



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:45 PM UTC

PDB ID : 2R3V / pdb_00002r3v
Title : The Biochemical and Structural Basis for Feedback Inhibition of Mevalonate Kinase and Isoprenoid Metabolism
Authors : Fu, Z.; Voynova, N.E.; Mizioro, H.M.; Kim, J.P.
Deposited on : 2007-08-30
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

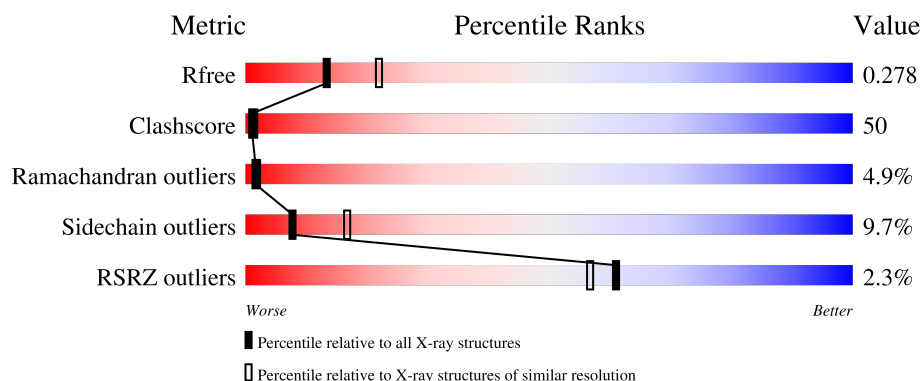
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of 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	396	2% 37% 52% 9% ..
1	B	396	% 36% 48% 13% ..
1	C	396	4% 35% 52% 11% .
1	D	396	2% 35% 55% 7% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11935 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 Mevalonate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2933	1849	519	552	13			
1	B	388	Total	C	N	O	S	0	0	0
			2918	1838	517	550	13			
1	C	390	Total	C	N	O	S	0	0	0
			2933	1849	519	552	13			
1	D	389	Total	C	N	O	S	0	0	0
			2926	1844	518	551	13			

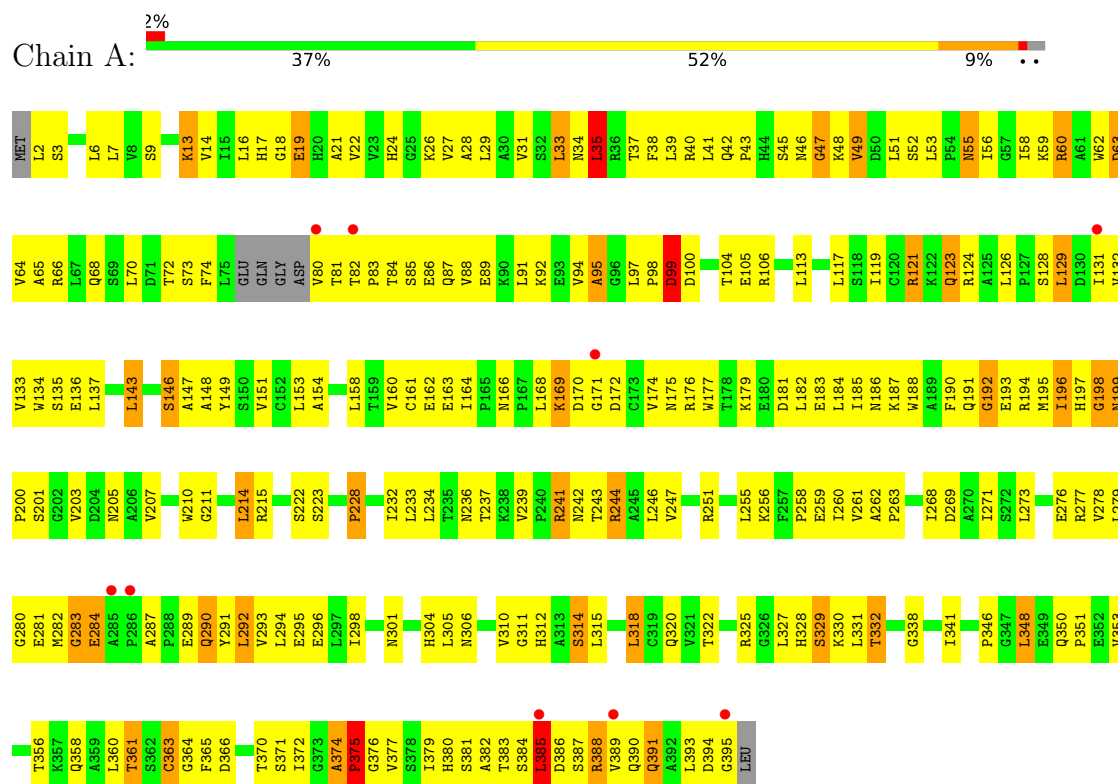
- Molecule 2 is water.

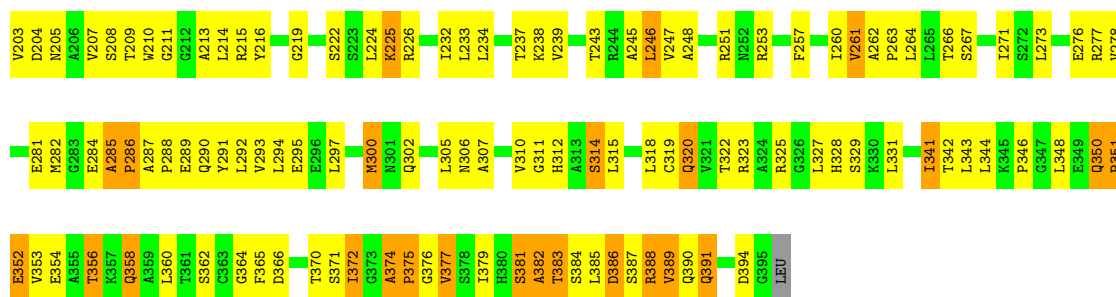
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		
2	B	63	Total	O	0	0
			63	63		
2	C	45	Total	O	0	0
			45	45		
2	D	45	Total	O	0	0
			45	45		

3 Residue-property plots

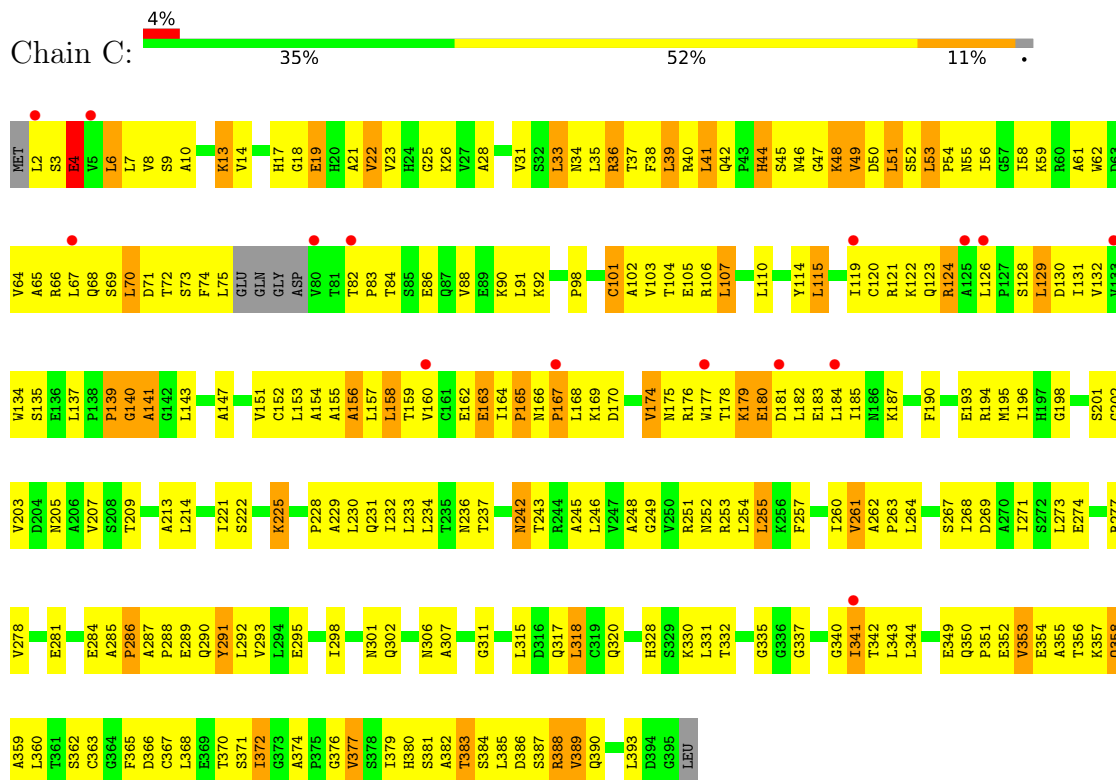
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Mevalonate kinase

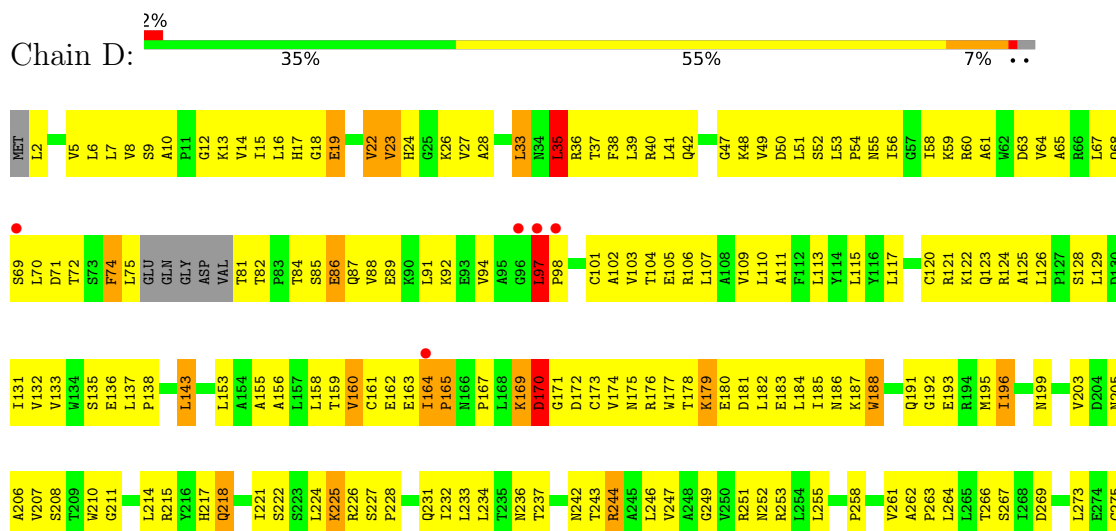


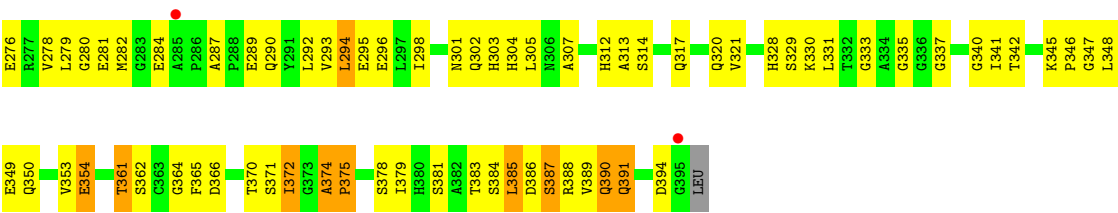


• Molecule 1: Mevalonate kinase



• Molecule 1: Mevalonate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.03Å 78.20Å 109.45Å 90.00° 113.33° 90.00°	Depositor
Resolution (Å)	29.37 – 2.50 29.37 – 2.50	Depositor EDS
% Data completeness (in resolution range)	84.1 (29.37-2.50) 84.1 (29.37-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.282 0.236 , 0.278	Depositor DCC
R_{free} test set	3916 reflections (8.45%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11935	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6120e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.51	0/2983	1.05	15/4055 (0.4%)
1	B	0.50	0/2968	1.01	16/4034 (0.4%)
1	C	0.44	0/2983	0.97	13/4055 (0.3%)
1	D	0.45	0/2976	0.99	11/4045 (0.3%)
All	All	0.48	0/11910	1.00	55/16189 (0.3%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	387	SER	N-CA-C	-10.19	101.52	112.93
1	D	97	LEU	N-CA-C	9.72	123.14	110.40
1	D	35	LEU	N-CA-C	-9.41	95.75	109.11
1	A	35	LEU	N-CA-C	-8.08	97.63	109.11
1	A	148	ALA	N-CA-C	-8.03	102.61	111.36
1	D	36	ARG	N-CA-C	7.85	120.72	110.43
1	C	383	THR	N-CA-C	-7.67	101.00	112.04
1	B	374	ALA	CA-C-N	7.38	129.07	119.84
1	B	374	ALA	C-N-CA	7.38	129.07	119.84
1	B	191	GLN	N-CA-C	-7.34	103.28	111.28
1	B	36	ARG	N-CA-C	7.32	120.02	110.43
1	C	363	CYS	N-CA-C	-7.29	103.98	113.17
1	B	72	THR	N-CA-C	7.00	125.70	110.80
1	C	291	TYR	N-CA-C	-6.82	104.82	113.01
1	A	363	CYS	N-CA-C	-6.53	104.71	114.64
1	C	261	VAL	N-CA-C	6.49	116.63	110.53
1	C	163	GLU	N-CA-C	-6.28	105.77	113.50
1	C	53	LEU	CA-C-N	6.26	125.75	119.24
1	C	53	LEU	C-N-CA	6.26	125.75	119.24
1	B	261	VAL	N-CA-C	6.25	116.42	110.42
1	D	196	ILE	N-CA-C	6.07	117.10	111.45
1	C	317	GLN	N-CA-C	-6.05	104.60	111.07
1	D	97	LEU	CA-C-N	5.89	125.89	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	97	LEU	C-N-CA	5.89	125.89	119.89
1	D	386	ASP	N-CA-C	-5.84	106.24	113.19
1	A	136	GLU	N-CA-C	-5.79	106.22	113.28
1	A	196	ILE	N-CA-C	5.75	116.50	111.56
1	A	353	VAL	N-CA-C	-5.72	103.77	111.44
1	A	374	ALA	CA-C-N	5.56	126.79	119.84
1	A	374	ALA	C-N-CA	5.56	126.79	119.84
1	B	35	LEU	N-CA-C	-5.52	101.92	109.71
1	D	296	GLU	N-CA-C	-5.50	105.39	111.71
1	C	388	ARG	N-CA-C	-5.49	107.23	114.04
1	C	229	ALA	N-CA-C	-5.49	100.75	109.59
1	A	163	GLU	N-CA-C	-5.47	105.70	112.38
1	B	53	LEU	CA-C-N	5.45	124.90	119.24
1	B	53	LEU	C-N-CA	5.45	124.90	119.24
1	A	391	GLN	N-CA-C	-5.39	105.48	111.36
1	A	364	GLY	N-CA-C	-5.38	106.26	115.08
1	A	45	SER	N-CA-C	-5.36	105.88	112.90
1	D	85	SER	N-CA-C	-5.36	106.25	112.89
1	B	109	VAL	N-CA-C	5.31	115.41	110.42
1	B	152	CYS	N-CA-C	-5.23	105.49	111.14
1	A	192	GLY	N-CA-C	-5.19	106.50	112.73
1	B	163	GLU	N-CA-C	-5.17	106.93	113.18
1	A	104	THR	N-CA-C	5.15	116.58	111.07
1	D	128	SER	N-CA-C	-5.13	101.34	109.96
1	A	27	VAL	N-CA-C	5.11	115.44	107.99
1	B	271	ILE	N-CA-C	-5.09	105.75	110.53
1	C	44	HIS	N-CA-C	-5.09	104.54	111.56
1	B	285	ALA	CA-C-N	5.08	126.19	119.84
1	B	285	ALA	C-N-CA	5.08	126.19	119.84
1	C	6	LEU	N-CA-C	5.06	117.86	109.46
1	D	354	GLU	N-CA-C	-5.05	106.28	112.90
1	B	4	GLU	N-CA-C	-5.00	107.57	113.97

There are no chirality outliers.

There are no planarity outliers.

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	2933	0	3003	294	0
1	B	2918	0	2983	292	0
1	C	2933	0	3003	315	0
1	D	2926	0	2994	289	0
2	A	72	0	0	7	0
2	B	63	0	0	5	0
2	C	45	0	0	4	0
2	D	45	0	0	5	0
All	All	11935	0	11983	1173	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 50.

All (1173) 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:C:119:ILE:HD11	1:C:158:LEU:HD13	1.27	1.08
1:C:50:ASP:HB2	1:C:130:ASP:HA	1.33	1.06
1:C:52:SER:HB3	1:C:132:VAL:HG22	1.35	1.06
1:B:232:ILE:HG12	1:B:372:ILE:HD13	1.36	1.04
1:A:52:SER:HB3	1:A:132:VAL:HG22	1.40	1.03
1:B:68:GLN:O	1:B:70:LEU:HD22	1.62	1.00
1:D:158:LEU:HD23	1:D:185:ILE:HD13	1.41	0.99
1:B:82:THR:HB	1:B:86:GLU:HB2	1.44	0.98
1:A:388:ARG:H	1:A:388:ARG:HE	1.02	0.97
1:B:115:LEU:HD23	1:B:153:LEU:HB3	1.43	0.96
1:C:386:ASP:HB2	1:C:389:VAL:HG23	1.47	0.96
1:B:55:ASN:HD21	1:B:135:SER:H	1.04	0.94
1:C:7:LEU:O	1:C:379:ILE:HD12	1.66	0.94
1:A:7:LEU:HD23	1:A:380:HIS:HB2	1.50	0.93
1:C:119:ILE:HD11	1:C:158:LEU:CD1	1.97	0.93
1:D:52:SER:HB3	1:D:132:VAL:HG22	1.50	0.93
1:D:164:ILE:HD11	1:D:181:ASP:CG	1.93	0.92
1:C:66:ARG:O	1:C:70:LEU:HD23	1.69	0.92
1:B:388:ARG:HH21	1:B:391:GLN:HG3	1.34	0.92
1:B:164:ILE:HD11	1:B:177:TRP:HD1	1.32	0.92
1:C:56:ILE:HG22	1:C:58:ILE:HG23	1.52	0.91
1:C:233:LEU:HD13	1:C:344:LEU:HD21	1.52	0.91
1:B:70:LEU:HG	1:B:72:THR:CG2	2.00	0.90
1:B:39:LEU:HD11	1:B:153:LEU:HD12	1.54	0.90
1:B:67:LEU:O	1:B:70:LEU:HD13	1.72	0.88
1:A:58:ILE:HD13	1:A:105:GLU:HB2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LEU:HD23	1:C:185:ILE:HD12	1.55	0.88
1:D:107:LEU:HD22	1:D:196:ILE:HG23	1.52	0.87
1:A:40:ARG:HH22	1:A:390:GLN:NE2	1.72	0.87
1:A:260:ILE:HG21	1:B:300:MET:HE3	1.56	0.87
1:B:211:GLY:HA3	1:B:375:PRO:O	1.75	0.87
1:B:39:LEU:HG	1:B:133:VAL:HG22	1.55	0.86
1:C:84:THR:HG22	1:C:86:GLU:H	1.39	0.86
1:B:287:ALA:HB3	1:B:290:GLN:HG3	1.57	0.86
1:B:122:LYS:H	1:B:122:LYS:HD3	1.41	0.85
1:C:6:LEU:HD13	1:C:379:ILE:HD11	1.58	0.85
1:B:33:LEU:HD11	1:B:234:LEU:HD22	1.57	0.85
1:C:385:LEU:HD23	1:C:390:GLN:HB2	1.57	0.85
1:B:13:LYS:HB2	1:B:207:VAL:HG11	1.58	0.84
1:C:141:ALA:HB3	1:C:143:LEU:HD23	1.57	0.84
1:D:243:THR:O	1:D:247:VAL:HG23	1.78	0.84
1:A:84:THR:HG22	1:A:86:GLU:H	1.40	0.83
1:A:175:ASN:HD22	1:A:176:ARG:H	1.25	0.83
1:A:386:ASP:HB2	1:A:389:VAL:HG23	1.60	0.83
1:D:39:LEU:HD21	1:D:131:ILE:HG23	1.59	0.83
1:A:81:THR:HA	1:A:194:ARG:NH1	1.91	0.83
1:A:39:LEU:HD11	1:A:153:LEU:HD23	1.58	0.83
1:C:53:LEU:HD12	1:C:58:ILE:HD11	1.61	0.82
1:A:385:LEU:CD2	1:A:389:VAL:HG11	2.10	0.82
1:A:385:LEU:HD23	1:A:389:VAL:HG11	1.61	0.82
1:B:164:ILE:HD11	1:B:177:TRP:CD1	2.14	0.82
1:D:12:GLY:HA2	1:D:137:LEU:HD11	1.60	0.82
1:B:164:ILE:HD13	1:B:165:PRO:N	1.95	0.81
1:B:70:LEU:HD23	1:B:70:LEU:O	1.79	0.81
1:D:37:THR:HG23	1:D:135:SER:HB2	1.62	0.81
1:D:49:VAL:HG23	1:D:64:VAL:HG12	1.62	0.81
1:D:388:ARG:HE	1:D:389:VAL:HG23	1.45	0.81
1:C:180:GLU:CD	1:C:180:GLU:H	1.88	0.81
1:D:12:GLY:CA	1:D:137:LEU:HD11	2.11	0.81
1:D:40:ARG:HD2	1:D:394:ASP:HB3	1.63	0.81
1:D:50:ASP:HB3	1:D:61:ALA:HB2	1.63	0.80
1:D:97:LEU:HB3	1:D:98:PRO:HD2	1.62	0.80
1:D:53:LEU:HD12	1:D:58:ILE:HD11	1.60	0.80
1:B:55:ASN:ND2	1:B:135:SER:H	1.79	0.79
1:C:225:LYS:HB2	1:C:225:LYS:HZ2	1.48	0.79
1:B:155:ALA:HA	1:B:185:ILE:HD12	1.64	0.79
1:D:39:LEU:HD11	1:D:153:LEU:HD23	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LEU:HA	1:B:169:LYS:HG3	1.65	0.79
1:C:350:GLN:HE21	1:C:354:GLU:HG2	1.48	0.78
1:A:60:ARG:HB2	1:A:60:ARG:NH1	1.99	0.78
1:B:55:ASN:HD21	1:B:135:SER:N	1.80	0.78
1:D:164:ILE:HD12	1:D:177:TRP:HD1	1.46	0.78
1:B:233:LEU:HD13	1:B:344:LEU:HD11	1.64	0.78
1:A:262:ALA:HB3	1:A:263:PRO:HD3	1.66	0.78
1:A:268:ILE:HD11	1:A:304:HIS:CB	2.13	0.78
1:A:46:ASN:HD21	1:A:48:LYS:HB2	1.48	0.77
1:A:374:ALA:HB1	1:A:375:PRO:HD2	1.67	0.77
1:A:84:THR:HG22	1:A:86:GLU:N	1.99	0.77
1:C:207:VAL:HG22	1:C:214:LEU:HD22	1.65	0.77
1:A:46:ASN:ND2	1:A:48:LYS:HB2	1.99	0.77
1:B:158:LEU:C	1:B:164:ILE:HG22	2.10	0.77
1:A:56:ILE:HG22	1:A:58:ILE:HG23	1.67	0.77
1:A:168:LEU:O	1:A:170:ASP:N	2.17	0.77
1:D:6:LEU:HB2	1:D:41:LEU:CD2	2.15	0.77
1:D:33:LEU:HD11	1:D:234:LEU:HD22	1.66	0.76
1:A:199:ASN:C	1:A:199:ASN:HD22	1.93	0.76
1:D:388:ARG:NE	1:D:389:VAL:HG23	2.00	0.76
1:A:81:THR:HA	1:A:194:ARG:HH11	1.46	0.76
1:A:40:ARG:HH22	1:A:390:GLN:HE21	1.31	0.76
1:A:97:LEU:HD13	1:A:106:ARG:HG3	1.68	0.76
1:B:119:ILE:O	1:B:122:LYS:HE2	1.86	0.76
1:A:287:ALA:H	1:A:290:GLN:NE2	1.83	0.75
1:A:147:ALA:HB2	1:A:193:GLU:OE2	1.86	0.75
1:B:12:GLY:HA3	1:B:137:LEU:HD11	1.69	0.75
1:A:84:THR:HB	1:A:87:GLN:HG3	1.69	0.75
1:C:147:ALA:O	1:C:151:VAL:HG23	1.87	0.75
1:D:244:ARG:H	1:D:244:ARG:NE	1.83	0.75
1:D:164:ILE:HD11	1:D:181:ASP:CB	2.17	0.75
1:D:251:ARG:O	1:D:255:LEU:HD23	1.87	0.74
1:A:35:LEU:O	1:A:137:LEU:HG	1.87	0.74
1:C:47:GLY:O	1:C:48:LYS:HG2	1.87	0.74
1:C:175:ASN:HD22	1:C:176:ARG:H	1.35	0.74
1:C:278:VAL:HG21	1:C:293:VAL:HG11	1.69	0.74
1:C:41:LEU:HD12	1:C:156:ALA:HB1	1.70	0.74
1:D:68:GLN:OE1	1:D:125:ALA:HB1	1.88	0.74
1:D:181:ASP:O	1:D:185:ILE:HG12	1.85	0.74
1:D:317:GLN:O	1:D:321:VAL:HG23	1.88	0.74
1:A:40:ARG:NH2	1:A:390:GLN:HE21	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ILE:HD11	1:D:181:ASP:HB3	1.70	0.74
1:D:164:ILE:HD13	1:D:165:PRO:CD	2.18	0.74
1:B:164:ILE:CD1	1:B:177:TRP:CD1	2.71	0.74
1:A:244:ARG:HD2	1:C:289:GLU:HG2	1.69	0.74
1:B:183:GLU:O	1:B:187:LYS:HG2	1.88	0.74
1:D:88:VAL:O	1:D:92:LYS:HB2	1.88	0.74
1:B:176:ARG:NH1	1:D:89:GLU:HG2	2.03	0.73
1:B:295:GLU:HB3	1:B:328:HIS:CD2	2.24	0.73
1:D:164:ILE:HD12	1:D:177:TRP:CD1	2.23	0.73
1:D:289:GLU:O	1:D:293:VAL:HG23	1.88	0.73
1:C:295:GLU:HB3	1:C:328:HIS:ND1	2.04	0.73
1:B:388:ARG:NH2	1:B:391:GLN:HG3	2.03	0.73
1:A:129:LEU:HD13	1:A:131:ILE:HD11	1.71	0.72
1:C:284:GLU:C	1:C:286:PRO:HD3	2.13	0.72
1:A:33:LEU:HD21	1:A:370:THR:HG21	1.71	0.72
1:B:158:LEU:O	1:B:164:ILE:HG22	1.87	0.72
1:A:241:ARG:HG2	1:A:241:ARG:HH11	1.55	0.72
1:C:193:GLU:HG3	1:C:205:ASN:HD22	1.53	0.72
1:D:105:GLU:O	1:D:109:VAL:HG23	1.90	0.72
1:C:332:THR:CG2	1:C:341:ILE:HD13	2.18	0.72
1:C:83:PRO:HG3	1:C:198:GLY:HA2	1.70	0.72
1:B:233:LEU:HB2	1:B:342:THR:HB	1.70	0.71
1:B:385:LEU:HB3	1:B:389:VAL:HG11	1.72	0.71
1:D:180:GLU:CD	1:D:180:GLU:H	1.98	0.71
1:A:22:VAL:HG11	1:A:28:ALA:HB2	1.72	0.71
1:A:41:LEU:C	1:A:41:LEU:HD23	2.15	0.71
1:C:41:LEU:HD13	1:C:160:VAL:HG21	1.73	0.71
1:D:164:ILE:HD11	1:D:181:ASP:OD1	1.90	0.71
1:D:231:GLN:NE2	1:D:371:SER:HB3	2.06	0.71
1:A:129:LEU:CD1	1:A:131:ILE:HD11	2.21	0.71
1:A:196:ILE:HG13	1:A:197:HIS:N	2.03	0.71
1:D:70:LEU:CD2	1:D:94:VAL:HG11	2.20	0.71
1:A:298:ILE:HG23	1:A:330:LYS:HB3	1.73	0.70
1:B:209:THR:HA	1:B:377:VAL:HG23	1.73	0.70
1:C:233:LEU:CD1	1:C:344:LEU:HD21	2.20	0.70
1:C:39:LEU:C	1:C:39:LEU:HD23	2.17	0.70
1:D:233:LEU:HB3	1:D:342:THR:HB	1.73	0.70
1:C:187:LYS:HD3	1:C:187:LYS:C	2.16	0.70
1:B:70:LEU:HG	1:B:72:THR:HG21	1.72	0.70
1:D:278:VAL:O	1:D:282:MET:HG3	1.92	0.70
1:C:51:LEU:O	1:C:59:LYS:HD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:SER:HA	1:D:37:THR:O	1.92	0.70
1:B:352:GLU:O	1:B:356:THR:HG23	1.92	0.69
1:C:121:ARG:HG3	1:C:122:LYS:H	1.57	0.69
1:D:207:VAL:HG22	1:D:214:LEU:HD12	1.73	0.69
1:A:22:VAL:CG1	1:A:28:ALA:HB2	2.22	0.69
1:D:51:LEU:HD21	1:D:53:LEU:HD21	1.72	0.69
1:B:112:PHE:HE1	1:B:131:ILE:HD12	1.54	0.69
1:D:6:LEU:HB2	1:D:41:LEU:HD21	1.74	0.69
1:D:203:VAL:O	1:D:207:VAL:HG23	1.92	0.69
1:D:236:ASN:HB3	1:D:366:ASP:HB2	1.72	0.69
1:B:233:LEU:CD1	1:B:344:LEU:HD11	2.23	0.69
1:B:348:LEU:HD21	2:B:431:HOH:O	1.93	0.69
1:A:13:LYS:HG2	1:A:14:VAL:N	2.07	0.69
1:A:117:LEU:O	1:A:121:ARG:HB2	1.93	0.69
1:A:73:SER:HA	1:A:121:ARG:HH22	1.58	0.69
1:D:86:GLU:O	1:D:89:GLU:HB3	1.93	0.69
1:D:22:VAL:HG13	1:D:28:ALA:HB2	1.73	0.69
1:C:41:LEU:HG	1:C:131:ILE:HG12	1.75	0.68
1:C:52:SER:HB3	1:C:132:VAL:CG2	2.20	0.68
1:A:360:LEU:O	1:A:365:PHE:HB2	1.93	0.68
1:B:176:ARG:HH11	1:D:89:GLU:HG2	1.58	0.68
1:C:154:ALA:O	1:C:158:LEU:HD22	1.93	0.68
1:C:232:ILE:HG12	1:C:372:ILE:HD13	1.75	0.68
1:B:39:LEU:HG	1:B:133:VAL:CG2	2.22	0.68
1:C:35:LEU:HB3	1:C:137:LEU:HD23	1.74	0.68
1:C:65:ALA:O	1:C:68:GLN:HB3	1.94	0.68
1:D:75:LEU:HD12	1:D:75:LEU:H	1.57	0.68
1:C:33:LEU:HD11	1:C:234:LEU:HD22	1.76	0.68
1:A:175:ASN:HD22	1:A:176:ARG:N	1.92	0.68
1:B:262:ALA:HB3	1:B:263:PRO:HD3	1.76	0.67
1:C:175:ASN:HD22	1:C:176:ARG:N	1.92	0.67
1:B:86:GLU:HG2	1:B:90:LYS:HD2	1.75	0.67
1:C:34:ASN:HB2	1:C:374:ALA:HB2	1.76	0.67
1:C:332:THR:HG21	1:C:341:ILE:HD13	1.75	0.67
1:D:84:THR:OG1	1:D:87:GLN:HG3	1.95	0.67
1:A:26:LYS:HD2	1:A:269:ASP:HB2	1.77	0.67
1:B:2:LEU:HA	1:B:169:LYS:CG	2.25	0.67
1:C:236:ASN:HB3	1:C:366:ASP:HB2	1.77	0.67
1:D:70:LEU:HD21	1:D:94:VAL:HG11	1.77	0.67
1:B:237:THR:HA	1:B:365:PHE:CD2	2.28	0.67
1:D:282:MET:HG2	1:D:290:GLN:NE2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:NH2	1:B:307:ALA:O	2.28	0.67
1:C:7:LEU:HD11	1:C:382:ALA:HB2	1.77	0.67
1:B:176:ARG:HH21	1:B:176:ARG:HG3	1.60	0.67
1:C:331:LEU:C	1:C:331:LEU:HD12	2.20	0.67
1:B:88:VAL:HG12	1:B:92:LYS:HE3	1.75	0.66
1:A:70:LEU:HD21	1:A:94:VAL:HG22	1.77	0.66
1:A:331:LEU:C	1:A:331:LEU:HD12	2.19	0.66
1:C:176:ARG:HB2	1:C:176:ARG:NH1	2.09	0.66
1:C:356:THR:HG22	1:C:360:LEU:CD1	2.25	0.66
1:D:12:GLY:HA3	1:D:137:LEU:HD21	1.77	0.66
1:D:122:LYS:HD2	1:D:163:GLU:OE1	1.95	0.66
1:A:33:LEU:HD11	1:A:234:LEU:HD22	1.76	0.66
1:B:160:VAL:C	1:B:162:GLU:H	2.03	0.66
1:C:306:ASN:HD22	1:C:311:GLY:HA3	1.61	0.66
1:A:381:SER:O	1:A:383:THR:N	2.27	0.66
1:A:268:ILE:HD11	1:A:304:HIS:HB2	1.76	0.66
1:B:67:LEU:O	1:B:70:LEU:HB3	1.95	0.66
1:A:322:THR:HG22	1:A:327:LEU:O	1.94	0.66
1:C:306:ASN:ND2	1:C:311:GLY:HA3	2.11	0.66
1:D:59:LYS:O	1:D:60:ARG:HG3	1.95	0.66
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.61	0.66
1:B:33:LEU:HD23	1:B:372:ILE:CD1	2.26	0.66
1:A:215:ARG:NH1	1:A:276:GLU:OE1	2.29	0.65
1:B:39:LEU:HD11	1:B:153:LEU:CD1	2.22	0.65
1:D:70:LEU:HG	1:D:72:THR:HG23	1.76	0.65
1:A:174:VAL:HG12	1:A:380:HIS:ND1	2.11	0.65
1:A:268:ILE:HD11	1:A:304:HIS:HB3	1.77	0.65
1:B:168:LEU:HD23	1:B:172:ASP:OD1	1.96	0.65
1:D:298:ILE:HG23	1:D:330:LYS:HB3	1.78	0.65
1:C:48:LYS:H	1:C:128:SER:CB	2.09	0.65
1:D:33:LEU:HD21	1:D:370:THR:HG21	1.79	0.65
1:B:121:ARG:HB3	1:B:121:ARG:HH21	1.61	0.65
1:A:322:THR:HG23	1:A:327:LEU:HB2	1.79	0.65
1:B:331:LEU:C	1:B:331:LEU:HD12	2.22	0.65
1:D:224:LEU:HB3	1:D:227:SER:HB2	1.79	0.65
1:B:158:LEU:HD21	1:B:184:LEU:HG	1.79	0.65
1:C:6:LEU:CD1	1:C:379:ILE:HD11	2.26	0.65
1:C:51:LEU:HA	1:C:131:ILE:O	1.97	0.65
1:B:22:VAL:HG13	1:B:28:ALA:HB2	1.77	0.65
1:C:64:VAL:HG11	1:C:128:SER:HB3	1.79	0.65
1:B:70:LEU:HG	1:B:72:THR:HG23	1.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:THR:HA	1:C:246:LEU:HD23	1.79	0.64
1:A:168:LEU:HG	1:A:379:ILE:HG23	1.78	0.64
1:A:291:TYR:CE1	1:A:346:PRO:HD2	2.32	0.64
1:B:37:THR:HG23	1:B:135:SER:HB2	1.79	0.64
1:D:39:LEU:HG	1:D:133:VAL:HG22	1.79	0.64
1:C:203:VAL:O	1:C:207:VAL:HG23	1.97	0.64
1:C:233:LEU:HB2	1:C:342:THR:HB	1.78	0.64
1:D:251:ARG:HG2	1:D:251:ARG:HH11	1.63	0.64
1:B:2:LEU:HD12	1:B:2:LEU:N	2.12	0.64
1:D:98:PRO:HG2	1:D:101:CYS:HA	1.78	0.64
1:A:277:ARG:HG2	1:A:281:GLU:OE1	1.98	0.63
1:C:193:GLU:HG3	1:C:205:ASN:ND2	2.13	0.63
1:A:287:ALA:H	1:A:290:GLN:HE21	1.43	0.63
1:C:390:GLN:HA	1:C:393:LEU:HD12	1.81	0.63
1:A:73:SER:HA	1:A:121:ARG:NH2	2.14	0.63
1:A:279:LEU:O	1:A:282:MET:HB3	1.98	0.63
1:C:298:ILE:HG23	1:C:330:LYS:HB3	1.80	0.63
1:D:53:LEU:HD12	1:D:58:ILE:CD1	2.27	0.63
1:D:41:LEU:HD13	1:D:156:ALA:HB1	1.79	0.63
1:D:255:LEU:O	1:D:258:PRO:HD3	1.99	0.63
1:B:325:ARG:HG2	1:B:356:THR:HG22	1.80	0.63
1:C:52:SER:HB2	1:C:59:LYS:HD3	1.81	0.63
1:C:262:ALA:HB3	1:C:263:PRO:HD3	1.80	0.63
1:D:176:ARG:HG2	1:D:378:SER:OG	1.99	0.63
1:B:389:VAL:HG12	1:B:390:GLN:N	2.13	0.63
1:D:215:ARG:NE	2:D:414:HOH:O	2.31	0.63
1:B:209:THR:HA	1:B:377:VAL:CG2	2.29	0.62
1:B:103:VAL:O	1:B:107:LEU:HD13	1.97	0.62
1:B:329:SER:HB2	1:B:341:ILE:O	1.99	0.62
1:B:260:ILE:O	1:B:263:PRO:HD2	1.97	0.62
1:C:62:TRP:HB2	1:C:67:LEU:HD11	1.80	0.62
1:B:263:PRO:O	1:B:266:THR:HB	1.99	0.62
1:C:52:SER:O	1:C:132:VAL:HA	1.99	0.62
1:C:71:ASP:O	1:C:73:SER:N	2.30	0.62
1:A:70:LEU:CD2	1:A:94:VAL:HG22	2.29	0.62
1:A:388:ARG:HE	1:A:388:ARG:N	1.87	0.62
1:C:166:ASN:HB3	1:C:169:LYS:HE2	1.80	0.62
1:B:186:ASN:OD1	1:B:210:TRP:HZ3	1.81	0.62
1:B:22:VAL:CG1	1:B:28:ALA:HB2	2.30	0.62
1:B:67:LEU:O	1:B:70:LEU:CD1	2.46	0.62
1:B:115:LEU:CD2	1:B:153:LEU:HB3	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:CD	1:C:289:GLU:HG2	2.29	0.62
1:A:22:VAL:HG11	1:A:28:ALA:CB	2.30	0.61
1:D:287:ALA:HB3	1:D:290:GLN:CD	2.26	0.61
1:C:55:ASN:HD21	1:C:134:TRP:CD1	2.18	0.61
1:D:81:THR:HG22	1:D:82:THR:N	2.15	0.61
1:B:89:GLU:HA	1:B:92:LYS:HD2	1.82	0.61
1:C:70:LEU:HD22	1:C:70:LEU:H	1.65	0.61
1:C:164:ILE:HG23	1:C:181:ASP:CG	2.24	0.61
1:A:325:ARG:HD3	1:A:356:THR:OG1	2.01	0.61
1:C:287:ALA:HB3	1:C:290:GLN:NE2	2.15	0.61
1:B:82:THR:HG22	1:B:83:PRO:HD2	1.83	0.61
1:C:6:LEU:CD1	1:C:379:ILE:CD1	2.78	0.61
1:C:51:LEU:N	1:C:59:LYS:HZ1	1.99	0.61
1:C:291:TYR:O	1:C:295:GLU:HG3	2.00	0.61
1:D:98:PRO:HG2	1:D:101:CYS:CB	2.31	0.61
1:A:70:LEU:H	1:A:70:LEU:HD12	1.66	0.61
1:B:168:LEU:HD13	1:B:168:LEU:O	2.01	0.61
1:B:208:SER:O	1:B:377:VAL:HG23	2.00	0.61
1:D:81:THR:HG22	1:D:82:THR:H	1.65	0.61
1:D:164:ILE:HD13	1:D:165:PRO:N	2.15	0.61
1:D:243:THR:HB	1:D:244:ARG:HH21	1.65	0.61
1:C:33:LEU:HD11	1:C:234:LEU:CD2	2.30	0.61
1:C:164:ILE:HG23	1:C:165:PRO:HD2	1.81	0.61
1:B:141:ALA:O	1:B:143:LEU:HD13	2.00	0.61
1:B:193:GLU:OE1	1:B:193:GLU:HA	2.01	0.61
1:D:35:LEU:O	1:D:137:LEU:HG	2.01	0.61
1:D:221:ILE:HG22	1:D:222:SER:N	2.16	0.61
1:C:42:GLN:NE2	1:C:44:HIS:NE2	2.49	0.61
1:C:165:PRO:O	1:C:166:ASN:HB2	2.01	0.61
1:C:176:ARG:HB2	1:C:176:ARG:HH11	1.65	0.61
1:A:81:THR:HB	1:C:225:LYS:NZ	2.16	0.60
1:D:70:LEU:CG	1:D:72:THR:HG23	2.31	0.60
1:D:173:CYS:CB	1:D:384:SER:HB3	2.30	0.60
1:A:13:LYS:HG3	1:A:207:VAL:HG21	1.83	0.60
1:A:119:ILE:C	1:A:121:ARG:H	2.10	0.60
1:B:52:SER:HB3	1:B:132:VAL:HG23	1.82	0.60
1:B:112:PHE:HA	1:B:153:LEU:HD21	1.82	0.60
1:C:175:ASN:O	1:C:379:ILE:HG22	2.01	0.60
1:A:182:LEU:HA	1:A:185:ILE:HD12	1.81	0.60
1:B:118:SER:HB3	1:B:188:TRP:CH2	2.36	0.60
1:B:122:LYS:HD3	1:B:122:LYS:N	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:VAL:O	1:D:211:GLY:N	2.33	0.60
1:A:374:ALA:HB1	1:A:375:PRO:CD	2.32	0.60
1:C:356:THR:HG22	1:C:360:LEU:HD11	1.84	0.60
1:C:233:LEU:HD12	1:C:344:LEU:HD11	1.84	0.60
1:D:22:VAL:HG23	1:D:23:VAL:H	1.67	0.60
1:A:53:LEU:CD2	1:A:133:VAL:HB	2.32	0.59
1:D:98:PRO:HG2	1:D:101:CYS:CA	2.32	0.59
1:A:49:VAL:HG13	1:A:62:TRP:HB2	1.84	0.59
1:A:387:SER:H	1:A:388:ARG:HH21	1.50	0.59
1:B:164:ILE:HD13	1:B:164:ILE:C	2.27	0.59
1:B:224:LEU:O	1:B:225:LYS:C	2.46	0.59
1:B:232:ILE:CG1	1:B:372:ILE:HD13	2.22	0.59
1:B:375:PRO:HG3	1:D:89:GLU:OE1	2.02	0.59
1:D:164:ILE:CD1	1:D:177:TRP:HD1	2.15	0.59
1:D:237:THR:HA	1:D:365:PHE:CD2	2.36	0.59
1:D:58:ILE:HD12	1:D:105:GLU:HG3	1.83	0.59
1:D:262:ALA:HB3	1:D:263:PRO:HD3	1.83	0.59
1:A:228:PRO:HD2	1:A:283:GLY:HA2	1.83	0.59
1:B:35:LEU:O	1:B:137:LEU:HG	2.02	0.59
1:C:82:THR:HB	1:C:83:PRO:HD2	1.82	0.59
1:C:139:PRO:O	1:C:140:GLY:C	2.45	0.59
1:D:187:LYS:C	1:D:187:LYS:HD3	2.28	0.59
1:C:8:VAL:HG23	1:C:39:LEU:HB3	1.84	0.59
1:D:40:ARG:HD3	1:D:394:ASP:O	2.02	0.59
1:D:7:LEU:O	1:D:379:ILE:HG13	2.03	0.59
1:D:243:THR:CB	1:D:244:ARG:HH21	2.16	0.59
1:A:192:GLY:O	1:A:195:MET:HB3	2.02	0.59
1:A:236:ASN:HB3	1:A:366:ASP:HB2	1.83	0.59
1:B:251:ARG:HG3	1:B:251:ARG:HH11	1.68	0.59
1:C:156:ALA:O	1:C:160:VAL:HG23	2.02	0.59
1:D:279:LEU:C	1:D:281:GLU:H	2.11	0.59
1:C:158:LEU:HD23	1:C:164:ILE:CD1	2.32	0.59
1:C:332:THR:HG21	1:C:341:ILE:CD1	2.33	0.59
1:C:62:TRP:CB	1:C:67:LEU:HD11	2.33	0.59
1:C:106:ARG:O	1:C:110:LEU:HD13	2.02	0.59
1:C:115:LEU:O	1:C:119:ILE:HG22	2.03	0.59
1:A:38:PHE:O	1:A:133:VAL:HG13	2.02	0.58
1:A:28:ALA:O	1:A:29:LEU:HD23	2.03	0.58
1:A:146:SER:O	1:A:149:TYR:HB3	2.03	0.58
1:B:33:LEU:HD23	1:B:372:ILE:HD12	1.85	0.58
1:C:180:GLU:CD	1:C:180:GLU:N	2.60	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:SER:HB2	1:D:383:THR:HG22	1.83	0.58
1:A:179:LYS:HE2	1:A:183:GLU:OE2	2.04	0.58
1:B:186:ASN:OD1	1:B:210:TRP:CZ3	2.57	0.58
1:C:178:THR:HB	1:C:180:GLU:OE2	2.03	0.58
1:A:386:ASP:HB2	1:A:389:VAL:CG2	2.33	0.58
1:B:9:SER:HB3	1:B:38:PHE:CD2	2.38	0.58
1:D:55:ASN:HB2	1:D:56:ILE:HD12	1.86	0.58
1:C:2:LEU:N	1:C:2:LEU:HD12	2.18	0.58
1:C:269:ASP:O	1:C:273:LEU:HD23	2.04	0.58
1:C:40:ARG:HH12	1:C:390:GLN:HG3	1.68	0.58
1:A:60:ARG:HB2	1:A:60:ARG:CZ	2.33	0.58
1:B:305:LEU:HD13	1:B:331:LEU:HD11	1.84	0.58
1:B:348:LEU:HD22	1:B:352:GLU:OE1	2.04	0.58
1:A:21:ALA:HB1	1:A:26:LYS:HB2	1.86	0.58
1:A:228:PRO:HG2	1:A:282:MET:HE3	1.86	0.58
1:B:44:HIS:CD2	1:B:46:ASN:HD21	2.22	0.58
1:C:73:SER:C	1:C:75:LEU:H	2.12	0.58
1:C:128:SER:C	1:C:129:LEU:HG	2.28	0.58
1:A:187:LYS:O	1:A:191:GLN:HG2	2.04	0.57
1:B:147:ALA:O	1:B:151:VAL:HG23	2.03	0.57
1:B:238:LYS:HE3	1:B:366:ASP:CG	2.28	0.57
1:B:257:PHE:HB3	1:B:260:ILE:HD12	1.84	0.57
1:C:55:ASN:ND2	1:C:134:TRP:CD1	2.71	0.57
1:C:141:ALA:HB3	1:C:143:LEU:CD2	2.29	0.57
1:C:350:GLN:HA	1:C:353:VAL:CG1	2.34	0.57
1:D:69:SER:C	1:D:71:ASP:H	2.11	0.57
1:A:168:LEU:C	1:A:170:ASP:H	2.11	0.57
1:A:388:ARG:H	1:A:388:ARG:NE	1.87	0.57
1:B:154:ALA:O	1:B:158:LEU:HB2	2.04	0.57
1:C:73:SER:O	1:C:75:LEU:N	2.38	0.57
1:B:386:ASP:O	1:B:389:VAL:HB	2.04	0.57
1:C:355:ALA:O	1:C:358:GLN:HB3	2.05	0.57
1:D:22:VAL:CG1	1:D:28:ALA:HB2	2.32	0.57
1:D:331:LEU:C	1:D:331:LEU:HD12	2.29	0.57
1:C:119:ILE:HG23	1:C:120:CYS:N	2.20	0.57
1:A:203:VAL:O	1:A:207:VAL:HG23	2.04	0.57
1:D:211:GLY:HA3	1:D:375:PRO:O	2.04	0.57
1:D:143:LEU:HD21	1:D:234:LEU:HD21	1.86	0.57
1:A:52:SER:OG	1:A:59:LYS:HE2	2.03	0.57
1:A:241:ARG:HG2	1:A:241:ARG:NH1	2.19	0.57
1:B:2:LEU:O	1:B:3:SER:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:TYR:CE2	1:B:346:PRO:HD3	2.40	0.57
1:D:39:LEU:HD23	1:D:40:ARG:N	2.19	0.57
1:D:164:ILE:CD1	1:D:181:ASP:HB3	2.35	0.57
1:D:295:GLU:HB2	1:D:328:HIS:CG	2.40	0.57
1:A:98:PRO:O	1:A:99:ASP:C	2.47	0.57
1:C:9:SER:HB3	1:C:38:PHE:CD2	2.40	0.57
1:A:158:LEU:HG	1:A:164:ILE:HD12	1.85	0.57
1:B:54:PRO:O	1:B:57:GLY:N	2.37	0.57
1:B:315:LEU:HD22	1:B:331:LEU:HB3	1.87	0.57
1:C:129:LEU:HD23	1:C:160:VAL:HG11	1.87	0.57
1:D:167:PRO:HG2	1:D:177:TRP:HA	1.86	0.57
1:A:21:ALA:HB1	1:A:26:LYS:CB	2.35	0.57
1:B:2:LEU:HA	1:B:169:LYS:CD	2.35	0.57
1:B:322:THR:CG2	1:B:360:LEU:HD11	2.35	0.56
1:C:274:GLU:O	1:C:278:VAL:HG23	2.05	0.56
1:A:201:SER:OG	1:A:203:VAL:HG23	2.06	0.56
1:A:295:GLU:HB3	1:A:328:HIS:CD2	2.40	0.56
1:B:38:PHE:O	1:B:133:VAL:HA	2.06	0.56
1:B:203:VAL:O	1:B:207:VAL:HG23	2.06	0.56
1:C:242:ASN:C	1:C:242:ASN:HD22	2.12	0.56
1:C:350:GLN:N	1:C:351:PRO:HD2	2.20	0.56
1:A:329:SER:HA	1:A:341:ILE:O	2.05	0.56
1:B:39:LEU:HD23	1:B:40:ARG:N	2.21	0.56
1:B:232:ILE:HD13	1:B:341:ILE:CD1	2.35	0.56
1:B:331:LEU:HD12	1:B:331:LEU:O	2.06	0.56
1:A:60:ARG:NH2	1:A:105:GLU:OE2	2.39	0.56
1:B:157:LEU:O	1:B:160:VAL:HG12	2.05	0.56
1:B:164:ILE:HD13	1:B:165:PRO:CD	2.36	0.56
1:D:173:CYS:HB3	1:D:384:SER:HB3	1.87	0.56
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.70	0.56
1:C:33:LEU:HD12	1:C:143:LEU:HD12	1.88	0.56
1:C:68:GLN:OE1	1:C:126:LEU:HD23	2.06	0.56
1:D:19:GLU:OE2	1:D:19:GLU:N	2.39	0.56
1:C:254:LEU:HD13	1:C:261:VAL:CG1	2.36	0.56
1:D:58:ILE:CD1	1:D:105:GLU:HG3	2.36	0.56
1:A:81:THR:HB	1:C:225:LYS:HZ1	1.71	0.56
1:C:39:LEU:HD23	1:C:40:ARG:N	2.21	0.56
1:D:178:THR:O	1:D:179:LYS:C	2.49	0.56
1:D:186:ASN:HD21	1:D:206:ALA:HA	1.70	0.56
1:A:13:LYS:HB2	1:A:207:VAL:HG11	1.88	0.56
1:A:92:LYS:O	1:A:95:ALA:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD23	1:A:389:VAL:CG1	2.34	0.56
1:A:387:SER:H	1:A:388:ARG:NH2	2.03	0.56
1:C:318:LEU:HD11	1:C:340:GLY:HA3	1.87	0.56
1:D:234:LEU:HD12	1:D:340:GLY:O	2.06	0.56
1:C:50:ASP:HB2	1:C:130:ASP:CA	2.23	0.55
1:A:322:THR:HG21	1:A:329:SER:OG	2.06	0.55
1:C:48:LYS:H	1:C:128:SER:HB2	1.70	0.55
1:C:233:LEU:CD1	1:C:344:LEU:HD11	2.36	0.55
1:A:232:ILE:HG13	1:A:233:LEU:N	2.19	0.55
1:C:18:GLY:HA3	1:C:28:ALA:CB	2.36	0.55
1:D:56:ILE:HG22	1:D:58:ILE:HG23	1.88	0.55
1:D:385:LEU:HD22	1:D:391:GLN:CD	2.31	0.55
1:A:41:LEU:HA	2:A:419:HOH:O	2.06	0.55
1:B:322:THR:HG22	1:B:360:LEU:HD11	1.87	0.55
1:C:167:PRO:C	1:C:169:LYS:H	2.14	0.55
1:D:50:ASP:HB3	1:D:61:ALA:CB	2.34	0.55
1:D:60:ARG:HG3	1:D:60:ARG:HH21	1.70	0.55
1:A:55:ASN:HD21	1:A:134:TRP:HE1	1.54	0.55
1:B:287:ALA:HB3	1:B:290:GLN:CG	2.33	0.55
1:B:158:LEU:CD2	1:B:185:ILE:HD13	2.36	0.55
1:C:167:PRO:HB2	1:C:379:ILE:HG21	1.89	0.55
1:A:121:ARG:HH11	1:A:121:ARG:CG	2.20	0.55
1:B:95:ALA:HB1	1:B:97:LEU:HG	1.88	0.55
1:B:232:ILE:C	1:B:232:ILE:HD12	2.32	0.55
1:B:248:ALA:O	1:B:251:ARG:HB3	2.05	0.55
1:D:266:THR:O	1:D:269:ASP:HB3	2.07	0.55
1:C:88:VAL:HG12	1:C:92:LYS:HE3	1.88	0.55
1:A:14:VAL:HG22	1:A:372:ILE:HD11	1.87	0.54
1:A:84:THR:HB	1:A:87:GLN:CG	2.36	0.54
1:A:199:ASN:HB2	1:C:281:GLU:HG3	1.89	0.54
1:B:318:LEU:HD23	1:B:318:LEU:C	2.31	0.54
1:B:168:LEU:HD11	1:B:381:SER:HA	1.89	0.54
1:C:51:LEU:C	1:C:59:LYS:HD2	2.32	0.54
1:C:390:GLN:HA	1:C:393:LEU:HB2	1.88	0.54
1:D:6:LEU:HB2	1:D:41:LEU:HD23	1.88	0.54
1:B:100:ASP:O	1:B:101:CYS:O	2.26	0.54
1:A:58:ILE:CD1	1:A:105:GLU:HB2	2.34	0.54
1:A:242:ASN:C	1:A:246:LEU:HD23	2.33	0.54
1:B:362:SER:C	1:B:364:GLY:H	2.15	0.54
1:D:226:ARG:HB2	1:D:280:GLY:HA2	1.88	0.54
1:A:282:MET:O	1:A:283:GLY:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LEU:HD23	1:B:91:LEU:O	2.07	0.54
1:C:207:VAL:CG2	1:C:214:LEU:HD22	2.36	0.54
1:C:343:LEU:HD12	1:C:344:LEU:H	1.73	0.54
1:A:85:SER:O	1:A:89:GLU:HB2	2.08	0.54
1:B:225:LYS:HD2	1:B:226:ARG:N	2.22	0.54
1:C:147:ALA:HB1	1:C:205:ASN:HA	1.88	0.54
1:C:158:LEU:HD23	1:C:164:ILE:HD11	1.89	0.54
1:C:251:ARG:HG3	1:C:251:ARG:HH11	1.73	0.54
1:D:188:TRP:O	1:D:191:GLN:HB2	2.07	0.54
1:A:38:PHE:CE2	1:A:385:LEU:HD21	2.42	0.54
1:C:41:LEU:HD13	1:C:160:VAL:CG2	2.37	0.54
1:A:197:HIS:O	1:A:200:PRO:HD3	2.08	0.54
1:B:158:LEU:HB3	1:B:164:ILE:HG21	1.88	0.54
1:B:5:VAL:HG22	1:B:42:GLN:HG3	1.89	0.54
1:C:349:GLU:C	1:C:351:PRO:HD2	2.33	0.54
1:C:384:SER:O	1:C:385:LEU:HD12	2.08	0.54
1:A:242:ASN:O	1:A:246:LEU:HD23	2.07	0.53
1:B:285:ALA:HB2	1:D:107:LEU:HD21	1.89	0.53
1:C:50:ASP:CB	1:C:130:ASP:HA	2.23	0.53
1:C:209:THR:O	1:C:376:GLY:HA3	2.09	0.53
1:D:295:GLU:HB2	1:D:328:HIS:CD2	2.43	0.53
1:B:101:CYS:O	1:B:102:ALA:C	2.52	0.53
1:D:385:LEU:C	1:D:387:SER:H	2.17	0.53
1:C:39:LEU:HD13	1:C:152:CYS:O	2.08	0.53
1:C:119:ILE:HD13	1:C:157:LEU:CB	2.38	0.53
1:C:6:LEU:HD12	1:C:379:ILE:HD13	1.90	0.53
1:C:13:LYS:O	1:C:13:LYS:HD3	2.08	0.53
1:A:282:MET:O	1:A:284:GLU:N	2.42	0.53
1:A:149:TYR:CZ	1:A:153:LEU:HD11	2.43	0.53
1:A:350:GLN:N	1:A:351:PRO:HD2	2.24	0.53
1:B:160:VAL:HG13	1:B:161:CYS:N	2.22	0.53
1:D:48:LYS:HE3	2:D:421:HOH:O	2.09	0.53
1:D:75:LEU:HD12	1:D:75:LEU:N	2.23	0.53
1:B:47:GLY:O	1:B:64:VAL:HG22	2.08	0.53
1:B:350:GLN:N	1:B:351:PRO:HD2	2.24	0.53
1:C:164:ILE:CG2	1:C:165:PRO:HD2	2.38	0.53
1:C:18:GLY:HA3	1:C:28:ALA:HB2	1.91	0.53
1:C:70:LEU:H	1:C:70:LEU:CD2	2.20	0.53
1:C:164:ILE:HG23	1:C:181:ASP:OD1	2.09	0.53
1:A:60:ARG:NH1	1:A:60:ARG:CB	2.71	0.53
1:A:123:GLN:HE21	1:A:123:GLN:CA	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HG	1:A:164:ILE:CD1	2.39	0.52
1:B:35:LEU:CD2	1:B:370:THR:HG21	2.39	0.52
1:B:306:ASN:ND2	1:B:311:GLY:HA3	2.24	0.52
1:C:164:ILE:HA	2:C:410:HOH:O	2.08	0.52
1:C:349:GLU:OE2	1:C:349:GLU:N	2.42	0.52
1:D:59:LYS:HD2	1:D:59:LYS:N	2.24	0.52
1:D:101:CYS:O	1:D:102:ALA:C	2.51	0.52
1:A:386:ASP:HB3	1:A:388:ARG:NE	2.24	0.52
1:B:52:SER:O	1:B:54:PRO:HD3	2.09	0.52
1:B:164:ILE:HD12	1:B:177:TRP:CD1	2.45	0.52
1:B:207:VAL:HG22	1:B:214:LEU:HD22	1.90	0.52
1:C:225:LYS:HZ2	1:C:225:LYS:CB	2.20	0.52
1:D:53:LEU:HB3	1:D:56:ILE:HD13	1.90	0.52
1:D:232:ILE:HG13	1:D:233:LEU:N	2.23	0.52
1:C:64:VAL:O	1:C:68:GLN:HB2	2.10	0.52
1:C:288:PRO:C	1:C:290:GLN:H	2.17	0.52
1:C:358:GLN:HG3	1:C:359:ALA:N	2.23	0.52
1:B:82:THR:CG2	1:B:83:PRO:HD2	2.39	0.52
1:C:175:ASN:ND2	1:C:176:ARG:N	2.57	0.52
1:C:386:ASP:C	1:C:388:ARG:H	2.17	0.52
1:D:164:ILE:HD13	1:D:165:PRO:HD2	1.90	0.52
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.25	0.52
1:D:75:LEU:HB2	1:D:121:ARG:CD	2.40	0.52
1:B:237:THR:O	1:B:238:LYS:HB2	2.10	0.52
1:C:10:ALA:HB2	1:C:377:VAL:HG13	1.91	0.52
1:D:47:GLY:C	1:D:64:VAL:HG13	2.35	0.52
1:D:52:SER:C	1:D:54:PRO:HD3	2.34	0.52
1:B:388:ARG:HH21	1:B:391:GLN:CG	2.16	0.52
1:D:12:GLY:HA3	1:D:137:LEU:HD11	1.90	0.52
1:C:237:THR:HA	1:C:365:PHE:CD2	2.45	0.52
1:C:356:THR:HG22	1:C:360:LEU:HD12	1.92	0.52
1:A:39:LEU:HD11	1:A:153:LEU:CD2	2.36	0.52
1:D:39:LEU:HD11	1:D:153:LEU:CD2	2.39	0.52
1:A:188:TRP:O	1:A:191:GLN:HB2	2.10	0.51
1:A:196:ILE:CG1	1:A:197:HIS:N	2.73	0.51
1:A:350:GLN:HG2	2:A:460:HOH:O	2.10	0.51
1:B:33:LEU:HD23	1:B:372:ILE:HD11	1.91	0.51
1:B:68:GLN:C	1:B:70:LEU:H	2.17	0.51
1:C:253:ARG:NH2	1:C:307:ALA:O	2.43	0.51
1:B:190:PHE:CE1	1:B:200:PRO:HG2	2.45	0.51
1:D:329:SER:HA	1:D:341:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:CG2	1:A:372:ILE:HD11	2.41	0.51
1:A:243:THR:O	1:A:247:VAL:HG23	2.10	0.51
1:D:158:LEU:HD23	1:D:185:ILE:CD1	2.27	0.51
1:D:186:ASN:ND2	1:D:206:ALA:HA	2.25	0.51
1:D:232:ILE:HD13	1:D:372:ILE:HD13	1.92	0.51
1:A:278:VAL:HG21	1:A:293:VAL:HG11	1.91	0.51
1:D:2:LEU:HD12	1:D:2:LEU:N	2.26	0.51
1:B:305:LEU:O	1:B:310:VAL:HG22	2.11	0.51
1:D:13:LYS:O	1:D:13:LYS:HD3	2.09	0.51
1:D:70:LEU:HD23	1:D:72:THR:HG21	1.92	0.51
1:A:164:ILE:HG23	1:A:181:ASP:CG	2.35	0.51
1:D:278:VAL:HG12	1:D:282:MET:SD	2.51	0.51
1:D:370:THR:OG1	1:D:371:SER:N	2.42	0.51
1:A:16:LEU:HG	1:A:17:HIS:CD2	2.46	0.51
1:A:284:GLU:N	1:A:284:GLU:OE1	2.43	0.51
1:B:70:LEU:HD23	1:B:70:LEU:C	2.36	0.51
1:B:176:ARG:HG3	1:B:176:ARG:NH2	2.23	0.51
1:C:73:SER:C	1:C:75:LEU:N	2.67	0.51
1:C:225:LYS:HB2	1:C:225:LYS:NZ	2.22	0.51
1:D:26:LYS:HD2	1:D:269:ASP:HB2	1.93	0.51
1:D:244:ARG:H	1:D:244:ARG:HE	1.59	0.51
1:D:374:ALA:HB1	1:D:375:PRO:HD2	1.93	0.51
1:C:163:GLU:HA	1:C:163:GLU:OE2	2.11	0.51
1:C:368:LEU:HD13	2:C:428:HOH:O	2.11	0.51
1:D:184:LEU:HG	1:D:188:TRP:CD1	2.46	0.51
1:B:13:LYS:HD3	1:B:13:LYS:O	2.11	0.51
1:B:293:VAL:O	1:B:297:LEU:HG	2.11	0.51
1:D:19:GLU:CD	1:D:19:GLU:H	2.19	0.51
1:D:54:PRO:HD2	1:D:133:VAL:O	2.11	0.51
1:D:387:SER:HA	1:D:391:GLN:HG2	1.93	0.51
1:A:182:LEU:HD23	1:A:185:ILE:HD12	1.93	0.50
1:A:258:PRO:HG2	1:A:259:GLU:OE1	2.11	0.50
1:B:39:LEU:HD21	1:B:131:ILE:HG23	1.92	0.50
1:B:165:PRO:O	1:B:167:PRO:HD3	2.12	0.50
1:D:40:ARG:HD2	1:D:394:ASP:CB	2.39	0.50
1:A:84:THR:O	1:A:88:VAL:HG23	2.11	0.50
1:B:232:ILE:HD11	1:B:370:THR:HG23	1.93	0.50
1:D:362:SER:C	1:D:364:GLY:H	2.17	0.50
1:A:80:VAL:HG13	1:A:82:THR:HG23	1.93	0.50
1:B:384:SER:O	1:B:385:LEU:HG	2.11	0.50
1:C:119:ILE:CG2	1:C:120:CYS:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:LEU:HD22	1:C:246:LEU:H	1.75	0.50
1:A:31:VAL:HG21	1:A:372:ILE:HG12	1.93	0.50
1:A:70:LEU:H	1:A:70:LEU:CD1	2.23	0.50
1:B:362:SER:C	1:B:364:GLY:N	2.67	0.50
1:A:41:LEU:HG	2:A:419:HOH:O	2.12	0.50
1:A:83:PRO:HD2	1:A:194:ARG:HH11	1.75	0.50
1:A:375:PRO:HA	2:A:406:HOH:O	2.11	0.50
1:A:228:PRO:CD	1:A:283:GLY:HA2	2.41	0.50
1:A:261:VAL:O	1:A:262:ALA:C	2.54	0.50
1:B:160:VAL:C	1:B:162:GLU:N	2.70	0.50
1:D:33:LEU:HD22	1:D:35:LEU:HD23	1.94	0.50
1:D:178:THR:O	1:D:181:ASP:N	2.44	0.50
1:D:249:GLY:HA3	2:D:428:HOH:O	2.12	0.50
1:A:60:ARG:CB	1:A:60:ARG:HH11	2.25	0.50
1:A:143:LEU:HD21	1:A:234:LEU:HD21	1.92	0.50
1:B:158:LEU:HD23	1:B:185:ILE:HD13	1.93	0.50
1:C:7:LEU:C	1:C:379:ILE:HD12	2.35	0.50
1:C:318:LEU:C	1:C:318:LEU:HD23	2.36	0.50
1:D:158:LEU:HD21	1:D:184:LEU:HD23	1.92	0.50
1:A:21:ALA:HB1	1:A:26:LYS:HG3	1.93	0.50
1:A:160:VAL:C	1:A:162:GLU:H	2.19	0.50
1:C:252:ASN:O	1:C:255:LEU:HD23	2.12	0.50
1:C:353:VAL:O	1:C:357:LYS:HG3	2.11	0.50
1:D:226:ARG:O	1:D:227:SER:C	2.53	0.50
1:C:354:GLU:OE2	1:C:357:LYS:HD3	2.11	0.49
1:D:279:LEU:HD23	1:D:282:MET:SD	2.52	0.49
1:A:306:ASN:ND2	1:A:311:GLY:HA3	2.27	0.49
1:C:48:LYS:H	1:C:128:SER:HB3	1.77	0.49
1:C:381:SER:C	1:C:383:THR:H	2.20	0.49
1:D:18:GLY:O	1:D:19:GLU:C	2.55	0.49
1:D:302:GLN:HE22	1:D:331:LEU:HD23	1.76	0.49
1:D:50:ASP:CB	1:D:61:ALA:HB2	2.39	0.49
1:B:215:ARG:HD2	1:B:276:GLU:OE1	2.12	0.49
1:B:264:LEU:O	1:B:267:SER:N	2.44	0.49
1:C:176:ARG:HG2	1:C:377:VAL:O	2.12	0.49
1:A:83:PRO:HB2	2:C:404:HOH:O	2.12	0.49
1:A:237:THR:O	1:A:239:VAL:HG23	2.11	0.49
1:A:259:GLU:OE1	1:A:259:GLU:N	2.46	0.49
1:B:121:ARG:HH21	1:B:121:ARG:CB	2.26	0.49
1:B:161:CYS:O	1:B:163:GLU:N	2.45	0.49
1:D:361:THR:O	1:D:364:GLY:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:CG	1:C:289:GLU:HG2	2.42	0.49
1:C:176:ARG:HH11	1:C:176:ARG:CB	2.26	0.49
1:C:292:LEU:O	1:C:293:VAL:C	2.55	0.49
1:A:123:GLN:CA	1:A:123:GLN:NE2	2.76	0.49
1:B:278:VAL:HG11	1:B:294:LEU:HD13	1.95	0.49
1:C:13:LYS:HD3	1:C:13:LYS:C	2.37	0.49
1:C:22:VAL:O	1:C:25:GLY:N	2.46	0.49
1:C:102:ALA:O	1:C:105:GLU:HB3	2.13	0.49
1:D:41:LEU:HB2	1:D:131:ILE:HG12	1.94	0.49
1:D:56:ILE:HD12	1:D:56:ILE:N	2.27	0.49
1:B:237:THR:C	1:B:239:VAL:H	2.20	0.49
1:C:52:SER:CB	1:C:132:VAL:HG22	2.25	0.49
1:A:22:VAL:HG12	1:A:26:LYS:O	2.13	0.49
1:A:131:ILE:HD12	1:A:131:ILE:N	2.27	0.49
1:D:199:ASN:C	1:D:199:ASN:HD22	2.19	0.49
1:A:22:VAL:C	1:A:24:HIS:N	2.71	0.48
1:A:86:GLU:HB2	2:A:449:HOH:O	2.12	0.48
1:A:164:ILE:HD11	1:A:184:LEU:HD23	1.95	0.48
1:B:32:SER:O	1:B:372:ILE:HA	2.14	0.48
1:B:52:SER:C	1:B:54:PRO:HD3	2.37	0.48
1:C:232:ILE:HG12	1:C:372:ILE:CD1	2.41	0.48
1:C:263:PRO:HB2	1:D:267:SER:HB2	1.94	0.48
1:D:37:THR:CG2	1:D:135:SER:HB2	2.40	0.48
1:D:242:ASN:C	1:D:246:LEU:HD23	2.37	0.48
1:B:121:ARG:C	1:B:123:GLN:H	2.21	0.48
1:B:278:VAL:O	1:B:282:MET:HG3	2.13	0.48
1:A:60:ARG:HG2	1:A:62:TRP:CZ2	2.49	0.48
1:A:88:VAL:HG22	1:A:195:MET:HE1	1.95	0.48
1:A:193:GLU:HA	1:A:193:GLU:OE1	2.13	0.48
1:A:376:GLY:O	1:A:377:VAL:C	2.55	0.48
1:B:4:GLU:HB3	1:B:43:PRO:HG2	1.95	0.48
1:B:47:GLY:HA2	1:B:128:SER:HB3	1.95	0.48
1:C:213:ALA:O	1:C:214:LEU:HD12	2.13	0.48
1:A:170:ASP:N	1:A:170:ASP:OD1	2.45	0.48
1:D:120:CYS:HA	1:D:161:CYS:SG	2.53	0.48
1:D:312:HIS:ND1	1:D:313:ALA:N	2.60	0.48
1:A:52:SER:CB	1:A:132:VAL:HG22	2.28	0.48
1:B:53:LEU:HD13	1:B:108:ALA:HB1	1.96	0.48
1:B:122:LYS:HE3	1:B:163:GLU:OE1	2.14	0.48
1:D:111:ALA:O	1:D:115:LEU:HD23	2.13	0.48
1:A:2:LEU:O	1:A:2:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:HH11	1:A:60:ARG:CA	2.27	0.48
1:B:41:LEU:HD23	1:B:41:LEU:C	2.38	0.48
1:D:91:LEU:HD11	1:D:117:LEU:HD12	1.95	0.48
1:A:22:VAL:C	1:A:24:HIS:H	2.21	0.48
1:A:66:ARG:O	1:A:70:LEU:CD1	2.62	0.48
1:A:134:TRP:HB3	1:A:393:LEU:HD21	1.96	0.48
1:A:135:SER:OG	1:A:137:LEU:HB2	2.14	0.48
1:A:280:GLY:O	1:A:281:GLU:C	2.57	0.48
1:A:384:SER:O	1:A:385:LEU:CB	2.60	0.48
1:B:180:GLU:HG3	1:B:181:ASP:N	2.29	0.48
1:B:232:ILE:HD13	1:B:341:ILE:HD12	1.95	0.48
1:B:278:VAL:HG11	1:B:294:LEU:CD1	2.44	0.48
1:B:291:TYR:O	1:B:295:GLU:HG3	2.14	0.48
1:C:174:VAL:HG13	1:C:380:HIS:ND1	2.28	0.48
1:C:290:GLN:C	1:C:292:LEU:N	2.70	0.48
1:A:55:ASN:HD21	1:A:134:TRP:NE1	2.10	0.48
1:A:83:PRO:HG2	1:A:194:ARG:HB3	1.96	0.48
1:B:103:VAL:HG12	1:B:107:LEU:HD13	1.96	0.48
1:D:50:ASP:HA	1:D:61:ALA:HA	1.95	0.48
1:A:390:GLN:HA	1:A:393:LEU:HB2	1.96	0.48
1:B:151:VAL:CG1	1:B:377:VAL:HG21	2.43	0.48
1:C:3:SER:OG	1:C:4:GLU:N	2.43	0.48
1:D:138:PRO:HD2	1:D:143:LEU:HD23	1.96	0.48
1:D:192:GLY:O	1:D:195:MET:HB3	2.14	0.48
1:A:68:GLN:HG3	1:A:126:LEU:HB2	1.96	0.48
1:B:40:ARG:HB3	1:B:132:VAL:CG1	2.44	0.48
1:B:52:SER:HB3	1:B:132:VAL:CG2	2.44	0.48
1:C:39:LEU:C	1:C:39:LEU:CD2	2.87	0.48
1:C:64:VAL:CG1	1:C:128:SER:HB3	2.43	0.48
1:D:158:LEU:HD21	1:D:184:LEU:HG	1.95	0.48
1:D:169:LYS:C	1:D:170:ASP:CG	2.82	0.48
1:D:374:ALA:HB1	1:D:375:PRO:CD	2.43	0.48
1:B:343:LEU:HG	1:B:344:LEU:N	2.29	0.47
1:C:302:GLN:HE21	1:C:302:GLN:HA	1.79	0.47
1:D:75:LEU:HB2	1:D:121:ARG:NE	2.30	0.47
1:D:155:ALA:HA	1:D:185:ILE:HD12	1.96	0.47
1:D:183:GLU:OE2	1:D:210:TRP:HZ2	1.97	0.47
1:B:370:THR:OG1	1:B:371:SER:N	2.38	0.47
1:C:7:LEU:HB2	1:C:380:HIS:O	2.13	0.47
1:C:119:ILE:HD13	1:C:157:LEU:HB2	1.95	0.47
1:C:234:LEU:HD12	1:C:341:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:THR:OG1	1:C:371:SER:N	2.46	0.47
1:A:55:ASN:ND2	1:A:134:TRP:NE1	2.63	0.47
1:A:129:LEU:HD12	1:A:131:ILE:HD11	1.97	0.47
1:B:113:LEU:O	1:B:114:TYR:C	2.58	0.47
1:C:83:PRO:HG3	1:C:198:GLY:O	2.14	0.47
1:C:166:ASN:HB3	1:C:169:LYS:CE	2.44	0.47
1:D:69:SER:C	1:D:71:ASP:N	2.72	0.47
1:A:119:ILE:C	1:A:121:ARG:N	2.70	0.47
1:A:305:LEU:O	1:A:310:VAL:HG22	2.15	0.47
1:C:21:ALA:HB1	1:C:26:LYS:HB2	1.96	0.47
1:C:22:VAL:O	1:C:23:VAL:C	2.57	0.47
1:C:157:LEU:C	1:C:159:THR:N	2.71	0.47
1:A:298:ILE:HD12	1:A:330:LYS:HG2	1.97	0.47
1:B:295:GLU:OE2	1:B:328:HIS:HD2	1.98	0.47
1:D:123:GLN:HG3	1:D:124:ARG:N	2.30	0.47
1:A:84:THR:CG2	1:A:86:GLU:H	2.20	0.47
1:B:13:LYS:HB2	1:B:207:VAL:CG1	2.39	0.47
1:B:348:LEU:HD22	1:B:352:GLU:CD	2.40	0.47
1:D:22:VAL:C	1:D:24:HIS:N	2.72	0.47
1:D:70:LEU:HD22	1:D:94:VAL:HG11	1.94	0.47
1:D:111:ALA:HB2	1:D:196:ILE:HD11	1.95	0.47
1:A:244:ARG:HG3	1:C:289:GLU:CB	2.45	0.47
1:A:260:ILE:N	1:A:260:ILE:HD12	2.30	0.47
1:A:268:ILE:O	1:A:271:ILE:HB	2.15	0.47
1:B:89:GLU:O	1:B:92:LYS:HB2	2.15	0.47
1:B:144:GLY:HA2	2:B:455:HOH:O	2.14	0.47
1:B:323:ARG:HD2	1:B:323:ARG:HA	1.72	0.47
1:C:36:ARG:HG2	1:C:36:ARG:HH11	1.79	0.47
1:C:343:LEU:HD12	1:C:344:LEU:N	2.29	0.47
1:D:113:LEU:O	1:D:117:LEU:HG	2.14	0.47
1:A:21:ALA:CB	1:A:26:LYS:HB2	2.44	0.47
1:B:54:PRO:C	1:B:57:GLY:H	2.22	0.47
1:C:261:VAL:O	1:C:264:LEU:HB3	2.15	0.47
1:A:13:LYS:C	1:A:13:LYS:HE2	2.40	0.47
1:C:221:ILE:HG22	1:C:222:SER:N	2.30	0.47
1:A:13:LYS:HE2	1:A:13:LYS:O	2.15	0.47
1:B:3:SER:H	1:B:169:LYS:CD	2.28	0.47
1:C:121:ARG:HG3	1:C:122:LYS:N	2.29	0.47
1:C:213:ALA:C	1:C:214:LEU:HD12	2.39	0.47
1:A:33:LEU:CD2	1:A:370:THR:HG21	2.41	0.46
1:B:312:HIS:ND1	1:B:314:SER:OG	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:VAL:HG13	1:C:104:THR:N	2.30	0.46
1:D:22:VAL:O	1:D:24:HIS:N	2.48	0.46
1:A:22:VAL:HG13	1:A:28:ALA:HB2	1.97	0.46
1:A:80:VAL:CG1	1:A:82:THR:HG23	2.45	0.46
1:A:97:LEU:CD1	1:A:106:ARG:HG3	2.41	0.46
1:B:12:GLY:CA	1:B:137:LEU:HD11	2.43	0.46
1:C:182:LEU:O	1:C:185:ILE:N	2.47	0.46
1:D:51:LEU:HD21	1:D:53:LEU:CD2	2.42	0.46
1:A:19:GLU:OE1	1:A:332:THR:HA	2.14	0.46
1:A:63:ASP:O	1:A:66:ARG:N	2.48	0.46
1:A:84:THR:CG2	1:A:86:GLU:HB3	2.45	0.46
1:A:315:LEU:HD13	1:A:331:LEU:HB3	1.97	0.46
1:A:318:LEU:C	1:A:318:LEU:HD23	2.40	0.46
1:B:147:ALA:O	1:B:148:ALA:C	2.58	0.46
1:C:182:LEU:O	1:C:183:GLU:C	2.58	0.46
1:D:64:VAL:HG23	1:D:65:ALA:N	2.30	0.46
1:D:160:VAL:CG1	1:D:161:CYS:N	2.78	0.46
1:D:269:ASP:O	1:D:273:LEU:HD13	2.14	0.46
1:A:332:THR:HB	1:A:341:ILE:CD1	2.46	0.46
1:B:11:PRO:CD	1:B:376:GLY:HA2	2.45	0.46
1:C:114:TYR:HD2	1:C:195:MET:HE2	1.81	0.46
1:C:228:PRO:HG2	1:C:230:LEU:HD21	1.98	0.46
1:D:74:PHE:CE1	1:D:75:LEU:HG	2.49	0.46
1:A:64:VAL:HG23	1:A:65:ALA:N	2.31	0.46
1:C:190:PHE:O	1:C:193:GLU:HB2	2.15	0.46
1:C:320:GLN:HG3	2:D:427:HOH:O	2.16	0.46
1:D:292:LEU:O	1:D:295:GLU:HG2	2.15	0.46
1:D:295:GLU:HA	1:D:298:ILE:HD12	1.97	0.46
1:A:166:ASN:OD1	1:A:168:LEU:HB2	2.16	0.46
1:A:174:VAL:HA	1:A:379:ILE:O	2.16	0.46
1:D:39:LEU:CD2	1:D:131:ILE:HG23	2.36	0.46
1:D:120:CYS:O	1:D:123:GLN:HB3	2.16	0.46
1:A:55:ASN:ND2	1:A:134:TRP:CD1	2.84	0.46
1:B:164:ILE:HG12	1:B:165:PRO:HD2	1.98	0.46
1:B:261:VAL:O	1:B:262:ALA:C	2.57	0.46
1:C:37:THR:OG1	1:C:135:SER:HB2	2.15	0.46
1:D:22:VAL:C	1:D:24:HIS:H	2.22	0.46
1:D:158:LEU:HD21	1:D:184:LEU:CG	2.46	0.46
1:D:164:ILE:CD1	1:D:165:PRO:HD2	2.46	0.46
1:D:193:GLU:HG3	1:D:205:ASN:HD22	1.81	0.46
1:A:181:ASP:O	1:A:185:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASN:C	1:A:199:ASN:ND2	2.66	0.46
1:A:330:LYS:O	1:A:330:LYS:HG3	2.15	0.46
1:D:261:VAL:O	1:D:262:ALA:C	2.59	0.46
1:D:349:GLU:O	1:D:353:VAL:HG12	2.16	0.46
1:A:237:THR:C	1:A:239:VAL:N	2.72	0.46
1:B:264:LEU:C	1:B:266:THR:N	2.71	0.46
1:B:277:ARG:HD3	2:B:443:HOH:O	2.16	0.46
1:C:26:LYS:HB3	1:C:269:ASP:HB2	1.97	0.46
1:C:42:GLN:HE21	1:C:44:HIS:CD2	2.34	0.45
1:A:38:PHE:CZ	1:A:385:LEU:HD21	2.51	0.45
1:A:237:THR:C	1:A:239:VAL:H	2.25	0.45
1:C:6:LEU:HD12	1:C:379:ILE:CD1	2.46	0.45
1:D:41:LEU:HD23	1:D:41:LEU:O	2.16	0.45
1:B:65:ALA:O	1:B:68:GLN:HB3	2.16	0.45
1:B:175:ASN:O	1:B:379:ILE:HG22	2.16	0.45
1:A:33:LEU:HA	1:A:372:ILE:HD12	1.97	0.45
1:B:261:VAL:O	1:B:264:LEU:N	2.50	0.45
1:A:124:ARG:NH1	2:A:421:HOH:O	2.48	0.45
1:A:215:ARG:NH1	1:A:276:GLU:CD	2.74	0.45
1:B:2:LEU:CA	1:B:169:LYS:HG3	2.42	0.45
1:B:51:LEU:HD11	1:B:112:PHE:CB	2.47	0.45
1:D:164:ILE:HD13	1:D:165:PRO:CG	2.46	0.45
1:D:312:HIS:CE1	1:D:314:SER:H	2.34	0.45
1:D:381:SER:CB	1:D:383:THR:HG22	2.46	0.45
1:D:387:SER:O	1:D:390:GLN:CB	2.65	0.45
1:A:64:VAL:HG11	1:A:128:SER:HB3	1.98	0.45
1:A:121:ARG:CG	1:A:121:ARG:NH1	2.80	0.45
1:C:151:VAL:HG12	1:C:377:VAL:HG11	1.98	0.45
1:C:252:ASN:HA	1:C:255:LEU:HD22	1.99	0.45
1:D:350:GLN:O	1:D:354:GLU:HB2	2.15	0.45
1:D:385:LEU:HD13	1:D:387:SER:HB3	1.98	0.45
1:A:214:LEU:HD12	1:A:223:SER:HA	1.99	0.45
1:A:377:VAL:O	1:A:377:VAL:HG13	2.15	0.45
1:B:157:LEU:HA	1:B:160:VAL:HG12	1.99	0.45
1:B:202:GLY:HA2	1:B:205:ASN:HD21	1.81	0.45
1:C:158:LEU:HD23	1:C:164:ILE:HD12	1.98	0.45
1:C:335:GLY:C	1:C:337:GLY:H	2.25	0.45
1:D:27:VAL:HG22	1:D:217:HIS:CD2	2.51	0.45
1:D:39:LEU:HD23	1:D:39:LEU:C	2.41	0.45
1:D:158:LEU:HD21	1:D:184:LEU:CD2	2.45	0.45
1:B:33:LEU:HD23	1:B:33:LEU:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:VAL:HG21	1:C:372:ILE:HG12	1.98	0.45
1:C:47:GLY:O	1:C:48:LYS:CG	2.62	0.45
1:C:167:PRO:HB2	1:C:379:ILE:CG2	2.46	0.45
1:C:257:PHE:HB3	1:C:260:ILE:HD12	1.98	0.45
1:C:352:GLU:O	1:C:355:ALA:N	2.50	0.45
1:D:225:LYS:HG3	1:D:226:ARG:N	2.32	0.45
1:A:17:HIS:ND1	1:A:301:ASN:ND2	2.61	0.45
1:A:63:ASP:O	1:A:64:VAL:C	2.59	0.45
1:A:196:ILE:HG13	1:A:197:HIS:CG	2.52	0.45
1:C:101:CYS:SG	1:C:106:ARG:HB2	2.57	0.45
1:C:385:LEU:CD2	1:C:390:GLN:HB2	2.40	0.45
1:B:42:GLN:OE1	1:B:44:HIS:HE1	1.99	0.45
1:B:54:PRO:O	1:B:55:ASN:C	2.58	0.45
1:B:167:PRO:HD3	1:B:177:TRP:NE1	2.32	0.45
1:B:306:ASN:HD22	1:B:311:GLY:HA3	1.81	0.45
1:B:388:ARG:HA	1:B:388:ARG:NE	2.32	0.45
1:C:160:VAL:HG12	1:C:160:VAL:O	2.16	0.45
1:C:254:LEU:HD12	1:C:254:LEU:O	2.17	0.45
1:C:268:ILE:HA	1:C:271:ILE:HD12	1.99	0.45
1:D:41:LEU:HD22	1:D:156:ALA:HB1	1.99	0.45
1:A:21:ALA:HB1	1:A:26:LYS:CG	2.46	0.44
1:A:168:LEU:C	1:A:170:ASP:N	2.73	0.44
1:A:169:LYS:O	1:A:169:LYS:HG2	2.17	0.44
1:A:280:GLY:O	1:A:282:MET:N	2.49	0.44
1:A:370:THR:OG1	1:A:371:SER:N	2.43	0.44
1:B:284:GLU:C	1:B:286:PRO:HD3	2.42	0.44
1:B:289:GLU:O	1:B:292:LEU:HB3	2.16	0.44
1:B:327:LEU:HD21	1:B:348:LEU:HD11	1.99	0.44
1:C:22:VAL:HA	1:C:26:LYS:O	2.17	0.44
1:D:5:VAL:HG13	1:D:42:GLN:HB3	1.98	0.44
1:A:190:PHE:HD1	1:A:205:ASN:HD21	1.66	0.44
1:B:49:VAL:HG11	1:B:116:TYR:CZ	2.52	0.44
1:B:158:LEU:HB3	1:B:164:ILE:CG2	2.47	0.44
1:B:383:THR:OG1	1:B:384:SER:N	2.50	0.44
1:C:350:GLN:O	1:C:353:VAL:HG13	2.17	0.44
1:D:385:LEU:HD12	1:D:385:LEU:O	2.17	0.44
1:B:160:VAL:CG1	1:B:161:CYS:N	2.81	0.44
1:B:243:THR:O	1:B:247:VAL:HG23	2.17	0.44
1:B:319:CYS:O	1:B:323:ARG:HB2	2.18	0.44
1:C:10:ALA:O	1:C:36:ARG:HA	2.17	0.44
1:C:209:THR:HA	1:C:377:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:GLU:C	1:C:354:GLU:N	2.72	0.44
1:C:362:SER:HB3	2:C:408:HOH:O	2.17	0.44
1:D:70:LEU:HD23	1:D:72:THR:CG2	2.48	0.44
1:A:41:LEU:C	1:A:41:LEU:CD2	2.86	0.44
1:A:55:ASN:ND2	1:A:134:TRP:HE1	2.15	0.44
1:A:199:ASN:CB	1:C:281:GLU:HG3	2.47	0.44
1:A:237:THR:HA	1:A:365:PHE:CD2	2.53	0.44
1:B:109:VAL:C	1:B:111:ALA:N	2.76	0.44
1:B:287:ALA:O	1:B:288:PRO:C	2.59	0.44
1:B:320:GLN:C	1:B:320:GLN:OE1	2.59	0.44
1:C:157:LEU:C	1:C:159:THR:H	2.25	0.44
1:C:367:CYS:C	1:C:368:LEU:HD22	2.42	0.44
1:D:110:LEU:HB3	1:D:195:MET:HE2	2.00	0.44
1:D:177:TRP:HB3	1:D:181:ASP:HB2	1.98	0.44
1:A:82:THR:N	1:A:83:PRO:CD	2.81	0.44
1:A:291:TYR:O	1:A:292:LEU:C	2.61	0.44
1:A:312:HIS:CE1	1:A:314:SER:HG	2.33	0.44
1:B:7:LEU:CD1	1:B:382:ALA:HA	2.48	0.44
1:B:60:ARG:HH22	1:B:97:LEU:HD23	1.83	0.44
1:C:179:LYS:O	1:C:182:LEU:HB2	2.18	0.44
1:D:97:LEU:CB	1:D:98:PRO:HD2	2.38	0.44
1:D:243:THR:N	1:D:244:ARG:NH2	2.65	0.44
1:D:278:VAL:HG11	1:D:294:LEU:HD13	2.00	0.44
1:A:55:ASN:CG	1:A:134:TRP:CD1	2.96	0.44
1:A:322:THR:HG23	1:A:327:LEU:CB	2.45	0.44
1:B:264:LEU:HD21	1:B:307:ALA:HB3	2.00	0.44
1:C:285:ALA:N	1:C:286:PRO:HD3	2.33	0.44
1:A:215:ARG:N	1:A:222:SER:O	2.43	0.44
1:B:181:ASP:O	1:B:185:ILE:HG12	2.17	0.44
1:B:381:SER:O	1:B:382:ALA:HB2	2.18	0.44
1:C:36:ARG:HG2	1:C:36:ARG:NH1	2.33	0.44
1:D:381:SER:C	1:D:383:THR:N	2.74	0.44
1:D:385:LEU:C	1:D:387:SER:N	2.72	0.44
1:A:18:GLY:O	1:A:19:GLU:C	2.60	0.44
1:A:197:HIS:O	1:A:199:ASN:N	2.51	0.44
1:B:164:ILE:HD12	1:B:177:TRP:NE1	2.33	0.44
1:A:177:TRP:HB3	1:A:181:ASP:HB2	1.99	0.44
1:B:92:LYS:HG2	1:B:110:LEU:HD21	2.00	0.44
1:B:164:ILE:CD1	1:B:164:ILE:C	2.91	0.44
1:B:285:ALA:O	1:B:286:PRO:O	2.36	0.44
1:C:35:LEU:HD12	1:C:35:LEU:HA	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:VAL:O	1:C:262:ALA:C	2.61	0.44
1:B:63:ASP:C	1:B:65:ALA:N	2.70	0.43
1:B:390:GLN:O	1:B:394:ASP:CB	2.66	0.43
1:C:350:GLN:HA	1:C:353:VAL:HG13	2.01	0.43
1:D:22:VAL:HG23	1:D:23:VAL:N	2.32	0.43
1:A:160:VAL:O	1:A:162:GLU:N	2.51	0.43
1:B:53:LEU:CD1	1:B:108:ALA:HB1	2.48	0.43
1:B:151:VAL:CG1	1:B:377:VAL:CG2	2.95	0.43
1:B:213:ALA:C	1:B:214:LEU:HD12	2.43	0.43
1:B:376:GLY:O	1:B:377:VAL:C	2.60	0.43
1:C:302:GLN:HA	1:C:302:GLN:NE2	2.32	0.43
1:A:358:GLN:HA	1:A:361:THR:OG1	2.18	0.43
1:B:38:PHE:O	1:B:133:VAL:HG13	2.17	0.43
1:B:83:PRO:HG2	1:B:84:THR:H	1.82	0.43
1:B:119:ILE:N	1:B:119:ILE:HD12	2.32	0.43
1:B:216:TYR:HE1	1:B:219:GLY:CA	2.31	0.43
1:C:48:LYS:N	1:C:128:SER:HB2	2.33	0.43
1:C:165:PRO:HD2	1:C:181:ASP:OD1	2.19	0.43
1:D:335:GLY:C	1:D:337:GLY:N	2.76	0.43
1:A:14:VAL:HG12	1:A:143:LEU:HD12	1.99	0.43
1:A:72:THR:HA	1:A:74:PHE:CE1	2.54	0.43
1:A:158:LEU:CB	1:A:164:ILE:HD12	2.48	0.43
1:B:371:SER:O	1:B:372:ILE:HD12	2.18	0.43
1:C:7:LEU:CD1	1:C:382:ALA:HB2	2.47	0.43
1:D:218:GLN:HE21	1:D:218:GLN:HB2	1.54	0.43
1:B:18:GLY:O	1:B:19:GLU:C	2.60	0.43
1:B:41:LEU:HD21	1:B:129:LEU:HD22	2.01	0.43
1:B:64:VAL:O	1:B:68:GLN:HB2	2.18	0.43
1:D:39:LEU:CD1	1:D:153:LEU:HD23	2.43	0.43
1:D:184:LEU:O	1:D:185:ILE:C	2.62	0.43
1:A:160:VAL:C	1:A:162:GLU:N	2.77	0.43
1:B:68:GLN:C	1:B:70:LEU:N	2.76	0.43
1:B:124:ARG:HD3	2:B:451:HOH:O	2.18	0.43
1:D:15:ILE:HD12	1:D:333:GLY:HA2	2.01	0.43
1:D:75:LEU:HD13	1:D:121:ARG:HE	1.83	0.43
1:A:97:LEU:HA	1:A:98:PRO:HD2	1.88	0.43
1:A:199:ASN:ND2	1:A:199:ASN:O	2.52	0.43
1:A:256:LYS:HZ1	1:B:292:LEU:HD12	1.84	0.43
1:A:262:ALA:HB3	1:A:263:PRO:CD	2.44	0.43
1:B:45:SER:C	1:B:47:GLY:H	2.27	0.43
1:C:70:LEU:HD22	1:C:70:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:TRP:HZ3	1:C:377:VAL:C	2.26	0.43
1:D:275:CYS:O	1:D:276:GLU:C	2.61	0.43
1:D:304:HIS:O	1:D:307:ALA:HB3	2.19	0.43
1:A:280:GLY:C	1:A:282:MET:N	2.75	0.43
1:B:278:VAL:HG21	1:B:293:VAL:HG11	2.00	0.43
1:B:379:ILE:HG23	1:B:379:ILE:O	2.19	0.43
1:D:35:LEU:HD12	1:D:136:GLU:HB3	2.00	0.43
1:D:164:ILE:HD13	1:D:165:PRO:HG2	2.01	0.43
1:A:9:SER:HA	1:A:37:THR:O	2.19	0.43
1:A:186:ASN:OD1	1:A:210:TRP:CH2	2.72	0.43
1:A:289:GLU:O	1:A:293:VAL:HG23	2.18	0.43
1:B:3:SER:H	1:B:169:LYS:HD2	1.84	0.43
1:D:70:LEU:O	1:D:71:ASP:C	2.62	0.43
1:D:302:GLN:O	1:D:303:HIS:C	2.61	0.43
1:A:70:LEU:HD12	1:A:70:LEU:N	2.33	0.43
1:A:197:HIS:O	1:A:198:GLY:C	2.59	0.43
1:B:32:SER:OG	1:B:374:ALA:N	2.52	0.43
1:C:182:LEU:CD2	1:C:185:ILE:HD12	2.38	0.43
1:C:287:ALA:HB3	1:C:290:GLN:HE21	1.82	0.43
1:A:53:LEU:HD21	1:A:133:VAL:HB	2.00	0.42
1:A:99:ASP:HB2	1:A:100:ASP:H	1.55	0.42
1:A:361:THR:C	1:A:363:CYS:H	2.26	0.42
1:B:351:PRO:O	1:B:354:GLU:N	2.52	0.42
1:C:17:HIS:ND1	1:C:301:ASN:ND2	2.67	0.42
1:C:248:ALA:O	1:C:251:ARG:HB3	2.20	0.42
1:C:252:ASN:O	1:C:255:LEU:CD2	2.67	0.42
1:D:64:VAL:CG2	1:D:65:ALA:N	2.82	0.42
1:D:160:VAL:O	1:D:162:GLU:HG3	2.19	0.42
1:D:177:TRP:HB2	1:D:182:LEU:HD21	2.00	0.42
1:B:245:ALA:O	1:B:246:LEU:C	2.62	0.42
1:C:147:ALA:HB1	1:C:205:ASN:CA	2.49	0.42
1:C:163:GLU:OE2	1:C:163:GLU:CA	2.67	0.42
1:D:92:LYS:NZ	1:D:106:ARG:CZ	2.82	0.42
1:D:173:CYS:SG	1:D:384:SER:HB3	2.59	0.42
1:B:33:LEU:HD13	1:B:35:LEU:HD23	2.01	0.42
1:B:116:TYR:HA	1:B:157:LEU:HD13	2.01	0.42
1:B:119:ILE:HD12	1:B:119:ILE:H	1.85	0.42
1:B:204:ASP:O	1:B:205:ASN:C	2.63	0.42
1:C:40:ARG:HH12	1:C:390:GLN:CG	2.32	0.42
1:C:166:ASN:HA	1:C:167:PRO:HD3	1.73	0.42
1:D:8:VAL:O	1:D:38:PHE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ALA:O	1:D:37:THR:N	2.43	0.42
1:D:252:ASN:O	1:D:253:ARG:C	2.62	0.42
1:A:287:ALA:N	1:A:290:GLN:HE21	2.14	0.42
1:B:84:THR:O	1:B:88:VAL:HG23	2.19	0.42
1:C:98:PRO:HG2	1:C:101:CYS:HB3	2.02	0.42
1:C:242:ASN:O	1:C:245:ALA:HB3	2.19	0.42
1:D:19:GLU:OE1	1:D:330:LYS:NZ	2.49	0.42
1:D:33:LEU:CD2	1:D:35:LEU:HD23	2.49	0.42
1:D:221:ILE:CG2	1:D:222:SER:N	2.82	0.42
1:C:155:ALA:O	1:C:157:LEU:N	2.53	0.42
1:D:188:TRP:HA	1:D:188:TRP:CE3	2.54	0.42
1:D:362:SER:C	1:D:364:GLY:N	2.78	0.42
1:B:284:GLU:OE1	1:D:92:LYS:HE2	2.20	0.42
1:C:22:VAL:HG23	1:C:23:VAL:H	1.84	0.42
1:C:141:ALA:CB	1:C:143:LEU:CD2	2.96	0.42
1:C:248:ALA:O	1:C:249:GLY:C	2.63	0.42
1:B:70:LEU:HB2	1:B:72:THR:HG22	2.01	0.42
1:B:207:VAL:CG2	1:B:214:LEU:HD22	2.50	0.42
1:C:50:ASP:N	1:C:129:LEU:O	2.40	0.42
1:C:66:ARG:HG3	1:C:70:LEU:HD21	2.01	0.42
1:C:231:GLN:C	1:C:232:ILE:CG2	2.93	0.42
1:D:174:VAL:HG12	1:D:175:ASN:H	1.84	0.42
1:D:279:LEU:C	1:D:281:GLU:N	2.76	0.42
1:A:287:ALA:O	1:A:290:GLN:HB2	2.20	0.42
1:B:119:ILE:CG2	1:B:158:LEU:HD12	2.50	0.42
1:C:153:LEU:O	1:C:154:ALA:C	2.61	0.42
1:D:60:ARG:HG3	1:D:60:ARG:NH2	2.35	0.42
1:D:177:TRP:HB2	1:D:182:LEU:CD2	2.49	0.42
1:A:33:LEU:C	1:A:35:LEU:H	2.28	0.42
1:A:168:LEU:HD11	1:A:380:HIS:C	2.45	0.42
1:A:268:ILE:HA	1:A:271:ILE:HD12	2.01	0.42
1:B:166:ASN:OD1	1:B:168:LEU:O	2.38	0.42
1:C:44:HIS:O	1:C:46:ASN:N	2.53	0.42
1:D:207:VAL:HA	1:D:214:LEU:HD11	2.02	0.42
1:A:35:LEU:HD12	1:A:35:LEU:HA	1.85	0.42
1:A:84:THR:HG21	1:A:86:GLU:HB3	2.01	0.42
1:B:60:ARG:HH21	1:B:60:ARG:HG3	1.85	0.42
1:B:108:ALA:O	1:B:149:TYR:OH	2.24	0.42
1:B:358:GLN:HE21	1:B:358:GLN:HB2	1.65	0.42
1:C:13:LYS:HG2	1:C:14:VAL:N	2.35	0.42
1:C:49:VAL:O	1:C:61:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ILE:HD13	1:C:105:GLU:HG3	2.01	0.42
1:C:201:SER:C	1:C:203:VAL:H	2.28	0.42
1:C:225:LYS:NZ	1:C:225:LYS:CB	2.80	0.42
1:C:242:ASN:O	1:C:243:THR:C	2.63	0.42
1:C:315:LEU:O	1:C:318:LEU:HB3	2.20	0.42
1:D:16:LEU:HG	1:D:17:HIS:CD2	2.55	0.42
1:D:179:LYS:HG2	1:D:180:GLU:N	2.34	0.42
1:D:231:GLN:HE22	1:D:371:SER:HB3	1.83	0.42
1:D:273:LEU:CD1	1:D:273:LEU:N	2.83	0.42
1:A:151:VAL:O	1:A:154:ALA:HB3	2.20	0.41
1:A:282:MET:C	1:A:284:GLU:N	2.77	0.41
1:C:91:LEU:O	1:C:91:LEU:HD12	2.20	0.41
1:D:9:SER:HB3	1:D:38:PHE:CD2	2.55	0.41
1:D:91:LEU:HD12	1:D:113:LEU:HB3	2.01	0.41
1:D:104:THR:HG23	2:D:441:HOH:O	2.18	0.41
1:D:184:LEU:HG	1:D:188:TRP:HD1	1.85	0.41
1:A:49:VAL:CG1	1:A:62:TRP:HB2	2.48	0.41
1:A:211:GLY:HA3	1:A:375:PRO:O	2.19	0.41
1:B:46:ASN:OD1	1:B:48:LYS:HB2	2.20	0.41
1:B:49:VAL:HG11	1:B:116:TYR:CE2	2.55	0.41
1:B:158:LEU:HD22	1:B:185:ILE:HD13	2.02	0.41
1:C:44:HIS:O	1:C:46:ASN:ND2	2.53	0.41
1:C:54:PRO:HD3	1:C:132:VAL:HG13	2.01	0.41
1:C:66:ARG:C	1:C:68:GLN:H	2.28	0.41
1:C:83:PRO:HD3	1:C:194:ARG:HG3	2.02	0.41
1:C:157:LEU:O	1:C:159:THR:N	2.53	0.41
1:C:232:ILE:HD12	1:C:233:LEU:C	2.46	0.41
1:D:75:LEU:HB2	1:D:121:ARG:HD2	2.00	0.41
1:C:381:SER:C	1:C:383:THR:N	2.78	0.41
1:D:41:LEU:CB	1:D:131:ILE:HG12	2.50	0.41
1:D:251:ARG:HG2	1:D:251:ARG:NH1	2.32	0.41
1:D:345:LYS:HA	1:D:346:PRO:HD3	1.87	0.41
1:A:318:LEU:HD23	1:A:318:LEU:O	2.20	0.41
1:B:94:VAL:HG12	1:B:94:VAL:O	2.21	0.41
1:B:174:VAL:HB	1:B:175:ASN:H	1.60	0.41
1:C:83:PRO:HG3	1:C:198:GLY:CA	2.45	0.41
1:C:201:SER:O	1:C:221:ILE:HD11	2.20	0.41
1:D:165:PRO:HG2	1:D:181:ASP:OD1	2.19	0.41
1:D:221:ILE:HG22	1:D:222:SER:H	1.86	0.41
1:D:242:ASN:O	1:D:246:LEU:HD23	2.20	0.41
1:D:381:SER:C	1:D:383:THR:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLY:HA2	1:A:195:MET:HB3	2.03	0.41
1:A:239:VAL:HG21	1:A:314:SER:OG	2.20	0.41
1:B:88:VAL:O	1:B:92:LYS:HG3	2.21	0.41
1:B:187:LYS:HD3	1:B:187:LYS:HA	1.79	0.41
1:C:86:GLU:O	1:C:90:LYS:HG2	2.20	0.41
1:C:119:ILE:CD1	1:C:158:LEU:HD13	2.20	0.41
1:A:255:LEU:O	1:A:258:PRO:HD3	2.21	0.41
1:B:351:PRO:O	1:B:352:GLU:C	2.63	0.41
1:C:350:GLN:HE21	1:C:354:GLU:CG	2.26	0.41
1:A:9:SER:O	1:A:377:VAL:HA	2.20	0.41
1:A:47:GLY:C	1:A:64:VAL:HG13	2.46	0.41
1:A:280:GLY:O	1:A:283:GLY:N	2.53	0.41
1:C:34:ASN:CB	1:C:374:ALA:HB2	2.49	0.41
1:C:190:PHE:CZ	1:C:194:ARG:NH1	2.88	0.41
1:C:264:LEU:O	1:C:267:SER:N	2.51	0.41
1:D:81:THR:CG2	1:D:82:THR:N	2.84	0.41
1:D:263:PRO:O	1:D:266:THR:HB	2.20	0.41
1:D:282:MET:C	1:D:284:GLU:N	2.79	0.41
1:B:16:LEU:HG	1:B:17:HIS:CD2	2.55	0.41
1:B:63:ASP:C	1:B:65:ALA:H	2.28	0.41
1:B:153:LEU:O	1:B:154:ALA:C	2.64	0.41
1:B:177:TRP:CH2	1:B:379:ILE:HB	2.55	0.41
1:C:254:LEU:HD13	1:C:261:VAL:HG12	2.01	0.41
1:C:354:GLU:OE2	1:C:354:GLU:HA	2.20	0.41
1:D:117:LEU:O	1:D:121:ARG:HB2	2.21	0.41
1:A:2:LEU:O	1:A:3:SER:HB2	2.21	0.41
1:A:6:LEU:HB2	1:A:41:LEU:HB3	2.03	0.41
1:A:348:LEU:N	1:A:348:LEU:HD12	2.36	0.41
1:A:394:ASP:O	1:A:395:GLY:O	2.39	0.41
1:B:44:HIS:HD2	1:B:46:ASN:HD21	1.68	0.41
1:B:60:ARG:HG3	1:B:60:ARG:NH2	2.36	0.41
1:B:109:VAL:O	1:B:111:ALA:N	2.54	0.41
1:B:162:GLU:HG3	2:B:404:HOH:O	2.21	0.41
1:C:13:LYS:C	1:C:13:LYS:CD	2.94	0.41
1:C:18:GLY:O	1:C:19:GLU:C	2.63	0.41
1:C:54:PRO:C	1:C:56:ILE:N	2.77	0.41
1:C:181:ASP:O	1:C:184:LEU:HB3	2.20	0.41
1:C:196:ILE:C	1:C:196:ILE:HD12	2.45	0.41
1:D:60:ARG:HE	1:D:97:LEU:HD23	1.86	0.41
1:D:264:LEU:HD21	1:D:307:ALA:HB3	2.03	0.41
1:D:287:ALA:HB3	1:D:290:GLN:NE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:ALA:O	1:D:290:GLN:HB2	2.20	0.41
1:A:28:ALA:C	1:A:29:LEU:HD23	2.46	0.41
1:C:242:ASN:O	1:C:245:ALA:N	2.49	0.41
1:A:42:GLN:HA	1:A:43:PRO:HD3	1.85	0.40
1:B:386:ASP:CG	1:B:387:SER:N	2.80	0.40
1:C:36:ARG:H	1:C:36:ARG:HG3	1.56	0.40
1:C:242:ASN:C	1:C:242:ASN:ND2	2.77	0.40
1:D:14:VAL:CG2	1:D:372:ILE:HD11	2.51	0.40
1:D:122:LYS:HD2	1:D:163:GLU:CD	2.46	0.40
1:D:155:ALA:O	1:D:156:ALA:C	2.63	0.40
1:D:273:LEU:N	1:D:273:LEU:HD12	2.36	0.40
1:D:389:VAL:O	1:D:389:VAL:HG12	2.22	0.40
1:B:52:SER:HB3	1:B:132:VAL:CB	2.51	0.40
1:B:67:LEU:HD13	1:B:116:TYR:HE2	1.86	0.40
1:B:260:ILE:C	1:B:263:PRO:HD2	2.45	0.40
1:C:231:GLN:C	1:C:232:ILE:HG23	2.46	0.40
1:C:340:GLY:O	1:C:341:ILE:HD12	2.20	0.40
1:D:137:LEU:HD22	1:D:143:LEU:HB3	2.02	0.40
1:D:301:ASN:O	1:D:305:LEU:HG	2.21	0.40
1:C:71:ASP:C	1:C:73:SER:N	2.79	0.40
1:C:107:LEU:HG	1:C:196:ILE:HB	2.03	0.40
1:C:349:GLU:HB2	1:C:352:GLU:HG3	2.04	0.40
1:A:241:ARG:HH12	1:A:338:GLY:HA3	1.87	0.40
1:A:278:VAL:O	1:A:282:MET:HB2	2.21	0.40
1:B:318:LEU:O	1:B:322:THR:HG23	2.20	0.40
1:C:6:LEU:CD1	1:C:379:ILE:HD13	2.46	0.40
1:D:63:ASP:OD2	1:D:65:ALA:HB3	2.22	0.40
1:D:67:LEU:O	1:D:68:GLN:C	2.62	0.40
1:D:385:LEU:HD22	1:D:391:GLN:CG	2.52	0.40
1:D:387:SER:O	1:D:388:ARG:C	2.64	0.40
1:A:256:LYS:NZ	1:B:292:LEU:HD12	2.37	0.40
1:A:292:LEU:HD21	2:A:420:HOH:O	2.20	0.40
1:A:312:HIS:CE1	1:A:314:SER:OG	2.73	0.40
1:B:158:LEU:C	1:B:164:ILE:CG2	2.90	0.40
1:C:37:THR:HG23	1:C:135:SER:HB3	2.04	0.40
1:C:123:GLN:O	1:C:124:ARG:C	2.64	0.40
1:C:153:LEU:C	1:C:155:ALA:N	2.77	0.40
1:C:164:ILE:HD13	1:C:181:ASP:HB3	2.04	0.40
1:C:287:ALA:O	1:C:290:GLN:HB2	2.22	0.40
1:D:67:LEU:HB3	1:D:126:LEU:CD1	2.52	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	386/396 (98%)	327 (85%)	44 (11%)	15 (4%)	2	3
1	B	384/396 (97%)	304 (79%)	58 (15%)	22 (6%)	1	1
1	C	386/396 (98%)	292 (76%)	73 (19%)	21 (5%)	1	1
1	D	385/396 (97%)	310 (80%)	58 (15%)	17 (4%)	2	2
All	All	1541/1584 (97%)	1233 (80%)	233 (15%)	75 (5%)	1	2

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	95	ALA
1	A	99	ASP
1	A	169	LYS
1	A	284	GLU
1	A	382	ALA
1	B	72	THR
1	B	83	PRO
1	B	101	CYS
1	B	162	GLU
1	B	286	PRO
1	B	381	SER
1	B	386	ASP
1	C	19	GLU
1	C	36	ARG
1	C	45	SER
1	C	48	LYS
1	C	70	LEU
1	C	101	CYS
1	C	165	PRO
1	D	19	GLU
1	D	169	LYS

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Mol	Chain	Res	Type
1	D	170	ASP
1	D	179	LYS
1	A	161	CYS
1	A	171	GLY
1	A	198	GLY
1	A	283	GLY
1	B	65	ALA
1	B	70	LEU
1	B	281	GLU
1	B	351	PRO
1	B	377	VAL
1	B	382	ALA
1	C	72	THR
1	C	74	PHE
1	C	124	ARG
1	C	140	GLY
1	C	156	ALA
1	C	286	PRO
1	D	165	PRO
1	D	171	GLY
1	D	375	PRO
1	A	34	ASN
1	A	375	PRO
1	A	385	LEU
1	B	100	ASP
1	B	352	GLU
1	C	141	ALA
1	C	167	PRO
1	C	168	LEU
1	D	228	PRO
1	D	387	SER
1	D	390	GLN
1	B	161	CYS
1	B	175	ASN
1	B	375	PRO
1	C	4	GLU
1	C	179	LYS
1	D	74	PHE
1	D	172	ASP
1	D	347	GLY
1	B	88	VAL
1	B	391	GLN

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Mol	Chain	Res	Type
1	C	389	VAL
1	D	23	VAL
1	D	225	LYS
1	B	3	SER
1	C	202	GLY
1	D	103	VAL
1	A	47	GLY
1	A	228	PRO
1	D	374	ALA
1	C	139	PRO
1	B	174	VAL

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	321/326 (98%)	284 (88%)	37 (12%)	5	11
1	B	319/326 (98%)	281 (88%)	38 (12%)	5	11
1	C	321/326 (98%)	294 (92%)	27 (8%)	10	22
1	D	320/326 (98%)	298 (93%)	22 (7%)	14	30
All	All	1281/1304 (98%)	1157 (90%)	124 (10%)	8	17

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	33	LEU
1	A	35	LEU
1	A	49	VAL
1	A	51	LEU
1	A	55	ASN
1	A	60	ARG
1	A	63	ASP
1	A	91	LEU
1	A	99	ASP

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Mol	Chain	Res	Type
1	A	113	LEU
1	A	121	ARG
1	A	123	GLN
1	A	129	LEU
1	A	143	LEU
1	A	146	SER
1	A	172	ASP
1	A	199	ASN
1	A	214	LEU
1	A	241	ARG
1	A	244	ARG
1	A	273	LEU
1	A	290	GLN
1	A	292	LEU
1	A	294	LEU
1	A	296	GLU
1	A	314	SER
1	A	318	LEU
1	A	320	GLN
1	A	329	SER
1	A	332	THR
1	A	348	LEU
1	A	361	THR
1	A	375	PRO
1	A	385	LEU
1	A	388	ARG
1	A	391	GLN
1	B	2	LEU
1	B	13	LYS
1	B	19	GLU
1	B	22	VAL
1	B	33	LEU
1	B	35	LEU
1	B	44	HIS
1	B	70	LEU
1	B	72	THR
1	B	82	THR
1	B	104	THR
1	B	121	ARG
1	B	122	LYS
1	B	153	LEU
1	B	158	LEU

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Mol	Chain	Res	Type
1	B	164	ILE
1	B	168	LEU
1	B	170	ASP
1	B	172	ASP
1	B	174	VAL
1	B	178	THR
1	B	222	SER
1	B	225	LYS
1	B	246	LEU
1	B	273	LEU
1	B	300	MET
1	B	302	GLN
1	B	314	SER
1	B	320	GLN
1	B	341	ILE
1	B	350	GLN
1	B	353	VAL
1	B	356	THR
1	B	358	GLN
1	B	372	ILE
1	B	383	THR
1	B	388	ARG
1	B	389	VAL
1	C	4	GLU
1	C	13	LYS
1	C	22	VAL
1	C	33	LEU
1	C	39	LEU
1	C	41	LEU
1	C	49	VAL
1	C	51	LEU
1	C	69	SER
1	C	107	LEU
1	C	115	LEU
1	C	129	LEU
1	C	158	LEU
1	C	162	GLU
1	C	170	ASP
1	C	174	VAL
1	C	180	GLU
1	C	225	LYS
1	C	242	ASN

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Mol	Chain	Res	Type
1	C	255	LEU
1	C	277	ARG
1	C	318	LEU
1	C	341	ILE
1	C	353	VAL
1	C	358	GLN
1	C	372	ILE
1	C	377	VAL
1	D	22	VAL
1	D	33	LEU
1	D	35	LEU
1	D	86	GLU
1	D	97	LEU
1	D	129	LEU
1	D	143	LEU
1	D	159	THR
1	D	160	VAL
1	D	164	ILE
1	D	170	ASP
1	D	188	TRP
1	D	208	SER
1	D	218	GLN
1	D	244	ARG
1	D	294	LEU
1	D	320	GLN
1	D	348	LEU
1	D	361	THR
1	D	372	ILE
1	D	385	LEU
1	D	391	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	46	ASN
1	A	55	ASN
1	A	87	GLN
1	A	123	GLN
1	A	175	ASN
1	A	186	ASN
1	A	199	ASN

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Mol	Chain	Res	Type
1	A	205	ASN
1	A	252	ASN
1	A	290	GLN
1	A	301	ASN
1	A	303	HIS
1	A	317	GLN
1	A	320	GLN
1	A	390	GLN
1	A	391	GLN
1	B	46	ASN
1	B	55	ASN
1	B	186	ASN
1	B	191	GLN
1	B	205	ASN
1	B	252	ASN
1	B	301	ASN
1	B	302	GLN
1	B	303	HIS
1	B	306	ASN
1	B	317	GLN
1	B	328	HIS
1	B	350	GLN
1	B	358	GLN
1	C	42	GLN
1	C	175	ASN
1	C	186	ASN
1	C	191	GLN
1	C	199	ASN
1	C	205	ASN
1	C	231	GLN
1	C	236	ASN
1	C	242	ASN
1	C	290	GLN
1	C	301	ASN
1	C	302	GLN
1	C	303	HIS
1	C	306	ASN
1	C	320	GLN
1	C	350	GLN
1	C	358	GLN
1	C	390	GLN
1	C	391	GLN

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Mol	Chain	Res	Type
1	D	42	GLN
1	D	44	HIS
1	D	46	ASN
1	D	55	ASN
1	D	186	ASN
1	D	199	ASN
1	D	205	ASN
1	D	217	HIS
1	D	218	GLN
1	D	231	GLN
1	D	252	ASN
1	D	290	GLN
1	D	301	ASN
1	D	302	GLN
1	D	306	ASN
1	D	350	GLN
1	D	391	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

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	390/396 (98%)	-0.07	9 (2%) 61 57	10, 37, 71, 90	0
1	B	388/396 (97%)	0.05	5 (1%) 75 71	9, 41, 74, 94	0
1	C	390/396 (98%)	0.48	15 (3%) 44 39	27, 56, 76, 86	0
1	D	389/396 (98%)	0.40	7 (1%) 67 64	27, 53, 77, 82	0
All	All	1557/1584 (98%)	0.21	36 (2%) 61 57	9, 49, 75, 94	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	THR	3.9
1	A	395	GLY	3.8
1	C	2	LEU	3.6
1	A	82	THR	3.4
1	B	74	PHE	3.4
1	A	389	VAL	3.2
1	C	341	ILE	3.1
1	D	96	GLY	2.9
1	D	395	GLY	2.9
1	C	67	LEU	2.9
1	C	160	VAL	2.8
1	A	171	GLY	2.8
1	C	184	LEU	2.8
1	D	69	SER	2.7
1	A	80	VAL	2.7
1	B	82	THR	2.7
1	A	285	ALA	2.7
1	D	285	ALA	2.6
1	D	97	LEU	2.6
1	D	98	PRO	2.3
1	A	385	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	181	ASP	2.3
1	C	133	VAL	2.3
1	C	5	VAL	2.3
1	C	125	ALA	2.3
1	A	131	ILE	2.3
1	B	88	VAL	2.3
1	C	177	TRP	2.2
1	C	82	THR	2.2
1	C	167	PRO	2.2
1	B	83	PRO	2.2
1	C	126	LEU	2.1
1	A	286	PRO	2.1
1	C	80	VAL	2.1
1	D	164	ILE	2.1
1	C	119	ILE	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 oligosaccharides 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.