



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:54 PM GMT

PDB ID : 3S7Y
Title : Crystal structure of mmNAGS in Space Group P3121 at 4.3 Å resolution
Authors : Shi, D.; Li, Y.; Cabrera-Luque, J.; Jin, Z.; Yu, X.; Allewell, N.M.; Tuchman, M.
Deposited on : 2011-05-27
Resolution : 4.31 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

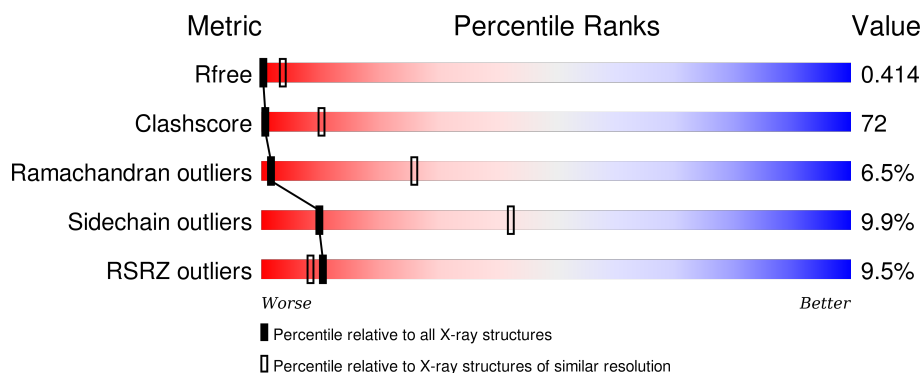
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.31 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	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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	461	
1	X	461	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6683 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 N-acetylglutamate kinase / N-acetylglutamate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	1	0
			3349	2107	605	631	6			
1	X	435	Total	C	N	O	S	0	0	0
			3334	2097	601	630	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q0ASS9
A	-18	GLY	-	EXPRESSION TAG	UNP Q0ASS9
A	-17	SER	-	EXPRESSION TAG	UNP Q0ASS9
A	-16	SER	-	EXPRESSION TAG	UNP Q0ASS9
A	-15	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-14	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-13	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-12	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-11	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-10	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-9	SER	-	EXPRESSION TAG	UNP Q0ASS9
A	-8	SER	-	EXPRESSION TAG	UNP Q0ASS9
A	-7	GLY	-	EXPRESSION TAG	UNP Q0ASS9
A	-6	LEU	-	EXPRESSION TAG	UNP Q0ASS9
A	-5	VAL	-	EXPRESSION TAG	UNP Q0ASS9
A	-4	PRO	-	EXPRESSION TAG	UNP Q0ASS9
A	-3	ARG	-	EXPRESSION TAG	UNP Q0ASS9
A	-2	GLY	-	EXPRESSION TAG	UNP Q0ASS9
A	-1	SER	-	EXPRESSION TAG	UNP Q0ASS9
A	0	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-19	MET	-	EXPRESSION TAG	UNP Q0ASS9
X	-18	GLY	-	EXPRESSION TAG	UNP Q0ASS9
X	-17	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	-16	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	-15	HIS	-	EXPRESSION TAG	UNP Q0ASS9

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-14	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-13	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-12	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-11	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-10	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-9	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	-8	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	-7	GLY	-	EXPRESSION TAG	UNP Q0ASS9
X	-6	LEU	-	EXPRESSION TAG	UNP Q0ASS9
X	-5	VAL	-	EXPRESSION TAG	UNP Q0ASS9
X	-4	PRO	-	EXPRESSION TAG	UNP Q0ASS9
X	-3	ARG	-	EXPRESSION TAG	UNP Q0ASS9
X	-2	GLY	-	EXPRESSION TAG	UNP Q0ASS9
X	-1	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	0	HIS	-	EXPRESSION TAG	UNP Q0ASS9

E438	G369	R307	A315	L296	G170	D103
A439	R370	L308	F316	M237	Q171	E104
PRO	V372	D309	G317	Q238	A172	A105
GLN	N373	N310	R318	A239	I174	I106
	N374	L311	P319	V242	I175	I107
	R375			N243	A176	I108
				G244	G177	I109
				M245	L178	L113
				G246	G179	T114
				R247	E180	Q115
				E251	T181	A116
				K254	P182	N117
				R255	D183	L118
				L256	G184	A119
				L257	T185	L120
				D258	L186	V121
				D259	V187	I124
				L260	M188	
				P261	I189	R130
				L262	N190	A131
				S263	D191	A132
				S264	V193	A133
				S265	A194	V134
				V266	V195	P135
				S267	R196	R136
				L268	A197	G137
				T269	H200	V138
				R270	A201	E140
				E273	L202	A141
				L274	Q203	D142
				A275	P204	I143
				R276	V205	V144
				E277	K206	D145
				L278	V207	A146
				F279	V208	D147
				G285	F209	K148
				T286	L210	L149
				L287	T211	G150
				I288	G212	R151
				R289	T213	V152
				G291	G214	G153
				E292	G215	E154
				A293	L216	P155
				R293	L217	R156
				A296	G221	I158
				T297	D222	H159
				D298	T223	L160
				D299	L224	D161
				K300	S225	L162
				S301	S226	V163
				S302	I227	G164
				L303	N228	S165
				G367	L229	A166
				L368	A230	A167
					T231	R168
					D232	A169

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.11Å 95.11Å 253.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.13 – 4.31 46.74 – 4.31	Depositor EDS
% Data completeness (in resolution range)	92.1 (31.13-4.31) 89.2 (46.74-4.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.274 , 0.419 0.262 , 0.414	Depositor DCC
R_{free} test set	867 reflections (9.93%)	DCC
Wilson B-factor (Å ²)	192.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 406.6	EDS
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 9472 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6683	wwPDB-VP
Average B, all atoms (Å ²)	456.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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	0.77	1/3412 (0.0%)	1.29	26/4639 (0.6%)
1	X	0.66	0/3393	0.99	12/4613 (0.3%)
All	All	0.72	1/6805 (0.0%)	1.15	38/9252 (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
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	ALA	CA-CB	-6.79	1.38	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	LEU	CB-CG-CD1	-9.50	94.86	111.00
1	A	236	LEU	CA-CB-CG	-9.06	94.45	115.30
1	A	260	LEU	CA-CB-CG	8.92	135.81	115.30
1	A	85	LEU	CB-CG-CD2	-8.54	96.49	111.00
1	A	354	LEU	CA-CB-CG	-7.52	98.01	115.30
1	X	354	LEU	CA-CB-CG	-7.21	98.72	115.30
1	A	236	LEU	CB-CG-CD1	7.12	123.11	111.00
1	A	344	ILE	N-CA-C	6.90	129.63	111.00
1	A	291	GLY	N-CA-C	-6.84	95.99	113.10
1	X	156	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	X	260	LEU	CA-CB-CG	6.75	130.83	115.30
1	A	115	GLN	CB-CG-CD	6.74	129.12	111.60
1	A	156	ARG	CG-CD-NE	6.73	125.93	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	156	ARG	CG-CD-NE	6.33	125.10	111.80
1	A	303	LEU	CA-CB-CG	-6.05	101.39	115.30
1	X	224	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	353	TYR	CB-CG-CD1	5.86	124.51	121.00
1	X	236	LEU	CB-CG-CD2	5.82	120.90	111.00
1	A	347	ARG	CA-CB-CG	-5.68	100.90	113.40
1	A	229	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	353	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	137	GLY	N-CA-C	5.55	126.98	113.10
1	A	257	LEU	CB-CG-CD2	-5.53	101.59	111.00
1	X	115	GLN	CB-CG-CD	5.47	125.83	111.60
1	A	95	VAL	N-CA-C	5.36	125.47	111.00
1	X	115	GLN	CA-CB-CG	-5.35	101.63	113.40
1	A	162	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	A	224	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	439	ALA	N-CA-C	5.32	125.36	111.00
1	A	354	LEU	CB-CG-CD1	-5.26	102.05	111.00
1	A	142	ASP	N-CA-CB	-5.20	101.24	110.60
1	A	360	LEU	CA-CB-CG	-5.18	103.39	115.30
1	A	344	ILE	CB-CA-C	-5.15	101.31	111.60
1	X	393	VAL	CB-CA-C	-5.13	101.65	111.40
1	X	368	LEU	CB-CG-CD1	-5.10	102.34	111.00
1	X	156	ARG	CD-NE-CZ	-5.09	116.48	123.60
1	X	360	LEU	CA-CB-CG	-5.05	103.68	115.30
1	A	268	ILE	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	GLN	Sidechain
1	A	413	PHE	Mainchain

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	3349	0	3352	533	0
1	X	3334	0	3332	462	0
All	All	6683	0	6684	956	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 72.

All (956) 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)
1:A:296:ALA:O	1:A:297:THR:HG22	1.21	1.26
1:A:398:PHE:CD1	1:X:398:PHE:CD1	2.33	1.15
1:A:95:VAL:H	1:A:100:VAL:CG1	1.59	1.14
1:A:295:VAL:HG22	1:A:335:VAL:O	1.46	1.14
1:A:266:VAL:O	1:A:287:LEU:HA	1.47	1.14
1:A:267:SER:HA	1:A:286:THR:O	1.48	1.13
1:A:398:PHE:CE2	1:X:406:ARG:HD2	1.85	1.10
1:X:266:VAL:O	1:X:287:LEU:HA	1.51	1.09
1:A:95:VAL:HG23	1:A:100:VAL:HG11	1.31	1.07
1:A:292:GLU:OE2	1:A:368:LEU:HD11	1.52	1.06
1:A:292:GLU:CD	1:A:368:LEU:HD11	1.78	1.03
1:X:332:ARG:HG3	1:X:332:ARG:HH11	1.24	1.02
1:A:29:LEU:HD21	1:A:68:GLY:HA3	1.41	1.02
1:A:37:GLN:O	1:A:40:PHE:HD2	1.41	1.02
1:X:267:SER:HA	1:X:286:THR:O	1.59	1.01
1:X:86:GLU:O	1:X:91:PRO:HD2	1.59	1.01
1:A:232:ASP:HB3	1:A:236:LEU:CD1	1.91	1.01
1:A:29:LEU:CD2	1:A:68:GLY:HA3	1.90	1.00
1:A:65:GLN:HE22	1:A:130:ARG:HB2	1.25	0.99
1:A:420:PRO:HB3	1:X:420:PRO:HB3	1.44	0.99
1:A:95:VAL:HB	1:A:149:LEU:HD23	1.43	0.99
1:X:65:GLN:HE22	1:X:130:ARG:HB2	1.22	0.98
1:A:296:ALA:O	1:A:297:THR:CG2	2.11	0.98
1:A:398:PHE:CD1	1:X:398:PHE:HD1	1.78	0.98
1:X:95:VAL:HG22	1:X:99:ARG:H	1.24	0.98
1:A:90:ILE:N	1:A:91:PRO:HD3	1.76	0.97
1:A:292:GLU:CD	1:A:368:LEU:CD1	2.33	0.97
1:X:232:ASP:HB3	1:X:236:LEU:HD23	1.46	0.96
1:A:13:VAL:CG1	1:A:26:ARG:HD3	1.94	0.96
1:A:95:VAL:CG1	1:A:148:LYS:HE2	1.94	0.95
1:A:95:VAL:CG2	1:A:100:VAL:HG11	1.97	0.95
1:A:196:ARG:HD3	1:A:255:ARG:HD2	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ARG:HD2	1:X:398:PHE:CE2	2.00	0.95
1:A:95:VAL:H	1:A:100:VAL:HG13	1.32	0.95
1:A:331:ASP:HB3	1:A:345:THR:OG1	1.66	0.94
1:X:36:ASP:HB2	1:X:39:ARG:HB2	1.47	0.94
1:A:50:ILE:HG13	1:A:80:GLN:HE22	1.30	0.94
1:A:173:ALA:C	1:A:174:ILE:HD13	1.88	0.94
1:X:133:ALA:C	1:X:135:PRO:HD3	1.89	0.93
1:X:297:THR:H	1:X:332:ARG:HH12	1.17	0.93
1:A:297:THR:N	1:A:332:ARG:HH12	1.65	0.92
1:A:297:THR:H	1:A:332:ARG:HH12	1.02	0.92
1:A:258:ASP:OD1	1:A:290:ARG:HD2	1.69	0.92
1:X:50:ILE:HG13	1:X:80:GLN:HE22	1.30	0.91
1:A:13:VAL:HG11	1:A:26:ARG:HD3	1.52	0.91
1:A:121:VAL:HG21	1:A:133:ALA:HB2	1.51	0.91
1:X:134:VAL:N	1:X:135:PRO:HD3	1.86	0.90
1:A:37:GLN:O	1:A:40:PHE:CD2	2.25	0.90
1:A:232:ASP:O	1:A:236:LEU:HD12	1.73	0.89
1:A:406:ARG:NH1	1:X:398:PHE:HE2	1.69	0.89
1:X:65:GLN:NE2	1:X:130:ARG:HB2	1.87	0.89
1:X:328:LEU:HG	1:X:330:VAL:HG23	1.54	0.89
1:X:258:ASP:OD1	1:X:290:ARG:HD2	1.71	0.89
1:A:404:ALA:HB3	1:X:404:ALA:HB3	1.56	0.88
1:A:406:ARG:HD2	1:X:398:PHE:CZ	2.09	0.88
1:A:372:VAL:HG12	1:A:373:TRP:N	1.89	0.88
1:A:143:ILE:HD12	1:A:152:VAL:O	1.74	0.88
1:A:77:GLY:O	1:A:81:LEU:HG	1.73	0.87
1:A:29:LEU:HD21	1:A:67:VAL:O	1.74	0.87
1:A:398:PHE:CE1	1:X:398:PHE:HD1	1.93	0.87
1:X:296:ALA:HB1	1:X:332:ARG:NH2	1.89	0.87
1:A:328:LEU:HG	1:A:330:VAL:HG23	1.55	0.87
1:X:64:LEU:HD22	1:X:69:LEU:HD12	1.56	0.86
1:A:203:GLN:OE1	1:A:261:PRO:HD3	1.75	0.86
1:A:404:ALA:O	1:A:405:VAL:HG23	1.73	0.86
1:X:232:ASP:HB3	1:X:236:LEU:CD2	2.04	0.86
1:A:229:LEU:HD22	1:A:254:LYS:HB2	1.58	0.86
1:X:332:ARG:HH11	1:X:332:ARG:CG	1.89	0.86
1:A:82:ASP:OD1	1:A:99:ARG:NH2	2.08	0.86
1:A:65:GLN:NE2	1:A:130:ARG:HB2	1.89	0.85
1:X:82:ASP:OD1	1:X:99:ARG:NH2	2.08	0.85
1:X:143:ILE:HD12	1:X:152:VAL:O	1.75	0.85
1:X:28:TYR:O	1:X:32:PHE:HB2	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:353:TYR:CE2	1:X:355:ASP:HA	2.11	0.85
1:A:64:LEU:HD12	1:A:71:PRO:HG3	1.57	0.85
1:A:97:GLY:O	1:A:98:LEU:HD23	1.76	0.85
1:X:121:VAL:HG21	1:X:133:ALA:HB2	1.57	0.84
1:X:292:GLU:OE1	1:X:337:GLU:HB3	1.77	0.84
1:A:85:LEU:HD21	1:A:108:ILE:HG21	1.59	0.84
1:X:12:ILE:O	1:X:16:LEU:HG	1.76	0.84
1:X:353:TYR:HE2	1:X:355:ASP:HA	1.43	0.84
1:A:51:GLN:OE1	1:A:80:GLN:HG3	1.77	0.84
1:A:229:LEU:HD12	1:A:289:ARG:O	1.78	0.84
1:A:85:LEU:CD2	1:A:108:ILE:HG21	2.08	0.83
1:X:232:ASP:CB	1:X:236:LEU:HD23	2.08	0.83
1:X:29:LEU:HD22	1:X:69:LEU:HD21	1.57	0.83
1:A:398:PHE:HD1	1:X:398:PHE:CD1	1.90	0.83
1:X:401:CYS:SG	1:X:403:GLY:O	2.37	0.83
1:A:157:HIS:C	1:A:158:ILE:HD13	1.98	0.83
1:A:133:ALA:C	1:A:135:PRO:HD3	1.98	0.83
1:A:12:ILE:HA	1:X:15:LEU:HD11	1.60	0.83
1:X:43:ILE:O	1:X:43:ILE:HG22	1.78	0.83
1:A:95:VAL:HG12	1:A:148:LYS:HE2	1.59	0.82
1:X:296:ALA:HB1	1:X:332:ARG:HH22	1.44	0.82
1:X:196:ARG:HD3	1:X:255:ARG:HD2	1.61	0.82
1:A:47:GLY:HA3	1:A:78:GLY:N	1.95	0.82
1:A:398:PHE:HD1	1:X:398:PHE:CE1	1.97	0.82
1:X:51:GLN:OE1	1:X:80:GLN:HG3	1.79	0.81
1:X:42:VAL:HB	1:X:207:VAL:HG22	1.63	0.81
1:A:42:VAL:HG23	1:A:204:PRO:HG2	1.60	0.81
1:A:95:VAL:N	1:A:100:VAL:CG1	2.42	0.81
1:A:96:ASP:OD1	1:A:148:LYS:NZ	2.13	0.81
1:A:95:VAL:HG11	1:A:148:LYS:HG2	1.63	0.81
1:X:77:GLY:O	1:X:81:LEU:HG	1.81	0.81
1:A:265:SER:O	1:A:266:VAL:HG23	1.80	0.80
1:A:265:SER:C	1:A:266:VAL:HG23	2.01	0.80
1:A:174:ILE:N	1:A:174:ILE:HD13	1.90	0.80
1:A:371:THR:O	1:A:374:ASN:HB2	1.80	0.80
1:X:398:PHE:CD2	1:X:398:PHE:O	2.34	0.80
1:X:297:THR:N	1:X:332:ARG:HH12	1.79	0.80
1:A:93:GLU:OE2	1:A:102:ARG:CZ	2.30	0.80
1:X:203:GLN:OE1	1:X:261:PRO:HD3	1.81	0.79
1:X:372:VAL:HG12	1:X:373:TRP:N	1.95	0.79
1:A:348:LEU:HD11	1:A:429:LYS:HD3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:PHE:HE2	1:X:406:ARG:HH11	1.30	0.79
1:A:45:VAL:HG22	1:A:210:LEU:HB2	1.64	0.79
1:A:106:ILE:HD13	1:A:186:LEU:HD23	1.63	0.79
1:A:64:LEU:HD22	1:A:69:LEU:HD12	1.64	0.79
1:X:157:HIS:C	1:X:158:ILE:HD13	2.03	0.79
1:A:42:VAL:HG23	1:A:204:PRO:CG	2.12	0.79
1:X:94:ARG:O	1:X:100:VAL:N	2.16	0.79
1:A:42:VAL:HB	1:A:207:VAL:HG22	1.64	0.78
1:X:67:VAL:HG12	1:X:69:LEU:HG	1.65	0.78
1:A:95:VAL:HB	1:A:149:LEU:CD2	2.14	0.78
1:A:63:PHE:O	1:A:67:VAL:HG13	1.82	0.78
1:A:93:GLU:HB3	1:A:100:VAL:HG22	1.65	0.78
1:A:404:ALA:O	1:A:405:VAL:CG2	2.31	0.78
1:A:214:GLY:HA2	1:A:269:THR:C	2.05	0.78
1:A:411:THR:HG22	1:A:413:PHE:CE2	2.19	0.78
1:A:48:ALA:N	1:A:79:PRO:HD2	1.98	0.78
1:A:94:ARG:HG2	1:A:99:ARG:HA	1.65	0.78
1:X:89:ASP:C	1:X:91:PRO:HD3	2.04	0.77
1:X:214:GLY:HA3	1:X:270:ARG:HB3	1.63	0.77
1:X:37:GLN:HG2	1:X:38:GLU:OE2	1.84	0.77
1:A:67:VAL:CG2	1:A:69:LEU:HG	2.14	0.77
1:A:372:VAL:CG1	1:A:373:TRP:N	2.48	0.77
1:A:214:GLY:HA3	1:A:270:ARG:HB3	1.65	0.77
1:X:318:ARG:CG	1:X:437:LEU:HB3	2.14	0.77
1:X:42:VAL:HG23	1:X:204:PRO:CG	2.15	0.76
1:X:214:GLY:HA2	1:X:269:THR:C	2.06	0.76
1:X:173:ALA:C	1:X:174:ILE:HD13	2.06	0.76
1:X:404:ALA:O	1:X:405:VAL:HG23	1.84	0.76
1:X:348:LEU:HD11	1:X:429:LYS:HD3	1.67	0.76
1:A:134:VAL:N	1:A:135:PRO:HD3	1.93	0.76
1:A:42:VAL:O	1:A:43:ILE:HG13	1.86	0.76
1:X:136:ARG:HH22	1:X:180:GLU:HB3	1.51	0.76
1:X:95:VAL:HG22	1:X:99:ARG:N	2.01	0.75
1:X:75:HIS:NE2	1:X:117:ASN:OD1	2.14	0.75
1:A:401:CYS:SG	1:A:403:GLY:O	2.44	0.75
1:A:266:VAL:O	1:A:287:LEU:CA	2.32	0.75
1:A:88:ALA:O	1:A:89:ASP:HB2	1.87	0.75
1:X:42:VAL:HG23	1:X:204:PRO:HG2	1.67	0.75
1:A:265:SER:O	1:A:266:VAL:CG2	2.35	0.75
1:A:353:TYR:CE2	1:A:355:ASP:HA	2.22	0.75
1:A:246:MET:HG3	1:A:246:MET:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:36:ASP:HB3	1:X:39:ARG:HG3	1.69	0.74
1:A:13:VAL:HG13	1:A:26:ARG:HD3	1.70	0.74
1:X:353:TYR:O	1:X:353:TYR:CD2	2.41	0.74
1:A:75:HIS:NE2	1:A:117:ASN:OD1	2.18	0.74
1:X:37:GLN:HB3	1:X:38:GLU:OE2	1.87	0.73
1:A:406:ARG:HH11	1:X:398:PHE:HE2	1.35	0.73
1:A:32:PHE:CD1	1:A:36:ASP:OD2	2.42	0.73
1:X:411:THR:CG2	1:X:413:PHE:CE2	2.71	0.73
1:A:95:VAL:HG23	1:A:100:VAL:CG1	2.17	0.73
1:A:197:ALA:O	1:A:200:HIS:HB3	1.89	0.73
1:A:390:ASN:O	1:A:392:PRO:N	2.22	0.73
1:A:311:LEU:CD1	1:A:360:LEU:HD11	2.19	0.73
1:X:47:GLY:HA3	1:X:78:GLY:N	2.04	0.73
1:X:357:PHE:HE1	1:X:372:VAL:HG11	1.53	0.73
1:A:42:VAL:C	1:A:43:ILE:HG13	2.09	0.72
1:A:136:ARG:HH11	1:A:136:ARG:HB3	1.54	0.72
1:X:132:ALA:HB2	1:X:171:GLN:OE1	1.88	0.72
1:X:239:ALA:HB3	1:X:242:VAL:HG23	1.70	0.72
1:X:229:LEU:HD12	1:X:289:ARG:O	1.90	0.72
1:A:85:LEU:HD21	1:A:108:ILE:CG2	2.19	0.72
1:X:106:ILE:HD13	1:X:186:LEU:HD23	1.71	0.72
1:A:398:PHE:HE2	1:X:406:ARG:NH1	1.87	0.72
1:A:357:PHE:HE1	1:A:372:VAL:HG11	1.53	0.72
1:X:329:ARG:O	1:X:330:VAL:HB	1.89	0.72
1:X:411:THR:HG22	1:X:413:PHE:CE2	2.25	0.71
1:X:64:LEU:HD12	1:X:71:PRO:HG3	1.71	0.71
1:A:398:PHE:CZ	1:X:406:ARG:HD2	2.23	0.71
1:X:296:ALA:CB	1:X:332:ARG:HH22	2.02	0.71
1:A:232:ASP:CB	1:A:236:LEU:CD1	2.69	0.71
1:A:155:PRO:HD3	1:A:189:ILE:HD12	1.73	0.71
1:A:136:ARG:HH22	1:A:180:GLU:HB3	1.56	0.71
1:A:131:ALA:HA	1:A:171:GLN:HB3	1.71	0.71
1:A:15:LEU:HD21	1:X:15:LEU:C	2.11	0.71
1:X:38:GLU:C	1:X:40:PHE:H	1.92	0.70
1:A:267:SER:CA	1:A:286:THR:O	2.35	0.70
1:A:292:GLU:OE2	1:A:368:LEU:CD1	2.33	0.70
1:X:351:TRP:CD1	1:X:426:VAL:HG11	2.26	0.70
1:X:48:ALA:N	1:X:79:PRO:HD2	2.07	0.70
1:X:157:HIS:O	1:X:158:ILE:HD13	1.92	0.70
1:X:136:ARG:HH11	1:X:136:ARG:HB3	1.56	0.70
1:A:132:ALA:HB2	1:A:171:GLN:OE1	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:67:VAL:CG1	1:X:69:LEU:HG	2.21	0.70
1:X:318:ARG:HG3	1:X:437:LEU:HB3	1.72	0.70
1:A:36:ASP:HB2	1:A:39:ARG:HB2	1.74	0.70
1:X:197:ALA:O	1:X:200:HIS:HB3	1.91	0.70
1:A:406:ARG:HG2	1:A:411:THR:OG1	1.92	0.70
1:A:38:GLU:C	1:A:40:PHE:H	1.95	0.70
1:A:51:GLN:HB2	1:A:80:GLN:NE2	2.07	0.70
1:A:328:LEU:CG	1:A:330:VAL:HG23	2.21	0.70
1:A:163:VAL:HG22	1:A:175:LEU:HD11	1.74	0.69
1:A:229:LEU:HD12	1:A:290:ARG:HA	1.74	0.69
1:X:412:VAL:HG23	1:X:431:PHE:CE1	2.27	0.69
1:X:155:PRO:HD3	1:X:189:ILE:HD12	1.74	0.69
1:X:51:GLN:HB2	1:X:80:GLN:NE2	2.08	0.69
1:A:90:ILE:HD12	1:A:104:GLU:OE1	1.92	0.69
1:X:37:GLN:CB	1:X:38:GLU:OE2	2.40	0.69
1:A:411:THR:CG2	1:A:413:PHE:CE2	2.75	0.69
1:A:145:ASP:OD2	1:A:149:LEU:HD12	1.93	0.69
1:A:29:LEU:HD21	1:A:68:GLY:CA	2.19	0.69
1:A:81:LEU:CD1	1:A:99:ARG:HH22	2.05	0.69
1:A:95:VAL:HG11	1:A:148:LYS:HE2	1.72	0.69
1:A:232:ASP:C	1:A:236:LEU:HD12	2.12	0.69
1:X:64:LEU:CD2	1:X:69:LEU:HD12	2.21	0.69
1:X:297:THR:N	1:X:332:ARG:NH1	2.39	0.69
1:A:32:PHE:HB2	1:A:40:PHE:CZ	2.28	0.69
1:A:420:PRO:HB3	1:X:420:PRO:CB	2.21	0.69
1:X:265:SER:HB2	1:X:287:LEU:HD21	1.74	0.69
1:A:5:ALA:HB3	1:A:6:PRO:HD3	1.75	0.69
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.57	0.69
1:X:81:LEU:O	1:X:86:GLU:HB2	1.92	0.69
1:A:47:GLY:C	1:A:79:PRO:HD2	2.13	0.69
1:X:113:LEU:O	1:X:117:ASN:N	2.26	0.69
1:A:85:LEU:HD21	1:A:108:ILE:CB	2.23	0.69
1:X:328:LEU:CG	1:X:330:VAL:HG23	2.23	0.68
1:A:229:LEU:HD22	1:A:254:LYS:CB	2.23	0.68
1:A:121:VAL:HG21	1:A:133:ALA:CB	2.24	0.68
1:X:117:ASN:OD1	1:X:176:ALA:HB2	1.93	0.68
1:A:43:ILE:O	1:A:43:ILE:HG22	1.93	0.68
1:A:353:TYR:HE2	1:A:355:ASP:HA	1.56	0.68
1:A:42:VAL:CG2	1:A:204:PRO:HG2	2.24	0.68
1:A:100:VAL:HB	1:A:149:LEU:O	1.94	0.68
1:A:295:VAL:CG2	1:A:335:VAL:O	2.35	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ILE:CD1	1:A:372:VAL:HA	2.23	0.68
1:X:181:THR:HG23	1:X:185:THR:O	1.94	0.68
1:X:266:VAL:O	1:X:287:LEU:CA	2.37	0.68
1:A:81:LEU:HD12	1:A:99:ARG:HH22	1.59	0.67
1:A:292:GLU:CD	1:A:368:LEU:HD13	2.13	0.67
1:A:95:VAL:CB	1:A:149:LEU:HD23	2.23	0.67
1:A:232:ASP:HB3	1:A:236:LEU:HD13	1.75	0.67
1:X:81:LEU:CD1	1:X:99:ARG:HH12	2.07	0.67
1:X:174:ILE:HD13	1:X:174:ILE:N	2.11	0.66
1:X:404:ALA:O	1:X:405:VAL:CG2	2.43	0.66
1:X:23:LYS:HE3	1:X:27:GLU:OE2	1.94	0.66
1:A:206:LYS:HZ1	1:A:287:LEU:HD22	1.61	0.66
1:X:37:GLN:CG	1:X:38:GLU:OE2	2.43	0.66
1:X:120:LEU:HD12	1:X:120:LEU:O	1.95	0.66
1:A:216:LEU:O	1:A:217:LEU:HD23	1.96	0.66
1:A:331:ASP:OD1	1:A:347:ARG:NE	2.28	0.66
1:A:311:LEU:HD12	1:A:360:LEU:HD11	1.76	0.66
1:X:81:LEU:HD12	1:X:99:ARG:HH22	1.61	0.66
1:X:61:LEU:HD22	1:X:73:VAL:HG21	1.77	0.66
1:X:227:ILE:HG22	1:X:228:ASN:N	2.11	0.66
1:X:229:LEU:HD12	1:X:290:ARG:HA	1.77	0.66
1:X:47:GLY:C	1:X:79:PRO:HD2	2.16	0.65
1:X:372:VAL:CG1	1:X:373:TRP:N	2.59	0.65
1:A:81:LEU:CD1	1:A:99:ARG:HH12	2.10	0.65
1:A:28:TYR:OH	1:A:205:TYR:HE2	1.78	0.65
1:A:93:GLU:CB	1:A:100:VAL:HG22	2.26	0.65
1:X:356:LYS:NZ	1:X:436:THR:HG21	2.12	0.65
1:X:332:ARG:NH1	1:X:332:ARG:CG	2.53	0.65
1:A:404:ALA:CB	1:X:404:ALA:HB3	2.25	0.65
1:X:100:VAL:HB	1:X:149:LEU:O	1.96	0.65
1:X:239:ALA:HB3	1:X:242:VAL:CG2	2.26	0.65
1:A:61:LEU:HD22	1:A:73:VAL:HG21	1.79	0.65
1:X:292:GLU:OE1	1:X:338:SER:N	2.29	0.65
1:A:426:VAL:O	1:A:429:LYS:HB2	1.97	0.65
1:A:292:GLU:HG3	1:A:336:THR:OG1	1.96	0.65
1:A:9:ARG:HA	1:A:12:ILE:HG22	1.78	0.65
1:X:81:LEU:CD1	1:X:99:ARG:HH22	2.09	0.65
1:A:329:ARG:O	1:A:330:VAL:HB	1.96	0.65
1:A:324:TYR:C	1:A:324:TYR:CD1	2.70	0.64
1:A:15:LEU:CD2	1:X:15:LEU:HG	2.27	0.64
1:X:239:ALA:O	1:X:242:VAL:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:133:ALA:O	1:X:135:PRO:HD3	1.97	0.64
1:X:318:ARG:HG2	1:X:437:LEU:HB3	1.79	0.64
1:X:175:LEU:HD12	1:X:175:LEU:N	2.11	0.64
1:A:295:VAL:HG22	1:A:335:VAL:C	2.16	0.64
1:A:196:ARG:O	1:A:197:ALA:C	2.36	0.64
1:X:136:ARG:NH2	1:X:180:GLU:HB3	2.12	0.64
1:A:292:GLU:OE1	1:A:336:THR:HG21	1.98	0.64
1:A:140:GLU:HG2	1:A:182:PRO:HG3	1.80	0.64
1:A:132:ALA:HB2	1:A:171:GLN:CD	2.18	0.64
1:X:174:ILE:O	1:X:174:ILE:HG22	1.97	0.64
1:A:9:ARG:HA	1:A:12:ILE:CG2	2.28	0.63
1:A:322:GLU:HG2	1:A:323:GLY:N	2.13	0.63
1:A:29:LEU:HD22	1:A:68:GLY:HA3	1.78	0.63
1:A:334:PHE:CE1	1:A:375:ARG:HB3	2.34	0.63
1:A:242:VAL:HG13	1:A:246:MET:HG2	1.78	0.63
1:A:136:ARG:NH2	1:A:180:GLU:HB3	2.13	0.63
1:A:229:LEU:CD2	1:A:254:LYS:HB2	2.29	0.63
1:A:109:ILE:HG22	1:A:178:LEU:HD21	1.80	0.63
1:A:181:THR:HG23	1:A:185:THR:O	1.99	0.63
1:A:304:ASP:CG	1:A:307:ARG:HB2	2.18	0.63
1:A:157:HIS:O	1:A:158:ILE:HD13	1.98	0.63
1:X:311:LEU:CD1	1:X:360:LEU:HD11	2.29	0.63
1:X:42:VAL:O	1:X:43:ILE:HG13	1.99	0.63
1:X:390:ASN:O	1:X:392:PRO:N	2.32	0.63
1:X:246:MET:O	1:X:246:MET:HG3	1.98	0.63
1:A:295:VAL:N	1:A:335:VAL:O	2.29	0.62
1:A:9:ARG:NH2	1:A:33:SER:HB2	2.13	0.62
1:A:28:TYR:OH	1:A:205:TYR:CE2	2.51	0.62
1:A:351:TRP:CD1	1:A:426:VAL:HG11	2.33	0.62
1:A:113:LEU:HD12	1:A:178:LEU:CD1	2.30	0.62
1:A:351:TRP:HD1	1:A:426:VAL:HB	1.64	0.62
1:A:95:VAL:CB	1:A:100:VAL:HG11	2.29	0.62
1:A:106:ILE:HG22	1:A:107:PRO:CD	2.30	0.62
1:A:144:VAL:O	1:A:144:VAL:HG13	2.00	0.62
1:A:196:ARG:NH1	1:A:255:ARG:HD2	2.15	0.62
1:X:334:PHE:CE1	1:X:375:ARG:HB3	2.35	0.62
1:X:398:PHE:C	1:X:398:PHE:CD2	2.73	0.62
1:X:132:ALA:HB2	1:X:171:GLN:CD	2.20	0.62
1:A:354:LEU:HB3	1:A:385:TRP:HB3	1.82	0.62
1:X:145:ASP:OD2	1:X:149:LEU:HD12	2.00	0.61
1:A:414:TRP:CE3	1:A:423:VAL:HG11	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:63:PHE:CE2	1:X:67:VAL:HG21	2.35	0.61
1:A:44:LYS:HG3	1:A:45:VAL:N	2.15	0.61
1:X:42:VAL:C	1:X:43:ILE:HG13	2.20	0.61
1:X:426:VAL:O	1:X:429:LYS:HB2	2.00	0.61
1:X:265:SER:C	1:X:266:VAL:HG23	2.20	0.61
1:A:232:ASP:HB3	1:A:236:LEU:HD12	1.80	0.61
1:X:414:TRP:CE3	1:X:423:VAL:HG11	2.35	0.61
1:X:106:ILE:HG23	1:X:186:LEU:HD23	1.82	0.61
1:X:121:VAL:HG21	1:X:133:ALA:CB	2.27	0.61
1:A:412:VAL:HG23	1:A:431:PHE:CE1	2.35	0.61
1:X:346:THR:HG23	1:X:355:ASP:HB2	1.83	0.61
1:A:34:GLY:O	1:A:36:ASP:N	2.34	0.61
1:X:132:ALA:HB3	1:X:166:ALA:CB	2.31	0.61
1:A:293:ARG:CZ	1:A:337:GLU:OE2	2.49	0.61
1:A:106:ILE:HG22	1:A:107:PRO:HD3	1.82	0.61
1:X:353:TYR:C	1:X:353:TYR:CD2	2.74	0.61
1:A:131:ALA:CA	1:A:171:GLN:HB3	2.30	0.61
1:A:16:LEU:HD23	1:X:19:MET:SD	2.41	0.60
1:A:63:PHE:CE2	1:A:67:VAL:HG11	2.35	0.60
1:X:77:GLY:O	1:X:78:GLY:C	2.39	0.60
1:A:77:GLY:O	1:A:78:GLY:C	2.38	0.60
1:A:120:LEU:O	1:A:120:LEU:HD12	2.02	0.60
1:X:140:GLU:HG2	1:X:182:PRO:HG3	1.82	0.60
1:X:232:ASP:C	1:X:236:LEU:HD23	2.20	0.60
1:X:88:ALA:C	1:X:90:ILE:H	2.03	0.60
1:X:292:GLU:CD	1:X:337:GLU:HB3	2.21	0.60
1:A:164:GLY:O	1:A:168:ARG:HB2	2.01	0.60
1:A:25:ILE:HG12	1:A:279:PHE:CE1	2.36	0.60
1:A:173:ALA:O	1:A:174:ILE:HD13	2.02	0.60
1:A:33:SER:O	1:A:37:GLN:NE2	2.34	0.60
1:A:196:ARG:CD	1:A:255:ARG:HD2	2.28	0.60
1:X:75:HIS:HE2	1:X:176:ALA:HB2	1.66	0.60
1:A:406:ARG:NH1	1:X:398:PHE:CE2	2.61	0.60
1:X:13:VAL:C	1:X:15:LEU:H	2.05	0.60
1:A:90:ILE:N	1:A:91:PRO:CD	2.52	0.60
1:X:94:ARG:O	1:X:100:VAL:HG13	2.01	0.60
1:A:65:GLN:NE2	1:A:170:GLY:O	2.35	0.60
1:A:77:GLY:O	1:A:78:GLY:O	2.18	0.60
1:A:90:ILE:CD1	1:A:104:GLU:OE1	2.50	0.60
1:A:356:LYS:NZ	1:A:436:THR:HG21	2.17	0.60
1:A:138:VAL:HG21	1:A:175:LEU:HG	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:356:LYS:CE	1:X:436:THR:OG1	2.50	0.60
1:X:42:VAL:CG2	1:X:204:PRO:HG2	2.32	0.59
1:A:106:ILE:HG23	1:A:186:LEU:HD23	1.83	0.59
1:X:371:THR:O	1:X:374:ASN:HB2	2.02	0.59
1:A:15:LEU:CD1	1:X:15:LEU:HG	2.32	0.59
1:A:227:ILE:HG22	1:A:228:ASN:N	2.16	0.59
1:X:75:HIS:NE2	1:X:176:ALA:HB2	2.17	0.59
1:A:113:LEU:O	1:A:117:ASN:N	2.21	0.59
1:X:26:ARG:O	1:X:30:HIS:CG	2.55	0.59
1:X:228:ASN:N	1:X:232:ASP:OD2	2.35	0.59
1:X:144:VAL:O	1:X:145:ASP:HB3	2.02	0.59
1:X:368:LEU:C	1:X:370:ARG:N	2.54	0.59
1:X:106:ILE:HG22	1:X:107:PRO:N	2.17	0.59
1:A:113:LEU:HD12	1:A:178:LEU:HD11	1.85	0.59
1:X:138:VAL:HG11	1:X:175:LEU:HD23	1.83	0.59
1:A:95:VAL:N	1:A:100:VAL:HG13	2.12	0.59
1:A:64:LEU:CD2	1:A:69:LEU:HD12	2.31	0.59
1:A:15:LEU:HD21	1:X:16:LEU:N	2.18	0.59
1:A:362:ASP:OD2	1:A:362:ASP:N	2.33	0.59
1:X:164:GLY:O	1:X:168:ARG:HB2	2.03	0.58
1:X:116:ALA:O	1:X:119:ALA:HB3	2.02	0.58
1:X:77:GLY:O	1:X:78:GLY:O	2.21	0.58
1:A:26:ARG:O	1:A:29:LEU:HB2	2.03	0.58
1:X:42:VAL:HG12	1:X:43:ILE:N	2.18	0.58
1:A:175:LEU:HD12	1:A:175:LEU:N	2.18	0.58
1:A:133:ALA:O	1:A:135:PRO:HD3	2.03	0.58
1:A:356:LYS:CE	1:A:436:THR:OG1	2.52	0.58
1:A:297:THR:N	1:A:332:ARG:NH1	2.47	0.58
1:X:29:LEU:CD1	1:X:67:VAL:HG13	2.34	0.58
1:A:47:GLY:O	1:A:50:ILE:HG12	2.04	0.58
1:X:113:LEU:HD12	1:X:178:LEU:HD11	1.83	0.58
1:X:36:ASP:CB	1:X:39:ARG:HG3	2.34	0.58
1:A:214:GLY:HA2	1:A:270:ARG:N	2.18	0.58
1:X:191:ALA:O	1:X:194:ALA:HB3	2.03	0.58
1:X:214:GLY:HA2	1:X:270:ARG:N	2.19	0.57
1:X:331:ASP:HB3	1:X:345:THR:OG1	2.04	0.57
1:A:47:GLY:HA3	1:A:78:GLY:H	1.68	0.57
1:X:44:LYS:HG2	1:X:209:PHE:CD1	2.39	0.57
1:A:90:ILE:H	1:A:91:PRO:HD3	1.64	0.57
1:A:174:ILE:HG22	1:A:174:ILE:O	2.03	0.57
1:X:229:LEU:HD22	1:X:254:LYS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:225:SER:O	1:X:226:SER:HB3	2.04	0.57
1:A:340:ARG:O	1:A:360:LEU:HD12	2.04	0.57
1:A:5:ALA:C	1:A:7:GLY:H	2.08	0.57
1:X:304:ASP:CG	1:X:307:ARG:HB2	2.25	0.57
1:A:94:ARG:HG2	1:A:99:ARG:H	1.70	0.57
1:A:203:GLN:N	1:A:204:PRO:HD3	2.19	0.57
1:A:138:VAL:HG11	1:A:175:LEU:HD23	1.86	0.57
1:A:48:ALA:CA	1:A:79:PRO:HG2	2.35	0.57
1:A:44:LYS:HG2	1:A:209:PHE:CD1	2.40	0.57
1:A:28:TYR:CE1	1:A:205:TYR:CD2	2.93	0.57
1:X:351:TRP:HD1	1:X:426:VAL:CB	2.18	0.57
1:X:322:GLU:HG2	1:X:323:GLY:N	2.19	0.57
1:X:48:ALA:CA	1:X:79:PRO:HG2	2.35	0.56
1:A:94:ARG:HA	1:A:99:ARG:HA	1.86	0.56
1:X:163:VAL:HG13	1:X:173:ALA:CB	2.35	0.56
1:A:239:ALA:O	1:A:242:VAL:HB	2.05	0.56
1:A:132:ALA:HB3	1:A:166:ALA:CB	2.35	0.56
1:X:296:ALA:C	1:X:332:ARG:HH22	2.08	0.56
1:A:228:ASN:N	1:A:232:ASP:OD2	2.36	0.56
1:X:64:LEU:HD22	1:X:69:LEU:CD1	2.31	0.56
1:X:109:ILE:HG22	1:X:178:LEU:HD21	1.87	0.56
1:X:307:ARG:O	1:X:310:ASN:HB2	2.05	0.56
1:X:54:LEU:HB3	1:X:55:PRO:HD3	1.88	0.56
1:X:48:ALA:HA	1:X:79:PRO:HG2	1.88	0.56
1:A:94:ARG:HG2	1:A:99:ARG:CA	2.34	0.56
1:A:42:VAL:O	1:A:43:ILE:CG1	2.52	0.56
1:X:368:LEU:O	1:X:369:GLY:C	2.43	0.56
1:X:106:ILE:HG22	1:X:107:PRO:CD	2.35	0.56
1:X:10:GLN:C	1:X:12:ILE:H	2.09	0.56
1:X:81:LEU:HD13	1:X:99:ARG:HH12	1.70	0.56
1:A:404:ALA:C	1:A:405:VAL:HG23	2.25	0.56
1:A:18:HIS:CE1	1:X:275:ALA:HB1	2.41	0.56
1:X:383:LEU:C	1:X:384:ILE:HD12	2.26	0.56
1:A:351:TRP:HD1	1:A:426:VAL:CB	2.17	0.56
1:X:139:PHE:CZ	1:X:194:ALA:HB1	2.40	0.56
1:A:32:PHE:HD1	1:A:36:ASP:OD2	1.87	0.56
1:X:47:GLY:O	1:X:50:ILE:HG12	2.06	0.56
1:A:232:ASP:CB	1:A:236:LEU:HD13	2.34	0.56
1:A:48:ALA:HB2	1:A:79:PRO:HG2	1.88	0.56
1:X:348:LEU:HD21	1:X:429:LYS:HB3	1.86	0.56
1:A:254:LYS:HG2	1:A:258:ASP:OD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:311:LEU:HD12	1:X:360:LEU:HD11	1.87	0.56
1:A:383:LEU:C	1:A:384:ILE:HD12	2.26	0.56
1:A:196:ARG:HH11	1:A:255:ARG:HD2	1.70	0.55
1:X:113:LEU:HD12	1:X:178:LEU:CD1	2.36	0.55
1:X:351:TRP:HD1	1:X:426:VAL:HB	1.70	0.55
1:A:54:LEU:N	1:A:55:PRO:CD	2.68	0.55
1:X:292:GLU:OE1	1:X:337:GLU:CB	2.50	0.55
1:X:175:LEU:CD1	1:X:175:LEU:H	2.19	0.55
1:X:391:ASN:C	1:X:393:VAL:H	2.09	0.55
1:A:13:VAL:HG13	1:A:26:ARG:CD	2.35	0.55
1:X:38:GLU:C	1:X:40:PHE:N	2.60	0.55
1:X:216:LEU:O	1:X:217:LEU:HD23	2.05	0.55
1:X:328:LEU:HG	1:X:330:VAL:CG2	2.31	0.55
1:A:356:LYS:HZ3	1:A:436:THR:HG21	1.70	0.55
1:A:331:ASP:CB	1:A:345:THR:OG1	2.49	0.55
1:A:145:ASP:O	1:A:147:ASP:N	2.39	0.55
1:A:32:PHE:HD1	1:A:36:ASP:CG	2.10	0.55
1:A:38:GLU:C	1:A:40:PHE:N	2.59	0.55
1:X:138:VAL:HG21	1:X:175:LEU:HG	1.87	0.55
1:A:132:ALA:HB3	1:A:166:ALA:HB2	1.89	0.55
1:X:391:ASN:O	1:X:393:VAL:N	2.38	0.55
1:A:112:THR:O	1:A:115:GLN:HB3	2.07	0.55
1:X:196:ARG:NH1	1:X:255:ARG:HD2	2.22	0.55
1:X:136:ARG:HH11	1:X:136:ARG:CB	2.20	0.55
1:A:136:ARG:CB	1:A:136:ARG:HH11	2.19	0.55
1:A:120:LEU:O	1:A:124:ILE:HG13	2.06	0.55
1:A:309:ASP:HA	1:A:325:TRP:HZ2	1.72	0.55
1:X:32:PHE:C	1:X:34:GLY:H	2.09	0.55
1:X:37:GLN:HB3	1:X:38:GLU:CD	2.27	0.55
1:A:15:LEU:HD22	1:X:15:LEU:HG	1.87	0.55
1:A:13:VAL:HA	1:A:16:LEU:HD12	1.88	0.55
1:A:196:ARG:HD3	1:A:255:ARG:CD	2.32	0.55
1:X:175:LEU:CD1	1:X:175:LEU:N	2.71	0.54
1:X:351:TRP:HZ3	1:X:382:GLN:OE1	1.90	0.54
1:X:5:ALA:N	1:X:6:PRO:CD	2.70	0.54
1:A:405:VAL:HG11	1:A:431:PHE:HE2	1.72	0.54
1:X:145:ASP:O	1:X:147:ASP:N	2.39	0.54
1:A:214:GLY:CA	1:A:270:ARG:N	2.70	0.54
1:A:53:ASP:O	1:A:54:LEU:C	2.44	0.54
1:A:357:PHE:CE1	1:A:372:VAL:HG11	2.37	0.54
1:X:159:HIS:HB3	1:X:161:ASP:OD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:29:LEU:CD2	1:X:69:LEU:HD21	2.34	0.54
1:A:40:PHE:CE1	1:A:69:LEU:HD22	2.43	0.54
1:A:163:VAL:HG13	1:A:173:ALA:CB	2.38	0.54
1:X:36:ASP:HB2	1:X:39:ARG:CB	2.29	0.54
1:X:132:ALA:HB3	1:X:166:ALA:HB2	1.90	0.54
1:X:351:TRP:CD1	1:X:426:VAL:CG1	2.90	0.54
1:X:134:VAL:HG11	1:X:162:LEU:HB3	1.90	0.54
1:X:411:THR:HG21	1:X:413:PHE:CE2	2.42	0.54
1:A:206:LYS:NZ	1:A:287:LEU:HD22	2.23	0.54
1:X:47:GLY:CA	1:X:79:PRO:HD2	2.38	0.54
1:X:203:GLN:N	1:X:204:PRO:HD3	2.22	0.54
1:A:28:TYR:CE1	1:A:205:TYR:HD2	2.24	0.54
1:A:307:ARG:O	1:A:310:ASN:HB2	2.07	0.54
1:X:65:GLN:NE2	1:X:170:GLY:O	2.41	0.53
1:A:94:ARG:CG	1:A:99:ARG:HA	2.35	0.53
1:A:28:TYR:CZ	1:A:205:TYR:CE2	2.96	0.53
1:X:35:ILE:C	1:X:37:GLN:N	2.61	0.53
1:A:390:ASN:O	1:A:391:ASN:C	2.45	0.53
1:A:295:VAL:O	1:A:334:PHE:HA	2.08	0.53
1:X:356:LYS:HZ3	1:X:436:THR:HG21	1.74	0.53
1:A:29:LEU:CD2	1:A:68:GLY:CA	2.77	0.53
1:X:167:ALA:O	1:X:170:GLY:N	2.29	0.53
1:X:43:ILE:CD1	1:X:71:PRO:HB3	2.38	0.53
1:X:292:GLU:OE1	1:X:337:GLU:CA	2.57	0.53
1:X:406:ARG:HG2	1:X:411:THR:OG1	2.08	0.53
1:X:262:LEU:HD21	1:X:290:ARG:CZ	2.39	0.53
1:A:131:ALA:C	1:A:171:GLN:HB3	2.29	0.53
1:X:254:LYS:HG2	1:X:258:ASP:OD2	2.07	0.53
1:A:191:ALA:O	1:A:194:ALA:HB3	2.08	0.53
1:X:163:VAL:HG22	1:X:175:LEU:HD11	1.90	0.53
1:X:354:LEU:HB3	1:X:385:TRP:CB	2.39	0.53
1:A:106:ILE:CB	1:A:107:PRO:HD3	2.38	0.53
1:X:383:LEU:O	1:X:384:ILE:HD12	2.08	0.53
1:X:296:ALA:CA	1:X:332:ARG:HH22	2.22	0.53
1:A:116:ALA:O	1:A:119:ALA:HB3	2.09	0.53
1:X:13:VAL:HG12	1:X:14:GLN:N	2.24	0.53
1:A:196:ARG:O	1:A:198:LEU:N	2.42	0.53
1:X:242:VAL:HG13	1:X:246:MET:HG2	1.90	0.53
1:A:352:VAL:O	1:A:383:LEU:HD12	2.09	0.53
1:X:287:LEU:HD23	1:X:288:ILE:N	2.23	0.52
1:A:81:LEU:HD13	1:A:99:ARG:HH12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:254:LYS:O	1:X:258:ASP:CG	2.47	0.52
1:X:138:VAL:HG11	1:X:175:LEU:CD2	2.39	0.52
1:A:372:VAL:HG12	1:A:373:TRP:H	1.73	0.52
1:A:351:TRP:CD1	1:A:426:VAL:HB	2.44	0.52
1:A:106:ILE:CG2	1:A:107:PRO:HD3	2.39	0.52
1:X:265:SER:O	1:X:266:VAL:CG2	2.58	0.52
1:X:84:ALA:O	1:X:88:ALA:N	2.42	0.52
1:X:289:ARG:HD2	1:X:366:GLU:HB3	1.90	0.52
1:A:106:ILE:HG22	1:A:107:PRO:N	2.24	0.52
1:A:311:LEU:HD13	1:A:360:LEU:HD11	1.92	0.52
1:A:19:MET:HE2	1:X:19:MET:HB2	1.91	0.52
1:X:292:GLU:OE1	1:X:337:GLU:N	2.42	0.52
1:A:351:TRP:HZ3	1:A:382:GLN:OE1	1.92	0.52
1:X:214:GLY:CA	1:X:270:ARG:N	2.72	0.52
1:A:354:LEU:HB3	1:A:385:TRP:CB	2.40	0.52
1:A:38:GLU:O	1:A:40:PHE:N	2.43	0.52
1:A:348:LEU:HD21	1:A:429:LYS:HB3	1.91	0.52
1:A:353:TYR:CD2	1:A:353:TYR:C	2.83	0.52
1:A:144:VAL:O	1:A:145:ASP:HB3	2.10	0.52
1:A:295:VAL:CG2	1:A:335:VAL:HB	2.40	0.52
1:A:294:ILE:HA	1:A:336:THR:HA	1.92	0.52
1:A:73:VAL:HB	1:A:174:ILE:HD12	1.92	0.52
1:A:158:ILE:HD13	1:A:158:ILE:N	2.23	0.52
1:A:106:ILE:HD13	1:A:186:LEU:CD2	2.38	0.52
1:A:340:ARG:CA	1:A:360:LEU:HD12	2.39	0.52
1:X:231:THR:CG2	1:X:293:ARG:HA	2.39	0.51
1:X:217:LEU:HD13	1:X:221:GLY:O	2.10	0.51
1:X:409:GLU:OE1	1:X:410:TRP:HD1	1.94	0.51
1:A:315:ALA:CB	1:A:358:ALA:HB1	2.41	0.51
1:X:13:VAL:C	1:X:15:LEU:N	2.64	0.51
1:A:189:ILE:HG22	1:A:190:ASN:O	2.10	0.51
1:A:217:LEU:HD13	1:A:221:GLY:O	2.10	0.51
1:A:47:GLY:CA	1:A:79:PRO:HD2	2.40	0.51
1:A:81:LEU:HD11	1:A:99:ARG:HH12	1.76	0.51
1:X:44:LYS:HE2	1:X:191:ALA:HB3	1.91	0.51
1:A:294:ILE:HD11	1:A:372:VAL:HA	1.92	0.51
1:X:383:LEU:HD12	1:X:384:ILE:H	1.76	0.51
1:X:27:GLU:O	1:X:31:ARG:HB3	2.10	0.51
1:A:32:PHE:HA	1:A:36:ASP:OD1	2.10	0.51
1:X:38:GLU:O	1:X:40:PHE:N	2.44	0.51
1:X:389:THR:O	1:X:394:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:297:THR:H	1:X:332:ARG:NH1	1.94	0.51
1:A:254:LYS:O	1:A:258:ASP:CG	2.50	0.51
1:X:106:ILE:CB	1:X:107:PRO:HD3	2.41	0.51
1:X:54:LEU:N	1:X:55:PRO:CD	2.74	0.51
1:A:174:ILE:N	1:A:174:ILE:CD1	2.56	0.51
1:A:19:MET:HA	1:X:21:ASP:HB2	1.93	0.51
1:X:289:ARG:NE	1:X:366:GLU:HB3	2.25	0.51
1:X:405:VAL:HG11	1:X:431:PHE:HE2	1.76	0.51
1:X:332:ARG:N	1:X:345:THR:OG1	2.44	0.50
1:A:17:SER:HA	1:A:26:ARG:HH21	1.75	0.50
1:A:205:TYR:O	1:A:264:SER:HA	2.11	0.50
1:A:140:GLU:OE2	1:A:182:PRO:HB3	2.11	0.50
1:A:409:GLU:OE1	1:A:410:TRP:HD1	1.94	0.50
1:X:353:TYR:CE2	1:X:355:ASP:CA	2.92	0.50
1:A:403:GLY:HA3	1:A:414:TRP:CE2	2.46	0.50
1:A:140:GLU:CG	1:A:182:PRO:HG3	2.41	0.50
1:A:15:LEU:HD13	1:X:15:LEU:HG	1.92	0.50
1:X:39:ARG:HD3	1:X:202:LEU:O	2.11	0.50
1:X:42:VAL:O	1:X:43:ILE:CG1	2.60	0.50
1:A:57:LEU:O	1:A:60:ALA:HB3	2.10	0.50
1:X:40:PHE:CE1	1:X:69:LEU:HD22	2.47	0.50
1:X:227:ILE:CG2	1:X:228:ASN:N	2.74	0.50
1:A:88:ALA:O	1:A:89:ASP:CB	2.56	0.50
1:X:120:LEU:O	1:X:124:ILE:HG13	2.12	0.50
1:X:106:ILE:HB	1:X:107:PRO:HD3	1.92	0.50
1:X:47:GLY:HA3	1:X:79:PRO:HD2	1.93	0.50
1:X:432:ALA:O	1:X:433:LEU:C	2.49	0.50
1:A:39:ARG:HD3	1:A:202:LEU:O	2.12	0.50
1:X:43:ILE:HD12	1:X:71:PRO:HB3	1.94	0.50
1:X:131:ALA:HA	1:X:171:GLN:HB3	1.94	0.50
1:X:357:PHE:CE1	1:X:372:VAL:HG11	2.41	0.50
1:A:139:PHE:CZ	1:A:194:ALA:HB1	2.47	0.50
1:A:48:ALA:N	1:A:79:PRO:CD	2.73	0.49
1:A:94:ARG:HG2	1:A:99:ARG:N	2.27	0.49
1:X:353:TYR:HD2	1:X:353:TYR:O	1.92	0.49
1:A:34:GLY:C	1:A:35:ILE:HG12	2.32	0.49
1:X:404:ALA:C	1:X:405:VAL:HG23	2.32	0.49
1:A:398:PHE:CD1	1:X:398:PHE:CE1	2.78	0.49
1:X:132:ALA:HB3	1:X:166:ALA:HB1	1.94	0.49
1:A:266:VAL:H	1:A:287:LEU:HD13	1.76	0.49
1:A:254:LYS:O	1:A:258:ASP:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TRP:CD1	1:A:426:VAL:CG1	2.95	0.49
1:A:80:GLN:O	1:A:84:ALA:CB	2.61	0.49
1:A:54:LEU:HB3	1:A:55:PRO:HD3	1.95	0.49
1:A:405:VAL:HG12	1:A:431:PHE:CZ	2.48	0.49
1:X:401:CYS:O	1:X:402:ASP:OD1	2.31	0.49
1:A:324:TYR:CD1	1:A:325:TRP:N	2.80	0.49
1:X:390:ASN:O	1:X:391:ASN:C	2.50	0.49
1:A:9:ARG:HG3	1:A:29:LEU:HD13	1.95	0.49
1:X:227:ILE:HG22	1:X:228:ASN:H	1.75	0.49
1:X:354:LEU:HB3	1:X:385:TRP:HB3	1.95	0.49
1:A:61:LEU:CD2	1:A:73:VAL:HG21	2.42	0.49
1:X:196:ARG:HH11	1:X:255:ARG:HD2	1.76	0.49
1:A:354:LEU:HG	1:A:355:ASP:N	2.24	0.49
1:X:140:GLU:CG	1:X:182:PRO:HG3	2.42	0.49
1:A:12:ILE:O	1:A:16:LEU:HG	2.12	0.49
1:A:196:ARG:O	1:A:199:VAL:N	2.46	0.49
1:A:138:VAL:HG11	1:A:175:LEU:CD2	2.43	0.49
1:A:106:ILE:CD1	1:A:186:LEU:HD23	2.36	0.49
1:A:64:LEU:HD22	1:A:69:LEU:CD1	2.37	0.48
1:X:289:ARG:CD	1:X:366:GLU:HB3	2.44	0.48
1:A:414:TRP:CZ3	1:A:423:VAL:HG11	2.48	0.48
1:X:183:ASP:C	1:X:183:ASP:OD2	2.52	0.48
1:A:232:ASP:CB	1:A:236:LEU:HD12	2.41	0.48
1:X:53:ASP:O	1:X:54:LEU:C	2.50	0.48
1:X:217:LEU:HD22	1:X:222:ASP:C	2.34	0.48
1:X:296:ALA:CB	1:X:332:ARG:NH2	2.67	0.48
1:A:64:LEU:CD1	1:A:71:PRO:HG3	2.37	0.48
1:A:262:LEU:HD21	1:A:290:ARG:CZ	2.43	0.48
1:X:232:ASP:CA	1:X:236:LEU:HD23	2.43	0.48
1:X:265:SER:C	1:X:266:VAL:CG2	2.82	0.48
1:A:232:ASP:O	1:A:236:LEU:CD1	2.56	0.48
1:X:65:GLN:NE2	1:X:130:ARG:O	2.44	0.48
1:X:35:ILE:O	1:X:37:GLN:N	2.47	0.48
1:X:120:LEU:HD12	1:X:120:LEU:C	2.31	0.48
1:X:387:SER:OG	1:X:388:ARG:N	2.45	0.48
1:A:65:GLN:NE2	1:A:130:ARG:O	2.44	0.48
1:A:117:ASN:O	1:A:121:VAL:HG23	2.13	0.48
1:A:391:ASN:O	1:A:393:VAL:N	2.46	0.48
1:A:93:GLU:HB3	1:A:100:VAL:CG2	2.42	0.48
1:A:19:MET:CE	1:X:19:MET:HB2	2.43	0.48
1:X:412:VAL:HG23	1:X:431:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ALA:O	1:A:433:LEU:C	2.51	0.48
1:A:368:LEU:O	1:A:369:GLY:C	2.52	0.48
1:A:63:PHE:CZ	1:A:67:VAL:HG11	2.49	0.48
1:X:143:ILE:HA	1:X:153:GLY:HA2	1.95	0.48
1:X:189:ILE:HG22	1:X:190:ASN:O	2.14	0.48
1:X:324:TYR:CD1	1:X:325:TRP:N	2.81	0.48
1:A:405:VAL:HG12	1:A:431:PHE:HZ	1.78	0.48
1:X:414:TRP:CZ3	1:X:423:VAL:HG11	2.49	0.48
1:A:106:ILE:HB	1:A:107:PRO:HD3	1.95	0.48
1:X:94:ARG:HB3	1:X:100:VAL:HG22	1.95	0.48
1:A:332:ARG:N	1:A:345:THR:OG1	2.46	0.48
1:X:10:GLN:O	1:X:12:ILE:N	2.39	0.48
1:X:391:ASN:CG	1:X:393:VAL:HG23	2.34	0.48
1:A:26:ARG:O	1:A:26:ARG:HG3	2.14	0.48
1:A:94:ARG:HA	1:A:99:ARG:CA	2.43	0.48
1:X:403:GLY:HA3	1:X:414:TRP:CE2	2.48	0.48
1:A:311:LEU:O	1:A:360:LEU:HD21	2.14	0.48
1:A:237:MET:O	1:A:247:ARG:NE	2.47	0.48
1:X:266:VAL:O	1:X:288:ILE:N	2.47	0.47
1:A:293:ARG:NH1	1:A:337:GLU:OE2	2.47	0.47
1:A:175:LEU:CD1	1:A:175:LEU:N	2.77	0.47
1:X:362:ASP:OD2	1:X:362:ASP:N	2.39	0.47
1:X:315:ALA:CB	1:X:358:ALA:HB1	2.44	0.47
1:X:227:ILE:HD12	1:X:288:ILE:CD1	2.44	0.47
1:A:332:ARG:HG3	1:A:332:ARG:NH1	2.26	0.47
1:X:262:LEU:C	1:X:264:SER:H	2.17	0.47
1:X:344:ILE:HG22	1:X:344:ILE:O	2.11	0.47
1:X:81:LEU:HD11	1:X:99:ARG:HH12	1.77	0.47
1:A:85:LEU:HD21	1:A:108:ILE:HG13	1.97	0.47
1:A:356:LYS:HE3	1:A:437:LEU:HD11	1.96	0.47
1:A:12:ILE:HD13	1:X:15:LEU:CD1	2.44	0.47
1:X:81:LEU:HD12	1:X:82:ASP:N	2.29	0.47
1:X:65:GLN:NE2	1:X:130:ARG:CB	2.70	0.47
1:X:29:LEU:HD13	1:X:67:VAL:HG13	1.96	0.47
1:X:409:GLU:OE1	1:X:410:TRP:CD1	2.68	0.47
1:X:274:LEU:HA	1:X:274:LEU:HD12	1.66	0.47
1:A:217:LEU:HD22	1:A:222:ASP:C	2.35	0.47
1:X:391:ASN:C	1:X:393:VAL:N	2.68	0.47
1:X:297:THR:O	1:X:332:ARG:NH1	2.47	0.47
1:A:9:ARG:O	1:A:12:ILE:HG22	2.14	0.47
1:A:232:ASP:CA	1:A:236:LEU:HD12	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:205:TYR:O	1:X:264:SER:HA	2.15	0.47
1:X:262:LEU:C	1:X:264:SER:N	2.67	0.47
1:X:196:ARG:O	1:X:197:ALA:C	2.52	0.47
1:X:106:ILE:HD13	1:X:186:LEU:CD2	2.44	0.47
1:X:324:TYR:C	1:X:324:TYR:CD1	2.87	0.47
1:X:315:ALA:HB3	1:X:358:ALA:HB1	1.96	0.47
1:X:232:ASP:O	1:X:236:LEU:HD23	2.13	0.47
1:A:26:ARG:HD2	1:A:30:HIS:HE1	1.80	0.47
1:X:24:GLU:OE1	1:X:279:PHE:O	2.33	0.47
1:X:42:VAL:CG1	1:X:43:ILE:N	2.77	0.47
1:A:45:VAL:HG12	1:A:46:GLY:O	2.15	0.47
1:X:356:LYS:HE2	1:X:436:THR:OG1	2.15	0.47
1:X:231:THR:HG22	1:X:293:ARG:HA	1.97	0.47
1:X:237:MET:O	1:X:247:ARG:NE	2.48	0.47
1:X:44:LYS:HE2	1:X:191:ALA:CB	2.44	0.46
1:A:295:VAL:O	1:A:335:VAL:N	2.49	0.46
1:A:13:VAL:CG1	1:A:26:ARG:CD	2.81	0.46
1:X:354:LEU:HG	1:X:355:ASP:N	2.30	0.46
1:X:106:ILE:HG22	1:X:107:PRO:HD3	1.96	0.46
1:A:183:ASP:OD2	1:A:183:ASP:C	2.53	0.46
1:X:48:ALA:HB2	1:X:79:PRO:HG2	1.97	0.46
1:A:353:TYR:O	1:A:353:TYR:CD2	2.68	0.46
1:X:154:GLU:HA	1:X:155:PRO:HD3	1.80	0.46
1:A:167:ALA:O	1:A:170:GLY:N	2.27	0.46
1:A:48:ALA:CB	1:A:79:PRO:HG2	2.45	0.46
1:A:299:ASP:OD2	1:A:302:SER:HB3	2.15	0.46
1:X:106:ILE:CD1	1:X:186:LEU:HD23	2.40	0.46
1:A:332:ARG:HD3	1:A:379:TYR:CE1	2.51	0.46
1:A:411:THR:HG22	1:A:413:PHE:CD2	2.50	0.46
1:A:406:ARG:CD	1:X:398:PHE:CE2	2.88	0.46
1:A:292:GLU:OE1	1:A:336:THR:CG2	2.63	0.46
1:A:36:ASP:HB2	1:A:39:ARG:CB	2.43	0.46
1:A:9:ARG:CA	1:A:12:ILE:HG22	2.43	0.46
1:A:113:LEU:HD12	1:A:178:LEU:HD12	1.97	0.46
1:X:356:LYS:HZ1	1:X:436:THR:HG21	1.81	0.46
1:A:64:LEU:HB2	1:A:71:PRO:HG3	1.98	0.46
1:A:81:LEU:HD12	1:A:82:ASP:N	2.31	0.46
1:X:229:LEU:HD22	1:X:254:LYS:CB	2.46	0.46
1:X:230:ALA:HB2	1:X:290:ARG:O	2.16	0.46
1:X:357:PHE:HE1	1:X:372:VAL:CG1	2.27	0.46
1:A:433:LEU:HA	1:A:434:PRO:HD3	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:OE2	1:A:102:ARG:NH1	2.49	0.46
1:A:85:LEU:HD21	1:A:108:ILE:HB	1.97	0.46
1:A:37:GLN:O	1:A:70:THR:HB	2.16	0.46
1:X:29:LEU:HD11	1:X:67:VAL:HG13	1.97	0.46
1:A:47:GLY:HA3	1:A:79:PRO:HD2	1.97	0.46
1:A:151:ARG:HH21	1:A:185:THR:HG23	1.80	0.46
1:A:273:GLU:HB3	1:A:284:SER:HB3	1.98	0.46
1:A:423:VAL:O	1:A:424:ALA:C	2.54	0.46
1:A:292:GLU:HG2	1:A:368:LEU:CD2	2.46	0.45
1:A:40:PHE:CE1	1:A:69:LEU:CD2	2.99	0.45
1:A:351:TRP:CD1	1:A:426:VAL:CB	2.98	0.45
1:A:398:PHE:CD2	1:A:398:PHE:C	2.89	0.45
1:A:389:THR:O	1:A:394:ASN:ND2	2.48	0.45
1:X:8:VAL:O	1:X:12:ILE:HG13	2.15	0.45
1:X:75:HIS:NE2	1:X:176:ALA:CB	2.78	0.45
1:A:270:ARG:NH1	1:A:273:GLU:CG	2.79	0.45
1:A:36:ASP:HB2	1:A:39:ARG:HG3	1.99	0.45
1:X:144:VAL:O	1:X:145:ASP:CB	2.64	0.45
1:A:292:GLU:OE1	1:A:368:LEU:HD13	2.16	0.45
1:A:328:LEU:HG	1:A:330:VAL:CG2	2.37	0.45
1:X:227:ILE:CG2	1:X:228:ASN:H	2.30	0.45
1:X:63:PHE:CZ	1:X:67:VAL:HG21	2.52	0.45
1:A:42:VAL:HG23	1:A:204:PRO:HG3	1.98	0.45
1:A:42:VAL:HG12	1:A:43:ILE:N	2.31	0.45
1:A:5:ALA:O	1:A:7:GLY:N	2.50	0.45
1:X:57:LEU:HD13	1:X:210:LEU:HD12	1.99	0.45
1:X:433:LEU:HA	1:X:434:PRO:HD3	1.59	0.45
1:A:65:GLN:HA	1:A:69:LEU:O	2.17	0.45
1:X:117:ASN:ND2	1:X:135:PRO:HG3	2.31	0.45
1:A:14:GLN:HA	1:A:14:GLN:NE2	2.32	0.45
1:A:292:GLU:CG	1:A:368:LEU:HD11	2.46	0.45
1:A:13:VAL:CG2	1:A:29:LEU:HD12	2.47	0.45
1:X:423:VAL:O	1:X:424:ALA:C	2.55	0.45
1:A:270:ARG:NH1	1:A:273:GLU:HG2	2.30	0.45
1:A:383:LEU:O	1:A:384:ILE:HD12	2.17	0.45
1:A:15:LEU:HD21	1:X:16:LEU:CA	2.47	0.45
1:A:19:MET:HB3	1:X:21:ASP:H	1.82	0.45
1:X:42:VAL:HG23	1:X:204:PRO:HG3	1.93	0.45
1:A:423:VAL:HG13	1:A:427:VAL:HG23	1.99	0.45
1:A:423:VAL:CG1	1:A:427:VAL:HG23	2.47	0.45
1:X:265:SER:O	1:X:266:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:THR:OG1	1:A:232:ASP:OD1	2.26	0.44
1:X:40:PHE:CE1	1:X:69:LEU:CD2	3.00	0.44
1:X:124:ILE:HG21	1:X:131:ALA:HB2	1.99	0.44
1:A:405:VAL:HG11	1:A:431:PHE:CE2	2.51	0.44
1:X:423:VAL:HG13	1:X:427:VAL:HG23	1.98	0.44
1:X:141:ALA:HB1	1:X:154:GLU:C	2.38	0.44
1:X:309:ASP:HA	1:X:325:TRP:HZ2	1.81	0.44
1:X:83:ALA:O	1:X:87:ALA:HB3	2.17	0.44
1:A:86:GLU:HA	1:A:91:PRO:HG3	2.00	0.44
1:A:42:VAL:C	1:A:43:ILE:CG1	2.84	0.44
1:A:401:CYS:HB2	1:A:414:TRP:O	2.17	0.44
1:A:257:LEU:HA	1:A:257:LEU:HD23	1.77	0.44
1:A:227:ILE:CG2	1:A:228:ASN:N	2.78	0.44
1:A:97:GLY:O	1:A:98:LEU:CD2	2.55	0.44
1:A:85:LEU:CD2	1:A:108:ILE:HG13	2.47	0.44
1:A:265:SER:HB2	1:A:287:LEU:HD11	1.99	0.44
1:X:232:ASP:O	1:X:236:LEU:CD2	2.65	0.44
1:X:346:THR:OG1	1:X:347:ARG:N	2.44	0.44
1:X:189:ILE:CG2	1:X:193:VAL:CG2	2.96	0.44
1:X:311:LEU:HD13	1:X:360:LEU:HD11	2.00	0.44
1:X:44:LYS:HG3	1:X:45:VAL:N	2.33	0.44
1:A:156:ARG:O	1:A:156:ARG:HG2	2.17	0.44
1:A:398:PHE:CE1	1:X:398:PHE:CD1	2.79	0.44
1:A:398:PHE:CD2	1:A:398:PHE:O	2.70	0.44
1:A:44:LYS:HE2	1:A:191:ALA:HB3	2.00	0.44
1:X:351:TRP:CD1	1:X:426:VAL:HB	2.50	0.44
1:A:409:GLU:OE1	1:A:410:TRP:CD1	2.70	0.44
1:A:89:ASP:C	1:A:91:PRO:HD3	2.36	0.44
1:A:141:ALA:HB1	1:A:154:GLU:C	2.38	0.44
1:A:239:ALA:HB3	1:A:242:VAL:HG23	2.00	0.44
1:X:340:ARG:CA	1:X:360:LEU:HD12	2.48	0.44
1:A:48:ALA:HA	1:A:79:PRO:HG2	1.98	0.44
1:X:403:GLY:HA3	1:X:414:TRP:CD2	2.53	0.44
1:A:270:ARG:HH11	1:A:273:GLU:HG2	1.82	0.44
1:X:74:VAL:HG12	1:X:75:HIS:N	2.32	0.44
1:A:328:LEU:HD11	1:A:346:THR:HG22	2.00	0.44
1:A:13:VAL:C	1:A:15:LEU:N	2.70	0.43
1:X:267:SER:CA	1:X:286:THR:O	2.47	0.43
1:X:32:PHE:CE1	1:X:40:PHE:HD1	2.36	0.43
1:X:299:ASP:OD1	1:X:301:SER:OG	2.30	0.43
1:A:368:LEU:C	1:A:370:ARG:N	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:37:GLN:CD	1:X:168:ARG:HG3	2.38	0.43
1:A:44:LYS:CG	1:A:45:VAL:N	2.79	0.43
1:A:9:ARG:HH22	1:A:33:SER:HB2	1.80	0.43
1:A:356:LYS:HE2	1:A:436:THR:OG1	2.18	0.43
1:A:15:LEU:HD21	1:X:15:LEU:O	2.19	0.43
1:X:83:ALA:O	1:X:87:ALA:CB	2.66	0.43
1:X:257:LEU:HA	1:X:257:LEU:HD23	1.76	0.43
1:A:132:ALA:N	1:A:171:GLN:HB3	2.33	0.43
1:X:90:ILE:N	1:X:91:PRO:HD3	2.33	0.43
1:X:427:VAL:O	1:X:430:ALA:N	2.52	0.43
1:X:26:ARG:HG2	1:X:30:HIS:NE2	2.33	0.43
1:X:411:THR:HG22	1:X:413:PHE:CD2	2.52	0.43
1:X:51:GLN:HB2	1:X:80:GLN:CD	2.39	0.43
1:X:44:LYS:O	1:X:45:VAL:HG12	2.19	0.43
1:A:391:ASN:C	1:A:393:VAL:H	2.21	0.43
1:A:144:VAL:O	1:A:144:VAL:CG1	2.66	0.43
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.87	0.43
1:X:78:GLY:O	1:X:82:ASP:CG	2.57	0.43
1:A:78:GLY:O	1:A:82:ASP:CG	2.57	0.43
1:X:57:LEU:O	1:X:60:ALA:HB3	2.19	0.42
1:A:13:VAL:HG22	1:A:29:LEU:HD12	2.01	0.42
1:A:67:VAL:HG23	1:A:69:LEU:HG	1.98	0.42
1:A:212:GLY:O	1:A:213:THR:C	2.57	0.42
1:A:85:LEU:HD21	1:A:108:ILE:CG1	2.49	0.42
1:X:299:ASP:OD2	1:X:302:SER:HB3	2.19	0.42
1:X:212:GLY:O	1:X:213:THR:C	2.57	0.42
1:X:42:VAL:HG12	1:X:43:ILE:H	1.84	0.42
1:A:163:VAL:CG2	1:A:175:LEU:HD21	2.49	0.42
1:A:166:ALA:HB1	1:A:171:GLN:HB2	2.01	0.42
1:A:120:LEU:O	1:A:124:ILE:N	2.51	0.42
1:A:356:LYS:HA	1:A:356:LYS:HD3	1.64	0.42
1:A:327:ARG:HB2	1:A:327:ARG:HE	1.56	0.42
1:X:120:LEU:O	1:X:124:ILE:N	2.48	0.42
1:X:270:ARG:NH1	1:X:273:GLU:CG	2.83	0.42
1:X:232:ASP:HB3	1:X:236:LEU:HD21	1.92	0.42
1:A:19:MET:HE2	1:X:19:MET:CB	2.50	0.42
1:A:36:ASP:HB2	1:A:39:ARG:CG	2.49	0.42
1:A:67:VAL:HG22	1:A:69:LEU:HG	1.96	0.42
1:X:423:VAL:CG1	1:X:427:VAL:HG23	2.50	0.42
1:X:297:THR:C	1:X:332:ARG:NH1	2.72	0.42
1:A:91:PRO:HD2	1:A:91:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:HIS:HB3	1:A:161:ASP:OD2	2.19	0.42
1:X:35:ILE:O	1:X:36:ASP:C	2.57	0.42
1:A:75:HIS:NE2	1:A:176:ALA:HB2	2.35	0.42
1:X:106:ILE:CG2	1:X:107:PRO:HD3	2.50	0.42
1:X:393:VAL:O	1:X:395:GLY:N	2.53	0.42
1:X:5:ALA:N	1:X:6:PRO:HD3	2.34	0.42
1:A:93:GLU:HG3	1:A:93:GLU:H	1.42	0.42
1:A:44:LYS:N	1:A:208:VAL:O	2.51	0.42
1:X:270:ARG:NH1	1:X:273:GLU:HG2	2.35	0.42
1:X:351:TRP:CD1	1:X:426:VAL:CB	3.00	0.42
1:X:81:LEU:HD11	1:X:99:ARG:NH1	2.35	0.42
1:A:44:LYS:HG2	1:A:209:PHE:HD1	1.85	0.42
1:A:15:LEU:HD21	1:X:16:LEU:HA	2.02	0.41
1:X:48:ALA:CB	1:X:79:PRO:HG2	2.50	0.41
1:X:98:LEU:O	1:X:99:ARG:O	2.38	0.41
1:A:328:LEU:HD21	1:A:330:VAL:CG2	2.49	0.41
1:A:141:ALA:O	1:A:181:THR:HG22	2.20	0.41
1:X:158:ILE:N	1:X:158:ILE:HD13	2.30	0.41
1:A:315:ALA:HB3	1:A:358:ALA:HB1	2.02	0.41
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.88	0.41
1:X:327:ARG:HE	1:X:327:ARG:HB2	1.56	0.41
1:A:95:VAL:H	1:A:100:VAL:HG11	1.65	0.41
1:X:287:LEU:C	1:X:287:LEU:HD23	2.41	0.41
1:X:78:GLY:O	1:X:82:ASP:OD1	2.38	0.41
1:X:262:LEU:O	1:X:264:SER:N	2.52	0.41
1:X:173:ALA:O	1:X:174:ILE:HD13	2.19	0.41
1:A:304:ASP:OD1	1:A:307:ARG:HB2	2.20	0.41
1:X:412:VAL:HG23	1:X:431:PHE:CD1	2.55	0.41
1:X:106:ILE:HD12	1:X:151:ARG:NH1	2.35	0.41
1:A:95:VAL:CG1	1:A:149:LEU:HD23	2.50	0.41
1:A:292:GLU:CG	1:A:336:THR:OG1	2.66	0.41
1:X:61:LEU:CD2	1:X:73:VAL:HG21	2.47	0.41
1:A:411:THR:HG21	1:A:413:PHE:CE2	2.55	0.41
1:X:332:ARG:HG3	1:X:333:ALA:H	1.84	0.41
1:A:231:THR:CG2	1:A:293:ARG:HA	2.51	0.41
1:X:42:VAL:CG1	1:X:43:ILE:H	2.34	0.41
1:A:75:HIS:HE2	1:A:176:ALA:HB2	1.84	0.41
1:X:190:ASN:C	1:X:190:ASN:OD1	2.58	0.41
1:A:118:LEU:O	1:A:119:ALA:C	2.57	0.41
1:A:265:SER:HB2	1:A:287:LEU:CD1	2.50	0.41
1:A:64:LEU:HD12	1:A:71:PRO:CG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:O	1:A:92:THR:HG23	2.20	0.41
1:A:47:GLY:CA	1:A:78:GLY:H	2.32	0.41
1:A:28:TYR:CZ	1:A:205:TYR:HE2	2.37	0.41
1:A:155:PRO:HG2	1:A:193:VAL:HG23	2.01	0.41
1:X:383:LEU:HD12	1:X:384:ILE:N	2.36	0.41
1:A:266:VAL:O	1:A:288:ILE:N	2.54	0.41
1:A:11:THR:C	1:A:13:VAL:N	2.73	0.41
1:A:227:ILE:HD13	1:A:250:LEU:HD21	2.02	0.41
1:A:262:LEU:C	1:A:264:SER:H	2.23	0.41
1:X:196:ARG:CD	1:X:255:ARG:HD2	2.43	0.41
1:X:231:THR:OG1	1:X:232:ASP:OD1	2.29	0.41
1:X:331:ASP:HB2	1:X:347:ARG:HG3	2.02	0.41
1:A:9:ARG:O	1:A:10:GLN:C	2.59	0.41
1:X:32:PHE:C	1:X:34:GLY:N	2.74	0.41
1:A:51:GLN:HB2	1:A:80:GLN:CD	2.39	0.41
1:X:134:VAL:N	1:X:135:PRO:CD	2.67	0.41
1:A:117:ASN:OD1	1:A:176:ALA:HB2	2.21	0.41
1:X:289:ARG:HE	1:X:366:GLU:HG2	1.85	0.41
1:A:340:ARG:HA	1:A:360:LEU:HD12	2.01	0.41
1:A:253:ILE:HD12	1:A:288:ILE:HD12	2.03	0.41
1:X:354:LEU:HB3	1:X:385:TRP:HB2	2.01	0.41
1:X:353:TYR:CE2	1:X:354:LEU:O	2.74	0.41
1:A:40:PHE:CD1	1:A:69:LEU:HD22	2.56	0.41
1:X:10:GLN:C	1:X:12:ILE:N	2.73	0.41
1:X:24:GLU:HG2	1:X:28:TYR:HD2	1.86	0.41
1:X:32:PHE:HD1	1:X:32:PHE:O	2.03	0.41
1:X:132:ALA:N	1:X:171:GLN:HB3	2.35	0.41
1:X:121:VAL:O	1:X:124:ILE:HB	2.20	0.41
1:A:28:TYR:CZ	1:A:205:TYR:CD2	3.08	0.41
1:X:254:LYS:O	1:X:258:ASP:N	2.49	0.41
1:A:154:GLU:HA	1:A:155:PRO:HD3	1.84	0.41
1:A:106:ILE:HD12	1:A:151:ARG:NH1	2.35	0.41
1:A:273:GLU:OE1	1:A:284:SER:CB	2.69	0.41
1:X:270:ARG:HH11	1:X:273:GLU:HG2	1.86	0.41
1:X:57:LEU:HG	1:X:61:LEU:HD11	2.03	0.41
1:X:340:ARG:HB3	1:X:360:LEU:HD12	2.02	0.41
1:X:26:ARG:O	1:X:30:HIS:CD2	2.73	0.41
1:X:81:LEU:CD1	1:X:99:ARG:NH1	2.81	0.41
1:A:255:ARG:HD3	1:A:255:ARG:HH11	1.73	0.41
1:X:336:THR:O	1:X:338:SER:N	2.54	0.41
1:A:348:LEU:O	1:A:351:TRP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TYR:CE2	1:A:355:ASP:CA	3.00	0.41
1:A:91:PRO:CD	1:A:91:PRO:O	2.69	0.40
1:X:40:PHE:CE1	1:X:69:LEU:HA	2.56	0.40
1:A:262:LEU:C	1:A:264:SER:N	2.74	0.40
1:A:131:ALA:O	1:A:171:GLN:NE2	2.54	0.40
1:A:132:ALA:HB3	1:A:166:ALA:HB1	2.03	0.40
1:A:120:LEU:C	1:A:120:LEU:HD12	2.41	0.40
1:A:165:SER:HA	1:A:168:ARG:HH21	1.86	0.40
1:A:292:GLU:HG2	1:A:368:LEU:HD21	2.02	0.40
1:A:403:GLY:HA3	1:A:414:TRP:CD2	2.57	0.40
1:A:394:ASN:HA	1:A:397:TYR:CD2	2.56	0.40
1:A:376:LEU:HG	1:A:376:LEU:O	2.19	0.40
1:A:294:ILE:HD13	1:A:372:VAL:HA	2.00	0.40
1:A:64:LEU:O	1:A:69:LEU:HB2	2.22	0.40
1:X:328:LEU:CD1	1:X:330:VAL:HG23	2.51	0.40
1:A:140:GLU:HA	1:A:180:GLU:O	2.21	0.40
1:A:309:ASP:HA	1:A:325:TRP:CZ2	2.53	0.40
1:X:65:GLN:HG3	1:X:66:THR:N	2.36	0.40
1:X:32:PHE:CD1	1:X:32:PHE:O	2.75	0.40
1:A:81:LEU:CD1	1:A:99:ARG:NH2	2.80	0.40
1:X:405:VAL:HG12	1:X:431:PHE:CZ	2.56	0.40
1:X:243:ASN:O	1:X:244:GLY:C	2.59	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	435/461 (94%)	360 (83%)	46 (11%)	29 (7%)	1	25
1	X	433/461 (94%)	349 (81%)	57 (13%)	27 (6%)	2	27
All	All	868/922 (94%)	709 (82%)	103 (12%)	56 (6%)	1	26

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	89	ASP
1	A	95	VAL
1	A	96	ASP
1	A	99	ARG
1	A	145	ASP
1	A	146	ALA
1	X	99	ARG
1	X	145	ASP
1	X	146	ALA
1	A	78	GLY
1	A	88	ALA
1	A	91	PRO
1	A	226	SER
1	A	330	VAL
1	A	405	VAL
1	X	36	ASP
1	X	39	ARG
1	X	43	ILE
1	X	78	GLY
1	X	316	PHE
1	A	23	LYS
1	A	39	ARG
1	A	92	THR
1	A	93	GLU
1	A	196	ARG
1	A	297	THR
1	A	316	PHE
1	A	349	ASP
1	X	84	ALA
1	X	89	ASP
1	X	103	ASP
1	X	226	SER
1	X	330	VAL
1	X	337	GLU
1	X	349	ASP
1	A	6	PRO
1	A	438	GLU
1	X	11	THR
1	X	91	PRO
1	X	92	THR
1	X	185	THR

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Mol	Chain	Res	Type
1	X	196	ARG
1	X	405	VAL
1	A	110	ARG
1	A	387	SER
1	X	8	VAL
1	X	33	SER
1	X	88	ALA
1	A	317	GLY
1	X	438	GLU
1	A	392	PRO
1	X	242	VAL
1	A	391	ASN
1	X	317	GLY
1	A	155	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	346/367 (94%)	310 (90%)	36 (10%)	9	40
1	X	344/367 (94%)	311 (90%)	33 (10%)	10	44
All	All	690/734 (94%)	621 (90%)	69 (10%)	10	41

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	35	ILE
1	A	65	GLN
1	A	89	ASP
1	A	92	THR
1	A	100	VAL
1	A	106	ILE
1	A	118	LEU
1	A	136	ARG

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Mol	Chain	Res	Type
1	A	143	ILE
1	A	144	VAL
1	A	190	ASN
1	A	196	ARG
1	A	206	LYS
1	A	224	LEU
1	A	236	LEU
1	A	246	MET
1	A	254	LYS
1	A	255	ARG
1	A	287	LEU
1	A	307	ARG
1	A	318	ARG
1	A	327	ARG
1	A	332	ARG
1	A	354	LEU
1	A	362	ASP
1	A	364[A]	ARG
1	A	364[B]	ARG
1	A	370	ARG
1	A	372	VAL
1	A	388	ARG
1	A	390	ASN
1	A	393	VAL
1	A	418	MET
1	A	421	VAL
1	A	437	LEU
1	X	10	GLN
1	X	32	PHE
1	X	37	GLN
1	X	45	VAL
1	X	65	GLN
1	X	89	ASP
1	X	100	VAL
1	X	106	ILE
1	X	115	GLN
1	X	136	ARG
1	X	143	ILE
1	X	144	VAL
1	X	190	ASN
1	X	196	ARG
1	X	206	LYS

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Mol	Chain	Res	Type
1	X	251	GLU
1	X	254	LYS
1	X	255	ARG
1	X	269	THR
1	X	307	ARG
1	X	318	ARG
1	X	327	ARG
1	X	332	ARG
1	X	346	THR
1	X	353	TYR
1	X	354	LEU
1	X	362	ASP
1	X	364	ARG
1	X	370	ARG
1	X	390	ASN
1	X	407	ARG
1	X	418	MET
1	X	421	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	18	HIS
1	A	30	HIS
1	A	65	GLN
1	A	80	GLN
1	X	14	GLN
1	X	65	GLN
1	X	80	GLN

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 [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	436/461 (94%)	0.37	33 (7%) 17 12	185, 422, 690, 893	0
1	X	435/461 (94%)	0.48	50 (11%) 6 6	209, 472, 685, 784	0
All	All	871/922 (94%)	0.42	83 (9%) 10 8	185, 455, 688, 893	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	VAL	16.9
1	A	5	ALA	13.2
1	X	342	ALA	11.6
1	A	17	SER	11.5
1	A	18	HIS	11.2
1	X	358	ALA	11.0
1	A	7	GLY	9.5
1	X	267	SER	9.1
1	A	14	GLN	6.9
1	X	357	PHE	6.9
1	X	20	ARG	6.7
1	X	187	VAL	6.5
1	X	10	GLN	6.4
1	X	22	GLY	6.0
1	X	341	ALA	5.9
1	X	19	MET	5.9
1	A	12	ILE	5.8
1	X	268	ILE	5.6
1	A	15	LEU	5.4
1	X	343	ALA	5.2
1	X	21	ASP	5.1
1	X	9	ARG	4.7
1	X	179	GLY	4.6
1	X	66	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	X	286	THR	4.4
1	X	287	LEU	4.4
1	X	285	GLY	4.3
1	A	19	MET	4.2
1	A	6	PRO	4.2
1	A	9	ARG	4.2
1	X	25	ILE	4.1
1	X	359	VAL	4.1
1	A	334	PHE	4.0
1	A	10	GLN	4.0
1	X	104	GLU	3.9
1	A	434	PRO	3.8
1	X	227	ILE	3.8
1	A	296	ALA	3.6
1	A	16	LEU	3.6
1	X	319	PRO	3.6
1	A	433	LEU	3.5
1	X	178	LEU	3.5
1	A	11	THR	3.4
1	X	18	HIS	3.4
1	A	333	ALA	3.4
1	A	297	THR	3.3
1	X	105	ALA	3.3
1	A	437	LEU	3.3
1	A	13	VAL	3.3
1	X	180	GLU	3.1
1	X	288	ILE	3.0
1	A	408	ASP	2.9
1	X	277	GLU	2.9
1	X	333	ALA	2.9
1	X	418	MET	2.9
1	A	66	THR	2.7
1	X	103	ASP	2.6
1	X	186	LEU	2.6
1	A	318	ARG	2.6
1	X	15	LEU	2.5
1	A	343	ALA	2.4
1	X	62	ALA	2.4
1	X	246	MET	2.4
1	X	189	ILE	2.4
1	X	16	LEU	2.4
1	X	318	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	20	ARG	2.4
1	X	278	LEU	2.3
1	X	177	CYS	2.3
1	X	226	SER	2.2
1	A	436	THR	2.2
1	X	188	ASN	2.2
1	X	102	ARG	2.2
1	X	247	ARG	2.2
1	X	209	PHE	2.2
1	A	99	ARG	2.2
1	X	289	ARG	2.1
1	A	105	ALA	2.1
1	A	342	ALA	2.1
1	X	316	PHE	2.1
1	A	94	ARG	2.0
1	X	101	THR	2.0
1	A	104	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.