



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:37 pm BST

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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

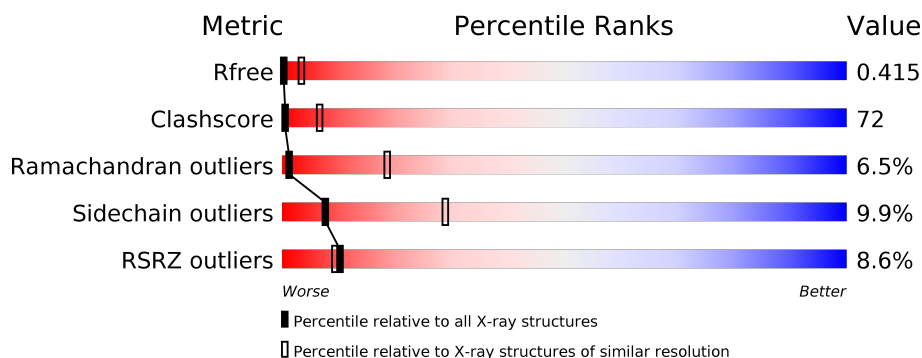
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	461	<div> <div>6%</div> <div>28% 54% 11% • 5%</div> </div>
1	X	461	<div> <div>10%</div> <div>31% 54% 10% • 6%</div> </div>

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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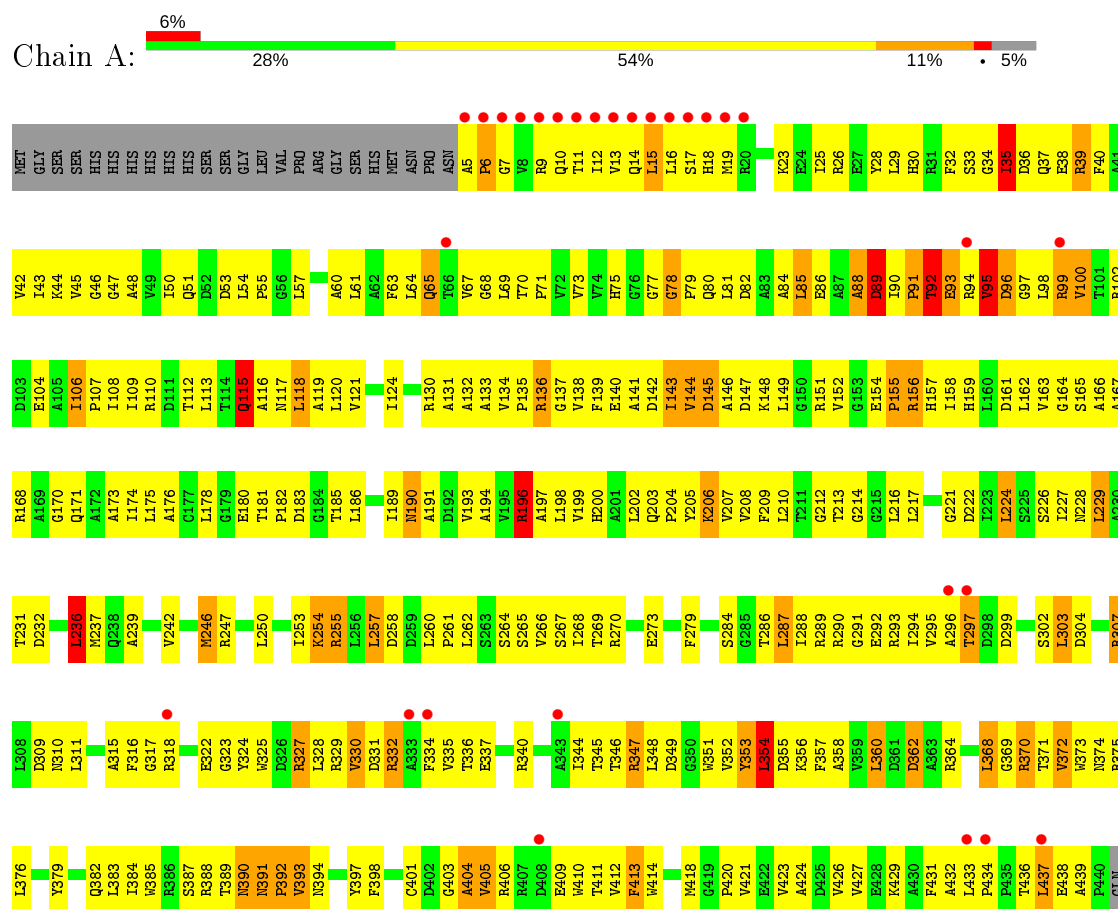
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Chain	Residue	Modelled	Actual	Comment	Reference
X	-14	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-13	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-12	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-11	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-10	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-9	SER	-	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

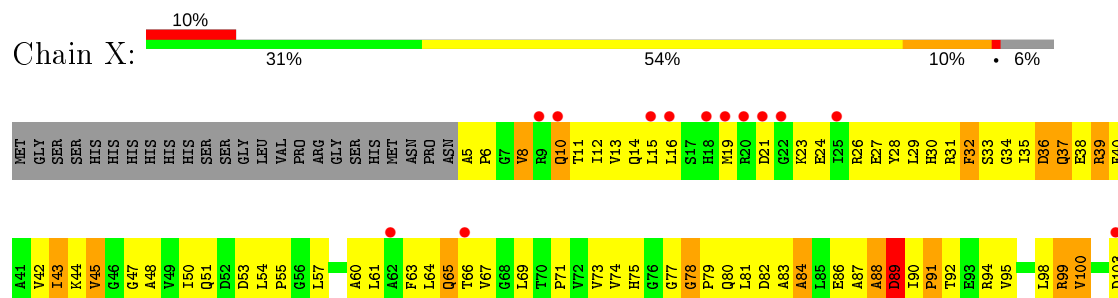
3 Residue-property plots

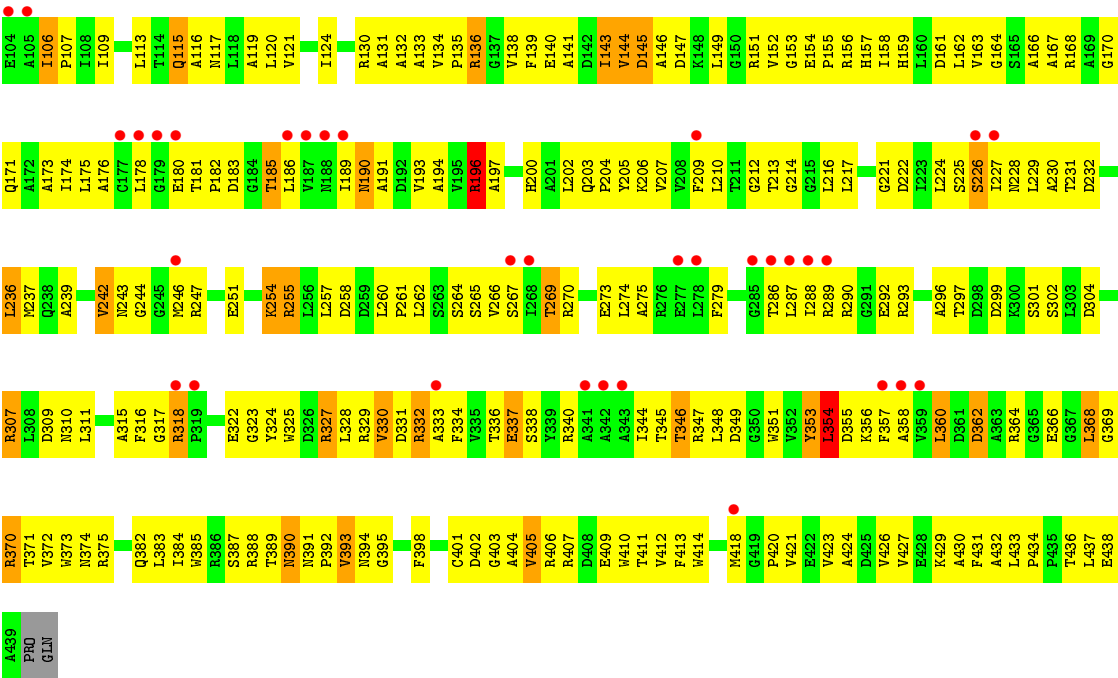
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: N-acetylglutamate kinase / N-acetylglutamate synthase



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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 1.6.4_486	Depositor
R, R_{free}	0.274 , 0.419 0.263 , 0.415	Depositor DCC
R_{free} test set	949 reflections (10.02%)	wwPDB-VP
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 , 406.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	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:A:13:VAL:CG1	1:A:26:ARG:HD3	1.94	0.96
1:X:232:ASP:HB3	1:X:236:LEU:HD23	1.46	0.96
1:A:95:VAL:CG1	1:A:148:LYS:HE2	1.94	0.95
1:A:196:ARG:HD3	1:A:255:ARG:HD2	1.48	0.95
1:A:95:VAL:CG2	1:A:100:VAL:HG11	1.97	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:258:ASP:OD1	1:A:290:ARG:HD2	1.69	0.92
1:A:297:THR:H	1:A:332:ARG:HH12	1.02	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:A:203:GLN:OE1	1:A:261:PRO:HD3	1.75	0.86
1:X:64:LEU:HD22	1:X:69:LEU:HD12	1.56	0.86
1:A:404:ALA:O	1:A:405:VAL:HG23	1.73	0.86
1:A:229:LEU:HD22	1:A:254:LYS:HB2	1.58	0.86
1:X:232:ASP:HB3	1:X:236:LEU:CD2	2.04	0.86
1:A:82:ASP:OD1	1:A:99:ARG:NH2	2.08	0.86
1:X:332:ARG:HH11	1:X:332:ARG:CG	1.89	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: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:353:TYR:CE2	1:X:355:ASP:HA	2.11	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:229:LEU:HD12	1:A:289:ARG:O	1.78	0.84
1:A:51:GLN:OE1	1:A:80:GLN:HG3	1.77	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:A:42:VAL:HG23	1:A:204:PRO:HG2	1.60	0.81
1:X:42:VAL:HB	1:X:207:VAL:HG22	1.63	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:174:ILE:N	1:A:174:ILE:HD13	1.90	0.80
1:A:265:SER:C	1:A:266:VAL:HG23	2.01	0.80
1:A:371:THR:O	1:A:374:ASN:HB2	1.80	0.80
1:X:297:THR:N	1:X:332:ARG:HH12	1.79	0.80
1:X:398:PHE:CD2	1:X:398:PHE:O	2.34	0.80
1:A:93:GLU:OE2	1:A:102:ARG:CZ	2.30	0.80
1:A:348:LEU:HD11	1:A:429:LYS:HD3	1.64	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HD13	1:A:186:LEU:HD23	1.63	0.79
1:A:45:VAL:HG22	1:A:210:LEU:HB2	1.64	0.79
1:A:398:PHE:HE2	1:X:406:ARG:HH11	1.30	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:63:PHE:O	1:A:67:VAL:HG13	1.82	0.78
1:A:95:VAL:HB	1:A:149:LEU:CD2	2.14	0.78
1:A:93:GLU:HB3	1:A:100:VAL:HG22	1.65	0.78
1:A:214:GLY:HA2	1:A:269:THR:C	2.05	0.78
1:A:404:ALA:O	1:A:405:VAL:CG2	2.31	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:214:GLY:HA3	1:A:270:ARG:HB3	1.65	0.77
1:A:372:VAL:CG1	1:A:373:TRP:N	2.48	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:75:HIS:NE2	1:X:117:ASN:OD1	2.14	0.75
1:X:95:VAL:HG22	1:X:99:ARG:N	2.01	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:A:75:HIS:NE2	1:A:117:ASN:OD1	2.18	0.74
1:X:353:TYR:O	1:X:353:TYR:CD2	2.41	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:A:95:VAL:HG23	1:A:100:VAL:CG1	2.17	0.73
1:X:411:THR:CG2	1:X:413:PHE:CE2	2.71	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:357:PHE:HE1	1:X:372:VAL:HG11	1.53	0.73
1:X:47:GLY:HA3	1:X:78:GLY:N	2.04	0.73
1:A:136:ARG:HH11	1:A:136:ARG:HB3	1.54	0.72
1:A:42:VAL:C	1:A:43:ILE:HG13	2.09	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: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:X:229:LEU:HD12	1:X:289:ARG:O	1.90	0.72
1:A:357:PHE:HE1	1:A:372:VAL:HG11	1.53	0.72
1:A:398:PHE:HE2	1:X:406:ARG:NH1	1.87	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:X:296:ALA:CB	1:X:332:ARG:HH22	2.02	0.71
1:A:398:PHE:CZ	1:X:406:ARG:HD2	2.23	0.71
1:A:136:ARG:HH22	1:A:180:GLU:HB3	1.56	0.71
1:A:155:PRO:HD3	1:A:189:ILE:HD12	1.73	0.71
1:A:232:ASP:CB	1:A:236:LEU:CD1	2.69	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:A:132:ALA:HB2	1:A:171:GLN:OE1	1.90	0.70
1:X:136:ARG:HH11	1:X:136:ARG:HB3	1.56	0.70
1:X:157:HIS:O	1:X:158:ILE:HD13	1.92	0.70
1:X:48:ALA:N	1:X:79:PRO:HD2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:318:ARG:HG3	1:X:437:LEU:HB3	1.72	0.70
1:X:67:VAL:CG1	1:X:69:LEU:HG	2.21	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:328:LEU:CG	1:A:330:VAL:HG23	2.21	0.70
1:A:38:GLU:C	1:A:40:PHE:H	1.95	0.70
1:A:406:ARG:HG2	1:A:411:THR:OG1	1.92	0.70
1:A:51:GLN:HB2	1:A:80:GLN:NE2	2.07	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:155:PRO:HD3	1:X:189:ILE:HD12	1.74	0.69
1:X:412:VAL:HG23	1:X:431:PHE:CE1	2.27	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:X:51:GLN:HB2	1:X:80:GLN:NE2	2.08	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:411:THR:CG2	1:A:413:PHE:CE2	2.75	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: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:297:THR:N	1:X:332:ARG:NH1	2.39	0.69
1:A:5:ALA:HB3	1:A:6:PRO:HD3	1.75	0.69
1:X:265:SER:HB2	1:X:287:LEU:HD21	1.74	0.69
1:A:85:LEU:HD21	1:A:108:ILE:CB	2.23	0.69
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.57	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:X:81:LEU:O	1:X:86:GLU:HB2	1.92	0.69
1:X:328:LEU:CG	1:X:330:VAL:HG23	2.23	0.68
1:A:121:VAL:HG21	1:A:133:ALA:CB	2.24	0.68
1:A:229:LEU:HD22	1:A:254:LYS:CB	2.23	0.68
1:A:353:TYR:HE2	1:A:355:ASP:HA	1.56	0.68
1:A:43:ILE:O	1:A:43:ILE:HG22	1.93	0.68
1:X:117:ASN:OD1	1:X:176:ALA:HB2	1.93	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:23:LYS:HE3	1:X:27:GLU:OE2	1.94	0.66
1:X:404:ALA:O	1:X:405:VAL:CG2	2.43	0.66
1:A:206:LYS:HZ1	1:A:287:LEU:HD22	1.61	0.66
1:X:120:LEU:HD12	1:X:120:LEU:O	1.95	0.66
1:X:37:GLN:CG	1:X:38:GLU:OE2	2.43	0.66
1:A:216:LEU:O	1:A:217:LEU:HD23	1.96	0.66
1:A:311:LEU:HD12	1:A:360:LEU:HD11	1.76	0.66
1:A:331:ASP:OD1	1:A:347:ARG:NE	2.28	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:372:VAL:CG1	1:X:373:TRP:N	2.59	0.65
1:X:47:GLY:C	1:X:79:PRO:HD2	2.16	0.65
1:A:28:TYR:OH	1:A:205:TYR:HE2	1.78	0.65
1:A:81:LEU:CD1	1:A:99:ARG:HH12	2.10	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: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: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:A:426:VAL:O	1:A:429:LYS:HB2	1.97	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:292:GLU:HG3	1:A:336:THR:OG1	1.96	0.65
1:A:329:ARG:O	1:A:330:VAL:HB	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: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:175:LEU:HD12	1:X:175:LEU:N	2.11	0.64
1:X:318:ARG:HG2	1:X:437:LEU:HB3	1.79	0.64
1:A:196:ARG:O	1:A:197:ALA:C	2.36	0.64
1:A:295:VAL:HG22	1:A:335:VAL:C	2.16	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:132:ALA:HB2	1:A:171:GLN:CD	2.18	0.64
1:A:140:GLU:HG2	1:A:182:PRO:HG3	1.80	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:242:VAL:HG13	1:A:246:MET:HG2	1.78	0.63
1:A:334:PHE:CE1	1:A:375:ARG:HB3	2.34	0.63
1:A:136:ARG:NH2	1:A:180:GLU:HB3	2.13	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:229:LEU:CD2	1:A:254:LYS:HB2	2.29	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:390:ASN:O	1:X:392:PRO:N	2.32	0.63
1:X:42:VAL:O	1:X:43:ILE:HG13	1.99	0.63
1:X:246:MET:O	1:X:246:MET:HG3	1.98	0.63
1:A:28:TYR:OH	1:A:205:TYR:CE2	2.51	0.62
1:A:295:VAL:N	1:A:335:VAL:O	2.29	0.62
1:A:351:TRP:CD1	1:A:426:VAL:HG11	2.33	0.62
1:A:9:ARG:NH2	1:A:33:SER:HB2	2.13	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:A:354:LEU:HB3	1:A:385:TRP:HB3	1.82	0.62
1:X:132:ALA:HB2	1:X:171:GLN:CD	2.20	0.62
1:X:398:PHE:C	1:X:398:PHE:CD2	2.73	0.62
1:A:414:TRP:CE3	1:A:423:VAL:HG11	2.35	0.61
1:X:145:ASP:OD2	1:X:149:LEU:HD12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:HG3	1:A:45:VAL:N	2.15	0.61
1:X:63:PHE:CE2	1:X:67:VAL:HG21	2.35	0.61
1:X:426:VAL:O	1:X:429:LYS:HB2	2.00	0.61
1:X:42:VAL:C	1:X:43:ILE:HG13	2.20	0.61
1:A:232:ASP:HB3	1:A:236:LEU:HD12	1.80	0.61
1:X:265:SER:C	1:X:266:VAL:HG23	2.20	0.61
1:X:106:ILE:HG23	1:X:186:LEU:HD23	1.82	0.61
1:X:414:TRP:CE3	1:X:423:VAL:HG11	2.35	0.61
1:A:412:VAL:HG23	1:A:431:PHE:CE1	2.35	0.61
1:X:121:VAL:HG21	1:X:133:ALA:CB	2.27	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:X:346:THR:HG23	1:X:355:ASP:HB2	1.83	0.61
1:A:106:ILE:HG22	1:A:107:PRO:HD3	1.82	0.61
1:A:293:ARG:CZ	1:A:337:GLU:OE2	2.49	0.61
1:A:131:ALA:CA	1:A:171:GLN:HB3	2.30	0.61
1:X:353:TYR:C	1:X:353:TYR:CD2	2.74	0.61
1:A:120:LEU:O	1:A:120:LEU:HD12	2.02	0.60
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:A:77:GLY:O	1:A:78:GLY:C	2.38	0.60
1:X:140:GLU:HG2	1:X:182:PRO:HG3	1.82	0.60
1:X:77:GLY:O	1:X:78:GLY:C	2.39	0.60
1:X:232:ASP:C	1:X:236:LEU:HD23	2.20	0.60
1:X:292:GLU:CD	1:X:337:GLU:HB3	2.21	0.60
1:X:88:ALA:C	1:X:90:ILE:H	2.03	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:196:ARG:CD	1:A:255:ARG:HD2	2.28	0.60
1:A:33:SER:O	1:A:37:GLN:NE2	2.34	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: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:X:13:VAL:C	1:X:15:LEU:H	2.05	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:356:LYS:NZ	1:A:436:THR:HG21	2.17	0.60
1:A:90:ILE:CD1	1:A:104:GLU:OE1	2.50	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:A:106:ILE:HG23	1:A:186:LEU:HD23	1.83	0.59
1:X:42:VAL:CG2	1:X:204:PRO:HG2	2.32	0.59
1:X:371:THR:O	1:X:374:ASN:HB2	2.02	0.59
1:A:227:ILE:HG22	1:A:228:ASN:N	2.16	0.59
1:A:15:LEU:CD1	1:X:15:LEU:HG	2.32	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:144:VAL:O	1:X:145:ASP:HB3	2.02	0.59
1:X:228:ASN:N	1:X:232:ASP:OD2	2.35	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:116:ALA:O	1:X:119:ALA:HB3	2.02	0.58
1:X:164:GLY:O	1:X:168:ARG:HB2	2.03	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:133:ALA:O	1:A:135:PRO:HD3	2.03	0.58
1:A:175:LEU:HD12	1:A:175:LEU:N	2.18	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: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:29:LEU:CD1	1:X:67:VAL:HG13	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:36:ASP:CB	1:X:39:ARG:HG3	2.34	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:174:ILE:HG22	1:A:174:ILE:O	2.03	0.57
1:A:90:ILE:H	1:A:91:PRO:HD3	1.64	0.57
1:X:225:SER:O	1:X:226:SER:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:229:LEU:HD22	1:X:254:LYS:HB2	1.86	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:44:LYS:HG2	1:A:209:PHE:CD1	2.40	0.57
1:A:48:ALA:CA	1:A:79:PRO:HG2	2.35	0.57
1:A:28:TYR:CE1	1:A:205:TYR:CD2	2.93	0.57
1:X:322:GLU:HG2	1:X:323:GLY:N	2.19	0.57
1:X:351:TRP:HD1	1:X:426:VAL:CB	2.18	0.57
1:A:132:ALA:HB3	1:A:166:ALA:CB	2.35	0.56
1:A:239:ALA:O	1:A:242:VAL:HB	2.05	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:X:48:ALA:CA	1:X:79:PRO:HG2	2.35	0.56
1:X:296:ALA:C	1:X:332:ARG:HH22	2.08	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:64:LEU:HD22	1:X:69:LEU:CD1	2.31	0.56
1:A:228:ASN:N	1:A:232:ASP:OD2	2.36	0.56
1:X:109:ILE:HG22	1:X:178:LEU:HD21	1.87	0.56
1:A:42:VAL:O	1:A:43:ILE:CG1	2.52	0.56
1:A:94:ARG:HG2	1:A:99:ARG:CA	2.34	0.56
1:X:368:LEU:O	1:X:369:GLY:C	2.43	0.56
1:X:48:ALA:HA	1:X:79:PRO:HG2	1.88	0.56
1:X:106:ILE:HG22	1:X:107:PRO:CD	2.35	0.56
1:A:404:ALA:C	1:A:405:VAL:HG23	2.25	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: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:232:ASP:CB	1:A:236:LEU:HD13	2.34	0.56
1:A:32:PHE:HD1	1:A:36:ASP:OD2	1.87	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:X:47:GLY:O	1:X:50:ILE:HG12	2.06	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:A:383:LEU:C	1:A:384:ILE:HD12	2.26	0.56
1:X:311:LEU:HD12	1:X:360:LEU:HD11	1.87	0.56
1:A:196:ARG:HH11	1:A:255:ARG:HD2	1.70	0.55
1:A:54:LEU:N	1:A:55:PRO:CD	2.68	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:X:175:LEU:CD1	1:X:175:LEU:H	2.19	0.55
1:X:292:GLU:OE1	1:X:337:GLU:CB	2.50	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:216:LEU:O	1:X:217:LEU:HD23	2.05	0.55
1:X:38:GLU:C	1:X:40:PHE:N	2.60	0.55
1:A:356:LYS:HZ3	1:A:436:THR:HG21	1.70	0.55
1:X:328:LEU:HG	1:X:330:VAL:CG2	2.31	0.55
1:A:112:THR:O	1:A:115:GLN:HB3	2.07	0.55
1:A:132:ALA:HB3	1:A:166:ALA:HB2	1.89	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:331:ASP:CB	1:A:345:THR:OG1	2.49	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:X:391:ASN:O	1:X:393:VAL:N	2.38	0.55
1:X:196:ARG:NH1	1:X:255:ARG:HD2	2.22	0.55
1:A:120:LEU:O	1:A:124:ILE:HG13	2.06	0.55
1:A:136:ARG:CB	1:A:136:ARG:HH11	2.19	0.55
1:X:136:ARG:HH11	1:X:136:ARG:CB	2.20	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: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:A:15:LEU:HD22	1:X:15:LEU:HG	1.87	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:214:GLY:CA	1:A:270:ARG:N	2.70	0.54
1:A:405:VAL:HG11	1:A:431:PHE:HE2	1.72	0.54
1:A:53:ASP:O	1:A:54:LEU:C	2.44	0.54
1:X:145:ASP:O	1:X:147:ASP:N	2.39	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:163:VAL:HG13	1:A:173:ALA:CB	2.38	0.54
1:A:40:PHE:CE1	1:A:69:LEU:HD22	2.43	0.54
1:X:132:ALA:HB3	1:X:166:ALA:HB2	1.90	0.54
1:X:36:ASP:HB2	1:X:39:ARG:CB	2.29	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:A:206:LYS:NZ	1:A:287:LEU:HD22	2.23	0.54
1:X:203:GLN:N	1:X:204:PRO:HD3	2.22	0.54
1:X:411:THR:HG21	1:X:413:PHE:CE2	2.42	0.54
1:X:47:GLY:CA	1:X:79:PRO:HD2	2.38	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:A:28:TYR:CZ	1:A:205:TYR:CE2	2.96	0.53
1:A:94:ARG:CG	1:A:99:ARG:HA	2.35	0.53
1:X:65:GLN:NE2	1:X:170:GLY:O	2.41	0.53
1:A:390:ASN:O	1:A:391:ASN:C	2.45	0.53
1:X:35:ILE:C	1:X:37:GLN:N	2.61	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:292:GLU:OE1	1:X:337:GLU:CA	2.57	0.53
1:X:43:ILE:CD1	1:X:71:PRO:HB3	2.38	0.53
1:A:131:ALA:C	1:A:171:GLN:HB3	2.29	0.53
1:X:262:LEU:HD21	1:X:290:ARG:CZ	2.39	0.53
1:X:406:ARG:HG2	1:X:411:THR:OG1	2.08	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:254:LYS:HG2	1:X:258:ASP:OD2	2.07	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:354:LEU:HB3	1:X:385:TRP:CB	2.39	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:A:196:ARG:O	1:A:198:LEU:N	2.42	0.53
1:A:352:VAL:O	1:A:383:LEU:HD12	2.09	0.53
1:X:13:VAL:HG12	1:X:14:GLN:N	2.24	0.53
1:X:242:VAL:HG13	1:X:246:MET:HG2	1.90	0.53
1:A:81:LEU:HD13	1:A:99:ARG:HH12	1.74	0.52
1:X:138:VAL:HG11	1:X:175:LEU:CD2	2.39	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:287:LEU:HD23	1:X:288:ILE:N	2.23	0.52
1:A:106:ILE:CG2	1:A:107:PRO:HD3	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: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:X:265:SER:O	1:X:266:VAL:CG2	2.58	0.52
1:X:289:ARG:HD2	1:X:366:GLU:HB3	1.90	0.52
1:X:84:ALA:O	1:X:88:ALA:N	2.42	0.52
1:A:19:MET:HE2	1:X:19:MET:HB2	1.91	0.52
1:A:351:TRP:HZ3	1:A:382:GLN:OE1	1.92	0.52
1:A:354:LEU:HB3	1:A:385:TRP:CB	2.40	0.52
1:X:214:GLY:CA	1:X:270:ARG:N	2.72	0.52
1:X:292:GLU:OE1	1:X:337:GLU:N	2.42	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:106:ILE:HD13	1:A:186:LEU:CD2	2.38	0.52
1:A:144:VAL:O	1:A:145:ASP:HB3	2.10	0.52
1:A:158:ILE:HD13	1:A:158:ILE:N	2.23	0.52
1:A:73:VAL:HB	1:A:174:ILE:HD12	1.92	0.52
1:A:294:ILE:HA	1:A:336:THR:HA	1.92	0.52
1:A:295:VAL:CG2	1:A:335:VAL:HB	2.40	0.52
1:A:340:ARG:CA	1:A:360:LEU:HD12	2.39	0.52
1:X:217:LEU:HD13	1:X:221:GLY:O	2.10	0.51
1:X:231:THR:CG2	1:X:293:ARG:HA	2.39	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: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:X:13:VAL:C	1:X:15:LEU:N	2.64	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: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:297:THR:H	1:X:332:ARG:NH1	1.94	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:A:140:GLU:OE2	1:A:182:PRO:HB3	2.11	0.50
1:A:205:TYR:O	1:A:264:SER:HA	2.11	0.50
1:A:17:SER:HA	1:A:26:ARG:HH21	1.75	0.50
1:A:409:GLU:OE1	1:A:410:TRP:HD1	1.94	0.50
1:X:332:ARG:N	1:X:345:THR:OG1	2.44	0.50
1:X:353:TYR:CE2	1:X:355:ASP:CA	2.92	0.50
1:A:140:GLU:CG	1:A:182:PRO:HG3	2.41	0.50
1:A:403:GLY:HA3	1:A:414:TRP:CE2	2.46	0.50
1:A:15:LEU:HD13	1:X:15:LEU:HG	1.92	0.50
1:A:57:LEU:O	1:A:60:ALA:HB3	2.10	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: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:106:ILE:HB	1:X:107:PRO:HD3	1.92	0.50
1:X:120:LEU:O	1:X:124:ILE:HG13	2.12	0.50
1:X:432:ALA:O	1:X:433:LEU:C	2.49	0.50
1:X:47:GLY:HA3	1:X:79:PRO:HD2	1.93	0.50
1:A:139:PHE:CZ	1:A:194:ALA:HB1	2.47	0.50
1:A:39:ARG:HD3	1:A:202:LEU:O	2.12	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:X:43:ILE:HD12	1:X:71:PRO:HB3	1.94	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:A:34:GLY:C	1:A:35:ILE:HG12	2.32	0.49
1:X:353:TYR:HD2	1:X:353:TYR:O	1.92	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:254:LYS:O	1:A:258:ASP:N	2.42	0.49
1:A:266:VAL:H	1:A:287:LEU:HD13	1.76	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:54:LEU:HB3	1:A:55:PRO:HD3	1.95	0.49
1:A:80:GLN:O	1:A:84:ALA:CB	2.61	0.49
1:A:324:TYR:CD1	1:A:325:TRP:N	2.80	0.49
1:A:405:VAL:HG12	1:A:431:PHE:CZ	2.48	0.49
1:X:390:ASN:O	1:X:391:ASN:C	2.50	0.49
1:X:401:CYS:O	1:X:402:ASP:OD1	2.31	0.49
1:A:9:ARG:HG3	1:A:29:LEU:HD13	1.95	0.49
1:A:354:LEU:HG	1:A:355:ASP:N	2.24	0.49
1:A:61:LEU:CD2	1:A:73:VAL:HG21	2.42	0.49
1:X:140:GLU:CG	1:X:182:PRO:HG3	2.42	0.49
1:X:196:ARG:HH11	1:X:255:ARG:HD2	1.76	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: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:414:TRP:CZ3	1:A:423:VAL:HG11	2.48	0.48
1:A:64:LEU:HD22	1:A:69:LEU:CD1	2.37	0.48
1:X:183:ASP:C	1:X:183:ASP:OD2	2.52	0.48
1:X:289:ARG:CD	1:X:366:GLU:HB3	2.44	0.48
1:A:232:ASP:CB	1:A:236:LEU:HD12	2.41	0.48
1:X:217:LEU:HD22	1:X:222:ASP:C	2.34	0.48
1:X:53:ASP:O	1:X:54:LEU:C	2.50	0.48
1:A:262:LEU:HD21	1:A:290:ARG:CZ	2.43	0.48
1:A:64:LEU:CD1	1:A:71:PRO:HG3	2.37	0.48
1:X:296:ALA:CB	1:X:332:ARG:NH2	2.67	0.48
1:A:232:ASP:O	1:A:236:LEU:CD1	2.56	0.48
1:X:120:LEU:HD12	1:X:120:LEU:C	2.31	0.48
1:X:65:GLN:NE2	1:X:130:ARG:O	2.44	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:X:35:ILE:O	1:X:37:GLN:N	2.47	0.48
1:X:387:SER:OG	1:X:388:ARG:N	2.45	0.48
1:A:117:ASN:O	1:A:121:VAL:HG23	2.13	0.48
1:A:65:GLN:NE2	1:A:130:ARG:O	2.44	0.48
1:A:391:ASN:O	1:A:393:VAL:N	2.46	0.48
1:A:432:ALA:O	1:A:433:LEU:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:412:VAL:HG23	1:X:431:PHE:CZ	2.49	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:106:ILE:HB	1:A:107:PRO:HD3	1.95	0.48
1:A:405:VAL:HG12	1:A:431:PHE:HZ	1.78	0.48
1:X:94:ARG:HB3	1:X:100:VAL:HG22	1.95	0.48
1:X:414:TRP:CZ3	1:X:423:VAL:HG11	2.49	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:237:MET:O	1:A:247:ARG:NE	2.47	0.48
1:A:26:ARG:O	1:A:26:ARG:HG3	2.14	0.48
1:A:311:LEU:O	1:A:360:LEU:HD21	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:175:LEU:CD1	1:A:175:LEU:N	2.77	0.47
1:A:293:ARG:NH1	1:A:337:GLU:OE2	2.47	0.47
1:X:266:VAL:O	1:X:288:ILE:N	2.47	0.47
1:X:315:ALA:CB	1:X:358:ALA:HB1	2.44	0.47
1:X:362:ASP:OD2	1:X:362:ASP:N	2.39	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: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:X:81:LEU:HD11	1:X:99:ARG:HH12	1.77	0.47
1:A:12:ILE:HD13	1:X:15:LEU:CD1	2.44	0.47
1:X:274:LEU:HA	1:X:274:LEU:HD12	1.66	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:65:GLN:NE2	1:X:130:ARG:CB	2.70	0.47
1:X:81:LEU:HD12	1:X:82:ASP:N	2.29	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:A:232:ASP:CA	1:A:236:LEU:HD12	2.44	0.47
1:X:196:ARG:O	1:X:197:ALA:C	2.52	0.47
1:X:324:TYR:C	1:X:324:TYR:CD1	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:315:ALA:HB3	1:X:358:ALA:HB1	1.96	0.47
1:A:9:ARG:O	1:A:12:ILE:HG22	2.14	0.47
1:X:106:ILE:HD13	1:X:186:LEU:CD2	2.44	0.47
1:X:262:LEU:C	1:X:264:SER:N	2.67	0.47
1:X:205:TYR:O	1:X:264:SER:HA	2.15	0.47
1:X:297:THR:O	1:X:332:ARG:NH1	2.47	0.47
1:A:26:ARG:HD2	1:A:30:HIS:HE1	1.80	0.47
1:X:232:ASP:O	1:X:236:LEU:HD23	2.13	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:13:VAL:CG1	1:A:26:ARG:CD	2.81	0.46
1:A:295:VAL:O	1:A:335:VAL:N	2.49	0.46
1:A:183:ASP:OD2	1:A:183:ASP:C	2.53	0.46
1:X:106:ILE:HG22	1:X:107:PRO:HD3	1.96	0.46
1:X:354:LEU:HG	1:X:355:ASP:N	2.30	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:X:48:ALA:HB2	1:X:79:PRO:HG2	1.97	0.46
1:A:167:ALA:O	1:A:170:GLY:N	2.27	0.46
1:A:299:ASP:OD2	1:A:302:SER:HB3	2.15	0.46
1:A:48:ALA:CB	1:A:79:PRO:HG2	2.45	0.46
1:X:106:ILE:CD1	1:X:186:LEU:HD23	2.40	0.46
1:A:113:LEU:HD12	1:A:178:LEU:HD12	1.97	0.46
1:A:292:GLU:OE1	1:A:336:THR:CG2	2.63	0.46
1:A:332:ARG:HD3	1:A:379:TYR:CE1	2.51	0.46
1:A:36:ASP:HB2	1:A:39:ARG:CB	2.43	0.46
1:A:411:THR:HG22	1:A:413:PHE:CD2	2.50	0.46
1:A:9:ARG:CA	1:A:12:ILE:HG22	2.43	0.46
1:X:356:LYS:HZ1	1:X:436:THR:HG21	1.81	0.46
1:A:406:ARG:CD	1:X:398:PHE:CE2	2.88	0.46
1:A:433:LEU:HA	1:A:434:PRO:HD3	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD21	1:A:108:ILE:HB	1.97	0.46
1:A:93:GLU:OE2	1:A:102:ARG:NH1	2.49	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:37:GLN:O	1:A:70:THR:HB	2.16	0.46
1:A:47:GLY:HA3	1:A:79:PRO:HD2	1.97	0.46
1:X:29:LEU:HD11	1:X:67:VAL:HG13	1.97	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:389:THR:O	1:A:394:ASN:ND2	2.48	0.45
1:A:398:PHE:CD2	1:A:398:PHE:C	2.89	0.45
1:A:270:ARG:NH1	1:A:273:GLU:CG	2.79	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: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:A:42:VAL:HG12	1:A:43:ILE:N	2.31	0.45
1:A:42:VAL:HG23	1:A:204:PRO:HG3	1.98	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:227:ILE:CG2	1:X:228:ASN:H	2.30	0.45
1:X:433:LEU:HA	1:X:434:PRO:HD3	1.59	0.45
1:X:63:PHE:CZ	1:X:67:VAL:HG21	2.52	0.45
1:A:14:GLN:HA	1:A:14:GLN:NE2	2.32	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:270:ARG:NH1	1:A:273:GLU:HG2	2.30	0.45
1:A:13:VAL:CG2	1:A:29:LEU:HD12	2.47	0.45
1:A:292:GLU:CG	1:A:368:LEU:HD11	2.46	0.45
1:X:423:VAL:O	1:X:424:ALA:C	2.55	0.45
1:A:383:LEU:O	1:A:384:ILE:HD12	2.17	0.45
1:A:19:MET:HB3	1:X:21:ASP:H	1.82	0.45
1:A:423:VAL:CG1	1:A:427:VAL:HG23	2.47	0.45
1:A:423:VAL:HG13	1:A:427:VAL:HG23	1.99	0.45
1:A:15:LEU:HD21	1:X:16:LEU:CA	2.47	0.45
1:X:42:VAL:HG23	1:X:204:PRO:HG3	1.93	0.45
1:A:231:THR:OG1	1:A:232:ASP:OD1	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:265:SER:O	1:X:266:VAL:HG23	2.16	0.44
1:A:405:VAL:HG11	1:A:431:PHE:CE2	2.51	0.44
1:X:124:ILE:HG21	1:X:131:ALA:HB2	1.99	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:423:VAL:HG13	1:X:427:VAL:HG23	1.98	0.44
1:X:40:PHE:CE1	1:X:69:LEU:CD2	3.00	0.44
1:X:83:ALA:O	1:X:87:ALA:HB3	2.17	0.44
1:A:257:LEU:HA	1:A:257:LEU:HD23	1.77	0.44
1:A:401:CYS:HB2	1:A:414:TRP:O	2.17	0.44
1:A:42:VAL:C	1:A:43:ILE:CG1	2.84	0.44
1:A:86:GLU:HA	1:A:91:PRO:HG3	2.00	0.44
1:A:85:LEU:CD2	1:A:108:ILE:HG13	2.47	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:156:ARG:O	1:A:156:ARG:HG2	2.17	0.44
1:A:265:SER:HB2	1:A:287:LEU:HD11	1.99	0.44
1:X:189:ILE:CG2	1:X:193:VAL:CG2	2.96	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: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:44:LYS:HE2	1:A:191:ALA:HB3	2.00	0.44
1:A:398:PHE:CD2	1:A:398:PHE:O	2.70	0.44
1:A:398:PHE:CE1	1:X:398:PHE:CD1	2.79	0.44
1:A:409:GLU:OE1	1:A:410:TRP:CD1	2.70	0.44
1:X:351:TRP:CD1	1:X:426:VAL:HB	2.50	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:A:89:ASP:C	1:A:91:PRO:HD3	2.36	0.44
1:X:340:ARG:CA	1:X:360:LEU:HD12	2.48	0.44
1:A:270:ARG:HH11	1:A:273:GLU:HG2	1.82	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:328:LEU:HD11	1:A:346:THR:HG22	2.00	0.44
1:X:74:VAL:HG12	1:X:75:HIS:N	2.32	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:299:ASP:OD1	1:X:301:SER:OG	2.30	0.43
1:X:32:PHE:CE1	1:X:40:PHE:HD1	2.36	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:A:44:LYS:CG	1:A:45:VAL:N	2.79	0.43
1:X:37:GLN:CD	1:X:168:ARG:HG3	2.38	0.43
1:A:356:LYS:HE2	1:A:436:THR:OG1	2.18	0.43
1:A:9:ARG:HH22	1:A:33:SER:HB2	1.80	0.43
1:A:15:LEU:HD21	1:X:15:LEU:O	2.19	0.43
1:X:257:LEU:HA	1:X:257:LEU:HD23	1.76	0.43
1:X:83:ALA:O	1:X:87:ALA:CB	2.66	0.43
1:A:132:ALA:N	1:A:171:GLN:HB3	2.33	0.43
1:X:26:ARG:HG2	1:X:30:HIS:NE2	2.33	0.43
1:X:427:VAL:O	1:X:430:ALA:N	2.52	0.43
1:X:90:ILE:N	1:X:91:PRO:HD3	2.33	0.43
1:X:411:THR:HG22	1:X:413:PHE:CD2	2.52	0.43
1:X:44:LYS:O	1:X:45:VAL:HG12	2.19	0.43
1:X:51:GLN:HB2	1:X:80:GLN:CD	2.39	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:A:78:GLY:O	1:A:82:ASP:CG	2.57	0.43
1:X:78:GLY:O	1:X: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:212:GLY:O	1:A:213:THR:C	2.57	0.42
1:A:67:VAL:HG23	1:A:69:LEU:HG	1.98	0.42
1:A:85:LEU:HD21	1:A:108:ILE:CG1	2.49	0.42
1:X:212:GLY:O	1:X:213:THR:C	2.57	0.42
1:X:299:ASP:OD2	1:X:302:SER:HB3	2.19	0.42
1:A:120:LEU:O	1:A:124:ILE:N	2.51	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:327:ARG:HE	1:A:327:ARG:HB2	1.56	0.42
1:A:356:LYS:HA	1:A:356:LYS:HD3	1.64	0.42
1:X:42:VAL:HG12	1:X:43:ILE:H	1.84	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: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:A:19:MET:HE2	1:X:19:MET:CB	2.50	0.42
1:X:232:ASP:HB3	1:X:236:LEU:HD21	1.92	0.42
1:X:423:VAL:CG1	1:X:427:VAL:HG23	2.50	0.42
1:A:159:HIS:HB3	1:A:161:ASP:OD2	2.19	0.42
1:A:91:PRO:O	1:A:91:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:297:THR:C	1:X:332:ARG:NH1	2.72	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:35:ILE:O	1:X:36:ASP:C	2.57	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:44:LYS:N	1:A:208:VAL:O	2.51	0.42
1:A:93:GLU:HG3	1:A:93:GLU:H	1.42	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:A:44:LYS:HG2	1:A:209:PHE:HD1	1.85	0.42
1:X:81:LEU:HD11	1:X:99:ARG:NH1	2.35	0.42
1:A:141:ALA:O	1:A:181:THR:HG22	2.20	0.41
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.88	0.41
1:A:328:LEU:HD21	1:A:330:VAL:CG2	2.49	0.41
1:A:315:ALA:HB3	1:A:358:ALA:HB1	2.02	0.41
1:X:158:ILE:N	1:X:158:ILE:HD13	2.30	0.41
1:A:15:LEU:HD21	1:X:16:LEU:HA	2.02	0.41
1:X:327:ARG:HE	1:X:327:ARG:HB2	1.56	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:304:ASP:OD1	1:A:307:ARG:HB2	2.20	0.41
1:A:95:VAL:H	1:A:100:VAL:HG11	1.65	0.41
1:X:173:ALA:O	1:X:174:ILE:HD13	2.19	0.41
1:X:262:LEU:O	1:X:264:SER:N	2.52	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:106:ILE:HD12	1:X:151:ARG:NH1	2.35	0.41
1:X:412:VAL:HG23	1:X:431:PHE:CD1	2.55	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:118:LEU:O	1:A:119:ALA:C	2.57	0.41
1:A:75:HIS:HE2	1:A:176:ALA:HB2	1.84	0.41
1:A:231:THR:CG2	1:A:293:ARG:HA	2.51	0.41
1:A:411:THR:HG21	1:A:413:PHE:CE2	2.55	0.41
1:X:190:ASN:C	1:X:190:ASN:OD1	2.58	0.41
1:X:332:ARG:HG3	1:X:333:ALA:H	1.84	0.41
1:X:42:VAL:CG1	1:X:43:ILE:H	2.34	0.41
1:A:155:PRO:HG2	1:A:193:VAL:HG23	2.01	0.41
1:A:265:SER:HB2	1:A:287:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:TYR:CZ	1:A:205:TYR:HE2	2.37	0.41
1:A:64:LEU:HD12	1:A:71:PRO:CG	2.39	0.41
1:A:47:GLY:CA	1:A:78:GLY:H	2.32	0.41
1:A:91:PRO:O	1:A:92:THR:HG23	2.20	0.41
1:X:383:LEU:HD12	1:X:384:ILE:N	2.36	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:A:266:VAL:O	1:A:288:ILE:N	2.54	0.41
1:X:196:ARG:CD	1:X:255:ARG:HD2	2.43	0.41
1:A:9:ARG:O	1:A:10:GLN:C	2.59	0.41
1:A:117:ASN:OD1	1:A:176:ALA:HB2	2.21	0.41
1:A:340:ARG:HA	1:A:360:LEU:HD12	2.01	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:X:231:THR:OG1	1:X:232:ASP:OD1	2.29	0.41
1:X:289:ARG:HE	1:X:366:GLU:HG2	1.85	0.41
1:X:32:PHE:C	1:X:34:GLY:N	2.74	0.41
1:X:331:ASP:HB2	1:X:347:ARG:HG3	2.02	0.41
1:A:154:GLU:HA	1:A:155:PRO:HD3	1.84	0.41
1:A:28:TYR:CZ	1:A:205:TYR:CD2	3.08	0.41
1:X:132:ALA:N	1:X:171:GLN:HB3	2.35	0.41
1:X:26:ARG:O	1:X:30:HIS:CD2	2.73	0.41
1:X:24:GLU:HG2	1:X:28:TYR:HD2	1.86	0.41
1:X:340:ARG:HB3	1:X:360:LEU:HD12	2.02	0.41
1:X:354:LEU:HB3	1:X:385:TRP:HB2	2.01	0.41
1:A:106:ILE:HD12	1:A:151:ARG:NH1	2.35	0.41
1:A:253:ILE:HD12	1:A:288:ILE:HD12	2.03	0.41
1:A:273:GLU:OE1	1:A:284:SER:CB	2.69	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:121:VAL:O	1:X:124:ILE:HB	2.20	0.41
1:X:254:LYS:O	1:X:258:ASP:N	2.49	0.41
1:X:270:ARG:HH11	1:X:273:GLU:HG2	1.86	0.41
1:X:32:PHE:HD1	1:X:32:PHE:O	2.03	0.41
1:X:353:TYR:CE2	1:X:354:LEU:O	2.74	0.41
1:X:57:LEU:HG	1:X:61:LEU:HD11	2.03	0.41
1:A:255:ARG:HD3	1:A:255:ARG:HH11	1.73	0.41
1:A:348:LEU:O	1:A:351:TRP:N	2.54	0.41
1:A:353:TYR:CE2	1:A:355:ASP:CA	3.00	0.41
1:X:336:THR:O	1:X:338:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:81:LEU:CD1	1:X:99:ARG:NH1	2.81	0.41
1:A:120:LEU:C	1:A:120:LEU:HD12	2.41	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:262:LEU:C	1:A:264:SER:N	2.74	0.40
1:A:91:PRO:O	1:A:91:PRO:CD	2.69	0.40
1:X:40:PHE:CE1	1:X:69:LEU:HA	2.56	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:376:LEU:HG	1:A:376:LEU:O	2.19	0.40
1:A:394:ASN:HA	1:A:397:TYR:CD2	2.56	0.40
1:A:403:GLY:HA3	1:A:414:TRP:CD2	2.57	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: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:81:LEU:CD1	1:A:99:ARG:NH2	2.80	0.40
1:X:243:ASN:O	1:X:244:GLY:C	2.59	0.40
1:X:32:PHE:CD1	1:X:32:PHE:O	2.75	0.40
1:X:405:VAL:HG12	1:X:431:PHE:CZ	2.56	0.40
1:X:65:GLN:HG3	1:X:66:THR:N	2.36	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	435/461 (94%)	360 (83%)	46 (11%)	29 (7%)	1	18
1	X	433/461 (94%)	349 (81%)	57 (13%)	27 (6%)	1	19
All	All	868/922 (94%)	709 (82%)	103 (12%)	56 (6%)	1	18

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%)	7	27
1	X	344/367 (94%)	311 (90%)	33 (10%)	8	30
All	All	690/734 (94%)	621 (90%)	69 (10%)	8	28

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%)	0.30	29 (6%) 17 15	185, 422, 690, 893	0
1	X	435/461 (94%)	0.42	46 (10%) 6 6	209, 472, 685, 784	0
All	All	871/922 (94%)	0.36	75 (8%) 10 9	185, 455, 688, 893	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	VAL	16.2
1	A	5	ALA	12.0
1	A	17	SER	11.9
1	X	342	ALA	10.7
1	A	18	HIS	10.5
1	X	358	ALA	10.3
1	A	7	GLY	8.9
1	X	267	SER	8.4
1	X	187	VAL	6.8
1	X	357	PHE	6.6
1	X	20	ARG	6.6
1	X	10	GLN	6.2
1	A	14	GLN	6.1
1	X	341	ALA	5.7
1	X	22	GLY	5.6
1	X	268	ILE	5.6
1	A	12	ILE	5.5
1	X	19	MET	5.2
1	A	15	LEU	4.8
1	X	21	ASP	4.8
1	X	286	THR	4.6
1	A	9	ARG	4.5
1	X	179	GLY	4.4
1	X	66	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	X	343	ALA	4.3
1	A	6	PRO	4.3
1	X	285	GLY	4.2
1	A	10	GLN	4.1
1	X	9	ARG	4.1
1	X	287	LEU	4.0
1	A	19	MET	4.0
1	X	359	VAL	3.9
1	X	227	ILE	3.7
1	A	334	PHE	3.7
1	X	25	ILE	3.6
1	X	104	GLU	3.5
1	A	434	PRO	3.4
1	A	16	LEU	3.4
1	X	319	PRO	3.4
1	X	178	LEU	3.3
1	A	296	ALA	3.2
1	A	11	THR	3.2
1	A	297	THR	3.2
1	X	180	GLU	3.0
1	X	18	HIS	3.0
1	A	433	LEU	2.9
1	A	333	ALA	2.9
1	A	13	VAL	2.9
1	X	277	GLU	2.9
1	A	437	LEU	2.8
1	X	288	ILE	2.8
1	A	408	ASP	2.8
1	A	318	ARG	2.7
1	X	103	ASP	2.7
1	X	418	MET	2.7
1	X	333	ALA	2.6
1	X	105	ALA	2.6
1	A	66	THR	2.6
1	X	16	LEU	2.4
1	X	186	LEU	2.3
1	X	62	ALA	2.3
1	X	15	LEU	2.3
1	X	189	ILE	2.3
1	X	246	MET	2.2
1	A	20	ARG	2.2
1	A	343	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	318	ARG	2.1
1	X	278	LEU	2.1
1	X	226	SER	2.1
1	A	94	ARG	2.1
1	X	289	ARG	2.1
1	X	177	CYS	2.1
1	X	209	PHE	2.0
1	X	188	ASN	2.0
1	A	99	ARG	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.