



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 06:06 AM EST

PDB ID : 1KQM
Title : SCALLOP MYOSIN S1-AMPPNP IN THE ACTIN-DETACHED CONFORMATION
Authors : Himmel, D.M.; Gourinath, S.; Reshetnikova, L.; Shen, Y.; Szent-Gyorgyi, G.; Cohen, C.
Deposited on : 2002-01-07
Resolution : 3.00 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

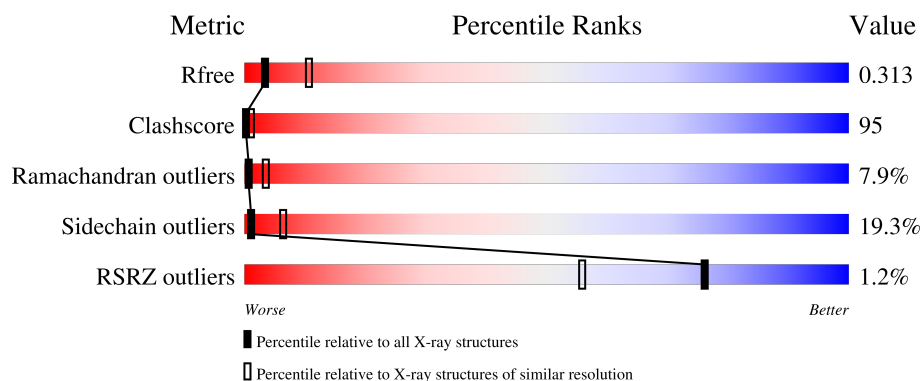
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	835	
2	B	156	
3	C	156	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ANP	A	999	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8276 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	777	Total	C	N	O	S	0	0	0
			5964	3781	1028	1120	35			

- Molecule 2 is a protein called MYOSIN REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			1097	691	176	223	7			

- Molecule 3 is a protein called MYOSIN ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1174	744	183	240	7			

- 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		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Ca 1 1	0	0

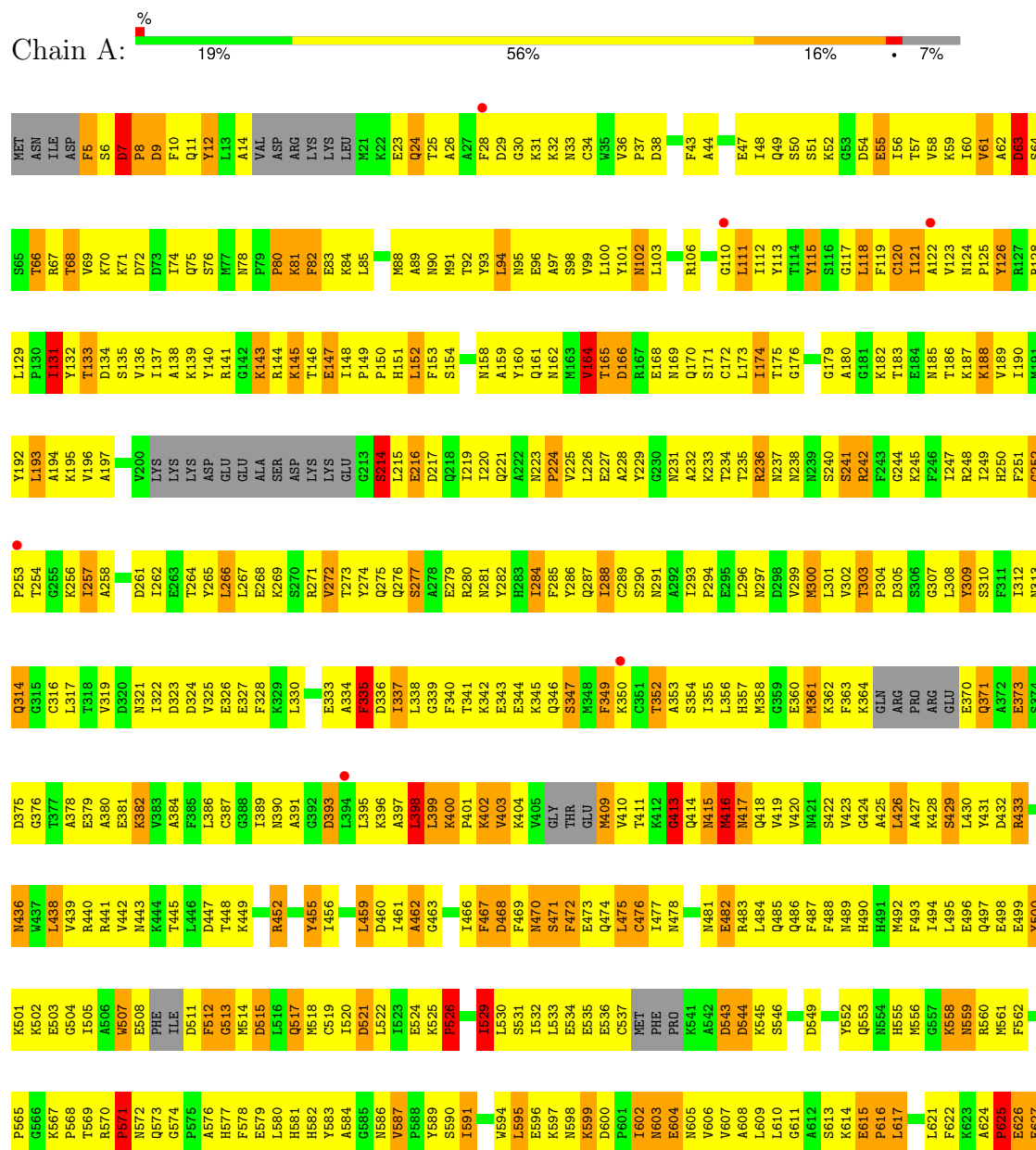
- Molecule 7 is water.

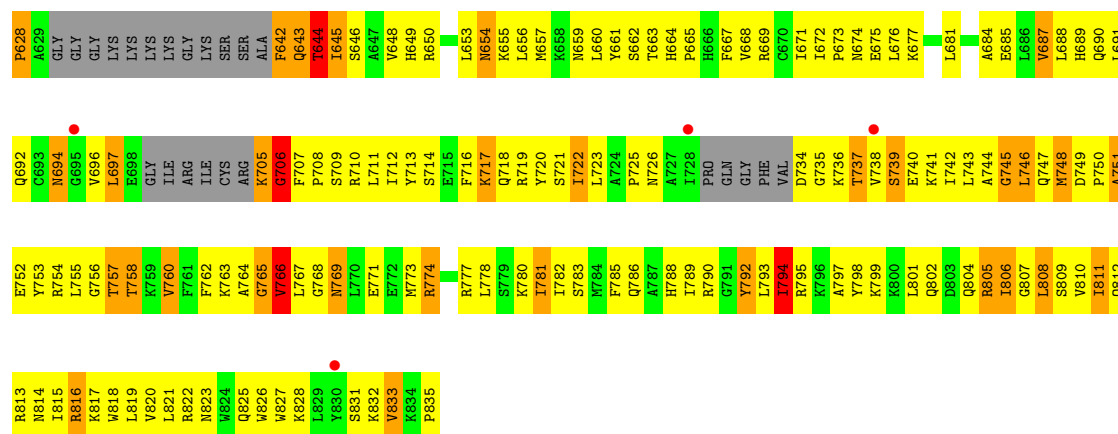
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	5	Total O 5 5	0	0
7	B	1	Total O 1 1	0	0
7	C	1	Total O 1 1	0	0

3 Residue-property plots

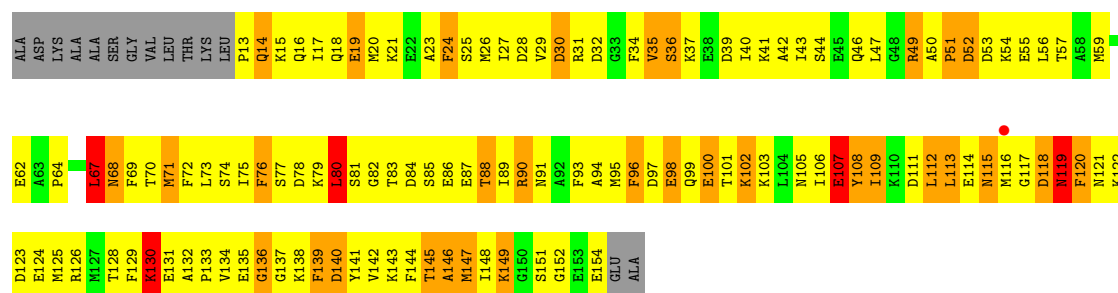
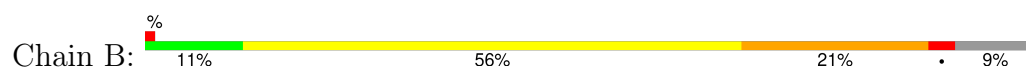
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

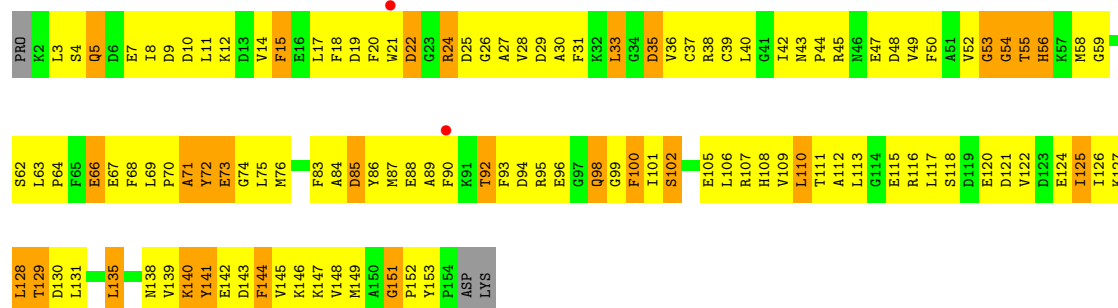




• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN



• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.40Å 58.64Å 148.87Å 81.64° 82.39° 87.43°	Depositor
Resolution (Å)	39.81 – 3.00 39.81 – 3.00	Depositor EDS
% Data completeness (in resolution range)	73.1 (39.81-3.00) 82.9 (39.81-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.01Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.277 , 0.316 0.279 , 0.313	Depositor DCC
R_{free} test set	1541 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8276	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	1/6074 (0.0%)	1.18	45/8217 (0.5%)
2	B	0.81	2/1114 (0.2%)	1.09	5/1494 (0.3%)
3	C	0.71	0/1198	0.89	1/1619 (0.1%)
All	All	0.77	3/8386 (0.0%)	1.13	51/11330 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	19	GLU	CG-CD	5.47	1.60	1.51
1	A	625	PRO	CA-C	-5.47	1.42	1.52
2	B	107	GLU	CD-OE1	5.01	1.31	1.25

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	643	GLN	N-CA-C	8.93	135.11	111.00
1	A	644	THR	N-CA-C	-8.88	87.04	111.00
1	A	706	GLY	N-CA-C	8.65	134.73	113.10
1	A	26	ALA	N-CA-C	-8.64	87.67	111.00
1	A	402	LYS	N-CA-C	8.46	133.83	111.00
1	A	705	LYS	CA-C-N	8.42	133.05	116.20
2	B	67	LEU	N-CA-C	8.02	132.65	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	A	833	VAL	CB-CA-C	-7.38	97.39	111.40
1	A	734	ASP	N-CA-C	7.23	130.51	111.00
1	A	626	GLU	N-CA-C	-7.18	91.61	111.00
1	A	513	GLY	N-CA-C	-7.05	95.47	113.10
1	A	236	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	413	GLY	N-CA-C	6.94	130.44	113.10
1	A	24	GLN	N-CA-C	-6.59	93.20	111.00
1	A	214	SER	N-CA-C	-6.57	93.25	111.00
1	A	628	PRO	N-CA-C	6.52	129.04	112.10
1	A	734	ASP	CA-C-N	-6.32	103.56	116.20
1	A	399	LEU	N-CA-C	-6.14	94.41	111.00
1	A	833	VAL	N-CA-C	6.13	127.55	111.00
2	B	152	GLY	N-CA-C	-6.12	97.79	113.10
1	A	471	SER	N-CA-CB	6.09	119.64	110.50
2	B	115	ASN	C-N-CA	6.07	136.88	121.70
1	A	751	ALA	N-CA-C	-6.04	94.69	111.00
1	A	67	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	B	118	ASP	N-CA-C	-5.83	95.25	111.00
1	A	66	THR	N-CA-C	5.83	126.74	111.00
1	A	571	PRO	N-CA-C	5.65	126.78	112.10
1	A	25	THR	CA-C-N	-5.62	104.84	117.20
1	A	398	LEU	CA-CB-CG	-5.62	102.38	115.30
1	A	25	THR	N-CA-C	5.60	126.11	111.00
1	A	252	GLY	C-N-CD	5.50	139.95	128.40
1	A	172	CYS	CA-CB-SG	-5.48	104.14	114.00
1	A	544	ASP	N-CA-C	5.46	125.74	111.00
1	A	642	PHE	N-CA-C	5.36	125.46	111.00
1	A	409	MET	CB-CG-SD	5.32	128.36	112.40
1	A	164	VAL	CB-CA-C	-5.29	101.35	111.40
1	A	642	PHE	C-N-CA	5.29	134.93	121.70
1	A	63	ASP	N-CA-C	-5.26	96.81	111.00
2	B	140	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	433	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	A	500	TYR	N-CA-C	-5.19	97.00	111.00
1	A	574	GLY	N-CA-C	5.17	126.03	113.10
1	A	544	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	303	THR	N-CA-C	-5.13	97.15	111.00
1	A	7	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	833	VAL	O-C-N	-5.08	114.57	122.70
1	A	749	ASP	N-CA-C	-5.08	97.29	111.00
1	A	25	THR	C-N-CA	5.04	134.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	TYR	N-CA-C	-5.02	97.44	111.00
3	C	151	GLY	N-CA-C	5.01	125.63	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	TYR	Sidechain

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	5964	0	5725	1178	1
2	B	1097	0	1040	215	0
3	C	1174	0	1061	215	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	13	16	0
6	C	1	0	0	0	0
7	A	5	0	0	5	0
7	B	1	0	0	1	0
7	C	1	0	0	0	0
All	All	8276	0	7839	1534	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 95.

All (1534) 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:472:PHE:HE1	1:A:476:CYS:SG	1.25	1.59
1:A:398:LEU:CA	1:A:401:PRO:HG2	1.36	1.53
1:A:398:LEU:N	1:A:401:PRO:CG	1.78	1.46
1:A:472:PHE:CE1	1:A:476:CYS:SG	2.11	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ALA:C	1:A:401:PRO:CG	1.94	1.35
1:A:398:LEU:N	1:A:401:PRO:HG2	1.02	1.34
1:A:397:ALA:C	1:A:401:PRO:HG2	1.50	1.30
1:A:395:LEU:O	1:A:399:LEU:HG	1.29	1.25
1:A:237:ASN:ND2	5:A:999:ANP:H5'2	1.54	1.23
1:A:472:PHE:HD1	1:A:472:PHE:O	1.18	1.22
1:A:397:ALA:O	1:A:401:PRO:HB2	1.33	1.22
1:A:197:ALA:HB2	1:A:256:LYS:CB	1.69	1.21
1:A:472:PHE:HD1	1:A:472:PHE:C	1.35	1.20
1:A:833:VAL:O	1:A:833:VAL:CG1	1.85	1.19
1:A:471:SER:OG	1:A:594:TRP:CZ2	1.97	1.18
1:A:14:ALA:HB2	1:A:149:PRO:CB	1.74	1.17
1:A:694:ASN:HD22	1:A:694:ASN:N	1.37	1.17
1:A:403:VAL:C	1:A:409:MET:HG3	1.66	1.15
1:A:397:ALA:O	1:A:398:LEU:HG	1.47	1.13
1:A:694:ASN:H	1:A:694:ASN:ND2	1.36	1.13
1:A:397:ALA:C	1:A:401:PRO:CB	2.18	1.13
1:A:363:PHE:HA	1:A:373:GLU:O	1.51	1.11
1:A:418:GLN:O	1:A:422:SER:N	1.82	1.11
1:A:402:LYS:N	1:A:411:THR:HG23	1.65	1.11
1:A:398:LEU:CA	1:A:401:PRO:CG	2.22	1.10
1:A:472:PHE:C	1:A:472:PHE:CD1	2.11	1.10
1:A:257:ILE:HD12	1:A:257:ILE:H	0.97	1.09
1:A:529:ILE:HG12	1:A:530:LEU:N	1.56	1.09
1:A:707:PHE:HB3	1:A:708:PRO:HD2	1.25	1.09
1:A:141:ARG:NH1	1:A:196:VAL:HB	1.67	1.08
2:B:44:SER:OG	2:B:50:ALA:HA	1.53	1.08
1:A:697:LEU:HD12	1:A:697:LEU:H	1.13	1.08
1:A:400:LYS:HA	1:A:414:GLN:HB2	1.15	1.08
1:A:197:ALA:CB	1:A:256:LYS:CB	2.31	1.08
1:A:257:ILE:HD12	1:A:257:ILE:N	1.59	1.07
1:A:100:LEU:HD22	1:A:688:LEU:HD21	1.29	1.07
1:A:123:VAL:HG12	1:A:673:PRO:HG3	1.28	1.07
1:A:296:LEU:HD22	1:A:299:VAL:HG11	1.37	1.07
1:A:417:ASN:HD22	1:A:417:ASN:N	1.47	1.07
1:A:461:ILE:CD1	1:A:462:ALA:H	1.67	1.07
1:A:472:PHE:O	1:A:472:PHE:CD1	2.06	1.07
1:A:416:MET:HG3	1:A:416:MET:O	1.53	1.06
1:A:598:ASN:ND2	1:A:644:THR:HB	1.68	1.06
1:A:400:LYS:N	1:A:401:PRO:HD3	1.72	1.05
1:A:417:ASN:H	1:A:417:ASN:ND2	1.54	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:TYR:HE2	1:A:757:THR:O	1.37	1.05
1:A:223:ASN:HB2	1:A:224:PRO:HD3	1.35	1.04
1:A:471:SER:OG	1:A:472:PHE:N	1.89	1.04
1:A:598:ASN:ND2	1:A:644:THR:CB	2.19	1.04
1:A:751:ALA:HA	1:A:754:ARG:HH12	1.17	1.04
1:A:400:LYS:N	1:A:401:PRO:CD	2.19	1.04
1:A:95:ASN:O	1:A:99:VAL:HG23	1.57	1.03
1:A:284:ILE:HD12	1:A:285:PHE:H	1.18	1.02
1:A:461:ILE:HD12	1:A:462:ALA:H	1.19	1.02
1:A:353:ALA:HA	1:A:356:LEU:HD12	1.42	1.01
1:A:598:ASN:HD21	1:A:644:THR:CB	1.71	1.00
2:B:119:ASN:HD22	2:B:119:ASN:N	1.51	1.00
1:A:48:ILE:HG23	1:A:58:VAL:HG12	1.38	1.00
1:A:398:LEU:HA	1:A:401:PRO:HG2	1.39	1.00
1:A:511:ASP:CA	1:A:514:MET:HB2	1.91	1.00
1:A:14:ALA:CB	1:A:149:PRO:HG3	1.92	1.00
1:A:511:ASP:N	1:A:514:MET:HB2	1.77	0.99
1:A:396:LYS:O	1:A:401:PRO:HG3	1.60	0.99
1:A:14:ALA:HB2	1:A:149:PRO:CG	1.91	0.99
1:A:131:ILE:HG13	1:A:132:TYR:CE1	1.98	0.98
1:A:237:ASN:HD21	5:A:999:ANP:H5'2	1.25	0.98
1:A:397:ALA:O	1:A:401:PRO:CB	2.11	0.98
1:A:384:ALA:HB2	1:A:391:ALA:HB2	1.47	0.97
1:A:399:LEU:N	1:A:401:PRO:CD	2.28	0.97
1:A:512:PHE:O	1:A:706:GLY:HA3	1.62	0.97
3:C:98:GLN:HE21	3:C:98:GLN:HA	1.28	0.97
3:C:135:LEU:HD12	3:C:135:LEU:H	1.30	0.97
1:A:515:ASP:OD2	1:A:515:ASP:N	1.96	0.97
1:A:805:ARG:HA	3:C:21:TRP:CZ2	2.00	0.96
1:A:257:ILE:H	1:A:257:ILE:CD1	1.64	0.96
1:A:82:PHE:CZ	1:A:91:MET:HA	2.00	0.96
1:A:753:TYR:O	1:A:754:ARG:HD3	1.64	0.96
1:A:833:VAL:O	1:A:835:PRO:HD3	1.63	0.96
1:A:395:LEU:O	1:A:399:LEU:CG	2.12	0.96
2:B:119:ASN:H	2:B:119:ASN:ND2	1.52	0.96
1:A:293:ILE:HD11	1:A:296:LEU:HD12	1.48	0.96
1:A:183:THR:HB	5:A:999:ANP:O1A	1.67	0.95
1:A:257:ILE:N	1:A:257:ILE:CD1	2.25	0.94
1:A:284:ILE:HA	1:A:287:GLN:OE1	1.67	0.94
1:A:420:VAL:O	1:A:423:VAL:HG12	1.65	0.94
1:A:400:LYS:H	1:A:401:PRO:HD3	1.27	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:VAL:HG12	2:B:143:LYS:NZ	1.82	0.94
2:B:143:LYS:HD3	2:B:146:ALA:HB3	1.50	0.94
1:A:555:HIS:HD2	1:A:558:LYS:HE3	1.29	0.94
1:A:530:LEU:O	1:A:534:GLU:HG3	1.68	0.93
1:A:11:GLN:HG2	1:A:12:TYR:HE1	1.32	0.93
2:B:93:PHE:CD2	2:B:141:TYR:HB2	2.03	0.93
3:C:42:ILE:HG22	3:C:44:PRO:HD3	1.51	0.93
1:A:364:LYS:CB	1:A:373:GLU:HG2	1.98	0.92
1:A:390:ASN:HD22	1:A:393:ASP:H	1.14	0.92
1:A:403:VAL:O	1:A:409:MET:HG3	1.67	0.92
2:B:114:GLU:HB2	2:B:125:MET:CE	2.00	0.92
1:A:812:GLN:NE2	2:B:118:ASP:O	2.02	0.92
1:A:555:HIS:CD2	1:A:558:LYS:HE3	2.03	0.92
1:A:237:ASN:ND2	5:A:999:ANP:O2A	2.01	0.92
1:A:400:LYS:HA	1:A:414:GLN:CB	2.00	0.91
1:A:529:ILE:HG12	1:A:530:LEU:H	1.29	0.91
2:B:118:ASP:OD2	3:C:24:ARG:NH2	2.02	0.91
1:A:397:ALA:O	1:A:398:LEU:CG	2.19	0.91
2:B:86:GLU:HG3	2:B:149:LYS:HD3	1.52	0.91
1:A:468:ASP:HB3	1:A:573:GLN:HA	1.51	0.90
1:A:395:LEU:CD2	1:A:399:LEU:HD21	2.02	0.90
1:A:397:ALA:CB	1:A:609:LEU:HD11	2.00	0.90
1:A:488:PHE:CE1	1:A:489:ASN:OD1	2.25	0.90
1:A:742:ILE:O	1:A:746:LEU:HD12	1.71	0.90
2:B:28:ASP:OD2	2:B:31:ARG:HA	1.70	0.90
1:A:470:ASN:N	1:A:470:ASN:HD22	1.70	0.89
1:A:126:TYR:CE1	1:A:677:LYS:HA	2.07	0.89
1:A:833:VAL:O	1:A:833:VAL:HG12	1.10	0.89
1:A:395:LEU:HD23	1:A:399:LEU:HD21	1.51	0.89
1:A:461:ILE:CG1	1:A:462:ALA:H	1.84	0.89
3:C:69:LEU:HB3	3:C:70:PRO:HD3	1.53	0.89
1:A:384:ALA:HA	1:A:389:ILE:HD12	1.53	0.89
1:A:398:LEU:C	1:A:401:PRO:HD2	1.92	0.89
1:A:398:LEU:N	1:A:401:PRO:HG3	1.87	0.89
2:B:25:SER:OG	2:B:26:MET:N	1.98	0.88
1:A:404:LYS:HA	1:A:409:MET:HA	1.56	0.88
1:A:720:TYR:HB3	1:A:723:LEU:HD12	1.53	0.88
1:A:512:PHE:N	1:A:512:PHE:CD2	2.40	0.88
1:A:713:TYR:CE2	1:A:757:THR:O	2.26	0.88
1:A:471:SER:OG	1:A:594:TRP:HZ2	1.55	0.88
1:A:712:ILE:HD12	1:A:714:SER:HB3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:C	1:A:371:GLN:HE21	1.77	0.88
2:B:53:ASP:HA	2:B:56:LEU:HD12	1.55	0.88
3:C:90:PHE:HB3	3:C:141:TYR:CE1	2.09	0.88
1:A:296:LEU:O	1:A:299:VAL:HG12	1.73	0.87
1:A:607:VAL:O	1:A:611:GLY:N	2.06	0.87
2:B:114:GLU:HB2	2:B:125:MET:HE1	1.55	0.87
1:A:488:PHE:CD1	1:A:489:ASN:OD1	2.28	0.87
1:A:402:LYS:CB	1:A:411:THR:OG1	2.23	0.87
1:A:115:TYR:CE1	1:A:150:PRO:HB3	2.09	0.86
1:A:795:ARG:HD2	3:C:38:ARG:O	1.75	0.86
1:A:234:THR:HG22	1:A:236:ARG:H	1.41	0.85
1:A:293:ILE:O	1:A:293:ILE:HG13	1.75	0.85
2:B:80:LEU:H	2:B:80:LEU:HD23	1.39	0.85
1:A:397:ALA:HB3	1:A:609:LEU:HD11	1.59	0.85
1:A:757:THR:OG1	1:A:758:THR:N	2.08	0.85
2:B:15:LYS:O	2:B:19:GLU:N	2.09	0.85
2:B:85:SER:HB2	2:B:88:THR:CG2	2.05	0.85
1:A:398:LEU:HD11	1:A:605:ASN:HB3	1.59	0.85
1:A:461:ILE:HD12	1:A:462:ALA:N	1.92	0.85
1:A:14:ALA:CB	1:A:149:PRO:CB	2.55	0.84
1:A:397:ALA:C	1:A:401:PRO:HB2	1.89	0.84
1:A:364:LYS:H	1:A:373:GLU:HB3	1.42	0.84
1:A:735:GLY:O	1:A:738:VAL:HG23	1.76	0.84
1:A:300:MET:HB2	1:A:302:VAL:HG22	1.60	0.84
1:A:389:ILE:HD12	1:A:389:ILE:O	1.78	0.84
1:A:598:ASN:HD22	1:A:644:THR:HB	1.35	0.84
1:A:778:LEU:HD11	3:C:89:ALA:HB1	1.58	0.84
1:A:14:ALA:HB2	1:A:149:PRO:HB3	1.56	0.84
1:A:361:MET:O	1:A:363:PHE:CE1	2.30	0.84
1:A:552:TYR:HA	1:A:556:MET:CB	2.06	0.84
1:A:242:ARG:O	1:A:267:LEU:HA	1.77	0.84
1:A:286:TYR:HE2	1:A:317:LEU:HA	1.40	0.84
1:A:313:ASN:HB2	1:A:317:LEU:HD21	1.59	0.84
1:A:805:ARG:CA	3:C:21:TRP:HZ2	1.89	0.84
3:C:98:GLN:HA	3:C:98:GLN:NE2	1.93	0.84
1:A:512:PHE:O	1:A:706:GLY:CA	2.26	0.84
1:A:707:PHE:HB3	1:A:708:PRO:CD	2.07	0.84
2:B:145:THR:HG22	2:B:146:ALA:N	1.92	0.84
2:B:80:LEU:HD23	2:B:80:LEU:N	1.93	0.83
1:A:763:LYS:O	1:A:766:VAL:CG2	2.26	0.83
1:A:511:ASP:HA	1:A:514:MET:HB2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:O	1:A:537:CYS:SG	2.36	0.83
1:A:697:LEU:H	1:A:697:LEU:CD1	1.89	0.83
3:C:4:SER:OG	3:C:7:GLU:HG3	1.79	0.83
1:A:82:PHE:HZ	1:A:91:MET:HA	1.40	0.82
1:A:833:VAL:HG22	2:B:47:LEU:CD1	2.09	0.82
2:B:142:VAL:HG12	2:B:143:LYS:HZ3	1.40	0.82
1:A:530:LEU:HD21	1:A:650:ARG:NE	1.95	0.82
1:A:145:LYS:NZ	1:A:158:ASN:OD1	2.12	0.82
1:A:403:VAL:C	1:A:409:MET:CG	2.47	0.82
1:A:124:ASN:O	1:A:673:PRO:HG2	1.79	0.82
1:A:284:ILE:CD1	1:A:285:PHE:H	1.93	0.82
2:B:24:PHE:HD1	2:B:24:PHE:O	1.63	0.82
2:B:135:GLU:HG3	2:B:136:GLY:H	1.43	0.82
1:A:697:LEU:HD12	1:A:697:LEU:N	1.95	0.82
1:A:507:TRP:HE3	1:A:508:GLU:H	1.28	0.81
1:A:475:LEU:HD23	1:A:475:LEU:C	2.00	0.81
1:A:722:ILE:HD11	1:A:781:ILE:HD12	1.63	0.81
2:B:109:ILE:O	2:B:112:LEU:HB2	1.80	0.81
1:A:11:GLN:HB3	1:A:12:TYR:CD1	2.15	0.81
2:B:111:ASP:O	2:B:115:ASN:ND2	2.14	0.81
1:A:269:LYS:NZ	1:A:600:ASP:OD2	2.13	0.81
1:A:242:ARG:NH1	1:A:268:GLU:OE1	2.13	0.81
1:A:14:ALA:CB	1:A:149:PRO:HB3	2.10	0.81
1:A:174:ILE:HG23	1:A:668:VAL:HB	1.63	0.81
2:B:106:ILE:HG22	2:B:137:GLY:O	1.81	0.80
1:A:232:ALA:HB1	1:A:271:ARG:NH1	1.96	0.80
1:A:111:LEU:C	1:A:112:ILE:HD12	2.00	0.80
1:A:14:ALA:CB	1:A:149:PRO:CG	2.56	0.80
1:A:166:ASP:OD1	1:A:166:ASP:C	2.19	0.80
1:A:570:ARG:CB	1:A:573:GLN:CB	2.60	0.80
1:A:778:LEU:O	1:A:782:ILE:HG13	1.81	0.80
1:A:286:TYR:OH	1:A:312:ILE:O	1.99	0.80
1:A:287:GLN:HE21	1:A:328:PHE:HA	1.46	0.80
1:A:398:LEU:HA	1:A:401:PRO:CG	2.02	0.80
2:B:121:ASN:ND2	2:B:124:GLU:HG3	1.97	0.80
1:A:59:LYS:HA	1:A:66:THR:HG22	1.63	0.79
1:A:521:ASP:HB3	1:A:525:LYS:HD3	1.63	0.79
1:A:738:VAL:HG12	1:A:738:VAL:O	1.80	0.79
1:A:402:LYS:CB	1:A:411:THR:CB	2.60	0.79
1:A:364:LYS:N	1:A:373:GLU:HB3	1.98	0.79
1:A:115:TYR:OH	1:A:150:PRO:HA	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:ALA:HA	1:A:754:ARG:NH1	1.96	0.79
3:C:131:LEU:HD13	3:C:144:PHE:HD1	1.48	0.79
1:A:175:THR:HG22	1:A:176:GLY:N	1.97	0.79
1:A:598:ASN:HA	1:A:645:ILE:HD12	1.63	0.79
1:A:404:LYS:N	1:A:409:MET:HG3	1.98	0.79
1:A:60:ILE:HG21	1:A:63:ASP:HB3	1.65	0.78
1:A:512:PHE:O	1:A:706:GLY:N	2.14	0.78
1:A:83:GLU:HG2	1:A:84:LYS:N	1.98	0.78
1:A:402:LYS:CB	1:A:411:THR:CA	2.61	0.78
1:A:402:LYS:CB	1:A:411:THR:HA	2.13	0.78
2:B:113:LEU:O	2:B:120:PHE:HB2	1.83	0.78
1:A:805:ARG:CA	3:C:21:TRP:CZ2	2.66	0.78
1:A:11:GLN:HB3	1:A:12:TYR:HD1	1.49	0.78
1:A:559:ASN:HD22	1:A:560:ARG:N	1.81	0.78
1:A:361:MET:O	1:A:363:PHE:HE1	1.66	0.78
1:A:684:ALA:O	1:A:687:VAL:HG23	1.83	0.78
1:A:363:PHE:CA	1:A:373:GLU:O	2.31	0.78
1:A:240:SER:OG	5:A:999:ANP:O2G	2.02	0.77
1:A:751:ALA:CA	1:A:754:ARG:HH12	1.97	0.77
1:A:399:LEU:N	1:A:401:PRO:HD2	1.97	0.77
1:A:360:GLU:O	1:A:362:LYS:HD2	1.84	0.77
1:A:808:LEU:HD21	1:A:812:GLN:OE1	1.84	0.77
1:A:833:VAL:HG12	1:A:835:PRO:HD3	1.67	0.77
1:A:11:GLN:C	1:A:12:TYR:CD1	2.58	0.77
1:A:384:ALA:HB2	1:A:391:ALA:CB	2.14	0.77
1:A:624:ALA:HB1	1:A:628:PRO:HG3	1.66	0.77
1:A:223:ASN:HB2	1:A:224:PRO:CD	2.11	0.77
3:C:64:PRO:HG2	3:C:66:GLU:OE2	1.84	0.77
1:A:49:GLN:HB2	1:A:57:THR:HG22	1.67	0.77
1:A:100:LEU:HD22	1:A:688:LEU:CD2	2.12	0.76
1:A:403:VAL:O	1:A:410:VAL:O	2.03	0.76
1:A:532:ILE:HA	1:A:535:GLU:HG2	1.66	0.76
3:C:144:PHE:O	3:C:148:VAL:HG12	1.84	0.76
1:A:410:VAL:CG1	1:A:411:THR:N	2.48	0.76
1:A:565:PRO:HA	1:A:579:GLU:HG3	1.68	0.76
1:A:798:TYR:OH	3:C:14:VAL:HG12	1.85	0.76
1:A:505:ILE:HD12	1:A:505:ILE:O	1.85	0.76
3:C:98:GLN:HE21	3:C:98:GLN:CA	1.96	0.76
1:A:466:ILE:HG23	1:A:587:VAL:HG12	1.68	0.76
1:A:503:GLU:O	1:A:505:ILE:HG13	1.86	0.76
2:B:145:THR:CG2	2:B:146:ALA:N	2.46	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HB3	1:A:102:ASN:HD21	1.49	0.76
1:A:461:ILE:CG1	1:A:462:ALA:N	2.48	0.76
2:B:35:VAL:C	2:B:67:LEU:HD23	2.06	0.76
1:A:296:LEU:HD22	1:A:299:VAL:CG1	2.15	0.76
1:A:100:LEU:CD2	1:A:688:LEU:HD21	2.14	0.76
1:A:256:LYS:CB	1:A:257:ILE:HD12	2.16	0.76
1:A:447:ASP:OD2	1:A:449:LYS:NZ	2.19	0.76
3:C:40:LEU:HB3	3:C:72:TYR:OH	1.85	0.76
1:A:233:LYS:HD2	1:A:238:ASN:HA	1.66	0.75
1:A:459:LEU:HD22	1:A:461:ILE:HG22	1.68	0.75
1:A:806:ILE:HG22	1:A:807:GLY:H	1.51	0.75
1:A:280:ARG:HH11	1:A:319:VAL:HG13	1.51	0.75
1:A:790:ARG:HH21	3:C:117:LEU:HD23	1.52	0.75
1:A:642:PHE:CG	1:A:643:GLN:N	2.54	0.75
3:C:42:ILE:HG22	3:C:43:ASN:N	2.01	0.75
1:A:60:ILE:CG2	1:A:63:ASP:HB3	2.16	0.75
1:A:743:LEU:HA	1:A:748:MET:CE	2.17	0.75
1:A:521:ASP:O	1:A:525:LYS:HG2	1.87	0.75
1:A:767:LEU:O	1:A:767:LEU:HD12	1.87	0.75
2:B:147:MET:HE3	2:B:151:SER:H	1.52	0.75
1:A:237:ASN:HD21	5:A:999:ANP:C5'	1.98	0.75
1:A:269:LYS:NZ	1:A:600:ASP:CG	2.41	0.75
1:A:398:LEU:CA	1:A:401:PRO:CD	2.65	0.75
1:A:226:LEU:CD2	1:A:439:VAL:HG22	2.16	0.75
1:A:148:ILE:HD12	1:A:149:PRO:HD2	1.69	0.74
2:B:32:ASP:OD2	7:B:503:HOH:O	2.05	0.74
3:C:33:LEU:O	3:C:36:VAL:HG13	1.87	0.74
1:A:398:LEU:HD13	1:A:606:VAL:N	2.01	0.74
1:A:642:PHE:CD1	1:A:643:GLN:N	2.53	0.74
1:A:403:VAL:O	1:A:409:MET:CG	2.34	0.74
1:A:415:ASN:ND2	1:A:417:ASN:HD21	1.85	0.74
1:A:433:ARG:HH21	1:A:602:ILE:CD1	2.00	0.74
1:A:615:GLU:OE1	1:A:616:PRO:HD2	1.86	0.74
1:A:112:ILE:HG23	1:A:123:VAL:O	1.88	0.74
1:A:808:LEU:C	1:A:808:LEU:HD23	2.08	0.74
2:B:143:LYS:HD3	2:B:146:ALA:CB	2.18	0.74
1:A:493:PHE:O	1:A:497:GLN:HG3	1.87	0.74
1:A:52:LYS:O	1:A:52:LYS:HG2	1.87	0.73
2:B:106:ILE:HD12	2:B:106:ILE:O	1.88	0.73
2:B:117:GLY:O	2:B:119:ASN:ND2	2.21	0.73
3:C:101:ILE:O	3:C:139:VAL:HG22	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ASN:HD22	1:A:393:ASP:N	1.86	0.73
3:C:90:PHE:HB3	3:C:141:TYR:CD1	2.23	0.73
1:A:559:ASN:HD22	1:A:560:ARG:H	1.36	0.73
2:B:118:ASP:CG	3:C:24:ARG:HH21	1.91	0.73
1:A:326:GLU:OE1	1:A:326:GLU:HA	1.89	0.73
2:B:85:SER:HB2	2:B:88:THR:HG22	1.70	0.73
1:A:398:LEU:CB	1:A:606:VAL:HG22	2.19	0.73
1:A:515:ASP:HA	1:A:518:MET:HB3	1.71	0.73
1:A:29:ASP:OD1	1:A:30:GLY:N	2.21	0.73
1:A:386:LEU:HD21	7:A:1000:HOH:O	1.87	0.73
1:A:499:GLU:HA	1:A:502:LYS:HB3	1.70	0.73
1:A:590:SER:O	1:A:594:TRP:CZ2	2.42	0.73
1:A:751:ALA:O	1:A:754:ARG:CZ	2.36	0.73
1:A:765:GLY:O	1:A:769:ASN:ND2	2.22	0.73
1:A:482:GLU:OE2	1:A:582:HIS:HA	1.89	0.72
1:A:396:LYS:C	1:A:401:PRO:HG3	2.08	0.72
3:C:122:VAL:O	3:C:126:ILE:HG13	1.88	0.72
1:A:358:MET:C	1:A:360:GLU:H	1.93	0.72
1:A:530:LEU:HG	1:A:650:ARG:HH21	1.55	0.72
1:A:707:PHE:CB	1:A:708:PRO:HD2	2.10	0.72
1:A:349:PHE:H	1:A:349:PHE:HD2	1.34	0.72
1:A:537:CYS:HB2	1:A:595:LEU:HD21	1.69	0.72
1:A:28:PHE:CE1	1:A:29:ASP:O	2.42	0.72
2:B:89:ILE:C	2:B:91:ASN:H	1.93	0.72
1:A:300:MET:O	1:A:302:VAL:HG13	1.90	0.72
1:A:399:LEU:N	1:A:401:PRO:HD3	2.05	0.72
1:A:403:VAL:O	1:A:410:VAL:N	2.22	0.72
1:A:350:LYS:HE2	1:A:386:LEU:HA	1.72	0.72
1:A:189:VAL:O	1:A:193:LEU:HG	1.90	0.72
1:A:447:ASP:OD1	1:A:447:ASP:O	2.07	0.72
1:A:234:THR:HG22	1:A:236:ARG:N	2.05	0.71
1:A:379:GLU:O	1:A:382:LYS:HB2	1.90	0.71
1:A:486:GLN:NE2	1:A:517:GLN:HG2	2.03	0.71
3:C:45:ARG:O	3:C:48:ASP:HB2	1.90	0.71
1:A:470:ASN:N	1:A:470:ASN:ND2	2.38	0.71
2:B:145:THR:HG22	2:B:146:ALA:H	1.53	0.71
1:A:81:LYS:HE2	1:A:81:LYS:N	2.04	0.71
1:A:598:ASN:HD21	1:A:644:THR:CA	2.03	0.71
1:A:376:GLY:C	1:A:378:ALA:H	1.91	0.71
1:A:511:ASP:N	1:A:514:MET:CB	2.54	0.71
1:A:402:LYS:CA	1:A:411:THR:HG23	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:SER:O	1:A:813:ARG:HB2	1.90	0.71
1:A:71:LYS:HA	1:A:74:ILE:HD12	1.73	0.71
1:A:23:GLU:O	1:A:81:LYS:NZ	2.24	0.70
3:C:109:VAL:HA	3:C:113:LEU:HD13	1.73	0.70
1:A:580:LEU:HD23	1:A:581:HIS:N	2.06	0.70
1:A:183:THR:OG1	7:A:1003:HOH:O	2.09	0.70
1:A:232:ALA:HB1	1:A:271:ARG:HH11	1.53	0.70
1:A:379:GLU:HA	1:A:382:LYS:HE3	1.72	0.70
1:A:529:ILE:CG1	1:A:530:LEU:N	2.45	0.70
1:A:133:THR:HG1	1:A:135:SER:HG	1.34	0.70
2:B:64:PRO:HD2	2:B:71:MET:SD	2.31	0.70
1:A:436:ASN:HB3	1:A:440:ARG:HH22	1.56	0.70
1:A:11:GLN:C	1:A:12:TYR:HD1	1.95	0.69
1:A:250:HIS:O	1:A:257:ILE:HG22	1.92	0.69
3:C:7:GLU:HA	3:C:10:ASP:OD2	1.92	0.69
1:A:806:ILE:CG2	1:A:807:GLY:N	2.55	0.69
1:A:33:ASN:OD1	1:A:47:GLU:HG2	1.92	0.69
1:A:626:GLU:C	1:A:627:GLU:HG3	2.11	0.69
1:A:131:ILE:HG13	1:A:132:TYR:CZ	2.27	0.69
1:A:400:LYS:CA	1:A:414:GLN:HB2	2.09	0.69
1:A:441:ARG:HH12	1:A:445:THR:HG23	1.57	0.69
1:A:241:SER:OG	7:A:1003:HOH:O	2.11	0.69
2:B:138:LYS:H	2:B:138:LYS:HD2	1.56	0.69
1:A:390:ASN:ND2	1:A:393:ASP:H	1.89	0.69
1:A:11:GLN:HG2	1:A:12:TYR:CE1	2.22	0.69
1:A:95:ASN:OD1	1:A:95:ASN:C	2.31	0.69
1:A:266:LEU:HD23	1:A:266:LEU:N	2.07	0.69
1:A:398:LEU:C	1:A:401:PRO:CD	2.59	0.69
1:A:398:LEU:HD11	1:A:605:ASN:CB	2.23	0.69
1:A:350:LYS:HE2	1:A:386:LEU:O	1.93	0.69
1:A:357:HIS:O	1:A:360:GLU:HB2	1.92	0.69
1:A:537:CYS:HB2	1:A:595:LEU:CD2	2.23	0.69
1:A:805:ARG:HA	3:C:21:TRP:CH2	2.28	0.69
2:B:93:PHE:O	2:B:95:MET:N	2.26	0.69
1:A:244:GLY:N	1:A:265:TYR:O	2.26	0.68
1:A:266:LEU:HD11	1:A:649:HIS:CD2	2.28	0.68
1:A:495:LEU:HD12	1:A:498:GLU:CB	2.23	0.68
1:A:537:CYS:CA	1:A:595:LEU:HD21	2.23	0.68
1:A:403:VAL:HG23	1:A:604:GLU:HB2	1.75	0.68
1:A:438:LEU:O	1:A:442:VAL:HG23	1.92	0.68
1:A:788:HIS:NE2	3:C:149:MET:HA	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:ARG:HG3	3:C:39:CYS:HA	1.75	0.68
1:A:826:TRP:HZ2	2:B:59:MET:O	1.76	0.68
1:A:169:ASN:CB	1:A:663:THR:HG22	2.24	0.68
1:A:507:TRP:HH2	1:A:763:LYS:CE	2.06	0.68
3:C:143:ASP:O	3:C:146:LYS:N	2.16	0.68
1:A:197:ALA:HB1	1:A:256:LYS:CB	2.22	0.68
1:A:398:LEU:HA	1:A:401:PRO:CD	2.22	0.68
3:C:30:ALA:HB3	3:C:55:THR:HB	1.75	0.68
1:A:169:ASN:HB3	1:A:663:THR:HG22	1.74	0.68
1:A:763:LYS:N	1:A:766:VAL:HG21	2.09	0.68
1:A:112:ILE:HD12	1:A:112:ILE:N	2.09	0.67
1:A:269:LYS:NZ	1:A:600:ASP:OD1	2.27	0.67
1:A:415:ASN:OD1	1:A:416:MET:N	2.27	0.67
1:A:717:LYS:O	1:A:719:ARG:N	2.27	0.67
1:A:769:ASN:HD22	1:A:769:ASN:N	1.90	0.67
1:A:815:ILE:HD11	2:B:144:PHE:HE2	1.57	0.67
3:C:107:ARG:O	3:C:110:LEU:HD12	1.94	0.67
1:A:763:LYS:O	1:A:766:VAL:HG23	1.94	0.67
3:C:8:ILE:O	3:C:12:LYS:HG3	1.94	0.67
1:A:415:ASN:CG	1:A:417:ASN:ND2	2.48	0.67
1:A:433:ARG:NH2	1:A:602:ILE:CD1	2.57	0.67
1:A:813:ARG:NH2	2:B:84:ASP:OD2	2.26	0.67
2:B:27:ILE:HG22	2:B:35:VAL:HG11	1.75	0.67
1:A:321:ASN:N	1:A:321:ASN:HD22	1.92	0.67
1:A:370:GLU:O	1:A:371:GLN:NE2	2.26	0.67
1:A:799:LYS:HA	1:A:802:GLN:HE21	1.58	0.67
1:A:398:LEU:CA	1:A:401:PRO:HD2	2.24	0.67
1:A:54:ASP:HB3	1:A:70:LYS:CD	2.24	0.67
1:A:266:LEU:HD11	1:A:649:HIS:NE2	2.10	0.67
1:A:397:ALA:O	1:A:398:LEU:CD1	2.43	0.67
1:A:466:ILE:HG23	1:A:587:VAL:CG1	2.25	0.67
3:C:90:PHE:HB3	3:C:141:TYR:HE1	1.60	0.67
1:A:299:VAL:HG13	1:A:300:MET:HG2	1.77	0.67
1:A:362:LYS:C	1:A:363:PHE:CD1	2.68	0.67
1:A:774:ARG:HG3	1:A:774:ARG:HH11	1.60	0.67
1:A:555:HIS:CD2	1:A:558:LYS:CE	2.76	0.66
1:A:488:PHE:HE1	1:A:489:ASN:OD1	1.75	0.66
1:A:817:LYS:C	1:A:819:LEU:H	1.98	0.66
1:A:819:LEU:HD23	1:A:822:ARG:HH21	1.60	0.66
1:A:5:PHE:N	1:A:5:PHE:CD2	2.63	0.66
1:A:422:SER:O	1:A:425:ALA:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:NH2	1:A:279:GLU:HG2	2.10	0.66
1:A:798:TYR:O	1:A:802:GLN:HG3	1.95	0.66
1:A:11:GLN:CG	1:A:12:TYR:HE1	2.07	0.66
1:A:215:LEU:HD12	1:A:215:LEU:O	1.96	0.66
1:A:441:ARG:NH1	1:A:445:THR:HG23	2.11	0.66
1:A:691:LEU:HA	1:A:694:ASN:HD21	1.61	0.66
1:A:410:VAL:HG13	1:A:411:THR:H	1.60	0.66
1:A:607:VAL:O	1:A:610:LEU:N	2.28	0.66
1:A:112:ILE:O	1:A:122:ALA:HA	1.95	0.65
1:A:461:ILE:HG13	1:A:462:ALA:N	2.11	0.65
1:A:743:LEU:HA	1:A:748:MET:HE3	1.78	0.65
1:A:792:TYR:HE1	3:C:128:LEU:HD13	1.61	0.65
1:A:806:ILE:HG22	1:A:807:GLY:N	2.10	0.65
2:B:143:LYS:HA	2:B:146:ALA:HB3	1.77	0.65
1:A:440:ARG:NH1	1:A:440:ARG:HB2	2.10	0.65
1:A:532:ILE:HG12	1:A:535:GLU:OE2	1.95	0.65
1:A:402:LYS:CB	1:A:411:THR:HG23	2.27	0.65
1:A:284:ILE:O	1:A:287:GLN:HG2	1.95	0.65
1:A:402:LYS:CB	1:A:410:VAL:O	2.45	0.65
2:B:24:PHE:O	2:B:24:PHE:CD1	2.49	0.65
2:B:114:GLU:HB2	2:B:125:MET:HE2	1.79	0.65
1:A:80:PRO:C	1:A:82:PHE:H	2.00	0.65
1:A:341:THR:HB	1:A:343:GLU:HG2	1.79	0.65
2:B:43:ILE:HD12	2:B:46:GLN:HB3	1.79	0.65
1:A:343:GLU:O	1:A:347:SER:OG	2.15	0.65
1:A:166:ASP:OD1	1:A:166:ASP:O	2.15	0.65
1:A:175:THR:HG22	1:A:176:GLY:H	1.60	0.65
1:A:175:THR:CG2	1:A:176:GLY:N	2.60	0.65
1:A:532:ILE:C	1:A:534:GLU:N	2.49	0.65
2:B:145:THR:C	2:B:147:MET:N	2.48	0.65
1:A:235:THR:N	1:A:279:GLU:OE1	2.24	0.64
1:A:254:THR:O	1:A:254:THR:HG23	1.96	0.64
1:A:537:CYS:O	1:A:595:LEU:HD21	1.97	0.64
1:A:54:ASP:HB3	1:A:70:LYS:HD3	1.78	0.64
1:A:415:ASN:ND2	1:A:417:ASN:ND2	2.45	0.64
1:A:531:SER:O	1:A:535:GLU:HB3	1.96	0.64
1:A:694:ASN:N	1:A:694:ASN:ND2	2.10	0.64
1:A:722:ILE:HD12	1:A:778:LEU:HD13	1.78	0.64
1:A:818:TRP:CD1	2:B:148:ILE:O	2.51	0.64
3:C:42:ILE:CG2	3:C:44:PRO:HD3	2.24	0.64
1:A:175:THR:CG2	1:A:176:GLY:H	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HD13	1:A:247:ILE:HD13	1.80	0.64
1:A:341:THR:CB	1:A:343:GLU:HG2	2.28	0.64
1:A:80:PRO:O	1:A:82:PHE:N	2.31	0.64
1:A:115:TYR:HH	1:A:150:PRO:HA	1.61	0.64
2:B:40:ILE:O	2:B:42:ALA:N	2.30	0.64
1:A:244:GLY:O	1:A:265:TYR:N	2.31	0.64
1:A:507:TRP:CH2	1:A:763:LYS:HE2	2.32	0.64
1:A:170:GLN:OE1	1:A:664:HIS:HB3	1.97	0.64
1:A:308:LEU:N	7:A:1004:HOH:O	2.31	0.64
1:A:507:TRP:CH2	1:A:763:LYS:CE	2.81	0.64
1:A:417:ASN:ND2	1:A:418:GLN:H	1.95	0.63
1:A:266:LEU:HD23	1:A:266:LEU:H	1.62	0.63
1:A:799:LYS:HA	1:A:802:GLN:NE2	2.13	0.63
1:A:778:LEU:HD11	3:C:89:ALA:CB	2.29	0.63
1:A:833:VAL:HG22	2:B:47:LEU:HD12	1.80	0.63
1:A:384:ALA:HA	1:A:389:ILE:CD1	2.27	0.63
1:A:822:ARG:HA	1:A:827:TRP:HD1	1.62	0.63
2:B:49:ARG:HD3	2:B:50:ALA:N	2.13	0.63
1:A:398:LEU:HA	1:A:401:PRO:HD2	1.80	0.63
1:A:286:TYR:CE2	1:A:317:LEU:HA	2.29	0.63
1:A:617:LEU:O	1:A:621:LEU:HG	1.97	0.63
1:A:743:LEU:O	1:A:748:MET:SD	2.57	0.63
1:A:805:ARG:CB	3:C:21:TRP:HZ2	2.10	0.63
2:B:90:ARG:HB2	2:B:145:THR:HG21	1.79	0.63
1:A:475:LEU:HD23	1:A:475:LEU:O	1.97	0.63
3:C:63:LEU:HD22	3:C:67:GLU:OE2	1.99	0.63
3:C:140:LYS:HE2	3:C:140:LYS:O	1.99	0.63
1:A:245:LYS:O	1:A:459:LEU:HD23	1.99	0.63
1:A:364:LYS:CB	1:A:373:GLU:CG	2.75	0.63
1:A:753:TYR:C	1:A:754:ARG:HD3	2.19	0.63
2:B:28:ASP:OD2	2:B:31:ARG:CA	2.46	0.62
2:B:135:GLU:HA	2:B:135:GLU:OE2	1.99	0.62
1:A:384:ALA:HB2	1:A:391:ALA:N	2.14	0.62
1:A:455:TYR:OH	1:A:659:ASN:HB3	1.99	0.62
1:A:490:HIS:O	1:A:494:ILE:HG12	1.99	0.62
1:A:286:TYR:CZ	1:A:312:ILE:O	2.51	0.62
1:A:397:ALA:HB1	1:A:605:ASN:ND2	2.14	0.62
1:A:763:LYS:C	1:A:766:VAL:CG2	2.66	0.62
1:A:126:TYR:CD1	1:A:677:LYS:HA	2.33	0.62
1:A:293:ILE:O	1:A:293:ILE:CG1	2.46	0.62
1:A:440:ARG:HB2	1:A:440:ARG:HH11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ILE:HG12	1:A:722:ILE:O	1.96	0.62
2:B:30:ASP:OD2	2:B:39:ASP:OD2	2.17	0.62
2:B:107:GLU:O	2:B:111:ASP:HB2	2.00	0.62
2:B:108:TYR:O	2:B:111:ASP:HB3	1.99	0.62
3:C:42:ILE:CG2	3:C:43:ASN:N	2.61	0.62
1:A:152:LEU:HD12	1:A:152:LEU:O	1.98	0.62
1:A:486:GLN:HE22	1:A:517:GLN:HG2	1.63	0.62
1:A:594:TRP:HA	1:A:597:LYS:HB3	1.80	0.62
1:A:252:GLY:O	1:A:253:PRO:C	2.33	0.62
1:A:403:VAL:HG13	1:A:404:LYS:N	2.15	0.62
1:A:404:LYS:HA	1:A:409:MET:HG3	1.80	0.62
3:C:84:ALA:O	3:C:87:MET:N	2.30	0.62
1:A:293:ILE:CD1	1:A:296:LEU:HD12	2.27	0.62
1:A:537:CYS:CB	1:A:595:LEU:HD21	2.30	0.62
1:A:387:CYS:HB2	1:A:389:ILE:HG13	1.81	0.62
1:A:403:VAL:HG22	1:A:404:LYS:H	1.63	0.62
1:A:410:VAL:HG12	1:A:411:THR:N	2.15	0.62
1:A:398:LEU:HD22	1:A:606:VAL:HG23	1.81	0.62
1:A:395:LEU:C	1:A:399:LEU:HG	2.18	0.62
1:A:397:ALA:HB3	1:A:609:LEU:CD1	2.29	0.62
1:A:669:ARG:NH1	1:A:694:ASN:HB2	2.15	0.62
1:A:805:ARG:HB2	3:C:21:TRP:HZ2	1.65	0.62
1:A:426:LEU:HG	1:A:427:ALA:N	2.15	0.61
2:B:36:SER:N	2:B:39:ASP:HB3	2.15	0.61
1:A:164:VAL:HG12	1:A:165:THR:N	2.14	0.61
1:A:275:GLN:HB2	1:A:314:GLN:HB2	1.81	0.61
1:A:475:LEU:C	1:A:475:LEU:CD2	2.68	0.61
1:A:743:LEU:C	1:A:748:MET:SD	2.79	0.61
2:B:145:THR:HA	2:B:148:ILE:HG22	1.81	0.61
3:C:135:LEU:HD12	3:C:135:LEU:N	2.08	0.61
1:A:404:LYS:CA	1:A:409:MET:HG3	2.29	0.61
1:A:604:GLU:O	1:A:607:VAL:HB	2.00	0.61
1:A:744:ALA:O	1:A:746:LEU:N	2.28	0.61
1:A:8:PRO:HG2	1:A:9:ASP:H	1.65	0.61
1:A:190:ILE:HD11	1:A:247:ILE:HG21	1.81	0.61
1:A:296:LEU:CA	1:A:299:VAL:HG12	2.29	0.61
3:C:36:VAL:HG21	3:C:68:PHE:CZ	2.35	0.61
1:A:738:VAL:O	1:A:738:VAL:CG1	2.48	0.61
2:B:53:ASP:CG	2:B:54:LYS:H	2.04	0.61
1:A:384:ALA:CB	1:A:391:ALA:H	2.13	0.61
1:A:429:SER:O	1:A:433:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:VAL:HG11	3:C:68:PHE:HZ	1.64	0.61
3:C:131:LEU:HD13	3:C:144:PHE:CD1	2.33	0.61
1:A:169:ASN:HB2	1:A:662:SER:O	2.00	0.61
1:A:441:ARG:HH12	1:A:445:THR:CG2	2.12	0.61
1:A:469:PHE:C	1:A:470:ASN:HD22	2.04	0.61
3:C:86:TYR:HB3	3:C:145:VAL:HG11	1.83	0.61
3:C:99:GLY:C	3:C:100:PHE:HD2	2.04	0.61
1:A:217:ASP:O	1:A:221:GLN:HG2	2.00	0.61
1:A:801:LEU:HD21	3:C:21:TRP:NE1	2.16	0.61
3:C:71:ALA:O	3:C:72:TYR:C	2.37	0.61
1:A:488:PHE:HD1	1:A:489:ASN:OD1	1.81	0.60
1:A:232:ALA:CB	1:A:271:ARG:NH1	2.64	0.60
1:A:313:ASN:CB	1:A:317:LEU:HD21	2.31	0.60
1:A:354:SER:O	1:A:358:MET:HG2	2.01	0.60
1:A:404:LYS:HA	1:A:409:MET:CA	2.30	0.60
1:A:14:ALA:HB3	1:A:149:PRO:HG3	1.78	0.60
1:A:801:LEU:HD22	3:C:17:LEU:HD11	1.82	0.60
2:B:27:ILE:CG2	2:B:35:VAL:HG11	2.31	0.60
3:C:40:LEU:HD12	3:C:72:TYR:CE1	2.36	0.60
1:A:535:GLU:CG	1:A:536:GLU:N	2.64	0.60
2:B:24:PHE:HE2	2:B:69:PHE:HA	1.66	0.60
2:B:35:VAL:O	2:B:67:LEU:HD23	2.01	0.60
1:A:323:ASP:OD1	1:A:325:VAL:HG22	2.00	0.60
1:A:425:ALA:O	1:A:429:SER:HB3	2.01	0.60
3:C:94:ASP:OD1	3:C:99:GLY:N	2.34	0.60
3:C:108:HIS:ND1	3:C:112:ALA:HB3	2.16	0.60
1:A:245:LYS:HB2	7:A:1002:HOH:O	2.01	0.60
1:A:399:LEU:H	1:A:401:PRO:CD	2.09	0.60
1:A:537:CYS:HA	1:A:595:LEU:HD11	1.84	0.60
1:A:398:LEU:HD11	1:A:605:ASN:ND2	2.17	0.60
1:A:569:THR:O	1:A:570:ARG:C	2.39	0.60
1:A:353:ALA:CA	1:A:356:LEU:HD12	2.27	0.60
1:A:807:GLY:H	2:B:95:MET:HE3	1.66	0.60
1:A:143:LYS:HE3	1:A:143:LYS:HA	1.83	0.60
1:A:598:ASN:ND2	1:A:644:THR:OG1	2.32	0.60
1:A:137:ILE:HG12	1:A:153:PHE:CE2	2.37	0.60
1:A:275:GLN:NE2	1:A:281:ASN:HD22	2.00	0.60
1:A:361:MET:O	1:A:363:PHE:CD1	2.55	0.60
1:A:397:ALA:CA	1:A:401:PRO:CB	2.79	0.60
1:A:423:VAL:HG13	1:A:424:GLY:N	2.17	0.60
1:A:535:GLU:CG	1:A:536:GLU:H	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:ALA:CA	1:A:754:ARG:NH1	2.60	0.60
2:B:98:GLU:H	2:B:98:GLU:CD	2.04	0.60
1:A:471:SER:OG	1:A:594:TRP:CE2	2.51	0.59
3:C:3:LEU:HB2	3:C:7:GLU:OE1	2.02	0.59
3:C:107:ARG:HD3	3:C:122:VAL:HG11	1.83	0.59
1:A:141:ARG:HH12	1:A:196:VAL:HB	1.60	0.59
1:A:274:TYR:CD1	1:A:275:GLN:N	2.70	0.59
1:A:325:VAL:HG23	1:A:326:GLU:N	2.17	0.59
1:A:342:LYS:HG2	1:A:346:GLN:HE21	1.66	0.59
1:A:400:LYS:N	1:A:401:PRO:HD2	2.12	0.59
1:A:415:ASN:CG	1:A:417:ASN:HD21	2.04	0.59
1:A:488:PHE:CD1	1:A:488:PHE:C	2.76	0.59
1:A:814:ASN:N	1:A:814:ASN:HD22	2.00	0.59
1:A:717:LYS:C	1:A:719:ARG:H	2.06	0.59
2:B:68:ASN:N	2:B:68:ASN:HD22	2.00	0.59
1:A:792:TYR:O	1:A:792:TYR:CD1	2.55	0.59
3:C:42:ILE:HG22	3:C:44:PRO:CD	2.27	0.59
3:C:64:PRO:CG	3:C:66:GLU:OE2	2.50	0.59
3:C:101:ILE:O	3:C:139:VAL:CG2	2.50	0.59
1:A:789:ILE:HG23	3:C:125:ILE:HG12	1.85	0.59
1:A:477:ILE:O	1:A:481:ASN:ND2	2.35	0.59
3:C:17:LEU:O	3:C:21:TRP:CD1	2.55	0.59
1:A:24:GLN:HA	1:A:81:LYS:HD2	1.85	0.59
2:B:145:THR:C	2:B:147:MET:H	2.05	0.59
3:C:18:PHE:C	3:C:20:PHE:N	2.51	0.59
1:A:55:GLU:O	1:A:56:ILE:HD13	2.03	0.59
1:A:124:ASN:C	1:A:124:ASN:OD1	2.40	0.59
1:A:233:LYS:O	1:A:279:GLU:HG3	2.03	0.59
1:A:269:LYS:HZ2	1:A:600:ASP:CG	2.04	0.59
1:A:397:ALA:C	1:A:401:PRO:HG3	2.12	0.59
3:C:9:ASP:C	3:C:11:LEU:H	2.05	0.59
1:A:517:GLN:O	1:A:517:GLN:NE2	2.36	0.58
1:A:720:TYR:OH	1:A:771:GLU:HG2	2.03	0.58
3:C:15:PHE:CD1	3:C:15:PHE:C	2.76	0.58
3:C:17:LEU:CD1	3:C:21:TRP:HE1	2.16	0.58
1:A:808:LEU:HD23	1:A:809:SER:N	2.17	0.58
1:A:438:LEU:C	1:A:438:LEU:CD2	2.71	0.58
1:A:496:GLU:OE2	1:A:710:ARG:NH2	2.37	0.58
1:A:777:ARG:NH1	1:A:780:LYS:HD3	2.17	0.58
2:B:24:PHE:HA	2:B:27:ILE:HD12	1.84	0.58
1:A:240:SER:CB	5:A:999:ANP:O2G	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:VAL:HG22	3:C:29:ASP:H	1.69	0.58
1:A:28:PHE:CD1	1:A:29:ASP:O	2.57	0.58
1:A:158:ASN:HA	1:A:161:GLN:HB2	1.84	0.58
1:A:801:LEU:O	1:A:801:LEU:HD23	2.02	0.58
3:C:37:CYS:O	3:C:42:ILE:HB	2.03	0.58
1:A:674:ASN:ND2	1:A:681:LEU:HB3	2.18	0.58
2:B:29:VAL:O	2:B:30:ASP:C	2.42	0.58
2:B:44:SER:OG	2:B:50:ALA:CA	2.42	0.58
3:C:3:LEU:H	3:C:3:LEU:HD23	1.68	0.58
3:C:18:PHE:C	3:C:20:PHE:H	2.05	0.58
1:A:288:ILE:HD12	1:A:352:THR:CG2	2.34	0.58
1:A:744:ALA:C	1:A:746:LEU:H	2.07	0.58
1:A:799:LYS:CA	1:A:802:GLN:HE21	2.17	0.58
2:B:29:VAL:C	2:B:31:ARG:N	2.55	0.58
2:B:67:LEU:N	2:B:67:LEU:CD1	2.66	0.58
2:B:142:VAL:HG12	2:B:143:LYS:HZ2	1.69	0.58
2:B:142:VAL:CG1	2:B:143:LYS:HZ3	2.15	0.58
3:C:28:VAL:HG22	3:C:29:ASP:N	2.18	0.58
3:C:145:VAL:O	3:C:149:MET:HB2	2.04	0.58
1:A:78:ASN:OD1	1:A:92:THR:HB	2.03	0.58
1:A:145:LYS:HB2	1:A:145:LYS:HZ3	1.68	0.58
1:A:166:ASP:OD1	1:A:168:GLU:HG2	2.04	0.58
1:A:459:LEU:HD22	1:A:461:ILE:CG2	2.34	0.58
1:A:598:ASN:ND2	1:A:644:THR:CA	2.63	0.58
1:A:735:GLY:C	1:A:737:THR:H	2.06	0.58
1:A:769:ASN:HD22	1:A:769:ASN:H	1.50	0.58
1:A:515:ASP:HA	1:A:518:MET:CB	2.34	0.58
2:B:90:ARG:O	2:B:90:ARG:HG2	2.04	0.58
1:A:94:LEU:HD12	1:A:94:LEU:O	2.03	0.58
1:A:379:GLU:O	1:A:382:LYS:CB	2.52	0.58
1:A:720:TYR:HB3	1:A:723:LEU:CD1	2.30	0.58
2:B:87:GLU:OE1	2:B:87:GLU:HA	2.03	0.58
1:A:121:ILE:O	1:A:121:ILE:HG22	2.04	0.57
1:A:221:GLN:O	1:A:224:PRO:HD2	2.04	0.57
1:A:225:VAL:HG11	1:A:438:LEU:HD21	1.86	0.57
1:A:384:ALA:HB2	1:A:391:ALA:H	1.68	0.57
1:A:396:LYS:O	1:A:401:PRO:CG	2.45	0.57
1:A:398:LEU:HD13	1:A:606:VAL:CA	2.33	0.57
1:A:410:VAL:CG1	1:A:411:THR:H	2.16	0.57
1:A:642:PHE:CZ	1:A:643:GLN:O	2.57	0.57
1:A:766:VAL:C	1:A:768:GLY:N	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASN:HD21	2:B:124:GLU:HG3	1.66	0.57
1:A:287:GLN:HE21	1:A:328:PHE:CA	2.16	0.57
1:A:515:ASP:OD1	1:A:560:ARG:NH2	2.38	0.57
1:A:580:LEU:HD23	1:A:581:HIS:H	1.68	0.57
1:A:789:ILE:HG12	3:C:148:VAL:HG21	1.85	0.57
1:A:792:TYR:CD1	1:A:792:TYR:C	2.78	0.57
1:A:313:ASN:OD1	1:A:313:ASN:O	2.22	0.57
2:B:145:THR:O	2:B:147:MET:N	2.37	0.57
3:C:109:VAL:O	3:C:113:LEU:HD13	2.04	0.57
1:A:56:ILE:HB	1:A:69:VAL:HG23	1.87	0.57
2:B:111:ASP:OD1	2:B:115:ASN:ND2	2.36	0.57
1:A:596:GLU:HG3	1:A:597:LYS:N	2.20	0.57
1:A:725:PRO:HG2	3:C:85:ASP:OD1	2.05	0.57
2:B:105:ASN:HB3	2:B:108:TYR:HB2	1.85	0.57
1:A:174:ILE:HG23	1:A:668:VAL:CB	2.34	0.57
1:A:517:GLN:NE2	1:A:521:ASP:OD2	2.37	0.57
1:A:36:VAL:CG1	1:A:37:PRO:HD2	2.35	0.57
1:A:363:PHE:HE2	1:A:399:LEU:HD22	1.69	0.57
1:A:696:VAL:HG13	1:A:697:LEU:N	2.19	0.57
1:A:774:ARG:HG3	1:A:774:ARG:NH1	2.17	0.57
1:A:805:ARG:HB2	3:C:21:TRP:CZ2	2.39	0.57
1:A:124:ASN:HB2	1:A:180:ALA:O	2.04	0.57
1:A:133:THR:OG1	1:A:135:SER:OG	2.12	0.57
1:A:833:VAL:CG2	2:B:47:LEU:HD12	2.35	0.57
2:B:121:ASN:O	2:B:124:GLU:HB2	2.04	0.57
1:A:287:GLN:NE2	1:A:328:PHE:HA	2.18	0.57
1:A:395:LEU:HD22	1:A:399:LEU:HD11	1.87	0.57
1:A:416:MET:O	1:A:420:VAL:HG23	2.04	0.57
1:A:537:CYS:HB2	1:A:595:LEU:CG	2.34	0.57
2:B:27:ILE:HG22	2:B:35:VAL:CG1	2.34	0.57
2:B:126:ARG:O	2:B:130:LYS:HB2	2.04	0.57
3:C:3:LEU:HD11	3:C:8:ILE:HD13	1.86	0.57
3:C:33:LEU:C	3:C:33:LEU:HD23	2.25	0.57
1:A:11:GLN:CG	1:A:12:TYR:CE1	2.84	0.56
1:A:113:TYR:HA	1:A:121:ILE:O	2.05	0.56
1:A:183:THR:OG1	5:A:999:ANP:O2B	2.23	0.56
1:A:345:LYS:O	1:A:349:PHE:CE2	2.58	0.56
1:A:423:VAL:CG1	1:A:424:GLY:N	2.68	0.56
1:A:507:TRP:HH2	1:A:763:LYS:HE3	1.68	0.56
1:A:532:ILE:O	1:A:535:GLU:N	2.38	0.56
1:A:376:GLY:C	1:A:378:ALA:N	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:HB2	1:A:606:VAL:HG22	1.86	0.56
1:A:517:GLN:O	1:A:521:ASP:HB2	2.05	0.56
1:A:817:LYS:HA	1:A:820:VAL:HG23	1.87	0.56
3:C:83:PHE:HA	3:C:149:MET:HE3	1.87	0.56
1:A:11:GLN:CB	1:A:12:TYR:CD1	2.88	0.56
1:A:397:ALA:HA	1:A:401:PRO:HB3	1.87	0.56
1:A:535:GLU:HG3	1:A:536:GLU:N	2.20	0.56
1:A:671:ILE:O	1:A:673:PRO:HD3	2.04	0.56
1:A:766:VAL:C	1:A:768:GLY:H	2.09	0.56
1:A:14:ALA:HB2	1:A:149:PRO:HB2	1.79	0.56
1:A:78:ASN:HD21	1:A:93:TYR:H	1.54	0.56
1:A:225:VAL:HG12	1:A:438:LEU:HD11	1.88	0.56
1:A:696:VAL:CG1	1:A:697:LEU:N	2.68	0.56
1:A:113:TYR:CE1	1:A:152:LEU:HB2	2.41	0.56
1:A:226:LEU:HD22	1:A:439:VAL:HG22	1.84	0.56
3:C:135:LEU:H	3:C:135:LEU:CD1	2.08	0.56
1:A:488:PHE:HD1	1:A:489:ASN:CG	2.09	0.56
1:A:617:LEU:HD22	1:A:621:LEU:HD11	1.88	0.56
3:C:72:TYR:O	3:C:76:MET:HB2	2.06	0.56
1:A:237:ASN:CG	5:A:999:ANP:H5'2	2.20	0.56
1:A:299:VAL:CG1	1:A:300:MET:HG2	2.36	0.56
1:A:353:ALA:HA	1:A:356:LEU:CD1	2.28	0.56
1:A:515:ASP:CA	1:A:518:MET:HB3	2.35	0.56
1:A:603:ASN:O	1:A:606:VAL:HG23	2.06	0.56
1:A:735:GLY:O	1:A:738:VAL:N	2.39	0.56
1:A:819:LEU:HD23	1:A:822:ARG:NH2	2.20	0.56
1:A:310:SER:HA	1:A:313:ASN:ND2	2.20	0.56
1:A:565:PRO:CA	1:A:579:GLU:HG3	2.36	0.56
2:B:14:GLN:OE1	2:B:18:GLN:HG3	2.06	0.56
2:B:40:ILE:C	2:B:42:ALA:H	2.10	0.56
1:A:124:ASN:HD21	1:A:126:TYR:HE2	1.54	0.55
1:A:362:LYS:O	1:A:363:PHE:CD1	2.58	0.55
1:A:397:ALA:HB1	1:A:609:LEU:HD11	1.88	0.55
1:A:672:ILE:HG23	1:A:672:ILE:O	2.06	0.55
2:B:85:SER:CB	2:B:88:THR:CG2	2.83	0.55
1:A:669:ARG:HH11	1:A:694:ASN:HB2	1.71	0.55
1:A:821:LEU:HD11	1:A:827:TRP:CD2	2.42	0.55
1:A:240:SER:HA	5:A:999:ANP:O2G	2.06	0.55
1:A:296:LEU:CD2	1:A:299:VAL:HG11	2.24	0.55
1:A:415:ASN:O	1:A:419:VAL:HG23	2.06	0.55
1:A:461:ILE:HG13	1:A:462:ALA:H	1.66	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ASN:CA	1:A:645:ILE:HD12	2.36	0.55
1:A:657:MET:HA	1:A:660:LEU:HD12	1.89	0.55
1:A:75:GLN:HE21	1:A:95:ASN:HB2	1.72	0.55
1:A:288:ILE:CD1	1:A:352:THR:CG2	2.84	0.55
1:A:477:ILE:HD12	1:A:477:ILE:N	2.22	0.55
1:A:795:ARG:CG	3:C:39:CYS:HA	2.36	0.55
2:B:114:GLU:OE1	2:B:125:MET:HE2	2.06	0.55
3:C:73:GLU:O	3:C:76:MET:HB3	2.06	0.55
1:A:190:ILE:CD1	1:A:247:ILE:HD13	2.36	0.55
1:A:280:ARG:NH1	1:A:319:VAL:HG13	2.18	0.55
1:A:417:ASN:N	1:A:417:ASN:ND2	2.21	0.55
1:A:469:PHE:C	1:A:470:ASN:ND2	2.60	0.55
1:A:691:LEU:C	1:A:694:ASN:HD21	2.10	0.55
2:B:79:LYS:C	2:B:81:SER:H	2.09	0.55
3:C:87:MET:CE	3:C:142:GLU:HG2	2.37	0.55
1:A:244:GLY:O	1:A:264:THR:HA	2.07	0.55
1:A:280:ARG:NH2	1:A:286:TYR:HB2	2.22	0.55
1:A:807:GLY:O	1:A:810:VAL:HB	2.06	0.55
1:A:141:ARG:HH11	1:A:196:VAL:HB	1.66	0.55
1:A:534:GLU:CD	1:A:650:ARG:HH22	2.10	0.55
1:A:160:TYR:O	1:A:161:GLN:C	2.44	0.55
1:A:481:ASN:O	1:A:484:LEU:HB2	2.07	0.55
2:B:24:PHE:CE2	2:B:69:PHE:HA	2.42	0.55
1:A:833:VAL:HG22	2:B:47:LEU:HD11	1.86	0.55
1:A:129:LEU:HB2	1:A:131:ILE:HD11	1.89	0.54
1:A:168:GLU:O	1:A:170:GLN:NE2	2.36	0.54
1:A:321:ASN:N	1:A:321:ASN:ND2	2.54	0.54
1:A:349:PHE:N	1:A:349:PHE:CD2	2.72	0.54
1:A:402:LYS:CB	1:A:411:THR:CG2	2.84	0.54
1:A:425:ALA:O	1:A:429:SER:CB	2.55	0.54
2:B:35:VAL:O	2:B:67:LEU:CD2	2.55	0.54
1:A:819:LEU:CD2	1:A:822:ARG:NH2	2.70	0.54
1:A:190:ILE:HG23	1:A:249:ILE:CD1	2.36	0.54
1:A:321:ASN:HD22	1:A:321:ASN:H	1.53	0.54
1:A:743:LEU:CA	1:A:748:MET:CE	2.85	0.54
1:A:746:LEU:O	1:A:747:GLN:HB2	2.08	0.54
1:A:785:PHE:HE1	3:C:148:VAL:HG11	1.72	0.54
1:A:794:ILE:HD13	3:C:35:ASP:HA	1.88	0.54
2:B:32:ASP:OD1	2:B:34:PHE:N	2.39	0.54
1:A:103:LEU:CD2	1:A:121:ILE:HG21	2.37	0.54
1:A:447:ASP:OD1	1:A:449:LYS:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:SER:C	1:A:741:LYS:N	2.58	0.54
1:A:751:ALA:O	1:A:754:ARG:NH1	2.40	0.54
1:A:417:ASN:HD22	1:A:417:ASN:H	0.70	0.54
1:A:789:ILE:HG23	3:C:125:ILE:CD1	2.38	0.54
1:A:136:VAL:HA	1:A:139:LYS:HD2	1.90	0.54
1:A:296:LEU:C	1:A:299:VAL:HG12	2.27	0.54
1:A:807:GLY:HA3	2:B:95:MET:HE3	1.89	0.54
3:C:28:VAL:O	3:C:62:SER:HA	2.08	0.54
1:A:343:GLU:CD	1:A:343:GLU:H	2.11	0.54
1:A:389:ILE:HG23	1:A:613:SER:OG	2.08	0.54
1:A:120:CYS:O	1:A:669:ARG:HB2	2.07	0.54
1:A:190:ILE:HG23	1:A:249:ILE:HD11	1.90	0.54
1:A:605:ASN:O	1:A:609:LEU:HG	2.08	0.54
1:A:762:PHE:HB3	1:A:766:VAL:HG21	1.90	0.54
2:B:89:ILE:C	2:B:91:ASN:N	2.57	0.54
2:B:106:ILE:O	2:B:106:ILE:CD1	2.56	0.54
3:C:31:PHE:CA	3:C:55:THR:HG22	2.37	0.54
1:A:11:GLN:CB	1:A:12:TYR:HD1	2.20	0.54
1:A:395:LEU:HD22	1:A:399:LEU:HD21	1.86	0.54
1:A:807:GLY:HA3	2:B:95:MET:CE	2.37	0.54
1:A:144:ARG:O	1:A:147:GLU:HG3	2.08	0.54
1:A:185:ASN:O	1:A:189:VAL:HG23	2.08	0.54
1:A:226:LEU:HD21	1:A:439:VAL:HG22	1.90	0.54
1:A:532:ILE:C	1:A:534:GLU:H	2.12	0.54
1:A:650:ARG:HH11	1:A:650:ARG:HB3	1.73	0.54
1:A:794:ILE:CD1	3:C:35:ASP:HA	2.38	0.54
1:A:124:ASN:ND2	1:A:126:TYR:CE2	2.75	0.53
1:A:258:ALA:O	1:A:448:THR:HG23	2.08	0.53
1:A:486:GLN:O	1:A:490:HIS:HB2	2.08	0.53
1:A:739:SER:O	1:A:740:GLU:C	2.45	0.53
1:A:790:ARG:HH21	3:C:117:LEU:CD2	2.19	0.53
1:A:269:LYS:O	1:A:428:LYS:HD2	2.08	0.53
1:A:284:ILE:HD12	1:A:285:PHE:N	2.04	0.53
1:A:355:ILE:HA	1:A:358:MET:CG	2.39	0.53
1:A:455:TYR:CD1	1:A:455:TYR:C	2.82	0.53
1:A:472:PHE:O	1:A:473:GLU:C	2.45	0.53
1:A:512:PHE:C	1:A:706:GLY:HA3	2.26	0.53
2:B:145:THR:O	2:B:148:ILE:HG22	2.08	0.53
1:A:511:ASP:CB	1:A:512:PHE:HD2	2.21	0.53
3:C:95:ARG:CZ	3:C:96:GLU:HG2	2.37	0.53
1:A:399:LEU:H	1:A:401:PRO:HD3	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:HA	1:A:502:LYS:CB	2.38	0.53
1:A:603:ASN:H	1:A:603:ASN:HD22	1.55	0.53
1:A:826:TRP:HB3	2:B:76:PHE:HE1	1.74	0.53
1:A:605:ASN:HA	1:A:608:ALA:HB3	1.90	0.53
1:A:719:ARG:HH21	1:A:771:GLU:CD	2.12	0.53
2:B:55:GLU:O	2:B:59:MET:HG3	2.08	0.53
1:A:234:THR:CG2	1:A:236:ARG:H	2.19	0.53
1:A:515:ASP:O	1:A:518:MET:HB3	2.09	0.53
1:A:691:LEU:CA	1:A:694:ASN:HD21	2.22	0.53
2:B:86:GLU:CG	2:B:149:LYS:HD3	2.30	0.53
3:C:15:PHE:C	3:C:15:PHE:HD1	2.12	0.53
1:A:256:LYS:CB	1:A:257:ILE:CD1	2.87	0.53
1:A:284:ILE:O	1:A:287:GLN:N	2.40	0.53
1:A:579:GLU:O	1:A:580:LEU:HB2	2.09	0.53
1:A:582:HIS:C	1:A:584:ALA:H	2.12	0.53
2:B:34:PHE:HA	2:B:67:LEU:O	2.08	0.53
3:C:42:ILE:CG2	3:C:43:ASN:H	2.21	0.53
1:A:120:CYS:HB3	1:A:668:VAL:HG13	1.91	0.53
1:A:240:SER:CA	5:A:999:ANP:O2G	2.57	0.53
1:A:537:CYS:HB2	1:A:595:LEU:HG	1.91	0.53
1:A:805:ARG:CB	3:C:21:TRP:CZ2	2.92	0.53
1:A:5:PHE:N	1:A:5:PHE:HD2	2.08	0.53
1:A:364:LYS:CA	1:A:373:GLU:HB3	2.39	0.53
1:A:801:LEU:HD23	1:A:801:LEU:C	2.30	0.53
1:A:179:GLY:H	5:A:999:ANP:HNB1	1.57	0.52
1:A:336:ASP:C	1:A:338:LEU:H	2.13	0.52
1:A:416:MET:O	1:A:416:MET:CG	2.40	0.52
1:A:530:LEU:HD11	1:A:650:ARG:NH2	2.23	0.52
1:A:719:ARG:O	1:A:774:ARG:NH1	2.42	0.52
2:B:16:GLN:O	2:B:20:MET:CG	2.57	0.52
2:B:139:PHE:CD1	2:B:139:PHE:C	2.82	0.52
3:C:36:VAL:HG11	3:C:68:PHE:CZ	2.44	0.52
3:C:84:ALA:O	3:C:85:ASP:C	2.48	0.52
1:A:106:ARG:HB3	1:A:111:LEU:HD12	1.91	0.52
1:A:507:TRP:CZ3	1:A:763:LYS:HE2	2.45	0.52
1:A:594:TRP:HA	1:A:597:LYS:CB	2.39	0.52
1:A:598:ASN:OD1	1:A:645:ILE:HB	2.09	0.52
1:A:492:MET:O	1:A:495:LEU:N	2.42	0.52
1:A:530:LEU:HD21	1:A:650:ARG:HE	1.72	0.52
3:C:17:LEU:O	3:C:20:PHE:HB3	2.09	0.52
3:C:140:LYS:HE2	3:C:143:ASP:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HA	1:A:193:LEU:HD12	1.90	0.52
1:A:778:LEU:O	1:A:782:ILE:CG1	2.56	0.52
2:B:97:ASP:OD2	2:B:100:GLU:HA	2.09	0.52
2:B:147:MET:CE	2:B:151:SER:OG	2.57	0.52
3:C:36:VAL:HG21	3:C:68:PHE:HZ	1.74	0.52
3:C:113:LEU:HD12	3:C:113:LEU:N	2.25	0.52
3:C:122:VAL:HA	3:C:125:ILE:CG2	2.39	0.52
1:A:705:LYS:O	1:A:707:PHE:N	2.43	0.52
3:C:31:PHE:N	3:C:55:THR:HG22	2.24	0.52
3:C:99:GLY:C	3:C:141:TYR:HE2	2.13	0.52
1:A:400:LYS:CB	1:A:414:GLN:N	2.73	0.52
1:A:556:MET:O	1:A:558:LYS:N	2.38	0.52
1:A:707:PHE:CB	1:A:708:PRO:CD	2.80	0.52
1:A:786:GLN:OE1	3:C:115:GLU:N	2.39	0.52
1:A:764:ALA:O	1:A:766:VAL:N	2.42	0.52
3:C:7:GLU:C	3:C:9:ASP:N	2.62	0.52
1:A:60:ILE:O	1:A:64:SER:HA	2.10	0.52
1:A:586:ASN:O	1:A:587:VAL:HG13	2.10	0.52
1:A:676:LEU:HD12	1:A:681:LEU:HD22	1.91	0.52
2:B:14:GLN:O	2:B:18:GLN:HG3	2.09	0.52
1:A:31:LYS:HD3	1:A:31:LYS:N	2.24	0.52
1:A:231:ASN:O	1:A:282:TYR:HD2	1.92	0.52
1:A:492:MET:O	1:A:496:GLU:N	2.40	0.52
1:A:795:ARG:C	1:A:797:ALA:N	2.62	0.52
3:C:9:ASP:C	3:C:11:LEU:N	2.63	0.52
1:A:14:ALA:HB1	1:A:149:PRO:HB3	1.92	0.51
1:A:300:MET:CB	1:A:302:VAL:HG22	2.37	0.51
1:A:822:ARG:HA	1:A:827:TRP:CD1	2.45	0.51
2:B:67:LEU:N	2:B:67:LEU:HD13	2.24	0.51
1:A:71:LYS:HA	1:A:74:ILE:CD1	2.38	0.51
1:A:143:LYS:HD3	1:A:147:GLU:OE2	2.10	0.51
1:A:363:PHE:CE2	1:A:399:LEU:HD22	2.45	0.51
1:A:387:CYS:HB2	1:A:389:ILE:CG1	2.40	0.51
1:A:487:PHE:HD1	1:A:661:TYR:CE1	2.27	0.51
1:A:341:THR:OG1	1:A:343:GLU:HG2	2.09	0.51
2:B:52:ASP:N	2:B:55:GLU:OE2	2.41	0.51
3:C:140:LYS:CE	3:C:143:ASP:H	2.24	0.51
1:A:345:LYS:O	1:A:349:PHE:CD2	2.63	0.51
1:A:512:PHE:N	1:A:512:PHE:HD2	2.01	0.51
3:C:95:ARG:NE	3:C:96:GLU:HG2	2.26	0.51
3:C:99:GLY:C	3:C:100:PHE:CD2	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:VAL:HA	3:C:125:ILE:HG22	1.93	0.51
1:A:192:TYR:O	1:A:194:ALA:N	2.43	0.51
1:A:395:LEU:O	1:A:399:LEU:CD1	2.59	0.51
1:A:399:LEU:N	1:A:401:PRO:CG	2.73	0.51
1:A:717:LYS:C	1:A:719:ARG:N	2.64	0.51
1:A:355:ILE:HA	1:A:358:MET:HG2	1.93	0.51
1:A:358:MET:C	1:A:360:GLU:N	2.58	0.51
1:A:543:ASP:O	1:A:546:SER:OG	2.28	0.51
3:C:3:LEU:HD12	3:C:7:GLU:HB3	1.91	0.51
1:A:146:THR:O	1:A:146:THR:HG22	2.11	0.51
1:A:766:VAL:O	1:A:768:GLY:N	2.44	0.51
3:C:92:THR:C	3:C:93:PHE:HD1	2.14	0.51
1:A:398:LEU:HD11	1:A:605:ASN:HD22	1.74	0.51
1:A:438:LEU:O	1:A:438:LEU:HD23	2.11	0.51
1:A:807:GLY:N	2:B:95:MET:HE3	2.26	0.51
1:A:817:LYS:C	1:A:819:LEU:N	2.62	0.51
2:B:68:ASN:N	2:B:68:ASN:ND2	2.58	0.51
3:C:4:SER:O	3:C:7:GLU:HB2	2.11	0.51
1:A:11:GLN:HB3	1:A:12:TYR:CE1	2.45	0.51
1:A:571:PRO:C	1:A:573:GLN:H	2.09	0.51
1:A:821:LEU:HD12	1:A:821:LEU:O	2.11	0.51
1:A:140:TYR:HE2	1:A:154:SER:HG	1.58	0.50
1:A:296:LEU:O	1:A:297:ASN:C	2.47	0.50
1:A:556:MET:C	1:A:558:LYS:H	2.14	0.50
1:A:743:LEU:HA	1:A:748:MET:HE1	1.91	0.50
1:A:103:LEU:HD22	1:A:121:ILE:HG21	1.92	0.50
1:A:428:LYS:C	1:A:430:LEU:H	2.15	0.50
1:A:488:PHE:CE1	1:A:492:MET:HG3	2.46	0.50
1:A:674:ASN:CG	1:A:681:LEU:HD23	2.31	0.50
2:B:67:LEU:HD13	2:B:67:LEU:H	1.77	0.50
1:A:50:SER:OG	1:A:57:THR:HB	2.10	0.50
1:A:61:VAL:HG12	1:A:62:ALA:N	2.24	0.50
1:A:93:TYR:O	1:A:98:SER:OG	2.29	0.50
1:A:663:THR:O	1:A:665:PRO:HD3	2.12	0.50
1:A:792:TYR:C	1:A:792:TYR:HD1	2.14	0.50
2:B:44:SER:C	2:B:46:GLN:H	2.14	0.50
1:A:145:LYS:NZ	1:A:145:LYS:HB2	2.27	0.50
1:A:272:VAL:HA	1:A:281:ASN:HD21	1.76	0.50
1:A:833:VAL:CG1	1:A:835:PRO:HD3	2.39	0.50
1:A:36:VAL:HG13	1:A:37:PRO:HD2	1.93	0.50
1:A:433:ARG:NH2	1:A:602:ILE:HD12	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASP:N	1:A:514:MET:SD	2.85	0.50
1:A:582:HIS:O	1:A:584:ALA:N	2.40	0.50
1:A:814:ASN:N	1:A:814:ASN:ND2	2.60	0.50
3:C:86:TYR:HB3	3:C:145:VAL:CG1	2.42	0.50
1:A:12:TYR:CD1	1:A:12:TYR:N	2.79	0.50
1:A:43:PHE:CD2	1:A:97:ALA:HB2	2.47	0.50
1:A:423:VAL:O	1:A:426:LEU:HD23	2.12	0.50
1:A:763:LYS:C	1:A:766:VAL:HG22	2.31	0.50
1:A:811:ILE:HD13	2:B:93:PHE:CD1	2.46	0.50
2:B:29:VAL:O	2:B:31:ARG:HG3	2.12	0.50
2:B:36:SER:O	2:B:39:ASP:HB3	2.12	0.50
1:A:112:ILE:N	1:A:112:ILE:CD1	2.74	0.50
1:A:537:CYS:C	1:A:595:LEU:HD21	2.31	0.50
1:A:626:GLU:C	1:A:627:GLU:CG	2.79	0.50
1:A:216:GLU:O	1:A:219:ILE:HG22	2.12	0.50
1:A:384:ALA:HB2	1:A:391:ALA:CA	2.41	0.50
1:A:390:ASN:ND2	1:A:393:ASP:OD1	2.45	0.50
1:A:602:ILE:HB	1:A:607:VAL:CG2	2.42	0.50
2:B:15:LYS:HE3	2:B:19:GLU:OE2	2.12	0.50
3:C:31:PHE:HB2	3:C:55:THR:HG22	1.94	0.50
3:C:67:GLU:O	3:C:70:PRO:HD2	2.11	0.50
1:A:530:LEU:HD11	1:A:646:SER:OG	2.12	0.49
3:C:92:THR:C	3:C:93:PHE:CD1	2.86	0.49
1:A:89:ALA:HB2	1:A:117:GLY:N	2.26	0.49
1:A:384:ALA:CB	1:A:391:ALA:HB2	2.32	0.49
1:A:522:LEU:HD21	1:A:562:PHE:CB	2.42	0.49
1:A:577:HIS:N	1:A:589:TYR:O	2.37	0.49
3:C:53:GLY:O	3:C:54:GLY:O	2.30	0.49
1:A:71:LYS:HG2	1:A:71:LYS:O	2.12	0.49
1:A:80:PRO:C	1:A:82:PHE:N	2.66	0.49
1:A:187:LYS:O	1:A:189:VAL:N	2.45	0.49
1:A:722:ILE:CD1	1:A:778:LEU:HD13	2.43	0.49
1:A:397:ALA:HB1	1:A:605:ASN:HD21	1.78	0.49
1:A:9:ASP:CG	1:A:139:LYS:NZ	2.66	0.49
1:A:288:ILE:CD1	1:A:352:THR:HG21	2.42	0.49
2:B:68:ASN:HD22	2:B:68:ASN:H	1.60	0.49
2:B:102:LYS:O	2:B:103:LYS:HG3	2.12	0.49
3:C:63:LEU:HD13	3:C:67:GLU:CB	2.43	0.49
3:C:69:LEU:HB3	3:C:70:PRO:CD	2.34	0.49
1:A:24:GLN:HA	1:A:81:LYS:CE	2.43	0.49
1:A:31:LYS:HD3	1:A:31:LYS:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLY:C	1:A:111:LEU:HD23	2.32	0.49
1:A:309:TYR:O	1:A:313:ASN:ND2	2.45	0.49
1:A:789:ILE:CG2	3:C:125:ILE:HG12	2.42	0.49
2:B:29:VAL:O	2:B:31:ARG:N	2.46	0.49
2:B:56:LEU:O	2:B:59:MET:HB2	2.13	0.49
3:C:86:TYR:N	3:C:86:TYR:CD1	2.80	0.49
1:A:401:PRO:C	1:A:411:THR:HG23	2.31	0.49
1:A:468:ASP:HB3	1:A:573:GLN:CA	2.33	0.49
2:B:147:MET:HE3	2:B:151:SER:OG	2.13	0.49
1:A:336:ASP:C	1:A:338:LEU:N	2.66	0.49
1:A:336:ASP:O	1:A:338:LEU:N	2.46	0.49
1:A:379:GLU:C	1:A:381:GLU:N	2.65	0.49
1:A:428:LYS:C	1:A:430:LEU:N	2.66	0.49
1:A:507:TRP:CH2	1:A:763:LYS:HE3	2.47	0.49
1:A:808:LEU:C	1:A:808:LEU:CD2	2.79	0.49
2:B:81:SER:O	2:B:83:THR:N	2.43	0.49
3:C:19:ASP:OD2	3:C:26:GLY:HA2	2.13	0.49
3:C:36:VAL:CG2	3:C:37:CYS:N	2.75	0.49
1:A:137:ILE:HG12	1:A:153:PHE:CZ	2.47	0.49
1:A:379:GLU:O	1:A:382:LYS:N	2.46	0.49
1:A:402:LYS:N	1:A:411:THR:CG2	2.57	0.49
1:A:525:LYS:HA	1:A:526:PRO:HD3	1.68	0.49
1:A:187:LYS:HD2	1:A:227:GLU:OE2	2.13	0.49
1:A:268:GLU:O	1:A:282:TYR:OH	2.30	0.49
1:A:380:ALA:HB1	1:A:395:LEU:HD11	1.94	0.49
1:A:556:MET:C	1:A:558:LYS:N	2.66	0.49
1:A:808:LEU:HD13	3:C:21:TRP:CZ3	2.48	0.49
2:B:80:LEU:N	2:B:80:LEU:CD2	2.65	0.49
3:C:28:VAL:O	3:C:62:SER:CA	2.61	0.49
3:C:107:ARG:O	3:C:111:THR:HG23	2.13	0.49
3:C:143:ASP:O	3:C:145:VAL:N	2.46	0.49
1:A:467:PHE:C	1:A:469:PHE:H	2.15	0.48
1:A:505:ILE:HG23	1:A:756:GLY:HA2	1.93	0.48
1:A:521:ASP:OD1	1:A:525:LYS:HB3	2.13	0.48
1:A:807:GLY:CA	2:B:95:MET:HE3	2.43	0.48
2:B:96:PHE:CD1	2:B:96:PHE:N	2.81	0.48
1:A:76:SER:HB3	1:A:93:TYR:CE1	2.48	0.48
1:A:101:TYR:O	1:A:102:ASN:C	2.51	0.48
1:A:335:PHE:O	1:A:340:PHE:HB2	2.14	0.48
1:A:535:GLU:HG2	1:A:536:GLU:H	1.78	0.48
2:B:14:GLN:OE1	2:B:14:GLN:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:GLU:HG3	2:B:136:GLY:N	2.22	0.48
3:C:28:VAL:O	3:C:63:LEU:N	2.41	0.48
1:A:225:VAL:CG1	1:A:438:LEU:HD11	2.43	0.48
2:B:35:VAL:H	2:B:67:LEU:HB3	1.77	0.48
3:C:36:VAL:HG22	3:C:37:CYS:N	2.28	0.48
3:C:128:LEU:C	3:C:130:ASP:H	2.16	0.48
1:A:83:GLU:HG3	1:A:101:TYR:HE2	1.78	0.48
1:A:94:LEU:O	1:A:94:LEU:CG	2.61	0.48
1:A:120:CYS:CB	1:A:668:VAL:HA	2.44	0.48
1:A:625:PRO:O	1:A:626:GLU:C	2.51	0.48
1:A:783:SER:CB	3:C:115:GLU:HG3	2.44	0.48
2:B:102:LYS:HD2	2:B:102:LYS:N	2.29	0.48
3:C:15:PHE:CD1	3:C:15:PHE:O	2.66	0.48
1:A:159:ALA:O	1:A:170:GLN:HG3	2.13	0.48
1:A:748:MET:O	1:A:748:MET:HG2	2.12	0.48
3:C:124:GLU:O	3:C:127:LYS:N	2.46	0.48
1:A:93:TYR:O	1:A:95:ASN:N	2.47	0.48
1:A:289:CYS:O	1:A:304:PRO:O	2.30	0.48
1:A:397:ALA:HA	1:A:401:PRO:CB	2.42	0.48
1:A:792:TYR:O	1:A:792:TYR:HD1	1.95	0.48
1:A:342:LYS:HE2	1:A:346:GLN:NE2	2.29	0.48
2:B:16:GLN:O	2:B:20:MET:HG2	2.14	0.48
3:C:74:GLY:C	3:C:76:MET:H	2.16	0.48
1:A:397:ALA:O	1:A:401:PRO:HG2	2.05	0.48
1:A:515:ASP:HB3	1:A:560:ARG:NH2	2.28	0.48
1:A:794:ILE:HG23	1:A:794:ILE:O	2.13	0.48
2:B:13:PRO:O	2:B:17:ILE:HG12	2.14	0.48
2:B:142:VAL:O	2:B:145:THR:HG22	2.14	0.48
1:A:256:LYS:C	1:A:257:ILE:HD12	2.29	0.48
1:A:88:MET:HE2	1:A:99:VAL:HA	1.96	0.48
1:A:140:TYR:CE2	1:A:154:SER:OG	2.67	0.48
1:A:143:LYS:HE3	1:A:143:LYS:CA	2.44	0.48
1:A:532:ILE:HA	1:A:535:GLU:CG	2.41	0.48
2:B:40:ILE:C	2:B:42:ALA:N	2.67	0.48
2:B:62:GLU:O	2:B:75:ILE:HG21	2.14	0.48
3:C:7:GLU:C	3:C:9:ASP:H	2.15	0.48
1:A:89:ALA:HB2	1:A:117:GLY:H	1.79	0.47
1:A:275:GLN:NE2	1:A:281:ASN:ND2	2.61	0.47
1:A:815:ILE:C	1:A:817:LYS:H	2.17	0.47
3:C:33:LEU:C	3:C:33:LEU:CD2	2.82	0.47
3:C:47:GLU:O	3:C:50:PHE:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PHE:CE2	1:A:90:ASN:O	2.67	0.47
1:A:719:ARG:NE	1:A:771:GLU:OE2	2.43	0.47
2:B:53:ASP:CG	2:B:54:LYS:N	2.68	0.47
2:B:53:ASP:O	2:B:56:LEU:HB2	2.14	0.47
2:B:140:ASP:OD2	2:B:142:VAL:HB	2.13	0.47
3:C:105:GLU:O	3:C:109:VAL:HG23	2.14	0.47
1:A:138:ALA:C	1:A:140:TYR:H	2.16	0.47
1:A:428:LYS:O	1:A:430:LEU:N	2.47	0.47
1:A:576:ALA:HB1	1:A:589:TYR:O	2.15	0.47
1:A:743:LEU:O	1:A:746:LEU:HB2	2.14	0.47
1:A:819:LEU:CD2	1:A:822:ARG:HH21	2.24	0.47
1:A:248:ARG:HB2	1:A:261:ASP:OD2	2.14	0.47
1:A:723:LEU:HD21	1:A:773:MET:HB3	1.95	0.47
2:B:136:GLY:C	2:B:138:LYS:HD2	2.34	0.47
3:C:90:PHE:CB	3:C:141:TYR:CE1	2.91	0.47
1:A:233:LYS:HA	1:A:238:ASN:C	2.35	0.47
1:A:515:ASP:C	1:A:518:MET:H	2.18	0.47
1:A:672:ILE:HG22	1:A:690:GLN:NE2	2.29	0.47
1:A:794:ILE:HD13	3:C:35:ASP:CA	2.44	0.47
1:A:826:TRP:CZ2	2:B:59:MET:HB3	2.50	0.47
3:C:108:HIS:ND1	3:C:112:ALA:CB	2.76	0.47
1:A:696:VAL:HG13	1:A:697:LEU:H	1.79	0.47
3:C:90:PHE:CB	3:C:141:TYR:HE1	2.27	0.47
1:A:120:CYS:HB3	1:A:668:VAL:HA	1.97	0.47
1:A:140:TYR:HE2	1:A:154:SER:OG	1.98	0.47
1:A:192:TYR:C	1:A:194:ALA:N	2.67	0.47
1:A:214:SER:O	1:A:217:ASP:N	2.47	0.47
1:A:403:VAL:HG13	1:A:404:LYS:O	2.14	0.47
1:A:430:LEU:HD12	1:A:622:PHE:CE2	2.50	0.47
1:A:511:ASP:CB	1:A:512:PHE:CD2	2.97	0.47
1:A:598:ASN:HD22	1:A:599:LYS:HD3	1.80	0.47
1:A:744:ALA:C	1:A:746:LEU:N	2.67	0.47
1:A:764:ALA:C	1:A:766:VAL:H	2.18	0.47
1:A:802:GLN:HG2	3:C:17:LEU:HD22	1.96	0.47
1:A:816:ARG:NH2	2:B:120:PHE:CD1	2.82	0.47
1:A:826:TRP:HB3	2:B:76:PHE:CE1	2.50	0.47
3:C:17:LEU:HD11	3:C:21:TRP:HE1	1.79	0.47
3:C:49:VAL:HA	3:C:52:VAL:CG2	2.45	0.47
1:A:135:SER:O	1:A:139:LYS:HG3	2.14	0.47
1:A:266:LEU:HD11	1:A:649:HIS:CE1	2.50	0.47
1:A:382:LYS:HB2	1:A:382:LYS:HE3	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASP:CG	1:A:449:LYS:HZ2	2.18	0.47
1:A:475:LEU:O	1:A:478:ASN:HB2	2.15	0.47
3:C:28:VAL:O	3:C:62:SER:HB2	2.15	0.47
3:C:69:LEU:C	3:C:71:ALA:H	2.18	0.47
3:C:95:ARG:HD2	3:C:95:ARG:C	2.35	0.47
3:C:141:TYR:H	3:C:141:TYR:HD2	1.61	0.47
1:A:48:ILE:HG23	1:A:58:VAL:CG1	2.27	0.47
1:A:128:ARG:HH12	1:A:188:LYS:NZ	2.13	0.47
1:A:237:ASN:ND2	5:A:999:ANP:PA	2.87	0.47
1:A:399:LEU:C	1:A:401:PRO:HD2	2.35	0.47
1:A:399:LEU:C	1:A:401:PRO:CD	2.83	0.47
1:A:473:GLU:O	1:A:477:ILE:HD13	2.15	0.47
1:A:520:ILE:O	1:A:524:GLU:HG2	2.15	0.47
1:A:795:ARG:CD	3:C:38:ARG:O	2.56	0.47
2:B:89:ILE:O	2:B:91:ASN:N	2.48	0.47
3:C:86:TYR:N	3:C:86:TYR:HD1	2.13	0.47
3:C:141:TYR:O	3:C:142:GLU:C	2.52	0.47
1:A:68:THR:O	1:A:69:VAL:HG13	2.15	0.47
1:A:173:LEU:HD21	1:A:660:LEU:HD21	1.96	0.47
1:A:716:PHE:CE1	1:A:720:TYR:HD2	2.33	0.47
2:B:72:PHE:C	2:B:74:SER:N	2.68	0.47
2:B:141:TYR:O	2:B:145:THR:HB	2.15	0.47
1:A:223:ASN:O	1:A:224:PRO:C	2.54	0.46
1:A:288:ILE:CD1	1:A:352:THR:HG22	2.44	0.46
2:B:68:ASN:ND2	2:B:68:ASN:H	2.13	0.46
1:A:783:SER:HA	1:A:786:GLN:OE1	2.15	0.46
1:A:828:LYS:O	1:A:832:LYS:N	2.43	0.46
1:A:169:ASN:HB2	1:A:663:THR:HG22	1.94	0.46
1:A:236:ARG:O	1:A:677:LYS:HE3	2.16	0.46
1:A:325:VAL:HG23	1:A:326:GLU:H	1.80	0.46
1:A:397:ALA:CA	1:A:401:PRO:CG	2.85	0.46
1:A:604:GLU:OE2	1:A:604:GLU:N	2.49	0.46
3:C:17:LEU:HD12	3:C:21:TRP:HE1	1.79	0.46
1:A:24:GLN:HA	1:A:81:LYS:HE3	1.98	0.46
1:A:95:ASN:OD1	1:A:98:SER:N	2.47	0.46
1:A:296:LEU:HA	1:A:299:VAL:HG12	1.98	0.46
1:A:492:MET:C	1:A:494:ILE:N	2.68	0.46
1:A:505:ILE:CG2	1:A:756:GLY:HA2	2.45	0.46
1:A:818:TRP:NE1	2:B:148:ILE:O	2.49	0.46
2:B:105:ASN:O	2:B:108:TYR:N	2.37	0.46
2:B:124:GLU:O	2:B:128:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:HA	1:A:297:ASN:ND2	2.30	0.46
1:A:653:LEU:O	1:A:656:LEU:HB3	2.15	0.46
2:B:21:LYS:O	2:B:24:PHE:N	2.47	0.46
2:B:136:GLY:HA3	2:B:138:LYS:HZ2	1.80	0.46
3:C:87:MET:C	3:C:89:ALA:H	2.19	0.46
1:A:24:GLN:HA	1:A:81:LYS:CD	2.46	0.46
1:A:430:LEU:O	1:A:433:ARG:N	2.48	0.46
1:A:488:PHE:CD1	1:A:489:ASN:N	2.84	0.46
1:A:644:THR:O	1:A:646:SER:N	2.48	0.46
1:A:713:TYR:CE1	1:A:760:VAL:HG22	2.50	0.46
1:A:54:ASP:CB	1:A:70:LYS:NZ	2.79	0.46
1:A:182:LYS:HZ2	5:A:999:ANP:PB	2.39	0.46
1:A:229:TYR:HA	1:A:284:ILE:CG1	2.46	0.46
1:A:514:MET:N	1:A:515:ASP:OD2	2.49	0.46
1:A:794:ILE:HG23	3:C:39:CYS:SG	2.55	0.46
1:A:816:ARG:NH2	2:B:120:PHE:HD1	2.13	0.46
1:A:140:TYR:CE2	1:A:151:HIS:HB3	2.51	0.46
1:A:143:LYS:HA	1:A:143:LYS:CE	2.43	0.46
1:A:237:ASN:ND2	5:A:999:ANP:C5'	2.47	0.46
1:A:336:ASP:O	1:A:339:GLY:N	2.44	0.46
1:A:653:LEU:O	1:A:654:ASN:C	2.53	0.46
1:A:789:ILE:HG23	3:C:125:ILE:CG1	2.45	0.46
1:A:271:ARG:HH22	1:A:279:GLU:CG	2.29	0.46
1:A:785:PHE:CE1	3:C:148:VAL:HG11	2.51	0.46
2:B:99:GLN:CG	2:B:99:GLN:O	2.64	0.46
3:C:8:ILE:O	3:C:12:LYS:HE3	2.16	0.46
1:A:131:ILE:HG13	1:A:132:TYR:CD1	2.47	0.46
1:A:430:LEU:C	1:A:432:ASP:N	2.69	0.46
1:A:443:ASN:O	1:A:447:ASP:HB2	2.16	0.46
1:A:785:PHE:O	1:A:789:ILE:HG13	2.15	0.46
2:B:80:LEU:H	2:B:80:LEU:CD2	2.09	0.46
3:C:93:PHE:CE2	3:C:109:VAL:HG13	2.50	0.46
1:A:106:ARG:CB	1:A:111:LEU:HD12	2.47	0.45
2:B:97:ASP:O	2:B:97:ASP:CG	2.55	0.45
3:C:18:PHE:O	3:C:20:PHE:N	2.49	0.45
1:A:236:ARG:NH2	1:A:672:ILE:HD13	2.29	0.45
1:A:387:CYS:CB	1:A:389:ILE:HG13	2.46	0.45
1:A:415:ASN:O	1:A:419:VAL:CG2	2.64	0.45
2:B:37:LYS:CE	2:B:57:THR:HG23	2.46	0.45
2:B:139:PHE:HE1	2:B:141:TYR:HA	1.80	0.45
1:A:232:ALA:CB	1:A:271:ARG:HH11	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:HH22	1:A:279:GLU:HG2	1.78	0.45
1:A:398:LEU:HB3	1:A:606:VAL:HG22	1.98	0.45
1:A:833:VAL:CG2	2:B:47:LEU:CD1	2.89	0.45
2:B:109:ILE:HA	2:B:112:LEU:HD12	1.98	0.45
3:C:63:LEU:HD13	3:C:67:GLU:HB3	1.99	0.45
1:A:125:PRO:O	1:A:125:PRO:HG2	2.16	0.45
1:A:187:LYS:C	1:A:189:VAL:N	2.68	0.45
1:A:234:THR:O	1:A:235:THR:C	2.54	0.45
1:A:477:ILE:HD12	1:A:477:ILE:H	1.81	0.45
1:A:8:PRO:HG2	1:A:9:ASP:N	2.29	0.45
1:A:285:PHE:HE2	1:A:431:TYR:CE2	2.35	0.45
1:A:473:GLU:O	1:A:477:ILE:CD1	2.64	0.45
1:A:603:ASN:HB2	1:A:606:VAL:CG2	2.46	0.45
1:A:781:ILE:HG21	3:C:89:ALA:HB2	1.97	0.45
2:B:21:LYS:C	2:B:23:ALA:N	2.70	0.45
2:B:37:LYS:C	2:B:39:ASP:H	2.19	0.45
1:A:337:ILE:H	1:A:337:ILE:HG13	1.53	0.45
1:A:818:TRP:CG	1:A:818:TRP:O	2.70	0.45
1:A:123:VAL:CG1	1:A:673:PRO:HG3	2.21	0.45
1:A:415:ASN:OD1	1:A:417:ASN:ND2	2.50	0.45
1:A:467:PHE:HE1	1:A:474:GLN:HB3	1.82	0.45
1:A:470:ASN:O	1:A:589:TYR:HA	2.17	0.45
1:A:719:ARG:C	1:A:774:ARG:HH12	2.20	0.45
3:C:67:GLU:C	3:C:69:LEU:H	2.19	0.45
1:A:578:PHE:O	1:A:589:TYR:N	2.49	0.45
1:A:788:HIS:HD2	3:C:148:VAL:HG22	1.82	0.45
2:B:71:MET:O	2:B:71:MET:HG3	2.17	0.45
2:B:105:ASN:O	2:B:108:TYR:HB3	2.16	0.45
2:B:119:ASN:C	2:B:120:PHE:O	2.53	0.45
2:B:142:VAL:CG1	2:B:143:LYS:NZ	2.67	0.45
3:C:22:ASP:OD1	3:C:22:ASP:O	2.35	0.45
1:A:140:TYR:CZ	1:A:148:ILE:HG12	2.52	0.45
2:B:121:ASN:CG	2:B:124:GLU:HG3	2.35	0.45
1:A:216:GLU:N	1:A:216:GLU:CD	2.70	0.45
1:A:300:MET:O	1:A:301:LEU:HB2	2.17	0.45
1:A:389:ILE:O	1:A:389:ILE:CD1	2.56	0.45
2:B:97:ASP:CG	2:B:101:THR:H	2.21	0.45
2:B:136:GLY:HA3	2:B:138:LYS:NZ	2.32	0.45
3:C:108:HIS:O	3:C:112:ALA:HB3	2.18	0.45
1:A:94:LEU:O	1:A:94:LEU:CD1	2.64	0.44
1:A:241:SER:O	1:A:242:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLU:HA	1:A:347:SER:OG	2.18	0.44
1:A:350:LYS:HE2	1:A:386:LEU:CA	2.45	0.44
1:A:463:GLY:O	1:A:477:ILE:HG22	2.17	0.44
1:A:483:ARG:NH1	1:A:657:MET:HG3	2.32	0.44
1:A:483:ARG:HH12	1:A:657:MET:HG3	1.82	0.44
1:A:530:LEU:HG	1:A:650:ARG:NH2	2.28	0.44
2:B:135:GLU:O	2:B:137:GLY:N	2.48	0.44
1:A:518:MET:O	1:A:518:MET:HG2	2.16	0.44
1:A:530:LEU:CD1	1:A:650:ARG:NH2	2.79	0.44
1:A:63:ASP:C	1:A:63:ASP:OD1	2.55	0.44
1:A:169:ASN:O	1:A:663:THR:HA	2.18	0.44
1:A:397:ALA:C	1:A:398:LEU:CG	2.83	0.44
1:A:549:ASP:O	1:A:553:GLN:HG2	2.17	0.44
1:A:676:LEU:HD12	1:A:681:LEU:CD2	2.47	0.44
1:A:688:LEU:O	1:A:689:HIS:C	2.56	0.44
1:A:735:GLY:O	1:A:737:THR:N	2.50	0.44
1:A:28:PHE:CZ	1:A:29:ASP:O	2.71	0.44
1:A:534:GLU:OE1	1:A:650:ARG:NH2	2.39	0.44
1:A:626:GLU:O	1:A:627:GLU:CG	2.65	0.44
1:A:785:PHE:O	1:A:785:PHE:CG	2.71	0.44
2:B:51:PRO:HB2	2:B:55:GLU:OE2	2.17	0.44
3:C:141:TYR:N	3:C:141:TYR:CD2	2.86	0.44
1:A:38:ASP:HB2	1:A:44:ALA:HB2	1.99	0.44
1:A:438:LEU:C	1:A:438:LEU:HD23	2.38	0.44
1:A:534:GLU:O	1:A:537:CYS:SG	2.76	0.44
2:B:72:PHE:O	2:B:74:SER:N	2.50	0.44
3:C:31:PHE:CD1	3:C:56:HIS:O	2.70	0.44
3:C:102:SER:HA	3:C:138:ASN:HA	2.00	0.44
1:A:182:LYS:O	1:A:186:THR:OG1	2.34	0.44
1:A:228:ALA:HB1	1:A:284:ILE:HG23	2.00	0.44
1:A:400:LYS:HA	1:A:414:GLN:CA	2.46	0.44
1:A:712:ILE:CD1	1:A:714:SER:HB3	2.36	0.44
2:B:118:ASP:CG	3:C:24:ARG:NH2	2.64	0.44
1:A:56:ILE:O	1:A:69:VAL:HG22	2.17	0.44
1:A:80:PRO:O	1:A:83:GLU:N	2.49	0.44
1:A:258:ALA:O	1:A:448:THR:CG2	2.66	0.44
1:A:284:ILE:HA	1:A:287:GLN:CD	2.36	0.44
1:A:341:THR:HB	1:A:343:GLU:OE2	2.17	0.44
1:A:398:LEU:HD13	1:A:606:VAL:HA	1.99	0.44
3:C:122:VAL:CA	3:C:125:ILE:HG22	2.48	0.44
3:C:129:THR:HB	3:C:147:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ALA:O	1:A:336:ASP:N	2.50	0.44
1:A:404:LYS:HA	1:A:409:MET:CB	2.48	0.44
1:A:495:LEU:HG	1:A:495:LEU:O	2.17	0.44
1:A:500:TYR:HA	1:A:505:ILE:CD1	2.47	0.44
1:A:831:SER:O	1:A:832:LYS:C	2.56	0.44
2:B:36:SER:N	2:B:39:ASP:CB	2.80	0.44
2:B:90:ARG:HH12	2:B:143:LYS:NZ	2.16	0.44
2:B:100:GLU:CA	2:B:102:LYS:HE3	2.47	0.44
3:C:100:PHE:CD2	3:C:100:PHE:N	2.85	0.44
1:A:94:LEU:O	1:A:94:LEU:HG	2.18	0.44
1:A:594:TRP:C	1:A:596:GLU:N	2.70	0.44
1:A:603:ASN:HB2	1:A:606:VAL:HG21	2.00	0.44
1:A:607:VAL:O	1:A:608:ALA:C	2.55	0.44
2:B:14:GLN:C	2:B:14:GLN:CD	2.76	0.44
2:B:37:LYS:HE3	2:B:57:THR:HG23	2.00	0.44
1:A:8:PRO:HD2	1:A:10:PHE:CD2	2.53	0.43
1:A:8:PRO:CG	1:A:9:ASP:H	2.31	0.43
1:A:32:LYS:NZ	3:C:95:ARG:HH22	2.16	0.43
1:A:276:GLN:O	1:A:277:SER:C	2.56	0.43
1:A:384:ALA:CB	1:A:391:ALA:N	2.76	0.43
1:A:577:HIS:HD2	1:A:591:ILE:H	1.65	0.43
1:A:610:LEU:O	1:A:611:GLY:C	2.54	0.43
1:A:140:TYR:O	1:A:141:ARG:C	2.55	0.43
1:A:780:LYS:O	1:A:782:ILE:N	2.51	0.43
1:A:801:LEU:C	1:A:801:LEU:CD2	2.87	0.43
3:C:109:VAL:O	3:C:113:LEU:HB2	2.18	0.43
3:C:128:LEU:O	3:C:130:ASP:N	2.51	0.43
1:A:280:ARG:HD3	1:A:319:VAL:CG1	2.48	0.43
1:A:413:GLY:O	1:A:414:GLN:C	2.55	0.43
1:A:511:ASP:HA	1:A:514:MET:CB	2.40	0.43
1:A:598:ASN:HD21	1:A:644:THR:C	2.22	0.43
1:A:806:ILE:HD12	1:A:806:ILE:HA	1.78	0.43
1:A:815:ILE:O	1:A:817:LYS:N	2.51	0.43
3:C:10:ASP:O	3:C:40:LEU:HD21	2.18	0.43
3:C:69:LEU:C	3:C:71:ALA:N	2.71	0.43
1:A:128:ARG:NH1	1:A:188:LYS:HZ3	2.17	0.43
1:A:229:TYR:HA	1:A:284:ILE:HG12	1.99	0.43
1:A:284:ILE:CD1	1:A:285:PHE:N	2.72	0.43
1:A:656:LEU:HD11	1:A:660:LEU:HD11	1.99	0.43
1:A:786:GLN:NE2	3:C:110:LEU:O	2.51	0.43
3:C:42:ILE:HG22	3:C:43:ASN:H	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:CYS:CB	1:A:668:VAL:HG13	2.48	0.43
1:A:499:GLU:HA	1:A:502:LYS:H	1.83	0.43
1:A:519:CYS:O	1:A:520:ILE:C	2.57	0.43
3:C:36:VAL:HG21	3:C:68:PHE:CE2	2.53	0.43
3:C:100:PHE:HD2	3:C:100:PHE:N	2.16	0.43
3:C:106:LEU:CA	3:C:109:VAL:HG23	2.48	0.43
1:A:598:ASN:ND2	1:A:598:ASN:O	2.52	0.43
1:A:646:SER:C	1:A:648:VAL:N	2.69	0.43
1:A:82:PHE:HE1	1:A:92:THR:H	1.66	0.43
1:A:399:LEU:H	1:A:401:PRO:CG	2.31	0.43
1:A:653:LEU:O	1:A:656:LEU:N	2.51	0.43
1:A:737:THR:C	1:A:739:SER:H	2.22	0.43
1:A:833:VAL:O	1:A:835:PRO:CD	2.51	0.43
3:C:62:SER:O	3:C:63:LEU:HD23	2.18	0.43
1:A:75:GLN:NE2	1:A:95:ASN:HB2	2.31	0.43
1:A:168:GLU:HG3	1:A:170:GLN:HE22	1.83	0.43
1:A:353:ALA:O	1:A:356:LEU:HB2	2.18	0.43
1:A:397:ALA:C	1:A:398:LEU:HD12	2.39	0.43
1:A:397:ALA:O	1:A:398:LEU:HD12	2.18	0.43
1:A:399:LEU:HA	1:A:399:LEU:HD23	1.68	0.43
1:A:667:PHE:N	1:A:667:PHE:CD2	2.87	0.43
1:A:286:TYR:CE1	1:A:312:ILE:HB	2.54	0.43
1:A:364:LYS:CB	1:A:373:GLU:CB	2.97	0.43
1:A:719:ARG:HD2	1:A:719:ARG:HA	1.71	0.43
1:A:773:MET:O	1:A:777:ARG:N	2.48	0.43
2:B:90:ARG:HH11	2:B:142:VAL:HG13	1.83	0.43
3:C:49:VAL:HA	3:C:52:VAL:HG23	2.00	0.43
1:A:272:VAL:HG12	1:A:273:THR:HG23	2.01	0.43
1:A:371:GLN:HE21	1:A:371:GLN:N	2.15	0.43
1:A:505:ILE:HD12	1:A:505:ILE:C	2.40	0.43
1:A:672:ILE:O	1:A:673:PRO:C	2.57	0.43
1:A:735:GLY:C	1:A:737:THR:N	2.72	0.43
1:A:43:PHE:CG	1:A:97:ALA:HB2	2.53	0.42
1:A:192:TYR:O	1:A:193:LEU:C	2.58	0.42
2:B:146:ALA:O	2:B:151:SER:HB3	2.18	0.42
1:A:288:ILE:HD12	1:A:352:THR:HG21	2.01	0.42
1:A:560:ARG:H	1:A:560:ARG:HG2	1.55	0.42
1:A:804:GLN:HB3	2:B:96:PHE:CZ	2.54	0.42
1:A:807:GLY:CA	2:B:95:MET:CE	2.97	0.42
3:C:5:GLN:O	3:C:9:ASP:OD1	2.37	0.42
3:C:109:VAL:CA	3:C:113:LEU:HD13	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD22	1:A:688:LEU:HD11	2.02	0.42
1:A:138:ALA:C	1:A:140:TYR:N	2.71	0.42
1:A:271:ARG:NH1	1:A:280:ARG:O	2.53	0.42
1:A:417:ASN:ND2	1:A:418:GLN:N	2.66	0.42
1:A:495:LEU:O	1:A:498:GLU:CB	2.68	0.42
1:A:794:ILE:O	1:A:794:ILE:CG2	2.65	0.42
1:A:812:GLN:HB2	2:B:120:PHE:CE1	2.54	0.42
2:B:24:PHE:CE2	2:B:69:PHE:CA	3.03	0.42
1:A:6:SER:OG	1:A:7:ASP:N	2.51	0.42
1:A:189:VAL:HG12	1:A:193:LEU:HD11	2.02	0.42
1:A:216:GLU:N	1:A:216:GLU:OE1	2.52	0.42
1:A:287:GLN:HB2	1:A:328:PHE:HB2	2.00	0.42
1:A:294:PRO:HB3	1:A:297:ASN:HD21	1.83	0.42
1:A:485:GLN:OE1	1:A:485:GLN:HA	2.19	0.42
1:A:764:ALA:O	1:A:766:VAL:HG22	2.20	0.42
3:C:143:ASP:O	3:C:144:PHE:C	2.56	0.42
1:A:362:LYS:C	1:A:363:PHE:HD1	2.19	0.42
1:A:379:GLU:HA	1:A:382:LYS:CE	2.45	0.42
1:A:750:PRO:O	1:A:751:ALA:C	2.54	0.42
2:B:97:ASP:OD1	2:B:101:THR:HG23	2.20	0.42
3:C:126:ILE:HG23	3:C:131:LEU:HB3	2.01	0.42
1:A:171:SER:HB3	1:A:663:THR:OG1	2.20	0.42
1:A:293:ILE:CD1	1:A:296:LEU:CD1	2.97	0.42
1:A:567:LYS:HA	1:A:568:PRO:HD2	1.70	0.42
1:A:762:PHE:CB	1:A:766:VAL:HG21	2.49	0.42
2:B:24:PHE:CE1	2:B:35:VAL:HG22	2.55	0.42
2:B:101:THR:OG1	2:B:103:LYS:O	2.37	0.42
1:A:28:PHE:CD1	1:A:29:ASP:N	2.87	0.42
1:A:223:ASN:O	1:A:225:VAL:N	2.52	0.42
1:A:229:TYR:O	1:A:431:TYR:OH	2.37	0.42
1:A:341:THR:OG1	1:A:344:GLU:HB2	2.18	0.42
1:A:530:LEU:CD1	1:A:646:SER:OG	2.68	0.42
1:A:530:LEU:CD2	1:A:650:ARG:HE	2.32	0.42
1:A:614:LYS:O	1:A:616:PRO:HD3	2.20	0.42
2:B:125:MET:O	2:B:128:THR:N	2.51	0.42
2:B:138:LYS:HD2	2:B:138:LYS:N	2.30	0.42
1:A:33:ASN:O	1:A:34:CYS:HB3	2.20	0.42
1:A:85:LEU:HB3	1:A:102:ASN:ND2	2.27	0.42
1:A:251:PHE:C	1:A:258:ALA:HB2	2.39	0.42
1:A:271:ARG:NH2	1:A:279:GLU:CG	2.79	0.42
1:A:404:LYS:HA	1:A:409:MET:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ASN:OD1	1:A:415:ASN:C	2.57	0.42
1:A:532:ILE:HG23	1:A:535:GLU:HG2	2.01	0.42
2:B:122:LYS:O	2:B:123:ASP:C	2.57	0.42
2:B:139:PHE:C	2:B:139:PHE:HD1	2.22	0.42
3:C:128:LEU:C	3:C:130:ASP:N	2.73	0.42
1:A:91:MET:HE1	1:A:94:LEU:HA	2.01	0.42
1:A:477:ILE:H	1:A:477:ILE:CD1	2.33	0.42
1:A:604:GLU:N	1:A:604:GLU:CD	2.72	0.42
2:B:54:LYS:HA	2:B:57:THR:OG1	2.20	0.42
1:A:11:GLN:O	1:A:12:TYR:CD1	2.73	0.42
1:A:24:GLN:O	1:A:81:LYS:HE3	2.20	0.42
1:A:118:LEU:C	1:A:119:PHE:CD1	2.93	0.42
1:A:400:LYS:HA	1:A:414:GLN:N	2.35	0.42
1:A:748:MET:O	1:A:750:PRO:HD3	2.20	0.42
1:A:237:ASN:HD21	5:A:999:ANP:PA	2.43	0.41
1:A:262:ILE:N	1:A:443:ASN:OD1	2.39	0.41
1:A:390:ASN:ND2	1:A:393:ASP:N	2.58	0.41
1:A:467:PHE:CD1	1:A:467:PHE:N	2.86	0.41
1:A:737:THR:C	1:A:739:SER:N	2.71	0.41
2:B:121:ASN:O	2:B:124:GLU:N	2.53	0.41
3:C:18:PHE:O	3:C:19:ASP:C	2.56	0.41
3:C:67:GLU:C	3:C:69:LEU:N	2.73	0.41
1:A:135:SER:HG	1:A:136:VAL:H	1.68	0.41
1:A:327:GLU:O	1:A:330:LEU:HB2	2.20	0.41
1:A:387:CYS:O	1:A:615:GLU:HB2	2.20	0.41
1:A:418:GLN:O	1:A:422:SER:HB2	2.20	0.41
1:A:535:GLU:O	1:A:537:CYS:N	2.46	0.41
1:A:783:SER:HB3	3:C:115:GLU:HG3	2.01	0.41
2:B:52:ASP:O	2:B:56:LEU:HG	2.20	0.41
2:B:52:ASP:O	2:B:55:GLU:HB2	2.19	0.41
1:A:85:LEU:CD2	1:A:91:MET:HG3	2.50	0.41
1:A:120:CYS:O	1:A:669:ARG:N	2.51	0.41
1:A:248:ARG:NE	1:A:261:ASP:OD2	2.53	0.41
1:A:429:SER:OG	1:A:602:ILE:HD13	2.19	0.41
1:A:447:ASP:O	1:A:447:ASP:CG	2.57	0.41
1:A:684:ALA:HB3	1:A:685:GLU:OE2	2.20	0.41
3:C:30:ALA:CB	3:C:55:THR:HB	2.46	0.41
3:C:40:LEU:CB	3:C:72:TYR:OH	2.64	0.41
3:C:106:LEU:HD23	3:C:110:LEU:HD11	2.02	0.41
1:A:95:ASN:O	1:A:95:ASN:OD1	2.38	0.41
1:A:214:SER:C	1:A:216:GLU:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:HA	1:A:279:GLU:OE1	2.21	0.41
1:A:251:PHE:HE1	1:A:456:ILE:HG12	1.86	0.41
1:A:418:GLN:O	1:A:422:SER:CB	2.68	0.41
1:A:429:SER:CB	1:A:602:ILE:HG23	2.51	0.41
1:A:716:PHE:HE1	1:A:720:TYR:HD2	1.68	0.41
1:A:763:LYS:O	1:A:766:VAL:HG21	2.18	0.41
1:A:798:TYR:CE1	3:C:17:LEU:HD23	2.55	0.41
1:A:805:ARG:HG2	3:C:20:PHE:CZ	2.55	0.41
2:B:43:ILE:HD12	2:B:43:ILE:O	2.20	0.41
3:C:122:VAL:O	3:C:126:ILE:CG1	2.65	0.41
1:A:472:PHE:HB2	1:A:594:TRP:CZ3	2.55	0.41
1:A:537:CYS:HA	1:A:595:LEU:HD21	2.01	0.41
1:A:685:GLU:H	1:A:685:GLU:CD	2.22	0.41
2:B:36:SER:O	2:B:39:ASP:N	2.53	0.41
2:B:129:PHE:O	2:B:131:GLU:N	2.53	0.41
3:C:106:LEU:O	3:C:110:LEU:CD1	2.69	0.41
3:C:120:GLU:O	3:C:121:ASP:C	2.57	0.41
1:A:134:ASP:OD2	1:A:195:LYS:HG2	2.21	0.41
1:A:291:ASN:HD21	1:A:297:ASN:HD21	1.68	0.41
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.61	0.41
1:A:488:PHE:O	1:A:492:MET:HG2	2.21	0.41
2:B:143:LYS:C	2:B:145:THR:N	2.73	0.41
3:C:70:PRO:HA	3:C:73:GLU:CG	2.51	0.41
1:A:12:TYR:HD1	1:A:12:TYR:N	2.16	0.41
1:A:186:THR:HG21	1:A:460:ASP:HB2	2.02	0.41
1:A:472:PHE:HB2	1:A:594:TRP:CE3	2.55	0.41
1:A:570:ARG:C	1:A:573:GLN:CB	2.88	0.41
1:A:721:SER:HA	1:A:742:ILE:HD13	2.03	0.41
2:B:114:GLU:O	2:B:114:GLU:HG2	2.20	0.41
2:B:125:MET:O	2:B:128:THR:HB	2.21	0.41
3:C:111:THR:HG22	3:C:122:VAL:HG21	2.02	0.41
1:A:7:ASP:O	1:A:7:ASP:CG	2.59	0.41
1:A:185:ASN:O	1:A:186:THR:C	2.58	0.41
1:A:219:ILE:CG2	1:A:220:ILE:N	2.83	0.41
1:A:290:SER:OG	1:A:325:VAL:HG12	2.21	0.41
1:A:398:LEU:HD11	1:A:605:ASN:CG	2.41	0.41
2:B:99:GLN:O	2:B:99:GLN:NE2	2.54	0.41
3:C:25:ASP:OD2	3:C:27:ALA:HB3	2.19	0.41
1:A:9:ASP:N	1:A:9:ASP:OD1	2.54	0.41
1:A:126:TYR:CD1	1:A:677:LYS:CA	3.02	0.41
1:A:129:LEU:HB2	1:A:131:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:C	1:A:162:ASN:N	2.72	0.41
1:A:334:ALA:O	1:A:338:LEU:HD23	2.20	0.41
1:A:496:GLU:C	1:A:498:GLU:H	2.24	0.41
1:A:521:ASP:O	1:A:522:LEU:C	2.59	0.41
1:A:537:CYS:CB	1:A:595:LEU:HD11	2.51	0.41
1:A:577:HIS:CD2	1:A:591:ILE:H	2.39	0.41
1:A:751:ALA:C	1:A:754:ARG:NH1	2.74	0.41
2:B:101:THR:O	2:B:102:LYS:HB2	2.21	0.41
2:B:108:TYR:C	2:B:108:TYR:CD1	2.95	0.41
2:B:121:ASN:ND2	2:B:124:GLU:CG	2.78	0.41
2:B:121:ASN:OD1	2:B:123:ASP:HB2	2.21	0.41
1:A:100:LEU:HB2	1:A:688:LEU:HD21	2.03	0.41
1:A:250:HIS:ND1	1:A:455:TYR:HB3	2.35	0.41
1:A:325:VAL:CG2	1:A:326:GLU:N	2.82	0.41
1:A:390:ASN:HB3	1:A:393:ASP:OD1	2.21	0.41
1:A:534:GLU:OE2	1:A:646:SER:HB3	2.22	0.41
1:A:788:HIS:CD2	3:C:149:MET:HA	2.56	0.41
2:B:132:ALA:HA	2:B:133:PRO:HD3	1.70	0.41
1:A:60:ILE:HG22	1:A:63:ASP:HB3	1.96	0.40
1:A:173:LEU:HD21	1:A:660:LEU:CD2	2.50	0.40
1:A:530:LEU:O	1:A:534:GLU:CG	2.53	0.40
1:A:790:ARG:O	1:A:793:LEU:HB2	2.21	0.40
2:B:24:PHE:HE2	2:B:69:PHE:CA	2.31	0.40
2:B:99:GLN:O	2:B:99:GLN:HG3	2.21	0.40
1:A:135:SER:O	1:A:138:ALA:HB3	2.22	0.40
1:A:398:LEU:C	1:A:401:PRO:CG	2.83	0.40
1:A:447:ASP:CG	1:A:449:LYS:NZ	2.73	0.40
1:A:645:ILE:O	1:A:645:ILE:HG22	2.20	0.40
1:A:815:ILE:C	1:A:817:LYS:N	2.75	0.40
1:A:66:THR:H	1:A:66:THR:HG23	1.63	0.40
1:A:91:MET:HB3	1:A:91:MET:HE2	1.94	0.40
1:A:323:ASP:OD1	1:A:323:ASP:C	2.59	0.40
1:A:615:GLU:O	1:A:616:PRO:C	2.60	0.40
1:A:737:THR:O	1:A:739:SER:N	2.54	0.40
3:C:106:LEU:HA	3:C:109:VAL:CG2	2.51	0.40
3:C:141:TYR:O	3:C:145:VAL:HG23	2.21	0.40
1:A:174:ILE:CG2	1:A:668:VAL:HB	2.41	0.40
1:A:288:ILE:HD11	1:A:352:THR:HG21	2.03	0.40
1:A:355:ILE:O	1:A:356:LEU:C	2.58	0.40
1:A:545:LYS:O	1:A:546:SER:C	2.56	0.40
1:A:741:LYS:O	1:A:745:GLY:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:ILE:HD11	3:C:35:ASP:CB	2.52	0.40
2:B:47:LEU:HD23	2:B:47:LEU:HA	1.75	0.40
2:B:102:LYS:HA	2:B:141:TYR:OH	2.20	0.40
2:B:106:ILE:O	2:B:106:ILE:CG1	2.69	0.40
3:C:40:LEU:CD1	3:C:72:TYR:CE1	3.03	0.40
3:C:109:VAL:O	3:C:113:LEU:CD1	2.69	0.40
1:A:136:VAL:O	1:A:137:ILE:C	2.59	0.40
1:A:187:LYS:O	1:A:188:LYS:C	2.60	0.40
1:A:319:VAL:HG23	1:A:322:ILE:HB	2.02	0.40
1:A:322:ILE:HD13	1:A:322:ILE:HA	1.87	0.40
1:A:468:ASP:OD1	1:A:468:ASP:N	2.54	0.40
1:A:496:GLU:OE1	1:A:496:GLU:HA	2.21	0.40
1:A:645:ILE:O	1:A:645:ILE:CG2	2.70	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)
1:A:452:ARG:O	1:A:572:ASN:OD1[1_655]	2.18	0.02

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	757/835 (91%)	551 (73%)	156 (21%)	50 (7%)	1	5
2	B	140/156 (90%)	93 (66%)	30 (21%)	17 (12%)	0	1
3	C	151/156 (97%)	100 (66%)	35 (23%)	16 (11%)	0	2
All	All	1048/1147 (91%)	744 (71%)	221 (21%)	83 (8%)	1	3

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	MET
1	A	413	GLY
1	A	504	GLY
1	A	526	PRO
1	A	604	GLU
1	A	645	ILE
1	A	718	GLN
2	B	41	LYS
2	B	94	ALA
3	C	54	GLY
1	A	8	PRO
1	A	81	LYS
1	A	164	VAL
1	A	193	LEU
1	A	272	VAL
1	A	307	GLY
1	A	316	CYS
1	A	335	PHE
1	A	373	GLU
1	A	375	ASP
1	A	416	MET
1	A	462	ALA
1	A	603	ASN
1	A	706	GLY
1	A	736	LYS
2	B	67	LEU
2	B	119	ASN
3	C	59	GLY
3	C	116	ARG
3	C	144	PHE
3	C	151	GLY
3	C	152	PRO
1	A	80	PRO
1	A	188	LYS
1	A	241	SER
1	A	429	SER
1	A	513	GLY
1	A	529	ILE
1	A	583	TYR
1	A	717	LYS
1	A	752	GLU
1	A	765	GLY
1	A	781	ILE

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Mol	Chain	Res	Type
2	B	73	LEU
2	B	77	SER
2	B	80	LEU
2	B	112	LEU
2	B	113	LEU
2	B	120	PHE
2	B	130	LYS
2	B	146	ALA
3	C	33	LEU
3	C	56	HIS
3	C	71	ALA
3	C	129	THR
1	A	214	SER
1	A	277	SER
1	A	794	ILE
1	A	816	ARG
1	A	825	GLN
2	B	90	ARG
3	C	53	GLY
3	C	72	TYR
3	C	75	LEU
1	A	337	ILE
1	A	616	PRO
2	B	82	GLY
1	A	61	VAL
1	A	102	ASN
1	A	242	ARG
1	A	400	LYS
1	A	571	PRO
1	A	625	PRO
2	B	98	GLU
3	C	85	ASP
3	C	128	LEU
3	C	125	ILE
2	B	136	GLY
1	A	745	GLY
2	B	51	PRO
1	A	811	ILE
1	A	131	ILE
1	A	766	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	614/728 (84%)	500 (81%)	114 (19%)	1	7
2	B	115/133 (86%)	85 (74%)	30 (26%)	0	2
3	C	119/132 (90%)	99 (83%)	20 (17%)	1	9
All	All	848/993 (85%)	684 (81%)	164 (19%)	1	6

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	7	ASP
1	A	9	ASP
1	A	12	TYR
1	A	51	SER
1	A	55	GLU
1	A	63	ASP
1	A	68	THR
1	A	72	ASP
1	A	82	PHE
1	A	94	LEU
1	A	96	GLU
1	A	111	LEU
1	A	115	TYR
1	A	118	LEU
1	A	120	CYS
1	A	121	ILE
1	A	131	ILE
1	A	133	THR
1	A	143	LYS
1	A	145	LYS
1	A	147	GLU
1	A	152	LEU
1	A	165	THR
1	A	166	ASP
1	A	174	ILE

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Mol	Chain	Res	Type
1	A	214	SER
1	A	216	GLU
1	A	224	PRO
1	A	257	ILE
1	A	266	LEU
1	A	284	ILE
1	A	288	ILE
1	A	300	MET
1	A	303	THR
1	A	305	ASP
1	A	314	GLN
1	A	324	ASP
1	A	333	GLU
1	A	335	PHE
1	A	347	SER
1	A	349	PHE
1	A	352	THR
1	A	371	GLN
1	A	382	LYS
1	A	393	ASP
1	A	398	LEU
1	A	403	VAL
1	A	415	ASN
1	A	416	MET
1	A	417	ASN
1	A	426	LEU
1	A	436	ASN
1	A	438	LEU
1	A	452	ARG
1	A	455	TYR
1	A	459	LEU
1	A	467	PHE
1	A	468	ASP
1	A	470	ASN
1	A	472	PHE
1	A	475	LEU
1	A	476	CYS
1	A	482	GLU
1	A	501	LYS
1	A	507	TRP
1	A	512	PHE
1	A	515	ASP

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Mol	Chain	Res	Type
1	A	517	GLN
1	A	521	ASP
1	A	526	PRO
1	A	529	ILE
1	A	543	ASP
1	A	544	ASP
1	A	558	LYS
1	A	559	ASN
1	A	561	MET
1	A	587	VAL
1	A	591	ILE
1	A	595	LEU
1	A	599	LYS
1	A	602	ILE
1	A	615	GLU
1	A	617	LEU
1	A	627	GLU
1	A	644	THR
1	A	654	ASN
1	A	655	LYS
1	A	675	GLU
1	A	687	VAL
1	A	692	GLN
1	A	694	ASN
1	A	697	LEU
1	A	709	SER
1	A	711	LEU
1	A	722	ILE
1	A	726	ASN
1	A	737	THR
1	A	739	SER
1	A	746	LEU
1	A	748	MET
1	A	755	LEU
1	A	757	THR
1	A	758	THR
1	A	760	VAL
1	A	766	VAL
1	A	769	ASN
1	A	774	ARG
1	A	792	TYR
1	A	794	ILE

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Mol	Chain	Res	Type
1	A	805	ARG
1	A	806	ILE
1	A	808	LEU
1	A	823	ASN
2	B	14	GLN
2	B	24	PHE
2	B	30	ASP
2	B	35	VAL
2	B	36	SER
2	B	49	ARG
2	B	52	ASP
2	B	67	LEU
2	B	68	ASN
2	B	70	THR
2	B	71	MET
2	B	76	PHE
2	B	78	ASP
2	B	80	LEU
2	B	88	THR
2	B	96	PHE
2	B	100	GLU
2	B	102	LYS
2	B	107	GLU
2	B	108	TYR
2	B	109	ILE
2	B	116	MET
2	B	119	ASN
2	B	130	LYS
2	B	134	VAL
2	B	139	PHE
2	B	145	THR
2	B	147	MET
2	B	149	LYS
2	B	154	GLU
3	C	5	GLN
3	C	15	PHE
3	C	22	ASP
3	C	24	ARG
3	C	35	ASP
3	C	55	THR
3	C	58	MET
3	C	66	GLU

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Mol	Chain	Res	Type
3	C	73	GLU
3	C	88	GLU
3	C	92	THR
3	C	98	GLN
3	C	100	PHE
3	C	102	SER
3	C	110	LEU
3	C	118	SER
3	C	135	LEU
3	C	140	LYS
3	C	141	TYR
3	C	153	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	161	GLN
1	A	218	GLN
1	A	223	ASN
1	A	237	ASN
1	A	275	GLN
1	A	276	GLN
1	A	291	ASN
1	A	297	ASN
1	A	313	ASN
1	A	314	GLN
1	A	321	ASN
1	A	346	GLN
1	A	371	GLN
1	A	390	ASN
1	A	417	ASN
1	A	421	ASN
1	A	478	ASN
1	A	486	GLN
1	A	517	GLN
1	A	554	ASN
1	A	559	ASN
1	A	577	HIS
1	A	586	ASN
1	A	598	ASN
1	A	603	ASN

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Mol	Chain	Res	Type
1	A	605	ASN
1	A	654	ASN
1	A	664	HIS
1	A	694	ASN
1	A	769	ASN
1	A	802	GLN
1	A	823	ASN
2	B	68	ASN
2	B	119	ASN
3	C	46	ASN
3	C	98	GLN
3	C	132	GLN
3	C	138	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are 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	ANP	A	999	4	29,33,33	1.68	6 (20%)	31,52,52	2.00	6 (19%)

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	ANP	A	999	4	-	6/14/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	ANP	PG-O1G	3.93	1.52	1.46
5	A	999	ANP	O4'-C1'	-3.42	1.36	1.40
5	A	999	ANP	PG-N3B	2.82	1.70	1.63
5	A	999	ANP	PB-O3A	2.64	1.62	1.59
5	A	999	ANP	PG-O2G	-2.13	1.51	1.56
5	A	999	ANP	C2'-C3'	-2.05	1.47	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	ANP	C5-C6-N6	6.76	130.62	120.31
5	A	999	ANP	O1G-PG-N3B	-4.45	105.22	111.77
5	A	999	ANP	C5-C6-N1	-3.85	111.06	120.23
5	A	999	ANP	N3-C2-N1	-3.32	124.17	128.67
5	A	999	ANP	O4'-C1'-N9	2.87	112.55	108.75
5	A	999	ANP	C1'-N9-C4	-2.02	123.10	126.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

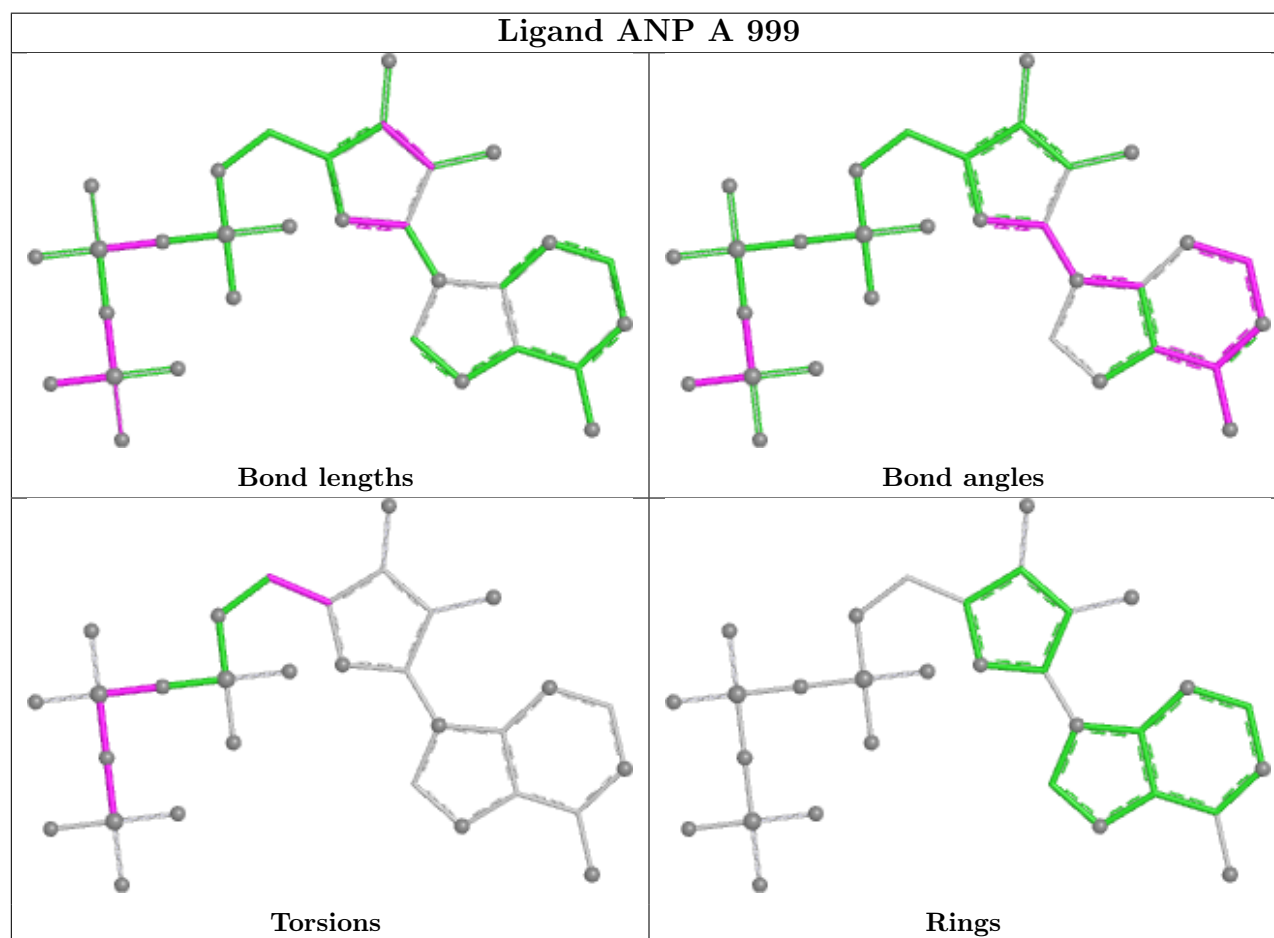
Mol	Chain	Res	Type	Atoms
5	A	999	ANP	PB-N3B-PG-O1G
5	A	999	ANP	PG-N3B-PB-O1B
5	A	999	ANP	C3'-C4'-C5'-O5'
5	A	999	ANP	O4'-C4'-C5'-O5'
5	A	999	ANP	PA-O3A-PB-O2B
5	A	999	ANP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	999	ANP	16	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 than 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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	777/835 (93%)	-0.07	10 (1%) 74 54	25, 81, 106, 108	0
2	B	142/156 (91%)	-0.30	1 (0%) 84 68	41, 76, 103, 108	0
3	C	153/156 (98%)	-0.38	2 (1%) 74 54	28, 75, 99, 105	0
All	All	1072/1147 (93%)	-0.15	13 (1%) 76 56	25, 79, 106, 108	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	695	GLY	4.1
2	B	116	MET	4.1
1	A	253	PRO	2.9
1	A	738	VAL	2.6
1	A	394	LEU	2.5
3	C	21	TRP	2.5
3	C	90	PHE	2.4
1	A	28	PHE	2.3
1	A	350	LYS	2.3
1	A	728	ILE	2.2
1	A	110	GLY	2.2
1	A	830	TYR	2.0
1	A	122	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

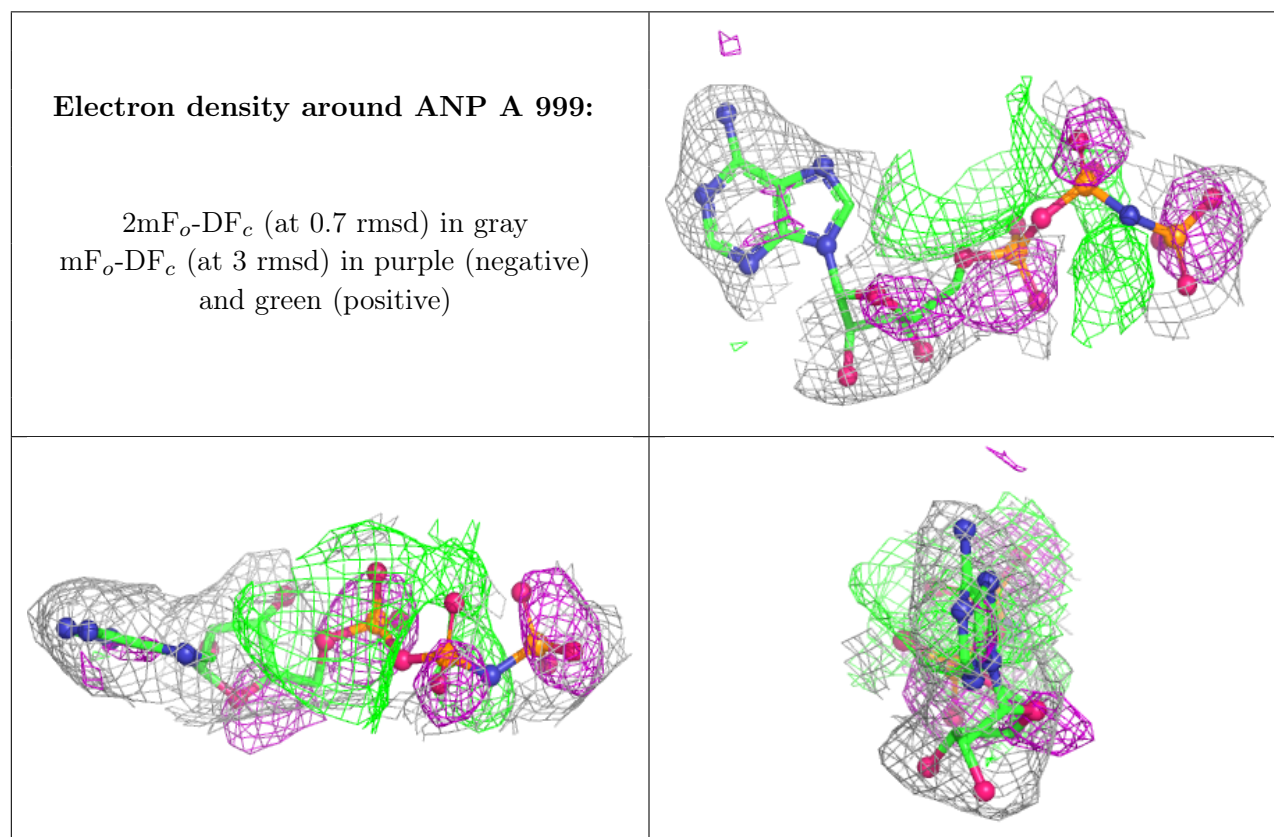
There are no monosaccharides in this entry.

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, 95th 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	903	1/1	0.82	0.18	58,58,58,58	0
5	ANP	A	999	31/31	0.85	0.12	9,22,37,49	0
4	MG	B	502	1/1	0.97	0.04	99,99,99,99	0
6	CA	C	501	1/1	0.97	0.06	70,70,70,70	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.