GLN:NE2	2.22	0.53
2:C:24:ASN:HD22	2:C:25:GLY:N	2.06	0.53
2:D:124:LEU:O	2:D:126:PRO:HD3	2.09	0.53
2:F:157:PHE:O	2:F:158:ARG:HD3	2.08	0.53
2:I:240:THR:HB	2:I:242:THR:HG22	1.89	0.53
2:Q:416:ARG:HD3	2:F:124:LEU:CD2	2.39	0.53
1:A:51:SER:HA	1:A:713:GLN:NE2	2.14	0.53
2:C:80:TYR:CE2	2:C:81:MET:HG3	2.43	0.53
2:D:214:TRP:CZ3	2:D:215:ALA:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:418:TYR:CE1	2:G:420:PRO:HG3	2.44	0.53
2:I:151:ILE:O	2:I:151:ILE:HD12	2.08	0.53
2:R:145:ILE:HD11	2:R:149:GLU:OE2	2.09	0.53
2:S:203:PRO:HG2	2:S:207:TYR:OH	2.08	0.53
2:P:31:LEU:HD21	2:D:45:GLN:HG3	1.91	0.53
2:I:329:LEU:HD23	2:I:412:ALA:CB	2.36	0.53
2:Q:282:LEU:HD11	2:Q:289:PHE:CE2	2.42	0.53
2:R:239:VAL:HG13	2:R:289:PHE:CA	2.39	0.53
1:A:945:ILE:O	1:A:948:TYR:HB3	2.08	0.53
1:B:280:MET:HB2	1:B:281:PRO:HD2	1.91	0.53
2:D:9:THR:HA	2:D:107:ARG:HD2	1.90	0.53
2:D:167:ILE:N	2:D:168:PRO:CD	2.71	0.53
2:E:144:ASP:OD1	2:E:302:ASN:HA	2.08	0.53
2:I:219:SER:HB2	2:I:300:LEU:CD2	2.39	0.53
2:P:225:VAL:HG12	2:P:263:VAL:HG13	1.91	0.53
2:Q:239:VAL:HA	2:Q:288:GLY:O	2.09	0.53
2:E:122:LEU:CD2	2:F:335:GLN:NE2	2.71	0.53
2:E:242:THR:HG23	2:F:175:THR:OG1	2.08	0.53
2:G:59:VAL:HG12	2:G:60:PRO:HD3	1.91	0.53
2:H:167:ILE:HB	2:H:168:PRO:HD3	1.91	0.53
2:P:146:PRO:HG2	2:P:149:GLU:HB2	1.91	0.53
1:A:326:ASP:O	1:A:330:VAL:HG23	2.08	0.52
1:A:361:ALA:O	1:A:364:MET:HE3	2.09	0.52
1:A:386:ILE:HG22	1:A:387:TYR:N	2.24	0.52
1:B:623:ARG:HG2	1:B:623:ARG:NH1	2.24	0.52
2:E:240:THR:HG22	2:E:242:THR:H	1.75	0.52
2:E:322:ASP:O	2:E:325:VAL:HG22	2.10	0.52
2:G:3:ARG:HD2	2:G:89:SER:O	2.09	0.52
2:R:107:ARG:HH11	2:R:107:ARG:HG2	1.73	0.52
1:A:450:ASN:O	1:A:452:ARG:N	2.42	0.52
2:C:121:ASN:HA	2:C:146:PRO:HA	1.90	0.52
2:D:107:ARG:HH11	2:D:107:ARG:HG2	1.75	0.52
2:E:82:LEU:HD11	2:E:352:LEU:HG	1.92	0.52
2:C:277:ASN:ND2	2:F:210:VAL:HB	2.23	0.52
2:G:268:ARG:HD2	2:H:321:ASP:HB2	1.91	0.52
2:Q:107:ARG:HH11	2:Q:107:ARG:HG2	1.73	0.52
2:Q:197:ARG:HD2	2:Q:237:ALA:O	2.08	0.52
2:R:229:ASN:HD21	2:G:235:ILE:H	1.57	0.52
2:T:140:MET:HE3	2:T:406:VAL:HG21	1.91	0.52
1:A:378:THR:HG22	1:A:379:LEU:N	2.24	0.52
1:B:1006:HIS:N	1:B:1006:HIS:CD2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:GLN:NE2	2:F:210:VAL:HG21	2.24	0.52
2:D:12:LEU:HD23	2:D:107:ARG:HD3	1.90	0.52
2:E:110:VAL:CG2	2:E:111:PRO:HA	2.39	0.52
2:E:337:ARG:NH1	2:E:337:ARG:HG3	2.24	0.52
2:G:192:ILE:HD11	2:G:218:LEU:HD13	1.90	0.52
2:H:230:SER:HA	2:H:234:THR:O	2.09	0.52
1:A:334:SER:C	1:A:336:ASN:H	2.13	0.52
1:B:489:LEU:HD13	1:B:514:PRO:HB3	1.92	0.52
1:B:531:LEU:O	1:B:532:ALA:HB3	2.10	0.52
2:J:407:ILE:HD12	2:J:407:ILE:H	1.73	0.52
1:B:851:GLU:OE2	1:B:854:ARG:NH1	2.42	0.52
2:D:210:VAL:HA	2:D:277:ASN:OD1	2.10	0.52
2:Q:14:GLU:HG3	2:F:124:LEU:HD12	1.92	0.52
2:F:1:MET:HG3	2:F:100:ILE:CG2	2.40	0.52
2:F:244:THR:HB	2:F:247:ASP:OD1	2.09	0.52
2:G:158:ARG:HG3	2:G:318:THR:HG21	1.90	0.52
2:R:239:VAL:HA	2:R:288:GLY:O	2.09	0.52
2:S:151:ILE:HD13	2:S:156:LEU:HD13	1.91	0.52
2:S:214:TRP:CZ3	2:S:215:ALA:HB2	2.45	0.52
2:T:31:LEU:HD23	2:T:36:PHE:CZ	2.44	0.52
1:B:970:THR:HG23	1:B:971:GLU:HG2	1.91	0.52
2:P:121:ASN:HA	2:P:146:PRO:HA	1.91	0.52
2:P:419:ARG:HD2	2:P:421:ASN:HD22	1.75	0.52
2:Q:197:ARG:HG2	2:Q:239:VAL:CG2	2.40	0.52
2:Q:211:VAL:HG12	2:Q:276:GLY:O	2.09	0.52
2:R:110:VAL:HG23	2:R:111:PRO:HA	1.91	0.52
1:A:565:MET:HG3	1:A:566:TYR:CD1	2.44	0.52
2:F:332:PHE:CE2	2:F:336:LEU:HD11	2.45	0.52
2:F:393:ASP:HB3	2:F:396:ILE:HG12	1.91	0.52
2:H:316:THR:CG2	2:H:397:ARG:HH12	2.23	0.52
2:S:1:MET:HB2	2:S:5:MET:SD	2.49	0.52
2:T:255:PRO:CB	2:T:275:GLY:HA3	2.40	0.52
1:A:340:PRO:HG2	1:A:341:ALA:H	1.75	0.52
2:D:121:ASN:HA	2:D:146:PRO:HA	1.91	0.52
2:E:24:ASN:HD22	2:E:25:GLY:N	2.07	0.52
2:E:350:ASP:OD2	2:E:382:ARG:NH2	2.39	0.52
2:J:57:PRO:O	2:J:61:LEU:HD23	2.10	0.52
2:P:202:ILE:HG22	2:P:207:TYR:OH	2.10	0.52
2:P:80:TYR:CZ	2:P:81:MET:HG3	2.45	0.52
1:A:124:ARG:NH1	1:A:128:SER:HB3	2.25	0.52
1:A:561:LEU:HG	1:A:565:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ARG:HG3	1:A:623:ARG:NH1	2.25	0.52
2:D:192:ILE:HD11	2:D:218:LEU:CD1	2.39	0.52
2:E:80:TYR:CE2	2:E:81:MET:HG3	2.44	0.52
2:F:252:PHE:CD1	2:F:278:ILE:HD11	2.45	0.52
2:G:379:PHE:HE1	2:G:404:LEU:HD22	1.74	0.52
2:T:137:ASN:HB3	2:T:143:LEU:HD12	1.90	0.52
2:T:225:VAL:HA	2:T:292:ALA:O	2.10	0.52
2:T:239:VAL:HA	2:T:288:GLY:O	2.09	0.52
1:B:127:TYR:OH	1:B:755:MET:HG2	2.10	0.52
2:C:329:LEU:CD2	2:C:412:ALA:HB2	2.40	0.52
2:E:191:ARG:HB3	2:E:294:GLU:HG3	1.91	0.52
2:E:386:ILE:HG21	2:E:400:ILE:CG2	2.40	0.52
2:G:160:VAL:HG22	2:G:161:ALA:H	1.75	0.52
2:G:69:VAL:HA	2:G:72:ILE:HG22	1.92	0.52
2:P:169:MET:O	2:P:173:LEU:HD13	2.09	0.52
2:Q:242:THR:HG23	2:E:175:THR:OG1	2.09	0.52
2:Q:323:PHE:HB2	2:Q:405:TRP:NE1	2.24	0.52
2:T:271:PHE:CZ	2:T:293:ILE:HD13	2.45	0.52
2:T:361:MET:HG2	2:T:392:VAL:HG11	1.90	0.52
1:A:695:HIS:HE1	1:B:653:GLN:HG3	1.74	0.51
1:B:19:VAL:C	1:B:21:GLU:H	2.13	0.51
1:B:37:GLU:O	1:B:41:ILE:HD13	2.10	0.51
2:F:325:VAL:HG22	2:F:329:LEU:HD21	1.92	0.51
2:G:239:VAL:HG13	2:G:289:PHE:CA	2.40	0.51
2:I:161:ALA:HA	2:I:315:GLN:OE1	2.10	0.51
2:P:148:SER:OG	2:C:331:THR:HG23	2.10	0.51
2:P:186:VAL:CG2	2:P:193:LEU:HB2	2.40	0.51
2:P:386:ILE:O	2:P:397:ARG:HG2	2.11	0.51
2:Q:342:TYR:HD2	2:Q:342:TYR:C	2.14	0.51
2:Q:82:LEU:HD11	2:Q:352:LEU:HD12	1.92	0.51
2:S:28:PHE:HB2	2:S:31:LEU:CD2	2.41	0.51
2:T:186:VAL:HG23	2:T:193:LEU:HB2	1.91	0.51
1:A:404:THR:HG22	1:A:406:ARG:H	1.76	0.51
1:A:714:LYS:HG3	1:B:18:LEU:HD21	1.91	0.51
1:B:269:LEU:HA	1:B:272:THR:CG2	2.40	0.51
1:A:116:PRO:HB3	2:E:53:TYR:CD2	2.46	0.51
2:G:124:LEU:HD21	2:H:416:ARG:HD3	1.92	0.51
2:H:110:VAL:HG23	2:H:111:PRO:HA	1.91	0.51
2:H:201:ALA:HA	2:H:287:THR:HA	1.92	0.51
2:H:339:CYS:CB	2:H:421:ASN:HD21	2.23	0.51
2:C:12:LEU:CD2	2:C:107:ARG:HD3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:375:PRO:CD	2:C:378:ARG:HD3	2.39	0.51
2:D:110:VAL:HG22	2:D:111:PRO:HA	1.91	0.51
2:D:151:ILE:HD12	2:D:151:ILE:C	2.30	0.51
2:I:6:TRP:CE3	2:I:410:LEU:HD13	2.45	0.51
2:S:137:ASN:HB3	2:S:143:LEU:HD12	1.91	0.51
2:T:43:PHE:HZ	2:T:60:PRO:HG3	1.74	0.51
2:C:9:THR:O	2:C:12:LEU:N	2.42	0.51
2:F:229:ASN:C	2:F:229:ASN:ND2	2.60	0.51
2:F:1:MET:CA	2:F:93:PRO:HG2	2.40	0.51
2:I:332:PHE:CE2	2:I:336:LEU:HD11	2.46	0.51
2:S:121:ASN:HA	2:S:146:PRO:HA	1.93	0.51
1:A:225:HIS:CE1	1:A:227:ILE:HG12	2.45	0.51
2:F:166:ASN:HD22	2:F:167:ILE:HD12	1.76	0.51
2:F:420:PRO:O	2:F:421:ASN:C	2.48	0.51
2:G:133:TYR:HA	2:G:136:GLN:OE1	2.11	0.51
2:I:381:GLU:O	2:I:384:ARG:HB3	2.11	0.51
2:Q:203:PRO:HG2	2:Q:207:TYR:OH	2.10	0.51
2:T:109:GLN:HG3	2:T:112:MET:HB3	1.92	0.51
1:A:780:ILE:HB	1:A:870:ILE:HB	1.91	0.51
2:C:132:LEU:HA	2:C:135:ARG:HD2	1.92	0.51
2:Q:12:LEU:HA	2:E:28:PHE:CZ	2.46	0.51
2:E:235:ILE:CD1	2:F:235:ILE:HD11	2.41	0.51
2:I:320:ILE:HD11	2:I:383:ALA:CB	2.40	0.51
2:I:261:LEU:CD2	2:J:378:ARG:CZ	2.89	0.51
2:Q:186:VAL:HG23	2:Q:193:LEU:HB2	1.92	0.51
2:S:107:ARG:CG	2:S:107:ARG:NH1	2.67	0.51
1:A:880:LEU:HG	1:A:881:GLN:N	2.26	0.51
2:E:182:GLN:NE2	2:E:183:PRO:HD2	2.22	0.51
2:G:132:LEU:O	2:G:136:GLN:HG3	2.10	0.51
2:G:309:THR:O	2:G:310:LEU:HB2	2.10	0.51
2:H:161:ALA:HA	2:H:315:GLN:HE22	1.76	0.51
2:J:211:VAL:HG23	2:J:277:ASN:HA	1.93	0.51
2:F:137:ASN:HB3	2:F:143:LEU:HD12	1.91	0.51
2:F:1:MET:O	2:F:2:SER:C	2.48	0.51
2:H:133:TYR:HA	2:H:136:GLN:HE21	1.75	0.51
2:J:403:HIS:HD2	2:J:407:ILE:CD1	2.24	0.51
2:P:115:THR:HG22	2:C:58:ARG:NH1	2.26	0.51
2:S:323:PHE:HB2	2:S:405:TRP:NE1	2.26	0.51
1:A:784:SER:HA	1:A:852:PHE:CZ	2.45	0.51
1:B:650:PRO:HB2	1:B:652:TYR:CE1	2.46	0.51
2:C:394:LEU:HG	2:C:398:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:117:ARG:O	2:Q:120:ASN:HB3	2.11	0.51
1:A:241:ILE:CD1	1:A:242:GLN:HG3	2.41	0.51
1:B:336:ASN:O	1:B:337:VAL:HG13	2.11	0.51
1:B:444:ILE:N	1:B:444:ILE:HD12	2.24	0.51
2:C:33:THR:HG23	2:C:36:PHE:CB	2.41	0.51
2:G:396:ILE:O	2:G:400:ILE:HG13	2.11	0.51
2:I:357:ILE:HD13	2:I:400:ILE:HG21	1.93	0.51
2:I:54:VAL:HG12	2:I:56:ASP:N	2.26	0.51
2:P:145:ILE:CG1	2:P:146:PRO:HD2	2.41	0.51
2:S:211:VAL:HG12	2:S:276:GLY:O	2.11	0.51
2:S:356:LEU:HD23	2:S:404:LEU:HD23	1.93	0.51
1:B:153:VAL:CG2	1:B:154:LYS:N	2.73	0.50
2:E:138:ALA:O	2:E:142:GLY:HA2	2.11	0.50
2:F:105:ARG:HB2	2:F:106:PRO:HD2	1.94	0.50
2:J:208:GLN:N	2:J:208:GLN:HE21	2.09	0.50
2:P:244:THR:HG22	2:P:245:ALA:N	2.26	0.50
2:R:163:GLN:HE22	2:R:185:PHE:H	1.59	0.50
2:R:254:VAL:CG1	2:R:255:PRO:HD2	2.39	0.50
1:A:432:LEU:CB	1:A:438:ILE:HG22	2.40	0.50
2:C:142:GLY:HA3	2:Q:344:ILE:CD1	2.36	0.50
2:D:329:LEU:CD2	2:D:412:ALA:HB2	2.40	0.50
2:E:185:PHE:HE2	2:E:192:ILE:HD11	1.76	0.50
2:I:352:LEU:HD21	2:I:407:ILE:HG21	1.93	0.50
2:I:357:ILE:HA	2:I:400:ILE:HD13	1.93	0.50
2:S:48:VAL:O	2:S:49:SER:HB3	2.10	0.50
1:B:259:ASN:O	1:B:260:PHE:HB2	2.10	0.50
2:D:349:MET:CE	2:D:349:MET:HA	2.41	0.50
2:E:151:ILE:HG12	2:E:152:GLU:N	2.25	0.50
2:F:112:MET:O	2:F:116:VAL:HG23	2.11	0.50
2:G:24:ASN:HD22	2:G:24:ASN:C	2.13	0.50
1:A:508:PRO:HG2	1:A:509:TYR:CD1	2.47	0.50
1:A:607:ALA:HA	1:A:654:ILE:HD13	1.92	0.50
1:A:822:ARG:HH12	1:A:904:LEU:HD13	1.75	0.50
1:B:20:THR:O	1:B:20:THR:HG22	2.11	0.50
2:S:124:LEU:HD21	2:I:416:ARG:HD3	1.92	0.50
2:J:394:LEU:HA	2:J:397:ARG:NE	2.26	0.50
2:Q:342:TYR:C	2:Q:342:TYR:CD2	2.84	0.50
1:A:108:ILE:HG22	1:A:774:ILE:CD1	2.40	0.50
1:A:85:ILE:HD12	1:A:85:ILE:N	2.26	0.50
2:D:220:VAL:HA	2:D:296:GLU:O	2.11	0.50
2:E:163:GLN:HE22	2:E:185:PHE:N	1.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:254:VAL:HG11	2:E:272:SER:O	2.12	0.50
2:E:375:PRO:HD2	2:E:378:ARG:HD3	1.93	0.50
2:F:167:ILE:N	2:F:167:ILE:HD12	2.26	0.50
2:H:2:SER:OG	2:H:5:MET:HG3	2.12	0.50
2:Q:361:MET:HE3	2:Q:365:ALA:O	2.10	0.50
1:A:210:VAL:CG2	1:A:276:ILE:HA	2.40	0.50
2:H:323:PHE:HB2	2:H:405:TRP:HE1	1.77	0.50
2:I:310:LEU:HD22	2:I:313:ILE:HD11	1.93	0.50
2:S:47:SER:HB2	2:S:51:ALA:CB	2.41	0.50
2:T:167:ILE:N	2:T:168:PRO:CD	2.75	0.50
1:A:389:ALA:HB1	1:A:562:ILE:HD13	1.92	0.50
2:C:87:PHE:CE1	2:C:140:MET:HG3	2.46	0.50
2:G:107:ARG:CG	2:G:107:ARG:HH11	2.23	0.50
2:I:203:PRO:HG2	2:I:207:TYR:OH	2.12	0.50
2:I:309:THR:O	2:I:310:LEU:HB2	2.12	0.50
2:J:104:ILE:N	2:J:104:ILE:HD12	2.27	0.50
2:P:110:VAL:CG2	2:P:111:PRO:HA	2.42	0.50
2:S:151:ILE:C	2:S:151:ILE:HD12	2.32	0.50
2:S:28:PHE:HB2	2:S:31:LEU:HD21	1.92	0.50
1:A:392:MET:CE	1:A:392:MET:HA	2.41	0.50
2:R:229:ASN:OD1	2:G:235:ILE:HG12	2.11	0.50
2:G:82:LEU:HD11	2:G:352:LEU:CD1	2.42	0.50
2:G:353:THR:CG2	2:G:404:LEU:HD11	2.39	0.50
2:I:225:VAL:HA	2:I:292:ALA:O	2.11	0.50
2:I:251:THR:O	2:I:280:LEU:HD12	2.12	0.50
2:P:254:VAL:HG12	2:P:256:THR:H	1.76	0.50
2:S:91:THR:O	2:S:93:PRO:HD3	2.12	0.50
2:T:337:ARG:HG3	2:T:337:ARG:HH11	1.76	0.50
1:B:406:ARG:O	1:B:409:LEU:HB3	2.12	0.50
1:B:85:ILE:CD1	1:B:933:THR:OG1	2.60	0.50
2:F:225:VAL:HG11	2:F:252:PHE:HE2	1.76	0.50
2:G:315:GLN:HE21	2:G:315:GLN:HA	1.77	0.50
2:G:230:SER:HB3	2:H:233:GLY:O	2.11	0.50
2:J:355:SER:O	2:J:358:THR:HB	2.12	0.50
2:P:378:ARG:O	2:P:380:SER:N	2.45	0.50
2:R:375:PRO:HD2	2:R:378:ARG:HD3	1.94	0.50
1:B:394:PHE:CE2	1:B:398:ILE:HD13	2.47	0.49
1:B:414:ARG:HG3	1:B:414:ARG:HH11	1.77	0.49
2:D:151:ILE:HD13	2:D:156:LEU:HD23	1.93	0.49
2:E:7:LEU:CD2	2:E:136:GLN:NE2	2.73	0.49
2:I:135:ARG:NH1	2:I:324:ASP:OD2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:163:GLN:HE22	2:I:185:PHE:H	1.59	0.49
2:I:252:PHE:CE1	2:I:261:LEU:HD12	2.47	0.49
2:I:344:ILE:N	2:I:344:ILE:HD12	2.23	0.49
1:A:400:PRO:HG3	1:A:509:TYR:HB2	1.95	0.49
1:A:533:LEU:HD13	1:A:663:PHE:CE2	2.47	0.49
2:G:109:GLN:HB2	2:H:29:SER:HA	1.94	0.49
2:J:139:ILE:O	2:J:402:ARG:NH1	2.45	0.49
1:A:147:PHE:CD1	1:A:147:PHE:N	2.80	0.49
1:A:654:ILE:HD12	1:A:1010:LEU:HD21	1.93	0.49
1:A:716:ASP:O	1:A:719:LYS:HG2	2.12	0.49
1:A:822:ARG:NH1	1:A:904:LEU:HD13	2.27	0.49
2:D:215:ALA:C	2:D:217:VAL:H	2.16	0.49
2:E:239:VAL:HG13	2:E:289:PHE:HA	1.94	0.49
2:E:352:LEU:HD23	2:E:352:LEU:C	2.32	0.49
2:G:110:VAL:HG22	2:G:111:PRO:CA	2.42	0.49
2:P:151:ILE:HD12	2:P:151:ILE:C	2.32	0.49
2:Q:374:SER:HB2	2:Q:375:PRO:HD2	1.94	0.49
2:C:120:ASN:O	2:C:122:LEU:N	2.46	0.49
2:D:132:LEU:O	2:D:136:GLN:HG3	2.12	0.49
2:E:360:TYR:CB	2:E:400:ILE:HD11	2.42	0.49
2:J:322:ASP:O	2:J:325:VAL:HG23	2.11	0.49
2:S:247:ASP:OD1	2:S:284:VAL:HG21	2.12	0.49
2:S:378:ARG:NH1	2:J:261:LEU:HD13	2.27	0.49
2:T:221:THR:HG22	2:T:270:SER:HB3	1.95	0.49
2:T:30:GLY:O	2:T:31:LEU:C	2.50	0.49
1:A:64:GLY:HA3	1:A:66:GLN:HE21	1.76	0.49
1:A:786:PHE:O	1:A:797:ALA:HA	2.13	0.49
1:B:623:ARG:HH11	1:B:623:ARG:HG2	1.77	0.49
2:C:277:ASN:HD21	2:F:210:VAL:HB	1.77	0.49
2:E:169:MET:O	2:E:173:LEU:HG	2.12	0.49
2:P:244:THR:HB	2:P:247:ASP:OD1	2.12	0.49
2:P:24:ASN:C	2:P:24:ASN:HD22	2.14	0.49
2:Q:361:MET:CE	2:Q:367:PRO:HG3	2.43	0.49
2:R:12:LEU:HD22	2:R:107:ARG:HD3	1.95	0.49
2:S:357:ILE:HD13	2:S:400:ILE:HG21	1.94	0.49
2:H:53:TYR:N	2:H:53:TYR:CD2	2.79	0.49
2:P:235:ILE:HD11	2:D:235:ILE:HD11	1.93	0.49
2:C:142:GLY:N	2:Q:344:ILE:HD11	2.27	0.49
2:S:87:PHE:HB2	2:S:403:HIS:CE1	2.47	0.49
1:A:307:LEU:HD21	1:A:365:LEU:HB3	1.94	0.49
2:C:156:LEU:HD21	2:C:299:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:MET:HB2	2:G:5:MET:SD	2.52	0.49
2:I:107:ARG:HH11	2:I:107:ARG:HG3	1.77	0.49
2:J:100:ILE:N	2:J:100:ILE:HD12	2.26	0.49
2:P:379:PHE:CE1	2:P:405:TRP:HA	2.47	0.49
2:P:82:LEU:O	2:P:356:LEU:HD12	2.13	0.49
1:A:278:THR:O	1:A:279:LEU:HD23	2.13	0.49
1:A:284:VAL:O	1:A:284:VAL:HG23	2.13	0.49
2:C:107:ARG:HH11	2:C:107:ARG:HG2	1.77	0.49
2:I:145:ILE:HD11	2:I:149:GLU:OE2	2.12	0.49
2:I:147:TYR:O	2:I:298:THR:HG21	2.11	0.49
2:J:158:ARG:NH2	2:J:321:ASP:OD1	2.46	0.49
2:S:14:GLU:OE1	2:S:131:LYS:HB3	2.13	0.49
2:C:133:TYR:HA	2:C:136:GLN:OE1	2.13	0.49
2:D:36:PHE:O	2:D:40:SER:HB2	2.12	0.49
2:Q:175:THR:OG1	2:F:242:THR:HG23	2.12	0.49
2:F:280:LEU:CD2	2:F:289:PHE:HE1	2.25	0.49
2:J:309:THR:O	2:J:310:LEU:HB2	2.13	0.49
2:J:358:THR:O	2:J:360:TYR:N	2.45	0.49
2:P:192:ILE:HD11	2:P:218:LEU:HD12	1.95	0.49
2:R:1:MET:O	2:R:2:SER:C	2.50	0.49
2:R:419:ARG:HG2	2:R:419:ARG:O	2.13	0.49
1:A:555:LEU:H	1:A:555:LEU:HD12	1.78	0.49
1:A:385:PHE:HA	1:A:566:TYR:CZ	2.47	0.49
1:A:783:ASN:ND2	1:A:784:SER:H	2.11	0.49
2:C:151:ILE:HD12	2:C:151:ILE:C	2.32	0.49
2:D:3:ARG:HG3	2:D:4:GLN:N	2.27	0.49
2:Q:170:MET:HE1	2:F:226:TYR:HD1	1.77	0.49
2:H:239:VAL:HG13	2:H:289:PHE:CA	2.43	0.49
2:P:120:ASN:C	2:P:122:LEU:N	2.66	0.49
2:P:91:THR:O	2:P:93:PRO:HD3	2.12	0.49
2:R:337:ARG:NH1	2:R:342:TYR:CE2	2.80	0.49
2:S:253:THR:HG22	2:S:279:ASN:HB3	1.95	0.49
2:E:132:LEU:HG	2:E:328:PHE:CE1	2.48	0.48
2:F:186:VAL:HB	2:F:231:PHE:CE1	2.48	0.48
2:F:202:ILE:HD12	2:F:202:ILE:N	2.28	0.48
2:F:357:ILE:HG23	2:F:400:ILE:HD13	1.95	0.48
2:P:31:LEU:HD21	2:D:45:GLN:HG2	1.95	0.48
2:R:244:THR:HG22	2:R:246:ALA:H	1.78	0.48
1:B:585:THR:O	1:B:589:SER:HB2	2.13	0.48
1:B:696:LEU:O	1:B:700:PHE:HD1	1.96	0.48
2:F:167:ILE:N	2:F:168:PRO:CD	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:396:ILE:O	2:F:400:ILE:HG13	2.13	0.48
2:H:169:MET:O	2:H:173:LEU:HG	2.12	0.48
2:Q:253:THR:HG22	2:Q:260:ASN:HA	1.94	0.48
2:Q:332:PHE:CE2	2:Q:336:LEU:HD11	2.49	0.48
2:T:396:ILE:O	2:T:400:ILE:HG13	2.13	0.48
1:A:591:PHE:HE1	1:A:642:LEU:HD12	1.76	0.48
1:B:675:ILE:HD13	1:B:717:VAL:HG13	1.94	0.48
2:C:329:LEU:HD23	2:C:412:ALA:HB2	1.93	0.48
2:G:56:ASP:OD1	2:G:58:ARG:HB2	2.12	0.48
2:H:323:PHE:HB2	2:H:405:TRP:NE1	2.29	0.48
2:S:362:ASP:OD1	2:S:362:ASP:C	2.51	0.48
1:B:19:VAL:C	1:B:21:GLU:N	2.66	0.48
1:B:561:LEU:O	1:B:565:MET:HG3	2.13	0.48
2:D:14:GLU:OE2	2:D:131:LYS:HB3	2.13	0.48
2:D:163:GLN:NE2	2:D:185:PHE:O	2.46	0.48
2:F:164:THR:HG23	2:F:165:GLY:N	2.29	0.48
2:J:387:LEU:HD21	2:J:401:VAL:HG21	1.94	0.48
2:T:271:PHE:HZ	2:T:293:ILE:HD13	1.78	0.48
1:A:641:LEU:HG	1:A:641:LEU:O	2.13	0.48
1:B:404:THR:HG22	1:B:406:ARG:H	1.78	0.48
1:B:459:TYR:CG	1:B:473:ILE:HG21	2.49	0.48
2:E:121:ASN:HA	2:E:146:PRO:HA	1.96	0.48
2:G:12:LEU:O	2:G:16:ILE:HG12	2.12	0.48
2:H:45:GLN:HE21	2:H:45:GLN:HB2	1.47	0.48
2:I:185:PHE:CD2	2:I:212:PRO:HD2	2.49	0.48
2:P:131:LYS:NZ	2:C:26:ASP:OD1	2.45	0.48
2:Q:186:VAL:HB	2:Q:231:PHE:CZ	2.49	0.48
2:Q:28:PHE:CZ	2:F:12:LEU:HA	2.48	0.48
2:R:167:ILE:N	2:R:168:PRO:CD	2.76	0.48
2:T:356:LEU:HD12	2:T:400:ILE:HG23	1.95	0.48
1:A:362:GLN:C	1:A:364:MET:H	2.16	0.48
1:A:523:ARG:NH2	1:A:609:THR:HG23	2.28	0.48
2:C:105:ARG:HG3	2:C:106:PRO:N	2.28	0.48
2:D:145:ILE:HD12	2:D:308:TYR:HE1	1.78	0.48
2:P:31:LEU:CD2	2:D:41:ASN:HB3	2.41	0.48
2:E:140:MET:CE	2:E:406:VAL:HG11	2.43	0.48
2:E:363:PRO:HA	2:E:364:PRO:HD3	1.71	0.48
2:F:325:VAL:HG13	2:F:326:SER:N	2.29	0.48
2:I:325:VAL:HG13	2:I:405:TRP:CZ2	2.48	0.48
2:I:47:SER:O	2:I:49:SER:N	2.47	0.48
2:S:158:ARG:HG3	2:S:313:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:379:PHE:CE1	2:S:404:LEU:HD12	2.49	0.48
2:T:56:ASP:C	2:T:58:ARG:N	2.66	0.48
2:F:239:VAL:HG13	2:F:288:GLY:O	2.13	0.48
2:F:378:ARG:NE	2:F:381:GLU:OE2	2.41	0.48
2:G:419:ARG:HD2	2:G:421:ASN:HD22	1.77	0.48
2:J:353:THR:HG22	2:J:404:LEU:HD11	1.95	0.48
2:P:132:LEU:HG	2:P:328:PHE:CE2	2.48	0.48
2:P:261:LEU:HD22	2:P:271:PHE:CD2	2.48	0.48
2:Q:235:ILE:HG12	2:F:229:ASN:HD21	1.78	0.48
2:S:173:LEU:HB3	2:S:236:ILE:HG23	1.95	0.48
1:A:468:VAL:O	1:A:472:LEU:HD23	2.13	0.48
2:D:121:ASN:HA	2:D:146:PRO:HB3	1.95	0.48
2:E:61:LEU:HD22	2:E:417:TYR:CE1	2.48	0.48
2:G:156:LEU:HD21	2:G:307:TYR:HB2	1.95	0.48
2:R:121:ASN:HA	2:R:146:PRO:HA	1.95	0.48
2:R:256:THR:HG22	2:G:337:ARG:NH1	2.28	0.48
2:R:361:MET:CE	2:R:367:PRO:HB3	2.44	0.48
2:R:361:MET:HE1	2:R:367:PRO:CG	2.44	0.48
2:S:309:THR:O	2:S:309:THR:HG22	2.14	0.48
2:T:1:MET:O	2:T:2:SER:C	2.52	0.48
2:T:332:PHE:CE2	2:T:336:LEU:HD11	2.49	0.48
1:B:165:ASN:ND2	1:B:168:ALA:H	2.12	0.48
1:B:666:GLY:O	1:B:667:GLU:C	2.52	0.48
2:C:225:VAL:HA	2:C:292:ALA:O	2.13	0.48
2:D:160:VAL:HG12	2:D:161:ALA:N	2.29	0.48
2:E:186:VAL:HG21	2:E:231:PHE:CZ	2.49	0.48
2:G:282:LEU:HD21	2:G:286:LYS:HD2	1.96	0.48
2:G:361:MET:HE1	2:G:367:PRO:CD	2.43	0.48
2:I:100:ILE:HG22	2:I:101:THR:N	2.28	0.48
2:I:104:ILE:HD12	2:I:104:ILE:N	2.28	0.48
2:Q:282:LEU:HD11	2:Q:289:PHE:CD2	2.49	0.48
2:C:5:MET:CE	2:C:106:PRO:HD3	2.43	0.48
2:C:14:GLU:HG2	2:C:131:LYS:HD3	1.94	0.48
2:D:121:ASN:HA	2:D:146:PRO:CB	2.44	0.48
2:D:166:ASN:N	2:D:168:PRO:HD2	2.29	0.48
2:D:254:VAL:HG12	2:D:256:THR:H	1.79	0.48
2:F:110:VAL:HG23	2:F:111:PRO:HA	1.96	0.48
2:F:244:THR:C	2:F:246:ALA:N	2.68	0.48
2:G:69:VAL:HG21	2:G:418:TYR:CZ	2.48	0.48
2:P:390:GLN:HG2	2:P:390:GLN:H	1.35	0.48
2:I:239:VAL:HG13	2:I:289:PHE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:341:GLN:HA	2:J:344:ILE:HD13	1.95	0.47
2:R:160:VAL:C	2:R:315:GLN:HE21	2.17	0.47
2:R:41:ASN:HD21	2:R:45:GLN:HE21	1.62	0.47
1:A:362:GLN:C	1:A:364:MET:N	2.68	0.47
1:B:297:PRO:HB3	1:B:630:TRP:CE2	2.48	0.47
2:C:254:VAL:HG12	2:C:256:THR:H	1.78	0.47
2:C:59:VAL:HB	2:C:60:PRO:HD3	1.95	0.47
2:D:182:GLN:HB3	2:D:183:PRO:HD2	1.96	0.47
2:D:239:VAL:HG13	2:D:289:PHE:CA	2.44	0.47
2:F:151:ILE:C	2:F:151:ILE:HD12	2.34	0.47
2:F:239:VAL:HG13	2:F:289:PHE:HA	1.97	0.47
2:H:14:GLU:OE2	2:H:131:LYS:HB3	2.14	0.47
2:S:378:ARG:HH11	2:J:261:LEU:HD13	1.78	0.47
2:E:122:LEU:HD21	2:F:335:GLN:NE2	2.10	0.47
2:G:363:PRO:HA	2:G:364:PRO:HD3	1.76	0.47
2:H:379:PHE:O	2:H:381:GLU:N	2.47	0.47
2:I:219:SER:HB2	2:I:300:LEU:HD23	1.97	0.47
2:P:157:PHE:C	2:P:158:ARG:HD2	2.35	0.47
2:Q:1:MET:HB2	2:Q:5:MET:SD	2.55	0.47
2:T:255:PRO:HG2	2:T:275:GLY:HA3	1.97	0.47
1:A:816:ASP:OD2	1:B:1005:VAL:HG12	2.13	0.47
1:A:861:VAL:HG12	1:A:862:PHE:N	2.29	0.47
1:B:245:HIS:CD2	1:B:246:PRO:HD2	2.50	0.47
1:B:541:ILE:HG23	1:B:542:THR:HG22	1.97	0.47
1:B:558:LYS:O	1:B:562:ILE:HG13	2.14	0.47
2:F:325:VAL:O	2:F:329:LEU:HD22	2.15	0.47
2:G:117:ARG:NH2	2:G:118:GLN:HE21	2.13	0.47
2:I:46:LEU:N	2:I:46:LEU:HD12	2.28	0.47
2:J:99:PHE:HD2	2:J:100:ILE:HD12	1.78	0.47
2:S:316:THR:HG21	2:S:397:ARG:HH12	1.79	0.47
1:A:334:SER:O	1:A:336:ASN:N	2.47	0.47
1:A:400:PRO:HB2	1:A:515:ILE:HG12	1.96	0.47
1:B:31:VAL:HG12	1:B:32:TYR:H	1.79	0.47
2:F:120:ASN:O	2:F:121:ASN:C	2.53	0.47
2:S:416:ARG:O	2:J:122:LEU:HD13	2.15	0.47
2:J:193:LEU:HD12	2:J:231:PHE:HD1	1.79	0.47
2:J:309:THR:HG22	2:J:309:THR:O	2.15	0.47
2:Q:272:SER:OG	2:Q:300:LEU:HD11	2.15	0.47
2:R:186:VAL:HG23	2:R:193:LEU:HB2	1.95	0.47
1:A:558:LYS:O	1:A:562:ILE:HG13	2.15	0.47
1:A:653:GLN:O	1:A:653:GLN:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:244:THR:C	2:F:246:ALA:H	2.17	0.47
2:I:110:VAL:CG2	2:I:111:PRO:HA	2.44	0.47
2:I:357:ILE:HD13	2:I:400:ILE:HD13	1.96	0.47
2:R:192:ILE:HD11	2:R:218:LEU:CD1	2.45	0.47
2:R:231:PHE:O	2:R:232:PHE:HB2	2.13	0.47
1:B:673:GLN:HE21	1:B:747:LEU:HD12	1.80	0.47
2:C:16:ILE:O	2:C:20:VAL:HG23	2.14	0.47
2:F:45:GLN:O	2:F:107:ARG:NH1	2.46	0.47
2:H:271:PHE:CZ	2:H:293:ILE:HD13	2.50	0.47
2:J:169:MET:O	2:J:173:LEU:HG	2.14	0.47
2:Q:82:LEU:HD11	2:Q:352:LEU:CD1	2.45	0.47
2:S:158:ARG:CG	2:S:313:ILE:HD13	2.44	0.47
2:S:221:THR:HG21	2:I:326:SER:O	2.15	0.47
1:A:104:LYS:HD3	1:B:23:THR:HG22	1.96	0.47
1:A:490:ILE:HB	1:A:501:GLU:HB2	1.96	0.47
1:A:364:MET:HE1	1:A:605:ILE:HG23	1.97	0.47
2:C:190:ARG:O	2:C:190:ARG:HG2	2.14	0.47
2:E:186:VAL:HG22	2:E:187:ALA:N	2.29	0.47
2:E:280:LEU:CD2	2:E:289:PHE:HE1	2.28	0.47
2:F:156:LEU:HD22	2:F:218:LEU:HD21	1.97	0.47
2:G:14:GLU:OE1	2:G:131:LYS:HB3	2.15	0.47
2:H:82:LEU:HD22	2:H:356:LEU:HD23	1.97	0.47
2:P:225:VAL:HA	2:P:292:ALA:O	2.15	0.47
2:P:363:PRO:HA	2:P:364:PRO:HD3	1.83	0.47
2:S:416:ARG:HD3	2:J:124:LEU:HD23	1.96	0.47
2:T:133:TYR:HA	2:T:136:GLN:OE1	2.14	0.47
1:A:241:ILE:HD12	1:A:242:GLN:N	2.30	0.47
1:A:356:LEU:O	1:A:360:ILE:HG13	2.14	0.47
1:A:303:LEU:HD22	1:A:369:ILE:HD11	1.97	0.47
1:A:767:GLN:C	1:A:769:THR:H	2.18	0.47
1:B:222:VAL:CG1	1:B:224:TYR:HD1	2.28	0.47
1:B:444:ILE:N	1:B:444:ILE:CD1	2.73	0.47
2:D:110:VAL:HG23	2:D:111:PRO:HA	1.97	0.47
2:C:123:SER:HB2	2:D:17:SER:OG	2.15	0.47
2:D:363:PRO:HA	2:D:364:PRO:HD3	1.81	0.47
2:F:203:PRO:HG2	2:F:207:TYR:OH	2.15	0.47
2:F:56:ASP:OD1	2:F:58:ARG:HB2	2.15	0.47
2:G:135:ARG:NH1	2:G:324:ASP:OD2	2.47	0.47
2:G:350:ASP:O	2:G:354:ASN:HB2	2.14	0.47
2:I:211:VAL:HG22	2:I:276:GLY:O	2.13	0.47
2:J:166:ASN:OD1	2:J:186:VAL:CG2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:230:SER:HB3	2:C:233:GLY:O	2.14	0.47
2:P:418:TYR:CE1	2:P:420:PRO:HG3	2.50	0.47
2:R:235:ILE:N	2:R:235:ILE:HD12	2.29	0.47
2:S:322:ASP:O	2:S:325:VAL:HG22	2.15	0.47
2:S:6:TRP:CZ2	2:S:81:MET:CE	2.98	0.47
2:T:132:LEU:O	2:T:136:GLN:HG3	2.14	0.47
1:A:484:GLN:NE2	2:D:29:SER:O	2.48	0.47
1:A:551:SER:OG	1:A:553:GLU:HB2	2.14	0.47
2:C:274:GLY:C	2:C:276:GLY:H	2.18	0.47
2:I:186:VAL:HG23	2:I:193:LEU:HB2	1.96	0.47
2:P:361:MET:CE	2:P:392:VAL:HG22	2.44	0.47
2:S:379:PHE:HE1	2:S:404:LEU:HD12	1.80	0.47
2:T:255:PRO:CG	2:T:275:GLY:HA3	2.45	0.47
2:T:420:PRO:O	2:T:421:ASN:C	2.53	0.47
1:A:222:VAL:HB	1:A:223:PRO:HD2	1.96	0.47
1:B:177:HIS:CD2	1:B:177:HIS:H	2.33	0.47
1:B:183:GLN:O	1:B:186:ASN:HB2	2.16	0.47
2:F:323:PHE:O	2:F:324:ASP:HB2	2.15	0.47
2:G:167:ILE:N	2:G:168:PRO:CD	2.78	0.47
2:T:59:VAL:N	2:T:60:PRO:HD2	2.30	0.47
1:A:679:TYR:CD1	1:A:703:ILE:HD11	2.50	0.46
2:F:164:THR:HG23	2:F:165:GLY:H	1.80	0.46
2:G:322:ASP:HB2	2:G:325:VAL:HG12	1.97	0.46
2:H:122:LEU:N	2:H:122:LEU:HD12	2.30	0.46
2:I:361:MET:HE3	2:I:361:MET:HB2	1.58	0.46
2:I:396:ILE:N	2:I:396:ILE:CD1	2.78	0.46
2:Q:84:LYS:HE2	2:S:351:GLN:HE22	1.79	0.46
2:R:154:CYS:HB3	2:R:188:GLU:O	2.14	0.46
2:S:13:LEU:HD21	2:S:64:MET:HE2	1.97	0.46
2:S:6:TRP:HZ2	2:S:81:MET:HE1	1.77	0.46
2:T:349:MET:HG2	2:T:376:TRP:CD2	2.51	0.46
2:C:337:ARG:HG3	2:C:337:ARG:NH1	2.28	0.46
2:E:9:THR:HA	2:E:107:ARG:HG3	1.97	0.46
2:Q:382:ARG:O	2:Q:386:ILE:HG12	2.15	0.46
2:S:22:ARG:HD3	2:S:35:ASP:OD2	2.15	0.46
2:T:361:MET:HE3	2:T:361:MET:HB2	1.64	0.46
1:A:787:VAL:HG21	1:A:853:VAL:HG12	1.97	0.46
1:B:63:ILE:HG12	1:B:64:GLY:N	2.29	0.46
1:B:74:ILE:HD11	1:B:979:PHE:CE1	2.50	0.46
2:C:83:ARG:HG2	2:C:359:ASN:ND2	2.30	0.46
2:F:226:TYR:CD2	2:F:226:TYR:N	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:140:MET:CE	2:H:406:VAL:HG11	2.45	0.46
2:J:39:LEU:HA	2:J:42:MET:CE	2.45	0.46
2:Q:329:LEU:O	2:Q:330:THR:C	2.54	0.46
2:R:271:PHE:CZ	2:R:293:ILE:HD13	2.50	0.46
2:R:337:ARG:HH12	2:H:256:THR:HG22	1.79	0.46
2:T:156:LEU:CD1	2:T:218:LEU:HD21	2.45	0.46
2:T:254:VAL:HG13	2:T:255:PRO:HD2	1.97	0.46
1:B:438:ILE:HG23	1:B:447:TRP:CZ2	2.48	0.46
2:D:16:ILE:HD11	2:D:42:MET:HB3	1.97	0.46
2:D:97:ASP:O	2:D:98:ASP:C	2.53	0.46
2:E:386:ILE:HG21	2:E:400:ILE:HG21	1.96	0.46
2:E:420:PRO:O	2:E:421:ASN:OXT	2.34	0.46
2:I:378:ARG:HB3	2:I:381:GLU:OE1	2.16	0.46
1:B:217:TYR:CE2	1:B:986:ARG:HB2	2.50	0.46
2:C:239:VAL:HG13	2:C:289:PHE:HA	1.98	0.46
2:F:217:VAL:HG22	2:F:303:ARG:HH21	1.81	0.46
2:F:271:PHE:CZ	2:F:293:ILE:HD13	2.50	0.46
2:F:69:VAL:HG21	2:F:418:TYR:CD1	2.51	0.46
2:G:361:MET:HE1	2:G:367:PRO:CG	2.44	0.46
2:H:5:MET:SD	2:H:106:PRO:HD3	2.56	0.46
2:J:250:THR:HG23	2:J:282:LEU:HA	1.98	0.46
2:P:167:ILE:N	2:P:168:PRO:CD	2.78	0.46
2:Q:145:ILE:HG12	2:Q:146:PRO:CD	2.42	0.46
2:S:271:PHE:CZ	2:S:293:ILE:HD13	2.50	0.46
1:A:591:PHE:HD2	1:A:592:LEU:HD23	1.80	0.46
1:A:805:VAL:HG12	1:A:805:VAL:O	2.16	0.46
1:B:429:THR:O	1:B:433:VAL:HG23	2.16	0.46
2:D:332:PHE:CE2	2:D:336:LEU:HD11	2.50	0.46
2:G:214:TRP:CZ3	2:G:215:ALA:HB2	2.50	0.46
2:H:1:MET:O	2:H:2:SER:C	2.53	0.46
2:H:363:PRO:HA	2:H:364:PRO:HD3	1.73	0.46
2:J:156:LEU:O	2:J:214:TRP:HB2	2.15	0.46
2:J:97:ASP:O	2:J:99:PHE:N	2.48	0.46
2:P:95:VAL:HG23	2:P:95:VAL:O	2.15	0.46
1:A:455:LEU:HD23	1:A:477:PHE:CZ	2.50	0.46
1:B:437:VAL:HG13	1:B:457:ALA:HB1	1.98	0.46
2:D:95:VAL:O	2:D:95:VAL:HG23	2.15	0.46
2:E:14:GLU:OE2	2:E:131:LYS:HB3	2.15	0.46
2:F:128:ALA:O	2:F:130:PRO:HD3	2.16	0.46
2:F:140:MET:CE	2:F:406:VAL:HG11	2.45	0.46
2:G:158:ARG:NH2	2:G:321:ASP:OD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:316:THR:HG21	2:P:397:ARG:HH12	1.81	0.46
2:R:361:MET:HE1	2:R:367:PRO:HB3	1.97	0.46
2:S:110:VAL:HG22	2:S:111:PRO:HA	1.97	0.46
2:T:9:THR:HG21	2:T:104:ILE:HA	1.98	0.46
1:A:210:VAL:HG23	1:A:276:ILE:CA	2.44	0.46
1:A:327:LEU:O	1:A:331:VAL:HG22	2.15	0.46
1:B:262:ARG:NH1	1:B:262:ARG:HB3	2.29	0.46
1:B:878:PHE:HA	1:B:921:VAL:O	2.16	0.46
2:C:110:VAL:HG23	2:C:111:PRO:HA	1.97	0.46
2:C:158:ARG:NH2	2:C:320:ILE:HG13	2.31	0.46
2:C:231:PHE:HB2	2:C:236:ILE:HD11	1.97	0.46
2:Q:378:ARG:NH1	2:F:257:ASP:OD1	2.46	0.46
2:F:87:PHE:HB2	2:F:403:HIS:ND1	2.31	0.46
2:G:284:VAL:O	2:G:284:VAL:HG23	2.16	0.46
2:G:318:THR:CG2	2:G:319:SER:N	2.78	0.46
2:H:156:LEU:HD22	2:H:218:LEU:HD21	1.97	0.46
2:J:227:PHE:HZ	2:J:250:THR:HG21	1.80	0.46
2:S:363:PRO:HA	2:S:364:PRO:HD3	1.74	0.46
1:A:108:ILE:H	1:A:108:ILE:CD1	2.22	0.46
1:A:349:ASN:N	1:A:349:ASN:ND2	2.63	0.46
1:A:537:SER:HB3	1:A:538:PRO:CD	2.46	0.46
1:A:928:ASN:C	1:A:928:ASN:OD1	2.55	0.46
1:A:93:PHE:CD2	1:A:975:LEU:HD22	2.51	0.46
1:B:175:PHE:O	1:B:176:GLU:C	2.54	0.46
1:B:60:LEU:HA	1:B:135:ALA:HB1	1.98	0.46
1:B:732:LYS:N	1:B:733:PRO:CD	2.79	0.46
2:D:69:VAL:HG21	2:D:418:TYR:CG	2.50	0.46
2:E:150:PRO:HA	2:E:297:PHE:O	2.16	0.46
2:S:211:VAL:O	2:S:211:VAL:HG13	2.15	0.46
2:T:396:ILE:HD12	2:T:396:ILE:N	2.31	0.46
1:A:410:ASP:O	1:A:414:ARG:HG2	2.16	0.46
1:B:810:HIS:CD2	1:B:840:MET:HG3	2.51	0.46
2:I:112:MET:O	2:I:112:MET:HE2	2.16	0.46
2:J:112:MET:HE2	2:J:116:VAL:CG2	2.46	0.46
2:P:68:PHE:HB2	2:P:99:PHE:CE1	2.51	0.46
2:R:160:VAL:HG12	2:R:161:ALA:N	2.30	0.46
2:R:349:MET:HA	2:R:349:MET:HE2	1.98	0.46
1:A:245:HIS:CD2	1:A:246:PRO:HD2	2.51	0.45
1:A:773:PRO:O	1:A:774:ILE:HG13	2.16	0.45
1:B:308:LEU:CD2	1:B:362:GLN:HB2	2.43	0.45
1:B:478:ARG:HD2	1:B:557:HIS:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:135:ARG:NH1	2:D:323:PHE:O	2.49	0.45
2:D:4:GLN:HE22	2:D:141:LYS:NZ	2.14	0.45
2:E:7:LEU:HD22	2:E:136:GLN:NE2	2.30	0.45
2:R:12:LEU:HA	2:G:28:PHE:CZ	2.51	0.45
2:I:310:LEU:HB3	2:I:313:ILE:HD12	1.98	0.45
2:I:322:ASP:HB2	2:I:325:VAL:CG2	2.47	0.45
2:T:240:THR:HB	2:T:242:THR:CG2	2.46	0.45
2:T:56:ASP:O	2:T:58:ARG:N	2.49	0.45
1:A:847:ILE:HG23	1:A:864:GLU:HG3	1.99	0.45
1:B:127:TYR:O	1:B:130:LEU:HB2	2.16	0.45
2:C:277:ASN:OD1	2:F:210:VAL:HG12	2.15	0.45
2:C:82:LEU:HD11	2:C:352:LEU:HD22	1.97	0.45
2:C:266:ASP:OD1	2:D:166:ASN:HB3	2.16	0.45
2:F:1:MET:HB3	2:F:93:PRO:HG2	1.98	0.45
2:I:153:PRO:O	2:I:156:LEU:N	2.48	0.45
2:J:378:ARG:HB3	2:J:381:GLU:OE1	2.16	0.45
2:P:28:PHE:CZ	2:D:12:LEU:HA	2.51	0.45
2:S:192:ILE:HG21	2:S:293:ILE:HD12	1.98	0.45
2:T:26:ASP:HA	2:T:28:PHE:CE1	2.52	0.45
1:A:360:ILE:HG23	1:A:397:LEU:O	2.15	0.45
1:A:697:GLU:HG3	1:A:718:ARG:NH2	2.31	0.45
1:B:227:ILE:HD11	1:B:768:LEU:CD2	2.46	0.45
2:C:125:GLN:HE22	2:D:131:LYS:HA	1.81	0.45
2:D:387:LEU:HG	2:D:401:VAL:HG21	1.98	0.45
2:F:193:LEU:HD12	2:F:231:PHE:CD1	2.50	0.45
2:Q:261:LEU:HD23	2:E:378:ARG:CZ	2.46	0.45
2:R:161:ALA:N	2:R:315:GLN:HE21	2.15	0.45
2:R:323:PHE:HB2	2:R:405:TRP:NE1	2.31	0.45
2:R:344:ILE:N	2:R:344:ILE:HD12	2.20	0.45
1:B:518:LEU:O	1:B:520:PRO:HD3	2.17	0.45
2:F:145:ILE:HG12	2:F:146:PRO:CD	2.46	0.45
2:F:211:VAL:HG23	2:F:277:ASN:N	2.32	0.45
2:G:13:LEU:HD21	2:G:64:MET:CE	2.47	0.45
2:J:133:TYR:HA	2:J:136:GLN:OE1	2.16	0.45
2:J:381:GLU:O	2:J:384:ARG:N	2.50	0.45
2:Q:31:LEU:CD1	2:F:42:MET:HG2	2.45	0.45
2:R:337:ARG:NH1	2:H:256:THR:CG2	2.80	0.45
2:T:169:MET:O	2:T:173:LEU:HD13	2.17	0.45
1:A:307:LEU:CD1	1:A:307:LEU:C	2.85	0.45
1:A:545:GLU:O	1:A:546:GLY:O	2.34	0.45
1:A:340:PRO:CG	1:A:584:ASN:HD21	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:GLN:O	1:A:713:GLN:HB2	2.17	0.45
2:C:254:VAL:HG13	2:C:255:PRO:HD2	1.98	0.45
2:D:387:LEU:HD23	2:D:397:ARG:HB3	1.97	0.45
2:E:394:LEU:HG	2:E:398:LYS:HE3	1.98	0.45
2:E:69:VAL:HG21	2:E:418:TYR:CD1	2.51	0.45
2:F:244:THR:O	2:F:246:ALA:N	2.49	0.45
2:F:322:ASP:HB2	2:F:325:VAL:CG1	2.40	0.45
2:F:140:MET:HE2	2:F:406:VAL:HG21	1.97	0.45
2:I:244:THR:HB	2:I:247:ASP:OD1	2.17	0.45
2:J:188:GLU:HA	2:J:232:PHE:CE1	2.51	0.45
2:J:346:SER:O	2:J:350:ASP:OD1	2.34	0.45
2:Q:3:ARG:HB2	2:Q:140:MET:HE3	1.97	0.45
2:R:151:ILE:C	2:R:151:ILE:HD12	2.35	0.45
2:T:207:TYR:N	2:T:207:TYR:CD1	2.84	0.45
1:A:531:LEU:O	1:A:532:ALA:CB	2.64	0.45
1:A:570:PHE:HE1	1:A:577:TRP:CE3	2.34	0.45
1:B:704:GLU:HG3	1:B:717:VAL:HG23	1.98	0.45
1:B:772:ILE:HD12	1:B:772:ILE:O	2.17	0.45
2:C:210:VAL:HG23	2:C:210:VAL:O	2.16	0.45
2:C:157:PHE:HD1	2:C:214:TRP:CE2	2.35	0.45
2:E:175:THR:O	2:E:176:PRO:C	2.55	0.45
2:F:421:ASN:HA	2:R:144:ASP:OD2	2.16	0.45
2:G:66:ASN:HD22	2:G:418:TYR:HD1	1.64	0.45
2:H:157:PHE:HD1	2:H:214:TRP:CE2	2.35	0.45
2:J:140:MET:HE1	2:J:406:VAL:HG11	1.96	0.45
2:S:175:THR:OG1	2:J:242:THR:HG23	2.16	0.45
2:J:59:VAL:O	2:J:62:GLN:HB3	2.16	0.45
2:R:120:ASN:O	2:R:121:ASN:C	2.55	0.45
2:S:356:LEU:O	2:S:357:ILE:C	2.54	0.45
2:T:5:MET:HB3	2:T:104:ILE:HG22	1.98	0.45
1:A:340:PRO:HG3	1:A:584:ASN:HD21	1.82	0.45
1:B:242:GLN:O	1:B:282:ARG:HG3	2.16	0.45
1:B:772:ILE:CD1	1:B:774:ILE:HB	2.47	0.45
2:C:349:MET:HA	2:C:349:MET:HE2	1.99	0.45
2:E:1:MET:O	2:E:2:SER:C	2.53	0.45
2:H:244:THR:HB	2:H:247:ASP:OD1	2.17	0.45
2:I:150:PRO:HA	2:I:297:PHE:O	2.17	0.45
2:Q:193:LEU:HD21	2:Q:292:ALA:HB2	1.99	0.45
2:Q:61:LEU:HD12	2:F:119:LEU:HD21	1.99	0.45
2:R:124:LEU:CD2	2:G:416:ARG:HD3	2.47	0.45
2:R:82:LEU:HD11	2:R:352:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:145:ILE:HD11	2:T:149:GLU:OE2	2.17	0.45
2:C:225:VAL:HG12	2:C:263:VAL:HG13	1.98	0.45
2:E:198:SER:HB3	2:E:202:ILE:HD11	1.99	0.45
2:E:156:LEU:CD1	2:E:218:LEU:HD21	2.47	0.45
2:Q:154:CYS:HB3	2:Q:187:ALA:O	2.17	0.45
2:R:1:MET:HB3	2:R:93:PRO:HD2	1.99	0.45
2:S:374:SER:HB2	2:S:375:PRO:HD2	1.99	0.45
1:A:731:SER:O	1:A:732:LYS:C	2.55	0.45
1:B:65:LEU:HD21	1:B:222:VAL:HG11	1.99	0.45
1:B:58:ILE:CG1	1:B:754:ILE:HD13	2.47	0.45
2:C:62:GLN:HG3	2:C:419:ARG:HB3	1.98	0.45
2:D:309:THR:CG2	2:D:309:THR:O	2.63	0.45
2:E:320:ILE:HD11	2:E:383:ALA:HB1	1.99	0.45
2:F:201:ALA:HA	2:F:287:THR:HA	1.98	0.45
2:H:156:LEU:HD11	2:H:299:ILE:HD11	1.99	0.45
2:J:140:MET:HE3	2:J:406:VAL:HG21	1.99	0.45
2:J:254:VAL:HG13	2:J:255:PRO:HD2	1.98	0.45
2:R:132:LEU:O	2:R:136:GLN:HG3	2.17	0.45
2:R:363:PRO:HA	2:R:364:PRO:HD3	1.85	0.45
1:A:125:VAL:O	1:A:126:ILE:C	2.55	0.45
1:A:170:ALA:C	1:A:172:HIS:H	2.20	0.45
1:A:286:GLN:CG	1:A:748:PRO:HA	2.46	0.45
1:A:311:ILE:HD11	1:A:362:GLN:HB3	1.98	0.45
1:A:669:ILE:N	1:A:669:ILE:CD1	2.79	0.45
1:A:914:TYR:O	1:B:1005:VAL:HG23	2.17	0.45
1:B:177:HIS:O	1:B:178:ASP:C	2.55	0.45
1:B:222:VAL:HG13	1:B:223:PRO:CD	2.46	0.45
2:C:169:MET:O	2:C:173:LEU:HD13	2.17	0.45
2:D:121:ASN:CB	2:D:146:PRO:HA	2.47	0.45
2:D:244:THR:HG22	2:D:245:ALA:N	2.31	0.45
2:D:132:LEU:HG	2:D:328:PHE:CE2	2.51	0.45
2:D:346:SER:O	2:D:349:MET:N	2.50	0.45
2:F:104:ILE:HD12	2:F:104:ILE:N	2.32	0.45
2:I:117:ARG:O	2:I:120:ASN:HB3	2.17	0.45
2:I:182:GLN:HG2	2:I:183:PRO:HD2	1.99	0.45
2:I:204:ALA:HB1	2:I:283:GLY:O	2.17	0.45
2:I:74:SER:HB3	2:I:77:ARG:HG3	1.99	0.45
2:Q:72:ILE:O	2:Q:72:ILE:HD13	2.17	0.45
2:R:167:ILE:HB	2:R:168:PRO:HD3	1.99	0.45
2:S:323:PHE:HB2	2:S:405:TRP:HE1	1.82	0.45
1:A:84:ARG:HD2	1:A:84:ARG:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LEU:HD23	1:B:298:LEU:C	2.37	0.44
1:B:627:PRO:HG2	1:B:630:TRP:CG	2.52	0.44
2:H:17:SER:O	2:H:21:VAL:HG23	2.17	0.44
2:R:235:ILE:HD11	2:H:235:ILE:CD1	2.46	0.44
2:I:186:VAL:HB	2:I:231:PHE:CZ	2.51	0.44
2:I:298:THR:HG22	2:I:299:ILE:H	1.79	0.44
2:I:348:ALA:O	2:I:351:GLN:HB3	2.17	0.44
2:Q:193:LEU:HD23	2:Q:292:ALA:HA	1.99	0.44
2:Q:49:SER:O	2:Q:50:SER:HB3	2.17	0.44
2:R:139:ILE:HD12	2:R:405:TRP:CE3	2.51	0.44
2:S:17:SER:O	2:S:21:VAL:HG23	2.16	0.44
1:A:311:ILE:CD1	1:A:362:GLN:HB3	2.47	0.44
1:A:327:LEU:HD11	1:A:646:PHE:CD1	2.53	0.44
1:B:463:LEU:HB3	1:B:464:PRO:HD2	2.00	0.44
1:B:550:ILE:HB	1:B:599:LEU:HD11	1.99	0.44
2:P:12:LEU:HA	2:C:28:PHE:CZ	2.52	0.44
2:D:24:ASN:C	2:D:24:ASN:ND2	2.68	0.44
2:E:172:ILE:HD12	2:E:172:ILE:N	2.32	0.44
2:E:3:ARG:HD3	2:E:89:SER:O	2.17	0.44
2:H:1:MET:HB2	2:H:5:MET:SD	2.57	0.44
2:I:254:VAL:HG13	2:I:255:PRO:HD2	1.98	0.44
2:P:14:GLU:OE2	2:P:131:LYS:HB3	2.17	0.44
2:Q:396:ILE:O	2:Q:400:ILE:HG13	2.18	0.44
2:R:140:MET:CE	2:R:406:VAL:HG11	2.47	0.44
2:S:170:MET:HE1	2:S:232:PHE:HB2	2.00	0.44
2:S:151:ILE:HG12	2:S:299:ILE:HG13	2.00	0.44
2:T:109:GLN:CG	2:T:112:MET:HB3	2.47	0.44
1:A:362:GLN:O	1:A:364:MET:N	2.50	0.44
1:A:834:THR:HG23	1:A:835:ASP:N	2.32	0.44
1:B:282:ARG:HA	1:B:283:PRO:HD3	1.85	0.44
1:B:800:SER:OG	1:B:801:VAL:N	2.50	0.44
2:D:107:ARG:HG2	2:D:107:ARG:NH1	2.32	0.44
2:E:49:SER:HB3	2:E:105:ARG:NH1	2.33	0.44
2:F:239:VAL:HA	2:F:288:GLY:CA	2.47	0.44
2:R:221:THR:HB	2:G:327:ASP:OD1	2.18	0.44
2:H:361:MET:HG2	2:H:392:VAL:HG11	1.99	0.44
2:J:100:ILE:HD12	2:J:100:ILE:H	1.83	0.44
2:Q:107:ARG:HG2	2:Q:107:ARG:NH1	2.32	0.44
2:Q:157:PHE:CG	2:Q:158:ARG:N	2.85	0.44
2:R:137:ASN:HB3	2:R:143:LEU:HD12	1.99	0.44
2:T:3:ARG:HG3	2:T:4:GLN:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:5:MET:O	2:T:9:THR:HG23	2.18	0.44
1:A:260:PHE:HA	1:A:1003:ILE:HD12	2.00	0.44
1:B:177:HIS:HA	1:B:180:VAL:CG1	2.42	0.44
2:E:271:PHE:CZ	2:E:293:ILE:HD13	2.53	0.44
2:G:176:PRO:HA	2:G:177:PRO:HD2	1.84	0.44
2:G:17:SER:O	2:G:21:VAL:HG23	2.17	0.44
2:G:188:GLU:HA	2:G:232:PHE:CE1	2.53	0.44
2:G:235:ILE:CD1	2:H:235:ILE:HD11	2.47	0.44
2:H:228:THR:CG2	2:H:229:ASN:H	2.21	0.44
2:I:164:THR:HG23	2:I:165:GLY:N	2.32	0.44
2:P:120:ASN:O	2:P:121:ASN:C	2.55	0.44
2:T:59:VAL:HG13	2:T:60:PRO:CD	2.45	0.44
1:A:264:ASP:HB3	1:A:267:VAL:HG23	2.00	0.44
1:A:286:GLN:CA	1:A:286:GLN:NE2	2.79	0.44
1:A:524:LEU:HD23	1:A:524:LEU:HA	1.85	0.44
1:B:110:HIS:C	1:B:112:SER:H	2.21	0.44
1:B:293:VAL:HG22	1:B:669:ILE:HG13	1.99	0.44
1:B:459:TYR:CD2	1:B:482:ALA:HA	2.53	0.44
1:B:86:VAL:HG22	1:B:88:GLU:H	1.81	0.44
1:B:880:LEU:HG	1:B:881:GLN:N	2.33	0.44
2:C:120:ASN:C	2:C:122:LEU:N	2.71	0.44
2:D:110:VAL:HG22	2:D:111:PRO:CA	2.48	0.44
2:F:214:TRP:CE3	2:F:215:ALA:HB2	2.53	0.44
2:H:337:ARG:HH11	2:H:337:ARG:HG3	1.83	0.44
2:I:132:LEU:HG	2:I:328:PHE:CE2	2.53	0.44
2:J:97:ASP:C	2:J:99:PHE:H	2.20	0.44
1:B:109:GLU:CD	1:B:109:GLU:H	2.20	0.44
1:B:439:TYR:O	1:B:440:PRO:C	2.56	0.44
1:B:601:ILE:HG13	1:B:648:ILE:HD13	1.99	0.44
1:B:65:LEU:HD21	1:B:222:VAL:CG1	2.47	0.44
1:B:711:VAL:O	1:B:711:VAL:HG12	2.18	0.44
2:E:110:VAL:HG23	2:E:111:PRO:HA	2.00	0.44
2:G:201:ALA:HA	2:G:287:THR:HA	2.00	0.44
2:I:344:ILE:H	2:I:344:ILE:CD1	2.26	0.44
2:P:31:LEU:HD22	2:D:41:ASN:CB	2.45	0.44
2:S:151:ILE:O	2:S:151:ILE:HD12	2.18	0.44
1:A:348:MET:CG	1:A:643:PHE:HB2	2.48	0.44
1:A:307:LEU:HD21	1:A:365:LEU:CB	2.48	0.44
1:A:63:ILE:HG13	1:A:64:GLY:N	2.33	0.44
1:A:732:LYS:HD3	1:A:736:ASP:OD2	2.17	0.44
2:D:184:PHE:HZ	2:D:290:CYS:HG	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:341:GLN:HA	2:E:344:ILE:HD13	2.00	0.44
2:G:341:GLN:HB3	2:G:341:GLN:HE21	1.53	0.44
2:P:12:LEU:HA	2:C:28:PHE:CE2	2.53	0.44
2:P:186:VAL:HB	2:P:231:PHE:CE1	2.53	0.44
2:P:254:VAL:CG1	2:P:255:PRO:HD2	2.46	0.44
2:Q:64:MET:HG3	2:Q:103:TYR:CD2	2.53	0.44
2:R:5:MET:CE	2:R:106:PRO:HD3	2.47	0.44
2:R:186:VAL:HB	2:R:231:PHE:CE1	2.53	0.44
2:R:28:PHE:N	2:R:28:PHE:CD1	2.86	0.44
2:S:132:LEU:HD23	2:S:132:LEU:HA	1.78	0.44
2:S:271:PHE:HZ	2:S:293:ILE:HD13	1.83	0.44
2:S:361:MET:HE2	2:S:361:MET:HB2	1.76	0.44
1:A:591:PHE:CE1	1:A:642:LEU:HD12	2.53	0.44
2:D:153:PRO:HD2	2:D:189:ARG:O	2.17	0.44
2:H:135:ARG:NH1	2:H:324:ASP:HB2	2.32	0.44
2:J:254:VAL:CG1	2:J:255:PRO:HD2	2.48	0.44
2:J:56:ASP:OD1	2:J:58:ARG:N	2.41	0.44
2:P:179:ALA:HA	2:P:199:ASN:OD1	2.18	0.44
2:P:24:ASN:ND2	2:P:24:ASN:C	2.70	0.44
2:S:419:ARG:NH1	2:S:419:ARG:HG2	2.33	0.44
2:S:72:ILE:O	2:S:72:ILE:HG23	2.17	0.44
2:T:394:LEU:O	2:T:397:ARG:HB2	2.18	0.44
1:A:201:ILE:HG22	1:A:201:ILE:O	2.18	0.44
1:A:595:THR:OG1	1:A:596:PRO:HD3	2.18	0.44
1:B:671:ILE:O	1:B:675:ILE:HG13	2.18	0.44
2:C:394:LEU:O	2:C:397:ARG:HB2	2.17	0.44
2:E:114:ASP:OD2	2:E:117:ARG:NH2	2.51	0.44
2:S:420:PRO:O	2:S:421:ASN:OXT	2.36	0.44
2:T:357:ILE:CD1	2:T:386:ILE:HD12	2.47	0.44
2:T:396:ILE:CD1	2:T:396:ILE:N	2.81	0.44
1:A:454:VAL:O	1:A:458:ILE:HG12	2.18	0.43
1:B:258:PRO:CG	1:B:261:LEU:HD12	2.43	0.43
1:B:443:ALA:O	1:B:444:ILE:C	2.57	0.43
1:B:97:TYR:CE2	1:B:771:ILE:HD12	2.51	0.43
2:D:225:VAL:HG23	2:D:269:LEU:HD12	2.00	0.43
2:E:91:THR:O	2:E:93:PRO:HD3	2.17	0.43
2:I:6:TRP:CE2	2:I:104:ILE:HG12	2.53	0.43
2:Q:325:VAL:HG13	2:Q:405:TRP:CE2	2.53	0.43
2:R:132:LEU:HG	2:R:328:PHE:CE2	2.53	0.43
2:S:1:MET:HG2	2:S:93:PRO:HD2	2.00	0.43
1:A:939:ARG:HG2	1:A:939:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ARG:NH1	1:B:187:ARG:CG	2.77	0.43
1:B:219:ARG:HD2	1:B:982:ASP:CG	2.38	0.43
2:C:186:VAL:HG23	2:C:193:LEU:HB2	2.00	0.43
2:D:84:LYS:HB3	2:D:360:TYR:CE2	2.53	0.43
2:F:361:MET:HE3	2:F:361:MET:HB2	1.70	0.43
2:G:140:MET:CE	2:G:406:VAL:HG11	2.48	0.43
2:G:145:ILE:HD12	2:G:308:TYR:HE1	1.83	0.43
2:I:166:ASN:N	2:I:168:PRO:HD2	2.33	0.43
2:S:343:GLU:HG2	2:S:344:ILE:HD12	2.00	0.43
1:A:489:LEU:HD11	1:A:503:ARG:HA	2.00	0.43
1:A:653:GLN:NE2	1:A:655:LEU:CD1	2.81	0.43
1:B:180:VAL:HG13	1:B:181:ASN:N	2.33	0.43
2:C:91:THR:O	2:C:93:PRO:HD3	2.18	0.43
2:E:202:ILE:HD12	2:E:202:ILE:N	2.33	0.43
2:E:250:THR:HG23	2:E:281:GLU:O	2.17	0.43
2:G:218:LEU:HA	2:G:218:LEU:HD23	1.85	0.43
2:G:226:TYR:HE1	2:G:228:THR:HG23	1.84	0.43
2:H:339:CYS:HB3	2:H:421:ASN:ND2	2.29	0.43
2:I:240:THR:HB	2:I:242:THR:CG2	2.49	0.43
2:J:71:PHE:CZ	2:J:78:CYS:HB3	2.53	0.43
2:Q:121:ASN:HA	2:Q:146:PRO:HA	2.01	0.43
2:Q:221:THR:HA	2:Q:270:SER:HB3	1.99	0.43
2:R:244:THR:HB	2:R:247:ASP:OD1	2.18	0.43
2:S:229:ASN:OD1	2:I:234:THR:HA	2.18	0.43
2:S:379:PHE:O	2:S:380:SER:C	2.55	0.43
1:B:597:ASN:C	1:B:599:LEU:N	2.70	0.43
2:D:272:SER:C	2:D:274:GLY:N	2.69	0.43
2:G:316:THR:HA	2:G:317:PRO:C	2.37	0.43
2:H:24:ASN:C	2:H:24:ASN:HD22	2.22	0.43
2:I:360:TYR:HB2	2:I:400:ILE:HD11	1.99	0.43
2:I:140:MET:HE3	2:I:406:VAL:HG11	2.00	0.43
2:J:415:GLY:O	2:J:418:TYR:N	2.49	0.43
2:Q:363:PRO:HA	2:Q:364:PRO:HD3	1.52	0.43
2:S:167:ILE:HB	2:S:168:PRO:HD3	2.00	0.43
2:S:1:MET:O	2:S:2:SER:C	2.55	0.43
2:S:361:MET:CE	2:S:367:PRO:CD	2.83	0.43
2:S:357:ILE:CD1	2:S:386:ILE:HD12	2.44	0.43
1:A:121:HIS:O	1:A:124:ARG:HB3	2.19	0.43
1:B:802:TYR:O	1:B:805:VAL:HG12	2.18	0.43
2:D:120:ASN:O	2:D:122:LEU:N	2.51	0.43
2:D:41:ASN:O	2:D:44:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:266:ASP:OD1	2:F:167:ILE:HD13	2.19	0.43
2:F:17:SER:O	2:F:21:VAL:HG23	2.18	0.43
2:G:261:LEU:HA	2:G:262:PRO:HD2	1.86	0.43
2:H:316:THR:HA	2:H:317:PRO:HA	1.88	0.43
2:I:310:LEU:HD22	2:I:313:ILE:CD1	2.48	0.43
2:J:82:LEU:HA	2:J:356:LEU:HD12	2.00	0.43
2:P:144:ASP:OD1	2:P:302:ASN:HA	2.19	0.43
2:Q:352:LEU:HD21	2:Q:407:ILE:HG21	2.01	0.43
2:R:418:TYR:CD1	2:R:420:PRO:HD3	2.54	0.43
2:T:254:VAL:CG1	2:T:255:PRO:HD2	2.48	0.43
1:A:220:TYR:N	1:A:220:TYR:CD1	2.86	0.43
1:A:358:VAL:HG13	1:A:359:PHE:N	2.33	0.43
1:A:488:ILE:HD12	1:A:488:ILE:N	2.33	0.43
1:A:903:PHE:O	1:A:906:PHE:HB3	2.19	0.43
2:C:346:SER:O	2:C:350:ASP:OD1	2.35	0.43
2:D:184:PHE:O	2:D:194:PHE:HA	2.19	0.43
2:F:337:ARG:NH1	2:F:337:ARG:HG3	2.12	0.43
2:F:359:ASN:ND2	2:F:359:ASN:H	2.14	0.43
2:G:325:VAL:HG13	2:G:326:SER:N	2.34	0.43
2:G:379:PHE:CE1	2:G:404:LEU:HD22	2.52	0.43
2:H:252:PHE:HA	2:H:279:ASN:O	2.18	0.43
2:I:217:VAL:O	2:I:300:LEU:HG	2.18	0.43
2:I:44:THR:O	2:I:44:THR:CG2	2.66	0.43
2:Q:254:VAL:HG12	2:Q:256:THR:H	1.84	0.43
2:Q:309:THR:O	2:Q:309:THR:CG2	2.66	0.43
2:S:201:ALA:HA	2:S:287:THR:HA	1.99	0.43
2:S:313:ILE:HB	2:S:398:LYS:HE2	2.01	0.43
2:T:329:LEU:HD13	2:T:412:ALA:HB2	2.00	0.43
1:A:307:LEU:HD22	1:A:617:TYR:HD1	1.84	0.43
1:A:715:ILE:HA	1:A:715:ILE:HD12	1.74	0.43
1:B:588:LEU:O	1:B:588:LEU:HD12	2.18	0.43
2:C:69:VAL:HG21	2:C:418:TYR:CD1	2.54	0.43
2:D:344:ILE:CD1	2:D:344:ILE:H	2.27	0.43
2:E:320:ILE:HD11	2:E:383:ALA:CB	2.49	0.43
2:E:83:ARG:HG2	2:E:359:ASN:HD22	1.83	0.43
2:F:220:VAL:CG1	2:F:223:ALA:HB2	2.49	0.43
2:G:16:ILE:CD1	2:G:42:MET:HB3	2.48	0.43
2:I:17:SER:O	2:I:21:VAL:HG23	2.19	0.43
2:J:145:ILE:HD11	2:J:149:GLU:OE2	2.18	0.43
2:Q:316:THR:HG21	2:Q:397:ARG:HH12	1.83	0.43
2:S:244:THR:HG22	2:S:246:ALA:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:378:ARG:NH2	2:J:259:ASN:HB2	2.34	0.43
1:B:225:HIS:ND1	1:B:227:ILE:CG2	2.62	0.43
2:C:235:ILE:HD12	2:C:235:ILE:N	2.33	0.43
2:E:190:ARG:HG2	2:E:190:ARG:O	2.19	0.43
2:I:262:PRO:HB2	2:I:265:THR:HG21	2.01	0.43
2:P:156:LEU:HD21	2:P:299:ILE:HD11	2.01	0.43
2:R:373:THR:O	2:R:373:THR:HG22	2.19	0.43
2:R:95:VAL:HG23	2:R:95:VAL:O	2.19	0.43
2:T:375:PRO:CD	2:T:378:ARG:HD3	2.48	0.43
1:A:252:TYR:CE1	1:A:256:ARG:NE	2.87	0.43
1:A:385:PHE:HA	1:A:566:TYR:CE2	2.54	0.43
1:B:845:ARG:NH2	1:B:864:GLU:OE1	2.42	0.43
2:D:197:ARG:HG3	2:D:197:ARG:HH11	1.84	0.43
2:F:46:LEU:HD12	2:F:46:LEU:HA	1.80	0.43
2:P:114:ASP:CG	2:P:117:ARG:HH12	2.22	0.43
2:Q:242:THR:HG22	2:Q:243:ALA:N	2.34	0.43
2:Q:325:VAL:HG13	2:Q:405:TRP:CZ2	2.54	0.43
2:S:303:ARG:HH11	2:S:303:ARG:CB	2.31	0.43
1:A:286:GLN:NE2	1:A:286:GLN:HA	2.34	0.43
1:A:366:ASN:HA	1:A:367:PRO:HD2	1.89	0.43
1:A:670:LEU:HD21	1:A:751:TYR:CE1	2.54	0.43
1:A:190:TYR:CE1	1:A:976:ARG:HG3	2.53	0.43
1:B:608:ASN:HA	1:B:612:ASN:HB2	2.00	0.43
1:B:781:VAL:HG21	1:B:784:SER:HB3	2.01	0.43
2:C:274:GLY:C	2:C:276:GLY:N	2.71	0.43
2:F:110:VAL:HG22	2:F:111:PRO:CA	2.47	0.43
2:H:341:GLN:HA	2:H:344:ILE:HD13	2.00	0.43
2:J:100:ILE:CD1	2:J:100:ILE:H	2.32	0.43
2:J:109:GLN:O	2:J:113:SER:CB	2.67	0.43
2:J:206:ALA:C	2:J:207:TYR:CD1	2.92	0.43
2:P:284:VAL:HG12	2:P:285:ALA:N	2.34	0.43
2:R:107:ARG:NH1	2:R:107:ARG:HG2	2.33	0.43
2:R:140:MET:HE3	2:R:406:VAL:HG11	2.01	0.43
2:S:361:MET:HG2	2:S:392:VAL:HG11	2.01	0.43
1:A:817:ALA:O	1:A:821:LEU:HG	2.18	0.42
1:A:887:GLY:HA2	1:A:930:LEU:CD1	2.48	0.42
2:C:310:LEU:HB3	2:C:313:ILE:HD12	2.01	0.42
2:D:214:TRP:CE3	2:D:215:ALA:HB2	2.53	0.42
2:E:186:VAL:HG22	2:E:187:ALA:H	1.83	0.42
2:H:210:VAL:O	2:H:210:VAL:HG23	2.18	0.42
2:J:358:THR:C	2:J:360:TYR:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:363:PRO:O	2:P:365:ALA:N	2.52	0.42
2:Q:177:PRO:HG2	2:Q:199:ASN:HB3	2.01	0.42
2:Q:41:ASN:O	2:Q:44:THR:HB	2.19	0.42
2:R:135:ARG:HG3	2:R:135:ARG:HH11	1.82	0.42
2:T:186:VAL:HB	2:T:231:PHE:CE1	2.53	0.42
2:T:82:LEU:HD11	2:T:352:LEU:HD22	2.01	0.42
1:A:392:MET:HE3	1:A:392:MET:HA	2.01	0.42
1:A:722:THR:CG2	1:A:728:GLY:HA2	2.49	0.42
1:A:781:VAL:HG21	1:A:867:ILE:HG22	2.01	0.42
2:D:316:THR:HG21	2:D:397:ARG:HH12	1.84	0.42
2:E:357:ILE:HD11	2:E:386:ILE:HD12	2.01	0.42
2:F:325:VAL:O	2:F:329:LEU:CD2	2.68	0.42
2:Q:254:VAL:HG11	2:Q:272:SER:O	2.19	0.42
1:A:667:GLU:O	1:A:671:ILE:HG12	2.19	0.42
1:B:31:VAL:HG21	1:B:1008:VAL:HG22	2.01	0.42
2:C:107:ARG:HG2	2:C:107:ARG:NH1	2.34	0.42
2:D:108:LEU:HA	2:D:108:LEU:HD23	1.84	0.42
2:D:244:THR:HG22	2:D:246:ALA:H	1.85	0.42
2:E:12:LEU:HA	2:F:28:PHE:CZ	2.54	0.42
2:G:231:PHE:HB2	2:G:236:ILE:HD11	2.00	0.42
2:H:59:VAL:HG13	2:H:60:PRO:HD3	2.01	0.42
2:J:166:ASN:OD1	2:J:186:VAL:HG22	2.18	0.42
2:J:418:TYR:CD1	2:J:420:PRO:HD3	2.55	0.42
2:R:210:VAL:HA	2:R:277:ASN:OD1	2.19	0.42
2:T:323:PHE:HB2	2:T:405:TRP:HE1	1.84	0.42
1:B:311:ILE:HD12	1:B:362:GLN:HB3	2.02	0.42
1:B:392:MET:HE3	1:B:561:LEU:HD21	2.00	0.42
1:B:599:LEU:O	1:B:603:GLU:HG3	2.19	0.42
2:D:186:VAL:HG23	2:D:193:LEU:HB2	2.01	0.42
2:C:221:THR:HB	2:D:327:ASP:OD2	2.19	0.42
2:E:309:THR:O	2:E:310:LEU:HB2	2.20	0.42
2:F:87:PHE:CE1	2:F:403:HIS:HA	2.54	0.42
2:G:121:ASN:HA	2:G:146:PRO:HA	2.00	0.42
2:I:132:LEU:O	2:I:136:GLN:HG3	2.20	0.42
2:S:147:TYR:HB2	2:I:331:THR:HG22	2.01	0.42
2:I:363:PRO:HA	2:I:364:PRO:HD3	1.74	0.42
2:P:152:GLU:OE1	2:P:189:ARG:HG2	2.19	0.42
2:Q:377:PHE:CD1	2:Q:377:PHE:C	2.93	0.42
2:T:9:THR:HA	2:T:107:ARG:HG3	2.02	0.42
1:A:988:ASP:HA	1:A:989:PRO:HD3	1.86	0.42
2:E:300:LEU:HD23	2:E:300:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:184:PHE:C	2:F:184:PHE:CD1	2.93	0.42
2:I:118:GLN:C	2:I:120:ASN:N	2.73	0.42
2:P:6:TRP:CD1	2:P:104:ILE:HG21	2.54	0.42
2:Q:337:ARG:HH21	2:Q:342:TYR:HE1	1.67	0.42
2:R:135:ARG:HG3	2:R:135:ARG:NH1	2.35	0.42
2:S:421:ASN:O	2:S:421:ASN:OD1	2.38	0.42
2:S:49:SER:C	2:S:51:ALA:N	2.67	0.42
1:A:192:ARG:HG3	1:A:220:TYR:CE2	2.55	0.42
1:A:459:TYR:CG	1:A:473:ILE:HG21	2.54	0.42
1:A:492:ALA:C	1:A:494:GLN:H	2.22	0.42
1:B:35:LEU:HD23	1:B:35:LEU:HA	1.81	0.42
1:B:2:ASP:C	1:B:4:THR:H	2.23	0.42
1:B:58:ILE:HG13	1:B:754:ILE:HD13	2.01	0.42
2:D:375:PRO:HD2	2:D:378:ARG:HD3	2.01	0.42
2:E:122:LEU:HD23	2:E:122:LEU:HA	1.82	0.42
2:E:375:PRO:CG	2:E:378:ARG:HD3	2.49	0.42
2:F:309:THR:O	2:F:310:LEU:HB2	2.20	0.42
2:F:363:PRO:HA	2:F:364:PRO:HD3	1.66	0.42
2:G:13:LEU:HD23	2:G:13:LEU:HA	1.85	0.42
2:G:186:VAL:HG23	2:G:193:LEU:HB2	2.02	0.42
2:I:309:THR:O	2:I:309:THR:HG22	2.20	0.42
2:J:157:PHE:HD1	2:J:214:TRP:CE2	2.36	0.42
2:J:24:ASN:C	2:J:24:ASN:HD22	2.20	0.42
2:I:12:LEU:HA	2:J:28:PHE:CZ	2.55	0.42
2:P:160:VAL:HG22	2:P:161:ALA:H	1.85	0.42
2:Q:410:LEU:HD12	2:Q:410:LEU:HA	1.83	0.42
2:R:343:GLU:N	2:R:343:GLU:OE2	2.52	0.42
2:S:418:TYR:CZ	2:S:420:PRO:HG3	2.55	0.42
1:A:126:ILE:HA	1:A:126:ILE:HD13	1.79	0.42
2:F:198:SER:HB3	2:F:202:ILE:HD11	2.01	0.42
2:F:132:LEU:HD21	2:F:328:PHE:CD1	2.54	0.42
2:I:298:THR:CG2	2:I:299:ILE:N	2.81	0.42
2:J:221:THR:HA	2:J:270:SER:HB3	2.01	0.42
2:P:154:CYS:HB3	2:P:188:GLU:O	2.19	0.42
2:P:160:VAL:HG22	2:P:161:ALA:N	2.35	0.42
2:P:210:VAL:HA	2:P:277:ASN:OD1	2.19	0.42
2:P:64:MET:HG3	2:P:103:TYR:CE2	2.55	0.42
2:R:105:ARG:O	2:R:107:ARG:HG3	2.18	0.42
2:R:305:GLN:O	2:R:309:THR:HB	2.20	0.42
2:R:396:ILE:O	2:R:400:ILE:HG13	2.19	0.42
2:S:152:GLU:HA	2:S:153:PRO:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:419:ARG:HH11	2:S:419:ARG:HG2	1.85	0.42
1:A:492:ALA:O	1:A:494:GLN:N	2.53	0.42
1:A:783:ASN:HD22	1:A:784:SER:H	1.66	0.42
1:A:878:PHE:HA	1:A:921:VAL:O	2.18	0.42
1:A:941:ARG:H	1:A:941:ARG:HG3	1.71	0.42
2:D:121:ASN:HA	2:D:146:PRO:CA	2.50	0.42
2:H:272:SER:C	2:H:274:GLY:H	2.22	0.42
2:H:379:PHE:O	2:H:380:SER:C	2.57	0.42
2:I:46:LEU:N	2:I:46:LEU:CD1	2.82	0.42
2:J:184:PHE:O	2:J:194:PHE:HA	2.20	0.42
2:P:394:LEU:O	2:P:397:ARG:HB2	2.20	0.42
2:P:6:TRP:CE3	2:P:410:LEU:HD13	2.54	0.42
2:Q:168:PRO:C	2:Q:170:MET:H	2.22	0.42
2:Q:244:THR:HG22	2:Q:245:ALA:N	2.35	0.42
2:S:322:ASP:O	2:S:323:PHE:HB2	2.20	0.42
1:B:956:GLN:C	1:B:957:ILE:HD12	2.40	0.42
2:C:110:VAL:HG22	2:C:111:PRO:HA	2.02	0.42
2:C:56:ASP:HA	2:C:57:PRO:HD2	1.79	0.42
2:E:119:LEU:HD23	2:E:119:LEU:HA	1.83	0.42
2:G:349:MET:HE3	2:G:352:LEU:CD2	2.48	0.42
2:H:107:ARG:CG	2:H:107:ARG:NH1	2.80	0.42
2:H:144:ASP:OD1	2:H:302:ASN:HA	2.20	0.42
1:A:826:ARG:HH11	1:A:826:ARG:HG2	1.85	0.42
1:B:308:LEU:HD22	1:B:362:GLN:CB	2.45	0.42
1:B:769:THR:O	1:B:772:ILE:HG13	2.19	0.42
1:B:892:PRO:HA	1:B:893:PRO:HD3	1.88	0.42
2:C:419:ARG:HA	2:C:420:PRO:HD2	1.74	0.42
2:C:56:ASP:O	2:C:60:PRO:HD2	2.19	0.42
2:D:33:THR:HG22	2:D:35:ASP:H	1.83	0.42
2:F:133:TYR:HA	2:F:136:GLN:OE1	2.20	0.42
2:F:166:ASN:N	2:F:168:PRO:HD2	2.34	0.42
2:G:107:ARG:NH1	2:G:107:ARG:CG	2.81	0.42
2:I:269:LEU:HD22	2:I:269:LEU:H	1.85	0.42
2:J:163:GLN:HE21	2:J:169:MET:HG3	1.77	0.42
2:P:110:VAL:HG23	2:P:111:PRO:HA	2.01	0.42
2:P:135:ARG:HG2	2:P:308:TYR:CE2	2.55	0.42
2:R:418:TYR:CG	2:R:420:PRO:HD3	2.55	0.42
2:S:268:ARG:HD2	2:I:321:ASP:HB2	2.02	0.42
1:A:170:ALA:C	1:A:172:HIS:N	2.74	0.41
1:A:533:LEU:CB	1:A:534:PRO:HD2	2.50	0.41
1:A:561:LEU:HG	1:A:565:MET:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LEU:HD13	1:B:477:PHE:CZ	2.55	0.41
1:B:458:ILE:O	1:B:462:LEU:HG	2.20	0.41
2:C:119:LEU:HA	2:C:119:LEU:HD23	1.90	0.41
2:C:309:THR:HG21	2:Q:343:GLU:HB3	2.01	0.41
2:E:109:GLN:O	2:E:113:SER:CB	2.67	0.41
2:Q:170:MET:HE1	2:F:227:PHE:O	2.20	0.41
2:F:278:ILE:O	2:F:278:ILE:HG23	2.19	0.41
2:H:214:TRP:CE3	2:H:215:ALA:HB2	2.54	0.41
2:J:228:THR:OG1	2:J:229:ASN:N	2.52	0.41
2:J:13:LEU:HD21	2:J:64:MET:HE2	2.02	0.41
2:P:264:GLN:O	2:C:168:PRO:HG3	2.19	0.41
2:R:12:LEU:HA	2:G:28:PHE:CE2	2.55	0.41
2:R:186:VAL:CG2	2:R:193:LEU:HB2	2.50	0.41
2:T:239:VAL:HG13	2:T:289:PHE:CA	2.50	0.41
1:A:151:LEU:HD12	1:A:152:PRO:CD	2.49	0.41
1:A:231:LEU:HA	1:A:231:LEU:HD23	1.84	0.41
1:A:783:ASN:ND2	1:A:784:SER:N	2.68	0.41
1:A:898:LEU:HD23	1:A:957:ILE:HG21	2.02	0.41
1:B:938:LEU:CD2	1:B:938:LEU:H	2.32	0.41
2:C:12:LEU:O	2:C:15:ALA:HB3	2.20	0.41
2:C:339:CYS:SG	2:C:420:PRO:HG3	2.61	0.41
2:D:311:ASN:C	2:D:313:ILE:H	2.24	0.41
2:E:8:ASP:OD2	2:E:108:LEU:HD12	2.21	0.41
2:F:114:ASP:C	2:F:116:VAL:N	2.74	0.41
2:F:271:PHE:HZ	2:F:293:ILE:HD13	1.84	0.41
2:G:374:SER:HB2	2:G:375:PRO:HD2	2.02	0.41
2:I:209:PHE:O	2:I:277:ASN:HB3	2.20	0.41
2:P:192:ILE:HD12	2:P:297:PHE:HE2	1.84	0.41
2:S:329:LEU:O	2:S:330:THR:C	2.58	0.41
2:S:3:ARG:HG3	2:S:4:GLN:N	2.35	0.41
1:A:394:PHE:CZ	1:A:636:VAL:HG11	2.55	0.41
1:A:552:ILE:HD11	1:A:556:ARG:HH21	1.86	0.41
1:A:653:GLN:NE2	1:A:655:LEU:HD11	2.35	0.41
1:A:732:LYS:N	1:A:733:PRO:CD	2.83	0.41
1:A:915:ARG:HA	1:B:1005:VAL:CG2	2.48	0.41
1:A:959:VAL:HA	1:A:960:PRO:HD3	1.85	0.41
1:B:296:SER:HB2	1:B:720:TYR:O	2.20	0.41
1:B:417:TYR:OH	1:B:421:LYS:HE3	2.21	0.41
1:B:747:LEU:HG	1:B:748:PRO:HD2	2.02	0.41
2:C:152:GLU:HA	2:C:153:PRO:HD2	1.87	0.41
2:C:329:LEU:O	2:C:330:THR:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:TYR:CE1	2:D:301:ALA:CB	3.04	0.41
2:D:215:ALA:O	2:D:217:VAL:N	2.53	0.41
2:D:46:LEU:HA	2:D:46:LEU:HD12	1.80	0.41
2:E:271:PHE:HZ	2:E:293:ILE:HD13	1.85	0.41
2:G:140:MET:HE1	2:G:406:VAL:HG11	2.02	0.41
2:H:203:PRO:HG2	2:H:207:TYR:OH	2.20	0.41
2:H:250:THR:HG22	2:H:251:THR:N	2.34	0.41
2:H:396:ILE:N	2:H:396:ILE:HD12	2.35	0.41
2:P:17:SER:O	2:P:21:VAL:HG23	2.20	0.41
2:S:1:MET:O	2:S:2:SER:O	2.39	0.41
2:T:179:ALA:HA	2:T:199:ASN:OD1	2.21	0.41
2:T:24:ASN:HD22	2:T:24:ASN:C	2.22	0.41
2:T:349:MET:HG2	2:T:376:TRP:CG	2.55	0.41
1:A:241:ILE:HD13	1:A:242:GLN:HG3	2.03	0.41
1:A:443:ALA:O	1:A:445:ASP:N	2.53	0.41
1:B:623:ARG:HH11	1:B:623:ARG:CG	2.33	0.41
1:B:212:GLU:CD	1:B:986:ARG:HH12	2.24	0.41
2:E:262:PRO:HB2	2:E:265:THR:HG21	2.01	0.41
2:E:379:PHE:O	2:E:380:SER:C	2.59	0.41
2:G:186:VAL:HB	2:G:231:PHE:CE1	2.55	0.41
2:H:244:THR:HG22	2:H:245:ALA:N	2.35	0.41
2:H:158:ARG:HD2	2:H:313:ILE:HG12	2.01	0.41
2:I:217:VAL:HG12	2:I:299:ILE:HG23	2.03	0.41
2:I:379:PHE:CE1	2:I:404:LEU:HD12	2.54	0.41
2:J:403:HIS:O	2:J:407:ILE:CD1	2.68	0.41
2:S:8:ASP:OD2	2:S:108:LEU:HB2	2.20	0.41
1:A:260:PHE:HA	1:A:1003:ILE:CD1	2.50	0.41
1:A:781:VAL:HG21	1:A:867:ILE:CG2	2.50	0.41
1:A:876:ALA:HA	1:A:918:LEU:HD12	2.03	0.41
1:B:459:TYR:HB2	1:B:473:ILE:HG21	2.01	0.41
1:B:949:PHE:C	1:B:951:SER:N	2.74	0.41
2:D:305:GLN:O	2:D:309:THR:HB	2.20	0.41
2:F:156:LEU:HD11	2:F:299:ILE:HD11	2.02	0.41
2:G:53:TYR:C	2:G:55:SER:N	2.73	0.41
2:H:59:VAL:N	2:H:60:PRO:HD2	2.36	0.41
2:J:132:LEU:HD23	2:J:132:LEU:HA	1.92	0.41
2:P:377:PHE:C	2:P:377:PHE:CD1	2.94	0.41
2:Q:239:VAL:HG13	2:Q:289:PHE:CA	2.50	0.41
2:R:124:LEU:HD21	2:G:416:ARG:HD3	2.03	0.41
2:R:202:ILE:HG22	2:R:207:TYR:OH	2.20	0.41
2:R:235:ILE:N	2:R:235:ILE:CD1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:58:ARG:HG3	2:H:115:THR:HG23	2.03	0.41
2:S:1:MET:HB3	2:S:2:SER:H	1.49	0.41
2:T:231:PHE:O	2:T:232:PHE:HB2	2.20	0.41
2:T:379:PHE:O	2:T:380:SER:C	2.59	0.41
1:A:198:VAL:HG13	1:A:199:PRO:HD2	2.02	0.41
1:A:219:ARG:CG	1:A:219:ARG:HH11	2.29	0.41
1:A:316:VAL:HG21	1:A:651:GLN:HE21	1.82	0.41
1:A:950:SER:O	1:A:953:VAL:HG22	2.20	0.41
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.80	0.41
1:B:31:VAL:CG1	1:B:32:TYR:N	2.81	0.41
1:B:362:GLN:C	1:B:364:MET:H	2.24	0.41
1:B:570:PHE:CD1	1:B:570:PHE:N	2.89	0.41
1:B:56:THR:HA	1:B:57:PRO:HD3	1.89	0.41
1:B:769:THR:C	1:B:771:ILE:H	2.24	0.41
2:C:16:ILE:N	2:C:42:MET:HE1	2.35	0.41
2:D:343:GLU:HB3	2:F:309:THR:HG21	2.03	0.41
2:E:151:ILE:HD11	2:E:156:LEU:HG	2.02	0.41
2:E:323:PHE:HB2	2:E:405:TRP:HE1	1.85	0.41
2:F:354:ASN:ND2	2:F:366:ILE:HD13	2.36	0.41
2:F:61:LEU:HD12	2:F:61:LEU:HA	1.91	0.41
2:G:12:LEU:HA	2:H:28:PHE:CZ	2.55	0.41
2:G:210:VAL:HA	2:G:277:ASN:CB	2.48	0.41
2:Q:163:GLN:NE2	2:Q:185:PHE:H	2.13	0.41
2:R:17:SER:O	2:R:21:VAL:HG23	2.20	0.41
2:S:178:ALA:O	2:S:199:ASN:ND2	2.53	0.41
2:T:45:GLN:O	2:T:46:LEU:C	2.59	0.41
1:A:111:ASP:OD2	1:A:875:ARG:HD2	2.21	0.41
1:B:238:LEU:HA	1:B:238:LEU:HD23	1.82	0.41
1:B:507:ALA:HB3	1:B:508:PRO:HD3	2.03	0.41
1:B:85:ILE:CG1	1:B:933:THR:OG1	2.66	0.41
2:D:169:MET:O	2:D:173:LEU:HD13	2.21	0.41
2:D:208:GLN:HG2	2:D:279:ASN:OD1	2.20	0.41
2:G:41:ASN:HB3	2:H:31:LEU:HD22	1.99	0.41
2:J:153:PRO:HB2	2:J:187:ALA:HB1	2.03	0.41
2:P:332:PHE:CE2	2:P:336:LEU:HD11	2.56	0.41
2:Q:132:LEU:HG	2:Q:328:PHE:CE2	2.56	0.41
2:Q:361:MET:HE1	2:Q:367:PRO:HG3	2.03	0.41
2:Q:404:LEU:HD22	2:Q:404:LEU:HA	1.91	0.41
2:Q:46:LEU:HA	2:Q:46:LEU:HD23	1.81	0.41
2:S:250:THR:HG23	2:S:282:LEU:HA	2.03	0.41
2:T:111:PRO:O	2:T:112:MET:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ILE:CD1	1:A:447:TRP:CZ2	2.96	0.41
1:A:541:ILE:HG23	1:A:542:THR:HG22	2.03	0.41
1:B:377:LEU:HD23	1:B:377:LEU:HA	1.84	0.41
1:B:801:VAL:O	1:B:961:ILE:HG13	2.20	0.41
2:C:222:GLY:HA2	2:C:268:ARG:HB3	2.02	0.41
2:C:46:LEU:HD12	2:C:46:LEU:N	2.36	0.41
2:D:139:ILE:HD12	2:D:405:TRP:CE3	2.56	0.41
2:E:166:ASN:N	2:E:168:PRO:HD2	2.36	0.41
2:E:185:PHE:CE2	2:E:192:ILE:HD11	2.54	0.41
2:F:211:VAL:HG23	2:F:276:GLY:C	2.41	0.41
2:F:325:VAL:HB	2:F:405:TRP:HE1	1.86	0.41
2:G:309:THR:CG2	2:G:309:THR:O	2.68	0.41
2:R:268:ARG:HD2	2:G:321:ASP:HB2	2.02	0.41
2:H:59:VAL:CG1	2:H:60:PRO:HD3	2.50	0.41
2:J:132:LEU:O	2:J:136:GLN:HG3	2.21	0.41
2:J:72:ILE:O	2:J:72:ILE:HG13	2.20	0.41
2:P:147:TYR:N	2:P:147:TYR:CD1	2.89	0.41
2:Q:9:THR:HA	2:Q:107:ARG:HD2	2.02	0.41
2:R:1:MET:O	2:R:2:SER:O	2.39	0.41
2:S:160:VAL:HG12	2:S:161:ALA:H	1.86	0.41
1:A:706:ILE:O	1:A:707:VAL:C	2.58	0.41
1:B:313:LEU:HD23	1:B:608:ASN:ND2	2.36	0.41
2:C:110:VAL:HG22	2:C:111:PRO:CA	2.51	0.41
2:D:203:PRO:HG2	2:D:207:TYR:OH	2.20	0.41
2:D:250:THR:HG23	2:D:281:GLU:O	2.21	0.41
2:F:215:ALA:C	2:F:217:VAL:H	2.25	0.41
2:S:124:LEU:HD12	2:I:14:GLU:HG3	2.03	0.41
2:I:201:ALA:HA	2:I:287:THR:HG22	2.03	0.41
1:A:317:MET:CE	3:K:294:ASP:OD2	2.69	0.41
2:P:214:TRP:CZ3	2:P:215:ALA:HB2	2.55	0.41
2:P:271:PHE:CZ	2:P:293:ILE:HD13	2.55	0.41
2:P:316:THR:HG21	2:P:397:ARG:NH1	2.35	0.41
2:Q:217:VAL:HG13	2:Q:303:ARG:HB3	2.02	0.41
2:Q:366:ILE:N	2:Q:366:ILE:CD1	2.79	0.41
2:S:13:LEU:HA	2:S:13:LEU:HD23	1.87	0.41
2:S:41:ASN:CB	2:I:31:LEU:HD11	2.51	0.41
2:T:82:LEU:HD22	2:T:356:LEU:HD23	2.03	0.41
1:A:307:LEU:HD22	1:A:617:TYR:CD1	2.55	0.41
1:A:676:ARG:HH11	1:A:676:ARG:HG2	1.86	0.41
1:B:177:HIS:C	1:B:179:VAL:N	2.73	0.41
2:C:150:PRO:HA	2:C:297:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:VAL:O	2:C:95:VAL:HG23	2.21	0.41
2:D:328:PHE:N	2:D:328:PHE:CD1	2.89	0.41
2:D:1:MET:HB3	2:D:93:PRO:HD2	2.03	0.41
2:E:203:PRO:O	2:E:204:ALA:C	2.59	0.41
2:E:24:ASN:HD22	2:E:24:ASN:C	2.24	0.41
2:E:196:ILE:HB	2:E:289:PHE:HE2	1.86	0.41
2:F:309:THR:HG22	2:F:309:THR:O	2.20	0.41
2:F:33:THR:O	2:F:34:GLY:C	2.60	0.41
2:F:80:TYR:CE2	2:F:81:MET:HG3	2.56	0.41
2:R:256:THR:CG2	2:G:337:ARG:HH12	2.33	0.41
2:G:361:MET:HE1	2:G:367:PRO:HD3	2.02	0.41
2:G:349:MET:HG2	2:G:376:TRP:CG	2.56	0.41
2:G:87:PHE:HB2	2:G:403:HIS:CE1	2.56	0.41
2:I:147:TYR:CD1	2:I:147:TYR:N	2.89	0.41
2:I:396:ILE:H	2:I:396:ILE:CD1	2.34	0.41
2:R:393:ASP:OD2	2:R:394:LEU:N	2.53	0.41
2:S:170:MET:CE	2:S:232:PHE:HB2	2.51	0.41
2:S:56:ASP:HA	2:S:57:PRO:HD2	1.88	0.41
2:T:186:VAL:CG2	2:T:193:LEU:HB2	2.51	0.41
1:A:286:GLN:HE21	1:A:286:GLN:C	2.23	0.41
1:A:223:PRO:HA	1:A:979:PHE:O	2.20	0.41
2:C:387:LEU:HG	2:C:401:VAL:HG21	2.03	0.41
2:D:120:ASN:O	2:D:121:ASN:C	2.59	0.41
2:D:160:VAL:HG12	2:D:161:ALA:H	1.86	0.41
2:E:82:LEU:HA	2:E:356:LEU:HD23	2.01	0.41
2:G:64:MET:HG3	2:G:103:TYR:CD2	2.55	0.41
2:G:145:ILE:HD12	2:G:308:TYR:CE1	2.55	0.41
2:G:272:SER:OG	2:G:272:SER:O	2.38	0.41
2:H:352:LEU:HD11	2:H:407:ILE:HG21	2.02	0.41
2:I:14:GLU:OE1	2:I:132:LEU:N	2.40	0.41
2:I:239:VAL:HG13	2:I:289:PHE:CA	2.51	0.41
2:J:271:PHE:CZ	2:J:293:ILE:HD13	2.56	0.41
2:P:208:GLN:HG2	2:P:279:ASN:OD1	2.20	0.41
2:P:2:SER:HB3	2:P:5:MET:CE	2.51	0.41
2:Q:326:SER:HA	2:Q:329:LEU:HD12	2.03	0.41
2:Q:3:ARG:HG3	2:Q:4:GLN:N	2.36	0.41
2:R:201:ALA:HA	2:R:287:THR:HA	2.03	0.41
2:R:48:VAL:HB	2:R:49:SER:H	1.68	0.41
2:T:272:SER:C	2:T:274:GLY:H	2.24	0.41
2:T:1:MET:HB3	2:T:2:SER:H	1.58	0.41
1:A:659:VAL:HG23	1:A:659:VAL:H	1.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:VAL:HG13	2:D:405:TRP:NE1	2.36	0.40
2:E:120:ASN:C	2:E:122:LEU:N	2.73	0.40
2:G:254:VAL:HG12	2:G:256:THR:H	1.86	0.40
2:I:131:LYS:NZ	2:J:26:ASP:OD1	2.52	0.40
2:J:408:THR:O	2:J:411:ILE:HB	2.20	0.40
2:P:2:SER:HB3	2:P:5:MET:HE2	2.04	0.40
2:R:387:LEU:HG	2:R:401:VAL:HG21	2.03	0.40
1:A:679:TYR:HD1	1:A:703:ILE:HD11	1.85	0.40
1:A:706:ILE:O	1:A:709:VAL:N	2.50	0.40
1:B:326:ASP:O	1:B:330:VAL:HG23	2.21	0.40
1:B:718:ARG:HG2	1:B:718:ARG:NH1	2.36	0.40
2:C:379:PHE:CE1	2:C:404:LEU:HD22	2.56	0.40
2:C:48:VAL:HG21	2:C:105:ARG:NH2	2.37	0.40
2:D:121:ASN:CA	2:D:146:PRO:HA	2.52	0.40
2:E:396:ILE:O	2:E:400:ILE:HG12	2.20	0.40
2:G:271:PHE:CZ	2:G:293:ILE:HD13	2.56	0.40
2:H:316:THR:HG23	2:H:397:ARG:HH12	1.87	0.40
2:I:158:ARG:HA	2:I:158:ARG:HD3	1.88	0.40
2:I:254:VAL:HG11	2:I:272:SER:O	2.20	0.40
2:P:167:ILE:HB	2:P:168:PRO:HD3	2.03	0.40
2:P:4:GLN:O	2:P:7:LEU:N	2.54	0.40
2:Q:188:GLU:HA	2:Q:232:PHE:CE1	2.56	0.40
2:Q:254:VAL:CG1	2:Q:255:PRO:HD2	2.50	0.40
2:Q:418:TYR:CZ	2:Q:420:PRO:HG3	2.56	0.40
2:R:353:THR:HG23	2:R:404:LEU:HD11	2.04	0.40
1:A:60:LEU:CD2	1:A:60:LEU:N	2.82	0.40
1:B:489:LEU:CD1	1:B:514:PRO:HB3	2.50	0.40
1:B:555:LEU:N	1:B:555:LEU:HD12	2.36	0.40
2:C:121:ASN:HA	2:C:146:PRO:HB3	2.03	0.40
2:C:182:GLN:HB3	2:C:183:PRO:HD2	2.03	0.40
2:C:309:THR:O	2:C:309:THR:CG2	2.67	0.40
2:C:323:PHE:HD1	2:C:405:TRP:CD1	2.39	0.40
2:C:363:PRO:HA	2:C:364:PRO:HD3	1.85	0.40
2:D:322:ASP:O	2:D:325:VAL:HG22	2.20	0.40
2:D:344:ILE:N	2:D:344:ILE:HD12	2.27	0.40
2:D:325:VAL:HG13	2:D:405:TRP:CE2	2.57	0.40
2:J:105:ARG:O	2:J:107:ARG:HG2	2.21	0.40
2:P:26:ASP:OD1	2:D:131:LYS:NZ	2.54	0.40
2:P:387:LEU:HG	2:P:401:VAL:HG21	2.03	0.40
2:Q:359:ASN:N	2:Q:359:ASN:ND2	2.68	0.40
2:R:341:GLN:O	2:R:342:TYR:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:157:PHE:HD1	2:S:214:TRP:CE2	2.39	0.40
2:T:9:THR:HG22	2:T:107:ARG:HE	1.86	0.40
1:B:108:ILE:HG12	1:B:109:GLU:N	2.37	0.40
1:B:364:MET:CE	1:B:541:ILE:HD12	2.50	0.40
1:B:6:ARG:CB	1:B:6:ARG:HH11	2.35	0.40
2:C:235:ILE:CD1	2:C:235:ILE:N	2.84	0.40
2:C:373:THR:O	2:C:373:THR:HG22	2.20	0.40
2:D:120:ASN:C	2:D:122:LEU:N	2.74	0.40
2:F:163:GLN:HE21	2:F:169:MET:HG3	1.86	0.40
2:G:87:PHE:HB2	2:G:403:HIS:ND1	2.36	0.40
2:H:121:ASN:HA	2:H:146:PRO:HA	2.04	0.40
2:H:132:LEU:HD23	2:H:132:LEU:HA	1.91	0.40
2:I:261:LEU:HA	2:I:262:PRO:HD2	1.85	0.40
2:I:194:PHE:CZ	2:I:291:VAL:HG11	2.56	0.40
2:I:358:THR:O	2:I:360:TYR:N	2.54	0.40
2:I:58:ARG:O	2:I:62:GLN:HB2	2.22	0.40
2:I:72:ILE:HA	2:I:72:ILE:HD12	1.86	0.40
2:J:418:TYR:CE1	2:J:420:PRO:HD3	2.57	0.40
2:P:197:ARG:HH11	2:P:197:ARG:HG3	1.86	0.40
2:P:244:THR:HG22	2:P:246:ALA:H	1.87	0.40
2:P:299:ILE:O	2:P:300:LEU:O	2.39	0.40
2:Q:396:ILE:N	2:Q:396:ILE:HD12	2.37	0.40
2:S:100:ILE:HG23	2:S:104:ILE:HB	2.03	0.40
2:T:282:LEU:HD11	2:T:289:PHE:CE2	2.57	0.40
1:B:263:LEU:O	1:B:264:ASP:C	2.60	0.40
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.84	0.40
1:B:575:PRO:HG2	1:B:576:ALA:H	1.86	0.40
2:D:186:VAL:HB	2:D:231:PHE:CZ	2.57	0.40
2:F:279:ASN:HA	2:F:279:ASN:HD22	1.51	0.40
2:F:310:LEU:HD21	2:F:320:ILE:HD11	2.03	0.40
2:I:140:MET:CE	2:I:406:VAL:HG11	2.50	0.40
2:Q:167:ILE:N	2:Q:168:PRO:CD	2.82	0.40
2:Q:17:SER:O	2:Q:18:GLU:C	2.58	0.40
2:R:64:MET:HG3	2:R:103:TYR:CE2	2.56	0.40
2:R:309:THR:O	2:R:309:THR:CG2	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	965/1019 (95%)	845 (88%)	105 (11%)	15 (2%)	9	43
1	B	1017/1019 (100%)	901 (89%)	97 (10%)	19 (2%)	8	40
2	C	411/421 (98%)	367 (89%)	38 (9%)	6 (2%)	10	45
2	D	413/421 (98%)	361 (87%)	46 (11%)	6 (2%)	10	45
2	E	419/421 (100%)	368 (88%)	41 (10%)	10 (2%)	6	35
2	F	411/421 (98%)	370 (90%)	34 (8%)	7 (2%)	9	42
2	G	413/421 (98%)	364 (88%)	43 (10%)	6 (2%)	10	45
2	H	419/421 (100%)	379 (90%)	34 (8%)	6 (1%)	11	46
2	I	415/421 (99%)	375 (90%)	34 (8%)	6 (1%)	11	46
2	J	409/421 (97%)	348 (85%)	47 (12%)	14 (3%)	3	28
2	P	410/421 (97%)	361 (88%)	40 (10%)	9 (2%)	6	37
2	Q	419/421 (100%)	365 (87%)	47 (11%)	7 (2%)	9	42
2	R	419/421 (100%)	376 (90%)	37 (9%)	6 (1%)	11	46
2	S	419/421 (100%)	366 (87%)	44 (10%)	9 (2%)	7	38
2	T	419/421 (100%)	369 (88%)	41 (10%)	9 (2%)	7	38
3	K	10/506 (2%)	8 (80%)	1 (10%)	1 (10%)	0	7
All	All	7388/8017 (92%)	6523 (88%)	729 (10%)	136 (2%)	8	41

All (136) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
1	A	451	GLY
1	A	546	GLY
1	B	24	SER
1	B	112	SER
1	B	379	LEU

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Mol	Chain	Res	Type
1	B	444	ILE
1	B	836	SER
1	B	931	GLY
1	B	934	ASN
2	P	364	PRO
2	P	379	PHE
2	P	416	ARG
2	C	364	PRO
2	C	379	PHE
2	D	47	SER
2	D	216	SER
2	Q	364	PRO
2	Q	379	PHE
2	Q	416	ARG
2	F	121	ASN
2	R	364	PRO
2	R	379	PHE
2	G	364	PRO
2	H	247	ASP
2	H	364	PRO
2	I	55	SER
2	J	98	ASP
2	T	95	VAL
3	K	297	ARG
1	A	215	ASN
1	A	335	SER
1	A	836	SER
1	A	1004	GLY
1	B	3	SER
1	B	10	GLY
1	B	20	THR
1	B	162	GLY
1	B	338	THR
1	B	612	ASN
1	B	662	PHE
2	P	300	LEU
2	C	340	GLY
2	D	364	PRO
2	D	376	TRP
2	D	379	PHE
2	E	162	GLY
2	E	364	PRO

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Mol	Chain	Res	Type
2	E	376	TRP
2	E	379	PHE
2	F	161	ALA
2	F	247	ASP
2	F	364	PRO
2	H	380	SER
2	S	2	SER
2	S	49	SER
2	S	364	PRO
2	I	364	PRO
2	J	57	PRO
2	J	359	ASN
2	J	364	PRO
2	J	416	ARG
2	T	364	PRO
2	T	416	ARG
1	A	493	ASP
1	A	931	GLY
1	B	499	ALA
1	B	653	GLN
2	P	121	ASN
2	C	121	ASN
2	Q	180	GLN
2	Q	203	PRO
2	E	330	THR
2	E	416	ARG
2	R	2	SER
2	R	51	ALA
2	R	201	ALA
2	G	161	ALA
2	G	201	ALA
2	H	86	TRP
2	H	330	THR
2	H	379	PHE
2	S	162	GLY
2	I	2	SER
2	I	359	ASN
2	I	416	ARG
2	J	180	GLN
2	T	29	SER
1	A	102	TYR
2	P	340	GLY

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Mol	Chain	Res	Type
2	P	420	PRO
2	C	420	PRO
2	D	201	ALA
2	F	2	SER
2	R	416	ARG
2	G	2	SER
2	S	330	THR
2	S	379	PHE
2	S	416	ARG
2	J	2	SER
2	T	359	ASN
1	A	378	THR
1	A	444	ILE
1	A	553	GLU
1	A	865	GLY
1	B	9	ASP
2	Q	376	TRP
2	E	2	SER
2	E	204	ALA
2	F	245	ALA
2	F	420	PRO
2	G	46	LEU
2	G	380	SER
2	S	50	SER
2	I	162	GLY
2	J	29	SER
2	J	212	PRO
2	J	247	ASP
2	J	367	PRO
2	J	379	PHE
1	B	824	GLN
2	P	2	SER
2	Q	330	THR
2	E	216	SER
2	S	359	ASN
2	T	300	LEU
1	B	148	VAL
2	E	203	PRO
2	T	162	GLY
2	T	420	PRO
2	P	162	GLY
2	J	203	PRO

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Mol	Chain	Res	Type
2	T	340	GLY
1	A	246	PRO
2	C	59	VAL
2	J	420	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	854/900 (95%)	793 (93%)	61 (7%)	14	46
1	B	900/900 (100%)	844 (94%)	56 (6%)	18	51
2	C	356/360 (99%)	338 (95%)	18 (5%)	24	57
2	D	358/360 (99%)	339 (95%)	19 (5%)	22	55
2	E	360/360 (100%)	340 (94%)	20 (6%)	21	54
2	F	356/360 (99%)	336 (94%)	20 (6%)	21	54
2	G	358/360 (99%)	337 (94%)	21 (6%)	19	53
2	H	360/360 (100%)	341 (95%)	19 (5%)	22	55
2	I	360/360 (100%)	333 (92%)	27 (8%)	13	43
2	J	354/360 (98%)	328 (93%)	26 (7%)	14	45
2	P	355/360 (99%)	335 (94%)	20 (6%)	21	54
2	Q	360/360 (100%)	334 (93%)	26 (7%)	14	45
2	R	360/360 (100%)	344 (96%)	16 (4%)	28	62
2	S	360/360 (100%)	334 (93%)	26 (7%)	14	45
2	T	360/360 (100%)	330 (92%)	30 (8%)	11	40
3	K	12/450 (3%)	10 (83%)	2 (17%)	2	12
All	All	6423/6930 (93%)	6016 (94%)	407 (6%)	18	51

All (407) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	84	ARG
1	A	85	ILE
1	A	87	ASP
1	A	108	ILE
1	A	124	ARG
1	A	147	PHE
1	A	184	ARG
1	A	192	ARG
1	A	241	ILE
1	A	259	ASN
1	A	269	LEU
1	A	278	THR
1	A	286	GLN
1	A	306	ARG
1	A	307	LEU
1	A	316	VAL
1	A	320	VAL
1	A	325	GLN
1	A	349	ASN
1	A	356	LEU
1	A	366	ASN
1	A	403	LEU
1	A	414	ARG
1	A	425	THR
1	A	452	ARG
1	A	460	ASN
1	A	478	ARG
1	A	483	GLN
1	A	526	THR
1	A	533	LEU
1	A	572	THR
1	A	588	LEU
1	A	590	ARG
1	A	593	ASP
1	A	629	GLU
1	A	674	LEU
1	A	688	ARG
1	A	694	PHE
1	A	718	ARG
1	A	722	THR
1	A	743	VAL
1	A	757	GLN

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Mol	Chain	Res	Type
1	A	759	ASP
1	A	766	THR
1	A	767	GLN
1	A	775	THR
1	A	792	THR
1	A	826	ARG
1	A	827	ARG
1	A	881	GLN
1	A	930	LEU
1	A	937	THR
1	A	940	MET
1	A	941	ARG
1	A	956	GLN
1	A	970	THR
1	A	983	VAL
1	A	988	ASP
1	A	994	ASP
1	A	1003	ILE
1	B	4	THR
1	B	6	ARG
1	B	12	SER
1	B	21	GLU
1	B	30	GLU
1	B	33	ASN
1	B	60	LEU
1	B	63	ILE
1	B	66	GLN
1	B	83	LEU
1	B	84	ARG
1	B	85	ILE
1	B	87	ASP
1	B	100	ASP
1	B	106	MET
1	B	124	ARG
1	B	134	CYS
1	B	163	ASP
1	B	165	ASN
1	B	169	LEU
1	B	177	HIS
1	B	204	ASP
1	B	206	LEU
1	B	262	ARG

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Mol	Chain	Res	Type
1	B	269	LEU
1	B	306	ARG
1	B	314	HIS
1	B	337	VAL
1	B	347	ARG
1	B	392	MET
1	B	438	ILE
1	B	455	LEU
1	B	460	ASN
1	B	478	ARG
1	B	496	SER
1	B	517	MET
1	B	536	ARG
1	B	543	THR
1	B	547	GLN
1	B	572	THR
1	B	621	VAL
1	B	623	ARG
1	B	653	GLN
1	B	676	ARG
1	B	680	ASP
1	B	681	THR
1	B	743	VAL
1	B	831	THR
1	B	842	ASN
1	B	854	ARG
1	B	859	ARG
1	B	881	GLN
1	B	938	LEU
1	B	939	ARG
1	B	943	GLU
1	B	1009	ARG
2	P	1	MET
2	P	24	ASN
2	P	27	THR
2	P	31	LEU
2	P	32	THR
2	P	33	THR
2	P	114	ASP
2	P	156	LEU
2	P	158	ARG
2	P	197	ARG

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Mol	Chain	Res	Type
2	P	221	THR
2	P	265	THR
2	P	279	ASN
2	P	281	GLU
2	P	287	THR
2	P	298	THR
2	P	325	VAL
2	P	352	LEU
2	P	390	GLN
2	P	419	ARG
2	C	8	ASP
2	C	24	ASN
2	C	27	THR
2	C	32	THR
2	C	105	ARG
2	C	114	ASP
2	C	144	ASP
2	C	156	LEU
2	C	158	ARG
2	C	197	ARG
2	C	221	THR
2	C	265	THR
2	C	287	THR
2	C	298	THR
2	C	325	VAL
2	C	352	LEU
2	C	361	MET
2	C	364	PRO
2	D	24	ASN
2	D	27	THR
2	D	32	THR
2	D	37	ASN
2	D	114	ASP
2	D	130	PRO
2	D	156	LEU
2	D	158	ARG
2	D	210	VAL
2	D	221	THR
2	D	247	ASP
2	D	265	THR
2	D	279	ASN
2	D	287	THR

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Mol	Chain	Res	Type
2	D	298	THR
2	D	314	THR
2	D	337	ARG
2	D	352	LEU
2	D	419	ARG
2	Q	24	ASN
2	Q	27	THR
2	Q	40	SER
2	Q	45	GLN
2	Q	62	GLN
2	Q	64	MET
2	Q	72	ILE
2	Q	94	THR
2	Q	144	ASP
2	Q	156	LEU
2	Q	164	THR
2	Q	185	PHE
2	Q	208	GLN
2	Q	247	ASP
2	Q	269	LEU
2	Q	287	THR
2	Q	298	THR
2	Q	325	VAL
2	Q	342	TYR
2	Q	354	ASN
2	Q	359	ASN
2	Q	373	THR
2	Q	392	VAL
2	Q	399	LEU
2	Q	410	LEU
2	Q	421	ASN
2	E	3	ARG
2	E	24	ASN
2	E	27	THR
2	E	56	ASP
2	E	98	ASP
2	E	114	ASP
2	E	158	ARG
2	E	197	ARG
2	E	247	ASP
2	E	253	THR
2	E	279	ASN

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Mol	Chain	Res	Type
2	E	289	PHE
2	E	303	ARG
2	E	314	THR
2	E	325	VAL
2	E	361	MET
2	E	370	LEU
2	E	391	ASN
2	E	395	ASN
2	E	419	ARG
2	F	24	ASN
2	F	31	LEU
2	F	33	THR
2	F	45	GLN
2	F	73	THR
2	F	114	ASP
2	F	144	ASP
2	F	185	PHE
2	F	197	ARG
2	F	229	ASN
2	F	265	THR
2	F	268	ARG
2	F	279	ASN
2	F	298	THR
2	F	315	GLN
2	F	316	THR
2	F	330	THR
2	F	335	GLN
2	F	337	ARG
2	F	359	ASN
2	R	10	SER
2	R	24	ASN
2	R	31	LEU
2	R	32	THR
2	R	114	ASP
2	R	144	ASP
2	R	156	LEU
2	R	221	THR
2	R	247	ASP
2	R	256	THR
2	R	265	THR
2	R	287	THR
2	R	298	THR

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Mol	Chain	Res	Type
2	R	352	LEU
2	R	361	MET
2	R	364	PRO
2	G	3	ARG
2	G	24	ASN
2	G	53	TYR
2	G	80	TYR
2	G	88	ASN
2	G	107	ARG
2	G	158	ARG
2	G	197	ARG
2	G	228	THR
2	G	264	GLN
2	G	273	LEU
2	G	279	ASN
2	G	282	LEU
2	G	303	ARG
2	G	315	GLN
2	G	334	SER
2	G	341	GLN
2	G	354	ASN
2	G	362	ASP
2	G	410	LEU
2	G	419	ARG
2	H	10	SER
2	H	24	ASN
2	H	45	GLN
2	H	49	SER
2	H	80	TYR
2	H	114	ASP
2	H	197	ARG
2	H	247	ASP
2	H	251	THR
2	H	265	THR
2	H	298	THR
2	H	305	GLN
2	H	309	THR
2	H	314	THR
2	H	315	GLN
2	H	331	THR
2	H	362	ASP
2	H	364	PRO

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Mol	Chain	Res	Type
2	H	392	VAL
2	S	31	LEU
2	S	72	ILE
2	S	80	TYR
2	S	105	ARG
2	S	107	ARG
2	S	114	ASP
2	S	160	VAL
2	S	182	GLN
2	S	197	ARG
2	S	208	GLN
2	S	221	THR
2	S	247	ASP
2	S	256	THR
2	S	265	THR
2	S	287	THR
2	S	298	THR
2	S	303	ARG
2	S	305	GLN
2	S	316	THR
2	S	325	VAL
2	S	334	SER
2	S	391	ASN
2	S	392	VAL
2	S	404	LEU
2	S	410	LEU
2	S	419	ARG
2	I	12	LEU
2	I	24	ASN
2	I	33	THR
2	I	40	SER
2	I	64	MET
2	I	77	ARG
2	I	100	ILE
2	I	107	ARG
2	I	114	ASP
2	I	144	ASP
2	I	148	SER
2	I	156	LEU
2	I	182	GLN
2	I	185	PHE
2	I	192	ILE

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Mol	Chain	Res	Type
2	I	197	ARG
2	I	242	THR
2	I	325	VAL
2	I	337	ARG
2	I	347	ASP
2	I	351	GLN
2	I	364	PRO
2	I	384	ARG
2	I	392	VAL
2	I	404	LEU
2	I	419	ARG
2	I	421	ASN
2	J	4	GLN
2	J	8	ASP
2	J	24	ASN
2	J	27	THR
2	J	33	THR
2	J	57	PRO
2	J	95	VAL
2	J	107	ARG
2	J	114	ASP
2	J	144	ASP
2	J	148	SER
2	J	151	ILE
2	J	156	LEU
2	J	158	ARG
2	J	184	PHE
2	J	185	PHE
2	J	197	ARG
2	J	208	GLN
2	J	220	VAL
2	J	229	ASN
2	J	247	ASP
2	J	261	LEU
2	J	265	THR
2	J	350	ASP
2	J	390	GLN
2	J	419	ARG
2	T	8	ASP
2	T	9	THR
2	T	24	ASN
2	T	27	THR

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Mol	Chain	Res	Type
2	T	42	MET
2	T	55	SER
2	T	64	MET
2	T	80	TYR
2	T	88	ASN
2	T	105	ARG
2	T	109	GLN
2	T	123	SER
2	T	158	ARG
2	T	185	PHE
2	T	192	ILE
2	T	197	ARG
2	T	210	VAL
2	T	242	THR
2	T	270	SER
2	T	298	THR
2	T	309	THR
2	T	312	SER
2	T	314	THR
2	T	315	GLN
2	T	325	VAL
2	T	334	SER
2	T	352	LEU
2	T	364	PRO
2	T	392	VAL
2	T	399	LEU
3	K	290	GLU
3	K	297	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (160) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	226	GLN
1	A	286	GLN
1	A	339	ASN
1	A	349	ASN
1	A	366	ASN
1	A	461	ASN
1	A	480	ASN
1	A	484	GLN
1	A	547	GLN

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Mol	Chain	Res	Type
1	A	573	GLN
1	A	584	ASN
1	A	651	GLN
1	A	653	GLN
1	A	673	GLN
1	A	695	HIS
1	A	757	GLN
1	A	767	GLN
1	A	783	ASN
1	A	810	HIS
1	A	830	ASN
1	A	1013	ASN
1	B	165	ASN
1	B	177	HIS
1	B	236	ASN
1	B	324	GLN
1	B	351	GLN
1	B	362	GLN
1	B	395	GLN
1	B	435	ASN
1	B	483	GLN
1	B	547	GLN
1	B	573	GLN
1	B	633	HIS
1	B	639	GLN
1	B	653	GLN
1	B	760	HIS
1	B	810	HIS
2	P	24	ASN
2	P	62	GLN
2	P	229	ASN
2	P	260	ASN
2	P	315	GLN
2	P	351	GLN
2	P	421	ASN
2	C	24	ASN
2	C	45	GLN
2	C	62	GLN
2	C	125	GLN
2	C	229	ASN
2	C	259	ASN
2	C	315	GLN

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Mol	Chain	Res	Type
2	C	335	GLN
2	C	351	GLN
2	C	359	ASN
2	D	4	GLN
2	D	24	ASN
2	D	45	GLN
2	D	62	GLN
2	D	229	ASN
2	D	351	GLN
2	Q	24	ASN
2	Q	125	GLN
2	Q	163	GLN
2	Q	180	GLN
2	Q	208	GLN
2	Q	279	ASN
2	Q	359	ASN
2	E	24	ASN
2	E	109	GLN
2	E	120	ASN
2	E	136	GLN
2	E	163	GLN
2	E	182	GLN
2	E	208	GLN
2	E	279	ASN
2	E	351	GLN
2	E	354	ASN
2	E	359	ASN
2	E	391	ASN
2	F	24	ASN
2	F	125	GLN
2	F	163	GLN
2	F	208	GLN
2	F	229	ASN
2	F	259	ASN
2	F	279	ASN
2	F	302	ASN
2	F	305	GLN
2	F	315	GLN
2	F	335	GLN
2	F	351	GLN
2	F	354	ASN
2	F	359	ASN

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Mol	Chain	Res	Type
2	R	41	ASN
2	R	62	GLN
2	R	163	GLN
2	R	315	GLN
2	R	395	ASN
2	G	4	GLN
2	G	24	ASN
2	G	37	ASN
2	G	41	ASN
2	G	66	ASN
2	G	109	GLN
2	G	118	GLN
2	G	120	ASN
2	G	163	GLN
2	G	180	GLN
2	G	264	GLN
2	G	315	GLN
2	G	341	GLN
2	G	421	ASN
2	H	24	ASN
2	H	37	ASN
2	H	41	ASN
2	H	45	GLN
2	H	118	GLN
2	H	121	ASN
2	H	136	GLN
2	H	259	ASN
2	H	305	GLN
2	H	315	GLN
2	H	421	ASN
2	S	24	ASN
2	S	109	GLN
2	S	120	ASN
2	S	208	GLN
2	S	259	ASN
2	S	279	ASN
2	S	305	GLN
2	S	351	GLN
2	S	354	ASN
2	S	395	ASN
2	S	421	ASN
2	I	24	ASN

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Mol	Chain	Res	Type
2	I	120	ASN
2	I	125	GLN
2	I	163	GLN
2	I	354	ASN
2	I	421	ASN
2	J	4	GLN
2	J	24	ASN
2	J	62	GLN
2	J	109	GLN
2	J	118	GLN
2	J	120	ASN
2	J	208	GLN
2	J	229	ASN
2	J	302	ASN
2	J	305	GLN
2	J	315	GLN
2	J	354	ASN
2	T	24	ASN
2	T	45	GLN
2	T	208	GLN
2	T	259	ASN
2	T	315	GLN
2	T	351	GLN
2	T	354	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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	967/1019 (94%)	-0.35	1 (0%) 95 95	1, 19, 50, 125	0
1	B	1019/1019 (100%)	-0.27	2 (0%) 95 93	1, 15, 49, 115	0
2	C	415/421 (98%)	-0.30	1 (0%) 95 93	44, 75, 99, 104	0
2	D	417/421 (99%)	-0.24	2 (0%) 91 88	18, 68, 106, 112	0
2	E	421/421 (100%)	-0.34	1 (0%) 95 93	3, 38, 71, 86	0
2	F	415/421 (98%)	-0.45	1 (0%) 95 93	6, 42, 76, 82	0
2	G	417/421 (99%)	-0.49	1 (0%) 95 93	1, 26, 59, 112	0
2	H	421/421 (100%)	-0.45	1 (0%) 95 93	1, 26, 59, 89	0
2	I	419/421 (99%)	-0.28	1 (0%) 95 93	12, 49, 82, 87	0
2	J	413/421 (98%)	-0.46	1 (0%) 95 93	18, 51, 77, 93	0
2	P	414/421 (98%)	0.07	3 (0%) 87 83	49, 93, 113, 118	0
2	Q	421/421 (100%)	-0.50	1 (0%) 95 93	11, 48, 76, 96	0
2	R	421/421 (100%)	-0.50	1 (0%) 95 93	1, 27, 58, 70	0
2	S	421/421 (100%)	-0.32	2 (0%) 91 88	6, 41, 72, 88	0
2	T	421/421 (100%)	-0.37	1 (0%) 95 93	1, 15, 44, 74	0
3	K	12/506 (2%)	0.63	1 (8%) 11 12	61, 67, 74, 80	0
All	All	7434/8017 (92%)	-0.34	21 (0%) 94 91	1, 35, 92, 125	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	1	MET	3.2
2	G	1	MET	3.2
2	T	1	MET	3.1
1	A	933	THR	3.0
2	D	1	MET	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	1	MET	2.8
2	C	1	MET	2.7
1	B	20	THR	2.7
2	I	1	MET	2.6
2	P	400	ILE	2.5
2	Q	1	MET	2.4
2	J	1	MET	2.4
2	R	1	MET	2.3
2	S	50	SER	2.2
2	H	1	MET	2.2
2	P	94	THR	2.2
2	D	225	VAL	2.1
3	K	289	SER	2.1
2	E	1	MET	2.0
2	S	1	MET	2.0
1	B	13	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.