



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:00 AM GMT

PDB ID : 3CW2
Title : Crystal structure of the intact archaeal translation initiation factor 2 from *Sulfolobus solfataricus* .
Authors : Stolboushkina, E.A.; Nikonov, S.V.; Nikulin, A.D; Blaesi, U; Manstein, D.J.; Fedorov, R.V.; Garber, M.B.; Nikonov, O.S.
Deposited on : 2008-04-21
Resolution : 2.80 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : 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

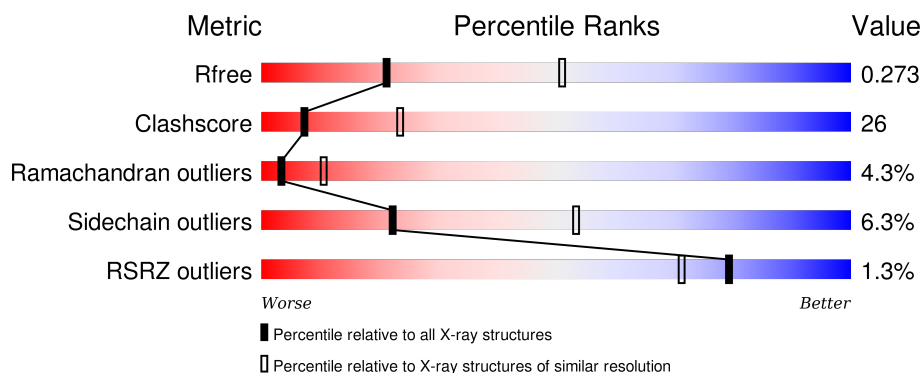
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 $\leq 5\%$. 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	415	<div> <div></div> <div>53% 42% 5%</div> </div>
1	B	415	<div> <div></div> <div>51% 43% . .</div> </div>
1	E	415	<div> <div></div> <div>51% 45% .</div> </div>
1	F	415	<div> <div></div> <div>44% 50% 5%</div> </div>
2	C	266	<div> <div></div> <div>53% 38% 8% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	266	<div><div></div><div>55%40%5%</div></div>
2	G	266	<div><div></div><div>54%40%6%</div></div>
2	H	266	<div><div></div><div>50%41%8%•</div></div>
3	K	139	<div><div>6%</div><div></div><div>42%37%9%•8%</div></div>
3	L	139	<div><div>7%8%</div><div></div><div>85%</div></div>
3	M	139	<div><div>7%</div><div></div><div>52%36%9%••</div></div>
3	N	139	<div><div>%</div><div></div><div>11%9%•78%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23823 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 Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3213	2058	548	595	12			
1	B	400	Total	C	N	O	S	0	0	0
			3096	1987	524	574	11			
1	E	414	Total	C	N	O	S	0	0	0
			3213	2058	548	595	12			
1	F	414	Total	C	N	O	S	0	0	0
			3213	2058	548	595	12			

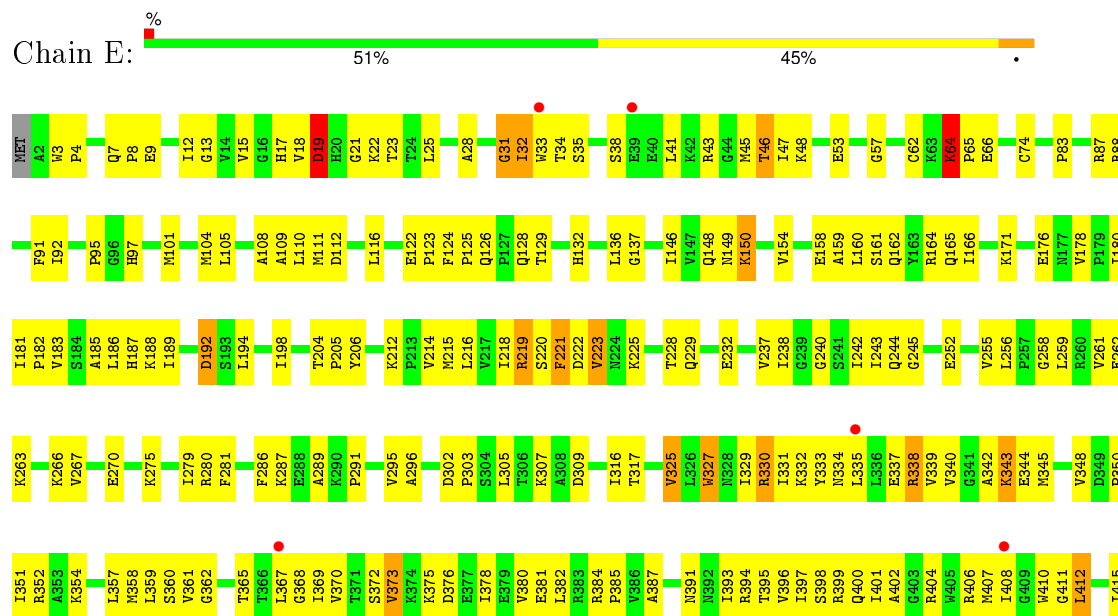
- Molecule 2 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	266	Total	C	N	O	S	0	0	0
			2134	1364	365	403	2			
2	D	266	Total	C	N	O	S	0	0	0
			2134	1364	365	403	2			
2	G	266	Total	C	N	O	S	0	0	0
			2134	1364	365	403	2			
2	H	266	Total	C	N	O	S	0	0	0
			2134	1364	365	403	2			

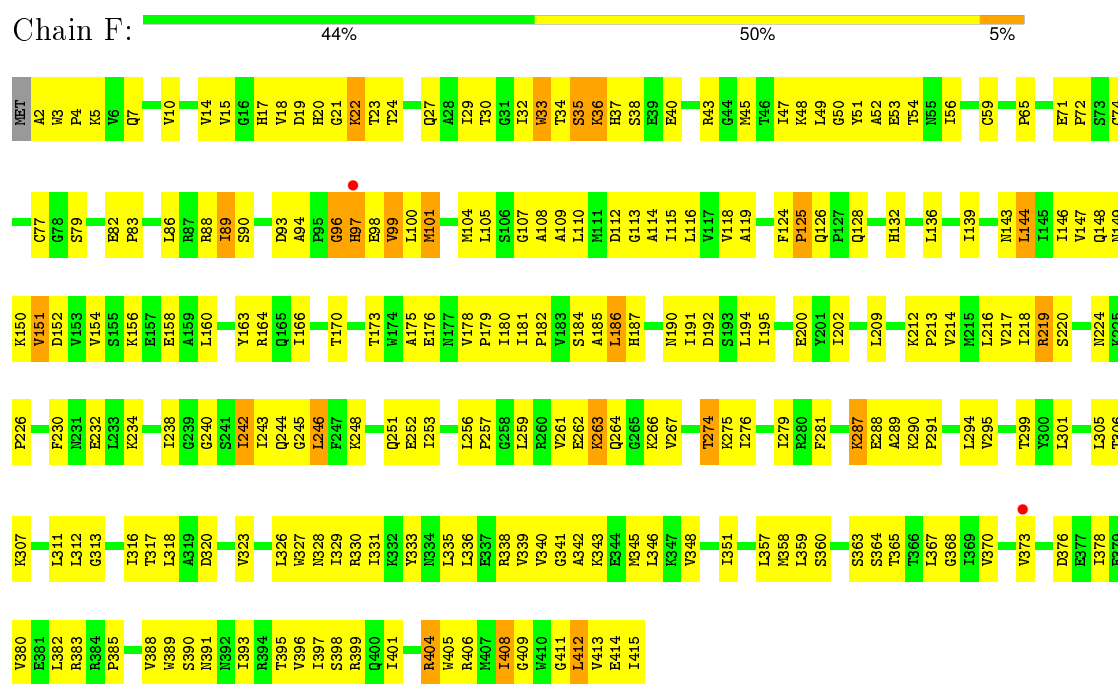
- Molecule 3 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	128	Total	C	N	O	S	0	0	0
			1032	655	174	194	9			
3	L	21	Total	C	N	O	S	0	0	0
			174	110	27	36	1			
3	M	138	Total	C	N	O	S	0	0	0
			1102	699	186	207	10			
3	N	30	Total	C	N	O	S	0	0	0
			244	152	41	50	1			

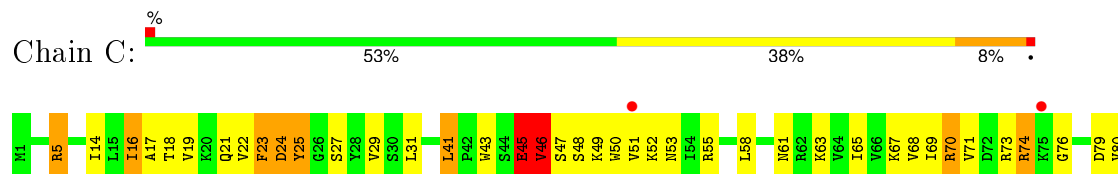
• Molecule 1: Translation initiation factor 2 subunit gamma

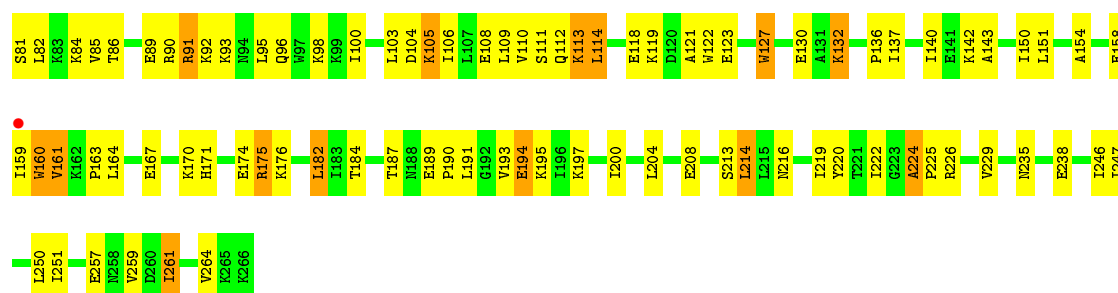


• Molecule 1: Translation initiation factor 2 subunit gamma



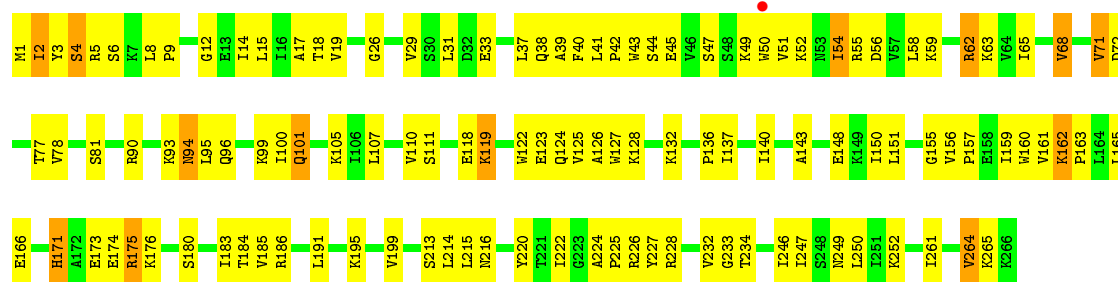
• Molecule 2: Translation initiation factor 2 subunit alpha





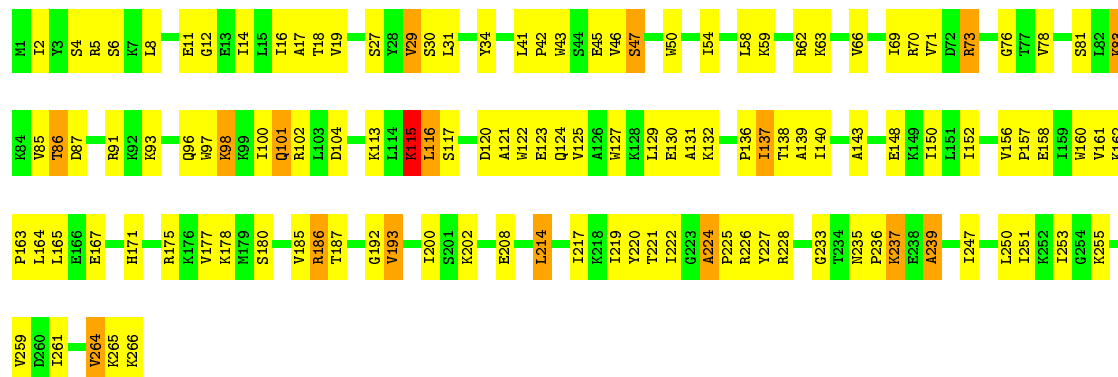
• Molecule 2: Translation initiation factor 2 subunit alpha

Chain D: 55% 40% 5%



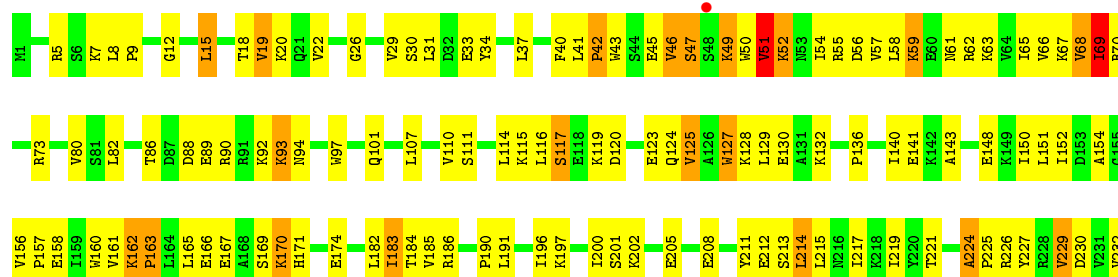
• Molecule 2: Translation initiation factor 2 subunit alpha

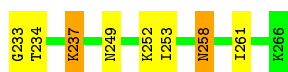
Chain G: 54% 40% 6%



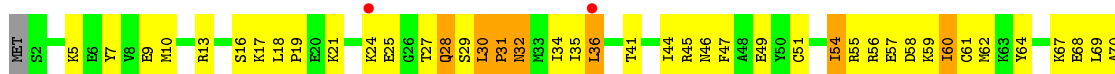
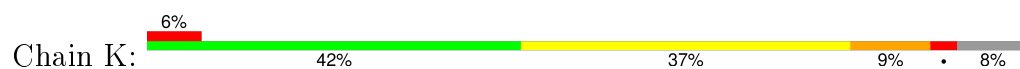
• Molecule 2: Translation initiation factor 2 subunit alpha

Chain H: 50% 41% 8%

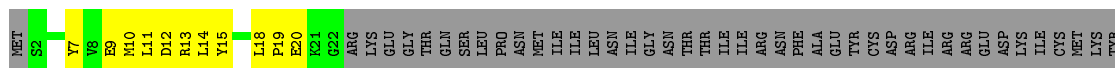




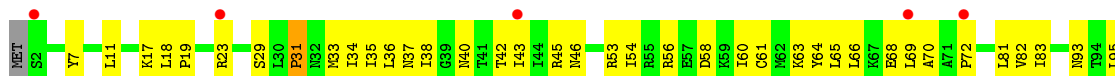
• Molecule 3: Translation initiation factor 2 subunit beta



• Molecule 3: Translation initiation factor 2 subunit beta



• Molecule 3: Translation initiation factor 2 subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.20 Å 162.92 Å 161.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.80 19.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (19.91-2.80) 98.5 (19.91-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.79 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.225 , 0.276 0.229 , 0.273	Depositor DCC
R_{free} test set	4940 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	72.0	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 49.6	EDS
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.449 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 98811 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23823	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.72% 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, 0.375 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	0.23	0/3272	0.42	0/4430
1	B	0.22	0/3152	0.41	0/4269
1	E	0.23	0/3272	0.42	0/4430
1	F	0.24	0/3272	0.41	0/4430
2	C	0.22	0/2164	0.39	0/2914
2	D	0.22	0/2164	0.39	0/2914
2	G	0.23	0/2164	0.40	0/2914
2	H	0.21	0/2164	0.38	0/2914
3	K	0.23	0/1045	0.39	0/1399
3	L	0.22	0/176	0.38	0/233
3	M	0.23	0/1117	0.47	0/1497
3	N	0.23	0/247	0.38	0/328
All	All	0.23	0/24209	0.41	0/32672

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	F	0	1
2	C	0	3
2	D	0	1
3	K	0	10
3	M	0	3
All	All	0	19

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	ARG	Peptide
2	C	158	GLU	Peptide
2	C	45	GLU	Peptide
2	C	46	VAL	Peptide
2	D	2	ILE	Peptide
1	F	96	GLY	Peptide
3	K	102	ALA	Peptide
3	K	103	TYR	Peptide
3	K	104	VAL	Peptide
3	K	108	THR	Peptide
3	K	111	SER	Peptide
3	K	114	THR	Peptide
3	K	115	ILE	Peptide
3	K	116	LEU	Peptide
3	K	117	LYS	Peptide
3	K	28	GLN	Peptide
3	M	110	LYS	Peptide
3	M	111	SER	Peptide
3	M	134	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3213	0	3332	159	0
1	B	3096	0	3207	160	0
1	E	3213	0	3332	203	0
1	F	3213	0	3334	197	0
2	C	2134	0	2242	96	0
2	D	2134	0	2242	101	0
2	G	2134	0	2242	109	0
2	H	2134	0	2242	106	0
3	K	1032	0	1073	59	0
3	L	174	0	173	10	0
3	M	1102	0	1148	89	0
3	N	244	0	246	12	0
All	All	23823	0	24813	1261	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 26.

All (1261) 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:D:5:ARG:HA	2:D:127:TRP:HE1	1.09	1.13
3:M:109:CYS:SG	3:M:127:CYS:HA	1.91	1.11
2:C:48:SER:HB2	2:C:50:TRP:HD1	1.18	1.08
3:M:111:SER:HB3	3:M:112:LEU:CG	1.84	1.07
1:E:330:ARG:HH11	1:E:330:ARG:HG3	1.16	1.06
3:M:126:VAL:O	3:M:126:VAL:HG13	1.59	1.02
3:K:84:GLN:HG3	3:K:84:GLN:O	1.58	1.00
1:E:35:SER:HB2	1:E:38:SER:HB2	1.44	0.99
3:M:111:SER:CB	3:M:112:LEU:HG	1.93	0.99
2:D:43:TRP:CD1	2:D:50:TRP:HA	1.97	0.99
1:B:360:SER:HA	1:B:365:THR:HG22	1.45	0.98
3:L:18:LEU:HG	3:L:19:PRO:HD2	1.43	0.98
3:M:125:ILE:HG12	3:M:126:VAL:H	1.27	0.97
3:M:111:SER:HB3	3:M:112:LEU:HG	0.99	0.97
1:E:48:LYS:HG3	1:E:219:ARG:HH22	1.28	0.97
2:C:48:SER:HB2	2:C:50:TRP:CD1	2.01	0.96
2:C:151:LEU:HD12	2:C:161:VAL:HG23	1.47	0.96
2:D:214:LEU:HA	2:D:233:GLY:HA2	1.48	0.95
1:A:207:ARG:HG3	1:A:207:ARG:HH11	1.28	0.95
1:A:17:HIS:HD2	1:A:128:GLN:HB2	1.30	0.95
1:A:48:LYS:HG2	1:A:219:ARG:HH11	1.33	0.94
3:N:30:LEU:HB3	3:N:31:PRO:HD3	1.50	0.93
2:G:157:PRO:HB2	2:G:160:TRP:CD1	2.03	0.92
1:A:207:ARG:CG	1:A:207:ARG:HH11	1.81	0.92
1:E:129:THR:HA	1:E:132:HIS:HD2	1.35	0.92
1:F:252:GLU:HG2	1:F:275:LYS:HG2	1.53	0.90
1:F:53:GLU:HG3	1:F:88:ARG:HH21	1.36	0.90
2:D:5:ARG:HA	2:D:127:TRP:NE1	1.88	0.89
2:C:90:ARG:HB3	2:C:91:ARG:HH11	1.37	0.89
3:M:137:LYS:HB3	3:M:138:PRO:HD3	1.55	0.89
1:E:335:LEU:HD21	1:E:348:VAL:HB	1.53	0.89
2:C:89:GLU:HA	2:C:92:LYS:HB3	1.54	0.89
2:C:45:GLU:HA	2:C:84:LYS:NZ	1.87	0.89
2:G:224:ALA:HB3	2:G:225:PRO:HD3	1.55	0.88
2:C:95:LEU:HA	2:C:98:LYS:HE2	1.55	0.88
1:A:124:PHE:HB3	1:A:125:PRO:HD3	1.55	0.88
1:E:330:ARG:HH11	1:E:330:ARG:CG	1.86	0.88
1:B:394:ARG:HG2	1:B:415:ILE:HB	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:VAL:O	1:A:340:VAL:HG13	1.71	0.88
2:H:224:ALA:HB3	2:H:225:PRO:HD3	1.52	0.87
1:E:338:ARG:HD2	1:E:345:MET:HG3	1.53	0.87
3:K:101:LYS:HB3	3:K:118:LYS:HE2	1.56	0.87
2:D:65:ILE:HG21	2:D:90:ARG:HE	1.40	0.87
1:E:22:LYS:HD3	1:E:97:HIS:CE1	2.08	0.86
3:M:54:ILE:HG13	3:M:56:ARG:HG2	1.55	0.86
2:G:161:VAL:HG22	2:G:165:LEU:HG	1.57	0.86
1:B:58:VAL:HG12	1:B:86:LEU:HD21	1.57	0.86
2:G:180:SER:HB3	2:G:228:ARG:HD2	1.58	0.86
2:G:186:ARG:HH11	2:G:186:ARG:CG	1.89	0.85
1:A:354:LYS:HA	1:A:369:ILE:HG23	1.57	0.85
1:B:367:LEU:HB2	1:B:383:ARG:NH1	1.92	0.85
1:E:398:SER:HA	1:E:407:MET:HA	1.57	0.85
3:K:70:ALA:O	3:K:72:PRO:HD3	1.77	0.84
2:G:186:ARG:HH11	2:G:186:ARG:HG3	1.38	0.84
2:G:137:ILE:HD12	2:G:138:THR:H	1.42	0.84
1:F:333:TYR:HA	1:F:411:GLY:HA2	1.60	0.83
1:E:242:ILE:HG23	1:E:291:PRO:HA	1.58	0.83
1:B:360:SER:HB2	1:B:396:VAL:HG12	1.60	0.83
1:B:287:LYS:HD2	1:B:288:GLU:HG3	1.58	0.83
1:B:107:GLY:HA2	1:B:110:LEU:HD13	1.60	0.83
2:H:8:LEU:HD12	2:H:73:ARG:HD2	1.58	0.83
2:C:90:ARG:HD3	2:C:91:ARG:HH12	1.44	0.83
1:A:99:VAL:HG21	1:A:103:THR:HG23	1.58	0.83
1:A:17:HIS:CD2	1:A:128:GLN:HB2	2.15	0.82
1:B:184:SER:HB2	1:B:187:HIS:HD2	1.45	0.82
1:B:367:LEU:HB2	1:B:383:ARG:HH12	1.41	0.82
2:H:20:LYS:HE3	2:H:30:SER:HB3	1.59	0.82
1:E:22:LYS:HD3	1:E:97:HIS:ND1	1.95	0.82
1:E:105:LEU:HA	1:E:109:ALA:HB3	1.61	0.81
1:F:151:VAL:HG11	1:F:182:PRO:HB3	1.63	0.81
1:E:339:VAL:HG12	1:E:406:ARG:HH22	1.46	0.81
1:E:394:ARG:H	1:E:394:ARG:HD2	1.45	0.81
1:B:392:ASN:HB3	1:B:415:ILE:HA	1.63	0.80
1:E:43:ARG:HG2	1:E:280:ARG:HG2	1.61	0.80
1:B:17:HIS:CE1	1:B:21:GLY:HA3	2.17	0.80
1:F:21:GLY:HA2	1:F:24:THR:HB	1.62	0.80
2:G:59:LYS:H	2:G:62:ARG:HD3	1.46	0.80
3:M:43:ILE:HG22	3:M:82:VAL:HA	1.63	0.79
1:A:399:ARG:HB3	1:A:406:ARG:HG2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:90:ARG:HB3	2:C:91:ARG:NH1	1.96	0.79
1:B:46:THR:HG21	1:B:49:LEU:HB2	1.64	0.79
1:F:53:GLU:HG3	1:F:88:ARG:NH2	1.97	0.79
2:G:157:PRO:HB2	2:G:160:TRP:NE1	1.97	0.78
1:F:154:VAL:HB	1:F:158:GLU:HB2	1.66	0.78
2:C:48:SER:CB	2:C:50:TRP:HD1	1.95	0.78
1:F:43:ARG:HB2	1:F:48:LYS:HA	1.65	0.78
1:B:329:ILE:HD11	1:B:380:VAL:HB	1.66	0.77
3:N:18:LEU:HB3	3:N:19:PRO:HD3	1.66	0.77
2:D:65:ILE:CG2	2:D:90:ARG:HE	1.97	0.77
1:E:48:LYS:CG	1:E:219:ARG:HH22	1.97	0.76
1:E:32:ILE:HG12	1:E:33:TRP:H	1.49	0.76
1:E:46:THR:HG23	1:E:219:ARG:HH11	1.51	0.75
1:B:19:ASP:HB3	1:B:96:GLY:HA2	1.68	0.75
1:E:48:LYS:HG2	1:E:219:ARG:HH12	1.50	0.75
1:E:129:THR:HA	1:E:132:HIS:CD2	2.19	0.75
1:A:73:SER:HB3	1:A:75:LYS:HG2	1.68	0.75
1:F:17:HIS:CE1	1:F:19:ASP:HB2	2.22	0.75
1:B:139:ILE:HA	1:B:394:ARG:HH12	1.52	0.75
2:G:11:GLU:HG3	2:G:70:ARG:NH1	2.02	0.74
1:A:401:ILE:HG12	1:A:402:ALA:H	1.50	0.74
1:B:105:LEU:HD21	1:B:394:ARG:HH11	1.53	0.74
1:F:20:HIS:HE1	1:F:150:LYS:NZ	1.86	0.74
1:F:242:ILE:HD12	1:F:242:ILE:H	1.53	0.74
2:D:132:LYS:HE2	2:D:150:ILE:HG23	1.68	0.74
2:H:184:THR:HG22	2:H:226:ARG:HG2	1.69	0.73
2:G:162:LYS:HB3	2:G:163:PRO:HD3	1.70	0.73
1:E:331:ILE:HG22	1:E:333:TYR:H	1.53	0.73
3:M:18:LEU:HB3	3:M:19:PRO:HD3	1.70	0.73
1:B:234:LYS:HD2	1:B:235:GLY:H	1.53	0.73
1:E:46:THR:HG22	1:E:219:ARG:HE	1.54	0.73
1:F:357:LEU:HB3	1:F:399:ARG:HA	1.70	0.72
3:M:137:LYS:CB	3:M:138:PRO:HD3	2.17	0.72
1:E:74:CYS:HB2	1:E:83:PRO:HG3	1.71	0.72
2:G:18:THR:HG22	2:G:63:LYS:HG2	1.69	0.72
1:E:342:ALA:HB1	1:E:343:LYS:HD2	1.71	0.72
1:E:149:ASN:HD21	1:E:185:ALA:H	1.38	0.72
1:B:329:ILE:O	1:B:379:GLU:HA	1.90	0.72
2:G:4:SER:HA	2:G:127:TRP:CH2	2.24	0.72
2:H:57:VAL:HB	2:H:62:ARG:HG3	1.70	0.72
2:C:105:LYS:HE3	2:C:105:LYS:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:LEU:HD21	2:G:186:ARG:HH12	1.53	0.72
1:F:329:ILE:HD13	1:F:331:ILE:HD13	1.71	0.71
1:E:339:VAL:CG1	1:E:406:ARG:HH22	2.04	0.71
1:E:406:ARG:HH11	1:E:406:ARG:HA	1.56	0.71
1:F:414:GLU:HG3	1:F:415:ILE:HG13	1.70	0.71
1:A:343:LYS:O	1:A:344:GLU:HB2	1.88	0.71
2:D:159:ILE:HG23	2:D:162:LYS:HE3	1.72	0.71
3:K:46:ASN:HD21	3:K:49:GLU:HB2	1.56	0.71
1:A:17:HIS:HD2	1:A:128:GLN:CB	2.02	0.71
1:E:401:ILE:HG12	1:E:402:ALA:H	1.55	0.71
1:E:48:LYS:HG3	1:E:219:ARG:NH2	2.05	0.71
1:E:104:MET:HA	1:E:108:ALA:HB3	1.72	0.71
2:C:45:GLU:HA	2:C:84:LYS:HZ1	1.54	0.71
1:F:330:ARG:NH1	1:F:415:ILE:HD12	2.06	0.70
1:B:120:ALA:HB2	1:B:151:VAL:HG12	1.74	0.70
3:M:126:VAL:O	3:M:126:VAL:CG1	2.33	0.70
1:F:313:GLY:HA2	1:F:363:SER:HB3	1.72	0.70
2:D:90:ARG:O	2:D:94:ASN:HB2	1.92	0.70
1:F:184:SER:HB2	1:F:187:HIS:HB2	1.73	0.70
1:E:334:ASN:HD22	1:E:411:GLY:HA2	1.55	0.70
2:D:123:GLU:HA	2:D:127:TRP:HE3	1.57	0.69
2:D:43:TRP:HD1	2:D:50:TRP:HA	1.56	0.69
3:K:44:ILE:HG22	3:K:46:ASN:H	1.57	0.69
1:E:19:ASP:O	1:E:22:LYS:HG2	1.92	0.69
1:E:357:LEU:HD22	1:E:370:VAL:HG21	1.75	0.69
2:H:249:ASN:HA	2:H:252:LYS:HB3	1.74	0.69
1:B:209:LEU:HD11	1:B:290:LYS:HE2	1.73	0.69
1:A:359:LEU:HD22	1:A:382:LEU:HD11	1.74	0.69
1:A:15:VAL:HB	1:A:132:HIS:CE1	2.27	0.69
2:H:213:SER:HB3	2:H:234:THR:HG22	1.72	0.69
2:C:224:ALA:HB3	2:C:225:PRO:HD3	1.74	0.69
3:M:108:THR:CG2	3:M:126:VAL:HG23	2.23	0.69
1:F:336:LEU:HD23	1:F:339:VAL:HG22	1.75	0.69
1:F:17:HIS:HA	1:F:128:GLN:HG3	1.74	0.69
1:E:333:TYR:CG	1:E:333:TYR:O	2.43	0.69
1:A:329:ILE:HG12	1:A:382:LEU:HD21	1.75	0.69
2:D:37:LEU:HD23	2:D:37:LEU:H	1.58	0.69
1:F:274:THR:HG22	1:F:275:LYS:H	1.57	0.68
1:B:250:ASP:HA	1:B:275:LYS:HD3	1.74	0.68
2:C:16:ILE:HG12	2:C:65:ILE:HG12	1.75	0.68
1:E:330:ARG:NH1	1:E:330:ARG:HG3	1.97	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:251:ILE:HG23	2:G:255:LYS:HE2	1.75	0.68
1:A:22:LYS:HD2	1:A:23:THR:N	2.07	0.68
1:E:64:LYS:HB3	1:E:65:PRO:HD3	1.75	0.68
1:F:287:LYS:H	1:F:287:LYS:HD3	1.58	0.68
1:F:329:ILE:HD11	1:F:380:VAL:HB	1.75	0.68
1:A:17:HIS:CE1	1:A:127:PRO:HD2	2.28	0.68
2:G:120:ASP:HA	2:G:123:GLU:HG2	1.73	0.68
3:M:56:ARG:HD2	3:M:60:ILE:HD13	1.75	0.68
1:E:339:VAL:HG12	1:E:406:ARG:NH2	2.08	0.68
1:A:287:LYS:H	1:A:287:LYS:HD3	1.58	0.68
2:C:17:ALA:HB2	2:C:31:LEU:HD23	1.75	0.68
2:G:200:ILE:HG23	2:G:219:ILE:HD12	1.76	0.68
2:H:15:LEU:HA	2:H:93:LYS:HE2	1.76	0.68
1:F:105:LEU:HD23	1:F:396:VAL:HG13	1.76	0.68
1:B:18:VAL:O	1:B:22:LYS:HD3	1.94	0.67
1:A:399:ARG:HE	1:A:406:ARG:HG2	1.58	0.67
1:E:17:HIS:ND1	1:E:128:GLN:HB3	2.08	0.67
1:A:327:TRP:CD2	1:A:385:PRO:HG3	2.29	0.67
1:F:99:VAL:HG12	1:F:104:MET:HG3	1.77	0.67
1:B:398:SER:HA	1:B:407:MET:HB3	1.76	0.67
1:F:40:GLU:HG2	3:M:137:LYS:CD	2.25	0.67
1:F:21:GLY:HA2	1:F:24:THR:CB	2.24	0.67
3:K:107:SER:O	3:K:108:THR:HG23	1.94	0.67
2:H:51:VAL:HG12	2:H:52:LYS:H	1.60	0.67
3:M:111:SER:HB2	3:M:129:ALA:CB	2.25	0.67
1:B:360:SER:HB3	1:B:395:THR:HA	1.76	0.67
2:H:5:ARG:HG2	2:H:127:TRP:NE1	2.09	0.67
1:B:213:PRO:HG2	1:B:318:LEU:HD11	1.77	0.66
2:H:120:ASP:HA	2:H:124:GLN:HG2	1.77	0.66
3:K:45:ARG:HA	3:K:78:LYS:HD2	1.76	0.66
2:G:86:THR:HG22	2:G:87:ASP:H	1.59	0.66
1:A:22:LYS:HB3	1:A:117:VAL:HG11	1.77	0.66
2:D:43:TRP:NE1	2:D:50:TRP:HA	2.09	0.66
2:H:186:ARG:HD3	2:H:225:PRO:HB3	1.76	0.66
2:D:162:LYS:HB2	2:D:163:PRO:HD3	1.75	0.66
1:E:333:TYR:CD2	1:E:333:TYR:O	2.49	0.66
1:E:124:PHE:CD1	1:E:125:PRO:HA	2.31	0.66
2:C:22:VAL:HG13	2:C:27:SER:HB2	1.78	0.66
1:A:22:LYS:HD2	1:A:23:THR:H	1.58	0.66
3:M:104:VAL:HG12	3:M:105:GLU:HG3	1.76	0.66
1:B:142:LYS:HD3	1:B:142:LYS:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:LYS:HB3	2:H:154:ALA:HB1	1.76	0.66
3:K:115:ILE:CG2	3:K:115:ILE:O	2.44	0.66
3:M:61:CYS:HA	3:M:64:TYR:HB3	1.77	0.65
3:M:98:ARG:O	3:M:99:PHE:HB2	1.96	0.65
1:A:340:VAL:O	1:A:340:VAL:CG1	2.42	0.65
1:A:164:ARG:NH1	3:K:5:LYS:HD2	2.11	0.65
1:F:97:HIS:CE1	1:F:101:MET:SD	2.90	0.65
2:D:49:LYS:HA	2:D:49:LYS:HE2	1.78	0.65
3:K:69:LEU:HB3	3:K:86:LYS:HG3	1.79	0.65
1:E:150:LYS:HZ3	1:E:186:LEU:HD11	1.61	0.65
2:H:110:VAL:HG11	2:H:161:VAL:HG23	1.77	0.65
1:A:64:LYS:HB3	1:A:65:PRO:HA	1.77	0.65
1:A:3:TRP:CD1	1:A:85:PHE:HB2	2.31	0.65
2:H:124:GLN:HB3	2:H:157:PRO:HG2	1.78	0.65
1:F:184:SER:CB	1:F:187:HIS:HB2	2.26	0.65
1:F:147:VAL:HG12	1:F:181:ILE:HB	1.79	0.65
1:E:360:SER:H	1:E:395:THR:HG23	1.62	0.65
1:A:37:HIS:CD2	1:A:40:GLU:HB2	2.31	0.65
3:K:41:THR:HG23	3:K:88:SER:HB2	1.77	0.65
2:C:45:GLU:HA	2:C:84:LYS:HZ3	1.62	0.64
3:M:108:THR:HG21	3:M:126:VAL:HG23	1.79	0.64
1:B:136:LEU:HA	1:B:139:ILE:HB	1.78	0.64
1:F:331:ILE:HG23	1:F:411:GLY:HA3	1.79	0.64
1:A:59:CYS:SG	1:A:83:PRO:HG3	2.38	0.64
1:E:146:ILE:HG12	1:E:178:VAL:HG11	1.79	0.64
2:G:157:PRO:HB2	2:G:160:TRP:HE1	1.62	0.64
1:A:220:SER:O	1:A:309:ASP:HA	1.98	0.64
1:A:94:ALA:N	1:A:95:PRO:HD3	2.12	0.64
1:F:253:ILE:HD12	1:F:316:ILE:HG21	1.80	0.64
1:B:10:VAL:HG11	1:B:205:PRO:HD2	1.79	0.64
2:C:110:VAL:HA	2:C:113:LYS:HD2	1.80	0.64
1:B:333:TYR:HB2	1:B:410:TRP:HB3	1.80	0.64
2:H:111:SER:HA	2:H:114:LEU:HB2	1.79	0.64
1:F:214:VAL:HG22	1:F:317:THR:HG22	1.80	0.64
1:E:243:ILE:HD12	1:E:244:GLN:HG2	1.78	0.64
2:D:4:SER:OG	2:D:5:ARG:N	2.31	0.63
1:F:43:ARG:HD3	1:F:48:LYS:HG2	1.80	0.63
1:B:101:MET:HG3	1:B:104:MET:HE3	1.78	0.63
1:B:17:HIS:CG	1:B:18:VAL:H	2.17	0.63
2:D:148:GLU:HB2	2:D:162:LYS:HD2	1.79	0.63
1:F:97:HIS:HE1	1:F:101:MET:CE	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:132:LYS:HD2	2:C:154:ALA:HB2	1.80	0.63
1:A:166:ILE:HD12	1:A:180:ILE:HD13	1.80	0.63
2:G:123:GLU:HA	2:G:127:TRP:CD1	2.33	0.63
2:D:184:THR:HG23	2:D:264:VAL:HG21	1.79	0.63
3:K:60:ILE:HA	3:K:64:TYR:HB2	1.81	0.63
1:F:15:VAL:HB	1:F:132:HIS:ND1	2.14	0.63
2:H:214:LEU:HA	2:H:233:GLY:HA2	1.79	0.63
1:A:254:LYS:HE3	1:A:256:LEU:HD11	1.78	0.63
1:F:368:GLY:HA3	1:F:382:LEU:HA	1.81	0.63
3:M:37:ASN:HD21	3:M:40:ASN:HB2	1.64	0.62
1:F:14:VAL:HG12	1:F:115:ILE:HB	1.81	0.62
1:E:351:ILE:HG22	1:E:352:ARG:H	1.64	0.62
2:H:116:LEU:HD22	2:H:120:ASP:H	1.64	0.62
1:E:305:LEU:HD21	2:G:186:ARG:NH1	2.12	0.62
2:H:86:THR:HB	2:H:89:GLU:HG3	1.81	0.62
3:M:118:LYS:HB2	3:M:124:TYR:HB3	1.82	0.62
1:A:112:ASP:HB3	1:A:205:PRO:HG2	1.81	0.62
3:M:63:LYS:HG3	3:M:66:LEU:HD13	1.80	0.62
2:C:160:TRP:C	2:C:163:PRO:HD2	2.19	0.62
1:E:34:THR:HG22	3:M:138:PRO:HB2	1.81	0.62
2:H:31:LEU:HD12	2:H:37:LEU:HD21	1.80	0.62
1:E:263:LYS:HE3	1:E:266:LYS:HZ3	1.62	0.62
1:B:150:LYS:HE3	1:B:186:LEU:HD11	1.81	0.62
2:D:159:ILE:HG22	2:D:163:PRO:HD3	1.82	0.62
1:E:358:MET:O	1:E:397:ILE:HA	2.00	0.62
1:B:335:LEU:HB2	1:B:410:TRP:HB2	1.81	0.62
3:K:54:ILE:HB	3:K:104:VAL:HG21	1.80	0.62
3:M:135:PRO:C	3:M:136:VAL:HG23	2.18	0.62
1:E:43:ARG:NE	1:E:280:ARG:HD3	2.15	0.62
1:A:215:MET:HA	1:A:242:ILE:HA	1.80	0.62
2:D:161:VAL:HG12	2:D:165:LEU:HG	1.82	0.62
2:H:65:ILE:HD13	2:H:90:ARG:HA	1.82	0.62
2:H:130:GLU:HG3	2:H:136:PRO:HG3	1.81	0.62
2:G:264:VAL:O	2:G:266:LYS:N	2.33	0.62
2:C:235:ASN:HB3	2:C:238:GLU:HB2	1.81	0.61
3:M:29:SER:HB3	3:M:53:ARG:HH21	1.64	0.61
3:M:109:CYS:SG	3:M:127:CYS:CA	2.79	0.61
1:A:73:SER:HB3	1:A:75:LYS:HE2	1.82	0.61
2:G:214:LEU:HA	2:G:233:GLY:CA	2.30	0.61
1:F:367:LEU:HB2	1:F:383:ARG:HD2	1.82	0.61
2:D:15:LEU:HA	2:D:93:LYS:HE2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:HIS:ND1	1:F:19:ASP:HB2	2.15	0.61
1:B:59:CYS:H	1:B:67:ALA:HB1	1.65	0.61
2:D:5:ARG:CA	2:D:127:TRP:HE1	1.99	0.61
1:E:351:ILE:HD12	1:E:357:LEU:HD21	1.82	0.61
2:C:118:GLU:O	2:C:122:TRP:HD1	1.84	0.61
2:C:214:LEU:H	2:C:214:LEU:HD13	1.64	0.61
1:E:218:ILE:HG12	1:E:240:GLY:HA2	1.81	0.61
1:A:175:ALA:HB1	1:A:178:VAL:HG21	1.82	0.61
1:E:223:VAL:HG23	1:E:237:VAL:HG21	1.83	0.61
1:B:163:TYR:HE2	3:L:11:LEU:HD22	1.66	0.61
1:F:150:LYS:HE2	1:F:186:LEU:HD22	1.83	0.61
2:C:122:TRP:HB3	2:C:127:TRP:CZ3	2.36	0.61
2:D:159:ILE:HA	2:D:162:LYS:HE2	1.83	0.61
2:G:214:LEU:HA	2:G:233:GLY:HA2	1.83	0.61
1:E:361:VAL:HB	1:E:393:ILE:HG21	1.82	0.61
2:D:44:SER:HB3	2:D:50:TRP:CH2	2.36	0.60
1:E:404:ARG:HH21	1:E:406:ARG:HD3	1.65	0.60
1:E:43:ARG:HG3	1:E:296:ALA:HB3	1.81	0.60
2:D:72:ASP:HB2	2:D:77:THR:HB	1.82	0.60
1:F:398:SER:HA	1:F:408:ILE:HD11	1.83	0.60
3:K:35:ILE:HG22	3:K:36:LEU:H	1.66	0.60
2:C:67:LYS:HB3	2:C:85:VAL:HG22	1.83	0.60
1:A:399:ARG:NE	1:A:406:ARG:HG2	2.16	0.60
2:D:42:PRO:HB2	2:D:45:GLU:HG2	1.84	0.60
1:E:46:THR:CG2	1:E:219:ARG:HE	2.14	0.60
1:B:349:ASP:O	1:B:351:ILE:HD12	2.01	0.60
3:M:133:GLN:HG3	3:M:133:GLN:O	2.01	0.60
2:G:59:LYS:N	2:G:62:ARG:HD3	2.15	0.60
1:A:399:ARG:HB3	1:A:406:ARG:CG	2.31	0.60
2:D:17:ALA:HB2	2:D:31:LEU:HD23	1.83	0.60
1:A:170:THR:HB	1:A:175:ALA:O	2.01	0.60
1:B:184:SER:HB2	1:B:187:HIS:CD2	2.32	0.60
2:H:213:SER:HB3	2:H:234:THR:CG2	2.32	0.60
1:F:263:LYS:HE2	1:F:264:GLN:HE21	1.65	0.60
2:G:160:TRP:CE2	2:G:161:VAL:HB	2.37	0.60
1:B:103:THR:HG23	1:B:107:GLY:HA3	1.83	0.60
2:D:125:VAL:HG21	2:D:165:LEU:HD21	1.83	0.60
1:A:336:LEU:HD13	1:A:409:GLY:H	1.67	0.59
2:H:116:LEU:HD21	2:H:119:LYS:HB3	1.83	0.59
1:E:214:VAL:HG22	1:E:317:THR:HG22	1.84	0.59
1:F:3:TRP:CZ3	1:F:72:PRO:HA	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:ILE:HA	1:E:399:ARG:HH12	1.66	0.59
2:G:4:SER:HA	2:G:127:TRP:HH2	1.65	0.59
2:C:184:THR:HG22	2:C:226:ARG:HB3	1.83	0.59
1:E:22:LYS:HG3	1:E:23:THR:N	2.18	0.59
1:B:24:THR:HG21	1:B:186:LEU:HD23	1.84	0.59
1:B:259:LEU:HG	1:B:272:ILE:HD11	1.85	0.59
2:G:41:LEU:HD13	2:G:81:SER:HA	1.84	0.59
1:F:373:VAL:HA	1:F:378:ILE:HG22	1.84	0.59
2:G:69:ILE:HD11	2:G:81:SER:HB2	1.84	0.59
1:A:124:PHE:CB	1:A:125:PRO:HD3	2.31	0.59
1:A:15:VAL:HG23	1:A:116:LEU:HA	1.84	0.59
1:F:191:ILE:HD12	1:F:192:ASP:N	2.18	0.59
1:B:242:ILE:H	1:B:242:ILE:HD12	1.68	0.59
1:E:187:HIS:HB2	1:E:189:ILE:HG13	1.85	0.58
1:F:32:ILE:HD11	1:F:52:ALA:HA	1.84	0.58
3:M:125:ILE:HG23	3:M:126:VAL:N	2.19	0.58
1:A:15:VAL:HB	1:A:132:HIS:HE1	1.68	0.58
2:D:41:LEU:CD1	2:D:81:SER:HA	2.33	0.58
1:F:156:LYS:O	1:F:160:LEU:HB2	2.04	0.58
1:F:317:THR:HG21	1:F:323:VAL:HG21	1.86	0.58
1:B:392:ASN:CB	1:B:415:ILE:HA	2.33	0.58
3:K:115:ILE:O	3:K:115:ILE:HG22	2.03	0.58
2:D:264:VAL:HG12	2:D:265:LYS:H	1.68	0.58
1:E:220:SER:HB3	1:E:309:ASP:HA	1.86	0.58
1:F:116:LEU:HB3	1:F:146:ILE:HG13	1.85	0.58
3:N:8:VAL:HB	3:N:11:LEU:HD12	1.84	0.58
1:E:43:ARG:HA	1:E:296:ALA:HB2	1.86	0.58
3:K:27:THR:HG21	3:K:31:PRO:HG3	1.85	0.58
1:A:373:VAL:HA	1:A:378:ILE:HD13	1.85	0.58
2:C:142:LYS:HE2	2:C:150:ILE:HD12	1.86	0.58
3:M:66:LEU:HD12	3:M:72:PRO:HB3	1.86	0.58
1:E:182:PRO:HG3	3:M:7:TYR:CE1	2.38	0.58
2:H:19:VAL:HA	2:H:29:VAL:HG23	1.86	0.58
2:D:191:LEU:O	2:D:195:LYS:HB2	2.03	0.58
1:A:307:LYS:HG3	1:A:308:ALA:H	1.68	0.58
1:E:329:ILE:HD11	1:E:380:VAL:HB	1.86	0.58
3:K:24:LYS:HB3	3:K:110:LYS:HB3	1.86	0.58
2:G:96:GLN:O	2:G:100:ILE:HG13	2.03	0.58
2:C:91:ARG:H	2:C:91:ARG:HD2	1.68	0.57
1:A:242:ILE:HD12	1:A:247:PHE:HD1	1.70	0.57
1:F:51:TYR:CE1	1:F:90:SER:HB2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:224:ALA:HB1	2:D:225:PRO:HD2	1.85	0.57
1:A:97:HIS:O	1:A:98:GLU:HB3	2.04	0.57
2:G:98:LYS:HA	2:G:101:GLN:HB2	1.87	0.57
2:G:186:ARG:NH1	2:G:186:ARG:CG	2.56	0.57
2:G:87:ASP:O	2:G:91:ARG:HG2	2.05	0.57
1:F:160:LEU:O	1:F:164:ARG:HG3	2.05	0.57
1:F:53:GLU:CG	1:F:88:ARG:HH21	2.12	0.57
2:C:74:ARG:NE	2:C:74:ARG:HA	2.18	0.57
1:F:218:ILE:HG12	1:F:240:GLY:HA2	1.86	0.57
1:A:125:PRO:HG2	1:A:130:ARG:HH21	1.68	0.57
1:E:351:ILE:HB	1:E:373:VAL:HG22	1.86	0.57
1:F:173:THR:O	1:F:176:GLU:HG3	2.03	0.57
1:E:368:GLY:HA2	1:E:382:LEU:HA	1.85	0.57
2:C:96:GLN:O	2:C:100:ILE:HG13	2.05	0.57
1:B:333:TYR:HE1	1:B:378:ILE:HD11	1.70	0.57
2:G:164:LEU:O	2:G:167:GLU:HG3	2.05	0.57
2:G:29:VAL:HG12	2:G:30:SER:H	1.69	0.57
1:E:238:ILE:HD13	1:E:316:ILE:HD11	1.87	0.57
2:C:81:SER:OG	2:C:84:LYS:HB2	2.04	0.57
1:B:351:ILE:HG13	1:B:399:ARG:HH22	1.68	0.57
3:K:57:GLU:HG3	3:K:59:LYS:HG3	1.86	0.57
2:H:183:ILE:HD13	2:H:183:ILE:H	1.70	0.57
3:M:68:GLU:HG3	3:M:95:LEU:HD13	1.87	0.56
1:A:146:ILE:O	1:A:180:ILE:HA	2.05	0.56
1:F:305:LEU:HD21	2:H:186:ARG:HH22	1.70	0.56
1:A:37:HIS:CD2	1:A:47:ILE:HG21	2.39	0.56
2:C:69:ILE:HD13	2:C:81:SER:HB2	1.87	0.56
1:E:259:LEU:HG	1:E:261:VAL:HG13	1.87	0.56
2:G:160:TRP:CD2	2:G:161:VAL:HB	2.40	0.56
1:F:274:THR:HG21	1:F:301:LEU:HG	1.87	0.56
2:C:204:LEU:HD21	2:C:219:ILE:HD11	1.87	0.56
2:C:114:LEU:HD23	2:C:114:LEU:H	1.69	0.56
2:C:193:VAL:HG12	2:C:197:LYS:HE2	1.86	0.56
2:D:95:LEU:O	2:D:99:LYS:HG3	2.03	0.56
2:C:187:THR:HB	2:C:259:VAL:HA	1.86	0.56
1:F:17:HIS:CD2	1:F:118:VAL:HA	2.41	0.56
1:B:118:VAL:HG23	1:B:148:GLN:HA	1.88	0.56
3:M:54:ILE:HG13	3:M:56:ARG:CG	2.33	0.56
1:E:404:ARG:NH2	1:E:406:ARG:HD3	2.19	0.56
2:H:157:PRO:HB2	2:H:160:TRP:HB3	1.88	0.56
2:D:143:ALA:HB1	2:D:151:LEU:HG	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:235:ASN:OD1	2:G:237:LYS:HB2	2.06	0.56
1:F:404:ARG:NH1	1:F:406:ARG:HD2	2.21	0.56
1:B:146:ILE:HB	1:B:180:ILE:HG12	1.87	0.56
3:K:34:ILE:HG12	3:K:44:ILE:HD13	1.86	0.56
2:D:19:VAL:HG11	2:D:58:LEU:HB3	1.87	0.56
2:H:46:VAL:HG13	2:H:47:SER:H	1.71	0.56
2:G:123:GLU:HG3	2:G:124:GLN:HG3	1.86	0.56
1:E:286:PHE:HA	1:F:232:GLU:HG2	1.87	0.56
3:N:13:ARG:N	3:N:13:ARG:HD2	2.20	0.56
1:B:33:TRP:H	3:K:125:ILE:HD13	1.70	0.56
1:F:359:LEU:H	1:F:359:LEU:HD12	1.71	0.56
1:A:368:GLY:HA3	1:A:382:LEU:HD13	1.88	0.56
1:A:116:LEU:HB2	1:A:144:LEU:HD11	1.86	0.56
1:A:37:HIS:HD2	1:A:40:GLU:H	1.54	0.56
1:E:281:PHE:HB2	1:E:286:PHE:HE2	1.71	0.56
1:A:207:ARG:CG	1:A:207:ARG:NH1	2.51	0.55
1:B:333:TYR:HB2	1:B:410:TRP:CD1	2.41	0.55
1:B:163:TYR:O	1:B:167:LYS:HG2	2.06	0.55
2:C:70:ARG:CB	2:C:79:ASP:HB2	2.37	0.55
3:K:25:GLU:OE2	3:K:109:CYS:HA	2.06	0.55
1:E:146:ILE:HG13	1:E:166:ILE:HD11	1.88	0.55
2:H:215:LEU:HB2	2:H:232:VAL:HG12	1.86	0.55
3:M:111:SER:HB3	3:M:112:LEU:CB	2.36	0.55
1:B:49:LEU:HD11	1:B:219:ARG:NH2	2.22	0.55
2:D:247:ILE:HA	2:D:250:LEU:HD12	1.87	0.55
1:E:225:LYS:N	1:E:225:LYS:HD2	2.22	0.55
2:D:55:ARG:NH1	2:D:59:LYS:HD3	2.22	0.55
2:D:68:VAL:HG21	2:D:71:VAL:HG13	1.87	0.55
1:A:366:THR:HB	1:A:384:ARG:CG	2.37	0.55
1:B:305:LEU:HD21	2:D:186:ARG:NH2	2.20	0.55
1:B:215:MET:SD	1:B:316:ILE:HD12	2.47	0.55
1:E:46:THR:HG22	1:E:219:ARG:NE	2.20	0.55
2:D:71:VAL:HG12	2:D:78:VAL:HG22	1.88	0.55
1:E:394:ARG:H	1:E:394:ARG:CD	2.19	0.55
1:E:334:ASN:HB3	1:E:410:TRP:CE2	2.41	0.55
1:E:161:SER:O	1:E:165:GLN:HG3	2.05	0.55
1:E:15:VAL:HG11	1:E:136:LEU:HD11	1.88	0.55
1:B:170:THR:HB	1:B:175:ALA:HB3	1.89	0.55
1:B:12:ILE:HG22	1:B:13:GLY:H	1.72	0.55
1:A:69:VAL:HG12	1:A:76:SER:HB3	1.89	0.55
1:B:175:ALA:HA	1:B:178:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:PRO:HD3	2:G:193:VAL:HG13	1.89	0.55
1:F:220:SER:HB2	1:F:306:THR:HB	1.89	0.55
1:E:332:LYS:HB2	1:E:412:LEU:HD13	1.89	0.55
1:A:214:VAL:O	1:A:243:ILE:HG13	2.06	0.54
1:B:17:HIS:HA	1:B:128:GLN:NE2	2.22	0.54
2:H:37:LEU:H	2:H:37:LEU:HD23	1.73	0.54
1:E:12:ILE:O	1:E:91:PHE:HA	2.08	0.54
2:H:136:PRO:O	2:H:140:ILE:HG13	2.08	0.54
1:B:12:ILE:HG21	1:B:115:ILE:HG13	1.89	0.54
1:B:97:HIS:HB2	1:B:99:VAL:HG22	1.90	0.54
1:F:238:ILE:HD13	1:F:316:ILE:HD11	1.90	0.54
1:A:242:ILE:O	1:A:291:PRO:HA	2.08	0.54
1:E:194:LEU:O	1:E:198:ILE:HG13	2.07	0.54
1:B:144:LEU:HG	1:B:145:ILE:N	2.23	0.54
1:F:327:TRP:CE2	1:F:385:PRO:HG3	2.43	0.54
3:M:125:ILE:HG12	3:M:126:VAL:N	2.10	0.54
1:A:224:ASN:HD21	1:A:234:LYS:H	1.54	0.54
1:F:34:THR:HB	1:F:50:GLY:HA3	1.90	0.54
1:E:48:LYS:HG2	1:E:219:ARG:NH1	2.21	0.54
1:B:397:ILE:HB	1:B:409:GLY:HA3	1.90	0.54
1:E:225:LYS:HD2	1:E:225:LYS:H	1.73	0.54
1:F:262:GLU:HA	1:F:267:VAL:HG12	1.90	0.54
2:G:115:LYS:HD3	2:G:115:LYS:H	1.72	0.54
1:F:49:LEU:HA	1:F:94:ALA:HB2	1.90	0.54
3:K:72:PRO:HD2	3:K:83:ILE:O	2.08	0.54
1:A:37:HIS:NE2	1:A:47:ILE:HG21	2.23	0.54
2:D:26:GLY:HA3	2:D:40:PHE:CZ	2.43	0.54
1:A:194:LEU:O	1:A:198:ILE:HG13	2.08	0.54
3:M:98:ARG:O	3:M:98:ARG:HD3	2.08	0.54
1:E:360:SER:HB3	1:E:365:THR:HG22	1.90	0.54
1:F:14:VAL:HG23	1:F:93:ASP:HB3	1.89	0.54
1:F:218:ILE:O	1:F:312:LEU:HD13	2.08	0.54
2:G:59:LYS:HG3	2:G:62:ARG:HH11	1.72	0.53
1:B:49:LEU:HD11	1:B:219:ARG:HH22	1.73	0.53
2:C:143:ALA:HA	2:C:150:ILE:HG13	1.89	0.53
2:D:18:THR:HB	2:D:63:LYS:HG2	1.90	0.53
1:A:259:LEU:O	1:A:269:TYR:HA	2.09	0.53
1:E:160:LEU:O	1:E:164:ARG:HG2	2.07	0.53
1:F:65:PRO:O	1:F:192:ASP:HB2	2.08	0.53
1:B:353:ALA:HA	1:B:370:VAL:HB	1.90	0.53
1:E:359:LEU:HD21	1:E:380:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:HB	1:A:384:ARG:HG2	1.90	0.53
2:H:202:LYS:HD2	2:H:253:ILE:HG12	1.91	0.53
2:G:187:THR:HB	2:G:259:VAL:HG13	1.89	0.53
2:G:17:ALA:HB2	2:G:31:LEU:HD23	1.90	0.53
2:H:54:ILE:HD12	2:H:55:ARG:NH1	2.24	0.53
1:B:75:LYS:HA	1:B:75:LYS:HE2	1.89	0.53
1:F:330:ARG:HH11	1:F:415:ILE:HD12	1.73	0.53
2:H:5:ARG:HG2	2:H:127:TRP:CD1	2.44	0.53
1:A:37:HIS:NE2	1:A:40:GLU:HB2	2.24	0.53
2:H:170:LYS:N	2:H:170:LYS:HE2	2.24	0.53
1:B:358:MET:HA	1:B:367:LEU:HD23	1.89	0.53
1:F:339:VAL:HG23	1:F:348:VAL:HG12	1.91	0.53
1:A:49:LEU:HD22	1:A:94:ALA:HA	1.89	0.53
2:D:184:THR:HA	2:D:225:PRO:O	2.09	0.53
1:E:25:LEU:HD21	1:E:194:LEU:HD11	1.90	0.53
1:B:19:ASP:O	1:B:23:THR:HB	2.09	0.53
1:B:410:TRP:CD1	1:B:411:GLY:N	2.74	0.53
1:F:218:ILE:HD11	1:F:219:ARG:NH1	2.23	0.53
1:B:13:GLY:HA3	1:B:111:MET:SD	2.48	0.53
3:K:18:LEU:HB3	3:K:19:PRO:HD3	1.91	0.53
1:E:399:ARG:HD3	1:E:408:ILE:HD13	1.90	0.53
2:H:15:LEU:HB2	2:H:33:GLU:OE2	2.09	0.53
3:K:27:THR:CG2	3:K:31:PRO:HG3	2.39	0.53
1:A:235:GLY:HA2	2:C:193:VAL:HG21	1.90	0.53
2:G:202:LYS:HB3	2:G:253:ILE:HD13	1.91	0.53
2:D:185:VAL:HB	2:D:227:TYR:CE1	2.44	0.53
1:B:4:PRO:HG3	2:C:220:TYR:CZ	2.43	0.53
2:H:56:ASP:CG	2:H:57:VAL:H	2.12	0.53
1:A:392:ASN:HB2	1:A:413:VAL:H	1.74	0.53
3:K:51:CYS:HB3	3:K:62:MET:HE1	1.89	0.53
3:K:82:VAL:HG13	3:K:83:ILE:N	2.24	0.53
1:E:404:ARG:HH21	1:E:406:ARG:CD	2.21	0.53
2:H:160:TRP:CG	2:H:161:VAL:N	2.75	0.53
1:F:263:LYS:C	1:F:264:GLN:HG2	2.28	0.53
1:A:404:ARG:O	1:A:404:ARG:HD3	2.09	0.52
1:B:10:VAL:HG13	1:B:204:THR:HG23	1.90	0.52
3:M:108:THR:HG23	3:M:126:VAL:HG23	1.92	0.52
1:F:359:LEU:HD11	1:F:380:VAL:HG11	1.91	0.52
1:A:401:ILE:HG12	1:A:402:ALA:N	2.22	0.52
2:D:31:LEU:HD12	2:D:37:LEU:HD21	1.92	0.52
1:A:117:VAL:HA	1:A:147:VAL:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:113:LYS:HB3	2:G:164:LEU:HD21	1.91	0.52
2:G:247:ILE:HA	2:G:250:LEU:HD12	1.91	0.52
2:H:97:TRP:O	2:H:101:GLN:HB2	2.09	0.52
2:G:130:GLU:HA	2:G:136:PRO:HD3	1.90	0.52
2:D:65:ILE:HG22	2:D:90:ARG:HH21	1.74	0.52
1:F:17:HIS:HD1	1:F:19:ASP:HB2	1.74	0.52
1:E:124:PHE:CG	1:E:125:PRO:HA	2.44	0.52
1:B:94:ALA:HB2	1:B:98:GLU:HB2	1.91	0.52
2:C:247:ILE:HA	2:C:250:LEU:HD12	1.91	0.52
1:A:257:PRO:HB3	1:A:325:VAL:HG21	1.92	0.52
3:M:127:CYS:O	3:M:128:LEU:HB2	2.10	0.52
2:D:50:TRP:CD1	2:D:51:VAL:HG23	2.44	0.52
2:C:49:LYS:O	2:C:49:LYS:HG2	2.09	0.52
3:M:104:VAL:O	3:M:105:GLU:HB2	2.09	0.52
1:B:215:MET:HB3	1:B:316:ILE:HB	1.91	0.52
1:A:218:ILE:O	1:A:312:LEU:HD13	2.10	0.52
1:F:40:GLU:HG2	3:M:137:LYS:HD2	1.90	0.52
1:F:335:LEU:HG	1:F:336:LEU:H	1.75	0.52
2:G:177:VAL:HG22	2:G:178:LYS:H	1.73	0.52
2:D:215:LEU:HB2	2:D:232:VAL:HG13	1.92	0.52
2:H:42:PRO:HB2	2:H:45:GLU:HG2	1.92	0.52
2:D:173:GLU:HG2	2:D:176:LYS:HD3	1.92	0.52
1:F:397:ILE:HG22	1:F:398:SER:H	1.75	0.52
1:F:360:SER:HB3	1:F:396:VAL:HG23	1.92	0.52
1:F:338:ARG:HG2	1:F:346:LEU:HD23	1.91	0.52
1:B:25:LEU:HD13	1:B:117:VAL:HG22	1.91	0.52
1:B:327:TRP:CD1	1:B:327:TRP:N	2.77	0.52
3:M:65:LEU:HA	3:M:68:GLU:HG2	1.91	0.52
1:E:358:MET:HB3	1:E:398:SER:HB2	1.91	0.52
1:B:25:LEU:HD11	1:B:147:VAL:HG11	1.91	0.52
1:E:154:VAL:HG12	1:E:158:GLU:HB3	1.91	0.52
3:K:67:LYS:HG3	3:K:67:LYS:O	2.09	0.52
1:E:206:TYR:HB2	2:H:170:LYS:HE3	1.92	0.52
3:M:54:ILE:HD12	3:M:56:ARG:HE	1.74	0.51
1:F:154:VAL:HB	1:F:158:GLU:CB	2.38	0.51
2:H:33:GLU:H	2:H:33:GLU:CD	2.14	0.51
2:H:163:PRO:O	2:H:166:GLU:HG2	2.10	0.51
2:C:74:ARG:HA	2:C:74:ARG:HE	1.75	0.51
2:C:119:LYS:O	2:C:123:GLU:HB2	2.09	0.51
2:H:68:VAL:HA	2:H:80:VAL:HA	1.91	0.51
3:M:105:GLU:CG	3:M:110:LYS:HE3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:ASN:OD1	1:F:185:ALA:HB2	2.11	0.51
1:F:287:LYS:HG2	1:F:288:GLU:HG3	1.93	0.51
2:D:45:GLU:HB3	2:D:81:SER:CB	2.41	0.51
1:E:368:GLY:CA	1:E:382:LEU:HA	2.40	0.51
2:C:70:ARG:HB2	2:C:79:ASP:HB2	1.92	0.51
1:A:321:ALA:HB1	1:A:323:VAL:HG23	1.93	0.51
1:E:327:TRP:N	1:E:327:TRP:CD1	2.79	0.51
1:B:394:ARG:NH2	1:B:412:LEU:CD1	2.73	0.51
1:B:22:LYS:HG2	1:B:23:THR:N	2.26	0.51
1:E:337:GLU:HB3	1:E:338:ARG:HD3	1.93	0.51
1:B:358:MET:O	1:B:397:ILE:HA	2.09	0.51
3:M:107:SER:O	3:M:108:THR:HG22	2.11	0.51
3:K:34:ILE:HG23	3:K:44:ILE:HG12	1.92	0.51
1:E:351:ILE:HG21	1:E:370:VAL:HG11	1.91	0.51
3:M:29:SER:HB3	3:M:53:ARG:NH2	2.25	0.51
1:B:146:ILE:O	1:B:180:ILE:HA	2.11	0.51
2:H:54:ILE:HD12	2:H:55:ARG:HH11	1.75	0.51
2:D:128:LYS:HG2	2:D:155:GLY:HA3	1.92	0.51
2:C:182:LEU:HD12	2:C:264:VAL:HG21	1.93	0.51
3:M:112:LEU:HB2	3:M:129:ALA:HB1	1.92	0.51
2:C:151:LEU:HD12	2:C:161:VAL:CG2	2.29	0.51
1:E:87:ARG:NH2	1:E:198:ILE:HG22	2.25	0.51
1:A:9:GLU:HG3	1:A:10:VAL:HG23	1.92	0.51
2:D:107:LEU:HA	2:D:110:VAL:HG12	1.92	0.51
2:D:136:PRO:O	2:D:140:ILE:HG13	2.10	0.51
1:E:46:THR:CG2	1:E:219:ARG:HH11	2.23	0.51
1:A:213:PRO:HG2	1:A:318:LEU:HD11	1.93	0.51
2:C:170:LYS:O	2:C:174:GLU:HG3	2.11	0.51
3:M:106:CYS:SG	3:M:107:SER:N	2.84	0.51
3:K:69:LEU:CB	3:K:86:LYS:HG3	2.40	0.51
1:A:312:LEU:HD12	1:A:313:GLY:H	1.75	0.51
2:H:202:LYS:HD3	2:H:202:LYS:O	2.10	0.51
1:F:230:PHE:O	2:H:197:LYS:HE2	2.11	0.51
1:F:4:PRO:HG3	2:G:220:TYR:CE2	2.46	0.51
1:E:17:HIS:CE1	1:E:128:GLN:HB3	2.45	0.51
3:K:10:MET:O	3:K:13:ARG:HB3	2.11	0.51
1:A:29:ILE:HD11	1:A:194:LEU:HD12	1.92	0.51
2:H:116:LEU:CD2	2:H:120:ASP:H	2.24	0.50
3:N:12:ASP:HB3	3:N:13:ARG:HH11	1.76	0.50
1:F:40:GLU:HG2	3:M:137:LYS:HD3	1.93	0.50
1:F:163:TYR:CE2	1:F:180:ILE:HD12	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:90:ARG:O	2:H:94:ASN:HB2	2.11	0.50
1:F:389:TRP:CD1	1:F:390:SER:N	2.78	0.50
1:F:148:GLN:HB2	1:F:182:PRO:HA	1.93	0.50
1:B:7:GLN:HE22	1:B:290:LYS:H	1.60	0.50
1:F:29:ILE:HG23	1:F:195:ILE:HD11	1.92	0.50
2:D:1:MET:CE	2:D:1:MET:HA	2.41	0.50
3:M:105:GLU:HG3	3:M:110:LYS:HE3	1.92	0.50
1:F:217:VAL:HG13	1:F:238:ILE:HG23	1.91	0.50
2:H:129:LEU:HB3	2:H:136:PRO:HA	1.94	0.50
3:M:7:TYR:HE2	3:M:11:LEU:HD22	1.76	0.50
2:D:171:HIS:HA	2:D:174:GLU:HG3	1.92	0.50
1:E:110:LEU:HB2	1:E:243:ILE:HG22	1.94	0.50
1:E:110:LEU:HD12	1:E:243:ILE:HG22	1.93	0.50
1:A:404:ARG:NH1	1:A:407:MET:HE3	2.27	0.50
2:H:26:GLY:HA2	2:H:40:PHE:HE1	1.76	0.50
1:B:279:ILE:O	1:B:285:GLU:HG3	2.12	0.50
1:B:146:ILE:HG22	1:B:180:ILE:HG23	1.94	0.50
1:B:123:PRO:O	1:B:126:GLN:HG2	2.11	0.50
1:F:170:THR:HB	1:F:175:ALA:O	2.12	0.50
2:D:224:ALA:HB1	2:D:225:PRO:CD	2.42	0.50
1:F:30:THR:HA	1:F:54:THR:HB	1.92	0.50
3:M:81:LEU:HG	3:M:83:ILE:HG12	1.94	0.50
1:A:5:LYS:HZ2	1:B:228:THR:HA	1.77	0.50
1:E:391:ASN:HA	1:E:415:ILE:CD1	2.42	0.50
3:M:125:ILE:CG1	3:M:126:VAL:H	2.05	0.50
3:M:126:VAL:O	3:M:127:CYS:HB2	2.10	0.50
3:L:18:LEU:CG	3:L:19:PRO:HD2	2.29	0.50
1:E:41:LEU:HD13	1:E:46:THR:O	2.12	0.50
2:D:99:LYS:HB3	2:D:137:ILE:HG21	1.93	0.50
1:A:214:VAL:HG22	1:A:317:THR:HG22	1.94	0.50
1:E:228:THR:HG23	1:E:232:GLU:HG3	1.94	0.50
1:F:339:VAL:HG21	1:F:408:ILE:HG22	1.93	0.50
3:K:58:ASP:HB3	3:K:61:CYS:HB3	1.94	0.50
1:E:41:LEU:HB3	1:E:46:THR:HA	1.94	0.49
3:K:56:ARG:HG2	3:K:57:GLU:H	1.76	0.49
3:K:18:LEU:HA	3:K:21:LYS:HE2	1.93	0.49
3:M:60:ILE:HG23	3:M:61:CYS:H	1.77	0.49
1:F:146:ILE:O	1:F:180:ILE:HA	2.12	0.49
1:F:287:LYS:N	1:F:287:LYS:HD3	2.26	0.49
1:A:287:LYS:HE2	1:A:288:GLU:HG2	1.93	0.49
2:H:15:LEU:HA	2:H:93:LYS:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:GLU:HA	1:E:275:LYS:HB3	1.94	0.49
2:C:106:ILE:HA	2:C:109:LEU:HD12	1.94	0.49
1:A:124:PHE:CE1	1:A:166:ILE:HG12	2.47	0.49
1:E:101:MET:O	1:E:104:MET:HG2	2.11	0.49
1:E:108:ALA:HA	1:E:362:GLY:HA2	1.94	0.49
3:K:54:ILE:HG13	3:K:58:ASP:OD2	2.12	0.49
2:C:18:THR:HG22	2:C:61:ASN:HA	1.93	0.49
1:F:10:VAL:HG23	1:F:112:ASP:HB2	1.94	0.49
1:F:136:LEU:HA	1:F:139:ILE:HG22	1.94	0.49
1:A:104:MET:HE1	1:A:136:LEU:HD22	1.94	0.49
2:D:43:TRP:HD1	2:D:50:TRP:CD1	2.30	0.49
1:E:338:ARG:NH1	1:E:345:MET:CE	2.75	0.49
2:D:29:VAL:O	2:D:39:ALA:HB3	2.12	0.49
2:H:161:VAL:O	2:H:165:LEU:HB2	2.13	0.49
1:E:360:SER:O	1:E:395:THR:HA	2.12	0.49
2:G:143:ALA:HA	2:G:150:ILE:HD12	1.94	0.49
1:F:143:ASN:HB3	1:F:202:ILE:HG12	1.94	0.49
2:G:116:LEU:HD13	2:G:117:SER:H	1.77	0.49
1:E:18:VAL:HG23	1:E:21:GLY:HA3	1.95	0.49
1:E:48:LYS:CG	1:E:219:ARG:NH2	2.72	0.49
1:A:65:PRO:HD2	3:K:13:ARG:NH1	2.26	0.49
2:G:171:HIS:HB3	2:G:175:ARG:NH1	2.28	0.49
2:H:162:LYS:HB3	2:H:163:PRO:HD3	1.93	0.49
1:E:116:LEU:HB3	1:E:146:ILE:HD13	1.95	0.49
1:A:238:ILE:HG21	1:A:316:ILE:HD11	1.94	0.49
2:C:14:ILE:HG22	2:C:93:LYS:HG2	1.95	0.49
1:A:100:LEU:O	1:A:101:MET:HB2	2.13	0.49
2:G:66:VAL:HA	2:G:85:VAL:HG21	1.94	0.49
1:E:154:VAL:HB	1:E:159:ALA:N	2.28	0.49
1:E:13:GLY:HA3	1:E:111:MET:SD	2.52	0.49
1:E:262:GLU:HB2	1:E:267:VAL:HG12	1.94	0.49
2:C:160:TRP:O	2:C:163:PRO:HD2	2.12	0.49
1:F:218:ILE:O	1:F:219:ARG:HB3	2.12	0.49
1:F:340:VAL:HG22	1:F:345:MET:HG2	1.95	0.49
1:B:161:SER:O	1:B:165:GLN:HG3	2.13	0.49
1:B:394:ARG:NH2	1:B:412:LEU:HD12	2.28	0.49
1:B:281:PHE:HB2	1:B:286:PHE:HE2	1.77	0.49
2:H:148:GLU:O	2:H:152:ILE:HD13	2.13	0.49
1:B:194:LEU:O	1:B:198:ILE:HG13	2.13	0.49
3:K:84:GLN:O	3:K:86:LYS:N	2.46	0.48
1:F:124:PHE:HA	1:F:125:PRO:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:69:LEU:HD12	3:M:83:ILE:HG22	1.95	0.48
1:B:212:LYS:HG2	1:B:244:GLN:HE21	1.78	0.48
2:G:221:THR:HA	2:G:227:TYR:CD2	2.47	0.48
2:G:16:ILE:HD13	2:G:97:TRP:CD1	2.47	0.48
1:E:351:ILE:O	1:E:373:VAL:HG11	2.13	0.48
2:H:116:LEU:HD23	2:H:117:SER:N	2.27	0.48
2:D:185:VAL:HG22	2:D:261:ILE:HG12	1.95	0.48
2:D:249:ASN:HA	2:D:252:LYS:HB3	1.95	0.48
2:C:48:SER:CB	2:C:50:TRP:CD1	2.82	0.48
3:M:54:ILE:CG1	3:M:56:ARG:HE	2.27	0.48
1:A:124:PHE:HE2	1:A:169:PHE:CG	2.30	0.48
1:B:328:ASN:HA	1:B:380:VAL:O	2.13	0.48
2:G:136:PRO:O	2:G:140:ILE:HG12	2.13	0.48
1:A:27:GLN:NE2	1:A:33:TRP:HA	2.28	0.48
2:H:237:LYS:HD3	2:H:237:LYS:H	1.79	0.48
1:E:307:LYS:HD2	2:G:224:ALA:HB3	1.96	0.48
1:F:331:ILE:CG2	1:F:411:GLY:HA3	2.43	0.48
1:A:243:ILE:HD12	1:A:244:GLN:HB3	1.95	0.48
2:G:185:VAL:HB	2:G:227:TYR:CE1	2.48	0.48
1:B:329:ILE:CD1	1:B:380:VAL:HB	2.41	0.48
1:E:329:ILE:HD12	1:E:329:ILE:O	2.14	0.48
1:E:281:PHE:CE2	1:E:295:VAL:HB	2.49	0.48
2:G:8:LEU:CD1	2:G:73:ARG:HA	2.43	0.48
2:H:59:LYS:HA	2:H:59:LYS:NZ	2.29	0.48
3:K:84:GLN:C	3:K:86:LYS:H	2.16	0.48
2:G:19:VAL:HB	2:G:59:LYS:O	2.13	0.48
1:E:370:VAL:HG13	1:E:378:ILE:HG23	1.95	0.48
3:K:35:ILE:HG22	3:K:36:LEU:N	2.27	0.48
1:E:189:ILE:HG23	3:M:17:LYS:HD2	1.95	0.48
1:A:321:ALA:O	1:A:322:GLU:HB2	2.13	0.48
1:B:215:MET:HG2	1:B:216:LEU:N	2.28	0.48
1:F:43:ARG:CD	1:F:48:LYS:HG2	2.43	0.48
1:E:110:LEU:CD1	1:E:243:ILE:HA	2.44	0.48
2:D:62:ARG:HD3	2:D:63:LYS:N	2.28	0.48
1:F:213:PRO:HB2	1:F:318:LEU:HD23	1.95	0.48
2:H:201:SER:O	2:H:205:GLU:HG3	2.13	0.48
3:M:110:LYS:HD3	3:M:111:SER:O	2.14	0.48
1:F:150:LYS:HE3	1:F:185:ALA:HB3	1.95	0.48
2:H:211:TYR:O	2:H:214:LEU:HD22	2.14	0.48
1:F:248:LYS:O	1:F:276:ILE:HD12	2.14	0.48
2:C:171:HIS:O	2:C:175:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:56:ARG:NH2	3:M:115:ILE:HD13	2.29	0.48
1:A:207:ARG:HG3	1:A:207:ARG:NH1	2.09	0.48
1:A:17:HIS:NE2	1:A:127:PRO:HD2	2.29	0.48
3:M:136:VAL:HG12	3:M:137:LYS:H	1.78	0.48
2:H:107:LEU:HD21	2:H:125:VAL:HG11	1.96	0.48
1:A:256:LEU:O	1:A:314:SER:HB2	2.13	0.48
2:G:2:ILE:HD13	2:G:100:ILE:HG22	1.96	0.48
1:E:394:ARG:N	1:E:394:ARG:HD2	2.23	0.48
1:F:327:TRP:CD2	1:F:385:PRO:HG3	2.49	0.48
3:M:38:ILE:HG23	3:M:42:THR:HG22	1.95	0.48
2:H:167:GLU:O	2:H:171:HIS:HB2	2.14	0.48
2:G:129:LEU:HD22	2:G:139:ALA:HB1	1.96	0.48
2:C:110:VAL:O	2:C:113:LYS:HB2	2.14	0.47
1:E:406:ARG:HH11	1:E:406:ARG:CA	2.26	0.47
1:E:149:ASN:ND2	1:E:183:VAL:HG23	2.29	0.47
1:F:99:VAL:CG1	1:F:104:MET:HG3	2.42	0.47
2:C:132:LYS:HE3	2:C:150:ILE:HG23	1.95	0.47
1:B:182:PRO:HD2	3:L:10:MET:HG2	1.96	0.47
2:C:200:ILE:HG23	2:C:219:ILE:HD12	1.95	0.47
1:E:28:ALA:HA	1:E:188:LYS:HE3	1.96	0.47
1:F:393:ILE:HB	1:F:413:VAL:HG21	1.95	0.47
1:B:333:TYR:HB2	1:B:410:TRP:HD1	1.77	0.47
2:D:41:LEU:HD11	2:D:45:GLU:O	2.14	0.47
2:D:18:THR:HA	2:D:63:LYS:HA	1.95	0.47
1:F:279:ILE:HG21	1:F:289:ALA:HB2	1.96	0.47
1:A:99:VAL:HG21	1:A:103:THR:CG2	2.37	0.47
1:B:163:TYR:CZ	3:L:7:TYR:HB2	2.48	0.47
1:F:51:TYR:HE1	1:F:90:SER:HB2	1.79	0.47
3:M:54:ILE:CD1	3:M:56:ARG:HE	2.27	0.47
2:H:61:ASN:O	2:H:62:ARG:HG2	2.14	0.47
2:H:158:GLU:HA	2:H:162:LYS:CB	2.44	0.47
3:M:7:TYR:CE2	3:M:11:LEU:HD22	2.49	0.47
2:C:251:ILE:HA	2:C:261:ILE:HG23	1.96	0.47
1:E:258:GLY:HA3	1:E:270:GLU:O	2.14	0.47
3:K:105:GLU:O	3:K:105:GLU:HG3	2.13	0.47
3:M:65:LEU:HA	3:M:68:GLU:CG	2.44	0.47
1:E:330:ARG:NH1	1:E:330:ARG:CG	2.55	0.47
1:E:214:VAL:HB	1:E:243:ILE:HD11	1.96	0.47
2:H:46:VAL:HG13	2:H:47:SER:N	2.29	0.47
1:A:286:PHE:HA	1:B:232:GLU:HG2	1.97	0.47
2:D:5:ARG:HG3	2:D:6:SER:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:ARG:HG2	2:H:127:TRP:CE2	2.50	0.47
1:E:361:VAL:HB	1:E:393:ILE:CG2	2.43	0.47
2:G:101:GLN:HE21	2:G:101:GLN:HA	1.78	0.47
1:E:368:GLY:HA2	1:E:381:GLU:O	2.14	0.47
2:G:102:ARG:HD3	2:G:175:ARG:NH1	2.29	0.47
1:F:388:VAL:HG11	1:F:413:VAL:HG11	1.97	0.47
1:F:23:THR:HG21	1:F:35:SER:HB2	1.96	0.47
3:K:116:LEU:HD23	3:K:120:LYS:HE2	1.96	0.47
1:B:135:ALA:O	1:B:139:ILE:HD13	2.15	0.47
1:F:335:LEU:HD13	1:F:351:ILE:HD11	1.97	0.47
1:F:331:ILE:O	1:F:378:ILE:HG12	2.14	0.47
1:F:357:LEU:CB	1:F:399:ARG:HA	2.41	0.47
1:F:146:ILE:N	1:F:146:ILE:HD12	2.29	0.47
1:F:114:ALA:HB3	1:F:144:LEU:HD22	1.97	0.47
2:D:54:ILE:HG23	2:D:55:ARG:H	1.80	0.47
2:D:174:GLU:HB2	2:D:175:ARG:HD3	1.97	0.47
2:H:185:VAL:HG22	2:H:261:ILE:HG12	1.96	0.47
3:K:28:GLN:O	3:K:30:LEU:N	2.48	0.47
2:D:118:GLU:O	2:D:122:TRP:HD1	1.97	0.47
1:F:266:LYS:H	1:F:266:LYS:HD2	1.79	0.47
1:B:203:LYS:O	1:B:205:PRO:HD3	2.15	0.47
3:M:29:SER:O	3:M:31:PRO:HD3	2.14	0.47
2:C:208:GLU:HA	2:C:214:LEU:HD21	1.95	0.47
2:H:12:GLY:H	2:H:68:VAL:HG13	1.80	0.47
1:E:66:GLU:HA	1:E:192:ASP:HB2	1.95	0.47
1:A:182:PRO:HG3	3:K:7:TYR:HE1	1.80	0.47
1:F:59:CYS:SG	1:F:83:PRO:HG3	2.54	0.47
1:E:74:CYS:HB2	1:E:83:PRO:CG	2.41	0.47
2:H:160:TRP:CD1	2:H:161:VAL:HB	2.50	0.47
1:B:259:LEU:O	1:B:269:TYR:HA	2.15	0.47
1:F:306:THR:HA	1:F:311:LEU:HD13	1.95	0.47
1:A:224:ASN:HD21	1:A:234:LYS:N	2.13	0.47
1:A:354:LYS:HA	1:A:369:ILE:CG2	2.36	0.47
1:E:373:VAL:HA	1:E:378:ILE:CD1	2.45	0.47
2:D:17:ALA:HB1	2:D:29:VAL:HG22	1.96	0.47
1:A:16:GLY:HA3	1:A:117:VAL:HG13	1.97	0.47
3:K:57:GLU:CG	3:K:59:LYS:HG3	2.45	0.47
2:H:49:LYS:HD2	2:H:49:LYS:O	2.15	0.47
3:M:64:TYR:O	3:M:68:GLU:HG2	2.16	0.46
1:B:138:ILE:HG22	1:B:412:LEU:HD13	1.96	0.46
3:M:42:THR:HB	3:M:83:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:ALA:HA	2:H:150:ILE:HD13	1.97	0.46
1:B:101:MET:HA	1:B:104:MET:HE3	1.97	0.46
2:H:208:GLU:HA	2:H:214:LEU:HD21	1.97	0.46
2:D:38:GLN:HG2	2:D:77:THR:HA	1.96	0.46
1:B:66:GLU:HG2	3:L:13:ARG:NH2	2.30	0.46
1:B:256:LEU:HA	1:B:257:PRO:C	2.35	0.46
3:M:108:THR:O	3:M:108:THR:HG23	2.14	0.46
1:E:339:VAL:HG12	1:E:340:VAL:H	1.80	0.46
2:D:100:ILE:HD11	2:D:122:TRP:HH2	1.81	0.46
2:H:7:LYS:HD3	2:H:7:LYS:H	1.80	0.46
1:B:105:LEU:HD21	1:B:394:ARG:HD3	1.97	0.46
2:G:121:ALA:O	2:G:125:VAL:HB	2.16	0.46
1:F:144:LEU:HD12	1:F:146:ILE:CD1	2.46	0.46
1:E:149:ASN:HD22	1:E:183:VAL:HG23	1.80	0.46
2:G:6:SER:HB2	2:G:34:TYR:HE2	1.80	0.46
1:F:125:PRO:O	1:F:126:GLN:HB2	2.16	0.46
1:F:125:PRO:HB2	1:F:126:GLN:H	1.46	0.46
2:H:125:VAL:HG22	2:H:161:VAL:HG11	1.97	0.46
2:H:154:ALA:HB3	2:H:156:VAL:HG23	1.97	0.46
1:F:261:VAL:HG12	1:F:263:LYS:HG3	1.96	0.46
1:B:111:MET:HG2	1:B:113:GLY:O	2.16	0.46
1:B:220:SER:OG	1:B:306:THR:HB	2.15	0.46
1:F:226:PRO:HA	2:H:221:THR:O	2.15	0.46
3:K:84:GLN:O	3:K:84:GLN:CG	2.41	0.46
2:G:71:VAL:HG22	2:G:78:VAL:HG23	1.97	0.46
2:D:156:VAL:HG13	2:D:161:VAL:H	1.80	0.46
1:A:404:ARG:HH12	1:A:407:MET:HE3	1.81	0.46
2:C:68:VAL:HA	2:C:80:VAL:HG12	1.98	0.46
2:C:53:ASN:HB2	2:C:55:ARG:CZ	2.46	0.46
1:B:184:SER:C	1:B:186:LEU:H	2.19	0.46
3:K:44:ILE:HD12	3:K:47:PHE:HD1	1.80	0.46
1:A:220:SER:HA	1:A:237:VAL:O	2.16	0.46
1:A:218:ILE:HG13	1:A:219:ARG:HG3	1.97	0.46
3:N:30:LEU:HB3	3:N:31:PRO:CD	2.35	0.46
2:H:224:ALA:CB	2:H:225:PRO:HD3	2.34	0.46
2:G:41:LEU:HG	2:G:46:VAL:HG22	1.98	0.46
2:G:42:PRO:O	2:G:46:VAL:HG23	2.16	0.46
1:F:82:GLU:HA	1:F:83:PRO:HD3	1.76	0.46
2:C:111:SER:HB3	2:C:121:ALA:HB2	1.98	0.46
2:G:157:PRO:HB2	2:G:160:TRP:HD1	1.72	0.46
1:F:148:GLN:O	1:F:151:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ARG:HE	1:A:406:ARG:CG	2.26	0.46
1:E:31:GLY:O	1:E:32:ILE:HG22	2.16	0.46
2:D:159:ILE:HG22	2:D:163:PRO:CD	2.44	0.46
1:A:117:VAL:HA	1:A:147:VAL:CG2	2.46	0.46
1:A:203:LYS:O	1:A:205:PRO:HD3	2.16	0.46
3:M:109:CYS:HG	3:M:127:CYS:HA	1.74	0.46
3:M:99:PHE:HD1	3:M:103:TYR:HB3	1.81	0.46
1:B:10:VAL:CG1	1:B:205:PRO:HD2	2.45	0.46
3:K:54:ILE:HB	3:K:104:VAL:CG2	2.45	0.46
3:K:16:SER:C	3:K:19:PRO:HD2	2.36	0.46
1:F:175:ALA:HB1	1:F:178:VAL:HG21	1.98	0.46
2:H:66:VAL:HG12	2:H:82:LEU:HG	1.98	0.46
1:A:262:GLU:HA	1:A:267:VAL:HG12	1.98	0.46
1:F:109:ALA:HB3	1:F:243:ILE:HB	1.98	0.46
2:C:5:ARG:NH1	2:C:130:GLU:HB3	2.31	0.45
2:C:24:ASP:HB3	2:C:25:TYR:H	1.46	0.45
1:B:119:ALA:HB3	1:B:122:GLU:CB	2.46	0.45
2:G:158:GLU:HA	2:G:162:LYS:HB2	1.99	0.45
1:B:234:LYS:HD2	1:B:235:GLY:N	2.26	0.45
1:A:173:THR:HB	1:A:174:TRP:CE3	2.51	0.45
1:E:148:GLN:HG2	3:M:7:TYR:OH	2.16	0.45
1:A:339:VAL:HG13	1:A:340:VAL:N	2.30	0.45
1:F:218:ILE:HG23	1:F:240:GLY:HA2	1.98	0.45
2:G:177:VAL:HG22	2:G:178:LYS:N	2.31	0.45
1:B:134:VAL:O	1:B:138:ILE:HG12	2.16	0.45
2:G:127:TRP:CE3	2:G:127:TRP:HA	2.52	0.45
1:A:173:THR:HB	1:A:174:TRP:HE3	1.82	0.45
1:E:279:ILE:HG21	1:E:289:ALA:HB2	1.98	0.45
1:F:224:ASN:HD21	1:F:234:LYS:H	1.64	0.45
2:H:69:ILE:HG13	2:H:70:ARG:H	1.81	0.45
1:F:336:LEU:HB2	1:F:409:GLY:N	2.30	0.45
1:B:150:LYS:CE	1:B:186:LEU:HD11	2.47	0.45
1:E:43:ARG:CZ	1:E:280:ARG:HD3	2.46	0.45
1:B:75:LYS:CA	1:B:75:LYS:HE2	2.47	0.45
2:G:97:TRP:O	2:G:97:TRP:CG	2.69	0.45
2:D:119:LYS:O	2:D:123:GLU:HB2	2.17	0.45
3:K:68:GLU:CB	3:K:86:LYS:HB3	2.47	0.45
2:D:50:TRP:HD1	2:D:51:VAL:HG23	1.81	0.45
1:F:37:HIS:NE2	3:M:118:LYS:HG2	2.31	0.45
3:M:56:ARG:NH2	3:M:99:PHE:CE1	2.85	0.45
1:E:218:ILE:HG12	1:E:240:GLY:CA	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:68:GLU:HB2	3:K:86:LYS:HB3	1.99	0.45
1:F:370:VAL:HA	1:F:380:VAL:HG22	1.99	0.45
1:E:64:LYS:CB	1:E:65:PRO:HD3	2.44	0.45
1:A:393:ILE:O	1:A:413:VAL:HG23	2.17	0.45
3:M:19:PRO:HA	3:M:23:ARG:HB3	1.99	0.45
2:C:246:ILE:O	2:C:250:LEU:HG	2.16	0.45
1:B:50:GLY:O	1:B:92:ILE:HA	2.15	0.45
1:F:405:TRP:CD1	1:F:405:TRP:N	2.85	0.45
3:N:17:LYS:NZ	3:N:17:LYS:HA	2.32	0.45
3:L:15:TYR:HA	3:L:18:LEU:HB2	1.99	0.45
1:B:19:ASP:HB3	1:B:96:GLY:CA	2.42	0.45
1:E:104:MET:CA	1:E:108:ALA:HB3	2.43	0.45
1:B:116:LEU:HD23	1:B:146:ILE:HG13	1.98	0.45
1:A:325:VAL:HA	1:A:387:ALA:HA	2.00	0.45
2:H:185:VAL:HB	2:H:227:TYR:CE1	2.52	0.45
1:F:96:GLY:HA3	1:F:100:LEU:HA	1.98	0.45
1:A:82:GLU:HA	1:A:83:PRO:HD3	1.78	0.44
1:F:263:LYS:HD3	1:F:263:LYS:O	2.16	0.44
1:E:181:ILE:CD1	1:E:194:LEU:HA	2.47	0.44
2:G:5:ARG:NH2	2:G:130:GLU:HG2	2.32	0.44
2:C:195:LYS:HE3	2:C:257:GLU:HB3	1.98	0.44
1:A:4:PRO:HG3	2:D:220:TYR:CE2	2.52	0.44
1:E:302:ASP:HB3	1:E:305:LEU:HG	1.99	0.44
2:G:264:VAL:O	2:G:264:VAL:HG12	2.18	0.44
2:H:150:ILE:HD12	2:H:150:ILE:H	1.83	0.44
2:C:53:ASN:HB2	2:C:55:ARG:NH1	2.32	0.44
1:B:124:PHE:CZ	1:B:166:ILE:HA	2.51	0.44
2:H:88:ASP:O	2:H:92:LYS:HG2	2.17	0.44
3:K:112:LEU:HD23	3:K:112:LEU:HA	1.81	0.44
2:D:65:ILE:CG2	2:D:90:ARG:HH21	2.30	0.44
1:B:84:LYS:HD3	1:B:85:PHE:N	2.32	0.44
1:B:17:HIS:CG	1:B:18:VAL:N	2.85	0.44
1:B:216:LEU:HD21	1:B:363:SER:HB2	1.99	0.44
1:F:397:ILE:HG22	1:F:398:SER:N	2.32	0.44
1:B:398:SER:HA	1:B:407:MET:CB	2.45	0.44
1:F:181:ILE:HD12	1:F:194:LEU:HD23	1.99	0.44
2:G:12:GLY:O	2:G:14:ILE:HD12	2.17	0.44
2:C:136:PRO:O	2:C:140:ILE:HG13	2.18	0.44
3:K:68:GLU:HB2	3:K:86:LYS:CB	2.47	0.44
1:B:105:LEU:HD13	1:B:105:LEU:O	2.17	0.44
1:E:215:MET:O	1:E:215:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:59:LYS:O	2:G:62:ARG:HG2	2.17	0.44
1:F:124:PHE:CE2	1:F:166:ILE:HA	2.53	0.44
2:H:41:LEU:HD13	2:H:80:VAL:HG23	1.99	0.44
1:E:13:GLY:HA2	1:E:92:ILE:HG13	1.98	0.44
1:B:124:PHE:HA	1:B:125:PRO:HA	1.74	0.44
1:B:312:LEU:HD12	1:B:313:GLY:H	1.83	0.44
1:E:9:GLU:HG2	1:E:204:THR:HG21	2.00	0.44
2:H:165:LEU:O	2:H:165:LEU:HD13	2.17	0.44
1:E:229:GLN:HB2	1:E:232:GLU:HG2	1.98	0.44
3:M:34:ILE:H	3:M:93:ASN:HD21	1.65	0.44
1:F:328:ASN:HA	1:F:380:VAL:O	2.18	0.44
1:F:105:LEU:HG	1:F:396:VAL:HG22	2.00	0.44
1:A:74:CYS:SG	1:A:83:PRO:HG3	2.58	0.44
1:E:25:LEU:HD11	1:E:194:LEU:HD13	1.99	0.44
1:E:222:ASP:CG	1:E:303:PRO:HB3	2.37	0.44
2:G:202:LYS:HD2	2:G:253:ILE:HD13	2.00	0.44
1:B:225:LYS:N	1:B:225:LYS:HD2	2.33	0.44
1:A:50:GLY:HA3	1:A:93:ASP:HB3	1.98	0.44
1:E:46:THR:HG23	1:E:47:ILE:HG13	2.00	0.44
3:K:101:LYS:CB	3:K:118:LYS:HE2	2.36	0.44
2:G:70:ARG:HG3	2:G:71:VAL:H	1.83	0.44
1:A:327:TRP:CE2	1:A:385:PRO:HG3	2.52	0.44
1:F:401:ILE:HG23	1:F:405:TRP:CZ2	2.53	0.44
2:H:20:LYS:H	2:H:29:VAL:HA	1.82	0.44
1:F:246:LEU:HB2	1:F:290:LYS:HG2	2.00	0.44
1:A:359:LEU:HD12	1:A:359:LEU:N	2.33	0.44
1:B:181:ILE:HA	1:B:182:PRO:HD3	1.88	0.44
2:G:93:LYS:HA	2:G:96:GLN:HG2	1.99	0.44
1:B:222:ASP:CG	1:B:303:PRO:HB3	2.38	0.44
1:A:349:ASP:HA	1:A:350:PRO:HD3	1.86	0.44
1:E:219:ARG:HD2	1:E:221:PHE:CE2	2.53	0.43
1:B:209:LEU:HD11	1:B:290:LYS:CE	2.45	0.43
2:D:119:LYS:O	2:D:119:LYS:HD2	2.18	0.43
1:A:29:ILE:HG22	1:A:54:THR:HG21	2.00	0.43
1:A:372:SER:HB3	1:A:379:GLU:HB2	2.01	0.43
1:E:338:ARG:NH1	1:E:345:MET:HE2	2.32	0.43
1:F:367:LEU:HD22	1:F:383:ARG:NH1	2.34	0.43
2:G:236:PRO:HA	2:G:239:ALA:HB2	2.00	0.43
1:A:118:VAL:HG12	1:A:149:ASN:H	1.83	0.43
1:F:74:CYS:HB3	1:F:79:SER:HB3	2.00	0.43
2:D:14:ILE:H	2:D:14:ILE:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:LYS:HD2	2:G:224:ALA:CB	2.48	0.43
1:A:327:TRP:CE3	1:A:385:PRO:HG3	2.54	0.43
2:H:43:TRP:HB3	2:H:51:VAL:HG23	2.00	0.43
2:H:119:LYS:O	2:H:123:GLU:HB2	2.18	0.43
1:E:181:ILE:HA	1:E:182:PRO:HD3	1.86	0.43
1:F:51:TYR:HB2	1:F:294:LEU:HD12	2.01	0.43
1:F:178:VAL:HA	1:F:179:PRO:HD3	1.74	0.43
1:F:113:GLY:HA3	1:F:202:ILE:HG23	1.99	0.43
1:F:234:LYS:HA	1:F:234:LYS:HD2	1.65	0.43
1:A:50:GLY:O	1:A:92:ILE:HA	2.19	0.43
1:A:189:ILE:HG21	3:K:17:LYS:HB3	2.00	0.43
1:E:255:VAL:C	1:E:256:LEU:HD12	2.37	0.43
1:A:60:GLU:O	1:A:61:SER:HB2	2.19	0.43
1:A:266:LYS:N	1:A:266:LYS:HD2	2.32	0.43
3:M:56:ARG:HH22	3:M:99:PHE:HE1	1.66	0.43
1:F:274:THR:HG21	1:F:299:THR:HB	2.00	0.43
3:M:137:LYS:N	3:M:138:PRO:CD	2.80	0.43
1:E:348:VAL:O	1:E:350:PRO:HD3	2.18	0.43
1:F:124:PHE:CG	1:F:125:PRO:HA	2.53	0.43
1:A:20:HIS:H	1:A:22:LYS:HZ1	1.65	0.43
1:E:212:LYS:O	1:E:244:GLN:HG3	2.18	0.43
2:G:235:ASN:HD22	2:G:236:PRO:HD2	1.83	0.43
1:E:412:LEU:C	1:E:412:LEU:HD22	2.39	0.43
2:D:124:GLN:O	2:D:128:LYS:HB2	2.18	0.43
1:A:155:SER:HB2	1:A:158:GLU:OE1	2.19	0.43
1:E:53:GLU:HG3	1:E:88:ARG:NH2	2.33	0.43
1:B:248:LYS:O	1:B:251:GLN:HG2	2.19	0.43
1:A:8:PRO:HD2	1:A:281:PHE:CD2	2.53	0.43
2:C:110:VAL:HG21	2:C:164:LEU:HA	2.01	0.43
1:B:329:ILE:HD12	1:B:331:ILE:HD12	2.00	0.43
1:F:242:ILE:HD13	1:F:290:LYS:O	2.19	0.43
1:A:290:LYS:HB3	1:A:291:PRO:HD2	2.01	0.43
1:F:3:TRP:CH2	1:F:72:PRO:HA	2.53	0.43
1:E:391:ASN:HA	1:E:415:ILE:HD12	1.99	0.43
1:E:252:GLU:HA	1:E:275:LYS:CB	2.49	0.43
1:B:119:ALA:HB3	1:B:122:GLU:HB2	2.01	0.43
2:G:208:GLU:CD	2:G:217:ILE:HD13	2.39	0.43
2:D:213:SER:OG	2:D:234:THR:HB	2.19	0.43
1:B:72:PRO:O	1:B:73:SER:HB2	2.18	0.43
1:B:105:LEU:HB3	1:B:360:SER:OG	2.17	0.43
1:B:396:VAL:HG23	1:B:408:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:134:THR:HA	3:M:135:PRO:HD3	1.62	0.43
1:B:110:LEU:HG	1:B:241:SER:OG	2.19	0.43
2:D:54:ILE:HG23	2:D:55:ARG:N	2.32	0.43
2:C:18:THR:HG23	2:C:63:LYS:HG2	1.99	0.43
2:C:104:ASP:O	2:C:108:GLU:HG3	2.18	0.43
3:K:83:ILE:O	3:K:84:GLN:HB3	2.17	0.43
3:L:18:LEU:O	3:L:20:GLU:HG3	2.19	0.43
1:A:336:LEU:HD11	1:A:339:VAL:HG21	2.01	0.43
1:E:338:ARG:NH1	1:E:345:MET:HE3	2.34	0.43
1:E:15:VAL:HG23	1:E:116:LEU:HD13	2.00	0.43
1:E:110:LEU:HD12	1:E:243:ILE:HA	2.00	0.43
2:G:214:LEU:HA	2:G:233:GLY:HA3	1.97	0.43
2:D:118:GLU:HG2	2:D:122:TRP:CD1	2.53	0.43
1:B:406:ARG:NH1	1:B:406:ARG:HB3	2.34	0.43
1:F:116:LEU:HB2	1:F:144:LEU:HD11	2.00	0.43
3:K:44:ILE:HD12	3:K:47:PHE:CD1	2.54	0.43
1:A:63:LYS:HG3	1:A:64:LYS:H	1.84	0.43
1:E:181:ILE:HD12	1:E:194:LEU:HA	2.01	0.43
1:F:218:ILE:HG13	1:F:219:ARG:HD2	2.00	0.43
2:D:107:LEU:O	2:D:111:SER:HB3	2.19	0.43
2:C:170:LYS:HE2	2:C:170:LYS:HB3	1.72	0.43
2:C:14:ILE:HD12	2:C:14:ILE:N	2.34	0.43
1:B:71:GLU:HA	1:B:72:PRO:HD3	1.85	0.43
1:A:18:VAL:HG21	1:A:150:LYS:HG3	2.01	0.43
1:E:3:TRP:CH2	1:E:57:GLY:HA3	2.54	0.43
1:B:280:ARG:HB3	1:B:296:ALA:HB3	2.00	0.43
1:A:20:HIS:HD2	1:A:24:THR:CG2	2.32	0.43
2:C:22:VAL:HG21	2:C:58:LEU:HB2	2.01	0.43
2:C:132:LYS:HE3	2:C:150:ILE:CG2	2.49	0.43
1:A:217:VAL:HB	1:A:314:SER:O	2.19	0.43
2:C:109:LEU:HD13	2:C:167:GLU:OE2	2.19	0.43
2:D:122:TRP:HA	2:D:126:ALA:HB3	2.00	0.43
2:D:2:ILE:HD12	2:D:2:ILE:N	2.33	0.43
2:H:7:LYS:N	2:H:7:LYS:HD3	2.33	0.43
3:L:9:GLU:O	3:L:12:ASP:HB3	2.18	0.43
2:D:8:LEU:HA	2:D:9:PRO:HD3	1.83	0.43
1:E:7:GLN:HG2	1:E:8:PRO:N	2.34	0.43
3:K:82:VAL:CG1	3:K:83:ILE:N	2.82	0.42
1:E:245:GLY:O	1:E:291:PRO:HD3	2.18	0.42
1:E:243:ILE:HG13	1:E:243:ILE:H	1.71	0.42
1:A:175:ALA:HB1	1:A:178:VAL:CG2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:116:LEU:CD1	2:G:117:SER:H	2.32	0.42
2:C:43:TRP:HD1	2:C:52:LYS:HE3	1.83	0.42
1:B:276:ILE:N	1:B:276:ILE:HD12	2.34	0.42
1:B:241:SER:HB3	1:B:294:LEU:HD23	2.01	0.42
2:C:105:LYS:CE	2:C:105:LYS:HA	2.46	0.42
1:E:410:TRP:CD1	1:E:410:TRP:N	2.86	0.42
2:H:160:TRP:O	2:H:163:PRO:HD2	2.19	0.42
2:D:2:ILE:HG23	2:D:122:TRP:CZ3	2.54	0.42
1:A:348:VAL:HG22	1:A:349:ASP:N	2.34	0.42
1:A:337:GLU:HB3	1:A:338:ARG:H	1.71	0.42
3:M:35:ILE:HG22	3:M:36:LEU:H	1.84	0.42
3:M:111:SER:HB2	3:M:129:ALA:HB3	1.99	0.42
2:G:125:VAL:HG22	2:G:161:VAL:HG11	2.01	0.42
2:C:90:ARG:HD3	2:C:91:ARG:NH1	2.23	0.42
3:N:20:GLU:HB3	3:N:24:LYS:HB2	2.01	0.42
2:H:249:ASN:HA	2:H:252:LYS:CB	2.47	0.42
2:H:196:ILE:O	2:H:200:ILE:HG13	2.20	0.42
1:A:222:ASP:OD1	1:A:303:PRO:HB3	2.19	0.42
3:M:54:ILE:HG13	3:M:56:ARG:HE	1.85	0.42
1:F:148:GLN:HG3	1:F:180:ILE:HG22	2.01	0.42
1:F:98:GLU:C	1:F:99:VAL:HG23	2.40	0.42
2:C:191:LEU:HB3	2:C:194:GLU:HB2	2.01	0.42
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.87	0.42
3:K:32:ASN:HD22	3:K:32:ASN:HA	1.66	0.42
1:E:401:ILE:HG22	1:E:404:ARG:O	2.20	0.42
1:E:43:ARG:HE	1:E:280:ARG:HB3	1.84	0.42
1:F:242:ILE:CD1	1:F:242:ILE:H	2.22	0.42
2:G:148:GLU:HB2	2:G:162:LYS:HD2	2.02	0.42
2:G:113:LYS:HE2	2:G:164:LEU:HD22	2.00	0.42
2:C:219:ILE:HG23	2:C:229:VAL:HG22	2.01	0.42
2:C:161:VAL:O	2:C:164:LEU:HB3	2.19	0.42
1:B:84:LYS:HD2	1:B:86:LEU:HD13	2.01	0.42
1:F:182:PRO:HG2	3:N:11:LEU:HG	2.02	0.42
3:M:118:LYS:HE3	3:M:119:GLU:HG2	2.02	0.42
2:C:5:ARG:H	2:C:5:ARG:HG2	1.67	0.42
1:F:307:LYS:HD3	2:H:224:ALA:CB	2.49	0.42
2:G:127:TRP:HE3	2:G:127:TRP:HA	1.83	0.42
2:D:49:LYS:CA	2:D:49:LYS:HE2	2.47	0.42
2:H:237:LYS:H	2:H:237:LYS:CD	2.32	0.42
1:E:112:ASP:HB3	1:E:205:PRO:HG2	2.01	0.42
2:C:189:GLU:HB3	2:C:190:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:ILE:H	1:F:89:ILE:HD13	1.84	0.42
1:B:163:TYR:OH	1:B:182:PRO:HG3	2.19	0.42
1:F:71:GLU:HA	1:F:72:PRO:HD3	1.85	0.42
2:D:96:GLN:HA	2:D:99:LYS:CD	2.49	0.42
1:F:406:ARG:HA	1:F:406:ARG:HD2	1.84	0.42
1:E:228:THR:HA	1:F:5:LYS:HE2	2.01	0.42
2:D:123:GLU:HA	2:D:127:TRP:CE3	2.45	0.42
2:G:160:TRP:CG	2:G:161:VAL:N	2.87	0.42
2:D:224:ALA:C	2:D:226:ARG:H	2.23	0.42
2:H:34:TYR:HB3	2:H:37:LEU:HD22	2.02	0.42
1:F:248:LYS:O	1:F:251:GLN:HB2	2.20	0.42
2:G:47:SER:HA	2:G:83:LYS:HG2	2.02	0.42
1:A:383:ARG:HA	1:A:383:ARG:HD2	1.83	0.42
1:E:22:LYS:HG3	1:E:23:THR:OG1	2.20	0.42
1:F:150:LYS:CD	1:F:185:ALA:HB3	2.50	0.42
2:G:42:PRO:HD2	2:G:45:GLU:HB2	2.02	0.42
2:G:41:LEU:CD1	2:G:81:SER:HA	2.50	0.42
1:F:412:LEU:CD2	1:F:413:VAL:H	2.33	0.42
1:F:256:LEU:HA	1:F:257:PRO:C	2.39	0.42
1:A:125:PRO:HB3	1:A:130:ARG:HB2	2.02	0.41
1:E:149:ASN:ND2	1:E:150:LYS:H	2.18	0.41
2:H:151:LEU:HD21	2:H:165:LEU:HD12	2.01	0.41
1:F:218:ILE:HD11	1:F:219:ARG:HH11	1.85	0.41
2:G:5:ARG:HH12	2:G:131:ALA:HB2	1.85	0.41
1:F:33:TRP:HB3	1:F:36:LYS:HG3	2.02	0.41
1:B:62:CYS:HB3	1:B:63:LYS:H	1.66	0.41
1:A:36:LYS:HA	1:A:36:LYS:HD2	1.82	0.41
1:A:297:ILE:N	1:A:297:ILE:HD12	2.35	0.41
2:C:86:THR:HB	2:C:89:GLU:CD	2.40	0.41
1:B:110:LEU:HD23	1:B:294:LEU:HD21	2.01	0.41
3:N:19:PRO:HB2	3:N:20:GLU:H	1.59	0.41
2:G:152:ILE:HD12	2:G:158:GLU:HG3	2.02	0.41
2:G:162:LYS:HB3	2:G:162:LYS:HE2	1.91	0.41
2:D:124:GLN:HE22	2:D:157:PRO:HD2	1.85	0.41
1:F:245:GLY:O	1:F:291:PRO:HD3	2.20	0.41
3:M:56:ARG:HB3	3:M:60:ILE:CG2	2.50	0.41
1:A:312:LEU:HD12	1:A:313:GLY:N	2.35	0.41
3:M:135:PRO:C	3:M:136:VAL:CG2	2.88	0.41
1:E:215:MET:HA	1:E:242:ILE:HA	2.02	0.41
1:F:17:HIS:NE2	1:F:119:ALA:N	2.68	0.41
1:E:351:ILE:HG22	1:E:352:ARG:N	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:TRP:O	1:A:382:LEU:HD23	2.20	0.41
2:G:98:LYS:HB2	2:G:98:LYS:HE3	1.77	0.41
1:A:181:ILE:HA	1:A:182:PRO:HD3	1.91	0.41
2:G:6:SER:HB2	2:G:34:TYR:CE2	2.55	0.41
3:L:15:TYR:HD2	3:L:18:LEU:HD22	1.85	0.41
2:C:90:ARG:CD	2:C:91:ARG:HH12	2.25	0.41
1:B:108:ALA:C	1:B:110:LEU:H	2.23	0.41
1:F:20:HIS:HE1	1:F:150:LYS:CE	2.34	0.41
1:F:404:ARG:HD2	1:F:406:ARG:HG2	2.02	0.41
2:D:2:ILE:HG13	2:D:122:TRP:CH2	2.56	0.41
1:B:137:GLY:HA3	1:B:174:TRP:CZ2	2.55	0.41
1:F:56:ILE:O	1:F:86:LEU:HB2	2.20	0.41
1:F:259:LEU:HA	1:F:259:LEU:HD23	1.84	0.41
1:F:22:LYS:HD3	1:F:22:LYS:H	1.86	0.41
1:E:22:LYS:HE3	1:E:95:PRO:O	2.20	0.41
1:F:333:TYR:CD2	1:F:335:LEU:HB2	2.56	0.41
1:F:335:LEU:HD11	1:F:399:ARG:HH21	1.85	0.41
2:G:19:VAL:HG11	2:G:58:LEU:HB3	2.01	0.41
1:B:120:ALA:HB3	1:B:154:VAL:HG11	2.01	0.41
3:M:63:LYS:O	3:M:66:LEU:HB3	2.21	0.41
2:C:238:GLU:HA	2:C:238:GLU:OE2	2.21	0.41
1:B:406:ARG:HB3	1:B:406:ARG:CZ	2.49	0.41
1:F:27:GLN:HB2	1:F:33:TRP:HD1	1.85	0.41
2:H:219:ILE:HD12	2:H:229:VAL:HB	2.03	0.41
1:B:410:TRP:CG	1:B:411:GLY:N	2.89	0.41
1:F:389:TRP:CG	1:F:390:SER:N	2.89	0.41
2:C:71:VAL:HG21	2:C:73:ARG:HH12	1.86	0.41
1:F:281:PHE:CZ	1:F:295:VAL:HB	2.55	0.41
1:B:27:GLN:HG3	1:B:32:ILE:C	2.40	0.41
2:H:258:ASN:HA	2:H:258:ASN:HD22	1.68	0.41
1:F:335:LEU:HD22	1:F:351:ILE:HG13	2.02	0.41
2:H:18:THR:HA	2:H:62:ARG:O	2.21	0.41
1:A:279:ILE:HD12	1:A:288:GLU:HA	2.03	0.41
1:E:87:ARG:HH21	1:E:198:ILE:HG22	1.85	0.41
2:D:246:ILE:O	2:D:250:LEU:HG	2.21	0.41
1:E:3:TRP:HA	1:E:4:PRO:HD3	1.81	0.41
1:F:190:ASN:HB2	3:N:14:LEU:HD13	2.02	0.41
2:C:103:LEU:HB2	2:C:137:ILE:HG22	2.03	0.41
1:A:17:HIS:HD2	1:A:128:GLN:CG	2.34	0.41
1:E:373:VAL:HA	1:E:378:ILE:HD13	2.02	0.41
1:F:360:SER:HA	1:F:364:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:183:ILE:O	2:D:226:ARG:HA	2.20	0.41
2:H:67:LYS:O	2:H:68:VAL:HB	2.20	0.41
1:E:375:LYS:HG3	1:E:376:ASP:H	1.84	0.41
1:F:107:GLY:HA2	1:F:110:LEU:HB2	2.03	0.41
2:C:19:VAL:HA	2:C:29:VAL:HG23	2.02	0.41
1:B:136:LEU:HB3	1:B:141:VAL:CG2	2.51	0.41
1:E:221:PHE:N	1:E:221:PHE:CD1	2.87	0.41
1:E:126:GLN:HB3	1:E:129:THR:OG1	2.21	0.41
2:G:137:ILE:CD1	2:G:138:THR:H	2.23	0.41
1:E:401:ILE:HG12	1:E:402:ALA:N	2.31	0.41
1:E:43:ARG:NE	1:E:280:ARG:CD	2.83	0.41
2:H:141:GLU:OE2	2:H:234:THR:HG21	2.21	0.41
2:C:224:ALA:H	2:C:225:PRO:CD	2.34	0.41
2:H:124:GLN:HA	2:H:128:LYS:HD3	2.02	0.41
2:C:27:SER:HB3	2:C:41:LEU:HD23	2.01	0.41
1:B:333:TYR:HA	1:B:410:TRP:HD1	1.86	0.41
3:K:36:LEU:HD21	3:K:90:GLN:OE1	2.21	0.41
1:A:260:ARG:HG2	1:A:269:TYR:CE1	2.55	0.41
1:B:212:LYS:HG2	1:B:244:GLN:NE2	2.36	0.41
1:A:189:ILE:HD12	3:K:17:LYS:HG2	2.03	0.41
2:G:83:LYS:HD2	2:G:83:LYS:O	2.20	0.41
1:F:33:TRP:HE3	1:F:36:LYS:HG3	1.85	0.41
1:F:358:MET:SD	1:F:365:THR:HB	2.61	0.41
2:D:180:SER:HB3	2:D:228:ARG:NH2	2.35	0.41
1:B:218:ILE:CG1	1:B:240:GLY:HA2	2.51	0.41
1:E:354:LYS:HA	1:E:369:ILE:HG22	2.03	0.41
2:D:101:GLN:NE2	2:D:105:LYS:HE3	2.35	0.41
2:G:43:TRP:CD1	2:G:54:ILE:HD12	2.56	0.41
1:F:2:ALA:N	2:G:222:ILE:HD11	2.36	0.41
1:B:363:SER:C	1:B:365:THR:H	2.25	0.41
2:C:16:ILE:CG1	2:C:65:ILE:HG12	2.45	0.41
2:D:12:GLY:H	2:D:68:VAL:HG13	1.84	0.41
2:G:185:VAL:HA	2:G:261:ILE:HG13	2.03	0.41
2:C:21:GLN:HB2	2:C:23:PHE:CD2	2.56	0.41
1:B:311:LEU:HA	1:B:311:LEU:HD12	1.83	0.41
1:F:97:HIS:CE1	1:F:101:MET:CE	2.98	0.40
3:M:66:LEU:HD12	3:M:72:PRO:HA	2.03	0.40
2:D:15:LEU:HD12	2:D:33:GLU:HB2	2.03	0.40
2:G:2:ILE:HG23	2:G:122:TRP:CZ2	2.56	0.40
1:B:109:ALA:HB1	1:B:243:ILE:HB	2.03	0.40
2:C:46:VAL:HG13	2:C:82:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:217:ILE:HG23	2:H:230:ASP:O	2.21	0.40
3:M:127:CYS:O	3:M:128:LEU:CB	2.69	0.40
1:B:357:LEU:HD13	1:B:397:ILE:HG23	2.04	0.40
1:E:359:LEU:HD12	1:E:359:LEU:N	2.36	0.40
1:A:174:TRP:CG	1:A:175:ALA:N	2.89	0.40
1:B:3:TRP:HA	1:B:4:PRO:HD3	1.94	0.40
1:A:19:ASP:C	1:A:21:GLY:H	2.25	0.40
1:F:212:LYS:O	1:F:244:GLN:HG3	2.21	0.40
1:E:219:ARG:HA	1:E:219:ARG:HD3	1.71	0.40
2:G:161:VAL:HG22	2:G:165:LEU:CG	2.39	0.40
1:E:396:VAL:HG13	1:E:407:MET:HE3	2.02	0.40
1:F:144:LEU:HD12	1:F:146:ILE:HD11	2.03	0.40
1:F:126:GLN:C	1:F:128:GLN:H	2.25	0.40
1:E:331:ILE:HD11	1:E:359:LEU:HD23	2.02	0.40
1:F:105:LEU:O	1:F:105:LEU:HD13	2.21	0.40
2:C:22:VAL:HG21	2:C:58:LEU:O	2.21	0.40
2:G:104:ASP:HA	2:G:122:TRP:CH2	2.56	0.40
3:N:12:ASP:HB3	3:N:13:ARG:NH1	2.36	0.40
1:E:384:ARG:HA	1:E:385:PRO:HD3	1.96	0.40
1:E:325:VAL:HB	1:E:387:ALA:HA	2.02	0.40
1:A:358:MET:HB3	1:A:398:SER:OG	2.21	0.40
3:M:103:TYR:CG	3:M:104:VAL:N	2.89	0.40
1:E:404:ARG:HH21	1:E:406:ARG:NE	2.19	0.40
2:H:116:LEU:HD21	2:H:119:LYS:N	2.36	0.40
2:H:130:GLU:HG3	2:H:136:PRO:CG	2.48	0.40
2:D:195:LYS:O	2:D:199:VAL:HG23	2.21	0.40
2:H:169:SER:C	2:H:171:HIS:H	2.23	0.40
1:A:159:ALA:O	1:A:163:TYR:HB3	2.22	0.40
1:B:270:GLU:HA	1:B:271:PRO:HD3	1.92	0.40
1:B:360:SER:HB2	1:B:396:VAL:H	1.86	0.40
1:A:404:ARG:HH12	1:A:407:MET:CE	2.35	0.40
1:A:372:SER:HB3	1:A:379:GLU:CG	2.52	0.40
3:M:45:ARG:HG3	3:M:46:ASN:N	2.37	0.40
1:E:122:GLU:HA	1:E:123:PRO:HD3	1.94	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	412/415 (99%)	312 (76%)	82 (20%)	18 (4%)	3	10
1	B	394/415 (95%)	322 (82%)	67 (17%)	5 (1%)	15	44
1	E	412/415 (99%)	325 (79%)	73 (18%)	14 (3%)	5	16
1	F	412/415 (99%)	323 (78%)	77 (19%)	12 (3%)	6	19
2	C	264/266 (99%)	212 (80%)	40 (15%)	12 (4%)	3	10
2	D	264/266 (99%)	224 (85%)	34 (13%)	6 (2%)	8	26
2	G	264/266 (99%)	219 (83%)	34 (13%)	11 (4%)	3	11
2	H	264/266 (99%)	202 (76%)	42 (16%)	20 (8%)	1	2
3	K	126/139 (91%)	74 (59%)	41 (32%)	11 (9%)	1	2
3	L	19/139 (14%)	12 (63%)	6 (32%)	1 (5%)	2	7
3	M	136/139 (98%)	85 (62%)	36 (26%)	15 (11%)	0	1
3	N	28/139 (20%)	20 (71%)	5 (18%)	3 (11%)	0	1
All	All	2995/3280 (91%)	2330 (78%)	537 (18%)	128 (4%)	3	10

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	MET
1	A	307	LYS
1	B	102	ALA
2	C	24	ASP
2	D	54	ILE
3	K	29	SER
3	K	31	PRO
3	K	102	ALA
3	K	117	LYS
1	E	19	ASP
1	E	32	ILE
1	E	62	CYS

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Mol	Chain	Res	Type
1	E	325	VAL
1	E	373	VAL
1	F	125	PRO
1	F	186	LEU
2	H	22	VAL
2	H	47	SER
2	H	115	LYS
3	M	99	PHE
3	M	111	SER
3	M	125	ILE
3	M	128	LEU
3	M	137	LYS
3	N	19	PRO
1	A	42	LYS
1	A	119	ALA
1	A	344	GLU
1	A	400	GLN
2	C	213	SER
2	D	160	TRP
3	K	103	TYR
1	E	31	GLY
1	E	367	LEU
1	E	372	SER
1	F	47	ILE
2	G	47	SER
2	G	115	LYS
2	G	132	LYS
2	H	51	VAL
2	H	52	LYS
2	H	163	PRO
2	H	174	GLU
3	M	58	ASP
3	M	135	PRO
3	M	136	VAL
3	N	26	GLY
1	A	95	PRO
1	A	124	PHE
1	A	410	TRP
2	C	23	PHE
2	C	25	TYR
2	C	47	SER
2	C	113	LYS

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Mol	Chain	Res	Type
2	D	52	LYS
2	D	56	ASP
3	K	55	ARG
3	K	116	LEU
1	E	64	LYS
1	F	18	VAL
1	F	36	LYS
1	F	342	ALA
1	F	343	LYS
2	G	98	LYS
2	G	265	LYS
2	H	9	PRO
2	H	46	VAL
2	H	93	LYS
2	H	117	SER
2	H	224	ALA
3	M	70	ALA
3	M	124	TYR
3	M	127	CYS
1	A	399	ARG
1	B	263	LYS
2	C	46	VAL
2	C	132	LYS
2	D	162	LYS
3	K	30	LEU
3	L	14	LEU
1	E	46	THR
1	E	137	GLY
1	E	176	GLU
1	F	35	SER
1	F	108	ALA
1	F	200	GLU
2	H	190	PRO
3	M	33	MET
3	M	120	LYS
3	N	8	VAL
1	A	120	ALA
1	A	123	PRO
1	A	159	ALA
1	A	337	GLU
1	B	379	GLU
2	C	224	ALA

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Mol	Chain	Res	Type
2	D	47	SER
3	K	113	ASP
1	F	341	GLY
2	G	27	SER
2	G	192	GLY
2	G	224	ALA
2	H	19	VAL
2	H	42	PRO
2	H	132	LYS
2	H	212	GLU
3	M	31	PRO
3	M	107	SER
1	A	408	ILE
1	B	325	VAL
3	K	112	LEU
1	F	77	CYS
2	G	239	ALA
2	G	264	VAL
1	A	44	GLY
2	C	51	VAL
2	C	76	GLY
1	E	180	ILE
2	H	68	VAL
2	H	69	ILE
2	H	125	VAL
3	K	60	ILE
1	B	411	GLY
2	C	159	ILE
1	E	223	VAL
2	G	76	GLY
1	A	151	VAL
1	A	65	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	356/357 (100%)	335 (94%)	21 (6%)	24	57
1	B	343/357 (96%)	330 (96%)	13 (4%)	40	74
1	E	356/357 (100%)	338 (95%)	18 (5%)	29	63
1	F	356/357 (100%)	328 (92%)	28 (8%)	15	40
2	C	237/239 (99%)	215 (91%)	22 (9%)	11	32
2	D	237/239 (99%)	223 (94%)	14 (6%)	24	57
2	G	237/239 (99%)	222 (94%)	15 (6%)	22	53
2	H	237/239 (99%)	219 (92%)	18 (8%)	16	42
3	K	117/126 (93%)	108 (92%)	9 (8%)	16	41
3	L	20/126 (16%)	20 (100%)	0	100	100
3	M	125/126 (99%)	119 (95%)	6 (5%)	31	66
3	N	28/126 (22%)	26 (93%)	2 (7%)	18	46
All	All	2649/2888 (92%)	2483 (94%)	166 (6%)	22	53

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	46	THR
1	A	103	THR
1	A	105	LEU
1	A	111	MET
1	A	116	LEU
1	A	142	LYS
1	A	143	ASN
1	A	168	GLN
1	A	207	ARG
1	A	218	ILE
1	A	232	GLU
1	A	266	LYS
1	A	287	LYS
1	A	307	LYS
1	A	315	ILE
1	A	325	VAL
1	A	352	ARG
1	A	383	ARG
1	A	395	THR
1	A	404	ARG
1	B	22	LYS

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Mol	Chain	Res	Type
1	B	105	LEU
1	B	142	LYS
1	B	144	LEU
1	B	192	ASP
1	B	203	LYS
1	B	217	VAL
1	B	225	LYS
1	B	231	ASN
1	B	234	LYS
1	B	243	ILE
1	B	251	GLN
1	B	405	TRP
2	C	5	ARG
2	C	16	ILE
2	C	41	LEU
2	C	45	GLU
2	C	46	VAL
2	C	70	ARG
2	C	74	ARG
2	C	91	ARG
2	C	105	LYS
2	C	112	GLN
2	C	114	LEU
2	C	127	TRP
2	C	160	TRP
2	C	161	VAL
2	C	175	ARG
2	C	176	LYS
2	C	182	LEU
2	C	194	GLU
2	C	214	LEU
2	C	216	ASN
2	C	222	ILE
2	C	261	ILE
2	D	3	TYR
2	D	4	SER
2	D	62	ARG
2	D	68	VAL
2	D	71	VAL
2	D	94	ASN
2	D	101	GLN
2	D	119	LYS

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Mol	Chain	Res	Type
2	D	166	GLU
2	D	171	HIS
2	D	175	ARG
2	D	216	ASN
2	D	222	ILE
2	D	264	VAL
3	K	9	GLU
3	K	32	ASN
3	K	36	LEU
3	K	54	ILE
3	K	103	TYR
3	K	105	GLU
3	K	108	THR
3	K	112	LEU
3	K	118	LYS
1	E	19	ASP
1	E	45	MET
1	E	64	LYS
1	E	150	LYS
1	E	162	GLN
1	E	171	LYS
1	E	192	ASP
1	E	216	LEU
1	E	219	ARG
1	E	221	PHE
1	E	287	LYS
1	E	327	TRP
1	E	330	ARG
1	E	338	ARG
1	E	343	LYS
1	E	344	GLU
1	E	400	GLN
1	E	412	LEU
1	F	7	GLN
1	F	22	LYS
1	F	33	TRP
1	F	38	SER
1	F	45	MET
1	F	89	ILE
1	F	97	HIS
1	F	99	VAL
1	F	101	MET

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Mol	Chain	Res	Type
1	F	144	LEU
1	F	151	VAL
1	F	152	ASP
1	F	209	LEU
1	F	216	LEU
1	F	219	ARG
1	F	242	ILE
1	F	246	LEU
1	F	263	LYS
1	F	274	THR
1	F	287	LYS
1	F	320	ASP
1	F	326	LEU
1	F	376	ASP
1	F	391	ASN
1	F	395	THR
1	F	404	ARG
1	F	408	ILE
1	F	412	LEU
2	G	29	VAL
2	G	50	TRP
2	G	73	ARG
2	G	83	LYS
2	G	86	THR
2	G	101	GLN
2	G	115	LYS
2	G	116	LEU
2	G	137	ILE
2	G	156	VAL
2	G	186	ARG
2	G	193	VAL
2	G	214	LEU
2	G	226	ARG
2	G	237	LYS
2	H	15	LEU
2	H	49	LYS
2	H	50	TRP
2	H	51	VAL
2	H	58	LEU
2	H	59	LYS
2	H	63	LYS
2	H	69	ILE

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Mol	Chain	Res	Type
2	H	127	TRP
2	H	162	LYS
2	H	170	LYS
2	H	182	LEU
2	H	183	ILE
2	H	191	LEU
2	H	214	LEU
2	H	229	VAL
2	H	237	LYS
2	H	258	ASN
3	M	98	ARG
3	M	108	THR
3	M	109	CYS
3	M	110	LYS
3	M	127	CYS
3	M	128	LEU
3	N	7	TYR
3	N	10	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	97	HIS
1	A	128	GLN
1	A	132	HIS
1	A	168	GLN
1	B	7	GLN
1	B	121	ASN
1	B	148	GLN
1	B	168	GLN
1	B	187	HIS
1	B	224	ASN
1	B	231	ASN
1	B	244	GLN
1	B	310	ASN
1	B	334	ASN
2	C	21	GLN
2	C	38	GLN
2	C	61	ASN
2	C	96	GLN
2	C	112	GLN

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Mol	Chain	Res	Type
2	C	124	GLN
2	C	171	HIS
2	C	206	ASN
2	C	216	ASN
2	D	21	GLN
2	D	61	ASN
2	D	94	ASN
2	D	96	GLN
2	D	101	GLN
2	D	209	GLN
2	D	216	ASN
2	D	244	ASN
2	D	258	ASN
3	K	32	ASN
3	K	46	ASN
1	E	126	GLN
1	E	132	HIS
1	E	149	ASN
1	E	162	GLN
1	E	177	ASN
1	E	187	HIS
1	E	310	ASN
1	E	334	ASN
1	E	392	ASN
1	E	400	GLN
1	F	20	HIS
1	F	97	HIS
1	F	126	GLN
1	F	143	ASN
1	F	165	GLN
1	F	177	ASN
1	F	211	GLN
1	F	224	ASN
1	F	231	ASN
1	F	264	GLN
1	F	310	ASN
1	F	391	ASN
1	F	392	ASN
2	G	38	GLN
2	G	101	GLN
2	G	206	ASN
2	G	235	ASN

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Mol	Chain	Res	Type
2	G	249	ASN
2	H	101	GLN
2	H	244	ASN
2	H	258	ASN
3	M	37	ASN
3	M	46	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	414/415 (99%)	-0.27	4 (0%) 84 77	47, 105, 152, 162	0
1	B	400/415 (96%)	-0.29	4 (1%) 84 77	37, 109, 149, 173	0
1	E	414/415 (99%)	-0.28	5 (1%) 81 73	46, 106, 150, 165	0
1	F	414/415 (99%)	-0.31	2 (0%) 91 88	47, 107, 147, 163	0
2	C	266/266 (100%)	-0.38	3 (1%) 82 74	42, 95, 133, 151	0
2	D	266/266 (100%)	-0.37	1 (0%) 93 90	38, 98, 135, 169	0
2	G	266/266 (100%)	-0.44	0 100 100	41, 90, 120, 138	0
2	H	266/266 (100%)	-0.31	1 (0%) 93 90	36, 102, 135, 146	0
3	K	128/139 (92%)	0.32	8 (6%) 23 14	124, 148, 168, 175	0
3	L	21/139 (15%)	-0.24	0 100 100	89, 119, 133, 134	0
3	M	138/139 (99%)	0.23	10 (7%) 18 10	108, 147, 172, 181	0
3	N	30/139 (21%)	0.01	1 (3%) 50 38	100, 139, 154, 155	0
All	All	3023/3280 (92%)	-0.27	39 (1%) 79 71	36, 106, 153, 181	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	LEU	7.4
3	M	128	LEU	6.6
3	K	36	LEU	4.8
3	N	28	GLN	4.6
3	K	126	VAL	4.0
3	K	96	MET	3.8
1	B	347	LYS	3.6
2	D	50	TRP	3.5
1	F	97	HIS	3.5
3	M	2	SER	3.5
1	A	120	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
3	M	69	LEU	3.3
3	K	123	TRP	3.3
3	K	24	LYS	3.2
3	K	84	GLN	2.9
2	C	159	ILE	2.9
1	B	103	THR	2.8
1	A	47	ILE	2.7
3	K	117	LYS	2.7
2	H	48	SER	2.7
1	A	345	MET	2.7
1	E	408	ILE	2.7
1	E	367	LEU	2.6
3	M	129	ALA	2.5
1	A	403	GLY	2.5
1	E	39	GLU	2.3
1	E	33	TRP	2.3
3	M	43	ILE	2.3
2	C	75	LYS	2.2
1	F	373	VAL	2.2
1	E	335	LEU	2.1
1	B	33	TRP	2.1
3	M	130	CYS	2.1
2	C	51	VAL	2.1
3	K	112	LEU	2.1
3	M	23	ARG	2.1
3	M	123	TRP	2.1
3	M	72	PRO	2.0
3	M	132	ALA	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.