Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 06:52 PM EDT

PDB ID	:	3I5F
Title	:	Crystal structure of squid MG.ADP myosin S1
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Deposited on	:	2009-07-05
Resolution	:	3.10 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:

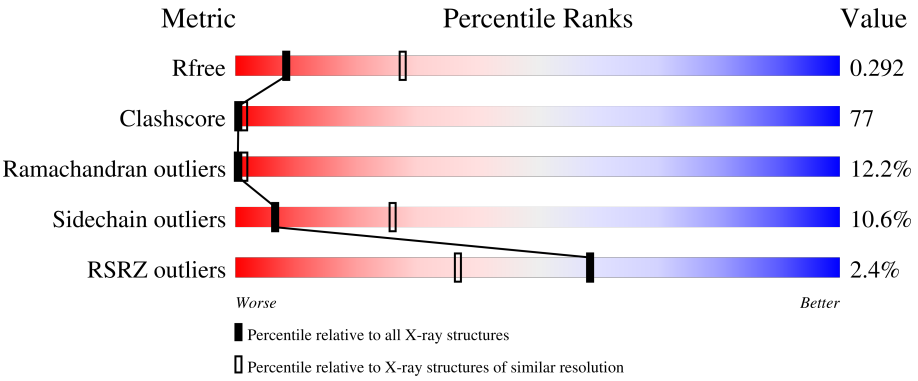
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	839	21% 59% 15%
2	B	153	8% 18% 49% 27% 5%
3	C	159	2% 20% 64% 15%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8971 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 Myosin heavy chain isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	S	0	0	0
			6514	4164	1114	1197	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	LYS	GLU	conflict	UNP O44934
A	744	ALA	VAL	conflict	UNP O44934

- Molecule 2 is a protein called Myosin regulatory light chain LC-2, mantle muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1166	733	191	233	9			

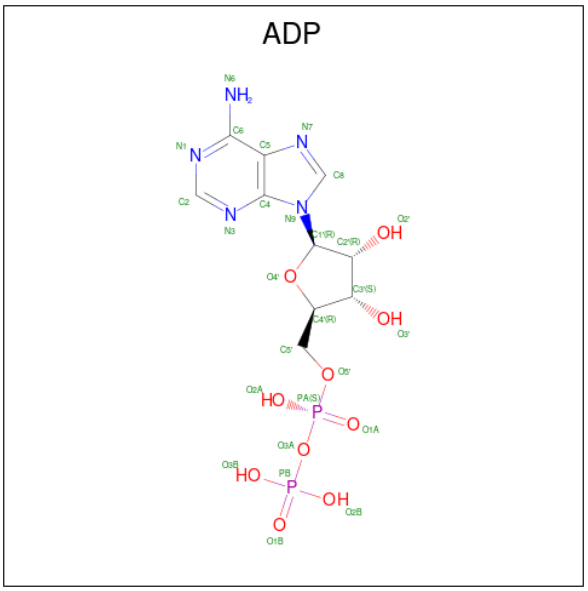
- Molecule 3 is a protein called Myosin catalytic light chain LC-1, mantle muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	159	Total	C	N	O	S	0	0	0
			1263	786	207	260	10			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



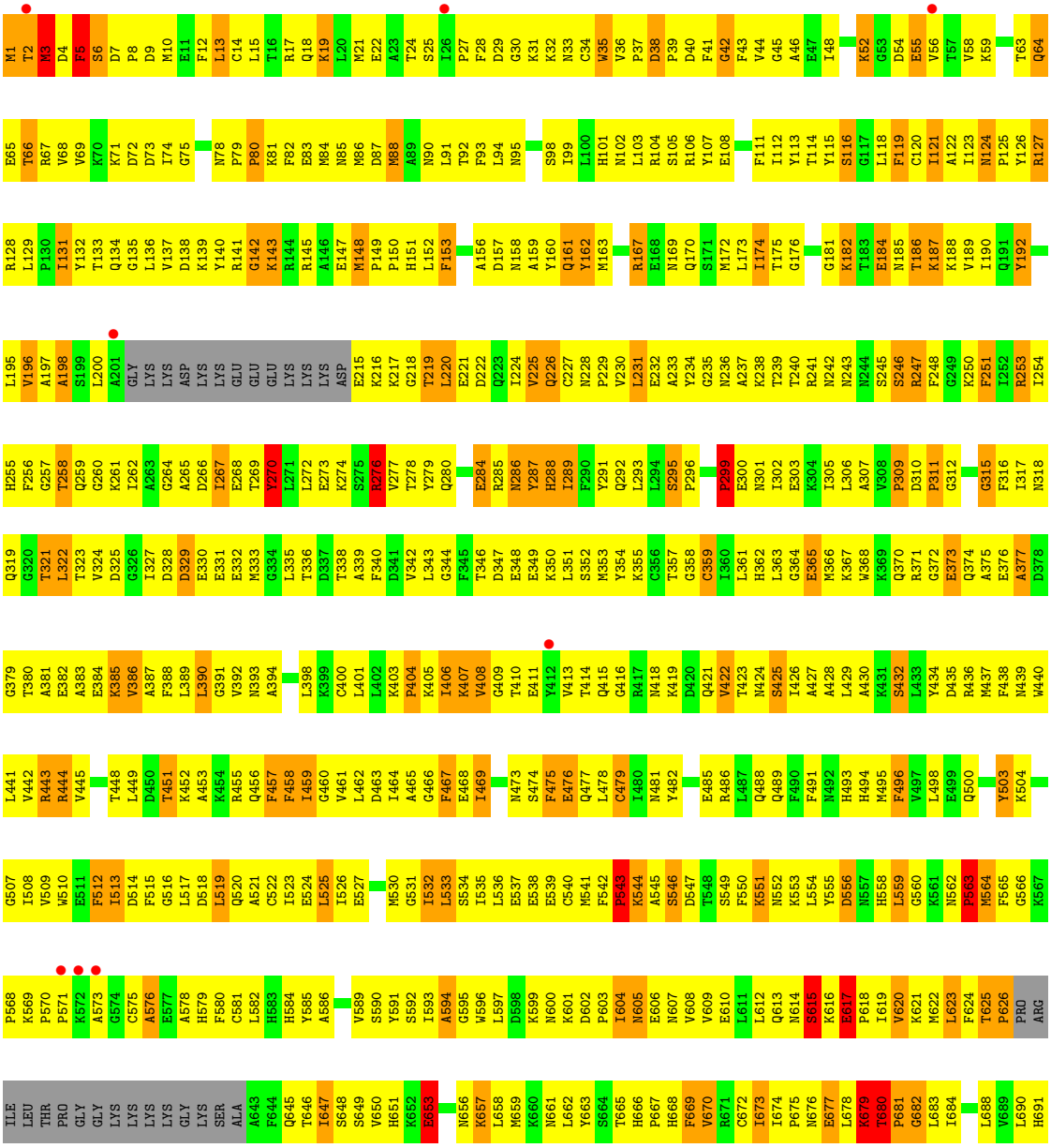
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

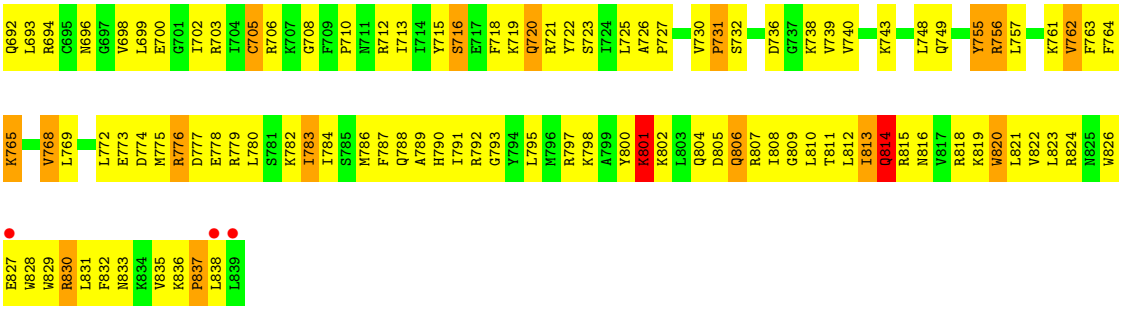
3 Residue-property plots (i)

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.

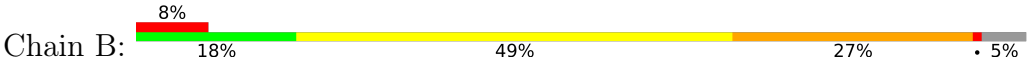
- Molecule 1: Myosin heavy chain isoform A

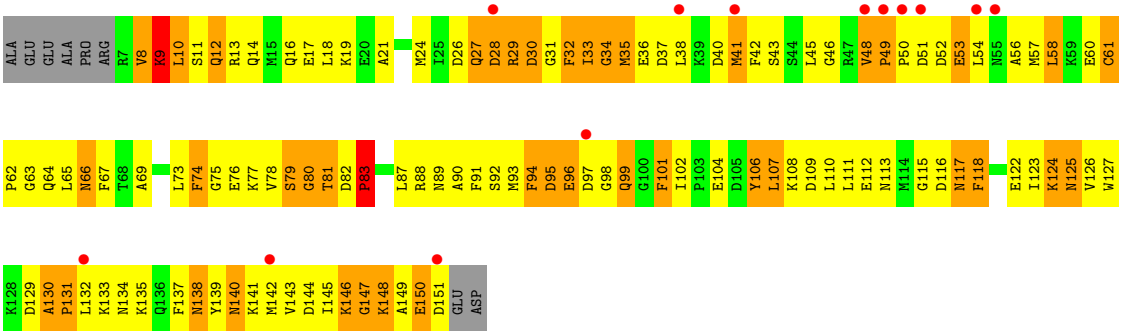
Chain A:



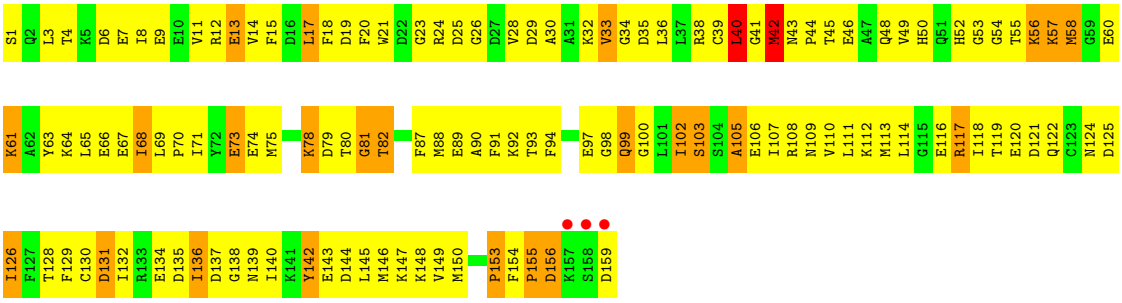


• Molecule 2: Myosin regulatory light chain LC-2, mantle muscle





• Molecule 3: Myosin catalytic light chain LC-1, mantle muscle



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	187.41Å 101.69Å 94.75Å 90.00° 119.75° 90.00°	Depositor
Resolution (Å)	43.23 – 3.10 43.25 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.6 (43.23-3.10) 83.4 (43.25-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.317 0.221 , 0.292	Depositor DCC
R_{free} test set	2552 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8971	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	0.68	2/6653 (0.0%)	1.10	21/8968 (0.2%)
2	B	0.63	0/1186	1.15	8/1588 (0.5%)
3	C	0.71	0/1282	1.11	3/1717 (0.2%)
All	All	0.68	2/9121 (0.0%)	1.11	32/12273 (0.3%)

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	4
2	B	0	1
3	C	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	653	GLU	CB-CG	5.83	1.63	1.52
1	A	820	TRP	CB-CG	-5.11	1.41	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	625	THR	C-N-CD	-8.50	101.89	120.60
1	A	626	PRO	CA-N-CD	-7.29	101.30	111.50
2	B	33	ILE	CB-CA-C	6.96	125.51	111.60
2	B	9	LYS	N-CA-C	6.86	129.51	111.00
1	A	623	LEU	CB-CG-CD1	-6.67	99.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	795	LEU	CA-CB-CG	6.30	129.79	115.30
1	A	680	THR	N-CA-C	6.29	128.00	111.00
1	A	220	LEU	CA-CB-CG	-6.29	100.83	115.30
1	A	466	GLY	N-CA-C	-6.08	97.91	113.10
1	A	453	ALA	N-CA-C	-6.00	94.81	111.00
3	C	114	LEU	N-CA-C	5.85	126.80	111.00
1	A	669	PHE	N-CA-C	5.85	126.79	111.00
2	B	150	GLU	N-CA-C	5.81	126.68	111.00
1	A	121	ILE	CB-CA-C	-5.70	100.20	111.60
1	A	459	ILE	N-CA-C	-5.65	95.74	111.00
1	A	251	PHE	N-CA-C	-5.63	95.81	111.00
1	A	726	ALA	C-N-CD	5.58	140.12	128.40
1	A	615	SER	N-CA-C	5.53	125.93	111.00
2	B	130	ALA	N-CA-C	5.52	125.91	111.00
1	A	143	LYS	N-CA-C	5.50	125.84	111.00
2	B	147	GLY	N-CA-C	-5.50	99.36	113.10
2	B	58	LEU	CB-CG-CD1	-5.48	101.68	111.00
1	A	617	GLU	N-CA-C	5.47	125.77	111.00
1	A	670	VAL	CB-CA-C	-5.44	101.06	111.40
3	C	40	LEU	N-CA-C	-5.35	96.56	111.00
1	A	276	ARG	CG-CD-NE	-5.33	100.62	111.80
2	B	101	PHE	N-CA-C	5.30	125.30	111.00
1	A	219	THR	N-CA-C	-5.24	96.87	111.00
2	B	28	ASP	N-CA-C	-5.22	96.90	111.00
1	A	625	THR	N-CA-C	5.22	125.09	111.00
1	A	13	LEU	CA-CB-CG	-5.19	103.36	115.30
3	C	17	LEU	CA-CB-CG	-5.05	103.69	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain
1	A	270	TYR	Sidechain
1	A	287	TYR	Sidechain
1	A	503	TYR	Sidechain
2	B	32	PHE	Sidechain
3	C	142	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6514	0	6519	1039	0
2	B	1166	0	1125	263	0
3	C	1263	0	1212	164	1
4	A	1	0	0	0	0
5	A	27	0	12	4	0
All	All	8971	0	8868	1382	1

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 77.

All (1382) 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:791:ILE:HG23	3:C:126:ILE:HD12	1.25	1.19
1:A:321:THR:O	1:A:322:LEU:HD23	1.41	1.17
1:A:550:PHE:CE2	1:A:554:LEU:HD11	1.82	1.14
2:B:143:VAL:O	2:B:146:LYS:HB3	1.46	1.13
1:A:792:ARG:HB3	3:C:38:ARG:NH1	1.62	1.11
1:A:406:ILE:HG22	1:A:407:LYS:H	1.14	1.11
1:A:1:MET:O	1:A:2:THR:HG23	1.51	1.09
1:A:436:ARG:NH1	1:A:623:LEU:HD22	1.66	1.09
1:A:814:GLN:HE22	2:B:116:ASP:N	1.50	1.09
1:A:674:ILE:HG22	1:A:692:GLN:HE22	1.10	1.08
1:A:816:ASN:HD22	2:B:87:LEU:HD13	0.97	1.08
1:A:372:GLY:O	1:A:374:GLN:N	1.85	1.08
1:A:612:LEU:HD13	1:A:623:LEU:HD11	1.29	1.08
1:A:359:CYS:SG	1:A:389:LEU:HB2	1.92	1.07
1:A:720:GLN:O	1:A:720:GLN:HG2	1.53	1.07
2:B:51:ASP:O	2:B:53:GLU:N	1.88	1.06
2:B:8:VAL:HG22	2:B:79:SER:HB3	1.37	1.06
1:A:175:THR:HG22	1:A:176:GLY:H	0.97	1.06
1:A:436:ARG:HH11	1:A:623:LEU:HD22	1.09	1.06
2:B:35:MET:HE2	2:B:54:LEU:HG	1.07	1.05
2:B:146:LYS:HG2	2:B:147:GLY:N	1.68	1.05
1:A:220:LEU:HD21	1:A:264:GLY:HA2	1.37	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:GLN:HG3	2:B:13:ARG:H	1.17	1.04
2:B:35:MET:HE1	2:B:54:LEU:O	1.58	1.03
1:A:764:PHE:CB	1:A:768:VAL:HG21	1.88	1.02
2:B:111:LEU:O	2:B:118:PHE:HB2	1.59	1.02
1:A:764:PHE:HB3	1:A:768:VAL:CG2	1.90	1.02
1:A:617:GLU:OE1	1:A:617:GLU:N	1.93	1.01
1:A:620:VAL:HG22	1:A:624:PHE:CE1	1.96	1.01
2:B:104:GLU:OE1	2:B:135:LYS:HD2	1.59	1.01
2:B:38:LEU:HD11	2:B:58:LEU:HD21	1.41	1.00
1:A:764:PHE:HB3	1:A:768:VAL:HG21	1.03	1.00
1:A:405:LYS:HA	1:A:413:VAL:O	1.61	1.00
1:A:536:LEU:HA	1:A:550:PHE:HE1	1.26	1.00
1:A:674:ILE:HG22	1:A:692:GLN:NE2	1.76	0.99
1:A:694:ARG:HG2	1:A:699:LEU:HD12	1.44	0.99
1:A:436:ARG:HH11	1:A:623:LEU:CD2	1.75	0.99
1:A:233:ALA:O	1:A:289:ILE:HB	1.63	0.99
1:A:274:LYS:O	1:A:277:VAL:HG23	1.62	0.98
1:A:816:ASN:HD22	2:B:87:LEU:CD1	1.76	0.98
1:A:52:LYS:HD2	1:A:55:GLU:HB3	1.45	0.98
1:A:86:MET:HE2	1:A:150:PRO:HD2	1.45	0.98
3:C:35:ASP:HA	3:C:38:ARG:HD2	1.43	0.98
3:C:78:LYS:HA	3:C:78:LYS:HE3	1.45	0.98
1:A:838:LEU:HG	2:B:24:MET:SD	2.04	0.97
2:B:35:MET:HE2	2:B:54:LEU:CG	1.95	0.97
1:A:88:MET:HB2	1:A:116:SER:HB2	1.43	0.97
1:A:406:ILE:HG22	1:A:407:LYS:N	1.80	0.96
2:B:35:MET:CE	2:B:54:LEU:HG	1.93	0.96
1:A:404:PRO:HB3	1:A:607:ASN:HD22	1.29	0.96
1:A:605:ASN:HB2	1:A:608:VAL:HG23	1.46	0.96
1:A:175:THR:HG22	1:A:176:GLY:N	1.80	0.96
1:A:269:THR:HG21	1:A:442:VAL:HG21	1.45	0.95
1:A:816:ASN:ND2	2:B:87:LEU:HD13	1.79	0.95
1:A:792:ARG:HB3	3:C:38:ARG:HH12	1.21	0.95
2:B:35:MET:CE	2:B:58:LEU:HD11	1.96	0.95
1:A:444:ARG:HH21	1:A:448:THR:HG23	1.31	0.94
1:A:646:THR:HG23	1:A:649:SER:H	1.32	0.93
1:A:175:THR:CG2	1:A:176:GLY:H	1.82	0.93
1:A:170:GLN:O	1:A:459:ILE:HA	1.68	0.93
1:A:250:LYS:O	1:A:462:LEU:HD12	1.68	0.93
1:A:131:ILE:HG23	1:A:151:HIS:CE1	2.04	0.92
1:A:620:VAL:HG22	1:A:624:PHE:HE1	1.26	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:GLN:HE22	2:B:116:ASP:H	1.00	0.92
1:A:232:GLU:HB3	1:A:236:ASN:HD22	1.33	0.91
2:B:27:GLN:C	2:B:29:ARG:H	1.73	0.90
1:A:85:ASN:HD22	1:A:91:LEU:HD23	1.35	0.90
1:A:151:HIS:NE2	1:A:153:PHE:CD1	2.38	0.90
1:A:818:ARG:HH21	2:B:118:PHE:HD1	0.93	0.90
1:A:256:PHE:CE1	1:A:459:ILE:HD12	2.07	0.89
1:A:355:LYS:HD2	1:A:616:LYS:NZ	1.86	0.89
1:A:355:LYS:HD2	1:A:616:LYS:HZ2	1.37	0.89
1:A:321:THR:HG22	1:A:322:LEU:H	1.35	0.89
1:A:235:GLY:HA3	1:A:248:PHE:HE1	1.38	0.89
1:A:832:PHE:CE1	2:B:18:LEU:HD23	2.08	0.89
2:B:150:GLU:HG2	2:B:151:ASP:H	1.37	0.89
1:A:78:ASN:OD1	1:A:93:PHE:HB2	1.74	0.88
1:A:184:GLU:OE2	1:A:184:GLU:HA	1.73	0.88
2:B:139:TYR:O	2:B:143:VAL:HG23	1.71	0.88
2:B:9:LYS:O	2:B:10:LEU:HG	1.73	0.88
1:A:531:GLY:HA2	1:A:558:HIS:NE2	1.87	0.88
1:A:550:PHE:HE2	1:A:554:LEU:HD11	1.35	0.88
1:A:94:LEU:O	1:A:706:ARG:NH2	2.06	0.88
1:A:235:GLY:O	1:A:247:ARG:HB2	1.73	0.88
3:C:66:GLU:OE1	3:C:66:GLU:N	2.07	0.87
1:A:169:ASN:HB3	1:A:665:THR:HG22	1.56	0.87
1:A:312:GLY:O	1:A:318:ASN:ND2	2.07	0.86
1:A:814:GLN:NE2	2:B:116:ASP:H	1.74	0.86
3:C:132:ILE:CD1	3:C:145:LEU:HD13	2.05	0.86
1:A:243:ASN:HB3	1:A:324:VAL:HG11	1.55	0.85
1:A:170:GLN:OE1	1:A:666:HIS:HB3	1.76	0.85
1:A:579:HIS:HD2	1:A:593:ILE:H	1.21	0.85
1:A:151:HIS:NE2	1:A:153:PHE:HD1	1.73	0.85
3:C:80:THR:O	3:C:82:THR:N	2.09	0.85
2:B:80:GLY:O	2:B:82:ASP:N	2.09	0.85
1:A:238:LYS:CD	1:A:324:VAL:HG22	2.06	0.84
2:B:28:ASP:HB3	2:B:37:ASP:OD2	1.77	0.84
2:B:26:ASP:O	2:B:29:ARG:C	2.15	0.84
1:A:95:ASN:O	1:A:99:ILE:HG12	1.77	0.84
1:A:593:ILE:O	1:A:595:GLY:N	2.11	0.84
1:A:536:LEU:HD12	1:A:550:PHE:CE1	2.12	0.84
1:A:612:LEU:O	1:A:614:ASN:N	2.09	0.84
1:A:612:LEU:CB	1:A:623:LEU:HD12	2.08	0.83
1:A:432:SER:HB2	1:A:604:ILE:HD11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:ARG:HB3	1:A:830:ARG:NH1	1.94	0.83
1:A:522:CYS:O	1:A:526:ILE:HG13	1.79	0.83
3:C:82:THR:HG21	3:C:87:PHE:CE2	2.13	0.83
1:A:71:LYS:HA	1:A:74:ILE:HD12	1.60	0.83
1:A:523:ILE:O	1:A:527:GLU:HG2	1.79	0.82
1:A:217:LYS:HD3	1:A:344:GLY:HA3	1.61	0.82
1:A:508:ILE:CG2	1:A:756:ARG:HG3	2.09	0.82
1:A:63:THR:O	1:A:64:GLN:HB2	1.77	0.82
1:A:181:GLY:HA2	5:A:1002:ADP:O1A	1.80	0.82
1:A:235:GLY:HA3	1:A:248:PHE:CE1	2.15	0.82
3:C:145:LEU:HD12	3:C:149:VAL:HG23	1.62	0.82
1:A:256:PHE:HE1	1:A:459:ILE:HD12	1.44	0.82
2:B:9:LYS:O	2:B:10:LEU:CG	2.28	0.82
1:A:346:THR:CB	1:A:349:GLU:HG3	2.10	0.82
2:B:35:MET:HE3	2:B:58:LEU:HD11	1.61	0.82
1:A:88:MET:CE	1:A:99:ILE:HA	2.10	0.81
3:C:88:MET:CE	3:C:143:GLU:HG3	2.10	0.81
1:A:612:LEU:CD1	1:A:623:LEU:HD11	2.10	0.81
1:A:536:LEU:CD2	1:A:600:ASN:ND2	2.42	0.81
2:B:12:GLN:HG3	2:B:13:ARG:N	1.95	0.81
1:A:2:THR:HG22	1:A:147:GLU:O	1.80	0.81
1:A:243:ASN:HD21	1:A:679:LYS:NZ	1.78	0.81
2:B:132:LEU:HD23	2:B:137:PHE:HB2	1.63	0.81
2:B:123:ILE:O	2:B:127:TRP:CD1	2.34	0.81
1:A:365:GLU:O	1:A:382:GLU:HG2	1.80	0.81
1:A:579:HIS:CD2	1:A:593:ILE:H	1.98	0.81
2:B:38:LEU:HD11	2:B:58:LEU:CD2	2.11	0.81
1:A:526:ILE:HG22	1:A:533:LEU:CD1	2.11	0.81
2:B:24:MET:HB3	2:B:41:MET:CE	2.10	0.81
2:B:26:ASP:CG	2:B:32:PHE:HA	2.01	0.81
1:A:317:ILE:HD11	1:A:361:LEU:HD21	1.63	0.81
1:A:831:LEU:CD1	1:A:835:VAL:HG21	2.11	0.81
1:A:432:SER:CB	1:A:604:ILE:HD11	2.10	0.80
2:B:26:ASP:O	2:B:29:ARG:N	2.14	0.80
2:B:127:TRP:CE3	2:B:132:LEU:HD13	2.16	0.80
1:A:128:ARG:O	1:A:129:LEU:HD23	1.81	0.80
1:A:151:HIS:CD2	1:A:153:PHE:HD1	1.99	0.80
1:A:616:LYS:O	1:A:619:ILE:HB	1.81	0.80
1:A:371:ARG:HG3	1:A:371:ARG:O	1.82	0.80
1:A:612:LEU:C	1:A:614:ASN:H	1.84	0.80
1:A:810:LEU:HD23	3:C:20:PHE:CZ	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ARG:HG2	1:A:443:ARG:HH11	1.44	0.80
1:A:617:GLU:H	1:A:617:GLU:CD	1.81	0.80
2:B:35:MET:HB3	2:B:54:LEU:HG	1.64	0.80
1:A:562:ASN:O	1:A:564:MET:N	2.15	0.79
2:B:143:VAL:O	2:B:146:LYS:CB	2.29	0.79
2:B:35:MET:HA	2:B:38:LEU:HG	1.62	0.79
1:A:220:LEU:O	1:A:224:ILE:HG13	1.82	0.79
1:A:508:ILE:HG21	1:A:756:ARG:HG3	1.62	0.79
2:B:28:ASP:HB2	2:B:37:ASP:HB3	1.64	0.79
2:B:141:LYS:O	2:B:145:ILE:N	2.14	0.79
2:B:12:GLN:CG	2:B:13:ARG:H	1.93	0.79
2:B:122:GLU:O	2:B:126:VAL:HG23	1.82	0.79
1:A:170:GLN:HB2	1:A:459:ILE:CG1	2.12	0.78
1:A:220:LEU:HD21	1:A:264:GLY:CA	2.13	0.78
1:A:353:MET:HE1	1:A:440:TRP:CZ3	2.18	0.78
2:B:28:ASP:O	2:B:37:ASP:OD1	2.00	0.78
2:B:8:VAL:CG1	2:B:9:LYS:N	2.47	0.78
1:A:232:GLU:CB	1:A:236:ASN:HD22	1.97	0.78
2:B:91:PHE:CD2	2:B:139:TYR:HB2	2.18	0.78
1:A:107:TYR:CD2	1:A:684:ILE:HD11	2.19	0.77
1:A:802:LYS:HE3	1:A:806:GLN:NE2	1.99	0.77
1:A:3:MET:HG3	1:A:148:MET:SD	2.23	0.77
1:A:52:LYS:HD2	1:A:55:GLU:CB	2.15	0.77
1:A:251:PHE:HE2	1:A:253:ARG:HD3	1.47	0.77
1:A:37:PRO:HG3	1:A:73:ASP:HB3	1.65	0.77
2:B:109:ASP:OD1	2:B:113:ASN:ND2	2.15	0.77
1:A:2:THR:HG21	1:A:148:MET:C	2.05	0.77
1:A:814:GLN:NE2	2:B:116:ASP:N	2.31	0.77
2:B:137:PHE:CE1	2:B:142:MET:SD	2.77	0.77
1:A:148:MET:HG3	1:A:149:PRO:CD	2.14	0.77
1:A:546:SER:O	1:A:549:SER:HB3	1.85	0.77
1:A:141:ARG:NH1	1:A:157:ASP:OD2	2.17	0.77
3:C:49:VAL:HG12	3:C:54:GLY:HA3	1.66	0.77
1:A:167:ARG:NH1	1:A:258:THR:HG23	1.99	0.77
1:A:352:SER:HB3	1:A:618:PRO:HG2	1.67	0.76
1:A:88:MET:HE1	1:A:99:ILE:HA	1.68	0.76
1:A:530:MET:HA	1:A:534:SER:OG	1.85	0.76
1:A:269:THR:HG21	1:A:442:VAL:CG2	2.15	0.76
1:A:827:GLU:OE1	1:A:830:ARG:NH2	2.17	0.76
1:A:618:PRO:O	1:A:622:MET:HG3	1.86	0.76
1:A:790:HIS:HE2	3:C:82:THR:HB	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ARG:NE	2:B:118:PHE:CE1	2.53	0.76
1:A:828:TRP:HZ2	2:B:57:MET:O	1.69	0.76
2:B:127:TRP:CZ3	2:B:132:LEU:HD13	2.21	0.76
1:A:176:GLY:O	1:A:182:LYS:NZ	2.18	0.76
1:A:219:THR:CG2	1:A:221:GLU:OE1	2.33	0.75
2:B:107:LEU:HD11	2:B:111:LEU:HD11	1.68	0.75
1:A:37:PRO:HD3	1:A:73:ASP:O	1.86	0.75
1:A:536:LEU:HD23	1:A:600:ASN:ND2	2.01	0.75
1:A:612:LEU:HD13	1:A:623:LEU:CD1	2.12	0.75
2:B:150:GLU:HG2	2:B:151:ASP:N	1.98	0.75
1:A:551:LYS:HB3	1:A:593:ILE:CD1	2.16	0.75
1:A:831:LEU:HD12	1:A:835:VAL:HG21	1.67	0.75
1:A:228:ASN:HB2	1:A:229:PRO:HD3	1.68	0.75
1:A:59:LYS:HA	1:A:65:GLU:O	1.85	0.75
1:A:551:LYS:HB3	1:A:593:ILE:HD13	1.68	0.75
1:A:614:ASN:O	1:A:615:SER:HB3	1.87	0.75
1:A:279:TYR:C	1:A:280:GLN:HG3	2.07	0.75
1:A:802:LYS:HE3	1:A:806:GLN:HE22	1.51	0.75
1:A:832:PHE:CZ	2:B:18:LEU:HD23	2.22	0.75
1:A:353:MET:HE1	1:A:440:TRP:CE3	2.22	0.75
1:A:519:LEU:O	1:A:523:ILE:HG13	1.87	0.75
1:A:827:GLU:CD	1:A:830:ARG:HH22	1.89	0.75
3:C:113:MET:O	3:C:117:ARG:HG2	1.86	0.75
1:A:148:MET:HG3	1:A:149:PRO:HD2	1.68	0.74
2:B:54:LEU:O	2:B:58:LEU:HG	1.86	0.74
2:B:126:VAL:O	2:B:130:ALA:HB2	1.87	0.74
1:A:140:TYR:OH	1:A:149:PRO:HD2	1.88	0.74
1:A:174:ILE:HG23	1:A:670:VAL:HB	1.68	0.74
1:A:536:LEU:CD2	1:A:600:ASN:HD22	2.00	0.74
3:C:50:HIS:CE1	3:C:56:LYS:HE3	2.22	0.74
1:A:41:PHE:HB3	1:A:104:ARG:HH12	1.52	0.74
1:A:818:ARG:NH2	2:B:118:PHE:HD1	1.78	0.74
2:B:137:PHE:CZ	2:B:142:MET:SD	2.81	0.74
1:A:444:ARG:HH21	1:A:448:THR:CG2	2.00	0.74
1:A:617:GLU:HB2	1:A:618:PRO:HD3	1.70	0.74
1:A:620:VAL:HG12	1:A:621:LYS:N	2.03	0.74
1:A:827:GLU:HA	1:A:830:ARG:NH2	2.03	0.74
1:A:786:MET:CE	3:C:80:THR:HG23	2.17	0.74
2:B:123:ILE:O	2:B:127:TRP:HD1	1.71	0.73
1:A:156:ALA:O	1:A:159:ALA:HB3	1.87	0.73
1:A:540:CYS:SG	1:A:601:LYS:HB3	2.29	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:PHE:O	1:A:544:LYS:N	2.21	0.73
1:A:646:THR:CG2	1:A:649:SER:HB3	2.18	0.73
1:A:118:LEU:HD11	1:A:498:LEU:HD23	1.69	0.73
2:B:104:GLU:HG2	2:B:127:TRP:HH2	1.53	0.73
1:A:267:ILE:N	1:A:267:ILE:HD12	2.04	0.73
1:A:318:ASN:OD1	1:A:318:ASN:O	2.05	0.73
2:B:26:ASP:O	2:B:29:ARG:CA	2.36	0.73
1:A:353:MET:CE	1:A:440:TRP:CZ3	2.70	0.73
1:A:678:LEU:O	1:A:680:THR:N	2.21	0.73
1:A:614:ASN:O	1:A:615:SER:CB	2.37	0.72
1:A:186:THR:OG1	1:A:463:ASP:OD1	2.06	0.72
1:A:69:VAL:CG1	1:A:73:ASP:HB2	2.19	0.72
1:A:181:GLY:HA2	5:A:1002:ADP:PA	2.30	0.72
1:A:788:GLN:HE21	3:C:111:LEU:HA	1.53	0.72
1:A:238:LYS:HD2	1:A:324:VAL:HG22	1.70	0.72
1:A:257:GLY:O	1:A:259:GLN:N	2.22	0.72
3:C:118:ILE:HG23	3:C:122:GLN:HB2	1.70	0.72
1:A:226:GLN:HG3	1:A:342:VAL:HG11	1.71	0.72
1:A:612:LEU:HB3	1:A:623:LEU:HD12	1.72	0.72
1:A:238:LYS:HD3	1:A:324:VAL:HG22	1.70	0.72
1:A:368:TRP:O	1:A:419:LYS:NZ	2.23	0.72
1:A:251:PHE:CE2	1:A:253:ARG:HD3	2.25	0.72
1:A:253:ARG:NH2	1:A:266:ASP:OD2	2.19	0.72
1:A:786:MET:HE1	3:C:80:THR:HG23	1.70	0.72
1:A:790:HIS:CD2	3:C:87:PHE:HZ	2.08	0.72
1:A:88:MET:HB2	1:A:116:SER:CB	2.18	0.71
1:A:346:THR:HB	1:A:349:GLU:HG3	1.72	0.71
1:A:768:VAL:HG23	1:A:769:LEU:H	1.55	0.71
2:B:28:ASP:CB	2:B:37:ASP:CG	2.58	0.71
2:B:35:MET:HB3	2:B:54:LEU:CG	2.20	0.71
3:C:105:ALA:O	3:C:108:ARG:N	2.23	0.71
1:A:78:ASN:HD21	1:A:91:LEU:HB3	1.54	0.71
3:C:66:GLU:H	3:C:66:GLU:CD	1.89	0.71
1:A:169:ASN:CB	1:A:665:THR:HG22	2.20	0.71
1:A:475:PHE:O	1:A:477:GLN:N	2.23	0.71
1:A:139:LYS:O	1:A:148:MET:HE1	1.91	0.71
1:A:219:THR:HG22	1:A:221:GLU:H	1.56	0.71
1:A:478:LEU:HB2	1:A:591:TYR:CE2	2.25	0.71
1:A:141:ARG:NH1	1:A:142:GLY:H	1.88	0.71
2:B:87:LEU:HD23	2:B:143:VAL:HG13	1.72	0.70
1:A:404:PRO:HB3	1:A:607:ASN:ND2	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LEU:HA	1:A:550:PHE:CE1	2.17	0.70
1:A:809:GLY:O	1:A:812:LEU:HB2	1.91	0.70
2:B:42:PHE:HA	2:B:45:LEU:HD12	1.73	0.70
1:A:822:VAL:HG12	1:A:822:VAL:O	1.90	0.70
1:A:288:HIS:O	1:A:292:GLN:HG3	1.91	0.70
1:A:9:ASP:HB3	1:A:136:LEU:HD21	1.73	0.70
1:A:555:TYR:O	1:A:559:LEU:HB2	1.91	0.70
2:B:24:MET:HB3	2:B:41:MET:HE2	1.74	0.70
1:A:85:ASN:HD22	1:A:91:LEU:CD2	2.04	0.70
1:A:88:MET:CB	1:A:116:SER:HB2	2.19	0.70
1:A:512:PHE:O	1:A:513:ILE:HG23	1.92	0.70
2:B:78:VAL:HG12	2:B:78:VAL:O	1.91	0.70
1:A:59:LYS:NZ	1:A:64:GLN:OE1	2.25	0.70
1:A:219:THR:HB	1:A:222:ASP:HB2	1.73	0.70
1:A:346:THR:HB	1:A:349:GLU:H	1.55	0.70
1:A:236:ASN:OD1	1:A:246:SER:HA	1.91	0.69
3:C:99:GLN:OE1	3:C:99:GLN:HA	1.89	0.69
1:A:170:GLN:HB2	1:A:459:ILE:HG12	1.73	0.69
1:A:826:TRP:CH2	2:B:73:LEU:HG	2.26	0.69
1:A:515:PHE:O	1:A:518:ASP:HB2	1.93	0.69
1:A:526:ILE:HG22	1:A:533:LEU:HD11	1.72	0.69
2:B:28:ASP:HB3	2:B:37:ASP:CG	2.12	0.69
1:A:1:MET:N	1:A:1:MET:HE2	2.07	0.69
1:A:680:THR:CG2	1:A:681:PRO:HD2	2.22	0.69
1:A:255:HIS:CD2	1:A:455:ARG:NH1	2.60	0.69
1:A:269:THR:CG2	1:A:442:VAL:HG21	2.20	0.69
1:A:390:LEU:HA	1:A:619:ILE:HD11	1.74	0.69
1:A:656:ASN:O	1:A:658:LEU:N	2.26	0.69
2:B:28:ASP:HB2	2:B:37:ASP:CB	2.23	0.69
3:C:112:LYS:HD3	3:C:120:GLU:OE1	1.92	0.69
1:A:69:VAL:HG11	1:A:73:ASP:HB2	1.74	0.69
1:A:805:ASP:C	2:B:93:MET:HE1	2.13	0.69
2:B:37:ASP:HA	2:B:40:ASP:HB2	1.75	0.69
1:A:276:ARG:O	1:A:286:ASN:ND2	2.26	0.69
1:A:493:HIS:ND1	1:A:514:ASP:OD2	2.26	0.69
1:A:124:ASN:HD22	1:A:124:ASN:C	1.96	0.68
1:A:359:CYS:O	1:A:363:LEU:HG	1.93	0.68
1:A:722:TYR:CE2	1:A:772:LEU:HB3	2.28	0.68
2:B:26:ASP:OD2	2:B:32:PHE:HA	1.92	0.68
1:A:488:GLN:HG2	1:A:585:TYR:CD2	2.28	0.68
2:B:19:LYS:HA	2:B:67:PHE:CE1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:LEU:O	1:A:584:HIS:CD2	2.46	0.68
1:A:243:ASN:ND2	1:A:679:LYS:NZ	2.41	0.68
1:A:251:PHE:CE1	1:A:662:LEU:HD21	2.29	0.68
2:B:29:ARG:HB2	2:B:33:ILE:HB	1.73	0.68
2:B:75:GLY:O	2:B:77:LYS:N	2.27	0.68
3:C:17:LEU:HD11	3:C:21:TRP:HE1	1.57	0.68
1:A:474:SER:O	1:A:477:GLN:HB2	1.93	0.68
1:A:226:GLN:HG3	1:A:342:VAL:CG1	2.24	0.68
2:B:28:ASP:CB	2:B:37:ASP:HB3	2.23	0.68
1:A:559:LEU:HG	1:A:560:GLY:H	1.58	0.68
1:A:137:VAL:HG13	1:A:192:TYR:HE1	1.58	0.67
1:A:405:LYS:O	1:A:405:LYS:HG3	1.94	0.67
1:A:17:ARG:O	1:A:21:MET:HG3	1.94	0.67
2:B:104:GLU:HG2	2:B:127:TRP:CH2	2.29	0.67
1:A:239:THR:HA	1:A:284:GLU:HG2	1.76	0.67
1:A:269:THR:C	1:A:270:TYR:HD1	1.97	0.67
1:A:289:ILE:HA	1:A:292:GLN:HG3	1.77	0.67
1:A:302:ILE:HD12	1:A:309:PRO:HG3	1.76	0.67
1:A:798:LYS:HE2	3:C:129:PHE:CE2	2.30	0.67
2:B:8:VAL:HG13	2:B:9:LYS:H	1.60	0.67
1:A:558:HIS:O	1:A:559:LEU:O	2.13	0.67
3:C:82:THR:CG2	3:C:87:PHE:CE2	2.78	0.67
1:A:293:LEU:HA	1:A:333:MET:CE	2.24	0.67
1:A:405:LYS:O	1:A:406:ILE:O	2.12	0.67
1:A:405:LYS:H	1:A:607:ASN:HD21	1.43	0.67
1:A:603:PRO:O	1:A:604:ILE:CB	2.43	0.67
1:A:163:MET:SD	1:A:256:PHE:CD1	2.88	0.67
1:A:157:ASP:OD1	1:A:161:GLN:NE2	2.25	0.67
1:A:219:THR:HG22	1:A:221:GLU:OE1	1.95	0.67
1:A:406:ILE:CG2	1:A:407:LYS:N	2.52	0.67
1:A:800:TYR:OH	3:C:14:VAL:HG22	1.95	0.67
1:A:403:LYS:HG2	1:A:415:GLN:O	1.94	0.67
2:B:31:GLY:C	2:B:32:PHE:CD1	2.69	0.67
2:B:33:ILE:HG22	2:B:37:ASP:OD1	1.94	0.67
1:A:126:TYR:O	1:A:681:PRO:HG3	1.95	0.66
1:A:170:GLN:O	1:A:459:ILE:CA	2.42	0.66
1:A:190:ILE:HD11	1:A:461:VAL:HG21	1.75	0.66
1:A:280:GLN:NE2	1:A:316:PHE:O	2.21	0.66
2:B:27:GLN:C	2:B:29:ARG:N	2.46	0.66
1:A:612:LEU:HB2	1:A:623:LEU:HD12	1.76	0.66
1:A:786:MET:HB3	3:C:82:THR:OG1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:ASP:OD2	3:C:58:MET:O	2.12	0.66
1:A:243:ASN:HD21	1:A:679:LYS:HZ3	1.43	0.66
1:A:269:THR:C	1:A:270:TYR:CD1	2.69	0.66
1:A:559:LEU:HG	1:A:560:GLY:N	2.11	0.66
1:A:300:GLU:O	1:A:303:GLU:N	2.29	0.66
1:A:550:PHE:CE2	1:A:554:LEU:CD1	2.72	0.66
1:A:2:THR:HG21	1:A:148:MET:O	1.96	0.66
1:A:167:ARG:HH12	1:A:258:THR:HA	1.60	0.66
1:A:539:GLU:OE1	1:A:539:GLU:HA	1.96	0.66
2:B:88:ARG:HG2	2:B:143:VAL:HG11	1.76	0.66
1:A:186:THR:HG22	1:A:187:LYS:N	2.09	0.66
1:A:649:SER:O	1:A:653:GLU:HG3	1.96	0.66
2:B:35:MET:CE	2:B:58:LEU:CD1	2.73	0.66
2:B:29:ARG:HB3	2:B:33:ILE:HD12	1.78	0.66
2:B:82:ASP:O	2:B:83:PRO:O	2.14	0.66
1:A:519:LEU:HD21	1:A:585:TYR:CD1	2.30	0.65
1:A:551:LYS:CB	1:A:593:ILE:CD1	2.74	0.65
1:A:413:VAL:HG12	1:A:414:THR:O	1.96	0.65
1:A:536:LEU:CA	1:A:550:PHE:HE1	2.06	0.65
1:A:546:SER:OG	1:A:549:SER:N	2.27	0.65
2:B:75:GLY:C	2:B:77:LYS:H	2.00	0.65
1:A:279:TYR:O	1:A:280:GLN:HG3	1.97	0.65
1:A:306:LEU:O	1:A:362:HIS:CE1	2.49	0.65
1:A:407:LYS:HA	1:A:411:GLU:O	1.97	0.65
1:A:605:ASN:HB2	1:A:608:VAL:CG2	2.24	0.65
1:A:421:GLN:O	1:A:423:THR:N	2.30	0.65
1:A:536:LEU:HD21	1:A:600:ASN:ND2	2.11	0.65
1:A:813:ILE:HG22	1:A:814:GLN:N	2.11	0.65
3:C:1:SER:HB3	3:C:73:GLU:OE1	1.97	0.65
1:A:359:CYS:SG	1:A:389:LEU:CB	2.79	0.65
1:A:798:LYS:NZ	3:C:129:PHE:CD2	2.64	0.65
1:A:831:LEU:HD12	1:A:835:VAL:CG2	2.25	0.65
2:B:132:LEU:CD2	2:B:137:PHE:HB2	2.26	0.65
1:A:65:GLU:CG	1:A:66:THR:H	2.10	0.65
1:A:646:THR:HG23	1:A:649:SER:N	2.07	0.65
3:C:14:VAL:HG12	3:C:36:LEU:CD1	2.26	0.65
1:A:41:PHE:HB3	1:A:104:ARG:NH1	2.12	0.65
1:A:276:ARG:HB2	1:A:286:ASN:ND2	2.12	0.65
1:A:550:PHE:O	1:A:554:LEU:HG	1.97	0.65
2:B:112:GLU:CD	2:B:123:ILE:HD13	2.16	0.65
3:C:15:PHE:O	3:C:18:PHE:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:HG13	1:A:113:TYR:H	1.61	0.65
1:A:137:VAL:HG13	1:A:192:TYR:CE1	2.32	0.65
1:A:429:LEU:HG	1:A:429:LEU:O	1.97	0.65
1:A:658:LEU:HG	1:A:659:MET:CE	2.27	0.65
1:A:813:ILE:HG12	2:B:91:PHE:CE1	2.32	0.65
2:B:9:LYS:O	2:B:10:LEU:CD2	2.45	0.65
1:A:2:THR:HG22	1:A:147:GLU:C	2.17	0.64
1:A:274:LYS:HE2	1:A:435:ASP:OD2	1.97	0.64
1:A:551:LYS:HD2	1:A:555:TYR:HE1	1.60	0.64
1:A:582:LEU:O	1:A:584:HIS:HD2	1.80	0.64
2:B:13:ARG:HG3	2:B:13:ARG:HH11	1.61	0.64
1:A:1:MET:N	1:A:1:MET:CE	2.61	0.64
1:A:332:GLU:OE1	1:A:332:GLU:HA	1.97	0.64
1:A:792:ARG:CB	3:C:38:ARG:HH12	2.05	0.64
1:A:736:ASP:O	1:A:739:VAL:HG23	1.97	0.64
1:A:278:THR:HA	1:A:316:PHE:CD2	2.32	0.64
1:A:551:LYS:HD2	1:A:555:TYR:CE1	2.32	0.64
1:A:551:LYS:HB2	1:A:593:ILE:HD11	1.80	0.64
1:A:830:ARG:CB	1:A:830:ARG:CZ	2.75	0.64
2:B:98:GLY:O	2:B:99:GLN:O	2.15	0.64
1:A:398:LEU:O	1:A:401:LEU:HB2	1.97	0.64
1:A:838:LEU:CG	2:B:24:MET:SD	2.84	0.64
1:A:41:PHE:O	1:A:43:PHE:N	2.28	0.64
1:A:273:GLU:OE1	1:A:276:ARG:NE	2.31	0.64
1:A:509:VAL:O	1:A:510:TRP:HB2	1.97	0.64
1:A:603:PRO:O	1:A:604:ILE:CG1	2.46	0.64
3:C:119:THR:OG1	3:C:122:GLN:HG3	1.96	0.64
1:A:112:ILE:HG13	1:A:113:TYR:N	2.13	0.63
1:A:170:GLN:HB2	1:A:459:ILE:HG13	1.78	0.63
1:A:274:LYS:NZ	1:A:647:ILE:CD1	2.61	0.63
1:A:620:VAL:HG12	1:A:621:LYS:H	1.64	0.63
3:C:57:LYS:O	3:C:60:GLU:HG3	1.97	0.63
1:A:346:THR:OG1	1:A:349:GLU:HG3	1.97	0.63
1:A:88:MET:HE3	1:A:99:ILE:HA	1.79	0.63
3:C:153:PRO:HD2	3:C:154:PHE:H	1.64	0.63
1:A:118:LEU:HD11	1:A:498:LEU:CD2	2.28	0.63
1:A:405:LYS:N	1:A:607:ASN:HD21	1.97	0.63
2:B:26:ASP:OD1	2:B:32:PHE:HA	1.98	0.63
2:B:113:ASN:O	2:B:117:ASN:OD1	2.15	0.63
3:C:82:THR:HG21	3:C:87:PHE:CZ	2.32	0.63
1:A:1:MET:O	1:A:2:THR:CG2	2.37	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASP:O	1:A:312:GLY:N	2.31	0.63
1:A:551:LYS:HG3	1:A:555:TYR:CD1	2.33	0.63
2:B:137:PHE:HE1	2:B:142:MET:SD	2.22	0.63
3:C:11:VAL:HA	3:C:40:LEU:HD21	1.81	0.63
3:C:57:LYS:HD2	3:C:58:MET:H	1.63	0.63
1:A:83:GLU:O	1:A:84:MET:HB2	1.98	0.63
1:A:482:TYR:O	1:A:485:GLU:HB3	1.98	0.63
2:B:9:LYS:O	2:B:10:LEU:HD23	1.99	0.63
1:A:722:TYR:CD2	1:A:772:LEU:HB3	2.34	0.63
3:C:144:ASP:OD1	3:C:148:LYS:HE3	1.99	0.63
1:A:134:GLN:HA	1:A:137:VAL:HG23	1.80	0.62
1:A:475:PHE:HB2	1:A:596:TRP:CD1	2.34	0.62
1:A:568:PRO:HG3	1:A:579:HIS:CA	2.29	0.62
1:A:830:ARG:HB3	1:A:830:ARG:CZ	2.27	0.62
1:A:756:ARG:HB2	1:A:763:PHE:HB2	1.81	0.62
1:A:666:HIS:CD2	1:A:668:HIS:CE1	2.87	0.62
2:B:137:PHE:O	2:B:137:PHE:CD2	2.52	0.62
1:A:251:PHE:HE2	1:A:253:ARG:CD	2.12	0.62
2:B:33:ILE:O	2:B:37:ASP:OD1	2.17	0.62
1:A:292:GLN:O	1:A:295:SER:HB3	1.99	0.62
1:A:666:HIS:HD2	1:A:668:HIS:CE1	2.18	0.62
1:A:141:ARG:O	1:A:143:LYS:N	2.32	0.62
1:A:293:LEU:HA	1:A:333:MET:HE3	1.79	0.62
1:A:836:LYS:C	1:A:838:LEU:H	2.02	0.62
1:A:1:MET:HE2	1:A:1:MET:H1	1.63	0.62
1:A:71:LYS:HA	1:A:74:ILE:CD1	2.29	0.62
1:A:500:GLN:HG3	1:A:512:PHE:CD1	2.34	0.62
1:A:605:ASN:C	1:A:607:ASN:N	2.50	0.62
1:A:317:ILE:HD11	1:A:361:LEU:CD2	2.28	0.62
1:A:457:PHE:CD1	1:A:457:PHE:N	2.66	0.62
3:C:36:LEU:CD2	3:C:68:ILE:HD12	2.28	0.62
1:A:2:THR:HG21	1:A:148:MET:CA	2.30	0.62
1:A:656:ASN:C	1:A:658:LEU:N	2.52	0.62
3:C:65:LEU:C	3:C:67:GLU:H	2.02	0.62
3:C:78:LYS:HE3	3:C:78:LYS:CA	2.26	0.62
1:A:296:PRO:HG2	1:A:330:GLU:CD	2.21	0.62
1:A:513:ILE:O	1:A:513:ILE:HG13	2.00	0.62
1:A:232:GLU:HG2	1:A:236:ASN:ND2	2.15	0.61
1:A:473:ASN:HB2	1:A:590:SER:O	2.00	0.61
1:A:526:ILE:HG22	1:A:533:LEU:HD12	1.82	0.61
1:A:267:ILE:HG22	1:A:268:GLU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:PHE:O	1:A:543:PRO:C	2.38	0.61
2:B:150:GLU:CG	2:B:151:ASP:H	2.09	0.61
1:A:272:LEU:HD22	1:A:438:PHE:CD2	2.35	0.61
1:A:676:ASN:ND2	1:A:683:LEU:HB3	2.15	0.61
2:B:131:PRO:HD2	2:B:142:MET:HG3	1.82	0.61
3:C:82:THR:CG2	3:C:87:PHE:CZ	2.83	0.61
1:A:579:HIS:HD2	1:A:593:ILE:N	1.97	0.61
1:A:604:ILE:HG22	1:A:609:VAL:HG23	1.82	0.61
1:A:115:TYR:CE1	1:A:150:PRO:HA	2.35	0.61
1:A:538:GLU:O	1:A:541:MET:N	2.25	0.61
2:B:8:VAL:HG12	2:B:9:LYS:N	2.14	0.61
1:A:469:ILE:HG23	1:A:589:VAL:HG22	1.82	0.61
1:A:539:GLU:HG3	1:A:550:PHE:HD1	1.65	0.61
1:A:721:ARG:CZ	1:A:776:ARG:NH1	2.64	0.61
2:B:14:GLN:O	2:B:18:LEU:HG	1.99	0.61
2:B:38:LEU:HB2	2:B:54:LEU:HD11	1.83	0.61
1:A:408:VAL:HG12	1:A:408:VAL:O	1.99	0.61
3:C:58:MET:O	3:C:58:MET:HG3	2.01	0.61
3:C:146:MET:O	3:C:150:MET:HG3	2.01	0.61
1:A:504:LYS:O	1:A:507:GLY:N	2.32	0.61
1:A:13:LEU:HD21	1:A:131:ILE:HG12	1.83	0.60
1:A:95:ASN:OD1	1:A:98:SER:OG	2.18	0.60
1:A:321:THR:HG22	1:A:322:LEU:N	2.13	0.60
1:A:666:HIS:CD2	1:A:668:HIS:HE1	2.18	0.60
3:C:132:ILE:HD11	3:C:145:LEU:HA	1.83	0.60
1:A:64:GLN:OE1	1:A:64:GLN:HA	2.01	0.60
1:A:422:VAL:HG12	1:A:422:VAL:O	2.01	0.60
1:A:730:VAL:O	1:A:731:PRO:O	2.18	0.60
3:C:132:ILE:HD12	3:C:145:LEU:HD13	1.82	0.60
1:A:38:ASP:OD1	1:A:40:ASP:N	2.34	0.60
1:A:126:TYR:O	1:A:127:ARG:HB3	2.01	0.60
1:A:321:THR:O	1:A:322:LEU:CD2	2.35	0.60
1:A:831:LEU:HD11	1:A:835:VAL:HG21	1.82	0.60
2:B:112:GLU:HG3	2:B:123:ILE:HD11	1.83	0.60
3:C:73:GLU:O	3:C:75:MET:N	2.34	0.60
1:A:801:LYS:O	1:A:804:GLN:HB2	2.01	0.60
2:B:66:ASN:OD1	2:B:69:ALA:CB	2.50	0.60
2:B:133:LYS:C	2:B:134:ASN:O	2.39	0.60
1:A:35:TRP:HA	1:A:35:TRP:CE3	2.36	0.60
1:A:232:GLU:HG2	1:A:236:ASN:HD21	1.66	0.60
1:A:764:PHE:CG	1:A:768:VAL:HG21	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:ARG:NH1	3:C:46:GLU:OE2	2.35	0.60
2:B:78:VAL:HG13	2:B:81:THR:OG1	2.01	0.60
2:B:95:ASP:O	2:B:97:ASP:N	2.34	0.60
3:C:153:PRO:CD	3:C:154:PHE:H	2.14	0.60
1:A:790:HIS:HD2	3:C:87:PHE:HZ	1.48	0.60
1:A:836:LYS:O	1:A:838:LEU:N	2.34	0.60
2:B:94:PHE:CD1	2:B:94:PHE:N	2.69	0.60
2:B:141:LYS:C	2:B:143:VAL:N	2.50	0.60
1:A:112:ILE:HG21	1:A:125:PRO:HD3	1.84	0.60
1:A:311:PRO:HG2	1:A:322:LEU:HD13	1.84	0.60
2:B:8:VAL:CG1	2:B:9:LYS:H	2.12	0.60
1:A:29:ASP:HB3	1:A:32:LYS:HB2	1.83	0.60
1:A:444:ARG:NH2	1:A:448:THR:CG2	2.65	0.60
1:A:539:GLU:HG3	1:A:550:PHE:CD1	2.37	0.60
1:A:617:GLU:O	1:A:620:VAL:N	2.34	0.60
3:C:12:ARG:O	3:C:14:VAL:N	2.34	0.59
1:A:243:ASN:ND2	1:A:679:LYS:HZ3	1.99	0.59
1:A:444:ARG:NH2	1:A:448:THR:HG23	2.11	0.59
1:A:65:GLU:HG3	1:A:66:THR:H	1.67	0.59
1:A:605:ASN:O	1:A:608:VAL:N	2.35	0.59
1:A:666:HIS:HD2	1:A:668:HIS:HE1	1.50	0.59
1:A:693:LEU:HA	1:A:696:ASN:HD22	1.67	0.59
1:A:121:ILE:HG22	1:A:122:ALA:N	2.17	0.59
2:B:35:MET:HA	2:B:38:LEU:CG	2.30	0.59
1:A:251:PHE:HD1	1:A:462:LEU:HD13	1.67	0.59
1:A:310:ASP:C	1:A:312:GLY:H	2.05	0.59
3:C:63:TYR:HD2	3:C:67:GLU:OE1	1.85	0.59
1:A:163:MET:SD	1:A:256:PHE:HD1	2.25	0.59
1:A:427:ALA:O	1:A:430:ALA:N	2.30	0.59
1:A:467:PHE:CZ	1:A:585:TYR:HB3	2.38	0.59
1:A:291:TYR:CZ	1:A:317:ILE:HG23	2.37	0.59
1:A:406:ILE:O	1:A:407:LYS:HG3	2.03	0.59
1:A:768:VAL:HG23	1:A:769:LEU:N	2.18	0.59
2:B:88:ARG:HD3	2:B:140:ASN:OD1	2.03	0.59
1:A:790:HIS:ND1	3:C:43:ASN:ND2	2.50	0.59
3:C:36:LEU:HD23	3:C:68:ILE:CD1	2.32	0.59
1:A:63:THR:O	1:A:64:GLN:CB	2.51	0.58
3:C:4:THR:O	3:C:8:ILE:HG13	2.03	0.58
1:A:28:PHE:HA	1:A:33:ASN:HD22	1.67	0.58
1:A:65:GLU:HG3	1:A:66:THR:N	2.17	0.58
1:A:792:ARG:HB3	3:C:38:ARG:HH11	1.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLU:O	1:A:332:GLU:C	2.41	0.58
1:A:536:LEU:CD1	1:A:550:PHE:CE1	2.83	0.58
1:A:811:THR:O	1:A:815:ARG:HB3	2.02	0.58
1:A:831:LEU:O	1:A:832:PHE:C	2.42	0.58
2:B:34:GLY:O	2:B:38:LEU:N	2.36	0.58
1:A:836:LYS:C	1:A:838:LEU:N	2.57	0.58
2:B:75:GLY:C	2:B:77:LYS:N	2.57	0.58
3:C:57:LYS:HZ2	3:C:58:MET:HB2	1.68	0.58
1:A:267:ILE:N	1:A:267:ILE:CD1	2.67	0.58
1:A:87:ASP:OD1	1:A:87:ASP:C	2.42	0.58
1:A:780:LEU:O	1:A:784:ILE:HG13	2.03	0.58
2:B:141:LYS:C	2:B:143:VAL:H	2.07	0.58
3:C:57:LYS:NZ	3:C:58:MET:HB2	2.19	0.58
1:A:606:GLU:O	1:A:610:GLU:HG2	2.04	0.58
1:A:823:LEU:HD21	2:B:77:LYS:HB3	1.85	0.58
1:A:826:TRP:HH2	2:B:73:LEU:HG	1.67	0.58
1:A:28:PHE:HA	1:A:33:ASN:ND2	2.18	0.58
1:A:305:ILE:HG22	1:A:355:LYS:HA	1.85	0.58
1:A:722:TYR:HB3	1:A:725:LEU:HD12	1.85	0.58
1:A:818:ARG:HE	2:B:118:PHE:HE1	1.43	0.58
3:C:80:THR:C	3:C:82:THR:H	2.07	0.58
1:A:86:MET:HE2	1:A:150:PRO:CD	2.29	0.57
1:A:232:GLU:CB	1:A:236:ASN:ND2	2.66	0.57
1:A:239:THR:HG22	1:A:240:THR:N	2.19	0.57
2:B:31:GLY:C	2:B:32:PHE:HD1	2.07	0.57
3:C:36:LEU:HD23	3:C:68:ILE:HD12	1.85	0.57
1:A:65:GLU:CG	1:A:66:THR:N	2.67	0.57
1:A:385:LYS:O	1:A:386:VAL:C	2.41	0.57
1:A:404:PRO:CB	1:A:607:ASN:ND2	2.68	0.57
1:A:486:ARG:O	1:A:489:GLN:N	2.36	0.57
1:A:836:LYS:N	1:A:837:PRO:HD2	2.19	0.57
1:A:40:ASP:HB2	1:A:41:PHE:CE1	2.38	0.57
1:A:167:ARG:HH12	1:A:258:THR:CA	2.17	0.57
1:A:373:GLU:O	1:A:373:GLU:HG2	2.04	0.57
1:A:830:ARG:HA	1:A:833:ASN:HD22	1.69	0.57
1:A:115:TYR:HB3	1:A:145:ARG:HH21	1.69	0.57
1:A:618:PRO:O	1:A:622:MET:CG	2.52	0.57
1:A:197:ALA:O	1:A:198:ALA:O	2.23	0.57
1:A:575:CYS:O	1:A:576:ALA:CB	2.52	0.57
1:A:789:ALA:HB1	3:C:44:PRO:O	2.03	0.57
2:B:106:TYR:O	2:B:108:LYS:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:TYR:CE1	3:C:17:LEU:HD23	2.40	0.57
1:A:826:TRP:HZ3	2:B:74:PHE:CD2	2.21	0.57
1:A:828:TRP:CZ2	2:B:57:MET:O	2.56	0.57
1:A:405:LYS:CA	1:A:413:VAL:O	2.46	0.57
1:A:835:VAL:O	1:A:838:LEU:HB3	2.03	0.57
1:A:104:ARG:HA	1:A:107:TYR:HB3	1.87	0.57
1:A:253:ARG:O	1:A:265:ALA:HB1	2.05	0.57
1:A:362:HIS:CE1	1:A:385:LYS:HD3	2.40	0.57
1:A:436:ARG:HD3	1:A:623:LEU:HD23	1.86	0.57
1:A:536:LEU:HD21	1:A:600:ASN:HD22	1.68	0.57
1:A:612:LEU:C	1:A:614:ASN:N	2.52	0.57
1:A:693:LEU:HA	1:A:696:ASN:ND2	2.19	0.57
1:A:830:ARG:HA	1:A:833:ASN:ND2	2.20	0.57
2:B:38:LEU:HD12	2:B:54:LEU:HD12	1.86	0.57
1:A:366:MET:HE2	1:A:383:ALA:CA	2.35	0.56
1:A:568:PRO:HG3	1:A:579:HIS:C	2.26	0.56
1:A:603:PRO:O	1:A:604:ILE:HB	2.04	0.56
2:B:147:GLY:O	2:B:148:LYS:HB2	2.05	0.56
1:A:167:ARG:HH12	1:A:258:THR:HG23	1.67	0.56
1:A:366:MET:HE2	1:A:383:ALA:HA	1.87	0.56
1:A:485:GLU:OE1	1:A:485:GLU:HA	2.05	0.56
1:A:773:GLU:HA	1:A:773:GLU:OE1	2.05	0.56
1:A:783:ILE:HG21	3:C:90:ALA:HB2	1.85	0.56
1:A:128:ARG:C	1:A:129:LEU:HD23	2.26	0.56
1:A:285:ARG:NH2	1:A:329:ASP:OD2	2.38	0.56
1:A:400:CYS:HB3	1:A:607:ASN:HB3	1.86	0.56
1:A:617:GLU:O	1:A:618:PRO:C	2.43	0.56
2:B:28:ASP:CB	2:B:37:ASP:CB	2.82	0.56
1:A:35:TRP:HA	1:A:35:TRP:HE3	1.71	0.56
1:A:99:ILE:HD11	1:A:702:ILE:HD13	1.86	0.56
1:A:273:GLU:HB3	1:A:287:TYR:OH	2.05	0.56
1:A:445:VAL:O	1:A:448:THR:N	2.37	0.56
1:A:617:GLU:O	1:A:620:VAL:HB	2.05	0.56
1:A:790:HIS:CD2	3:C:87:PHE:CZ	2.92	0.56
1:A:792:ARG:NH2	3:C:116:GLU:O	2.38	0.56
2:B:13:ARG:HG3	2:B:13:ARG:NH1	2.20	0.56
1:A:197:ALA:O	1:A:198:ALA:C	2.43	0.56
1:A:719:LYS:HD2	1:A:740:VAL:HG21	1.86	0.56
1:A:755:TYR:HA	1:A:763:PHE:O	2.06	0.56
1:A:819:LYS:HE3	2:B:77:LYS:O	2.06	0.56
2:B:19:LYS:HA	2:B:67:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:MET:SD	2:B:58:LEU:HD11	2.46	0.56
1:A:385:LYS:O	1:A:388:PHE:N	2.39	0.56
1:A:708:GLY:O	1:A:765:LYS:NZ	2.33	0.56
1:A:29:ASP:C	1:A:31:LYS:H	2.08	0.56
1:A:54:ASP:O	1:A:56:VAL:N	2.36	0.56
1:A:266:ASP:C	1:A:267:ILE:HD12	2.26	0.56
1:A:688:LEU:O	1:A:691:HIS:HB3	2.05	0.56
1:A:826:TRP:HZ3	2:B:74:PHE:CE2	2.24	0.56
2:B:35:MET:HE1	2:B:54:LEU:C	2.26	0.56
1:A:232:GLU:CG	1:A:236:ASN:ND2	2.69	0.56
1:A:620:VAL:HA	1:A:624:PHE:CD1	2.40	0.56
1:A:36:VAL:HG22	1:A:44:VAL:O	2.06	0.56
1:A:536:LEU:O	1:A:540:CYS:HB2	2.06	0.56
3:C:92:LYS:C	3:C:94:PHE:H	2.10	0.56
1:A:285:ARG:HG2	1:A:286:ASN:H	1.71	0.56
1:A:537:GLU:OE2	1:A:648:SER:OG	2.22	0.56
1:A:798:LYS:NZ	3:C:129:PHE:HD2	2.04	0.56
1:A:226:GLN:CG	1:A:342:VAL:HG11	2.36	0.55
1:A:612:LEU:CD1	1:A:623:LEU:CD1	2.80	0.55
2:B:29:ARG:HB2	2:B:33:ILE:CB	2.36	0.55
1:A:37:PRO:CD	1:A:73:ASP:O	2.54	0.55
1:A:44:VAL:CG1	1:A:45:GLY:N	2.69	0.55
1:A:355:LYS:CD	1:A:616:LYS:HZ2	2.15	0.55
1:A:680:THR:HG22	1:A:681:PRO:HD2	1.87	0.55
2:B:29:ARG:HB2	2:B:33:ILE:CG2	2.37	0.55
2:B:141:LYS:O	2:B:144:ASP:N	2.39	0.55
2:B:112:GLU:HG3	2:B:123:ILE:CD1	2.36	0.55
3:C:39:CYS:C	3:C:41:GLY:H	2.08	0.55
2:B:66:ASN:OD1	2:B:69:ALA:HB3	2.07	0.55
1:A:34:CYS:HB2	1:A:75:GLY:O	2.06	0.55
1:A:291:TYR:CE2	1:A:317:ILE:CG2	2.90	0.55
1:A:547:ASP:HB3	1:A:593:ILE:HG22	1.88	0.55
2:B:146:LYS:HG2	2:B:147:GLY:H	1.66	0.55
1:A:226:GLN:OE1	1:A:226:GLN:HA	2.07	0.55
1:A:434:TYR:O	1:A:437:MET:N	2.40	0.55
1:A:228:ASN:O	1:A:232:GLU:HG3	2.05	0.55
1:A:558:HIS:O	1:A:559:LEU:C	2.44	0.55
1:A:620:VAL:HA	1:A:624:PHE:HD1	1.72	0.55
1:A:721:ARG:NH2	1:A:776:ARG:NH1	2.53	0.55
2:B:18:LEU:HD22	2:B:74:PHE:CD1	2.42	0.55
2:B:124:LYS:O	2:B:126:VAL:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	1:A:1:MET:H3	2.19	0.55
1:A:440:TRP:HE1	1:A:621:LYS:HD2	1.71	0.55
1:A:543:PRO:C	1:A:545:ALA:H	2.10	0.55
1:A:659:MET:CE	1:A:659:MET:N	2.70	0.55
1:A:675:PRO:HD2	1:A:676:ASN:H	1.72	0.55
1:A:612:LEU:HD22	1:A:619:ILE:HG23	1.89	0.55
1:A:646:THR:CG2	1:A:649:SER:CB	2.85	0.55
1:A:835:VAL:HG13	1:A:838:LEU:HD23	1.89	0.55
2:B:35:MET:HB3	2:B:54:LEU:CD2	2.37	0.55
1:A:478:LEU:O	1:A:479:CYS:O	2.25	0.54
1:A:680:THR:HG23	1:A:681:PRO:HD2	1.89	0.54
1:A:38:ASP:N	1:A:42:GLY:O	2.40	0.54
1:A:125:PRO:O	1:A:126:TYR:HB2	2.07	0.54
1:A:190:ILE:HD11	1:A:461:VAL:CG2	2.38	0.54
1:A:276:ARG:HA	1:A:279:TYR:O	2.06	0.54
1:A:605:ASN:C	1:A:607:ASN:H	2.10	0.54
1:A:151:HIS:HD2	1:A:153:PHE:H	1.56	0.54
1:A:220:LEU:HD23	1:A:262:ILE:HG22	1.89	0.54
1:A:563:PRO:C	1:A:565:PHE:H	2.09	0.54
2:B:29:ARG:HB3	2:B:33:ILE:CD1	2.36	0.54
3:C:49:VAL:CG1	3:C:54:GLY:HA3	2.36	0.54
3:C:88:MET:HE1	3:C:143:GLU:HG3	1.87	0.54
1:A:251:PHE:HE1	1:A:662:LEU:HD21	1.72	0.54
1:A:730:VAL:O	1:A:731:PRO:C	2.44	0.54
3:C:148:LYS:O	3:C:149:VAL:C	2.44	0.54
1:A:44:VAL:HG12	1:A:45:GLY:N	2.22	0.54
1:A:358:GLY:O	1:A:361:LEU:HB2	2.08	0.54
1:A:464:ILE:HG13	1:A:465:ALA:N	2.21	0.54
1:A:656:ASN:O	1:A:657:LYS:C	2.46	0.54
2:B:26:ASP:HB3	2:B:29:ARG:O	2.07	0.54
1:A:258:THR:C	1:A:260:GLY:N	2.59	0.54
1:A:375:ALA:HB3	1:A:422:VAL:HG21	1.90	0.54
1:A:519:LEU:HD21	1:A:585:TYR:HD1	1.71	0.54
1:A:761:LYS:HB2	1:A:763:PHE:HE1	1.72	0.54
1:A:4:ASP:C	1:A:6:SER:H	2.11	0.54
1:A:134:GLN:HA	1:A:137:VAL:CG2	2.37	0.54
1:A:274:LYS:HZ1	1:A:647:ILE:CD1	2.21	0.54
1:A:353:MET:HE3	1:A:440:TRP:CZ3	2.42	0.54
1:A:31:LYS:O	1:A:48:ILE:HD12	2.07	0.54
1:A:339:ALA:O	1:A:343:LEU:HG	2.07	0.54
1:A:524:GLU:O	1:A:525:LEU:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:CYS:HB3	1:A:710:PRO:HB3	1.89	0.54
2:B:28:ASP:HB2	2:B:37:ASP:CG	2.29	0.54
1:A:531:GLY:HA2	1:A:558:HIS:CE1	2.43	0.54
1:A:174:ILE:HD12	1:A:186:THR:HG1	1.72	0.53
1:A:190:ILE:CD1	1:A:461:VAL:HG21	2.37	0.53
1:A:786:MET:HE1	3:C:80:THR:CG2	2.37	0.53
2:B:127:TRP:CE3	2:B:132:LEU:CD1	2.90	0.53
3:C:145:LEU:CD1	3:C:149:VAL:HG23	2.37	0.53
1:A:126:TYR:O	1:A:127:ARG:CB	2.55	0.53
1:A:813:ILE:O	1:A:815:ARG:N	2.41	0.53
2:B:35:MET:HE1	2:B:58:LEU:CD1	2.37	0.53
2:B:127:TRP:CD1	2:B:127:TRP:N	2.76	0.53
3:C:135:ASP:O	3:C:138:GLY:N	2.33	0.53
1:A:239:THR:HG23	1:A:284:GLU:OE2	2.09	0.53
1:A:382:GLU:O	1:A:385:LYS:HG3	2.08	0.53
1:A:219:THR:HB	1:A:222:ASP:CB	2.38	0.53
1:A:659:MET:N	1:A:659:MET:HE3	2.24	0.53
1:A:818:ARG:NH2	2:B:118:PHE:CD1	2.61	0.53
1:A:267:ILE:HD11	1:A:449:LEU:HD12	1.89	0.53
1:A:370:GLN:OE1	1:A:418:ASN:HB2	2.08	0.53
1:A:380:THR:O	1:A:384:GLU:HG3	2.09	0.53
2:B:16:GLN:O	2:B:19:LYS:HB3	2.09	0.53
1:A:15:LEU:HD22	1:A:19:LYS:HG3	1.91	0.53
1:A:521:ALA:HB1	1:A:564:MET:HG3	1.91	0.53
1:A:12:PHE:O	1:A:111:PHE:HD2	1.91	0.53
1:A:52:LYS:HG3	1:A:55:GLU:O	2.09	0.53
1:A:826:TRP:CZ2	2:B:73:LEU:HG	2.44	0.53
1:A:151:HIS:CD2	1:A:153:PHE:CD1	2.86	0.53
1:A:215:GLU:HG3	1:A:216:LYS:N	2.23	0.53
1:A:291:TYR:CE2	1:A:317:ILE:HG23	2.44	0.53
1:A:434:TYR:O	1:A:435:ASP:C	2.47	0.53
1:A:692:GLN:O	1:A:693:LEU:C	2.46	0.53
1:A:790:HIS:HD2	3:C:87:PHE:CZ	2.25	0.53
1:A:230:VAL:HG23	1:A:339:ALA:HB3	1.91	0.53
1:A:374:GLN:NE2	1:A:416:GLY:HA2	2.24	0.53
1:A:519:LEU:O	1:A:523:ILE:CD1	2.57	0.53
1:A:601:LYS:O	1:A:601:LYS:HG3	2.09	0.53
1:A:659:MET:O	1:A:663:TYR:HD1	1.91	0.53
3:C:65:LEU:C	3:C:67:GLU:N	2.62	0.53
1:A:157:ASP:O	1:A:158:ASN:C	2.44	0.53
1:A:500:GLN:HG3	1:A:512:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:CYS:O	1:A:576:ALA:HB2	2.08	0.53
1:A:605:ASN:CB	1:A:608:VAL:HG23	2.28	0.52
1:A:306:LEU:HB3	1:A:385:LYS:NZ	2.25	0.52
2:B:137:PHE:HZ	2:B:142:MET:SD	2.29	0.52
1:A:148:MET:HG3	1:A:149:PRO:HD3	1.91	0.52
1:A:251:PHE:CE2	1:A:253:ARG:CD	2.91	0.52
1:A:438:PHE:O	1:A:441:LEU:HB3	2.08	0.52
1:A:288:HIS:O	1:A:292:GLN:CG	2.56	0.52
1:A:374:GLN:HE22	1:A:416:GLY:HA2	1.73	0.52
1:A:488:GLN:HG2	1:A:585:TYR:CE2	2.45	0.52
1:A:812:LEU:O	1:A:813:ILE:C	2.47	0.52
2:B:101:PHE:HD2	2:B:137:PHE:C	2.12	0.52
3:C:52:HIS:CD2	3:C:75:MET:HG2	2.44	0.52
1:A:162:TYR:O	1:A:163:MET:C	2.47	0.52
1:A:217:LYS:HD3	1:A:344:GLY:CA	2.38	0.52
2:B:29:ARG:HB2	2:B:33:ILE:HG21	1.92	0.52
3:C:69:LEU:N	3:C:70:PRO:HD2	2.25	0.52
1:A:24:THR:HG23	1:A:81:LYS:HA	1.91	0.52
1:A:172:MET:SD	1:A:189:VAL:HG11	2.49	0.52
1:A:421:GLN:C	1:A:423:THR:N	2.63	0.52
1:A:658:LEU:O	1:A:661:ASN:HB2	2.10	0.52
1:A:373:GLU:O	1:A:373:GLU:CG	2.57	0.52
1:A:605:ASN:O	1:A:607:ASN:N	2.43	0.52
1:A:7:ASP:HB3	1:A:10:MET:HG2	1.90	0.52
1:A:428:ALA:O	1:A:432:SER:N	2.42	0.52
2:B:31:GLY:O	2:B:32:PHE:HB2	2.09	0.52
2:B:28:ASP:O	2:B:37:ASP:CG	2.47	0.52
3:C:132:ILE:HD13	3:C:145:LEU:HB2	1.92	0.52
1:A:458:PHE:CD1	1:A:458:PHE:C	2.83	0.51
1:A:475:PHE:C	1:A:477:GLN:N	2.64	0.51
3:C:80:THR:C	3:C:82:THR:N	2.64	0.51
1:A:274:LYS:NZ	1:A:647:ILE:HD13	2.25	0.51
1:A:568:PRO:HB2	1:A:578:ALA:HB3	1.90	0.51
3:C:81:GLY:O	3:C:82:THR:CB	2.58	0.51
1:A:239:THR:CG2	1:A:240:THR:N	2.73	0.51
1:A:350:LYS:O	1:A:351:LEU:C	2.49	0.51
1:A:489:GLN:HB2	1:A:516:GLY:HA2	1.91	0.51
1:A:568:PRO:HB2	1:A:578:ALA:CB	2.41	0.51
1:A:620:VAL:CG1	1:A:621:LYS:N	2.73	0.51
1:A:478:LEU:O	1:A:479:CYS:C	2.46	0.51
1:A:830:ARG:HB3	1:A:830:ARG:HH11	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:HG2	1:A:286:ASN:N	2.25	0.51
1:A:715:TYR:CD2	1:A:738:LYS:HA	2.46	0.51
2:B:38:LEU:CD1	2:B:58:LEU:HD21	2.29	0.51
2:B:133:LYS:O	2:B:134:ASN:O	2.28	0.51
1:A:95:ASN:OD1	1:A:98:SER:N	2.42	0.51
1:A:243:ASN:HB3	1:A:324:VAL:CG1	2.35	0.51
1:A:255:HIS:ND1	1:A:458:PHE:HB3	2.26	0.51
1:A:317:ILE:CD1	1:A:361:LEU:HD21	2.39	0.51
2:B:112:GLU:CG	2:B:123:ILE:CD1	2.89	0.51
3:C:30:ALA:HB1	3:C:55:THR:HG23	1.92	0.51
3:C:57:LYS:HD2	3:C:58:MET:N	2.26	0.51
3:C:135:ASP:O	3:C:136:ILE:C	2.49	0.51
1:A:2:THR:HB	1:A:148:MET:HA	1.93	0.51
1:A:782:LYS:O	1:A:786:MET:HG3	2.10	0.51
1:A:788:GLN:NE2	3:C:111:LEU:HA	2.24	0.51
1:A:443:ARG:HH11	1:A:443:ARG:CG	2.14	0.51
1:A:551:LYS:CB	1:A:593:ILE:HD11	2.39	0.51
2:B:32:PHE:CD1	2:B:32:PHE:N	2.79	0.51
1:A:253:ARG:NH1	1:A:661:ASN:OD1	2.44	0.50
1:A:423:THR:O	1:A:426:ILE:N	2.44	0.50
2:B:139:TYR:O	2:B:143:VAL:CG2	2.52	0.50
1:A:185:ASN:O	1:A:188:LYS:HB2	2.10	0.50
1:A:519:LEU:O	1:A:523:ILE:CG1	2.56	0.50
1:A:388:PHE:CD2	1:A:388:PHE:O	2.64	0.50
1:A:489:GLN:HB2	1:A:516:GLY:CA	2.42	0.50
1:A:736:ASP:HB3	1:A:739:VAL:CG2	2.42	0.50
2:B:122:GLU:O	2:B:126:VAL:CG2	2.56	0.50
2:B:143:VAL:O	2:B:146:LYS:N	2.40	0.50
3:C:43:ASN:N	3:C:44:PRO:HD3	2.27	0.50
1:A:4:ASP:O	1:A:6:SER:N	2.44	0.50
1:A:568:PRO:HD3	1:A:579:HIS:O	2.11	0.50
1:A:604:ILE:CG2	1:A:609:VAL:HG23	2.41	0.50
1:A:34:CYS:SG	1:A:46:ALA:HB3	2.51	0.50
1:A:170:GLN:CB	1:A:459:ILE:HG12	2.41	0.50
1:A:494:HIS:ND1	1:A:667:PRO:HG3	2.27	0.50
1:A:88:MET:HB2	1:A:116:SER:HA	1.92	0.50
1:A:537:GLU:OE1	1:A:646:THR:HG21	2.12	0.50
2:B:35:MET:CA	2:B:38:LEU:HG	2.37	0.50
3:C:52:HIS:CD2	3:C:75:MET:CG	2.95	0.50
3:C:57:LYS:CD	3:C:58:MET:H	2.24	0.50
1:A:36:VAL:HB	1:A:37:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:THR:OG1	1:A:456:GLN:HG3	2.11	0.50
1:A:439:ASN:O	1:A:443:ARG:HB2	2.11	0.50
2:B:109:ASP:CG	2:B:113:ASN:HD22	2.10	0.50
1:A:473:ASN:O	1:A:592:SER:N	2.44	0.50
1:A:769:LEU:O	1:A:773:GLU:HG2	2.12	0.50
1:A:786:MET:HE2	3:C:80:THR:O	2.11	0.50
1:A:832:PHE:HE1	2:B:18:LEU:HA	1.77	0.50
2:B:95:ASP:C	2:B:95:ASP:OD1	2.50	0.50
1:A:224:ILE:HD13	1:A:254:ILE:HD13	1.94	0.50
1:A:359:CYS:SG	1:A:389:LEU:HD12	2.51	0.50
1:A:778:GLU:HG2	1:A:778:GLU:O	2.11	0.50
1:A:276:ARG:HB2	1:A:286:ASN:HD21	1.77	0.49
1:A:467:PHE:HD1	1:A:467:PHE:H	1.59	0.49
1:A:721:ARG:HG2	1:A:722:TYR:CE1	2.47	0.49
2:B:98:GLY:C	2:B:99:GLN:O	2.49	0.49
1:A:99:ILE:CD1	1:A:702:ILE:HD13	2.42	0.49
1:A:366:MET:CE	1:A:383:ALA:HB2	2.42	0.49
1:A:372:GLY:C	1:A:374:GLN:H	2.03	0.49
3:C:48:GLN:HB3	3:C:75:MET:HE3	1.93	0.49
3:C:97:GLU:HA	3:C:97:GLU:OE1	2.12	0.49
1:A:29:ASP:OD1	1:A:31:LYS:HB2	2.13	0.49
1:A:124:ASN:ND2	5:A:1002:ADP:C8	2.81	0.49
1:A:139:LYS:O	1:A:143:LYS:HE3	2.12	0.49
1:A:242:ASN:ND2	1:A:245:SER:HA	2.28	0.49
1:A:597:LEU:HD23	1:A:597:LEU:N	2.27	0.49
1:A:124:ASN:HD22	1:A:125:PRO:N	2.09	0.49
3:C:57:LYS:NZ	3:C:58:MET:CB	2.75	0.49
1:A:134:GLN:O	1:A:137:VAL:N	2.43	0.49
1:A:366:MET:HE2	1:A:383:ALA:HB2	1.95	0.49
1:A:800:TYR:HE1	3:C:17:LEU:HD23	1.77	0.49
2:B:13:ARG:O	2:B:17:GLU:HG3	2.12	0.49
2:B:95:ASP:O	2:B:96:GLU:C	2.49	0.49
3:C:121:ASP:O	3:C:124:ASN:N	2.46	0.49
1:A:88:MET:HB2	1:A:116:SER:CA	2.43	0.49
1:A:615:SER:OG	1:A:619:ILE:HG21	2.13	0.49
1:A:217:LYS:CD	1:A:344:GLY:HA3	2.39	0.49
1:A:832:PHE:CE2	1:A:836:LYS:HE2	2.48	0.49
2:B:131:PRO:HG2	2:B:141:LYS:HB3	1.94	0.49
1:A:2:THR:CG2	1:A:147:GLU:C	2.81	0.49
1:A:125:PRO:HG2	5:A:1002:ADP:C6	2.48	0.49
1:A:316:PHE:CE1	1:A:364:GLY:CA	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLN:O	1:A:422:VAL:C	2.48	0.49
1:A:680:THR:HA	1:A:681:PRO:HD3	1.73	0.49
3:C:14:VAL:HG12	3:C:36:LEU:HD12	1.92	0.49
1:A:104:ARG:O	1:A:108:GLU:N	2.34	0.49
1:A:227:CYS:SG	1:A:445:VAL:HG11	2.53	0.49
2:B:10:LEU:O	2:B:11:SER:OG	2.30	0.48
2:B:102:ILE:HG22	2:B:107:LEU:HB2	1.95	0.48
2:B:145:ILE:O	2:B:145:ILE:HG22	2.13	0.48
1:A:37:PRO:HG3	1:A:73:ASP:CB	2.41	0.48
1:A:404:PRO:CB	1:A:607:ASN:HD22	2.10	0.48
1:A:603:PRO:O	1:A:604:ILE:HD12	2.14	0.48
1:A:826:TRP:HH2	2:B:73:LEU:O	1.96	0.48
1:A:423:THR:O	1:A:424:ASN:C	2.49	0.48
1:A:827:GLU:HG3	2:B:57:MET:CE	2.43	0.48
1:A:832:PHE:CE1	2:B:18:LEU:CD2	2.89	0.48
1:A:4:ASP:C	1:A:6:SER:N	2.67	0.48
1:A:135:GLY:O	1:A:139:LYS:HG3	2.14	0.48
1:A:316:PHE:CD1	1:A:364:GLY:HA3	2.48	0.48
1:A:389:LEU:O	1:A:391:GLY:N	2.45	0.48
1:A:494:HIS:CG	1:A:667:PRO:HG3	2.48	0.48
1:A:810:LEU:HD23	3:C:20:PHE:CE2	2.49	0.48
2:B:73:LEU:HG	2:B:73:LEU:O	2.13	0.48
1:A:368:TRP:HB2	1:A:419:LYS:HG2	1.94	0.48
1:A:648:SER:O	1:A:651:HIS:N	2.46	0.48
3:C:79:ASP:C	3:C:81:GLY:H	2.15	0.48
1:A:538:GLU:O	1:A:539:GLU:C	2.52	0.48
1:A:589:VAL:HB	1:A:591:TYR:CE1	2.49	0.48
2:B:64:GLN:O	2:B:66:ASN:N	2.42	0.48
2:B:91:PHE:HD1	2:B:91:PHE:H	1.60	0.48
1:A:84:MET:CE	1:A:105:SER:HB2	2.44	0.48
1:A:131:ILE:HG23	1:A:151:HIS:HE1	1.68	0.48
1:A:376:GLU:C	1:A:377:ALA:O	2.51	0.48
1:A:797:ARG:NH2	3:C:43:ASN:OD1	2.47	0.48
3:C:119:THR:O	3:C:121:ASP:N	2.46	0.48
1:A:106:ARG:NE	1:A:114:THR:OG1	2.44	0.48
1:A:351:LEU:HD12	1:A:351:LEU:HA	1.63	0.48
1:A:658:LEU:HB3	1:A:659:MET:HE3	1.96	0.48
3:C:132:ILE:HD11	3:C:145:LEU:HD13	1.91	0.48
1:A:2:THR:CG2	1:A:148:MET:CA	2.91	0.48
1:A:124:ASN:C	1:A:124:ASN:ND2	2.67	0.48
1:A:150:PRO:O	1:A:151:HIS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:HZ3	1:A:647:ILE:CD1	2.27	0.48
1:A:592:SER:OG	1:A:594:ALA:HB3	2.13	0.48
1:A:798:LYS:HZ3	3:C:129:PHE:HD2	1.51	0.48
2:B:8:VAL:HA	2:B:79:SER:HA	1.96	0.48
2:B:111:LEU:O	2:B:118:PHE:CB	2.47	0.48
2:B:26:ASP:C	2:B:28:ASP:N	2.66	0.48
2:B:35:MET:CE	2:B:54:LEU:O	2.47	0.48
3:C:119:THR:C	3:C:121:ASP:N	2.67	0.48
1:A:287:TYR:O	1:A:289:ILE:N	2.46	0.47
1:A:299:PRO:O	1:A:300:GLU:C	2.52	0.47
1:A:748:LEU:O	1:A:749:GLN:HB2	2.14	0.47
2:B:28:ASP:O	2:B:29:ARG:HB2	2.14	0.47
2:B:141:LYS:HA	2:B:144:ASP:HB2	1.96	0.47
3:C:134:GLU:HB3	3:C:138:GLY:HA2	1.96	0.47
1:A:170:GLN:O	1:A:460:GLY:N	2.44	0.47
1:A:278:THR:HB	1:A:316:PHE:HE2	1.79	0.47
1:A:646:THR:C	1:A:648:SER:N	2.67	0.47
1:A:813:ILE:HG12	2:B:91:PHE:CZ	2.49	0.47
2:B:61:CYS:SG	2:B:65:LEU:HD13	2.54	0.47
2:B:89:ASN:O	2:B:92:SER:HB2	2.15	0.47
1:A:276:ARG:NH1	1:A:284:GLU:OE1	2.42	0.47
1:A:488:GLN:HA	1:A:488:GLN:OE1	2.13	0.47
1:A:521:ALA:O	1:A:522:CYS:C	2.52	0.47
1:A:122:ALA:O	1:A:673:ILE:HB	2.14	0.47
1:A:139:LYS:O	1:A:148:MET:CE	2.62	0.47
1:A:317:ILE:CD1	1:A:361:LEU:CD2	2.92	0.47
1:A:537:GLU:CD	1:A:646:THR:HG21	2.34	0.47
3:C:153:PRO:CD	3:C:154:PHE:N	2.77	0.47
1:A:195:LEU:O	1:A:196:VAL:C	2.51	0.47
1:A:335:LEU:O	1:A:338:THR:N	2.44	0.47
1:A:475:PHE:HE2	1:A:647:ILE:HG21	1.80	0.47
1:A:519:LEU:CD2	1:A:585:TYR:HD1	2.28	0.47
1:A:683:LEU:C	1:A:684:ILE:HD13	2.35	0.47
2:B:50:PRO:HD2	2:B:53:GLU:OE2	2.14	0.47
3:C:154:PHE:N	3:C:155:PRO:HD3	2.30	0.47
1:A:270:TYR:CD1	1:A:270:TYR:N	2.82	0.47
1:A:808:ILE:O	1:A:809:GLY:C	2.52	0.47
1:A:824:ARG:NH1	2:B:129:ASP:OD2	2.47	0.47
1:A:296:PRO:HG2	1:A:330:GLU:CG	2.45	0.47
1:A:406:ILE:O	1:A:407:LYS:CG	2.62	0.47
1:A:467:PHE:CE2	1:A:585:TYR:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:PHE:O	1:A:478:LEU:N	2.47	0.47
1:A:566:GLY:O	1:A:581:CYS:N	2.39	0.47
1:A:782:LYS:HE2	1:A:786:MET:CE	2.44	0.47
1:A:805:ASP:HB3	2:B:93:MET:CE	2.45	0.47
2:B:8:VAL:HG12	2:B:9:LYS:HB2	1.95	0.47
1:A:29:ASP:O	1:A:31:LYS:N	2.48	0.47
1:A:366:MET:SD	1:A:426:ILE:CD1	3.02	0.47
1:A:674:ILE:HG23	1:A:688:LEU:HD21	1.97	0.47
2:B:112:GLU:CG	2:B:123:ILE:HD13	2.45	0.47
3:C:67:GLU:O	3:C:71:ILE:HD12	2.14	0.47
1:A:267:ILE:CG2	1:A:268:GLU:N	2.77	0.47
2:B:38:LEU:HB2	2:B:54:LEU:CD1	2.45	0.47
2:B:131:PRO:HD2	2:B:142:MET:CG	2.44	0.47
1:A:237:ALA:HA	1:A:288:HIS:CE1	2.50	0.47
1:A:537:GLU:OE2	1:A:646:THR:HG21	2.15	0.47
1:A:12:PHE:O	1:A:111:PHE:CD2	2.68	0.46
1:A:278:THR:HG22	1:A:316:PHE:CE2	2.50	0.46
1:A:559:LEU:CG	1:A:560:GLY:H	2.18	0.46
2:B:102:ILE:O	2:B:137:PHE:HB3	2.15	0.46
2:B:124:LYS:O	2:B:125:ASN:C	2.53	0.46
1:A:237:ALA:HB2	1:A:287:TYR:HA	1.98	0.46
1:A:274:LYS:NZ	1:A:647:ILE:HD11	2.30	0.46
1:A:440:TRP:HE1	1:A:621:LYS:CD	2.28	0.46
1:A:826:TRP:HZ2	2:B:73:LEU:HD11	1.80	0.46
3:C:100:GLY:O	3:C:142:TYR:CD2	2.67	0.46
3:C:119:THR:C	3:C:121:ASP:H	2.17	0.46
1:A:256:PHE:HA	1:A:261:LYS:O	2.16	0.46
1:A:468:GLU:N	1:A:481:ASN:OD1	2.47	0.46
2:B:78:VAL:O	2:B:78:VAL:CG1	2.63	0.46
3:C:6:ASP:O	3:C:9:GLU:HB2	2.15	0.46
1:A:94:LEU:HB2	1:A:706:ARG:HE	1.80	0.46
1:A:123:ILE:O	1:A:125:PRO:HD3	2.14	0.46
1:A:157:ASP:O	1:A:160:TYR:N	2.48	0.46
1:A:174:ILE:HG23	1:A:670:VAL:CB	2.41	0.46
1:A:538:GLU:OE1	1:A:553:LYS:NZ	2.46	0.46
1:A:543:PRO:O	1:A:545:ALA:N	2.42	0.46
1:A:552:ASN:O	1:A:556:ASP:HB2	2.16	0.46
1:A:774:ASP:O	1:A:776:ARG:N	2.48	0.46
1:A:787:PHE:O	1:A:790:HIS:N	2.47	0.46
3:C:60:GLU:O	3:C:61:LYS:HB3	2.15	0.46
1:A:43:PHE:HE1	1:A:690:LEU:CD2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:PRO:CG	1:A:322:LEU:HD13	2.46	0.46
3:C:7:GLU:O	3:C:8:ILE:C	2.52	0.46
1:A:251:PHE:CD1	1:A:658:LEU:HD11	2.50	0.46
1:A:167:ARG:NH1	1:A:258:THR:HA	2.27	0.46
1:A:278:THR:HB	1:A:316:PHE:CE2	2.50	0.46
1:A:286:ASN:O	1:A:291:TYR:HE1	1.97	0.46
1:A:302:ILE:HG22	1:A:307:ALA:O	2.16	0.46
1:A:328:ASP:O	1:A:331:GLU:N	2.47	0.46
1:A:332:GLU:O	1:A:333:MET:C	2.53	0.46
1:A:426:ILE:HG22	1:A:426:ILE:O	2.15	0.46
1:A:592:SER:O	1:A:596:TRP:NE1	2.49	0.46
2:B:29:ARG:C	2:B:31:GLY:H	2.19	0.46
1:A:65:GLU:CD	1:A:66:THR:H	2.18	0.46
1:A:231:LEU:O	1:A:235:GLY:N	2.49	0.46
1:A:353:MET:HG3	1:A:353:MET:O	2.15	0.46
1:A:523:ILE:O	1:A:527:GLU:CG	2.60	0.46
1:A:617:GLU:HB2	1:A:618:PRO:CD	2.41	0.46
1:A:721:ARG:CZ	1:A:776:ARG:HH12	2.28	0.46
1:A:88:MET:HE1	1:A:99:ILE:CD1	2.45	0.46
1:A:151:HIS:HD2	1:A:153:PHE:N	2.12	0.46
1:A:296:PRO:HG2	1:A:330:GLU:HG2	1.98	0.46
1:A:348:GLU:HA	1:A:348:GLU:OE1	2.16	0.46
1:A:354:TYR:O	1:A:357:THR:N	2.48	0.46
1:A:458:PHE:C	1:A:458:PHE:HD1	2.19	0.46
1:A:585:TYR:O	1:A:586:ALA:C	2.55	0.46
1:A:827:GLU:HA	1:A:830:ARG:HH22	1.76	0.46
2:B:96:GLU:HA	2:B:96:GLU:OE1	2.15	0.46
3:C:81:GLY:O	3:C:82:THR:OG1	2.34	0.46
1:A:826:TRP:CH2	2:B:73:LEU:O	2.69	0.46
1:A:285:ARG:HG2	1:A:291:TYR:CE1	2.51	0.45
1:A:530:MET:HE3	1:A:538:GLU:OE1	2.16	0.45
1:A:715:TYR:CE2	1:A:738:LYS:HA	2.51	0.45
1:A:38:ASP:HB2	1:A:67:ARG:HH12	1.81	0.45
1:A:88:MET:HE3	1:A:102:ASN:HB3	1.98	0.45
1:A:328:ASP:O	1:A:330:GLU:N	2.50	0.45
1:A:736:ASP:O	1:A:740:VAL:HG23	2.17	0.45
1:A:774:ASP:C	1:A:774:ASP:OD1	2.55	0.45
1:A:812:LEU:HD23	1:A:812:LEU:HA	1.70	0.45
2:B:116:ASP:OD1	3:C:24:ARG:HD3	2.17	0.45
1:A:656:ASN:O	1:A:659:MET:N	2.49	0.45
1:A:657:LYS:O	1:A:661:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:MET:HB3	2:B:54:LEU:HD21	1.99	0.45
3:C:102:ILE:O	3:C:103:SER:C	2.55	0.45
1:A:270:TYR:OH	1:A:658:LEU:HD22	2.17	0.45
1:A:363:LEU:HD12	1:A:430:ALA:HB2	1.98	0.45
1:A:379:GLY:C	1:A:381:ALA:N	2.69	0.45
1:A:554:LEU:O	1:A:555:TYR:C	2.53	0.45
1:A:793:GLY:O	1:A:797:ARG:HB2	2.17	0.45
1:A:822:VAL:O	1:A:822:VAL:CG1	2.61	0.45
3:C:92:LYS:C	3:C:94:PHE:N	2.70	0.45
3:C:109:ASN:O	3:C:110:VAL:C	2.54	0.45
3:C:137:ASP:HB2	3:C:139:ASN:ND2	2.31	0.45
1:A:232:GLU:C	1:A:234:TYR:N	2.70	0.45
1:A:215:GLU:HG3	1:A:216:LYS:H	1.80	0.45
1:A:521:ALA:CB	1:A:564:MET:HG3	2.47	0.45
1:A:536:LEU:O	1:A:536:LEU:HG	2.16	0.45
1:A:36:VAL:O	1:A:43:PHE:HA	2.17	0.45
1:A:140:TYR:OH	1:A:149:PRO:O	2.25	0.45
1:A:158:ASN:O	1:A:162:TYR:HD1	1.99	0.45
2:B:37:ASP:O	2:B:41:MET:N	2.48	0.45
1:A:15:LEU:HB3	1:A:19:LYS:HB3	1.97	0.45
1:A:385:LYS:O	1:A:387:ALA:N	2.50	0.45
1:A:456:GLN:HB2	1:A:457:PHE:CE1	2.52	0.45
1:A:676:ASN:OD1	1:A:678:LEU:O	2.34	0.45
2:B:35:MET:SD	2:B:54:LEU:HG	2.54	0.45
1:A:525:LEU:HG	1:A:532:ILE:HD12	1.99	0.45
1:A:568:PRO:HG3	1:A:579:HIS:HA	1.99	0.45
1:A:806:GLN:O	3:C:21:TRP:HH2	1.99	0.45
2:B:101:PHE:CD2	2:B:138:ASN:N	2.85	0.45
1:A:92:THR:HG23	1:A:93:PHE:N	2.32	0.45
1:A:105:SER:OG	1:A:106:ARG:N	2.49	0.45
1:A:255:HIS:CD2	1:A:455:ARG:HH11	2.34	0.45
1:A:346:THR:HG22	1:A:347:ASP:N	2.32	0.45
1:A:740:VAL:O	1:A:743:LYS:N	2.50	0.45
2:B:95:ASP:OD1	2:B:97:ASP:HB3	2.17	0.45
1:A:79:PRO:HG2	1:A:82:PHE:CE1	2.52	0.44
1:A:185:ASN:O	1:A:188:LYS:N	2.46	0.44
1:A:236:ASN:HA	1:A:245:SER:O	2.16	0.44
1:A:451:THR:O	1:A:452:LYS:HB2	2.16	0.44
1:A:569:LYS:HA	1:A:570:PRO:HD3	1.83	0.44
1:A:592:SER:OG	1:A:594:ALA:CB	2.65	0.44
1:A:656:ASN:C	1:A:658:LEU:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:ARG:HG2	1:A:777:ASP:N	2.29	0.44
1:A:828:TRP:HZ2	2:B:57:MET:C	2.20	0.44
1:A:512:PHE:O	1:A:513:ILE:CG2	2.64	0.44
1:A:531:GLY:O	1:A:532:ILE:C	2.56	0.44
1:A:535:ILE:HD12	1:A:554:LEU:HD23	2.00	0.44
3:C:53:GLY:O	3:C:63:TYR:OH	2.21	0.44
1:A:141:ARG:HG3	1:A:142:GLY:H	1.82	0.44
1:A:200:LEU:HA	1:A:200:LEU:HD23	1.43	0.44
1:A:247:ARG:NE	1:A:247:ARG:HA	2.32	0.44
1:A:620:VAL:O	1:A:621:LYS:C	2.55	0.44
1:A:788:GLN:HG2	3:C:118:ILE:HD12	1.98	0.44
1:A:119:PHE:H	1:A:119:PHE:HD1	1.65	0.44
1:A:131:ILE:HG22	1:A:132:TYR:CD2	2.52	0.44
1:A:134:GLN:O	1:A:137:VAL:HB	2.17	0.44
1:A:296:PRO:HG2	1:A:330:GLU:OE2	2.17	0.44
1:A:646:THR:HG23	1:A:646:THR:O	2.17	0.44
3:C:12:ARG:C	3:C:14:VAL:N	2.70	0.44
1:A:79:PRO:O	1:A:82:PHE:HD1	2.01	0.44
1:A:192:TYR:CE2	1:A:196:VAL:HG21	2.53	0.44
1:A:243:ASN:OD1	1:A:324:VAL:HG13	2.18	0.44
2:B:12:GLN:CG	2:B:13:ARG:N	2.61	0.44
2:B:65:LEU:HA	2:B:65:LEU:HD12	1.54	0.44
2:B:139:TYR:C	2:B:141:LYS:H	2.20	0.44
2:B:142:MET:HA	2:B:145:ILE:HB	1.99	0.44
1:A:1:MET:H3	1:A:1:MET:HE3	1.82	0.44
1:A:85:ASN:ND2	1:A:91:LEU:HD23	2.17	0.44
1:A:236:ASN:OD1	1:A:246:SER:CA	2.62	0.44
1:A:238:LYS:HB3	1:A:285:ARG:HB3	1.99	0.44
1:A:306:LEU:O	1:A:362:HIS:HE1	2.01	0.44
1:A:358:GLY:O	1:A:361:LEU:N	2.43	0.44
1:A:491:PHE:O	1:A:493:HIS:N	2.50	0.44
1:A:659:MET:HE2	1:A:659:MET:HA	2.00	0.44
1:A:706:ARG:C	1:A:708:GLY:H	2.20	0.44
2:B:109:ASP:OD1	2:B:113:ASN:HB2	2.18	0.44
3:C:12:ARG:O	3:C:13:GLU:C	2.56	0.44
3:C:28:VAL:O	3:C:63:TYR:N	2.49	0.44
3:C:155:PRO:O	3:C:156:ASP:O	2.36	0.44
1:A:315:GLY:O	1:A:319:GLN:NE2	2.46	0.44
1:A:366:MET:HE2	1:A:383:ALA:CB	2.48	0.44
1:A:405:LYS:O	1:A:405:LYS:CG	2.61	0.44
1:A:406:ILE:O	1:A:407:LYS:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ILE:HG23	1:A:553:LYS:HG2	2.00	0.44
1:A:755:TYR:CD2	1:A:755:TYR:N	2.86	0.44
1:A:790:HIS:CE1	3:C:43:ASN:ND2	2.84	0.44
2:B:35:MET:HA	2:B:38:LEU:HB2	1.99	0.44
2:B:74:PHE:HD2	2:B:74:PHE:HA	1.57	0.44
3:C:23:GLY:O	3:C:24:ARG:C	2.55	0.44
1:A:121:ILE:CG2	1:A:122:ALA:N	2.79	0.44
1:A:332:GLU:O	1:A:335:LEU:HB2	2.17	0.44
1:A:366:MET:SD	1:A:426:ILE:HD13	2.58	0.44
1:A:535:ILE:HD12	1:A:554:LEU:CD2	2.48	0.44
1:A:134:GLN:O	1:A:137:VAL:HG23	2.18	0.44
1:A:438:PHE:O	1:A:441:LEU:N	2.51	0.44
1:A:603:PRO:O	1:A:604:ILE:HG13	2.18	0.44
1:A:646:THR:CG2	1:A:649:SER:H	2.16	0.44
1:A:698:VAL:HG12	1:A:699:LEU:HD23	2.00	0.44
2:B:132:LEU:HD21	2:B:137:PHE:CD1	2.53	0.44
1:A:162:TYR:O	1:A:163:MET:O	2.36	0.43
1:A:253:ARG:O	1:A:265:ALA:CB	2.66	0.43
1:A:495:MET:O	1:A:496:PHE:C	2.55	0.43
1:A:782:LYS:HE2	1:A:786:MET:HE1	2.00	0.43
1:A:807:ARG:O	1:A:807:ARG:HG2	2.16	0.43
2:B:141:LYS:HB2	2:B:141:LYS:HE3	1.84	0.43
3:C:29:ASP:O	3:C:32:LYS:HB2	2.18	0.43
1:A:167:ARG:HH12	1:A:258:THR:CG2	2.30	0.43
1:A:173:LEU:HD12	1:A:669:PHE:CE2	2.53	0.43
1:A:310:ASP:C	1:A:312:GLY:N	2.69	0.43
1:A:328:ASP:O	1:A:329:ASP:C	2.57	0.43
1:A:818:ARG:NE	2:B:118:PHE:HE1	2.04	0.43
2:B:95:ASP:OD2	2:B:101:PHE:O	2.36	0.43
2:B:124:LYS:O	2:B:127:TRP:N	2.34	0.43
1:A:138:ASP:O	1:A:139:LYS:C	2.54	0.43
1:A:185:ASN:O	1:A:186:THR:C	2.56	0.43
1:A:461:VAL:HG12	1:A:462:LEU:N	2.33	0.43
1:A:559:LEU:HA	1:A:565:PHE:CE2	2.53	0.43
1:A:720:GLN:O	1:A:720:GLN:CG	2.41	0.43
2:B:89:ASN:O	2:B:90:ALA:C	2.57	0.43
2:B:95:ASP:OD1	2:B:97:ASP:N	2.45	0.43
3:C:154:PHE:CD2	3:C:159:ASP:HB3	2.53	0.43
1:A:152:LEU:O	1:A:153:PHE:C	2.56	0.43
1:A:184:GLU:OE2	1:A:184:GLU:CA	2.50	0.43
1:A:669:PHE:N	1:A:669:PHE:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:PHE:O	1:A:718:PHE:CD2	2.71	0.43
1:A:748:LEU:HA	1:A:748:LEU:HD23	1.79	0.43
1:A:58:VAL:O	1:A:66:THR:HA	2.19	0.43
1:A:286:ASN:HD22	1:A:286:ASN:HA	1.62	0.43
1:A:355:LYS:CD	1:A:616:LYS:NZ	2.71	0.43
1:A:683:LEU:O	1:A:684:ILE:HD13	2.19	0.43
1:A:5:PHE:N	1:A:5:PHE:CD2	2.87	0.43
1:A:251:PHE:CE1	1:A:658:LEU:HD11	2.54	0.43
1:A:579:HIS:CD2	1:A:593:ILE:HB	2.53	0.43
3:C:32:LYS:O	3:C:33:VAL:C	2.57	0.43
1:A:2:THR:OG1	1:A:149:PRO:HG3	2.18	0.43
1:A:18:GLN:O	1:A:22:GLU:HG3	2.19	0.43
1:A:141:ARG:HG3	1:A:142:GLY:N	2.34	0.43
1:A:363:LEU:CD1	1:A:430:ALA:HB2	2.48	0.43
1:A:444:ARG:O	1:A:444:ARG:NE	2.37	0.43
1:A:645:GLN:O	1:A:646:THR:C	2.55	0.43
2:B:102:ILE:CG2	2:B:107:LEU:HB2	2.49	0.43
2:B:146:LYS:CG	2:B:147:GLY:N	2.49	0.43
1:A:86:MET:CE	1:A:149:PRO:HB3	2.49	0.43
1:A:508:ILE:CG2	1:A:756:ARG:CG	2.91	0.43
1:A:757:LEU:HD23	1:A:762:VAL:HB	2.01	0.43
1:A:810:LEU:O	1:A:814:GLN:HB2	2.19	0.43
2:B:132:LEU:CD2	2:B:137:PHE:HD1	2.32	0.43
1:A:582:LEU:HB3	1:A:591:TYR:HE1	1.83	0.43
3:C:100:GLY:O	3:C:142:TYR:CE2	2.71	0.43
1:A:226:GLN:HB3	1:A:339:ALA:HB1	2.00	0.43
1:A:270:TYR:HD1	1:A:270:TYR:N	2.16	0.43
1:A:272:LEU:HD22	1:A:438:PHE:CG	2.54	0.43
1:A:475:PHE:C	1:A:477:GLN:H	2.21	0.43
1:A:525:LEU:HD13	1:A:562:ASN:HD22	1.84	0.43
1:A:602:ASP:OD1	1:A:604:ILE:HD12	2.18	0.43
1:A:835:VAL:CG1	1:A:838:LEU:HD23	2.49	0.43
2:B:91:PHE:CD1	2:B:91:PHE:N	2.86	0.43
3:C:42:MET:HE3	3:C:42:MET:HB3	1.89	0.43
1:A:84:MET:O	1:A:85:ASN:C	2.57	0.42
1:A:410:THR:O	1:A:410:THR:HG22	2.19	0.42
2:B:50:PRO:HD2	2:B:53:GLU:CD	2.39	0.42
2:B:82:ASP:O	2:B:83:PRO:C	2.57	0.42
3:C:91:PHE:CB	3:C:142:TYR:CD1	3.01	0.42
3:C:107:ILE:HD12	3:C:140:ILE:HB	2.01	0.42
1:A:119:PHE:CD1	1:A:119:PHE:N	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:TRP:O	1:A:419:LYS:CE	2.67	0.42
1:A:464:ILE:HG23	1:A:464:ILE:O	2.18	0.42
1:A:681:PRO:O	1:A:682:GLY:C	2.58	0.42
3:C:19:ASP:OD2	3:C:26:GLY:N	2.52	0.42
3:C:57:LYS:CE	3:C:58:MET:H	2.32	0.42
1:A:187:LYS:HE2	1:A:232:GLU:OE2	2.18	0.42
1:A:324:VAL:HB	1:A:327:ILE:HG13	2.00	0.42
1:A:423:THR:C	1:A:425:SER:N	2.71	0.42
1:A:476:GLU:OE2	1:A:599:LYS:HD3	2.19	0.42
1:A:789:ALA:HB1	3:C:43:ASN:O	2.18	0.42
1:A:41:PHE:CB	1:A:104:ARG:HH12	2.25	0.42
1:A:286:ASN:O	1:A:287:TYR:C	2.57	0.42
1:A:309:PRO:O	1:A:310:ASP:HB2	2.19	0.42
1:A:310:ASP:HA	1:A:311:PRO:HD2	1.79	0.42
1:A:322:LEU:C	1:A:323:THR:HG23	2.40	0.42
1:A:338:THR:O	1:A:339:ALA:C	2.58	0.42
1:A:491:PHE:C	1:A:493:HIS:N	2.72	0.42
1:A:520:GLN:OE1	1:A:523:ILE:HD12	2.19	0.42
1:A:580:PHE:HZ	1:A:596:TRP:HH2	1.67	0.42
1:A:646:THR:O	1:A:648:SER:N	2.52	0.42
2:B:31:GLY:O	2:B:32:PHE:CB	2.68	0.42
2:B:56:ALA:O	2:B:60:GLU:HG3	2.19	0.42
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.20	0.42
1:A:467:PHE:N	1:A:467:PHE:CD1	2.87	0.42
1:A:543:PRO:C	1:A:545:ALA:N	2.72	0.42
1:A:800:TYR:CE1	3:C:17:LEU:CD2	3.02	0.42
3:C:125:ASP:O	3:C:128:THR:HB	2.19	0.42
1:A:2:THR:HG21	1:A:148:MET:N	2.34	0.42
1:A:140:TYR:CZ	1:A:149:PRO:HD2	2.55	0.42
1:A:175:THR:CG2	1:A:176:GLY:N	2.53	0.42
1:A:220:LEU:O	1:A:220:LEU:HG	2.19	0.42
1:A:285:ARG:HH21	1:A:291:TYR:CB	2.33	0.42
1:A:489:GLN:O	1:A:493:HIS:N	2.50	0.42
1:A:584:HIS:HB3	1:A:585:TYR:H	1.37	0.42
1:A:645:GLN:O	1:A:645:GLN:HG3	2.19	0.42
1:A:79:PRO:HG2	1:A:82:PHE:HE1	1.85	0.42
1:A:175:THR:O	1:A:672:CYS:HB2	2.20	0.42
1:A:748:LEU:O	1:A:749:GLN:CB	2.67	0.42
1:A:761:LYS:HB2	1:A:763:PHE:CE1	2.55	0.42
1:A:779:ARG:HA	1:A:779:ARG:HD2	1.88	0.42
1:A:790:HIS:CE1	3:C:43:ASN:HD22	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLN:OE1	2:B:19:LYS:HD3	2.20	0.42
2:B:106:TYR:O	2:B:109:ASP:N	2.53	0.42
2:B:106:TYR:HB3	2:B:107:LEU:H	1.63	0.42
1:A:524:GLU:O	1:A:526:ILE:N	2.52	0.42
1:A:615:SER:HG	1:A:619:ILE:HG21	1.85	0.42
1:A:832:PHE:CE1	2:B:21:ALA:HB2	2.54	0.42
2:B:104:GLU:CG	2:B:127:TRP:CH2	3.01	0.42
3:C:69:LEU:HA	3:C:69:LEU:HD23	1.68	0.42
3:C:130:CYS:O	3:C:131:ASP:C	2.58	0.42
3:C:155:PRO:C	3:C:156:ASP:O	2.58	0.42
1:A:38:ASP:OD1	1:A:38:ASP:C	2.57	0.42
1:A:225:VAL:C	1:A:227:CYS:H	2.22	0.42
1:A:230:VAL:CG1	1:A:441:LEU:HD11	2.49	0.42
1:A:535:ILE:CD1	1:A:554:LEU:HD23	2.50	0.42
1:A:551:LYS:HG3	1:A:555:TYR:CE1	2.55	0.42
3:C:14:VAL:CG1	3:C:36:LEU:HD12	2.49	0.42
1:A:24:THR:HA	1:A:80:PRO:O	2.20	0.42
1:A:38:ASP:HA	1:A:39:PRO:HD3	1.79	0.42
1:A:236:ASN:OD1	1:A:245:SER:O	2.37	0.42
1:A:791:ILE:C	1:A:793:GLY:H	2.23	0.42
1:A:822:VAL:O	1:A:823:LEU:HD23	2.20	0.42
1:A:838:LEU:CD2	2:B:24:MET:SD	3.07	0.42
2:B:95:ASP:C	2:B:97:ASP:N	2.73	0.42
1:A:253:ARG:O	1:A:265:ALA:HA	2.20	0.41
3:C:153:PRO:HG2	3:C:154:PHE:CD1	2.54	0.41
1:A:140:TYR:CE2	1:A:148:MET:HB3	2.55	0.41
1:A:791:ILE:CG2	3:C:126:ILE:HD12	2.18	0.41
1:A:831:LEU:HG	1:A:832:PHE:N	2.35	0.41
2:B:33:ILE:O	2:B:37:ASP:HB2	2.20	0.41
2:B:40:ASP:O	2:B:43:SER:OG	2.38	0.41
1:A:157:ASP:C	1:A:159:ALA:N	2.72	0.41
1:A:380:THR:HG22	1:A:384:GLU:CG	2.50	0.41
1:A:532:ILE:H	1:A:532:ILE:HG13	1.66	0.41
1:A:605:ASN:O	1:A:606:GLU:C	2.59	0.41
1:A:677:GLU:O	1:A:678:LEU:C	2.59	0.41
1:A:713:ILE:CG2	1:A:718:PHE:HB2	2.50	0.41
2:B:35:MET:O	2:B:36:GLU:C	2.58	0.41
2:B:48:VAL:HA	2:B:49:PRO:HD3	1.80	0.41
3:C:89:GLU:HA	3:C:89:GLU:OE1	2.21	0.41
3:C:112:LYS:CD	3:C:120:GLU:OE1	2.62	0.41
1:A:82:PHE:HE2	1:A:90:ASN:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:THR:O	1:A:136:LEU:HB2	2.21	0.41
1:A:134:GLN:O	1:A:137:VAL:CB	2.69	0.41
1:A:274:LYS:HZ3	1:A:647:ILE:HD13	1.84	0.41
1:A:276:ARG:CB	1:A:286:ASN:ND2	2.83	0.41
1:A:535:ILE:HG21	1:A:554:LEU:HD23	2.02	0.41
2:B:8:VAL:HG13	2:B:9:LYS:HG2	2.02	0.41
2:B:49:PRO:HA	2:B:50:PRO:HD3	1.95	0.41
3:C:118:ILE:CG2	3:C:122:GLN:HB2	2.44	0.41
1:A:78:ASN:HD22	1:A:91:LEU:HD22	1.85	0.41
1:A:376:GLU:O	1:A:377:ALA:O	2.38	0.41
1:A:217:LYS:HE2	1:A:344:GLY:HA2	2.02	0.41
1:A:413:VAL:HG12	1:A:414:THR:N	2.36	0.41
1:A:582:LEU:HD23	1:A:584:HIS:NE2	2.36	0.41
1:A:604:ILE:O	1:A:606:GLU:N	2.53	0.41
1:A:716:SER:O	1:A:719:LYS:N	2.52	0.41
1:A:786:MET:HE2	3:C:80:THR:HG23	1.98	0.41
2:B:147:GLY:O	2:B:148:LYS:CB	2.68	0.41
1:A:414:THR:HG22	1:A:415:GLN:H	1.86	0.41
1:A:648:SER:O	1:A:649:SER:C	2.58	0.41
1:A:809:GLY:HA3	2:B:93:MET:SD	2.61	0.41
1:A:826:TRP:CZ3	2:B:74:PHE:CE2	3.08	0.41
3:C:12:ARG:O	3:C:15:PHE:N	2.53	0.41
3:C:19:ASP:OD2	3:C:26:GLY:HA2	2.20	0.41
1:A:124:ASN:HA	1:A:125:PRO:HD2	1.78	0.41
1:A:232:GLU:C	1:A:234:TYR:H	2.23	0.41
1:A:292:GLN:O	1:A:333:MET:HE3	2.20	0.41
1:A:322:LEU:O	1:A:323:THR:HG23	2.20	0.41
1:A:372:GLY:C	1:A:374:GLN:N	2.66	0.41
1:A:810:LEU:HD23	3:C:20:PHE:HZ	1.75	0.41
3:C:33:VAL:O	3:C:34:GLY:C	2.57	0.41
1:A:35:TRP:O	1:A:75:GLY:N	2.46	0.41
1:A:228:ASN:HB2	1:A:229:PRO:CD	2.45	0.41
1:A:292:GLN:HB2	1:A:333:MET:HE2	2.02	0.41
1:A:494:HIS:ND1	1:A:667:PRO:CG	2.84	0.41
1:A:503:TYR:HE1	1:A:712:ARG:NH2	2.18	0.41
1:A:547:ASP:O	1:A:550:PHE:N	2.54	0.41
2:B:29:ARG:O	2:B:31:GLY:N	2.54	0.41
2:B:53:GLU:O	2:B:57:MET:N	2.32	0.41
2:B:127:TRP:HA	2:B:130:ALA:HB3	2.03	0.41
3:C:102:ILE:HB	3:C:107:ILE:HD11	2.02	0.41
3:C:143:GLU:OE2	3:C:147:LYS:NZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:PRO:C	3:C:155:PRO:HD3	2.41	0.41
1:A:5:PHE:H	1:A:5:PHE:HD2	1.68	0.41
1:A:19:LYS:HA	1:A:19:LYS:HD2	1.51	0.41
1:A:79:PRO:HA	1:A:80:PRO:HD3	1.86	0.41
1:A:86:MET:CE	1:A:149:PRO:HA	2.51	0.41
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.84	0.41
1:A:220:LEU:HD23	1:A:262:ILE:CG2	2.51	0.41
1:A:285:ARG:NE	1:A:291:TYR:CD1	2.89	0.41
1:A:565:PHE:CD2	1:A:565:PHE:C	2.95	0.41
1:A:647:ILE:HD12	1:A:647:ILE:HA	1.72	0.41
3:C:145:LEU:HD12	3:C:149:VAL:CG2	2.43	0.41
1:A:5:PHE:N	1:A:5:PHE:HD2	2.19	0.40
1:A:83:GLU:O	1:A:84:MET:CB	2.68	0.40
1:A:98:SER:O	1:A:101:HIS:N	2.54	0.40
1:A:115:TYR:CD1	1:A:150:PRO:HG3	2.56	0.40
1:A:293:LEU:C	1:A:295:SER:H	2.23	0.40
1:A:493:HIS:CE1	1:A:514:ASP:OD2	2.74	0.40
1:A:606:GLU:H	1:A:606:GLU:HG3	1.58	0.40
1:A:774:ASP:C	1:A:776:ARG:N	2.74	0.40
2:B:18:LEU:HD22	2:B:74:PHE:CE1	2.56	0.40
2:B:127:TRP:HA	2:B:130:ALA:CB	2.51	0.40
3:C:66:GLU:N	3:C:66:GLU:CD	2.67	0.40
3:C:88:MET:HE3	3:C:143:GLU:HG3	1.99	0.40
1:A:7:ASP:O	1:A:8:PRO:C	2.58	0.40
1:A:86:MET:CE	1:A:150:PRO:HD2	2.33	0.40
1:A:398:LEU:HD23	1:A:398:LEU:HA	1.83	0.40
1:A:414:THR:HG22	1:A:415:GLN:N	2.37	0.40
1:A:719:LYS:O	1:A:721:ARG:N	2.55	0.40
2:B:28:ASP:O	2:B:29:ARG:CB	2.68	0.40
2:B:29:ARG:CB	2:B:33:ILE:HB	2.48	0.40
2:B:31:GLY:O	2:B:32:PHE:HD1	2.04	0.40
2:B:107:LEU:CD1	2:B:111:LEU:HD11	2.45	0.40
1:A:10:MET:HB3	1:A:14:CYS:SG	2.62	0.40
1:A:292:GLN:C	1:A:333:MET:HE2	2.41	0.40
1:A:353:MET:HE3	1:A:353:MET:HB2	1.85	0.40
1:A:534:SER:OG	1:A:535:ILE:N	2.55	0.40
1:A:718:PHE:CD2	1:A:718:PHE:C	2.95	0.40
1:A:820:TRP:O	1:A:821:LEU:C	2.59	0.40
1:A:830:ARG:CZ	1:A:830:ARG:HB2	2.50	0.40
1:A:831:LEU:O	1:A:835:VAL:HG23	2.21	0.40
1:A:601:LYS:O	1:A:603:PRO:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:TRP:HB3	1:A:829:TRP:HB2	2.03	0.40
2:B:115:GLY:C	2:B:117:ASN:H	2.24	0.40
1:A:21:MET:O	1:A:25:SER:HB3	2.21	0.40
1:A:161:GLN:O	1:A:162:TYR:C	2.60	0.40
1:A:333:MET:O	1:A:336:THR:N	2.54	0.40
1:A:349:GLU:OE1	1:A:444:ARG:NH1	2.55	0.40
1:A:713:ILE:O	1:A:761:LYS:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:LEU:O	3:C:64:LYS:NZ[2_656]	2.03	0.17

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	804/839 (96%)	536 (67%)	184 (23%)	84 (10%)	0	3
2	B	143/153 (94%)	86 (60%)	28 (20%)	29 (20%)	0	0
3	C	157/159 (99%)	108 (69%)	27 (17%)	22 (14%)	0	1
All	All	1104/1151 (96%)	730 (66%)	239 (22%)	135 (12%)	0	1

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	27	PRO
1	A	127	ARG
1	A	142	GLY
1	A	198	ALA

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Mol	Chain	Res	Type
1	A	218	GLY
1	A	258	THR
1	A	309	PRO
1	A	373	GLU
1	A	406	ILE
1	A	407	LYS
1	A	475	PHE
1	A	476	GLU
1	A	532	ILE
1	A	543	PRO
1	A	559	LEU
1	A	563	PRO
1	A	571	PRO
1	A	576	ALA
1	A	594	ALA
1	A	604	ILE
1	A	613	GLN
1	A	615	SER
1	A	620	VAL
1	A	625	THR
1	A	679	LYS
1	A	814	GLN
2	B	8	VAL
2	B	9	LYS
2	B	10	LEU
2	B	29	ARG
2	B	30	ASP
2	B	52	ASP
2	B	81	THR
2	B	83	PRO
2	B	96	GLU
2	B	99	GLN
2	B	106	TYR
2	B	107	LEU
2	B	117	ASN
3	C	74	GLU
3	C	81	GLY
3	C	156	ASP
1	A	5	PHE
1	A	42	GLY
1	A	64	GLN
1	A	88	MET

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Mol	Chain	Res	Type
1	A	288	HIS
1	A	311	PRO
1	A	315	GLY
1	A	377	ALA
1	A	390	LEU
1	A	409	GLY
1	A	479	CYS
1	A	533	LEU
1	A	605	ASN
1	A	653	GLU
1	A	657	LYS
1	A	682	GLY
1	A	727	PRO
1	A	731	PRO
1	A	813	ILE
2	B	12	GLN
2	B	34	GLY
2	B	62	PRO
2	B	76	GLU
2	B	79	SER
2	B	138	ASN
2	B	148	LYS
3	C	13	GLU
3	C	25	ASP
3	C	58	MET
3	C	73	GLU
3	C	103	SER
3	C	117	ARG
3	C	136	ILE
3	C	155	PRO
1	A	55	GLU
1	A	131	ILE
1	A	161	GLN
1	A	167	ARG
1	A	284	GLU
1	A	329	ASP
1	A	394	ALA
1	A	422	VAL
1	A	544	LYS
1	A	556	ASP
1	A	573	ALA
1	A	617	GLU

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Mol	Chain	Res	Type
1	A	720	GLN
1	A	765	LYS
1	A	806	GLN
2	B	125	ASN
3	C	42	MET
3	C	61	LYS
3	C	82	THR
3	C	93	THR
3	C	98	GLY
3	C	131	ASP
1	A	153	PHE
1	A	196	VAL
1	A	299	PRO
1	A	301	ASN
1	A	496	PHE
1	A	564	MET
1	A	677	GLU
2	B	46	GLY
2	B	140	ASN
2	B	149	ALA
1	A	30	GLY
1	A	68	VAL
1	A	192	TYR
1	A	226	GLN
1	A	404	PRO
1	A	513	ILE
1	A	519	LEU
1	A	525	LEU
2	B	49	PRO
2	B	80	GLY
2	B	95	ASP
2	B	124	LYS
3	C	33	VAL
3	C	106	GLU
1	A	80	PRO
1	A	681	PRO
1	A	775	MET
1	A	801	LYS
3	C	105	ALA
1	A	392	VAL
1	A	768	VAL
1	A	386	VAL

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Mol	Chain	Res	Type
3	C	153	PRO
1	A	837	PRO
2	B	63	GLY
3	C	102	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	707/731 (97%)	628 (89%)	79 (11%)	6 24
2	B	128/134 (96%)	113 (88%)	15 (12%)	5 22
3	C	137/137 (100%)	128 (93%)	9 (7%)	16 47
All	All	972/1002 (97%)	869 (89%)	103 (11%)	6 26

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	3	MET
1	A	5	PHE
1	A	6	SER
1	A	19	LYS
1	A	35	TRP
1	A	38	ASP
1	A	52	LYS
1	A	66	THR
1	A	72	ASP
1	A	116	SER
1	A	119	PHE
1	A	120	CYS
1	A	124	ASN
1	A	148	MET
1	A	174	ILE
1	A	182	LYS

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Mol	Chain	Res	Type
1	A	184	GLU
1	A	186	THR
1	A	187	LYS
1	A	225	VAL
1	A	231	LEU
1	A	241	ARG
1	A	246	SER
1	A	247	ARG
1	A	253	ARG
1	A	267	ILE
1	A	270	TYR
1	A	276	ARG
1	A	286	ASN
1	A	289	ILE
1	A	295	SER
1	A	299	PRO
1	A	321	THR
1	A	322	LEU
1	A	325	ASP
1	A	340	PHE
1	A	359	CYS
1	A	365	GLU
1	A	367	LYS
1	A	385	LYS
1	A	393	ASN
1	A	408	VAL
1	A	425	SER
1	A	432	SER
1	A	443	ARG
1	A	444	ARG
1	A	451	THR
1	A	457	PHE
1	A	458	PHE
1	A	467	PHE
1	A	469	ILE
1	A	512	PHE
1	A	517	LEU
1	A	543	PRO
1	A	546	SER
1	A	551	LYS
1	A	563	PRO
1	A	626	PRO

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Mol	Chain	Res	Type
1	A	647	ILE
1	A	650	VAL
1	A	673	ILE
1	A	679	LYS
1	A	680	THR
1	A	700	GLU
1	A	703	ARG
1	A	705	CYS
1	A	716	SER
1	A	723	SER
1	A	732	SER
1	A	755	TYR
1	A	756	ARG
1	A	762	VAL
1	A	776	ARG
1	A	783	ILE
1	A	801	LYS
1	A	814	GLN
1	A	830	ARG
2	B	27	GLN
2	B	30	ASP
2	B	35	MET
2	B	41	MET
2	B	48	VAL
2	B	53	GLU
2	B	61	CYS
2	B	66	ASN
2	B	74	PHE
2	B	83	PRO
2	B	94	PHE
2	B	110	LEU
2	B	118	PHE
2	B	131	PRO
2	B	146	LYS
3	C	40	LEU
3	C	42	MET
3	C	45	THR
3	C	56	LYS
3	C	57	LYS
3	C	68	ILE
3	C	78	LYS
3	C	99	GLN

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Mol	Chain	Res	Type
3	C	126	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	124	ASN
1	A	236	ASN
1	A	243	ASN
1	A	255	HIS
1	A	286	ASN
1	A	318	ASN
1	A	374	GLN
1	A	557	ASN
1	A	579	HIS
1	A	607	ASN
1	A	666	HIS
1	A	668	HIS
1	A	696	ASN
1	A	788	GLN
1	A	806	GLN
1	A	814	GLN
1	A	816	ASN
1	A	833	ASN
3	C	43	ASN
3	C	48	GLN
3	C	50	HIS
3	C	52	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ADP	A	1002	4	24,29,29	1.48	4 (16%)	29,45,45	1.64	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	1002	4	-	6/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	ADP	C2-N3	3.24	1.37	1.32
5	A	1002	ADP	C5'-C4'	2.81	1.60	1.51
5	A	1002	ADP	C2-N1	2.54	1.38	1.33
5	A	1002	ADP	C5-N7	-2.37	1.31	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1002	ADP	N3-C2-N1	-6.73	118.15	128.68
5	A	1002	ADP	C2-N1-C6	2.56	123.14	118.75
5	A	1002	ADP	C1'-N9-C4	2.14	130.41	126.64
5	A	1002	ADP	PA-O5'-C5'	2.10	134.00	121.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

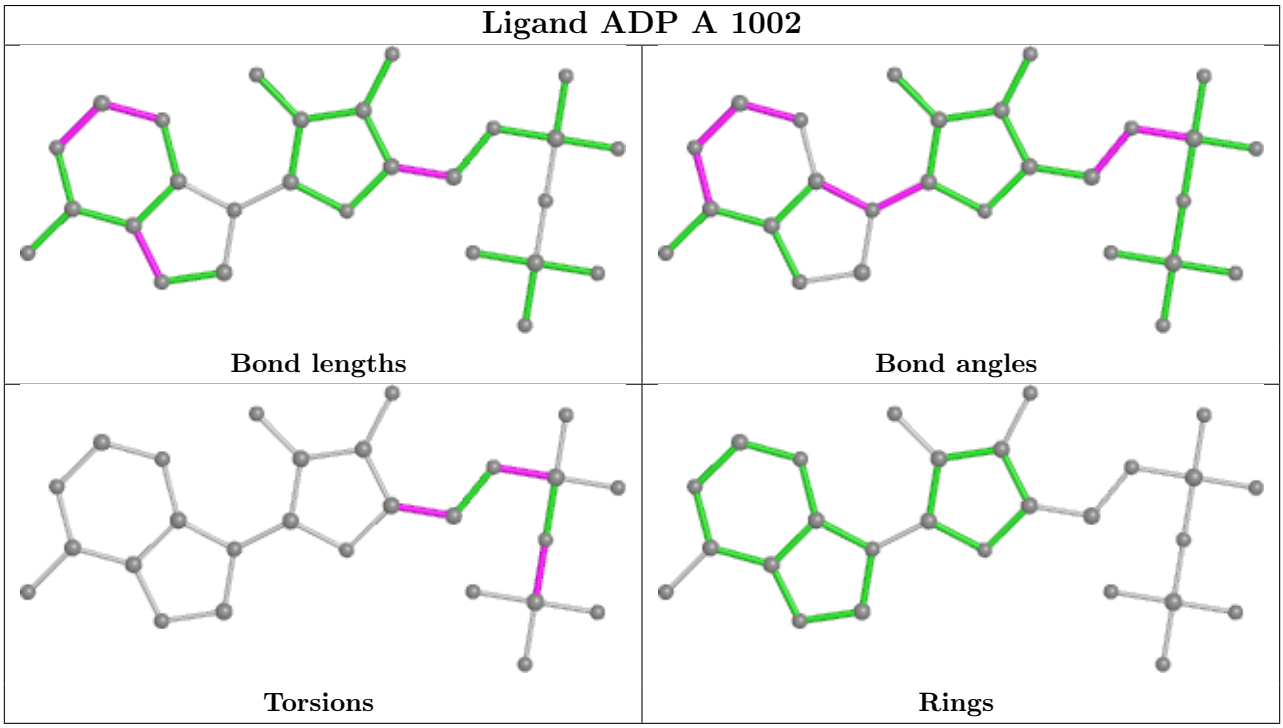
Mol	Chain	Res	Type	Atoms
5	A	1002	ADP	C5'-O5'-PA-O1A
5	A	1002	ADP	C5'-O5'-PA-O2A
5	A	1002	ADP	C5'-O5'-PA-O3A
5	A	1002	ADP	O4'-C4'-C5'-O5'
5	A	1002	ADP	C3'-C4'-C5'-O5'
5	A	1002	ADP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	810/839 (96%)	-0.27	11 (1%) 75 56	12, 36, 82, 105	0
2	B	145/153 (94%)	0.57	13 (8%) 9 3	44, 83, 107, 127	0
3	C	159/159 (100%)	-0.24	3 (1%) 66 46	13, 43, 72, 112	0
All	All	1114/1151 (96%)	-0.16	27 (2%) 59 37	12, 42, 93, 127	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	159	ASP	5.8
2	B	48	VAL	5.0
3	C	158	SER	3.7
2	B	54	LEU	3.6
3	C	157	LYS	3.6
1	A	572	LYS	3.5
2	B	38	LEU	3.5
2	B	142	MET	3.4
2	B	49	PRO	3.2
1	A	839	LEU	3.0
2	B	55	ASN	3.0
2	B	51	ASP	3.0
2	B	28	ASP	2.9
1	A	571	PRO	2.7
1	A	26	ILE	2.7
1	A	412	TYR	2.4
1	A	827	GLU	2.4
2	B	132	LEU	2.4
2	B	50	PRO	2.3
2	B	97	ASP	2.2
1	A	838	LEU	2.2
1	A	2	THR	2.2
1	A	56	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	573	ALA	2.2
1	A	201	ALA	2.1
2	B	41	MET	2.1
2	B	151	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

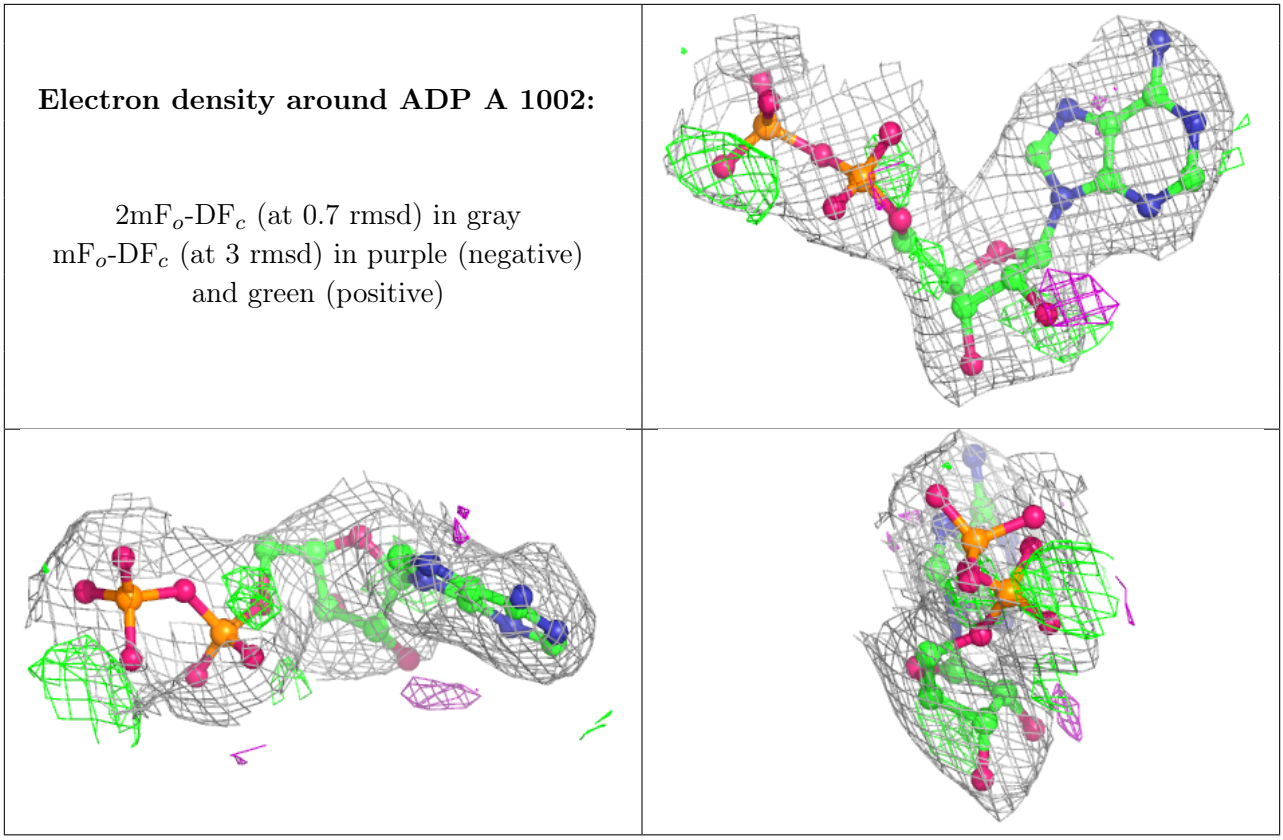
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	1001	1/1	0.85	0.52	43,43,43,43	0
5	ADP	A	1002	27/27	0.94	0.28	11,30,47,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.