Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:33 PM GMT

PDB ID	:	1U5T
Title	:	Structure of the ESCRT-II endosomal trafficking complex
Authors	:	Hierro, A.; Sun, J.; Rusnak, A.S.; Kim, J.; Prag, G.; Emr, S.D.; Hurley, J.H.
Deposited on	:	2004-07-28
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

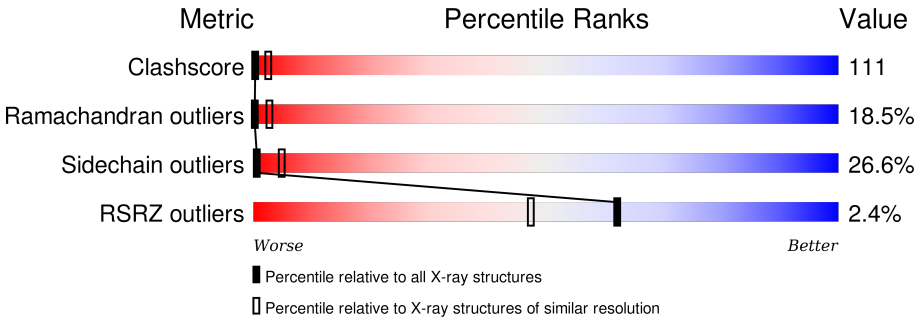
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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

Mol	Chain	Length	Quality of chain
1	A	233	3% 15% 50% 23% • 9%
2	B	169	% 17% 56% 21% 6%
3	C	202	3% 6% 45% 33% • 12%
3	D	202	2% 8% 42% 30% 8% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6055 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 appears to be functionally related to SNF7; Snf8p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1732	1108	290	323	11			

- Molecule 2 is a protein called Defective in vacuolar protein sorting; Vps36p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1377	879	222	267	9			

- Molecule 3 is a protein called Hypothetical 23.6 kDa protein in YUH1-URA8 intergenic region.

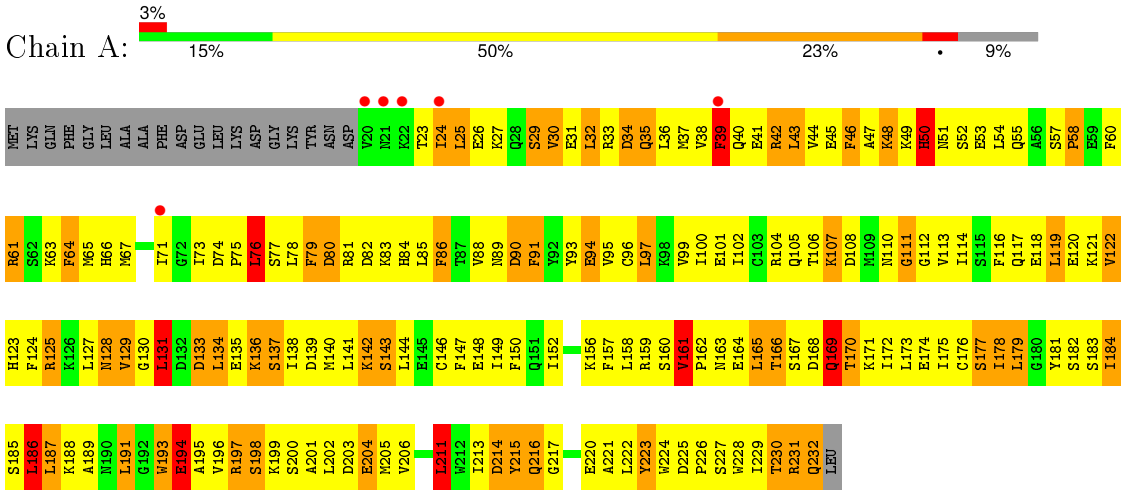
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	178	Total	C	N	O	S	0	0	0
			1473	939	247	279	8			
3	D	178	Total	C	N	O	S	0	0	0
			1473	939	247	279	8			

3 Residue-property plots (i)

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

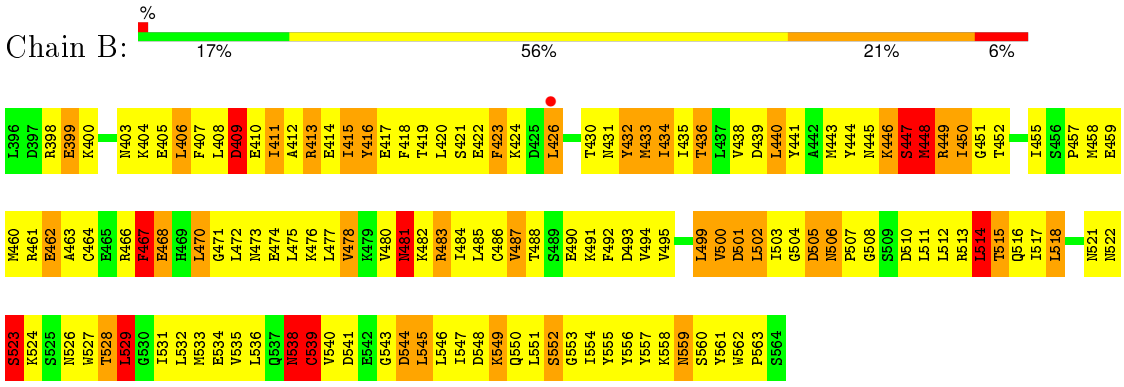
- Molecule 1: appears to be functionally related to SNF7; Snf8p

Chain A:



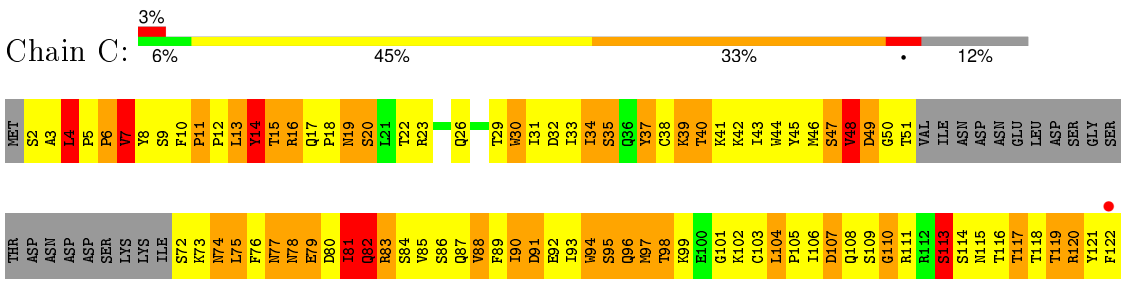
- Molecule 2: Defective in vacuolar protein sorting; Vps36p

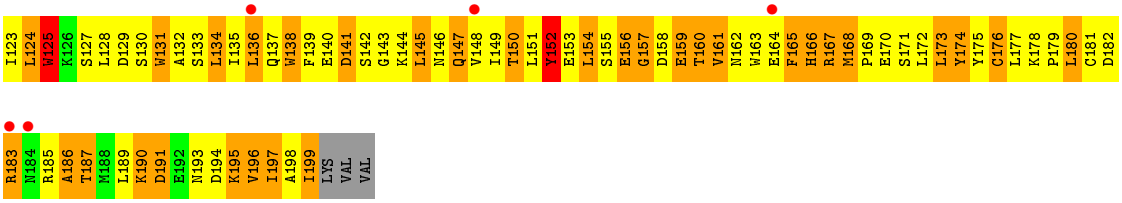
Chain B:



- Molecule 3: Hypothetical 23.6 kDa protein in YUH1-URA8 intergenic region

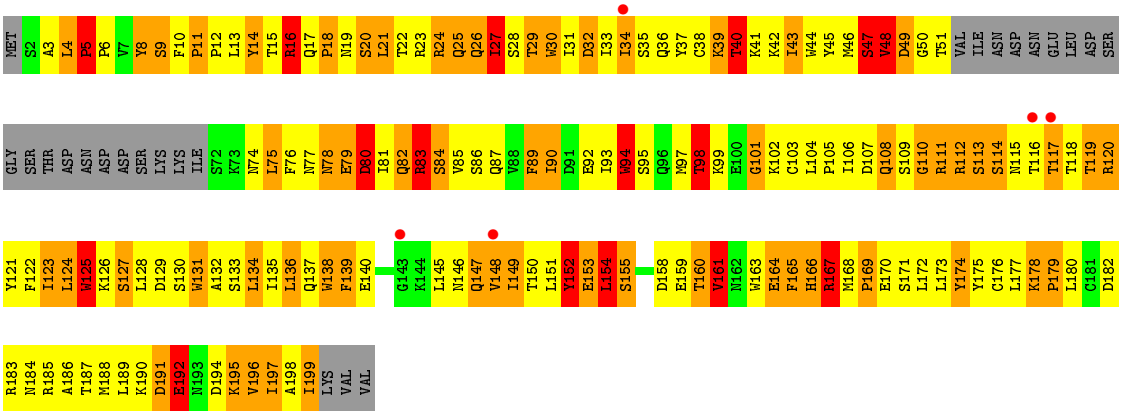
Chain C:





• Molecule 3: Hypothetical 23.6 kDa protein in YUH1-URA8 intergenic region

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	150.04Å 150.04Å 185.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.60 48.29 – 3.41	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-3.60) 86.3 (48.29-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 3.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.288 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	109.8	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 128.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 48297 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6055	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.72	1/1764 (0.1%)	1.05	6/2372 (0.3%)
2	B	0.80	1/1398 (0.1%)	1.15	7/1882 (0.4%)
3	C	0.71	0/1508	1.19	13/2045 (0.6%)
3	D	0.72	1/1508 (0.1%)	1.16	9/2045 (0.4%)
All	All	0.74	3/6178 (0.0%)	1.13	35/8344 (0.4%)

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
3	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	VAL	CA-CB	-5.99	1.42	1.54
3	D	192	GLU	CB-CG	-5.67	1.41	1.52
2	B	433	MET	SD-CE	5.65	2.09	1.77

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	84	SER	N-CA-C	7.83	132.14	111.00
3	C	49	ASP	N-CA-C	-7.55	90.63	111.00
3	D	48	VAL	N-CA-C	-7.37	91.10	111.00
3	C	197	ILE	N-CA-C	7.11	130.18	111.00
2	B	434	ILE	N-CA-C	-6.74	92.80	111.00
1	A	97	LEU	CA-CB-CG	-6.64	100.02	115.30
1	A	131	LEU	CA-CB-CG	-6.54	100.26	115.30
3	D	195	LYS	N-CA-C	6.47	128.46	111.00
2	B	481	ASN	N-CA-C	-6.34	93.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	191	ASP	CB-CG-OD1	5.80	123.52	118.30
2	B	524	LYS	N-CA-C	5.75	126.52	111.00
1	A	129	VAL	N-CA-C	-5.71	95.57	111.00
3	C	4	LEU	CA-CB-CG	5.69	128.39	115.30
3	C	125	TRP	N-CA-C	-5.69	95.64	111.00
3	C	186	ALA	N-CA-C	-5.68	95.67	111.00
3	C	183	ARG	N-CA-C	-5.62	95.82	111.00
1	A	211	LEU	CA-CB-CG	5.61	128.20	115.30
2	B	529	LEU	CA-CB-CG	-5.59	102.45	115.30
2	B	433	MET	CG-SD-CE	5.58	109.13	100.20
3	C	187	THR	N-CA-C	5.54	125.95	111.00
3	C	104	LEU	CA-CB-CG	-5.50	102.66	115.30
2	B	523	SER	CB-CA-C	-5.46	99.72	110.10
3	D	83	ARG	NE-CZ-NH1	-5.40	117.60	120.30
3	C	7	VAL	CB-CA-C	-5.38	101.17	111.40
3	C	50	GLY	N-CA-C	-5.36	99.71	113.10
3	D	80	ASP	C-N-CA	-5.30	108.45	121.70
3	C	113	SER	N-CA-C	-5.26	96.80	111.00
1	A	134	LEU	CA-CB-CG	5.21	127.28	115.30
3	C	79	GLU	N-CA-C	-5.20	96.96	111.00
1	A	165	LEU	N-CA-C	-5.16	97.07	111.00
2	B	426	LEU	CA-CB-CG	5.14	127.12	115.30
3	D	5	PRO	C-N-CA	-5.10	100.60	122.00
3	C	147	GLN	N-CA-C	5.08	124.72	111.00
3	D	197	ILE	N-CA-C	5.08	124.71	111.00
3	D	160	THR	N-CA-C	-5.05	97.35	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	165	PHE	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	1732	0	1741	369	0
2	B	1377	0	1388	282	0
3	C	1473	0	1449	351	0
3	D	1473	0	1449	386	0
All	All	6055	0	6027	1338	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 111.

All (1338) 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:B:433:MET:CE	2:B:433:MET:SD	2.09	1.40
3:C:76:PHE:HB3	3:C:85:VAL:CG1	1.79	1.12
2:B:415:ILE:HD12	2:B:460:MET:HE3	1.24	1.12
3:D:123:ILE:HG22	3:D:124:LEU:H	1.00	1.12
3:C:120:ARG:HH12	3:C:172:LEU:HD21	1.18	1.09
3:C:195:LYS:O	3:C:196:VAL:HG13	1.49	1.09
1:A:172:ILE:H	1:A:172:ILE:HD12	1.14	1.09
1:A:45:GLU:HA	1:A:48:LYS:HB2	1.23	1.09
3:C:150:THR:HA	3:C:196:VAL:HB	1.34	1.08
2:B:416:TYR:CE1	2:B:472:LEU:HB3	1.88	1.08
1:A:181:TYR:CD1	1:A:222:LEU:HD12	1.87	1.08
2:B:416:TYR:CD1	2:B:472:LEU:HB3	1.89	1.08
3:D:105:PRO:O	3:D:106:ILE:HG13	1.52	1.08
3:D:160:THR:HA	3:D:166:HIS:HB2	1.37	1.06
1:A:125:ARG:HA	1:A:125:ARG:HE	0.92	1.05
3:D:125:TRP:N	3:D:125:TRP:HE3	1.55	1.04
3:C:76:PHE:CD1	3:C:90:ILE:HG12	1.92	1.03
3:D:16:ARG:HD2	3:D:23:ARG:NH2	1.71	1.03
2:B:464:CYS:HA	2:B:467:PHE:HE1	1.21	1.03
3:D:166:HIS:HD2	3:D:167:ARG:HB2	1.17	1.03
3:D:74:ASN:O	3:D:78:ASN:HB3	1.59	1.02
3:D:104:LEU:O	3:D:121:TYR:HA	1.59	1.02
3:D:77:ASN:HA	3:D:84:SER:HB3	1.38	1.01
2:B:474:GLU:O	2:B:475:LEU:HD23	1.58	1.01
3:D:166:HIS:CD2	3:D:167:ARG:HB2	1.95	1.01
3:C:166:HIS:O	3:C:168:MET:N	1.94	1.00
3:C:197:ILE:HG22	3:C:198:ALA:N	1.75	1.00
2:B:503:ILE:HG12	2:B:514:LEU:HD21	1.42	1.00
3:D:24:ARG:O	3:D:26:GLN:N	1.94	0.99
1:A:125:ARG:HA	1:A:125:ARG:NE	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:ILE:HD12	2:B:534:GLU:HB3	1.43	0.99
3:D:189:LEU:HB2	3:D:196:VAL:HG13	1.44	0.99
3:D:125:TRP:N	3:D:125:TRP:CE3	2.31	0.98
3:D:151:LEU:HA	3:D:154:LEU:HD11	1.43	0.98
3:C:48:VAL:HG12	3:C:87:GLN:HE22	1.25	0.98
3:C:82:GLN:HE21	3:C:82:GLN:HA	1.25	0.98
1:A:112:GLY:HA3	1:A:161:VAL:HG22	1.43	0.98
3:D:46:MET:HG3	3:D:51:THR:HG22	1.45	0.97
1:A:122:VAL:HG12	1:A:123:HIS:N	1.79	0.97
3:C:82:GLN:HA	3:C:82:GLN:NE2	1.75	0.97
3:C:122:PHE:CG	3:C:172:LEU:HD22	1.98	0.97
3:D:123:ILE:HG22	3:D:124:LEU:N	1.79	0.96
1:A:211:LEU:HB3	1:A:224:TRP:O	1.64	0.96
2:B:416:TYR:HD1	2:B:472:LEU:HD13	1.30	0.96
2:B:407:PHE:O	2:B:411:ILE:HB	1.64	0.96
1:A:125:ARG:HE	1:A:125:ARG:CA	1.78	0.95
2:B:464:CYS:HA	2:B:467:PHE:CE1	2.01	0.95
3:D:188:MET:HB3	3:D:197:ILE:HG12	1.48	0.94
2:B:544:ASP:O	2:B:545:LEU:HD23	1.67	0.94
1:A:229:ILE:HD11	3:C:10:PHE:CG	2.02	0.94
3:C:45:TYR:HA	3:C:121:TYR:O	1.66	0.94
1:A:226:PRO:O	1:A:229:ILE:HB	1.68	0.94
3:C:152:TYR:HD2	3:C:152:TYR:O	1.50	0.94
2:B:434:ILE:HG23	2:B:531:ILE:HG12	1.47	0.94
2:B:485:LEU:HD12	2:B:486:CYS:N	1.83	0.94
3:C:106:ILE:HG22	3:C:107:ASP:H	1.32	0.93
3:D:30:TRP:HA	3:D:33:ILE:HD12	1.46	0.93
1:A:110:ASN:ND2	1:A:111:GLY:H	1.66	0.93
1:A:172:ILE:H	1:A:172:ILE:CD1	1.82	0.93
3:C:161:VAL:HG12	3:C:162:ASN:H	1.35	0.92
3:C:120:ARG:NH1	3:C:172:LEU:HD21	1.84	0.92
3:D:38:CYS:SG	3:D:123:ILE:HG12	2.09	0.92
3:D:74:ASN:HB3	3:D:78:ASN:H	1.31	0.92
1:A:181:TYR:HD1	1:A:222:LEU:HD12	1.26	0.91
2:B:450:ILE:HD13	2:B:450:ILE:H	1.30	0.91
2:B:546:LEU:HA	3:D:17:GLN:NE2	1.86	0.91
2:B:561:TYR:C	2:B:563:PRO:HD3	1.91	0.91
2:B:506:ASN:N	2:B:506:ASN:HD22	1.65	0.91
3:D:135:ILE:HG12	3:D:165:PHE:CE1	2.05	0.90
3:D:106:ILE:HB	3:D:120:ARG:CG	2.02	0.90
3:D:76:PHE:HB3	3:D:85:VAL:HG12	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:550:GLN:HE22	3:D:83:ARG:HG3	1.35	0.89
3:C:74:ASN:O	3:C:78:ASN:HB3	1.71	0.89
1:A:110:ASN:ND2	1:A:112:GLY:H	1.71	0.89
3:C:104:LEU:HB3	3:C:122:PHE:HB3	1.55	0.89
3:C:77:ASN:C	3:C:79:GLU:H	1.76	0.89
2:B:547:ILE:HD12	3:D:17:GLN:HE22	1.38	0.89
3:C:165:PHE:O	3:C:168:MET:HB3	1.72	0.88
3:D:149:ILE:HG22	3:D:153:GLU:HG3	1.56	0.88
3:D:77:ASN:HA	3:D:84:SER:CB	2.02	0.88
1:A:172:ILE:HD12	1:A:172:ILE:N	1.88	0.88
2:B:549:LYS:N	3:D:15:THR:HG21	1.89	0.88
3:C:136:LEU:HB2	3:C:180:LEU:HD21	1.56	0.88
2:B:450:ILE:CD1	2:B:450:ILE:H	1.86	0.88
3:C:76:PHE:HB3	3:C:85:VAL:HG11	1.53	0.88
3:C:34:ILE:HG21	3:C:97:MET:CE	2.03	0.88
1:A:50:HIS:HB3	1:A:53:GLU:HB2	1.54	0.87
3:C:110:GLY:HA3	3:C:175:TYR:CE1	2.10	0.86
2:B:484:ILE:CD1	2:B:534:GLU:HB3	2.05	0.86
3:D:123:ILE:CG2	3:D:124:LEU:H	1.87	0.86
3:D:16:ARG:HH11	3:D:16:ARG:HB3	1.38	0.86
3:D:76:PHE:HB3	3:D:85:VAL:CG1	2.05	0.86
1:A:205:MET:HB3	1:A:211:LEU:CD1	2.06	0.85
3:C:197:ILE:HG22	3:C:198:ALA:H	1.35	0.85
1:A:179:LEU:HD22	1:A:179:LEU:H	1.39	0.85
3:C:152:TYR:CD2	3:C:152:TYR:O	2.30	0.85
2:B:550:GLN:HE22	3:D:83:ARG:CG	1.90	0.84
3:D:107:ASP:HB3	3:D:116:THR:O	1.77	0.84
3:C:106:ILE:HB	3:C:120:ARG:HD2	1.59	0.84
2:B:470:LEU:HB2	2:B:472:LEU:HG	1.58	0.84
1:A:161:VAL:HB	1:A:162:PRO:HD2	1.59	0.84
3:D:29:THR:O	3:D:33:ILE:HG13	1.78	0.84
2:B:436:THR:HG22	2:B:531:ILE:HB	1.58	0.84
2:B:468:GLU:OE1	2:B:476:LYS:HD3	1.78	0.84
3:C:177:LEU:O	3:C:180:LEU:HB2	1.78	0.83
1:A:232:GLN:HG3	1:A:232:GLN:O	1.78	0.83
3:C:48:VAL:CG1	3:C:87:GLN:HE22	1.92	0.83
1:A:196:VAL:C	1:A:198:SER:H	1.82	0.83
3:C:148:VAL:HG23	3:C:198:ALA:HB2	1.60	0.82
3:D:85:VAL:HG22	3:D:86:SER:N	1.91	0.82
2:B:517:ILE:H	2:B:517:ILE:HD12	1.42	0.82
3:D:191:ASP:OD1	3:D:191:ASP:O	1.98	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:O	1:A:198:SER:N	2.11	0.82
3:D:98:THR:HG22	3:D:99:LYS:N	1.93	0.82
3:C:151:LEU:O	3:C:153:GLU:N	2.13	0.81
3:C:161:VAL:HB	3:C:163:TRP:HD1	1.43	0.81
2:B:502:LEU:HD21	2:B:518:LEU:HD21	1.62	0.81
3:C:197:ILE:CG2	3:C:198:ALA:H	1.92	0.81
1:A:110:ASN:ND2	1:A:113:VAL:H	1.78	0.81
2:B:439:ASP:C	2:B:441:TYR:H	1.83	0.81
1:A:175:ILE:O	1:A:178:ILE:HD11	1.80	0.81
3:D:178:LYS:O	3:D:178:LYS:HD3	1.81	0.81
1:A:137:SER:HA	1:A:140:MET:HG3	1.62	0.80
1:A:112:GLY:HA3	1:A:161:VAL:CG2	2.12	0.80
1:A:97:LEU:H	1:A:97:LEU:HD12	1.45	0.80
3:C:87:GLN:HA	3:C:90:ILE:HD12	1.64	0.80
3:D:30:TRP:CE3	3:D:33:ILE:HD12	2.17	0.80
1:A:78:LEU:O	1:A:80:ASP:N	2.14	0.80
3:D:165:PHE:H	3:D:165:PHE:HD2	1.28	0.79
3:C:98:THR:O	3:C:101:GLY:N	2.14	0.79
1:A:141:LEU:O	1:A:143:SER:N	2.15	0.79
3:C:148:VAL:HG21	3:C:189:LEU:HD11	1.65	0.79
2:B:399:GLU:O	2:B:400:LYS:HG3	1.83	0.79
2:B:420:LEU:HD11	2:B:475:LEU:HD21	1.64	0.79
1:A:113:VAL:HG11	1:A:165:LEU:HD11	1.65	0.79
2:B:549:LYS:H	3:D:15:THR:HG21	1.46	0.79
1:A:178:ILE:HB	1:A:179:LEU:HD13	1.64	0.79
3:C:30:TRP:CE3	3:C:33:ILE:HD12	2.17	0.79
3:D:107:ASP:OD1	3:D:117:THR:HG23	1.83	0.79
2:B:416:TYR:CE2	2:B:420:LEU:HD22	2.18	0.79
1:A:178:ILE:HD13	1:A:178:ILE:H	1.47	0.79
3:C:151:LEU:C	3:C:153:GLU:H	1.85	0.78
2:B:550:GLN:NE2	3:D:83:ARG:HG3	1.97	0.78
3:C:176:CYS:O	3:C:179:PRO:HD2	1.81	0.78
2:B:515:THR:HG22	2:B:516:GLN:N	1.97	0.78
1:A:229:ILE:HD11	3:C:10:PHE:CB	2.14	0.78
3:C:161:VAL:HB	3:C:163:TRP:CD1	2.18	0.78
1:A:131:LEU:HD23	1:A:135:GLU:HG3	1.66	0.78
3:C:14:TYR:H	3:C:14:TYR:HD1	1.30	0.78
2:B:419:THR:HG21	2:B:475:LEU:HD13	1.66	0.78
1:A:222:LEU:N	1:A:222:LEU:HD22	1.99	0.78
3:D:191:ASP:CG	3:D:191:ASP:O	2.21	0.78
3:C:160:THR:OG1	3:C:166:HIS:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:PHE:CD1	3:C:172:LEU:HD22	2.19	0.77
3:C:155:SER:O	3:C:157:GLY:N	2.17	0.77
2:B:480:VAL:HB	2:B:484:ILE:HB	1.66	0.77
1:A:161:VAL:CB	1:A:162:PRO:HD2	2.10	0.77
3:C:132:ALA:HB1	3:C:180:LEU:HG	1.67	0.77
2:B:467:PHE:HD1	2:B:467:PHE:H	1.30	0.77
2:B:476:LYS:O	2:B:487:VAL:HA	1.84	0.77
1:A:183:SER:OG	1:A:186:LEU:HB2	1.85	0.77
3:D:170:GLU:O	3:D:173:LEU:HB2	1.85	0.77
1:A:150:PHE:CZ	1:A:157:PHE:HD2	2.03	0.77
3:C:76:PHE:HD1	3:C:90:ILE:HG12	1.47	0.76
3:D:119:THR:O	3:D:119:THR:HG22	1.84	0.76
2:B:514:LEU:HD12	2:B:532:LEU:HD11	1.65	0.76
1:A:32:LEU:O	1:A:32:LEU:HD12	1.85	0.76
3:C:83:ARG:HH11	3:C:83:ARG:HG3	1.51	0.76
3:C:125:TRP:CE3	3:C:125:TRP:N	2.53	0.76
1:A:120:GLU:HG3	1:A:131:LEU:HD12	1.66	0.76
2:B:480:VAL:HG11	2:B:492:PHE:CG	2.21	0.76
3:C:2:SER:O	3:C:5:PRO:HD3	1.86	0.76
3:C:195:LYS:O	3:C:196:VAL:CG1	2.33	0.76
3:D:173:LEU:O	3:D:177:LEU:HD23	1.86	0.75
1:A:106:THR:O	1:A:108:ASP:N	2.18	0.75
2:B:450:ILE:N	2:B:450:ILE:HD13	2.01	0.75
3:D:86:SER:O	3:D:90:ILE:HD12	1.85	0.75
2:B:416:TYR:CE1	2:B:472:LEU:CB	2.67	0.75
3:D:105:PRO:C	3:D:106:ILE:HG13	2.07	0.75
2:B:513:ARG:HG3	2:B:517:ILE:HD11	1.68	0.75
3:D:102:LYS:O	3:D:124:LEU:HB2	1.85	0.75
3:C:152:TYR:HB2	3:C:170:GLU:OE2	1.86	0.75
3:D:78:ASN:O	3:D:80:ASP:N	2.19	0.75
1:A:95:VAL:HG12	1:A:137:SER:OG	1.87	0.75
3:D:150:THR:HA	3:D:196:VAL:HG23	1.69	0.75
1:A:152:ILE:HG13	1:A:173:LEU:HD22	1.69	0.74
3:C:38:CYS:HA	3:C:43:ILE:HB	1.69	0.74
2:B:547:ILE:H	3:D:17:GLN:HE22	1.34	0.74
1:A:112:GLY:CA	1:A:161:VAL:HG22	2.17	0.74
1:A:205:MET:HB3	1:A:211:LEU:HD11	1.67	0.74
2:B:423:PHE:HB3	2:B:526:ASN:HD21	1.52	0.74
3:C:34:ILE:HG21	3:C:97:MET:HE2	1.67	0.74
1:A:166:THR:H	1:A:169:GLN:HB2	1.50	0.74
1:A:116:PHE:CD1	1:A:156:LYS:HB2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASN:CG	1:A:111:GLY:H	1.90	0.74
2:B:419:THR:HG21	2:B:475:LEU:CD1	2.18	0.74
3:D:16:ARG:NH1	3:D:16:ARG:HB3	2.01	0.74
3:D:131:TRP:NE1	3:D:168:MET:HE2	2.03	0.74
2:B:491:LYS:HB2	2:B:494:VAL:HG22	1.69	0.74
2:B:416:TYR:HE1	2:B:472:LEU:HA	1.53	0.73
3:D:110:GLY:HA3	3:D:175:TYR:HE1	1.53	0.73
2:B:440:LEU:O	2:B:440:LEU:HG	1.88	0.73
3:C:125:TRP:N	3:C:125:TRP:HE3	1.86	0.73
3:C:127:SER:O	3:C:131:TRP:HB2	1.88	0.73
3:D:106:ILE:HG23	3:D:109:SER:C	2.08	0.73
1:A:221:ALA:C	1:A:222:LEU:HD22	2.08	0.73
2:B:480:VAL:HG11	2:B:492:PHE:CD2	2.24	0.73
3:C:19:ASN:C	3:C:19:ASN:HD22	1.91	0.73
1:A:110:ASN:HD21	1:A:112:GLY:H	1.37	0.73
3:D:188:MET:CB	3:D:197:ILE:HG12	2.17	0.73
3:D:189:LEU:HB2	3:D:196:VAL:CG1	2.19	0.73
3:C:166:HIS:C	3:C:168:MET:H	1.93	0.72
1:A:188:LYS:HA	1:A:193:TRP:O	1.88	0.72
3:C:37:TYR:CD2	3:C:75:LEU:HD21	2.24	0.72
3:C:39:LYS:O	3:C:41:LYS:N	2.22	0.72
3:C:155:SER:OG	3:C:156:GLU:N	2.21	0.72
3:D:45:TYR:HB3	3:D:122:PHE:CE2	2.25	0.72
3:D:188:MET:HG3	3:D:195:LYS:HE3	1.71	0.72
3:D:34:ILE:HG23	3:D:46:MET:CE	2.19	0.72
3:D:131:TRP:CE3	3:D:131:TRP:HA	2.24	0.72
3:D:34:ILE:HG23	3:D:46:MET:HE1	1.69	0.72
3:D:150:THR:CA	3:D:196:VAL:HG23	2.20	0.72
3:C:102:LYS:O	3:C:124:LEU:HG	1.89	0.72
2:B:411:ILE:HD11	2:B:455:ILE:HD13	1.70	0.72
2:B:485:LEU:HD12	2:B:486:CYS:H	1.51	0.72
3:C:177:LEU:CD1	3:C:180:LEU:HD12	2.20	0.71
2:B:423:PHE:CE1	2:B:424:LYS:HG2	2.25	0.71
3:C:160:THR:HG22	3:C:160:THR:O	1.90	0.71
1:A:166:THR:HB	1:A:168:ASP:H	1.56	0.71
3:C:9:SER:O	3:C:11:PRO:HD3	1.90	0.71
3:D:177:LEU:C	3:D:179:PRO:HD2	2.10	0.71
3:D:43:ILE:N	3:D:43:ILE:HD12	2.05	0.71
3:C:150:THR:HA	3:C:196:VAL:CB	2.17	0.71
3:D:43:ILE:HG22	3:D:44:TRP:N	2.04	0.71
3:C:76:PHE:HB3	3:C:85:VAL:HG12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:PHE:CE2	3:D:12:PRO:HG2	2.25	0.71
1:A:75:PRO:O	1:A:77:SER:N	2.24	0.71
1:A:137:SER:O	1:A:140:MET:HB2	1.90	0.71
3:D:163:TRP:HB3	3:D:165:PHE:HE2	1.55	0.71
1:A:102:ILE:HD13	1:A:123:HIS:CB	2.20	0.71
3:D:126:LYS:HB3	3:D:130:SER:HB2	1.71	0.71
2:B:518:LEU:HD12	2:B:527:TRP:CG	2.25	0.70
3:C:78:ASN:O	3:C:78:ASN:ND2	2.24	0.70
1:A:146:CYS:SG	1:A:147:PHE:CD2	2.82	0.70
1:A:37:MET:O	1:A:41:GLU:HG2	1.90	0.70
3:D:128:LEU:O	3:D:131:TRP:HB2	1.90	0.70
3:D:85:VAL:CG2	3:D:86:SER:N	2.54	0.70
1:A:211:LEU:HD12	1:A:211:LEU:N	2.06	0.70
3:D:138:TRP:CZ2	3:D:159:GLU:OE1	2.45	0.70
2:B:529:LEU:O	2:B:532:LEU:HB3	1.91	0.70
3:C:2:SER:C	3:C:4:LEU:H	1.93	0.70
3:C:76:PHE:HE1	3:C:90:ILE:HG23	1.57	0.70
1:A:179:LEU:HD13	1:A:179:LEU:N	2.06	0.70
2:B:483:ARG:HG3	2:B:483:ARG:HH11	1.56	0.70
3:C:16:ARG:HB2	3:C:89:PHE:CE1	2.27	0.70
3:D:161:VAL:C	3:D:163:TRP:H	1.93	0.70
2:B:513:ARG:O	2:B:515:THR:N	2.25	0.70
3:C:97:MET:HG3	3:C:103:CYS:SG	2.31	0.69
2:B:423:PHE:CB	2:B:526:ASN:HD21	2.05	0.69
3:D:27:ILE:HG22	3:D:28:SER:N	2.07	0.69
1:A:100:ILE:HD11	1:A:141:LEU:HD22	1.73	0.69
1:A:205:MET:HB3	1:A:211:LEU:HD13	1.74	0.69
2:B:546:LEU:HD12	3:D:10:PHE:CE2	2.27	0.69
3:D:28:SER:O	3:D:31:ILE:HB	1.92	0.69
3:D:165:PHE:N	3:D:165:PHE:HD2	1.89	0.69
3:D:136:LEU:HD11	3:D:180:LEU:HD11	1.74	0.69
2:B:416:TYR:HE1	2:B:472:LEU:CA	2.06	0.69
1:A:110:ASN:HD22	1:A:113:VAL:H	1.39	0.69
3:D:104:LEU:HD12	3:D:105:PRO:HD2	1.73	0.69
3:D:122:PHE:CD1	3:D:172:LEU:HD13	2.28	0.69
1:A:179:LEU:HD22	1:A:179:LEU:N	2.06	0.69
1:A:32:LEU:C	1:A:32:LEU:HD12	2.12	0.69
2:B:416:TYR:O	2:B:416:TYR:HD2	1.74	0.69
3:D:166:HIS:O	3:D:168:MET:N	2.25	0.69
3:C:120:ARG:HH12	3:C:172:LEU:CD2	2.01	0.69
3:C:128:LEU:C	3:C:130:SER:H	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:ILE:O	3:C:138:TRP:N	2.25	0.69
3:C:31:ILE:HG12	3:C:97:MET:HB2	1.75	0.68
3:D:136:LEU:HD11	3:D:180:LEU:CD1	2.22	0.68
2:B:513:ARG:HG3	2:B:517:ILE:CD1	2.23	0.68
3:C:85:VAL:HG13	3:C:90:ILE:HD11	1.73	0.68
3:D:139:PHE:CZ	3:D:199:ILE:HD12	2.28	0.68
1:A:79:PHE:CE1	1:A:88:VAL:HG11	2.28	0.68
2:B:415:ILE:HG21	2:B:460:MET:HE1	1.75	0.68
3:D:106:ILE:HB	3:D:120:ARG:HG3	1.75	0.68
3:D:48:VAL:O	3:D:49:ASP:C	2.32	0.68
1:A:146:CYS:SG	1:A:147:PHE:CE2	2.86	0.68
1:A:229:ILE:HD11	3:C:10:PHE:CD2	2.28	0.68
3:C:14:TYR:N	3:C:14:TYR:CD1	2.60	0.68
3:D:50:GLY:HA3	3:D:74:ASN:OD1	1.93	0.68
3:D:133:SER:O	3:D:137:GLN:HG2	1.94	0.68
3:C:106:ILE:CB	3:C:120:ARG:HD2	2.22	0.68
3:C:177:LEU:HD12	3:C:180:LEU:HD12	1.73	0.68
3:C:77:ASN:C	3:C:79:GLU:N	2.47	0.68
3:D:85:VAL:HG13	3:D:90:ILE:HD11	1.76	0.68
1:A:100:ILE:HD12	2:B:438:VAL:CG1	2.24	0.68
3:D:188:MET:HE2	3:D:195:LYS:HD2	1.76	0.68
2:B:502:LEU:CD2	2:B:518:LEU:HD21	2.24	0.68
3:C:138:TRP:HA	3:C:163:TRP:CH2	2.29	0.68
1:A:196:VAL:HG12	1:A:197:ARG:N	2.07	0.68
3:C:168:MET:HG2	3:C:173:LEU:HG	1.76	0.68
3:D:16:ARG:CD	3:D:23:ARG:NH2	2.54	0.68
1:A:175:ILE:C	1:A:178:ILE:HD11	2.14	0.68
1:A:53:GLU:O	1:A:57:SER:OG	2.12	0.67
3:D:131:TRP:HE3	3:D:131:TRP:HA	1.58	0.67
2:B:416:TYR:CD1	2:B:472:LEU:HD13	2.22	0.67
3:D:3:ALA:HB1	3:D:37:TYR:CD1	2.29	0.67
3:C:16:ARG:O	3:C:16:ARG:HG2	1.92	0.67
2:B:415:ILE:HD12	2:B:460:MET:CE	2.15	0.67
3:D:122:PHE:O	3:D:123:ILE:O	2.13	0.67
3:D:85:VAL:CG2	3:D:86:SER:H	2.08	0.67
3:D:31:ILE:C	3:D:33:ILE:H	1.98	0.67
3:C:174:TYR:CE1	3:C:178:LYS:HD2	2.29	0.67
2:B:399:GLU:HG3	2:B:407:PHE:CZ	2.29	0.67
1:A:124:PHE:CE2	1:A:134:LEU:HD23	2.29	0.67
1:A:34:ASP:O	1:A:38:VAL:HG23	1.95	0.67
3:C:37:TYR:HD2	3:C:75:LEU:HD21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:PHE:CE1	3:C:172:LEU:HD13	2.30	0.67
1:A:166:THR:HG22	1:A:167:SER:H	1.59	0.67
1:A:50:HIS:N	1:A:50:HIS:ND1	2.42	0.67
2:B:439:ASP:C	2:B:441:TYR:N	2.49	0.67
2:B:449:ARG:O	2:B:449:ARG:HG2	1.93	0.66
3:D:85:VAL:HG22	3:D:86:SER:H	1.58	0.66
3:D:139:PHE:N	3:D:139:PHE:CD2	2.61	0.66
1:A:104:ARG:O	1:A:106:THR:N	2.28	0.66
1:A:175:ILE:HD13	1:A:187:LEU:HD23	1.78	0.66
2:B:506:ASN:N	2:B:506:ASN:ND2	2.39	0.66
3:C:115:ASN:C	3:C:117:THR:H	1.99	0.66
2:B:510:ASP:OD2	2:B:511:LEU:N	2.27	0.66
3:C:17:GLN:NE2	3:C:18:PRO:HD2	2.09	0.66
3:D:8:TYR:CD2	3:D:8:TYR:O	2.49	0.66
3:C:177:LEU:O	3:C:180:LEU:N	2.26	0.66
2:B:547:ILE:HD12	2:B:547:ILE:H	1.59	0.66
3:D:16:ARG:HD2	3:D:23:ARG:HH21	1.59	0.66
3:D:106:ILE:HB	3:D:120:ARG:HD2	1.76	0.66
3:C:179:PRO:C	3:C:181:CYS:H	1.99	0.66
3:C:109:SER:O	3:C:111:ARG:N	2.26	0.66
2:B:411:ILE:CD1	2:B:455:ILE:HD13	2.26	0.66
1:A:100:ILE:HD12	2:B:438:VAL:HG13	1.75	0.66
1:A:48:LYS:HD2	1:A:82:ASP:OD2	1.96	0.66
3:D:31:ILE:HG22	3:D:32:ASP:N	2.10	0.66
3:D:3:ALA:C	3:D:5:PRO:HD3	2.16	0.66
1:A:216:GLN:HE21	3:C:84:SER:H	1.43	0.65
3:D:48:VAL:HA	3:D:94:TRP:HE1	1.60	0.65
3:C:82:GLN:CA	3:C:82:GLN:HE21	2.05	0.65
2:B:423:PHE:HB3	2:B:526:ASN:ND2	2.11	0.65
3:C:177:LEU:HG	3:C:197:ILE:HD12	1.77	0.65
2:B:408:LEU:O	2:B:409:ASP:C	2.34	0.65
3:D:106:ILE:HB	3:D:120:ARG:CD	2.25	0.65
1:A:122:VAL:CG1	1:A:123:HIS:N	2.53	0.65
2:B:433:MET:HG3	2:B:526:ASN:HB3	1.78	0.65
2:B:515:THR:CG2	2:B:516:GLN:N	2.59	0.65
3:C:198:ALA:C	3:C:199:ILE:HD13	2.16	0.65
1:A:31:GLU:O	1:A:34:ASP:HB2	1.96	0.65
1:A:50:HIS:HA	1:A:53:GLU:OE1	1.97	0.65
3:D:151:LEU:O	3:D:153:GLU:N	2.29	0.65
1:A:75:PRO:HG2	1:A:76:LEU:H	1.62	0.65
2:B:547:ILE:N	2:B:547:ILE:HD12	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:C	1:A:179:LEU:HD13	2.16	0.65
3:C:128:LEU:O	3:C:130:SER:N	2.30	0.65
2:B:415:ILE:CD1	2:B:460:MET:HE3	2.15	0.65
3:D:45:TYR:HB3	3:D:122:PHE:CD2	2.32	0.65
1:A:46:PHE:HD1	1:A:46:PHE:O	1.80	0.65
2:B:562:TRP:N	2:B:563:PRO:HD3	2.12	0.65
3:C:43:ILE:HD13	3:C:51:THR:HG21	1.79	0.65
3:D:98:THR:HG22	3:D:99:LYS:H	1.61	0.65
2:B:439:ASP:O	2:B:441:TYR:N	2.28	0.65
3:D:19:ASN:O	3:D:20:SER:C	2.35	0.65
2:B:422:GLU:O	2:B:423:PHE:HB3	1.95	0.65
3:C:48:VAL:HG12	3:C:87:GLN:NE2	2.07	0.64
3:D:151:LEU:HB2	3:D:170:GLU:OE2	1.98	0.64
3:C:132:ALA:O	3:C:134:LEU:N	2.30	0.64
3:C:138:TRP:O	3:C:138:TRP:CE3	2.50	0.64
3:C:19:ASN:ND2	3:C:19:ASN:C	2.50	0.64
3:D:165:PHE:N	3:D:165:PHE:CD2	2.62	0.64
3:C:135:ILE:HD13	3:C:165:PHE:CZ	2.32	0.64
3:D:128:LEU:HD12	3:D:129:ASP:N	2.13	0.64
1:A:222:LEU:N	1:A:222:LEU:CD2	2.61	0.64
3:C:45:TYR:CA	3:C:121:TYR:O	2.45	0.63
3:D:166:HIS:CD2	3:D:166:HIS:C	2.70	0.63
2:B:506:ASN:H	2:B:506:ASN:HD22	1.45	0.63
3:C:153:GLU:C	3:C:155:SER:H	2.02	0.63
1:A:216:GLN:O	3:C:83:ARG:CZ	2.47	0.63
3:D:74:ASN:N	3:D:78:ASN:HB2	2.13	0.63
1:A:141:LEU:C	1:A:143:SER:N	2.49	0.63
2:B:503:ILE:CG1	2:B:514:LEU:HD21	2.23	0.63
1:A:178:ILE:HB	1:A:179:LEU:CD1	2.28	0.63
1:A:27:LYS:O	1:A:30:VAL:HG22	1.97	0.63
1:A:146:CYS:CB	2:B:438:VAL:HG21	2.28	0.63
1:A:53:GLU:O	1:A:60:PHE:HD2	1.80	0.63
3:C:138:TRP:HE3	3:C:138:TRP:C	2.01	0.63
3:C:14:TYR:N	3:C:14:TYR:HD1	1.97	0.63
1:A:61:ARG:NH2	1:A:91:PHE:CZ	2.66	0.63
1:A:79:PHE:HD2	1:A:85:LEU:HD13	1.64	0.63
1:A:110:ASN:ND2	1:A:111:GLY:N	2.43	0.63
3:C:135:ILE:O	3:C:138:TRP:CB	2.46	0.63
3:C:122:PHE:CZ	3:C:172:LEU:HB3	2.34	0.63
3:D:30:TRP:HB3	3:D:93:ILE:HD13	1.81	0.62
1:A:93:TYR:N	1:A:93:TYR:CD2	2.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:149:ILE:C	3:D:196:VAL:HG23	2.20	0.62
1:A:76:LEU:HG	1:A:89:ASN:ND2	2.14	0.62
3:D:110:GLY:HA3	3:D:175:TYR:CE1	2.34	0.62
1:A:224:TRP:CH2	3:C:11:PRO:HG2	2.34	0.62
1:A:46:PHE:O	1:A:46:PHE:CD1	2.51	0.62
3:D:30:TRP:HA	3:D:33:ILE:CD1	2.26	0.62
3:D:90:ILE:O	3:D:93:ILE:N	2.33	0.62
1:A:77:SER:O	1:A:78:LEU:C	2.37	0.62
2:B:398:ARG:O	2:B:400:LYS:N	2.32	0.62
3:D:34:ILE:HD11	3:D:76:PHE:CZ	2.34	0.62
3:D:94:TRP:CZ3	3:D:97:MET:CE	2.83	0.62
3:D:16:ARG:HG3	3:D:23:ARG:HH21	1.64	0.62
3:C:159:GLU:HA	3:C:159:GLU:OE1	2.00	0.62
3:C:77:ASN:HB2	3:C:84:SER:OG	2.00	0.62
3:D:114:SER:HA	3:D:118:THR:HG21	1.81	0.62
1:A:229:ILE:HD11	3:C:10:PHE:HB2	1.81	0.62
3:C:190:LYS:HB3	3:C:190:LYS:NZ	2.15	0.62
3:C:187:THR:C	3:C:197:ILE:HG23	2.19	0.62
3:D:94:TRP:HZ3	3:D:97:MET:CE	2.12	0.62
1:A:43:LEU:HD12	1:A:64:PHE:HE1	1.64	0.62
1:A:49:LYS:HB3	1:A:50:HIS:ND1	2.15	0.62
1:A:23:THR:O	1:A:27:LYS:HG3	2.00	0.62
1:A:64:PHE:CG	1:A:64:PHE:O	2.52	0.61
3:D:126:LYS:HB3	3:D:130:SER:CB	2.28	0.61
3:D:98:THR:CG2	3:D:99:LYS:N	2.62	0.61
3:C:138:TRP:CE3	3:C:138:TRP:C	2.73	0.61
2:B:416:TYR:HD1	2:B:472:LEU:CD1	2.07	0.61
2:B:448:MET:O	2:B:449:ARG:HB2	2.00	0.61
2:B:539:CYS:HA	2:B:544:ASP:HB2	1.82	0.61
1:A:162:PRO:HA	2:B:483:ARG:CZ	2.30	0.61
3:C:34:ILE:HG21	3:C:97:MET:HE1	1.80	0.61
3:D:123:ILE:O	3:D:124:LEU:HG	1.99	0.61
3:C:43:ILE:O	3:C:125:TRP:HH2	1.82	0.61
2:B:416:TYR:CD2	2:B:416:TYR:O	2.53	0.61
3:D:194:ASP:O	3:D:195:LYS:HG2	2.01	0.61
3:C:111:ARG:HH11	3:C:111:ARG:HG3	1.65	0.61
3:C:135:ILE:HD13	3:C:165:PHE:CE1	2.36	0.61
3:C:134:LEU:HD13	3:C:163:TRP:CE3	2.36	0.61
3:D:106:ILE:HG22	3:D:107:ASP:N	2.14	0.61
3:C:114:SER:HA	3:C:118:THR:HG23	1.83	0.61
1:A:215:TYR:HD1	1:A:215:TYR:N	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLN:C	1:A:42:ARG:N	2.50	0.61
2:B:436:THR:HG22	2:B:531:ILE:CB	2.29	0.61
3:C:191:ASP:C	3:C:193:ASN:H	2.03	0.61
3:C:98:THR:CG2	3:C:99:LYS:N	2.64	0.61
3:D:89:PHE:O	3:D:90:ILE:C	2.38	0.61
3:D:138:TRP:HA	3:D:138:TRP:CE3	2.36	0.61
2:B:409:ASP:O	2:B:412:ALA:HB3	2.01	0.61
2:B:418:PHE:CD2	2:B:444:TYR:HA	2.36	0.61
3:C:173:LEU:O	3:C:177:LEU:CD2	2.49	0.60
3:C:34:ILE:HD11	3:C:76:PHE:CZ	2.36	0.60
3:C:76:PHE:CE1	3:C:90:ILE:HG23	2.36	0.60
3:D:27:ILE:CG2	3:D:28:SER:N	2.64	0.60
3:D:148:VAL:HG12	3:D:148:VAL:O	2.01	0.60
3:C:150:THR:HG23	3:C:153:GLU:CG	2.32	0.60
1:A:178:ILE:H	1:A:178:ILE:CD1	2.05	0.60
3:D:138:TRP:HA	3:D:138:TRP:HE3	1.66	0.60
2:B:538:ASN:O	2:B:541:ASP:N	2.34	0.60
3:D:26:GLN:O	3:D:29:THR:N	2.34	0.60
3:D:43:ILE:N	3:D:43:ILE:CD1	2.64	0.60
3:D:4:LEU:C	3:D:5:PRO:O	2.39	0.60
3:D:10:PHE:CZ	3:D:12:PRO:HG3	2.37	0.60
2:B:438:VAL:O	2:B:438:VAL:HG12	2.01	0.60
1:A:65:MET:C	1:A:67:MET:H	2.05	0.60
1:A:227:SER:C	1:A:229:ILE:N	2.52	0.60
3:C:138:TRP:O	3:C:138:TRP:HE3	1.83	0.60
2:B:418:PHE:CE2	2:B:444:TYR:HA	2.37	0.60
3:D:123:ILE:HG22	3:D:125:TRP:CZ3	2.36	0.60
1:A:175:ILE:O	1:A:175:ILE:HG12	2.02	0.60
2:B:434:ILE:HG13	2:B:488:THR:OG1	2.02	0.60
3:C:34:ILE:HG22	3:C:35:SER:N	2.16	0.60
2:B:513:ARG:O	2:B:514:LEU:C	2.39	0.60
3:C:122:PHE:CE2	3:C:172:LEU:HB3	2.36	0.60
3:C:150:THR:HB	3:C:196:VAL:HG11	1.83	0.60
3:D:16:ARG:HD2	3:D:23:ARG:HH22	1.61	0.60
1:A:215:TYR:CD1	1:A:215:TYR:N	2.69	0.59
3:D:118:THR:O	3:D:119:THR:OG1	2.20	0.59
3:C:169:PRO:HD2	3:C:172:LEU:HD12	1.84	0.59
3:C:173:LEU:O	3:C:177:LEU:HD22	2.02	0.59
3:D:123:ILE:CG2	3:D:124:LEU:N	2.52	0.59
3:D:186:ALA:HB1	3:D:199:ILE:HA	1.84	0.59
3:D:122:PHE:CG	3:D:172:LEU:HD13	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HD13	1:A:178:ILE:N	2.16	0.59
1:A:63:LYS:HG3	1:A:64:PHE:N	2.17	0.59
1:A:23:THR:HA	1:A:26:GLU:HG2	1.84	0.59
2:B:408:LEU:O	2:B:411:ILE:N	2.36	0.59
1:A:171:LYS:HA	1:A:174:GLU:HB3	1.85	0.59
1:A:181:TYR:O	1:A:181:TYR:CD1	2.55	0.59
3:D:135:ILE:HG12	3:D:165:PHE:HE1	1.64	0.59
3:C:177:LEU:HD12	3:C:180:LEU:CD1	2.32	0.59
3:C:19:ASN:O	3:C:22:THR:N	2.35	0.59
3:C:145:LEU:HB2	3:C:199:ILE:HB	1.83	0.59
2:B:420:LEU:CD1	2:B:475:LEU:HD21	2.30	0.59
3:D:74:ASN:HB3	3:D:78:ASN:N	2.09	0.59
3:D:30:TRP:CD1	3:D:93:ILE:HD11	2.37	0.59
1:A:141:LEU:C	1:A:143:SER:H	2.06	0.59
1:A:196:VAL:C	1:A:198:SER:N	2.47	0.59
3:C:128:LEU:C	3:C:130:SER:N	2.55	0.59
3:C:39:LYS:HG2	3:C:40:THR:H	1.67	0.59
3:C:143:GLY:O	3:C:145:LEU:N	2.28	0.59
1:A:161:VAL:CB	1:A:162:PRO:CD	2.81	0.59
3:C:89:PHE:O	3:C:90:ILE:C	2.40	0.59
1:A:146:CYS:SG	2:B:438:VAL:HG21	2.42	0.59
3:C:199:ILE:HD13	3:C:199:ILE:N	2.18	0.59
3:C:76:PHE:O	3:C:85:VAL:HG12	2.02	0.59
2:B:416:TYR:HE2	2:B:420:LEU:HD22	1.64	0.59
3:D:90:ILE:HG22	3:D:94:TRP:CD1	2.38	0.59
3:C:132:ALA:O	3:C:135:ILE:N	2.36	0.58
3:D:136:LEU:CD1	3:D:136:LEU:N	2.66	0.58
3:C:139:PHE:O	3:C:143:GLY:N	2.36	0.58
2:B:432:TYR:O	2:B:432:TYR:HD1	1.87	0.58
2:B:546:LEU:HA	3:D:17:GLN:HE22	1.63	0.58
3:D:87:GLN:HA	3:D:90:ILE:HD13	1.84	0.58
1:A:125:ARG:HH21	1:A:128:ASN:HA	1.69	0.58
1:A:229:ILE:CD1	3:C:10:PHE:CG	2.83	0.58
3:C:187:THR:O	3:C:197:ILE:HG23	2.02	0.58
3:C:19:ASN:HD22	3:C:22:THR:H	1.49	0.58
3:D:104:LEU:CD1	3:D:105:PRO:HD2	2.32	0.58
3:D:138:TRP:HB3	3:D:139:PHE:CE2	2.39	0.58
3:D:43:ILE:CG2	3:D:44:TRP:N	2.66	0.58
1:A:152:ILE:CG2	1:A:174:GLU:HA	2.34	0.58
1:A:114:ILE:HG22	1:A:158:LEU:O	2.04	0.58
1:A:169:GLN:CG	1:A:205:MET:HG3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:194:ASP:O	3:D:195:LYS:NZ	2.27	0.58
1:A:232:GLN:CG	1:A:232:GLN:O	2.51	0.58
2:B:547:ILE:HD12	3:D:17:GLN:NE2	2.15	0.58
1:A:223:TYR:CD2	1:A:223:TYR:N	2.72	0.58
3:D:138:TRP:HB3	3:D:139:PHE:CD2	2.39	0.58
3:C:43:ILE:HG22	3:C:44:TRP:N	2.18	0.58
2:B:408:LEU:HA	2:B:411:ILE:HG22	1.84	0.58
3:D:74:ASN:H	3:D:78:ASN:HB2	1.69	0.58
1:A:114:ILE:O	1:A:157:PHE:HA	2.04	0.58
1:A:150:PHE:CZ	1:A:157:PHE:CD2	2.89	0.58
2:B:480:VAL:HG11	2:B:492:PHE:CD1	2.39	0.58
3:C:135:ILE:HA	3:C:165:PHE:CZ	2.38	0.58
3:C:154:LEU:HD11	3:C:173:LEU:HD13	1.86	0.58
3:D:147:GLN:O	3:D:148:VAL:HG23	2.04	0.58
1:A:174:GLU:O	1:A:177:SER:OG	2.17	0.58
1:A:45:GLU:O	1:A:48:LYS:N	2.37	0.58
3:C:38:CYS:SG	3:C:123:ILE:HD12	2.44	0.58
1:A:159:ARG:HD2	1:A:163:ASN:O	2.03	0.57
1:A:141:LEU:O	1:A:142:LYS:C	2.41	0.57
1:A:38:VAL:O	1:A:40:GLN:N	2.37	0.57
3:D:10:PHE:CD1	3:D:12:PRO:HD2	2.38	0.57
3:D:188:MET:CG	3:D:195:LYS:HE3	2.35	0.57
3:C:95:SER:O	3:C:98:THR:N	2.31	0.57
3:D:16:ARG:CG	3:D:23:ARG:HH21	2.17	0.57
3:C:138:TRP:HZ3	3:C:142:SER:HG	1.50	0.57
3:C:77:ASN:CB	3:C:84:SER:HB2	2.34	0.57
1:A:102:ILE:HD13	1:A:123:HIS:HB2	1.85	0.57
3:D:95:SER:O	3:D:98:THR:HB	2.04	0.57
3:C:137:GLN:HG2	3:C:137:GLN:O	2.05	0.57
3:C:153:GLU:C	3:C:155:SER:N	2.57	0.57
3:C:23:ARG:O	3:C:26:GLN:HB3	2.04	0.57
3:D:166:HIS:HD2	3:D:167:ARG:CB	2.06	0.57
2:B:435:ILE:O	2:B:486:CYS:HB2	2.05	0.57
3:D:113:SER:O	3:D:115:ASN:N	2.37	0.57
1:A:216:GLN:NE2	3:C:84:SER:H	2.01	0.57
3:D:10:PHE:CD2	3:D:12:PRO:HG2	2.39	0.57
3:D:150:THR:O	3:D:153:GLU:HB2	2.04	0.57
3:D:150:THR:HG22	3:D:153:GLU:HG2	1.85	0.57
3:D:151:LEU:O	3:D:154:LEU:HD12	2.05	0.57
3:D:139:PHE:HE1	3:D:199:ILE:HG21	1.68	0.57
2:B:547:ILE:CD1	3:D:17:GLN:HE22	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:30:TRP:CE3	3:D:30:TRP:HA	2.39	0.57
3:D:30:TRP:HE3	3:D:33:ILE:HD12	1.66	0.57
1:A:24:ILE:HG22	1:A:24:ILE:O	2.05	0.57
3:C:22:THR:O	3:C:23:ARG:C	2.42	0.57
1:A:141:LEU:O	1:A:144:LEU:N	2.38	0.57
3:D:135:ILE:HG12	3:D:165:PHE:CD1	2.39	0.57
3:C:161:VAL:HG12	3:C:162:ASN:N	2.13	0.57
3:C:172:LEU:O	3:C:175:TYR:N	2.38	0.57
1:A:95:VAL:CG2	1:A:129:VAL:HG11	2.34	0.57
1:A:124:PHE:HB3	1:A:129:VAL:HG22	1.86	0.57
1:A:161:VAL:HB	1:A:162:PRO:CD	2.34	0.56
1:A:223:TYR:HD2	1:A:223:TYR:N	2.02	0.56
1:A:42:ARG:O	1:A:45:GLU:HG2	2.05	0.56
3:D:191:ASP:O	3:D:192:GLU:HB2	2.05	0.56
3:C:197:ILE:CG2	3:C:198:ALA:N	2.45	0.56
3:C:10:PHE:C	3:C:12:PRO:HD2	2.25	0.56
1:A:213:ILE:HD11	1:A:223:TYR:CE2	2.40	0.56
1:A:162:PRO:HG2	1:A:163:ASN:H	1.69	0.56
2:B:517:ILE:N	2:B:517:ILE:HD12	2.15	0.56
3:D:146:ASN:O	3:D:147:GLN:O	2.23	0.56
1:A:65:MET:O	1:A:67:MET:N	2.38	0.56
3:C:148:VAL:CG2	3:C:189:LEU:HD11	2.34	0.56
1:A:170:THR:O	1:A:174:GLU:N	2.32	0.56
3:C:43:ILE:O	3:C:125:TRP:CH2	2.59	0.56
3:C:106:ILE:HG13	3:C:120:ARG:HH11	1.70	0.56
2:B:552:SER:HA	3:C:18:PRO:O	2.06	0.56
1:A:193:TRP:O	1:A:194:GLU:O	2.22	0.56
3:D:139:PHE:HZ	3:D:199:ILE:HD12	1.69	0.56
1:A:32:LEU:O	1:A:33:ARG:C	2.44	0.56
3:C:34:ILE:HD11	3:C:76:PHE:CE2	2.40	0.56
3:D:43:ILE:O	3:D:125:TRP:HH2	1.88	0.56
1:A:136:LYS:O	1:A:139:ASP:N	2.39	0.56
2:B:399:GLU:C	2:B:400:LYS:HG3	2.26	0.56
2:B:472:LEU:HD23	2:B:472:LEU:N	2.20	0.56
1:A:184:ILE:HG22	1:A:220:GLU:CD	2.26	0.56
3:D:187:THR:O	3:D:197:ILE:HG23	2.06	0.56
2:B:502:LEU:HD11	2:B:517:ILE:HG21	1.88	0.56
2:B:517:ILE:H	2:B:517:ILE:CD1	2.14	0.56
3:C:160:THR:O	3:C:160:THR:CG2	2.54	0.56
3:D:43:ILE:O	3:D:125:TRP:CH2	2.59	0.56
3:D:154:LEU:HD12	3:D:154:LEU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:166:HIS:C	3:D:168:MET:H	2.09	0.56
3:D:34:ILE:HD13	3:D:75:LEU:CD1	2.36	0.56
3:D:39:LYS:HA	3:D:125:TRP:NE1	2.21	0.56
1:A:101:GLU:O	1:A:102:ILE:C	2.44	0.56
1:A:205:MET:CE	1:A:211:LEU:HD11	2.36	0.56
2:B:491:LYS:HB2	2:B:494:VAL:CG2	2.36	0.56
3:C:77:ASN:HB2	3:C:84:SER:CB	2.37	0.55
2:B:449:ARG:HH12	2:B:452:THR:HG21	1.71	0.55
3:D:16:ARG:CD	3:D:23:ARG:HH21	2.17	0.55
1:A:169:GLN:HG2	1:A:205:MET:CG	2.37	0.55
3:D:129:ASP:C	3:D:131:TRP:N	2.59	0.55
3:D:160:THR:O	3:D:160:THR:HG22	2.05	0.55
2:B:538:ASN:O	2:B:539:CYS:C	2.43	0.55
1:A:227:SER:O	1:A:229:ILE:N	2.39	0.55
1:A:185:SER:O	1:A:187:LEU:N	2.40	0.55
3:D:105:PRO:HG2	3:D:112:ARG:HG2	1.87	0.55
3:D:10:PHE:CZ	3:D:12:PRO:CG	2.90	0.55
2:B:508:GLY:HA2	2:B:557:TYR:CE2	2.42	0.55
3:D:122:PHE:CB	3:D:172:LEU:HD13	2.37	0.55
1:A:119:LEU:HD13	1:A:134:LEU:HD21	1.87	0.55
2:B:419:THR:CG2	2:B:475:LEU:CD1	2.85	0.55
3:D:110:GLY:O	3:D:111:ARG:O	2.24	0.55
2:B:492:PHE:O	2:B:495:VAL:HG23	2.06	0.55
3:C:165:PHE:O	3:C:166:HIS:O	2.25	0.55
3:C:122:PHE:CD2	3:C:172:LEU:HD22	2.40	0.55
2:B:416:TYR:HE1	2:B:472:LEU:CB	2.19	0.55
2:B:470:LEU:HD23	2:B:470:LEU:N	2.21	0.55
3:D:13:LEU:HD23	3:D:14:TYR:HE1	1.72	0.55
3:D:16:ARG:O	3:D:17:GLN:C	2.42	0.55
3:C:176:CYS:C	3:C:179:PRO:HD2	2.27	0.55
3:D:83:ARG:N	3:D:83:ARG:CD	2.68	0.55
1:A:117:GLN:O	1:A:121:LYS:N	2.40	0.55
3:C:106:ILE:O	3:C:118:THR:HA	2.06	0.55
1:A:162:PRO:HG2	1:A:163:ASN:N	2.21	0.55
2:B:512:LEU:O	2:B:515:THR:HB	2.07	0.55
3:C:37:TYR:HE1	3:C:41:LYS:HD2	1.72	0.55
1:A:65:MET:C	1:A:67:MET:N	2.60	0.55
2:B:408:LEU:O	2:B:411:ILE:HG22	2.06	0.55
2:B:499:LEU:O	2:B:500:VAL:C	2.46	0.55
2:B:561:TYR:O	2:B:563:PRO:HD3	2.06	0.55
3:C:168:MET:CG	3:C:173:LEU:HG	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASN:ND2	1:A:113:VAL:N	2.53	0.55
3:D:132:ALA:HB2	3:D:176:CYS:O	2.07	0.55
3:D:151:LEU:HD11	3:D:195:LYS:CB	2.36	0.55
2:B:503:ILE:HD12	2:B:545:LEU:HD11	1.89	0.55
1:A:139:ASP:O	1:A:142:LYS:HG2	2.06	0.54
3:D:150:THR:N	3:D:196:VAL:HG23	2.22	0.54
3:C:17:GLN:HE21	3:C:18:PRO:HD2	1.72	0.54
3:D:14:TYR:CD1	3:D:14:TYR:N	2.74	0.54
3:C:135:ILE:O	3:C:138:TRP:HB2	2.07	0.54
1:A:202:LEU:HB3	1:A:223:TYR:CE1	2.43	0.54
3:D:153:GLU:O	3:D:155:SER:N	2.41	0.54
2:B:495:VAL:HG12	2:B:527:TRP:HZ2	1.73	0.54
2:B:417:GLU:O	2:B:418:PHE:C	2.45	0.54
2:B:445:ASN:O	2:B:447:SER:N	2.40	0.54
1:A:205:MET:CB	1:A:211:LEU:HD11	2.37	0.54
3:C:106:ILE:CG2	3:C:107:ASP:H	2.11	0.54
3:C:115:ASN:C	3:C:117:THR:N	2.57	0.54
3:D:151:LEU:C	3:D:153:GLU:N	2.57	0.54
3:C:76:PHE:CD2	3:C:76:PHE:N	2.75	0.54
3:C:83:ARG:NH1	3:C:83:ARG:HG3	2.19	0.54
3:C:94:TRP:HA	3:C:94:TRP:CE3	2.43	0.54
3:D:3:ALA:HB1	3:D:37:TYR:HD1	1.72	0.54
1:A:102:ILE:HG21	1:A:123:HIS:CD2	2.42	0.54
3:D:149:ILE:HG22	3:D:153:GLU:CG	2.35	0.54
2:B:515:THR:HG22	2:B:516:GLN:H	1.71	0.54
1:A:79:PHE:CZ	1:A:88:VAL:HG11	2.43	0.54
3:D:104:LEU:O	3:D:121:TYR:CA	2.46	0.54
3:D:31:ILE:O	3:D:33:ILE:N	2.41	0.54
1:A:225:ASP:OD1	1:A:227:SER:OG	2.22	0.54
3:C:186:ALA:HB1	3:C:199:ILE:HA	1.90	0.54
3:C:13:LEU:O	3:C:26:GLN:NE2	2.36	0.54
3:D:105:PRO:HA	3:D:120:ARG:O	2.08	0.54
3:D:170:GLU:HA	3:D:173:LEU:HD12	1.89	0.54
1:A:93:TYR:O	1:A:96:CYS:HB2	2.08	0.54
3:D:114:SER:HA	3:D:118:THR:CG2	2.38	0.54
3:C:106:ILE:HG22	3:C:107:ASP:N	2.13	0.53
3:D:27:ILE:HG22	3:D:28:SER:H	1.73	0.53
1:A:39:PHE:O	1:A:42:ARG:HB3	2.07	0.53
1:A:75:PRO:C	1:A:77:SER:N	2.60	0.53
2:B:464:CYS:O	2:B:467:PHE:CD1	2.62	0.53
3:D:77:ASN:O	3:D:79:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASN:ND2	1:A:113:VAL:O	2.41	0.53
3:D:168:MET:SD	3:D:173:LEU:HG	2.48	0.53
1:A:79:PHE:HA	1:A:85:LEU:HB3	1.90	0.53
3:C:98:THR:C	3:C:101:GLY:H	2.12	0.53
3:D:129:ASP:C	3:D:131:TRP:H	2.11	0.53
2:B:539:CYS:CB	2:B:545:LEU:HG	2.38	0.53
3:C:110:GLY:HA3	3:C:175:TYR:CZ	2.43	0.53
2:B:440:LEU:HD23	2:B:487:VAL:HG11	1.91	0.53
3:D:76:PHE:HB3	3:D:85:VAL:HG11	1.88	0.53
1:A:185:SER:OG	1:A:186:LEU:N	2.41	0.53
2:B:513:ARG:C	2:B:515:THR:N	2.61	0.53
3:C:77:ASN:CG	3:C:84:SER:HB2	2.28	0.53
3:D:151:LEU:HD11	3:D:195:LYS:HB2	1.90	0.53
3:D:150:THR:CG2	3:D:153:GLU:HG2	2.39	0.53
3:C:73:LYS:HB2	3:C:78:ASN:HB2	1.91	0.53
1:A:29:SER:O	1:A:32:LEU:N	2.42	0.53
1:A:25:LEU:C	1:A:27:LYS:N	2.61	0.53
3:C:139:PHE:N	3:C:139:PHE:CD2	2.75	0.53
2:B:461:ARG:O	2:B:462:GLU:C	2.46	0.53
3:D:39:LYS:O	3:D:41:LYS:N	2.41	0.53
3:C:132:ALA:C	3:C:134:LEU:H	2.12	0.53
1:A:43:LEU:HD12	1:A:64:PHE:CE1	2.42	0.53
3:D:34:ILE:HD12	3:D:46:MET:HE1	1.90	0.53
3:C:114:SER:O	3:C:118:THR:OG1	2.26	0.52
3:C:177:LEU:HD13	3:C:180:LEU:HD12	1.91	0.52
3:C:76:PHE:CB	3:C:85:VAL:HG11	2.32	0.52
3:D:14:TYR:HD1	3:D:14:TYR:N	2.07	0.52
3:D:34:ILE:HG21	3:D:97:MET:HE3	1.91	0.52
3:C:37:TYR:O	3:C:37:TYR:HD1	1.92	0.52
1:A:25:LEU:C	1:A:27:LYS:H	2.13	0.52
3:C:13:LEU:HD11	3:C:30:TRP:CD1	2.44	0.52
3:C:150:THR:HG23	3:C:153:GLU:HG2	1.91	0.52
2:B:415:ILE:HG21	2:B:460:MET:CE	2.39	0.52
1:A:184:ILE:HD11	1:A:195:ALA:O	2.09	0.52
2:B:432:TYR:N	2:B:432:TYR:CD1	2.75	0.52
3:C:29:THR:O	3:C:33:ILE:HG13	2.10	0.52
1:A:40:GLN:C	1:A:42:ARG:H	2.12	0.52
1:A:53:GLU:O	1:A:60:PHE:CD2	2.62	0.52
3:D:197:ILE:CG2	3:D:198:ALA:N	2.72	0.52
3:C:169:PRO:HB2	3:C:172:LEU:HD12	1.91	0.52
3:D:34:ILE:HD11	3:D:76:PHE:HZ	1.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLN:O	1:A:42:ARG:N	2.42	0.52
1:A:225:ASP:O	1:A:226:PRO:C	2.47	0.52
1:A:100:ILE:HD11	1:A:141:LEU:CD2	2.39	0.52
1:A:146:CYS:HB3	2:B:438:VAL:HG21	1.91	0.52
1:A:34:ASP:O	1:A:38:VAL:N	2.41	0.52
3:D:136:LEU:HD21	3:D:180:LEU:CD2	2.40	0.52
2:B:503:ILE:CD1	2:B:545:LEU:HD11	2.39	0.52
3:D:171:SER:O	3:D:174:TYR:HB3	2.10	0.52
1:A:227:SER:C	1:A:229:ILE:H	2.12	0.52
3:C:136:LEU:CB	3:C:180:LEU:HD21	2.35	0.52
3:D:13:LEU:HD23	3:D:14:TYR:CE1	2.45	0.52
3:D:151:LEU:HA	3:D:154:LEU:CD1	2.29	0.52
1:A:107:LYS:HD2	2:B:533:MET:CE	2.39	0.52
2:B:536:LEU:HD22	2:B:556:TYR:CE2	2.44	0.52
1:A:203:ASP:O	1:A:206:VAL:N	2.37	0.52
3:C:106:ILE:HB	3:C:120:ARG:CD	2.36	0.52
1:A:187:LEU:HD13	1:A:193:TRP:CD1	2.45	0.52
3:D:151:LEU:C	3:D:153:GLU:H	2.12	0.52
3:D:114:SER:O	3:D:118:THR:OG1	2.27	0.52
3:C:37:TYR:CE1	3:C:41:LYS:HD2	2.45	0.52
1:A:104:ARG:C	1:A:106:THR:H	2.13	0.52
3:C:13:LEU:HB3	3:C:14:TYR:HD1	1.75	0.52
3:D:16:ARG:HG2	3:D:16:ARG:O	2.10	0.52
3:D:38:CYS:O	3:D:39:LYS:O	2.27	0.52
3:D:34:ILE:HA	3:D:75:LEU:HD11	1.90	0.52
3:D:127:SER:HB3	3:D:130:SER:OG	2.09	0.52
3:D:136:LEU:CD1	3:D:136:LEU:H	2.22	0.52
1:A:77:SER:O	1:A:80:ASP:HB2	2.09	0.52
3:C:124:LEU:HD23	3:C:124:LEU:N	2.24	0.52
2:B:443:MET:O	2:B:447:SER:HB2	2.10	0.52
3:C:14:TYR:CZ	3:C:79:GLU:HG2	2.45	0.52
2:B:477:LEU:C	2:B:478:VAL:HG22	2.30	0.52
2:B:466:ARG:O	2:B:467:PHE:C	2.48	0.51
3:D:123:ILE:CG2	3:D:125:TRP:CZ3	2.93	0.51
3:D:29:THR:O	3:D:33:ILE:CG1	2.54	0.51
1:A:124:PHE:HE2	1:A:134:LEU:HD23	1.74	0.51
3:C:102:LYS:C	3:C:124:LEU:HG	2.30	0.51
3:C:150:THR:CB	3:C:196:VAL:CG1	2.88	0.51
2:B:547:ILE:H	3:D:17:GLN:NE2	2.04	0.51
1:A:39:PHE:HD2	1:A:39:PHE:O	1.93	0.51
1:A:93:TYR:N	1:A:93:TYR:HD2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:THR:CG2	2:B:475:LEU:HD11	2.41	0.51
2:B:547:ILE:HD13	3:D:18:PRO:CD	2.41	0.51
3:D:94:TRP:HZ3	3:D:97:MET:HE3	1.74	0.51
3:D:167:ARG:O	3:D:169:PRO:HD3	2.10	0.51
2:B:408:LEU:O	2:B:410:GLU:N	2.43	0.51
3:D:123:ILE:O	3:D:124:LEU:CB	2.58	0.51
3:D:43:ILE:HG22	3:D:44:TRP:H	1.75	0.51
1:A:144:LEU:HB3	2:B:438:VAL:HG22	1.91	0.51
1:A:172:ILE:O	1:A:175:ILE:HG22	2.10	0.51
2:B:558:LYS:O	2:B:560:SER:N	2.42	0.51
3:D:24:ARG:O	3:D:27:ILE:N	2.44	0.51
1:A:46:PHE:C	1:A:46:PHE:CD1	2.83	0.51
2:B:434:ILE:HA	2:B:488:THR:OG1	2.11	0.51
3:C:96:GLN:HG3	3:C:96:GLN:O	2.10	0.51
3:C:10:PHE:CZ	3:C:12:PRO:HG3	2.46	0.51
3:C:195:LYS:C	3:C:196:VAL:HG13	2.26	0.51
1:A:58:PRO:HD3	1:A:61:ARG:NH2	2.26	0.51
1:A:231:ARG:HB2	1:A:231:ARG:HH11	1.76	0.51
2:B:416:TYR:CE1	2:B:472:LEU:CA	2.88	0.51
1:A:91:PHE:HZ	1:A:133:ASP:OD2	1.92	0.51
3:D:123:ILE:HG22	3:D:125:TRP:HZ3	1.75	0.51
3:D:29:THR:C	3:D:31:ILE:N	2.65	0.51
3:D:161:VAL:C	3:D:163:TRP:N	2.64	0.51
2:B:480:VAL:HG11	2:B:492:PHE:CE2	2.46	0.51
1:A:75:PRO:O	1:A:78:LEU:N	2.44	0.51
3:C:134:LEU:HD13	3:C:163:TRP:HE3	1.75	0.51
2:B:414:GLU:OE2	2:B:449:ARG:NH1	2.43	0.51
1:A:45:GLU:O	1:A:46:PHE:C	2.48	0.51
1:A:23:THR:HG22	1:A:27:LYS:HG3	1.92	0.51
1:A:45:GLU:O	1:A:47:ALA:N	2.44	0.50
3:D:195:LYS:C	3:D:196:VAL:HG12	2.31	0.50
3:C:4:LEU:N	3:C:5:PRO:CD	2.74	0.50
2:B:552:SER:O	3:C:19:ASN:HA	2.11	0.50
2:B:407:PHE:O	2:B:411:ILE:CB	2.50	0.50
1:A:171:LYS:O	1:A:175:ILE:N	2.30	0.50
3:D:150:THR:HA	3:D:196:VAL:HA	1.94	0.50
1:A:93:TYR:O	1:A:97:LEU:HD12	2.11	0.50
3:C:4:LEU:N	3:C:5:PRO:HD3	2.26	0.50
1:A:110:ASN:ND2	1:A:112:GLY:N	2.52	0.50
3:D:186:ALA:CB	3:D:199:ILE:O	2.59	0.50
2:B:514:LEU:CD1	2:B:532:LEU:HD11	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:C	1:A:106:THR:N	2.64	0.50
3:C:46:MET:O	3:C:121:TYR:N	2.44	0.50
2:B:416:TYR:HE2	2:B:420:LEU:CD2	2.24	0.50
3:D:46:MET:HG3	3:D:51:THR:CG2	2.32	0.50
3:D:136:LEU:N	3:D:136:LEU:HD12	2.26	0.50
1:A:34:ASP:O	1:A:37:MET:N	2.45	0.50
1:A:45:GLU:C	1:A:47:ALA:N	2.62	0.50
3:C:10:PHE:CE2	3:C:12:PRO:HG2	2.47	0.50
2:B:410:GLU:O	2:B:413:ARG:HB2	2.10	0.50
2:B:449:ARG:O	2:B:449:ARG:CG	2.58	0.50
3:D:43:ILE:CG2	3:D:44:TRP:H	2.24	0.50
1:A:139:ASP:O	1:A:140:MET:C	2.49	0.50
1:A:48:LYS:HE2	1:A:48:LYS:HA	1.92	0.50
1:A:23:THR:C	1:A:25:LEU:H	2.14	0.50
3:C:31:ILE:CD1	3:C:97:MET:HA	2.41	0.50
1:A:175:ILE:HD13	1:A:187:LEU:CD2	2.42	0.50
1:A:211:LEU:CD1	1:A:211:LEU:N	2.73	0.50
1:A:213:ILE:HD11	1:A:223:TYR:CZ	2.46	0.50
1:A:52:SER:C	1:A:54:LEU:N	2.64	0.50
3:C:150:THR:OG1	3:C:196:VAL:HG12	2.12	0.50
3:C:151:LEU:C	3:C:153:GLU:N	2.55	0.50
3:C:170:GLU:O	3:C:173:LEU:N	2.45	0.50
3:D:197:ILE:HG22	3:D:198:ALA:N	2.27	0.50
1:A:206:VAL:HB	2:B:551:LEU:CD1	2.42	0.49
3:C:114:SER:HA	3:C:118:THR:CG2	2.42	0.49
3:C:135:ILE:HA	3:C:165:PHE:CE2	2.47	0.49
3:D:111:ARG:HG2	3:D:175:TYR:OH	2.12	0.49
1:A:146:CYS:HB3	2:B:438:VAL:CG2	2.41	0.49
3:D:136:LEU:H	3:D:136:LEU:HD13	1.76	0.49
3:D:163:TRP:HB3	3:D:165:PHE:CE2	2.42	0.49
3:D:177:LEU:C	3:D:179:PRO:CD	2.80	0.49
3:C:14:TYR:HD2	3:C:84:SER:HA	1.78	0.49
2:B:546:LEU:HD12	3:D:10:PHE:HE2	1.73	0.49
2:B:547:ILE:HD13	3:D:18:PRO:HD3	1.95	0.49
1:A:168:ASP:OD2	1:A:193:TRP:HZ2	1.96	0.49
1:A:34:ASP:C	1:A:38:VAL:HG23	2.33	0.49
3:C:104:LEU:CB	3:C:122:PHE:HB3	2.34	0.49
3:D:29:THR:C	3:D:31:ILE:H	2.15	0.49
3:D:135:ILE:O	3:D:138:TRP:HB3	2.12	0.49
3:D:164:GLU:C	3:D:166:HIS:H	2.15	0.49
3:C:16:ARG:HG3	3:C:23:ARG:NH2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:LEU:HD11	3:C:30:TRP:NE1	2.27	0.49
2:B:455:ILE:HG22	2:B:459:GLU:OE2	2.13	0.49
3:D:106:ILE:HG12	3:D:110:GLY:HA2	1.94	0.49
3:D:24:ARG:O	3:D:25:GLN:C	2.48	0.49
3:D:33:ILE:O	3:D:37:TYR:HB2	2.13	0.49
3:D:41:LYS:O	3:D:43:ILE:CD1	2.61	0.49
1:A:185:SER:N	1:A:220:GLU:OE2	2.31	0.49
2:B:538:ASN:O	2:B:540:VAL:N	2.45	0.49
3:C:111:ARG:HG3	3:C:111:ARG:NH1	2.26	0.49
3:C:104:LEU:O	3:C:121:TYR:HA	2.12	0.49
3:C:138:TRP:CZ3	3:C:142:SER:OG	2.61	0.49
3:C:150:THR:OG1	3:C:151:LEU:N	2.45	0.49
3:C:172:LEU:O	3:C:175:TYR:HB2	2.13	0.49
2:B:408:LEU:HA	2:B:411:ILE:CG2	2.42	0.49
2:B:491:LYS:O	2:B:495:VAL:HG23	2.12	0.49
3:C:151:LEU:O	3:C:154:LEU:HD12	2.11	0.49
3:C:94:TRP:O	3:C:97:MET:HB3	2.13	0.49
3:C:97:MET:CG	3:C:103:CYS:HB3	2.43	0.49
3:D:31:ILE:C	3:D:33:ILE:N	2.64	0.49
3:D:34:ILE:HD13	3:D:75:LEU:HD13	1.94	0.49
1:A:213:ILE:HG23	1:A:214:ASP:N	2.28	0.49
3:C:173:LEU:HA	3:C:176:CYS:SG	2.53	0.49
2:B:554:ILE:N	2:B:554:ILE:HD12	2.27	0.49
1:A:231:ARG:CB	1:A:231:ARG:HH11	2.26	0.49
3:D:154:LEU:HA	3:D:159:GLU:HG3	1.93	0.49
2:B:485:LEU:C	2:B:485:LEU:HD12	2.23	0.49
3:C:137:GLN:O	3:C:163:TRP:HH2	1.96	0.49
3:C:179:PRO:C	3:C:181:CYS:N	2.65	0.49
2:B:416:TYR:OH	2:B:474:GLU:HB2	2.13	0.49
2:B:467:PHE:O	2:B:468:GLU:C	2.51	0.49
1:A:130:GLY:O	1:A:133:ASP:N	2.46	0.49
1:A:193:TRP:CE3	1:A:193:TRP:HA	2.48	0.49
3:D:137:GLN:O	3:D:163:TRP:CH2	2.66	0.49
3:D:188:MET:SD	3:D:195:LYS:HE3	2.53	0.49
3:D:34:ILE:HA	3:D:75:LEU:CD1	2.43	0.48
3:D:85:VAL:CG1	3:D:90:ILE:HD11	2.42	0.48
1:A:200:SER:OG	1:A:201:ALA:N	2.45	0.48
3:D:186:ALA:HB1	3:D:199:ILE:O	2.12	0.48
3:C:90:ILE:O	3:C:93:ILE:HB	2.13	0.48
2:B:460:MET:CE	2:B:464:CYS:SG	3.01	0.48
1:A:112:GLY:O	1:A:160:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:135:ILE:O	3:D:138:TRP:CB	2.61	0.48
2:B:561:TYR:O	2:B:563:PRO:CD	2.60	0.48
1:A:79:PHE:HA	1:A:85:LEU:HD13	1.95	0.48
3:C:19:ASN:ND2	3:C:22:THR:H	2.10	0.48
2:B:467:PHE:CD1	2:B:467:PHE:N	2.78	0.48
1:A:23:THR:O	1:A:25:LEU:N	2.46	0.48
3:C:87:GLN:O	3:C:89:PHE:N	2.46	0.48
3:C:90:ILE:HG22	3:C:94:TRP:CD1	2.48	0.48
3:D:123:ILE:O	3:D:124:LEU:CG	2.60	0.48
1:A:119:LEU:CD1	1:A:134:LEU:HD21	2.43	0.48
1:A:36:LEU:C	1:A:38:VAL:N	2.64	0.48
3:D:164:GLU:C	3:D:166:HIS:N	2.67	0.48
3:C:44:TRP:HZ3	3:C:131:TRP:CH2	2.32	0.48
1:A:23:THR:HG22	1:A:27:LYS:HD2	1.96	0.48
2:B:555:TYR:CD1	2:B:555:TYR:N	2.81	0.48
3:D:83:ARG:N	3:D:83:ARG:HD2	2.29	0.48
1:A:222:LEU:C	1:A:223:TYR:HD2	2.17	0.48
2:B:502:LEU:HD21	2:B:518:LEU:CD2	2.39	0.48
2:B:495:VAL:HG12	2:B:527:TRP:CZ2	2.48	0.48
2:B:415:ILE:HD13	2:B:444:TYR:CE2	2.48	0.48
3:D:183:ARG:HG3	3:D:184:ASN:N	2.28	0.48
3:C:177:LEU:CD1	3:C:180:LEU:CD1	2.91	0.48
3:C:77:ASN:HB2	3:C:84:SER:HB2	1.95	0.48
2:B:411:ILE:O	2:B:415:ILE:CG1	2.61	0.48
3:D:23:ARG:O	3:D:26:GLN:HB3	2.14	0.48
3:D:34:ILE:HG23	3:D:46:MET:HE2	1.94	0.48
3:C:4:LEU:O	3:C:5:PRO:C	2.51	0.48
2:B:548:ASP:OD2	3:D:83:ARG:NH1	2.46	0.48
3:C:87:GLN:O	3:C:88:VAL:C	2.51	0.48
3:C:91:ASP:O	3:C:94:TRP:N	2.47	0.48
2:B:415:ILE:HD13	2:B:444:TYR:CZ	2.48	0.48
2:B:445:ASN:O	2:B:446:LYS:C	2.52	0.48
2:B:539:CYS:HB3	2:B:545:LEU:HG	1.96	0.48
3:C:2:SER:C	3:C:4:LEU:N	2.65	0.48
2:B:423:PHE:CD1	2:B:424:LYS:HG2	2.48	0.48
3:C:97:MET:HG3	3:C:103:CYS:HB3	1.94	0.48
3:C:77:ASN:OD1	3:C:84:SER:HB2	2.14	0.48
2:B:408:LEU:HD13	2:B:462:GLU:HB3	1.95	0.48
1:A:185:SER:HB3	1:A:220:GLU:OE1	2.14	0.48
1:A:41:GLU:C	1:A:44:VAL:HG22	2.33	0.48
2:B:518:LEU:HD23	2:B:518:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:ASN:O	2:B:406:LEU:HB2	2.13	0.48
2:B:500:VAL:O	2:B:501:ASP:C	2.52	0.48
3:C:132:ALA:C	3:C:134:LEU:N	2.67	0.47
3:D:90:ILE:H	3:D:90:ILE:HD12	1.79	0.47
3:D:94:TRP:O	3:D:97:MET:N	2.38	0.47
1:A:159:ARG:NH1	1:A:161:VAL:O	2.47	0.47
1:A:181:TYR:CE1	1:A:222:LEU:HD12	2.45	0.47
2:B:503:ILE:O	2:B:504:GLY:C	2.52	0.47
2:B:518:LEU:CD1	2:B:527:TRP:CG	2.96	0.47
3:D:106:ILE:HG22	3:D:107:ASP:H	1.77	0.47
1:A:161:VAL:CG1	1:A:162:PRO:HD2	2.44	0.47
1:A:198:SER:O	1:A:199:LYS:C	2.52	0.47
1:A:97:LEU:HD12	1:A:97:LEU:N	2.23	0.47
3:C:43:ILE:CG2	3:C:44:TRP:N	2.77	0.47
2:B:505:ASP:O	2:B:507:PRO:HD3	2.14	0.47
3:C:135:ILE:HG21	3:C:177:LEU:HD11	1.96	0.47
3:D:106:ILE:O	3:D:120:ARG:HG2	2.14	0.47
1:A:95:VAL:HG21	1:A:129:VAL:HG11	1.95	0.47
2:B:432:TYR:CD1	2:B:432:TYR:C	2.87	0.47
3:C:12:PRO:O	3:C:13:LEU:C	2.51	0.47
3:C:149:ILE:HD11	3:C:153:GLU:HB3	1.97	0.47
3:D:34:ILE:HG21	3:D:97:MET:CE	2.43	0.47
1:A:124:PHE:HB3	1:A:129:VAL:CG2	2.43	0.47
3:D:128:LEU:O	3:D:131:TRP:CB	2.60	0.47
2:B:547:ILE:CD1	2:B:547:ILE:H	2.26	0.47
1:A:113:VAL:HG11	1:A:165:LEU:CD1	2.41	0.47
1:A:35:GLN:O	1:A:38:VAL:HB	2.15	0.47
2:B:450:ILE:HD13	2:B:451:GLY:H	1.80	0.47
3:C:148:VAL:O	3:C:148:VAL:HG12	2.15	0.47
3:C:150:THR:CG2	3:C:153:GLU:CG	2.92	0.47
3:C:165:PHE:C	3:C:166:HIS:O	2.51	0.47
3:D:123:ILE:CG2	3:D:125:TRP:HZ3	2.28	0.47
3:D:3:ALA:HB1	3:D:37:TYR:CE1	2.48	0.47
1:A:169:GLN:HG2	1:A:205:MET:HG3	1.94	0.47
2:B:561:TYR:C	2:B:563:PRO:CD	2.76	0.47
1:A:93:TYR:O	1:A:94:GLU:C	2.53	0.47
3:C:8:TYR:CE1	3:C:75:LEU:HD13	2.50	0.47
2:B:521:ASN:O	2:B:523:SER:N	2.48	0.47
3:C:150:THR:CB	3:C:196:VAL:HG11	2.45	0.47
1:A:147:PHE:CB	1:A:158:LEU:HD11	2.45	0.47
2:B:518:LEU:CD1	2:B:527:TRP:CD1	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:HD2	2:B:533:MET:HE3	1.96	0.47
2:B:481:ASN:HB3	2:B:482:LYS:H	1.43	0.47
3:D:9:SER:O	3:D:11:PRO:HD3	2.15	0.47
3:D:97:MET:HG2	3:D:103:CYS:SG	2.55	0.47
1:A:114:ILE:CG2	1:A:158:LEU:HB3	2.45	0.47
1:A:227:SER:O	1:A:228:TRP:C	2.52	0.47
3:C:104:LEU:HA	3:C:104:LEU:HD12	1.61	0.47
3:C:13:LEU:HB3	3:C:14:TYR:CD1	2.50	0.47
3:C:79:GLU:O	3:C:83:ARG:O	2.33	0.47
2:B:419:THR:OG1	2:B:440:LEU:HD11	2.15	0.47
1:A:164:GLU:C	1:A:165:LEU:O	2.43	0.47
1:A:150:PHE:CE2	1:A:165:LEU:HD22	2.50	0.47
1:A:173:LEU:O	1:A:176:CYS:HB2	2.15	0.47
1:A:107:LYS:O	1:A:107:LYS:HG2	2.13	0.47
2:B:449:ARG:HG3	2:B:452:THR:HB	1.96	0.46
3:D:177:LEU:CD1	3:D:180:LEU:HD12	2.44	0.46
3:D:178:LYS:N	3:D:179:PRO:CD	2.79	0.46
3:C:104:LEU:CD1	3:C:105:PRO:HD2	2.45	0.46
3:C:91:ASP:O	3:C:92:GLU:C	2.51	0.46
2:B:411:ILE:O	2:B:415:ILE:HG12	2.16	0.46
3:D:30:TRP:CE3	3:D:33:ILE:CD1	2.96	0.46
1:A:61:ARG:CZ	1:A:91:PHE:CZ	2.98	0.46
2:B:484:ILE:HD13	2:B:534:GLU:OE1	2.14	0.46
3:D:98:THR:O	3:D:101:GLY:N	2.37	0.46
1:A:116:PHE:CE1	1:A:156:LYS:HB2	2.51	0.46
2:B:547:ILE:CD1	3:D:17:GLN:NE2	2.77	0.46
3:D:166:HIS:C	3:D:168:MET:N	2.68	0.46
3:C:136:LEU:C	3:C:138:TRP:H	2.19	0.46
3:C:170:GLU:O	3:C:172:LEU:N	2.47	0.46
1:A:168:ASP:OD1	1:A:193:TRP:HZ2	1.98	0.46
2:B:546:LEU:CD1	3:D:10:PHE:HE2	2.27	0.46
3:D:105:PRO:C	3:D:106:ILE:CG1	2.81	0.46
3:D:10:PHE:CE2	3:D:12:PRO:CG	2.97	0.46
1:A:41:GLU:O	1:A:44:VAL:CG2	2.63	0.46
1:A:232:GLN:HA	1:A:232:GLN:HE21	1.80	0.46
3:C:113:SER:HB3	3:C:117:THR:OG1	2.15	0.46
2:B:416:TYR:CD1	2:B:472:LEU:CB	2.79	0.46
3:D:106:ILE:C	3:D:120:ARG:HG2	2.35	0.46
1:A:114:ILE:HG23	1:A:158:LEU:HB3	1.96	0.46
3:C:37:TYR:C	3:C:37:TYR:CD1	2.88	0.46
1:A:138:ILE:HA	1:A:141:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:199:ILE:HG12	3:D:199:ILE:H	1.27	0.46
3:D:22:THR:O	3:D:23:ARG:C	2.54	0.46
3:D:76:PHE:O	3:D:77:ASN:C	2.52	0.46
3:D:149:ILE:O	3:D:196:VAL:HG23	2.16	0.46
1:A:199:LYS:O	1:A:202:LEU:N	2.49	0.46
2:B:502:LEU:HD12	2:B:502:LEU:O	2.16	0.46
3:C:128:LEU:O	3:C:131:TRP:N	2.49	0.46
3:D:46:MET:HB2	3:D:123:ILE:HD11	1.96	0.46
3:D:89:PHE:O	3:D:92:GLU:N	2.50	0.46
1:A:205:MET:CG	1:A:211:LEU:HD11	2.46	0.46
3:D:187:THR:O	3:D:198:ALA:N	2.48	0.46
3:C:150:THR:CA	3:C:196:VAL:HB	2.25	0.45
3:C:145:LEU:O	3:C:199:ILE:HG12	2.16	0.45
1:A:136:LYS:O	1:A:137:SER:C	2.55	0.45
1:A:40:GLN:O	1:A:43:LEU:N	2.49	0.45
1:A:50:HIS:CD2	1:A:60:PHE:CZ	3.03	0.45
3:D:165:PHE:O	3:D:168:MET:CB	2.64	0.45
3:D:195:LYS:O	3:D:196:VAL:HG12	2.15	0.45
1:A:76:LEU:HG	1:A:89:ASN:HD21	1.81	0.45
1:A:149:ILE:O	1:A:149:ILE:HG13	2.15	0.45
1:A:206:VAL:HB	2:B:551:LEU:HD11	1.98	0.45
1:A:102:ILE:HG21	1:A:123:HIS:CG	2.51	0.45
3:D:135:ILE:C	3:D:137:GLN:H	2.19	0.45
2:B:480:VAL:CG1	2:B:492:PHE:CD2	2.97	0.45
2:B:513:ARG:O	2:B:516:GLN:N	2.48	0.45
2:B:555:TYR:N	2:B:555:TYR:HD1	2.14	0.45
3:D:106:ILE:HB	3:D:120:ARG:HG2	1.94	0.45
3:D:14:TYR:HE2	3:D:79:GLU:CB	2.29	0.45
1:A:44:VAL:O	1:A:48:LYS:N	2.43	0.45
3:C:81:ILE:O	3:C:82:GLN:HG2	2.17	0.45
2:B:547:ILE:HG23	2:B:554:ILE:HG23	1.98	0.45
2:B:546:LEU:HD21	2:B:559:ASN:OD1	2.15	0.45
3:D:39:LYS:HG3	3:D:125:TRP:CD1	2.52	0.45
1:A:199:LYS:O	1:A:200:SER:C	2.55	0.45
3:D:166:HIS:HD2	3:D:166:HIS:C	2.18	0.45
3:D:187:THR:OG1	3:D:188:MET:N	2.49	0.45
2:B:512:LEU:O	2:B:512:LEU:HD23	2.16	0.45
2:B:539:CYS:O	2:B:543:GLY:N	2.49	0.45
3:C:37:TYR:HD2	3:C:75:LEU:CD2	2.26	0.45
2:B:474:GLU:C	2:B:475:LEU:HD23	2.32	0.45
1:A:152:ILE:CG1	1:A:173:LEU:HD22	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:483:ARG:CG	2:B:483:ARG:HH11	2.24	0.45
2:B:435:ILE:HD12	2:B:435:ILE:HA	1.72	0.45
3:D:191:ASP:O	3:D:192:GLU:CB	2.64	0.45
3:C:105:PRO:O	3:C:106:ILE:HD13	2.17	0.45
3:D:4:LEU:O	3:D:5:PRO:O	2.35	0.45
1:A:198:SER:O	1:A:202:LEU:N	2.46	0.45
3:D:139:PHE:HE1	3:D:199:ILE:CG2	2.30	0.45
3:C:138:TRP:HZ3	3:C:142:SER:OG	1.99	0.45
1:A:122:VAL:HG12	1:A:123:HIS:CG	2.51	0.45
1:A:166:THR:OG1	1:A:169:GLN:CD	2.55	0.45
1:A:171:LYS:O	1:A:174:GLU:HB3	2.17	0.45
2:B:513:ARG:HG2	2:B:513:ARG:HH11	1.82	0.45
3:C:73:LYS:HE3	3:C:78:ASN:CG	2.37	0.45
3:C:174:TYR:HE1	3:C:178:LYS:HD2	1.80	0.45
1:A:229:ILE:HG22	1:A:230:THR:N	2.32	0.45
3:D:105:PRO:CG	3:D:112:ARG:HG2	2.46	0.45
3:D:15:THR:O	3:D:17:GLN:N	2.50	0.45
3:D:151:LEU:O	3:D:152:TYR:C	2.56	0.45
3:C:104:LEU:HG	3:C:105:PRO:HD2	1.99	0.45
3:C:14:TYR:OH	3:C:79:GLU:HG2	2.17	0.45
3:D:30:TRP:CA	3:D:33:ILE:HD12	2.33	0.45
3:D:41:LYS:C	3:D:42:LYS:HG2	2.36	0.45
3:D:77:ASN:HA	3:D:84:SER:HB2	1.92	0.45
1:A:39:PHE:O	1:A:43:LEU:HD23	2.17	0.45
1:A:75:PRO:C	1:A:77:SER:H	2.18	0.45
1:A:106:THR:C	1:A:108:ASP:N	2.70	0.45
3:C:116:THR:O	3:C:116:THR:HG22	2.17	0.45
3:C:138:TRP:HZ3	3:C:142:SER:CB	2.29	0.44
2:B:460:MET:HE2	2:B:464:CYS:SG	2.57	0.44
3:D:47:SER:HB2	3:D:48:VAL:H	1.53	0.44
1:A:40:GLN:O	1:A:41:GLU:C	2.55	0.44
1:A:75:PRO:O	1:A:76:LEU:C	2.55	0.44
1:A:203:ASP:HA	1:A:206:VAL:HG23	1.98	0.44
1:A:202:LEU:HG	1:A:223:TYR:CD1	2.53	0.44
3:D:139:PHE:N	3:D:139:PHE:HD2	2.10	0.44
2:B:550:GLN:HG3	2:B:551:LEU:H	1.81	0.44
3:C:137:GLN:O	3:C:141:ASP:HB2	2.17	0.44
1:A:130:GLY:O	1:A:131:LEU:C	2.55	0.44
1:A:23:THR:HG22	1:A:27:LYS:CG	2.47	0.44
3:C:97:MET:HG3	3:C:103:CYS:CB	2.48	0.44
3:D:39:LYS:HA	3:D:125:TRP:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLN:HA	1:A:172:ILE:HD13	1.99	0.44
1:A:168:ASP:CG	1:A:193:TRP:HZ2	2.20	0.44
3:C:73:LYS:HB2	3:C:78:ASN:CB	2.47	0.44
3:D:104:LEU:CG	3:D:105:PRO:HD2	2.47	0.44
1:A:169:GLN:HG3	1:A:205:MET:HG3	1.99	0.44
1:A:165:LEU:HD21	1:A:173:LEU:CD1	2.47	0.44
1:A:181:TYR:CD1	1:A:222:LEU:CD1	2.79	0.44
3:C:37:TYR:CD2	3:C:75:LEU:CD2	2.98	0.44
3:C:189:LEU:O	3:C:190:LYS:O	2.35	0.44
3:C:191:ASP:C	3:C:193:ASN:N	2.69	0.44
1:A:89:ASN:O	1:A:90:ASP:C	2.56	0.44
3:C:39:LYS:CG	3:C:40:THR:H	2.31	0.44
3:C:79:GLU:HG3	3:C:79:GLU:O	2.18	0.44
3:C:98:THR:HG23	3:C:99:LYS:N	2.33	0.44
3:D:77:ASN:O	3:D:78:ASN:C	2.55	0.44
1:A:61:ARG:NH2	1:A:91:PHE:CE1	2.86	0.44
2:B:502:LEU:O	2:B:503:ILE:C	2.56	0.44
2:B:477:LEU:HD12	2:B:477:LEU:HA	1.73	0.44
2:B:556:TYR:O	2:B:557:TYR:CD2	2.71	0.44
3:C:46:MET:HE2	3:C:94:TRP:CZ2	2.53	0.44
1:A:205:MET:SD	1:A:211:LEU:HD11	2.57	0.44
3:D:127:SER:OG	3:D:128:LEU:N	2.51	0.44
2:B:500:VAL:O	2:B:503:ILE:N	2.51	0.44
2:B:434:ILE:CG2	2:B:531:ILE:HG12	2.34	0.44
2:B:423:PHE:CD1	2:B:424:LYS:N	2.85	0.43
1:A:203:ASP:O	1:A:204:GLU:C	2.56	0.43
3:C:97:MET:HE3	3:C:103:CYS:HB3	2.00	0.43
3:D:159:GLU:O	3:D:161:VAL:HG23	2.17	0.43
3:D:176:CYS:HB2	3:D:177:LEU:HD22	2.00	0.43
1:A:71:ILE:HG21	1:A:73:ILE:HD11	2.00	0.43
1:A:73:ILE:HG21	1:A:78:LEU:HD21	2.00	0.43
3:C:13:LEU:CD1	3:C:30:TRP:NE1	2.81	0.43
3:D:39:LYS:O	3:D:40:THR:C	2.57	0.43
3:D:94:TRP:HA	3:D:94:TRP:CE3	2.53	0.43
1:A:102:ILE:HD13	1:A:123:HIS:HB3	1.98	0.43
3:D:131:TRP:HE1	3:D:168:MET:HE2	1.80	0.43
3:D:177:LEU:HD12	3:D:180:LEU:HD12	1.99	0.43
2:B:499:LEU:C	2:B:499:LEU:HD12	2.39	0.43
2:B:499:LEU:O	2:B:499:LEU:HD12	2.17	0.43
2:B:518:LEU:CD2	2:B:518:LEU:N	2.79	0.43
2:B:529:LEU:HA	2:B:529:LEU:HD12	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:536:LEU:HD23	2:B:536:LEU:HA	1.55	0.43
1:A:229:ILE:HG13	3:C:10:PHE:CD1	2.53	0.43
3:C:45:TYR:CD1	3:C:45:TYR:C	2.92	0.43
3:C:95:SER:O	3:C:97:MET:N	2.52	0.43
3:D:46:MET:CE	3:D:94:TRP:HH2	2.31	0.43
1:A:49:LYS:O	1:A:51:ASN:N	2.42	0.43
3:D:136:LEU:HD21	3:D:180:LEU:HD22	1.99	0.43
2:B:491:LYS:O	2:B:494:VAL:CG2	2.66	0.43
2:B:516:GLN:O	2:B:517:ILE:C	2.56	0.43
3:D:14:TYR:CE2	3:D:79:GLU:HG2	2.53	0.43
2:B:551:LEU:O	2:B:551:LEU:HD12	2.18	0.43
1:A:185:SER:O	1:A:186:LEU:C	2.57	0.43
3:C:39:LYS:O	3:C:40:THR:C	2.54	0.43
3:C:13:LEU:O	3:C:15:THR:N	2.52	0.43
3:C:95:SER:O	3:C:98:THR:HG22	2.19	0.43
1:A:110:ASN:CG	1:A:111:GLY:N	2.56	0.43
1:A:125:ARG:CA	1:A:125:ARG:NE	2.53	0.43
2:B:502:LEU:CD1	2:B:517:ILE:HG21	2.48	0.43
1:A:216:GLN:O	3:C:83:ARG:NE	2.51	0.43
2:B:410:GLU:O	2:B:413:ARG:N	2.52	0.43
1:A:46:PHE:HE1	1:A:60:PHE:HZ	1.67	0.43
3:D:137:GLN:OE1	3:D:137:GLN:HA	2.19	0.43
2:B:529:LEU:O	2:B:532:LEU:N	2.50	0.43
1:A:25:LEU:HG	1:A:26:GLU:N	2.34	0.43
3:D:174:TYR:C	3:D:174:TYR:CD1	2.92	0.43
1:A:225:ASP:CG	1:A:227:SER:HG	2.20	0.43
3:C:30:TRP:CE3	3:C:30:TRP:HA	2.53	0.43
1:A:130:GLY:O	1:A:133:ASP:HB2	2.19	0.43
2:B:556:TYR:C	2:B:557:TYR:HD2	2.22	0.43
3:C:190:LYS:HB3	3:C:190:LYS:HZ2	1.83	0.43
2:B:448:MET:O	2:B:448:MET:CG	2.65	0.43
3:D:106:ILE:HG22	3:D:108:GLN:H	1.83	0.43
1:A:175:ILE:HG21	1:A:187:LEU:HD21	2.01	0.43
3:D:138:TRP:C	3:D:139:PHE:HD2	2.23	0.43
2:B:528:THR:O	2:B:529:LEU:C	2.57	0.43
2:B:404:LYS:C	2:B:406:LEU:H	2.21	0.43
3:C:170:GLU:O	3:C:173:LEU:HB2	2.18	0.43
2:B:445:ASN:C	2:B:447:SER:N	2.72	0.43
2:B:550:GLN:HE22	3:D:83:ARG:HG2	1.77	0.42
1:A:229:ILE:CD1	3:C:10:PHE:HB2	2.48	0.42
3:C:88:VAL:O	3:C:91:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:447:SER:O	2:B:449:ARG:N	2.45	0.42
1:A:133:ASP:O	1:A:134:LEU:C	2.57	0.42
1:A:171:LYS:O	1:A:174:GLU:N	2.52	0.42
3:D:163:TRP:O	3:D:166:HIS:HB3	2.19	0.42
2:B:499:LEU:HD11	2:B:514:LEU:HD11	2.00	0.42
3:C:19:ASN:ND2	3:C:19:ASN:O	2.42	0.42
2:B:460:MET:HE1	2:B:464:CYS:SG	2.59	0.42
1:A:144:LEU:HG	2:B:457:PRO:HB3	2.00	0.42
1:A:165:LEU:CD2	1:A:173:LEU:HD13	2.49	0.42
3:C:78:ASN:CG	3:C:78:ASN:O	2.58	0.42
3:C:47:SER:HA	3:C:119:THR:O	2.19	0.42
3:C:163:TRP:C	3:C:165:PHE:H	2.21	0.42
2:B:416:TYR:CE2	2:B:420:LEU:CD2	2.96	0.42
2:B:420:LEU:HA	2:B:420:LEU:HD12	1.74	0.42
3:D:38:CYS:O	3:D:42:LYS:N	2.52	0.42
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.67	0.42
1:A:39:PHE:C	1:A:42:ARG:HB3	2.39	0.42
3:C:10:PHE:CE2	3:C:12:PRO:CG	3.02	0.42
2:B:416:TYR:C	2:B:416:TYR:CD2	2.92	0.42
2:B:471:GLY:C	2:B:472:LEU:HD23	2.39	0.42
2:B:420:LEU:HD13	2:B:475:LEU:HD11	2.00	0.42
3:D:74:ASN:H	3:D:78:ASN:CB	2.32	0.42
1:A:171:LYS:O	1:A:172:ILE:C	2.56	0.42
1:A:152:ILE:HG23	1:A:174:GLU:HA	2.00	0.42
3:C:173:LEU:O	3:C:177:LEU:HD23	2.17	0.42
3:C:17:GLN:NE2	3:C:18:PRO:CD	2.78	0.42
3:C:34:ILE:O	3:C:35:SER:C	2.58	0.42
1:A:117:GLN:O	1:A:118:GLU:C	2.56	0.42
1:A:168:ASP:O	1:A:169:GLN:C	2.56	0.42
1:A:232:GLN:CA	1:A:232:GLN:HE21	2.31	0.42
3:C:75:LEU:HA	3:C:75:LEU:HD22	1.25	0.42
3:C:3:ALA:C	3:C:5:PRO:CD	2.87	0.42
3:C:13:LEU:HD12	3:C:13:LEU:C	2.40	0.42
3:C:166:HIS:CD2	3:C:167:ARG:HB2	2.55	0.42
3:C:34:ILE:HD12	3:C:46:MET:HE1	2.02	0.42
1:A:76:LEU:HD21	1:A:93:TYR:HE2	1.84	0.42
2:B:556:TYR:C	2:B:557:TYR:CD2	2.92	0.42
3:C:107:ASP:O	3:C:108:GLN:HG3	2.20	0.42
3:D:124:LEU:C	3:D:125:TRP:HE3	2.16	0.42
3:D:173:LEU:HD23	3:D:173:LEU:HA	1.91	0.42
1:A:23:THR:C	1:A:25:LEU:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:51:THR:O	3:D:51:THR:HG23	2.19	0.42
1:A:168:ASP:O	1:A:170:THR:N	2.53	0.42
1:A:175:ILE:HD12	1:A:191:LEU:HD12	2.01	0.42
3:D:176:CYS:O	3:D:179:PRO:HD2	2.20	0.42
2:B:515:THR:O	2:B:518:LEU:N	2.52	0.42
3:C:139:PHE:O	3:C:140:GLU:C	2.57	0.42
2:B:551:LEU:HG	3:C:18:PRO:HB2	2.01	0.42
3:D:90:ILE:CG2	3:D:94:TRP:CD1	3.02	0.42
1:A:60:PHE:CD1	1:A:63:LYS:HD3	2.55	0.42
3:C:185:ARG:H	3:C:185:ARG:HG2	1.61	0.42
3:D:106:ILE:HG22	3:D:108:GLN:N	2.35	0.42
3:D:110:GLY:C	3:D:111:ARG:O	2.57	0.42
1:A:181:TYR:O	1:A:182:SER:C	2.56	0.42
1:A:191:LEU:HB3	1:A:193:TRP:HB2	2.02	0.42
3:D:159:GLU:C	3:D:161:VAL:H	2.23	0.42
3:C:95:SER:C	3:C:97:MET:N	2.73	0.41
3:D:29:THR:O	3:D:31:ILE:N	2.53	0.41
1:A:118:GLU:O	1:A:122:VAL:HB	2.20	0.41
1:A:168:ASP:O	1:A:171:LYS:N	2.53	0.41
3:D:132:ALA:O	3:D:135:ILE:HB	2.19	0.41
3:D:174:TYR:HD1	3:D:174:TYR:C	2.24	0.41
3:C:106:ILE:CG2	3:C:107:ASP:N	2.80	0.41
1:A:187:LEU:O	1:A:188:LYS:C	2.58	0.41
1:A:213:ILE:CG2	1:A:215:TYR:HE1	2.32	0.41
1:A:211:LEU:HD22	1:A:223:TYR:HB3	2.02	0.41
3:D:184:ASN:O	3:D:185:ARG:HB2	2.20	0.41
3:C:146:ASN:HD22	3:C:146:ASN:N	2.16	0.41
3:D:45:TYR:HA	3:D:121:TYR:O	2.20	0.41
1:A:185:SER:C	1:A:187:LEU:N	2.72	0.41
1:A:99:VAL:O	1:A:100:ILE:C	2.56	0.41
2:B:483:ARG:NH1	2:B:483:ARG:CG	2.83	0.41
3:D:150:THR:HG22	3:D:153:GLU:CG	2.50	0.41
3:C:74:ASN:O	3:C:78:ASN:CB	2.57	0.41
3:C:190:LYS:O	3:C:191:ASP:HB2	2.20	0.41
2:B:411:ILE:O	2:B:415:ILE:HG13	2.20	0.41
2:B:418:PHE:O	2:B:421:SER:OG	2.36	0.41
3:D:46:MET:HE3	3:D:94:TRP:CH2	2.56	0.41
1:A:150:PHE:CE1	1:A:157:PHE:CB	3.03	0.41
2:B:480:VAL:CG1	2:B:492:PHE:CG	2.98	0.41
2:B:398:ARG:HA	2:B:452:THR:O	2.20	0.41
3:D:134:LEU:HA	3:D:137:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:165:PHE:O	3:D:168:MET:HB3	2.21	0.41
3:C:19:ASN:O	3:C:20:SER:C	2.58	0.41
3:D:110:GLY:O	3:D:111:ARG:C	2.59	0.41
3:D:30:TRP:O	3:D:34:ILE:HG12	2.20	0.41
3:D:79:GLU:HG3	3:D:82:GLN:HG3	2.03	0.41
1:A:169:GLN:CA	1:A:172:ILE:HD13	2.51	0.41
1:A:34:ASP:O	1:A:36:LEU:N	2.53	0.41
1:A:46:PHE:CE1	1:A:60:PHE:HZ	2.38	0.41
1:A:106:THR:C	1:A:108:ASP:H	2.24	0.41
2:B:432:TYR:HD1	2:B:432:TYR:H	1.68	0.41
2:B:438:VAL:O	2:B:438:VAL:CG1	2.67	0.41
3:D:135:ILE:C	3:D:137:GLN:N	2.71	0.41
3:D:105:PRO:HG2	3:D:112:ARG:CG	2.50	0.41
3:D:30:TRP:CD1	3:D:93:ILE:CD1	3.03	0.41
3:D:41:LYS:O	3:D:42:LYS:CG	2.69	0.41
3:D:78:ASN:O	3:D:79:GLU:C	2.58	0.41
1:A:198:SER:O	1:A:202:LEU:HB2	2.21	0.41
3:D:139:PHE:CE1	3:D:199:ILE:HG21	2.52	0.41
2:B:484:ILE:CD1	2:B:534:GLU:OE1	2.68	0.41
3:C:74:ASN:N	3:C:78:ASN:HB3	2.35	0.41
2:B:481:ASN:HD22	2:B:481:ASN:HA	1.56	0.41
3:C:77:ASN:O	3:C:77:ASN:CG	2.59	0.41
3:C:138:TRP:HB3	3:C:139:PHE:CD2	2.55	0.41
2:B:447:SER:HB3	2:B:448:MET:H	1.38	0.41
3:D:77:ASN:CA	3:D:84:SER:HB3	2.27	0.41
3:D:111:ARG:O	3:D:117:THR:HG22	2.21	0.41
3:D:90:ILE:O	3:D:93:ILE:HB	2.21	0.41
1:A:100:ILE:CD1	2:B:438:VAL:HG13	2.49	0.41
1:A:58:PRO:O	1:A:61:ARG:HB2	2.21	0.41
1:A:39:PHE:CD2	1:A:43:LEU:CD2	3.04	0.41
1:A:53:GLU:C	1:A:60:PHE:HD2	2.24	0.41
1:A:63:LYS:CG	1:A:64:PHE:N	2.83	0.41
3:D:131:TRP:O	3:D:135:ILE:HG13	2.21	0.41
1:A:78:LEU:HA	1:A:78:LEU:HD23	1.58	0.41
3:C:38:CYS:C	3:C:39:LYS:O	2.57	0.41
3:C:38:CYS:SG	3:C:123:ILE:CD1	3.09	0.41
1:A:107:LYS:HE3	1:A:108:ASP:OD1	2.21	0.41
1:A:79:PHE:HA	1:A:85:LEU:CD1	2.51	0.41
3:C:182:ASP:HB3	3:C:183:ARG:H	1.70	0.41
2:B:423:PHE:HB2	2:B:526:ASN:HD21	1.82	0.41
3:C:177:LEU:HA	3:C:177:LEU:HD13	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:31:ILE:O	3:D:34:ILE:N	2.54	0.41
3:D:16:ARG:HA	3:D:89:PHE:CE2	2.55	0.41
1:A:118:GLU:O	1:A:119:LEU:C	2.58	0.41
1:A:169:GLN:CG	1:A:205:MET:CG	2.98	0.41
3:D:128:LEU:HD12	3:D:129:ASP:H	1.85	0.41
3:D:180:LEU:HD23	3:D:180:LEU:HA	1.81	0.41
1:A:230:THR:O	1:A:231:ARG:C	2.59	0.40
3:C:33:ILE:O	3:C:34:ILE:C	2.60	0.40
3:C:89:PHE:C	3:C:91:ASP:N	2.74	0.40
2:B:546:LEU:HG	2:B:559:ASN:HA	2.03	0.40
2:B:547:ILE:N	3:D:17:GLN:HE22	2.09	0.40
3:D:42:LYS:C	3:D:43:ILE:HD12	2.41	0.40
1:A:38:VAL:C	1:A:40:GLN:N	2.72	0.40
3:C:73:LYS:HE3	3:C:78:ASN:OD1	2.22	0.40
1:A:89:ASN:HB3	1:A:93:TYR:CZ	2.56	0.40
2:B:432:TYR:C	2:B:432:TYR:HD1	2.24	0.40
3:C:132:ALA:HB2	3:C:176:CYS:O	2.20	0.40
3:C:153:GLU:O	3:C:155:SER:N	2.54	0.40
3:D:29:THR:O	3:D:33:ILE:CD1	2.69	0.40
1:A:213:ILE:CG1	1:A:215:TYR:HE1	2.35	0.40
3:C:7:VAL:C	3:C:9:SER:H	2.25	0.40
1:A:74:ASP:HA	1:A:75:PRO:HD2	1.84	0.40
2:B:550:GLN:HG3	2:B:551:LEU:N	2.36	0.40
2:B:552:SER:OG	2:B:553:GLY:N	2.52	0.40
3:C:135:ILE:HD13	3:C:165:PHE:CE2	2.56	0.40
3:C:180:LEU:O	3:C:181:CYS:SG	2.76	0.40
1:A:176:CYS:O	1:A:178:ILE:N	2.54	0.40
1:A:64:PHE:O	1:A:64:PHE:CD1	2.73	0.40
3:D:186:ALA:HB1	3:D:198:ALA:O	2.22	0.40
3:C:8:TYR:HE1	3:C:75:LEU:HD13	1.86	0.40
3:C:34:ILE:CG2	3:C:97:MET:HE1	2.51	0.40
1:A:222:LEU:HD13	1:A:222:LEU:HA	1.74	0.40
2:B:478:VAL:N	2:B:486:CYS:O	2.52	0.40
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.95	0.40
1:A:120:GLU:OE2	1:A:121:LYS:CG	2.70	0.40
1:A:34:ASP:O	1:A:35:GLN:C	2.59	0.40
1:A:32:LEU:HD13	1:A:32:LEU:HA	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	211/233 (91%)	131 (62%)	51 (24%)	29 (14%)	0 6
2	B	167/169 (99%)	104 (62%)	41 (25%)	22 (13%)	0 6
3	C	174/202 (86%)	78 (45%)	56 (32%)	40 (23%)	0 1
3	D	174/202 (86%)	91 (52%)	40 (23%)	43 (25%)	0 1
All	All	726/806 (90%)	404 (56%)	188 (26%)	134 (18%)	0 3

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	PHE
1	A	76	LEU
1	A	79	PHE
1	A	107	LYS
1	A	142	LYS
1	A	177	SER
1	A	194	GLU
1	A	197	ARG
2	B	448	MET
2	B	449	ARG
2	B	500	VAL
2	B	522	ASN
2	B	529	LEU
3	C	14	TYR
3	C	34	ILE
3	C	40	THR
3	C	82	GLN
3	C	110	GLY
3	C	113	SER
3	C	144	LYS
3	C	147	GLN
3	C	152	TYR

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Mol	Chain	Res	Type
3	C	156	GLU
3	C	166	HIS
3	C	167	ARG
3	C	171	SER
3	C	190	LYS
3	D	20	SER
3	D	24	ARG
3	D	25	GLN
3	D	27	ILE
3	D	35	SER
3	D	39	LYS
3	D	48	VAL
3	D	79	GLU
3	D	111	ARG
3	D	114	SER
3	D	123	ILE
3	D	124	LEU
3	D	127	SER
3	D	147	GLN
3	D	148	VAL
3	D	154	LEU
3	D	167	ARG
3	D	196	VAL
1	A	24	ILE
1	A	61	ARG
1	A	83	LYS
1	A	105	GLN
1	A	122	VAL
1	A	128	ASN
1	A	186	LEU
2	B	399	GLU
2	B	423	PHE
2	B	467	PHE
2	B	468	GLU
2	B	514	LEU
2	B	523	SER
2	B	539	CYS
3	C	35	SER
3	C	39	LYS
3	C	47	SER
3	C	77	ASN
3	C	91	ASP

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Mol	Chain	Res	Type
3	C	129	ASP
3	C	133	SER
3	C	191	ASP
3	C	196	VAL
3	D	16	ARG
3	D	32	ASP
3	D	40	THR
3	D	98	THR
3	D	108	GLN
3	D	110	GLY
3	D	119	THR
3	D	152	TYR
1	A	29	SER
1	A	50	HIS
1	A	66	HIS
1	A	189	ALA
2	B	409	ASP
2	B	440	LEU
2	B	538	ASN
3	C	20	SER
3	C	95	SER
3	D	26	GLN
3	D	34	ILE
3	D	78	ASN
3	D	90	ILE
3	D	94	TRP
3	D	125	TRP
3	D	153	GLU
1	A	35	GLN
1	A	80	ASP
1	A	86	PHE
1	A	111	GLY
1	A	133	ASP
1	A	169	GLN
2	B	405	GLU
2	B	426	LEU
2	B	430	THR
2	B	446	LYS
2	B	559	ASN
3	C	42	LYS
3	C	88	VAL
3	C	96	GLN

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Mol	Chain	Res	Type
3	C	195	LYS
3	D	21	LEU
1	A	217	GLY
2	B	447	SER
2	B	463	ALA
3	C	4	LEU
3	C	6	PRO
3	C	11	PRO
3	C	107	ASP
3	C	157	GLY
3	C	180	LEU
3	D	8	TYR
3	D	47	SER
1	A	58	PRO
1	A	64	PHE
3	C	194	ASP
3	D	5	PRO
3	D	6	PRO
3	D	101	GLY
3	D	113	SER
3	C	48	VAL
3	D	178	LYS
3	C	90	ILE
3	D	179	PRO
1	A	30	VAL
3	C	81	ILE
3	D	161	VAL
3	C	161	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	195/211 (92%)	148 (76%)	47 (24%)	1 6
2	B	158/158 (100%)	119 (75%)	39 (25%)	1 6
3	C	169/192 (88%)	121 (72%)	48 (28%)	0 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	169/192 (88%)	119 (70%)	50 (30%)	0 3
All	All	691/753 (92%)	507 (73%)	184 (27%)	0 5

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	32	LEU
1	A	34	ASP
1	A	39	PHE
1	A	42	ARG
1	A	43	LEU
1	A	46	PHE
1	A	48	LYS
1	A	50	HIS
1	A	55	GLN
1	A	76	LEU
1	A	81	ARG
1	A	84	HIS
1	A	86	PHE
1	A	90	ASP
1	A	91	PHE
1	A	94	GLU
1	A	119	LEU
1	A	125	ARG
1	A	127	LEU
1	A	131	LEU
1	A	136	LYS
1	A	137	SER
1	A	143	SER
1	A	148	GLU
1	A	161	VAL
1	A	166	THR
1	A	169	GLN
1	A	170	THR
1	A	178	ILE
1	A	179	LEU
1	A	184	ILE
1	A	186	LEU
1	A	187	LEU
1	A	191	LEU
1	A	193	TRP

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Mol	Chain	Res	Type
1	A	194	GLU
1	A	198	SER
1	A	204	GLU
1	A	211	LEU
1	A	214	ASP
1	A	215	TYR
1	A	216	GLN
1	A	223	TYR
1	A	230	THR
1	A	231	ARG
1	A	232	GLN
2	B	406	LEU
2	B	409	ASP
2	B	411	ILE
2	B	413	ARG
2	B	415	ILE
2	B	416	TYR
2	B	431	ASN
2	B	432	TYR
2	B	436	THR
2	B	447	SER
2	B	448	MET
2	B	450	ILE
2	B	458	MET
2	B	462	GLU
2	B	467	PHE
2	B	470	LEU
2	B	473	ASN
2	B	478	VAL
2	B	481	ASN
2	B	483	ARG
2	B	487	VAL
2	B	490	GLU
2	B	493	ASP
2	B	499	LEU
2	B	501	ASP
2	B	502	LEU
2	B	505	ASP
2	B	506	ASN
2	B	514	LEU
2	B	515	THR
2	B	518	LEU

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Mol	Chain	Res	Type
2	B	528	THR
2	B	535	VAL
2	B	538	ASN
2	B	539	CYS
2	B	544	ASP
2	B	545	LEU
2	B	549	LYS
2	B	552	SER
3	C	4	LEU
3	C	6	PRO
3	C	7	VAL
3	C	13	LEU
3	C	14	TYR
3	C	15	THR
3	C	16	ARG
3	C	19	ASN
3	C	30	TRP
3	C	32	ASP
3	C	37	TYR
3	C	48	VAL
3	C	49	ASP
3	C	72	SER
3	C	74	ASN
3	C	75	LEU
3	C	78	ASN
3	C	80	ASP
3	C	81	ILE
3	C	82	GLN
3	C	83	ARG
3	C	86	SER
3	C	94	TRP
3	C	97	MET
3	C	98	THR
3	C	117	THR
3	C	119	THR
3	C	120	ARG
3	C	124	LEU
3	C	125	TRP
3	C	131	TRP
3	C	134	LEU
3	C	136	LEU
3	C	138	TRP

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Mol	Chain	Res	Type
3	C	141	ASP
3	C	145	LEU
3	C	150	THR
3	C	152	TYR
3	C	154	LEU
3	C	158	ASP
3	C	159	GLU
3	C	160	THR
3	C	164	GLU
3	C	168	MET
3	C	173	LEU
3	C	174	TYR
3	C	176	CYS
3	C	199	ILE
3	D	4	LEU
3	D	9	SER
3	D	11	PRO
3	D	14	TYR
3	D	16	ARG
3	D	18	PRO
3	D	21	LEU
3	D	27	ILE
3	D	29	THR
3	D	30	TRP
3	D	36	GLN
3	D	40	THR
3	D	43	ILE
3	D	47	SER
3	D	49	ASP
3	D	75	LEU
3	D	80	ASP
3	D	81	ILE
3	D	82	GLN
3	D	83	ARG
3	D	89	PHE
3	D	94	TRP
3	D	98	THR
3	D	112	ARG
3	D	117	THR
3	D	120	ARG
3	D	125	TRP
3	D	131	TRP

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Mol	Chain	Res	Type
3	D	134	LEU
3	D	136	LEU
3	D	138	TRP
3	D	139	PHE
3	D	140	GLU
3	D	145	LEU
3	D	149	ILE
3	D	152	TYR
3	D	154	LEU
3	D	155	SER
3	D	158	ASP
3	D	161	VAL
3	D	164	GLU
3	D	165	PHE
3	D	166	HIS
3	D	167	ARG
3	D	169	PRO
3	D	174	TYR
3	D	182	ASP
3	D	190	LYS
3	D	192	GLU
3	D	199	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	51	ASN
1	A	66	HIS
1	A	89	ASN
1	A	110	ASN
1	A	117	GLN
1	A	151	GLN
1	A	216	GLN
2	B	445	ASN
2	B	469	HIS
2	B	481	ASN
2	B	506	ASN
2	B	526	ASN
2	B	538	ASN
2	B	550	GLN
3	C	17	GLN

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Mol	Chain	Res	Type
3	C	19	ASN
3	C	74	ASN
3	C	78	ASN
3	C	82	GLN
3	C	87	GLN
3	C	137	GLN
3	C	146	ASN
3	C	166	HIS
3	D	17	GLN
3	D	82	GLN
3	D	166	HIS

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, 95^{th} 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	213/233 (91%)	-0.13	6 (2%)	56	42	27, 76, 182, 199	0
2	B	169/169 (100%)	-0.19	1 (0%)	90	83	29, 66, 192, 200	0
3	C	178/202 (88%)	-0.05	6 (3%)	49	35	36, 118, 184, 193	0
3	D	178/202 (88%)	-0.03	5 (2%)	56	42	46, 129, 185, 200	0
All	All	738/806 (91%)	-0.10	18 (2%)	62	47	27, 100, 184, 200	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	ASN	7.1
3	D	116	THR	4.7
3	C	164	GLU	4.5
3	C	148	VAL	4.2
1	A	20	VAL	4.0
1	A	24	ILE	3.6
1	A	39	PHE	3.3
3	D	34	ILE	3.1
3	D	117	THR	3.1
3	D	143	GLY	2.9
1	A	71	ILE	2.8
3	D	148	VAL	2.7
3	C	136	LEU	2.5
1	A	22	LYS	2.2
3	C	184	ASN	2.2
2	B	426	LEU	2.1
3	C	183	ARG	2.1
3	C	122	PHE	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.