Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:12 AM BST

PDB ID	:	3B60
Title	:	Crystal Structure of MsbA from Salmonella typhimurium with AMPPNP, higher resolution form
Authors	:	Ward, A.; Reyes, C.L.; Yu, J.; Roth, C.B.; Chang, G.
Deposited on	:	2007-10-26
Resolution	:	3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

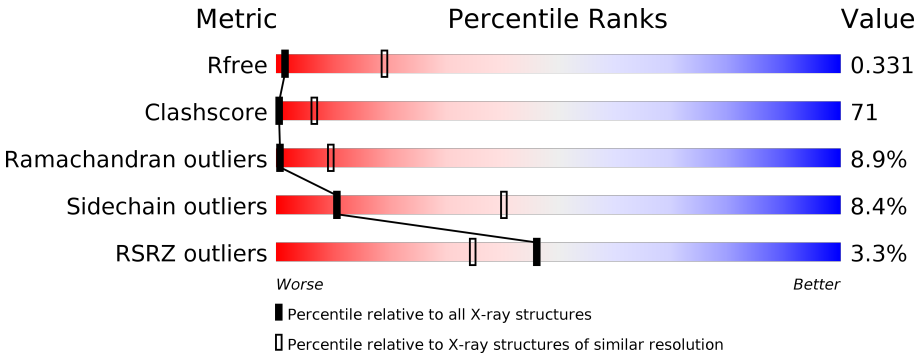
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	582	5% 24% 61% 12%
1	B	582	3% 25% 61% 11%
1	C	582	3% 25% 61% 11%
1	D	582	2% 25% 60% 12%

2 Entry composition

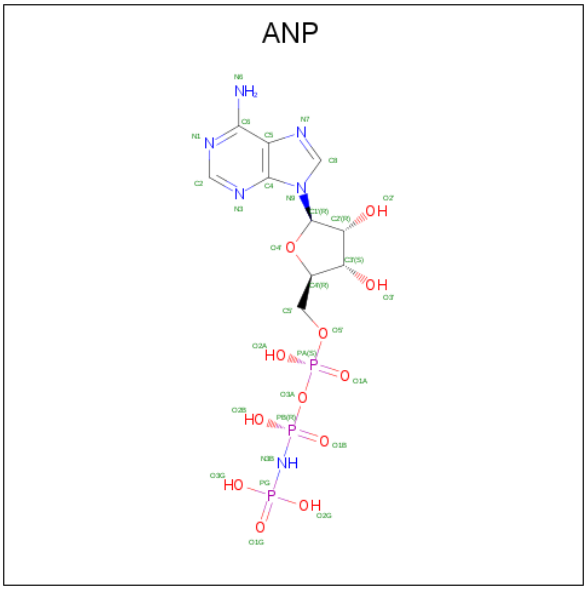
There are 2 unique types of molecules in this entry. The entry contains 17844 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lipid A export ATP-binding/permease protein msbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4430	2813	768	822	27			
1	B	572	Total	C	N	O	S	0	0	0
			4430	2813	768	822	27			
1	C	572	Total	C	N	O	S	0	0	0
			4430	2813	768	822	27			
1	D	572	Total	C	N	O	S	0	0	0
			4430	2813	768	822	27			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

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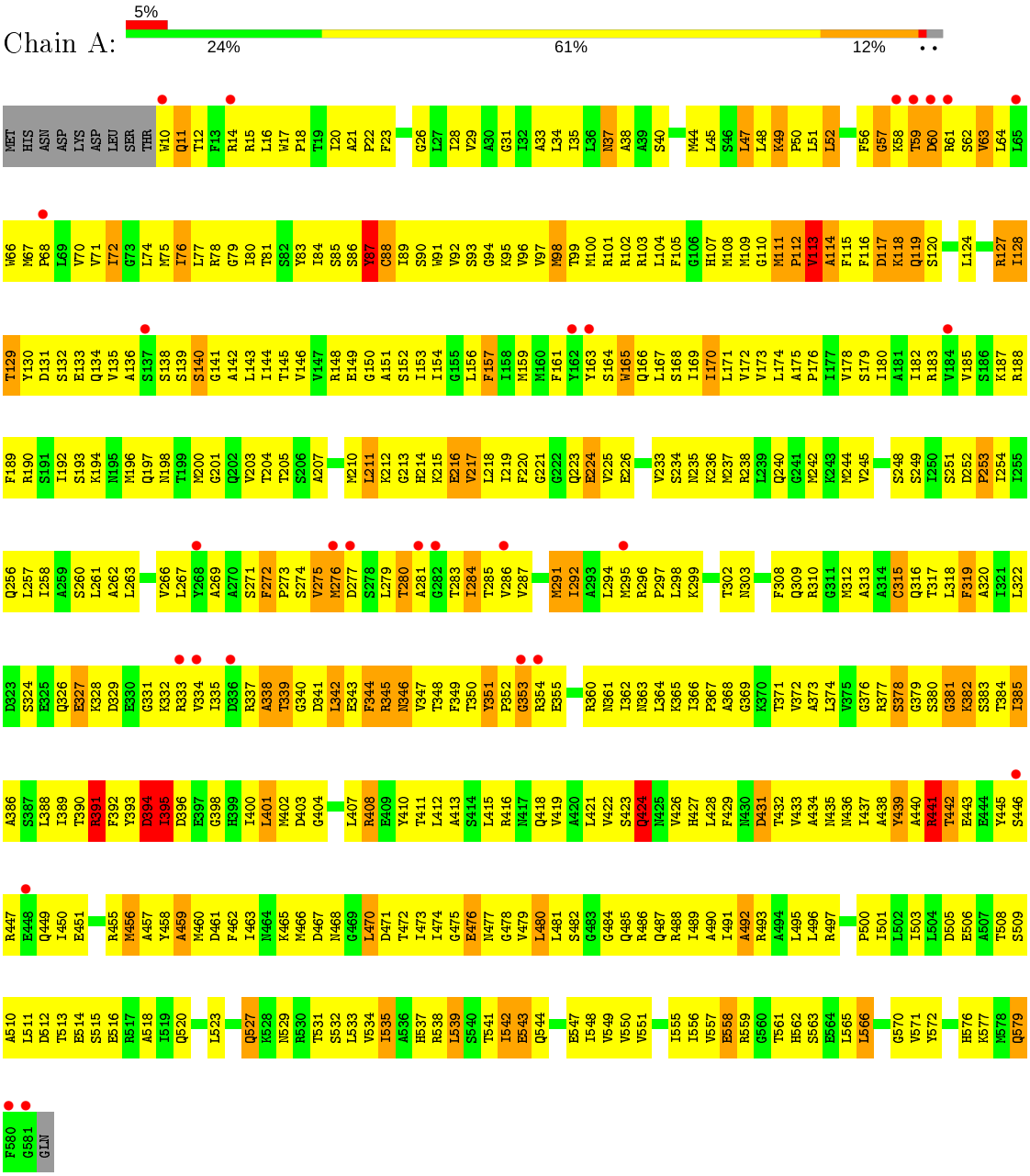
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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.

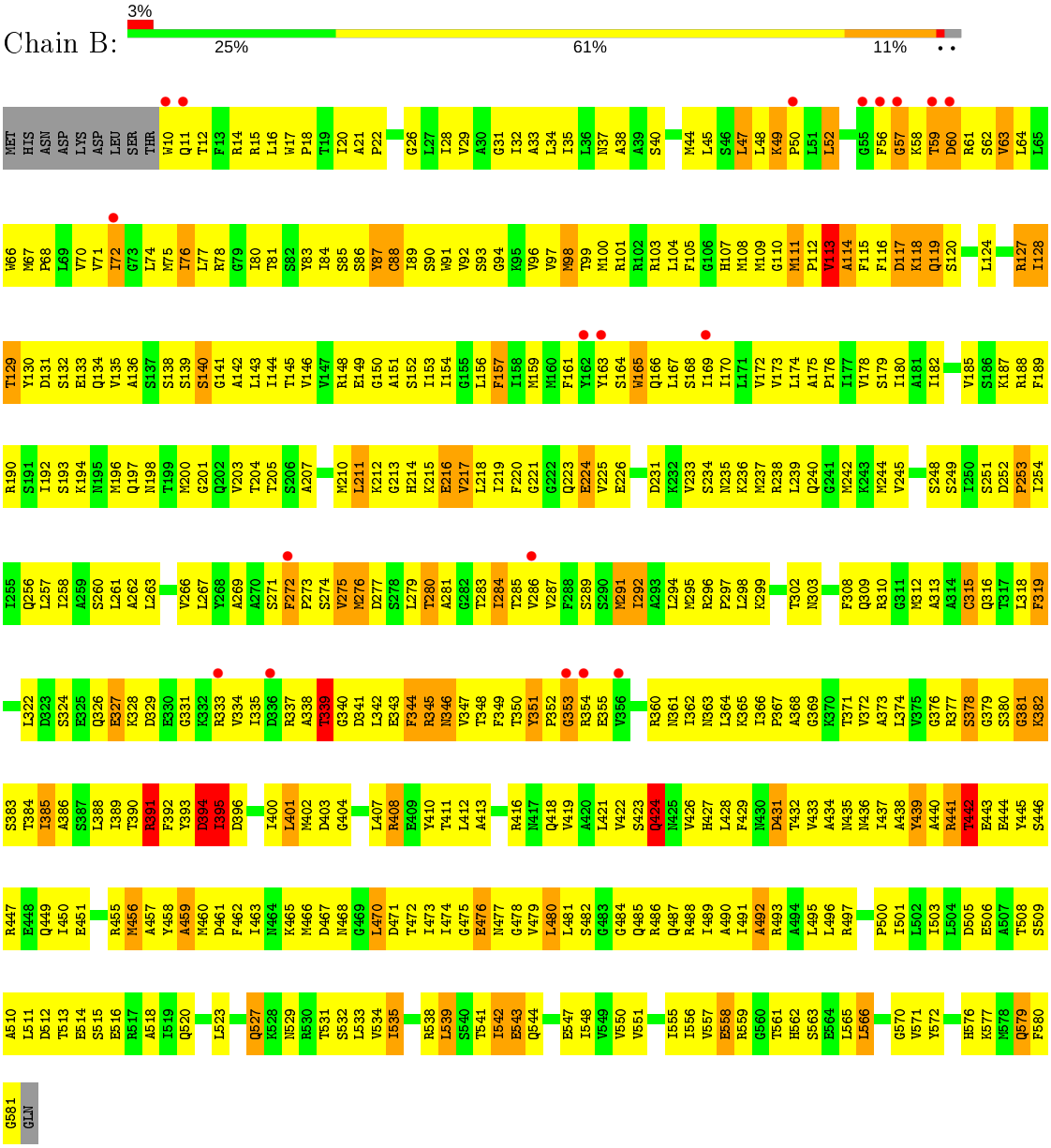
- Molecule 1: Lipid A export ATP-binding/permease protein msbA

Chain A:



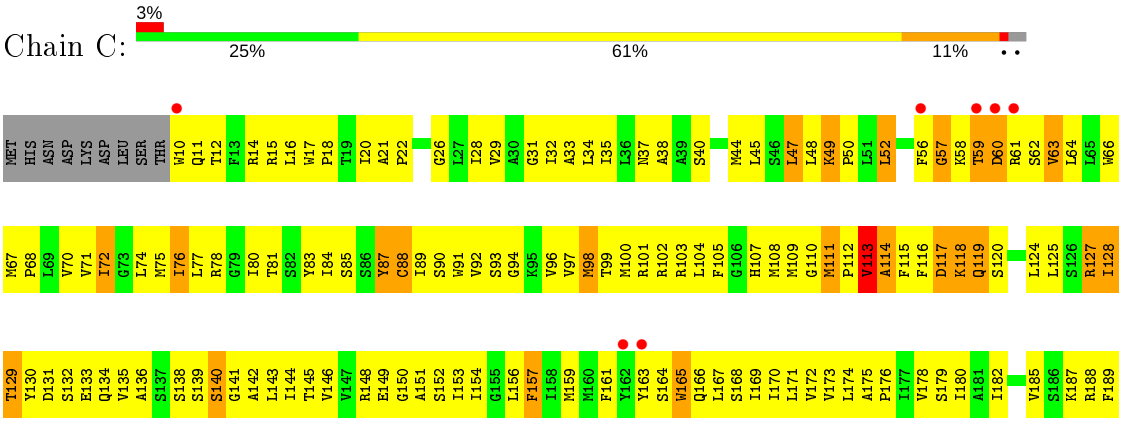
• Molecule 1: Lipid A export ATP-binding/permease protein msbA

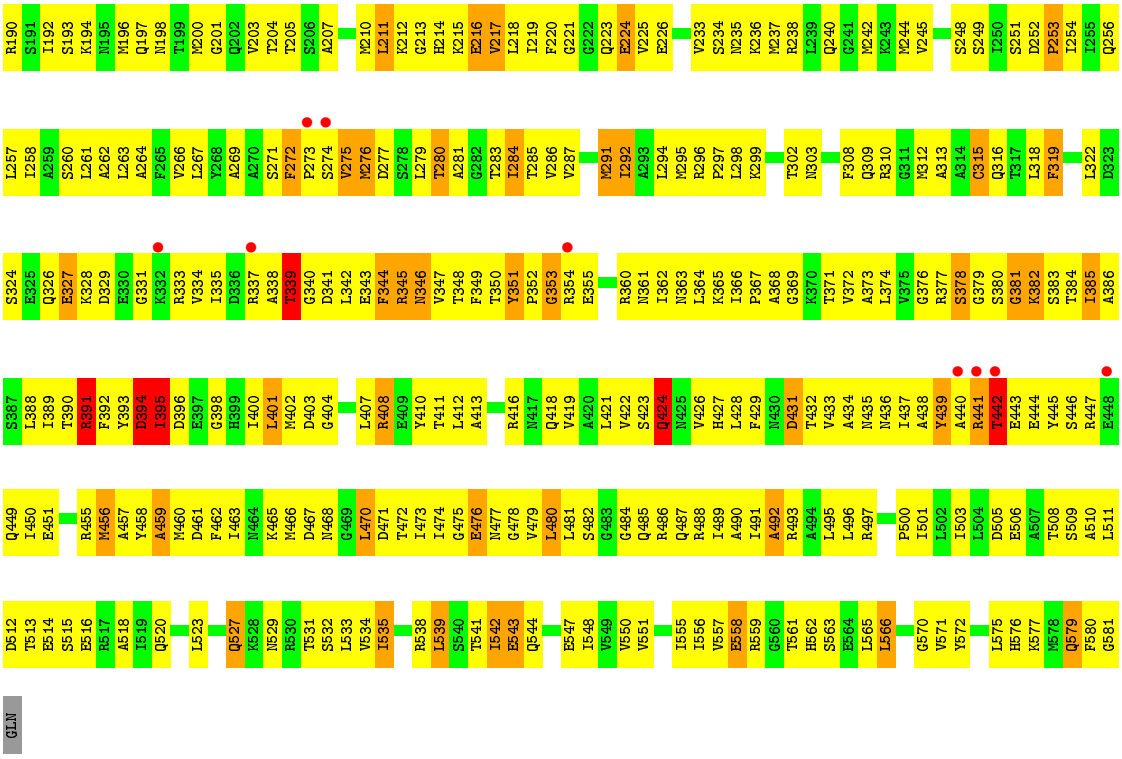
Chain B:



• Molecule 1: Lipid A export ATP-binding/permease protein msbA

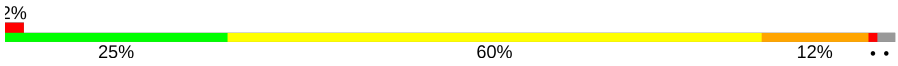
Chain C:

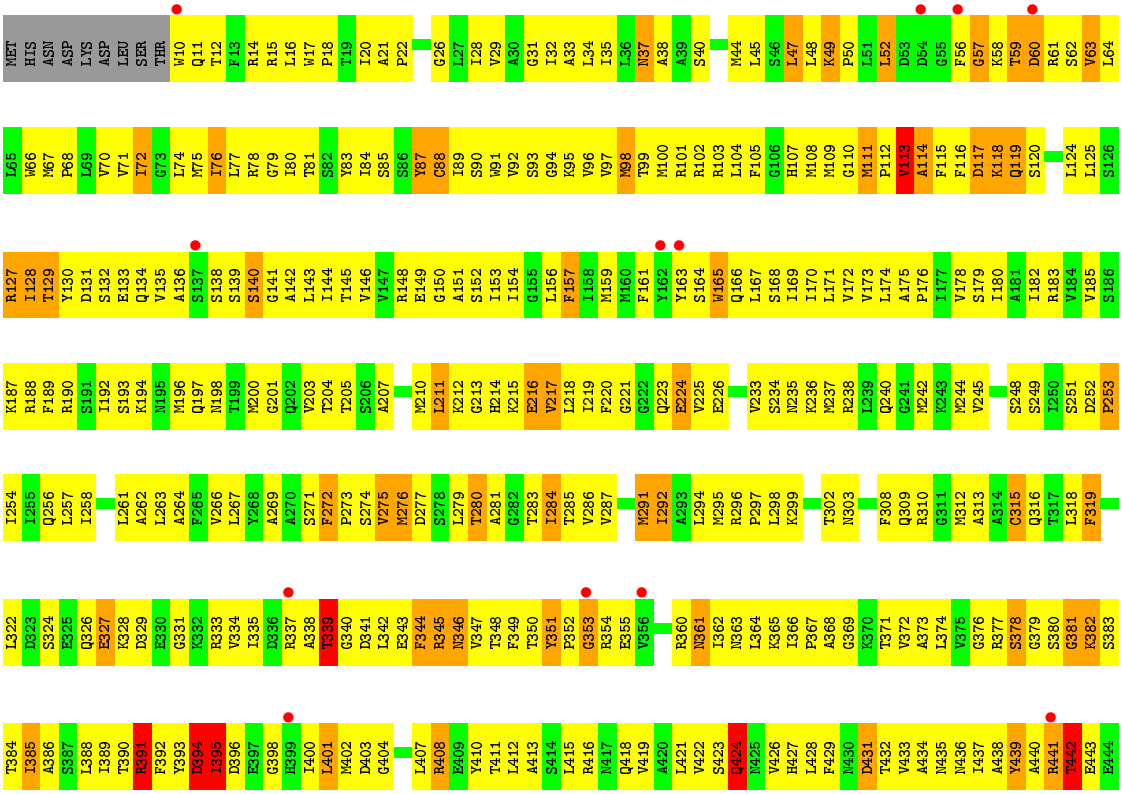


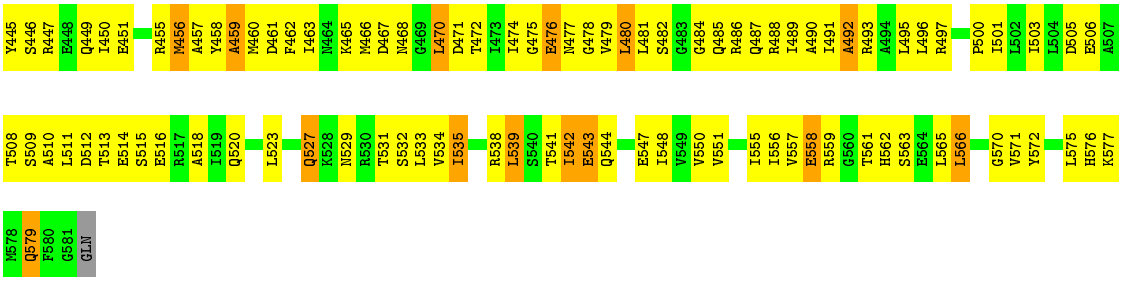


• Molecule 1: Lipid A export ATP-binding/permease protein msbA

Chain D:






Y445 S446 R447 E448 Q449 I450 E451 R455 M456 A457 Y458 A459 M460 D461 F462 I463 N464 K465 M466 D467 N468 G469 L470 D471 T472 I473 I474 G475 E476 N477 G478 V479 L480 L481 S482 G483 G484 Q485 R486 Q487 R488 I489 A490 I491 A492 R493 A494 L495 L496 R497 P500 I501 L502 I503 L504 D505 E506 A507
T508 S509 A510 L511 D512 T513 E514 S515 E516 R517 A518 I519 Q520 L523 Q527 K528 N529 R530 T531 S532 L533 V534 I535 R538 L539 S540 T541 I542 E543 Q544 E547 I548 V549 V550 V551 I555 I556 V557 E558 R559 G560 T561 H562 S563 E564 L565 L566 G570 V571 Y572 L575 H576 K577
M578 Q579 F580 G581 GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	249.64Å 119.90Å 168.80Å 90.00° 120.61° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	87.7 (20.00-3.70) 87.7 (20.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 3.71Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.307 , 0.343 0.294 , 0.331	Depositor DCC
R_{free} test set	2019 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	118.5	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 98.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	17844	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: ANP

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	0.45	0/4497	0.73	4/6076 (0.1%)
1	B	0.33	0/4497	0.68	4/6076 (0.1%)
1	C	0.33	0/4497	0.68	4/6076 (0.1%)
1	D	0.33	0/4497	0.68	4/6076 (0.1%)
All	All	0.37	0/17988	0.69	16/24304 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	441	ARG	C-N-CA	12.51	152.96	121.70
1	D	441	ARG	C-N-CA	7.75	141.07	121.70
1	C	441	ARG	C-N-CA	7.72	141.01	121.70
1	B	441	ARG	C-N-CA	7.71	140.97	121.70
1	A	338	ALA	C-N-CA	-7.59	102.73	121.70
1	A	395	ILE	N-CA-C	5.66	126.28	111.00
1	A	353	GLY	N-CA-C	5.37	126.53	113.10
1	B	395	ILE	N-CA-C	5.30	125.31	111.00
1	B	353	GLY	N-CA-C	5.29	126.33	113.10
1	C	395	ILE	N-CA-C	5.29	125.29	111.00
1	D	395	ILE	N-CA-C	5.29	125.27	111.00
1	D	353	GLY	N-CA-C	5.28	126.29	113.10
1	C	353	GLY	N-CA-C	5.26	126.26	113.10
1	B	442	THR	N-CA-CB	5.20	120.18	110.30
1	C	442	THR	N-CA-CB	5.19	120.17	110.30
1	D	442	THR	N-CA-CB	5.16	120.10	110.30

There are no chirality outliers.

There are no planarity outliers.

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	4430	0	4555	719	0
1	B	4430	0	4556	689	0
1	C	4430	0	4556	714	0
1	D	4430	0	4556	711	0
2	A	31	0	13	5	0
2	B	31	0	13	6	0
2	C	31	0	13	3	0
2	D	31	0	13	5	0
All	All	17844	0	18275	2575	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 71.

All (2575) 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:221:GLY:HA3	1:B:441:ARG:CD	1.57	1.35
1:A:221:GLY:CA	1:B:441:ARG:HD3	1.67	1.22
1:C:11:GLN:HG2	1:C:12:THR:H	1.10	1.17
1:C:281:ALA:HB2	1:D:56:PHE:HB3	1.24	1.17
1:C:441:ARG:CD	1:D:221:GLY:HA3	1.75	1.16
1:C:441:ARG:HD3	1:D:221:GLY:CA	1.77	1.15
1:A:441:ARG:HD3	1:B:221:GLY:HA3	1.17	1.14
1:D:11:GLN:HG2	1:D:12:THR:H	1.10	1.13
1:A:11:GLN:N	1:A:14:ARG:HB3	1.62	1.12
1:C:56:PHE:HB3	1:D:281:ALA:HB2	1.26	1.12
1:B:338:ALA:HB3	1:B:500:PRO:HG2	1.12	1.11
1:B:11:GLN:HG2	1:B:12:THR:H	1.10	1.11
1:A:10:TRP:HA	1:A:14:ARG:HB2	1.33	1.10
1:C:221:GLY:HA3	1:D:441:ARG:CD	1.80	1.10
1:C:221:GLY:HA3	1:D:441:ARG:HD3	1.15	1.10
1:A:11:GLN:HG2	1:A:12:THR:H	1.06	1.07
1:D:338:ALA:HB3	1:D:500:PRO:HG2	1.12	1.07
1:C:10:TRP:HA	1:C:14:ARG:HB2	1.37	1.07
1:C:338:ALA:HB3	1:C:500:PRO:HG2	1.12	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLY:CA	1:D:441:ARG:HD3	1.85	1.06
1:A:338:ALA:O	1:A:339:THR:C	1.92	1.06
1:A:441:ARG:CD	1:B:221:GLY:HA3	1.84	1.06
1:C:441:ARG:HD3	1:D:221:GLY:HA3	1.09	1.05
1:B:10:TRP:HA	1:B:14:ARG:HB2	1.37	1.05
1:D:10:TRP:HA	1:D:14:ARG:HB2	1.37	1.05
1:A:220:PHE:HA	1:B:497:ARG:HH21	1.22	1.04
1:A:338:ALA:HB3	1:A:500:PRO:HG2	1.08	1.03
1:D:351:TYR:HB3	1:D:352:PRO:HD3	1.41	1.02
1:A:351:TYR:HB3	1:A:352:PRO:HD3	1.42	1.01
1:B:351:TYR:HB3	1:B:352:PRO:HD3	1.41	1.01
1:C:351:TYR:HB3	1:C:352:PRO:HD3	1.41	1.01
1:A:441:ARG:HD3	1:B:221:GLY:CA	1.91	1.00
1:C:497:ARG:HH21	1:D:220:PHE:HA	1.26	1.00
1:B:80:ILE:O	1:B:84:ILE:HG12	1.63	0.99
1:B:11:GLN:N	1:B:14:ARG:HB3	1.78	0.98
1:D:11:GLN:N	1:D:14:ARG:HB3	1.78	0.98
1:D:80:ILE:O	1:D:84:ILE:HG12	1.63	0.98
1:C:512:ASP:OD1	1:D:377:ARG:HA	1.61	0.98
1:C:395:ILE:HG12	1:C:396:ASP:H	1.28	0.98
1:B:395:ILE:HG12	1:B:396:ASP:H	1.27	0.98
1:A:338:ALA:HB3	1:A:500:PRO:CG	1.93	0.97
1:A:80:ILE:O	1:A:84:ILE:HG12	1.63	0.97
1:C:80:ILE:O	1:C:84:ILE:HG12	1.63	0.97
1:A:395:ILE:HG12	1:A:396:ASP:H	1.28	0.97
1:D:395:ILE:HG12	1:D:396:ASP:H	1.27	0.97
1:B:338:ALA:O	1:B:339:THR:C	2.02	0.97
1:C:11:GLN:N	1:C:14:ARG:HB3	1.78	0.96
1:A:91:TRP:HA	1:B:242:MET:CE	1.95	0.96
1:B:347:VAL:HG13	1:B:395:ILE:HD11	1.47	0.96
1:D:347:VAL:HG13	1:D:395:ILE:HD11	1.47	0.96
1:C:347:VAL:HG13	1:C:395:ILE:HD11	1.47	0.95
1:A:539:LEU:HA	1:A:542:ILE:HD13	1.46	0.95
1:A:272:PHE:HB2	1:A:273:PRO:HD3	1.49	0.94
1:C:338:ALA:O	1:C:339:THR:C	2.02	0.94
1:C:377:ARG:HA	1:D:512:ASP:OD1	1.65	0.94
1:A:347:VAL:HG13	1:A:395:ILE:HD11	1.44	0.94
1:B:338:ALA:HB3	1:B:500:PRO:CG	1.97	0.94
1:D:272:PHE:HB2	1:D:273:PRO:HD3	1.50	0.93
1:D:338:ALA:HB3	1:D:500:PRO:CG	1.97	0.93
1:C:338:ALA:HB3	1:C:500:PRO:CG	1.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:HA	1:B:497:ARG:NH2	1.83	0.93
1:C:497:ARG:NH2	1:D:220:PHE:HA	1.83	0.93
1:B:272:PHE:HB2	1:B:273:PRO:HD3	1.50	0.93
1:A:220:PHE:CZ	1:B:429:PHE:HE1	1.87	0.93
1:D:338:ALA:O	1:D:339:THR:C	2.02	0.92
1:A:11:GLN:N	1:A:14:ARG:CB	2.32	0.92
1:B:539:LEU:HA	1:B:542:ILE:HD13	1.51	0.92
1:A:98:MET:HB3	1:B:238:ARG:NH2	1.83	0.92
1:C:272:PHE:HB2	1:C:273:PRO:HD3	1.50	0.91
1:A:11:GLN:HG2	1:A:12:THR:N	1.85	0.91
1:A:470:LEU:H	1:A:470:LEU:HD12	1.36	0.90
1:A:429:PHE:HE1	1:B:220:PHE:CZ	1.90	0.90
1:C:220:PHE:HA	1:D:497:ARG:HH21	1.36	0.89
1:A:116:PHE:HE1	1:B:211:LEU:HD12	1.37	0.89
1:C:116:PHE:HE1	1:D:211:LEU:HD12	1.38	0.89
1:C:539:LEU:HA	1:C:542:ILE:HD13	1.53	0.89
1:D:539:LEU:HA	1:D:542:ILE:HD13	1.53	0.89
1:A:98:MET:HB3	1:B:238:ARG:CZ	2.03	0.89
1:A:10:TRP:CA	1:A:14:ARG:HB2	2.03	0.88
1:A:21:ALA:HB3	1:A:22:PRO:HD3	1.56	0.87
1:A:20:ILE:HD13	1:A:96:VAL:HG21	1.56	0.87
1:A:221:GLY:HA3	1:B:441:ARG:NE	1.89	0.87
1:A:211:LEU:HD12	1:B:116:PHE:HE1	1.40	0.87
1:A:220:PHE:CZ	1:B:439:TYR:HB3	2.08	0.87
1:C:459:ALA:O	1:C:463:ILE:HG12	1.75	0.87
1:B:21:ALA:HB3	1:B:22:PRO:HD3	1.57	0.87
1:D:11:GLN:HG2	1:D:12:THR:N	1.90	0.87
1:B:459:ALA:O	1:B:463:ILE:HG12	1.75	0.87
1:A:221:GLY:HA3	1:B:441:ARG:HD3	0.90	0.86
1:D:459:ALA:O	1:D:463:ILE:HG12	1.75	0.86
1:C:439:TYR:HB3	1:D:220:PHE:CZ	2.10	0.86
1:A:497:ARG:HH21	1:B:220:PHE:HA	1.37	0.86
1:C:21:ALA:HB3	1:C:22:PRO:HD3	1.57	0.86
1:C:505:ASP:HA	1:C:535:ILE:HG23	1.57	0.86
1:A:238:ARG:NH2	1:B:98:MET:HB3	1.90	0.86
1:C:11:GLN:HG2	1:C:12:THR:N	1.90	0.85
1:D:505:ASP:HA	1:D:535:ILE:HG23	1.57	0.85
1:A:459:ALA:O	1:A:463:ILE:HG12	1.74	0.85
1:B:426:VAL:HG11	1:B:490:ALA:HB2	1.59	0.85
1:A:433:VAL:HG11	1:A:463:ILE:HD12	1.59	0.85
1:D:433:VAL:HG11	1:D:463:ILE:HD12	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:N	1:A:470:LEU:HD12	1.91	0.85
1:C:433:VAL:HG11	1:C:463:ILE:HD12	1.59	0.85
1:C:292:ILE:HD12	1:D:48:LEU:HD12	1.59	0.85
1:B:433:VAL:HG11	1:B:463:ILE:HD12	1.57	0.85
1:B:11:GLN:HG2	1:B:12:THR:N	1.90	0.84
1:C:292:ILE:HD12	1:D:48:LEU:CD1	2.07	0.84
1:D:436:ASN:ND2	1:D:474:ILE:HG21	1.91	0.84
1:A:436:ASN:ND2	1:A:474:ILE:HG21	1.92	0.84
1:B:505:ASP:HA	1:B:535:ILE:HG23	1.57	0.84
1:D:113:VAL:HG22	1:D:114:ALA:H	1.42	0.84
1:D:174:LEU:HD22	1:D:262:ALA:HB2	1.59	0.84
1:A:505:ASP:HA	1:A:535:ILE:HG23	1.59	0.84
1:D:21:ALA:HB3	1:D:22:PRO:HD3	1.57	0.84
1:B:67:MET:O	1:B:70:VAL:HG12	1.78	0.84
1:C:436:ASN:ND2	1:C:474:ILE:HG21	1.91	0.84
1:B:436:ASN:ND2	1:B:474:ILE:HG21	1.91	0.84
1:A:67:MET:O	1:A:70:VAL:HG12	1.78	0.84
1:B:113:VAL:HG22	1:B:114:ALA:H	1.42	0.84
1:C:113:VAL:HG22	1:C:114:ALA:H	1.42	0.84
1:C:119:GLN:HE21	1:C:119:GLN:H	1.26	0.84
1:A:316:GLN:OE1	1:A:319:PHE:HD1	1.61	0.83
1:D:470:LEU:HD12	1:D:470:LEU:H	1.42	0.83
1:C:426:VAL:HG11	1:C:490:ALA:HB2	1.59	0.83
1:C:470:LEU:HD12	1:C:470:LEU:H	1.42	0.83
1:C:211:LEU:HD12	1:D:116:PHE:HE1	1.42	0.83
1:D:67:MET:O	1:D:70:VAL:HG12	1.78	0.83
1:B:174:LEU:HD22	1:B:262:ALA:HB2	1.60	0.83
1:C:67:MET:O	1:C:70:VAL:HG12	1.78	0.83
1:A:395:ILE:HG12	1:A:396:ASP:N	1.94	0.83
1:B:470:LEU:HD12	1:B:470:LEU:H	1.42	0.83
1:A:238:ARG:CZ	1:B:98:MET:HB3	2.08	0.83
1:D:119:GLN:HE21	1:D:119:GLN:H	1.26	0.83
1:A:113:VAL:HG22	1:A:114:ALA:H	1.44	0.83
1:D:426:VAL:HG11	1:D:490:ALA:HB2	1.59	0.83
1:A:470:LEU:H	1:A:470:LEU:CD1	1.92	0.83
1:C:512:ASP:HB2	1:D:378:SER:H	1.43	0.83
1:B:20:ILE:HD13	1:B:96:VAL:HG21	1.61	0.83
1:D:284:ILE:O	1:D:284:ILE:HD13	1.79	0.82
1:A:426:VAL:HG11	1:A:490:ALA:HB2	1.62	0.82
1:A:242:MET:CE	1:B:91:TRP:HA	2.09	0.82
1:A:174:LEU:HD22	1:A:262:ALA:HB2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HD13	1:A:284:ILE:O	1.80	0.82
1:C:284:ILE:HD13	1:C:284:ILE:O	1.80	0.82
1:B:284:ILE:HD13	1:B:284:ILE:O	1.79	0.82
1:C:174:LEU:HD22	1:C:262:ALA:HB2	1.59	0.82
1:A:56:PHE:HA	1:A:59:THR:HG23	1.62	0.81
1:C:220:PHE:HA	1:D:497:ARG:NH2	1.93	0.81
1:D:151:ALA:HA	1:D:154:ILE:HD12	1.62	0.81
1:A:512:ASP:OD1	1:B:377:ARG:HA	1.81	0.81
1:B:345:ARG:HD2	1:B:345:ARG:N	1.96	0.81
1:C:220:PHE:CZ	1:D:429:PHE:HE1	1.99	0.81
1:C:378:SER:H	1:D:512:ASP:HB2	1.45	0.81
1:A:151:ALA:HA	1:A:154:ILE:HD12	1.61	0.81
1:B:119:GLN:HE21	1:B:119:GLN:H	1.26	0.81
1:A:221:GLY:CA	1:B:441:ARG:CD	2.42	0.81
1:D:20:ILE:HD13	1:D:96:VAL:HG21	1.61	0.81
1:D:345:ARG:HD2	1:D:345:ARG:N	1.96	0.81
1:D:412:LEU:HD21	1:D:416:ARG:NH1	1.96	0.81
1:C:20:ILE:HD13	1:C:96:VAL:HG21	1.61	0.81
1:D:10:TRP:CA	1:D:14:ARG:HB2	2.11	0.81
1:C:441:ARG:NE	1:D:221:GLY:HA3	1.96	0.81
1:A:344:PHE:HD1	1:A:400:ILE:HG12	1.44	0.80
1:C:220:PHE:CZ	1:D:439:TYR:HB3	2.15	0.80
1:D:344:PHE:HD1	1:D:400:ILE:HG12	1.47	0.80
1:B:412:LEU:HD21	1:B:416:ARG:NH1	1.97	0.80
1:C:221:GLY:HA3	1:D:441:ARG:NE	1.97	0.80
1:A:441:ARG:HD3	1:B:220:PHE:O	1.81	0.80
1:B:395:ILE:HG12	1:B:396:ASP:N	1.96	0.80
1:A:119:GLN:H	1:A:119:GLN:HE21	1.27	0.80
1:A:412:LEU:HD21	1:A:416:ARG:NH1	1.97	0.80
1:A:497:ARG:NH2	1:B:220:PHE:HA	1.96	0.80
1:C:426:VAL:HG11	1:C:490:ALA:CB	2.12	0.80
1:A:156:LEU:HB2	1:A:294:LEU:HD13	1.64	0.80
1:B:151:ALA:HA	1:B:154:ILE:HD12	1.62	0.80
1:C:220:PHE:O	1:D:441:ARG:HD3	1.81	0.80
1:C:349:PHE:HA	1:C:396:ASP:HB2	1.63	0.80
1:A:210:MET:HG3	1:A:211:LEU:HD13	1.62	0.80
1:A:345:ARG:N	1:A:345:ARG:HD2	1.97	0.80
1:B:382:LYS:HB2	2:B:5002:ANP:O1B	1.82	0.80
1:D:210:MET:HG3	1:D:211:LEU:HD13	1.64	0.80
1:D:351:TYR:CB	1:D:352:PRO:HD3	2.12	0.80
1:C:10:TRP:CA	1:C:14:ARG:HB2	2.11	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:PHE:HD1	1:B:400:ILE:HG12	1.46	0.79
1:C:412:LEU:HD21	1:C:416:ARG:NH1	1.96	0.79
1:D:395:ILE:HG12	1:D:396:ASP:N	1.96	0.79
1:D:470:LEU:HD12	1:D:470:LEU:N	1.97	0.79
1:A:112:PRO:O	1:A:113:VAL:HG12	1.82	0.79
1:C:344:PHE:HD1	1:C:400:ILE:HG12	1.47	0.79
1:B:351:TYR:CB	1:B:352:PRO:HD3	2.12	0.79
1:C:345:ARG:N	1:C:345:ARG:HD2	1.96	0.79
1:B:349:PHE:HA	1:B:396:ASP:HB2	1.63	0.79
1:A:350:THR:HG22	1:A:396:ASP:OD2	1.83	0.79
1:A:74:LEU:HD22	1:A:75:MET:HE2	1.65	0.79
1:D:349:PHE:HA	1:D:396:ASP:HB2	1.63	0.79
1:D:56:PHE:HA	1:D:59:THR:HG23	1.63	0.79
1:B:16:LEU:HD12	1:B:315:CYS:SG	2.23	0.79
1:B:426:VAL:HG11	1:B:490:ALA:CB	2.12	0.79
1:C:151:ALA:HA	1:C:154:ILE:HD12	1.62	0.79
1:C:349:PHE:HA	1:C:396:ASP:CB	2.13	0.79
1:C:429:PHE:HE1	1:D:220:PHE:CZ	2.01	0.79
1:C:210:MET:HG3	1:C:211:LEU:HD13	1.64	0.79
1:D:349:PHE:HA	1:D:396:ASP:CB	2.13	0.79
1:D:426:VAL:HG11	1:D:490:ALA:CB	2.12	0.79
1:B:156:LEU:HB2	1:B:294:LEU:HD13	1.65	0.79
1:C:351:TYR:CB	1:C:352:PRO:HD3	2.12	0.79
1:B:10:TRP:CA	1:B:14:ARG:HB2	2.11	0.78
1:B:478:GLY:O	1:B:486:ARG:HD2	1.83	0.78
1:D:348:THR:O	1:D:396:ASP:HB3	1.84	0.78
1:A:349:PHE:HA	1:A:396:ASP:CB	2.13	0.78
1:C:16:LEU:HD12	1:C:315:CYS:SG	2.23	0.78
1:D:16:LEU:HD12	1:D:315:CYS:SG	2.23	0.78
1:D:93:SER:HB3	1:D:140:SER:HB3	1.65	0.78
1:B:348:THR:O	1:B:396:ASP:HB3	1.83	0.78
1:B:56:PHE:HA	1:B:59:THR:HG23	1.63	0.78
1:C:93:SER:HB3	1:C:140:SER:HB3	1.65	0.78
1:C:56:PHE:HA	1:C:59:THR:HG23	1.63	0.78
1:C:395:ILE:HG12	1:C:396:ASP:N	1.96	0.78
1:A:154:ILE:HA	1:A:157:PHE:CE2	2.18	0.78
1:A:377:ARG:HA	1:B:512:ASP:OD1	1.83	0.78
1:C:470:LEU:HD12	1:C:470:LEU:N	1.97	0.78
1:C:478:GLY:O	1:C:486:ARG:HD2	1.84	0.78
1:C:48:LEU:CD1	1:D:292:ILE:HD12	2.14	0.78
1:A:349:PHE:HA	1:A:396:ASP:HB2	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ILE:HA	1:D:157:PHE:CE2	2.19	0.78
1:A:426:VAL:HG11	1:A:490:ALA:CB	2.14	0.78
1:B:349:PHE:HA	1:B:396:ASP:CB	2.13	0.78
1:C:242:MET:CE	1:D:91:TRP:HA	2.13	0.78
1:C:350:THR:HG22	1:C:396:ASP:OD2	1.84	0.78
1:B:112:PRO:O	1:B:113:VAL:HG12	1.84	0.77
1:D:156:LEU:HB2	1:D:294:LEU:HD13	1.65	0.77
1:B:470:LEU:N	1:B:470:LEU:HD12	1.97	0.77
1:D:112:PRO:O	1:D:113:VAL:HG12	1.84	0.77
1:D:478:GLY:O	1:D:486:ARG:HD2	1.84	0.77
1:C:112:PRO:O	1:C:113:VAL:HG12	1.84	0.77
1:A:93:SER:HB3	1:A:140:SER:HB3	1.65	0.77
1:A:439:TYR:HB3	1:B:220:PHE:CZ	2.20	0.77
1:C:156:LEU:HB2	1:C:294:LEU:HD13	1.65	0.77
1:A:315:CYS:SG	1:A:316:GLN:NE2	2.57	0.77
1:A:220:PHE:CE1	1:B:439:TYR:HB3	2.20	0.77
1:C:154:ILE:HA	1:C:157:PHE:CE2	2.19	0.77
1:C:348:THR:O	1:C:396:ASP:HB3	1.83	0.77
1:A:316:GLN:OE1	1:A:319:PHE:CD1	2.37	0.77
1:B:93:SER:HB3	1:B:140:SER:HB3	1.65	0.77
1:B:210:MET:HG3	1:B:211:LEU:HD13	1.64	0.77
1:A:348:THR:O	1:A:396:ASP:HB3	1.84	0.77
1:A:438:ALA:C	1:A:440:ALA:H	1.87	0.77
1:B:350:THR:HG22	1:B:396:ASP:OD2	1.84	0.77
1:A:476:GLU:O	1:A:479:VAL:HG23	1.85	0.77
1:A:20:ILE:CD1	1:A:96:VAL:HG21	2.15	0.76
1:A:478:GLY:O	1:A:486:ARG:HD2	1.84	0.76
1:B:438:ALA:C	1:B:440:ALA:H	1.88	0.76
1:C:441:ARG:CZ	1:D:221:GLY:O	2.33	0.76
1:D:26:GLY:HA2	1:D:88:CYS:SG	2.25	0.76
1:A:401:LEU:N	1:A:401:LEU:HD23	2.00	0.76
1:B:26:GLY:HA2	1:B:88:CYS:SG	2.25	0.76
1:C:68:PRO:O	1:C:72:ILE:HD13	1.86	0.76
1:D:350:THR:HG22	1:D:396:ASP:OD2	1.84	0.76
1:D:119:GLN:NE2	1:D:119:GLN:H	1.84	0.76
1:B:119:GLN:NE2	1:B:119:GLN:H	1.84	0.76
1:B:535:ILE:O	1:B:535:ILE:HD13	1.86	0.76
1:D:476:GLU:O	1:D:479:VAL:HG23	1.86	0.76
1:A:256:GLN:HA	1:A:299:LYS:HD3	1.68	0.76
1:A:351:TYR:CB	1:A:352:PRO:HD3	2.14	0.76
1:B:58:LYS:HB3	1:B:62:SER:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:ILE:O	1:C:535:ILE:HD13	1.86	0.76
1:C:316:GLN:OE1	1:C:319:PHE:HD1	1.69	0.76
1:B:68:PRO:O	1:B:72:ILE:HD13	1.86	0.75
1:C:470:LEU:CD1	1:C:470:LEU:H	1.98	0.75
1:C:58:LYS:HB3	1:C:62:SER:HB3	1.68	0.75
1:D:68:PRO:O	1:D:72:ILE:HD13	1.86	0.75
1:B:154:ILE:HA	1:B:157:PHE:CE2	2.19	0.75
1:C:218:LEU:HD23	1:D:416:ARG:NH1	2.02	0.75
1:C:238:ARG:NH2	1:D:98:MET:HB3	2.01	0.75
1:C:26:GLY:HA2	1:C:88:CYS:SG	2.25	0.75
1:A:58:LYS:HB3	1:A:62:SER:HB3	1.68	0.75
1:A:63:VAL:HG12	1:B:271:SER:HB2	1.66	0.75
1:C:48:LEU:HD12	1:D:292:ILE:HD12	1.67	0.75
1:C:281:ALA:CB	1:D:56:PHE:HB3	2.13	0.75
1:B:252:ASP:HB2	1:B:253:PRO:HD3	1.69	0.75
1:A:220:PHE:O	1:B:441:ARG:HD3	1.87	0.75
1:A:83:TYR:O	1:A:87:TYR:HB3	1.87	0.75
1:C:438:ALA:C	1:C:440:ALA:H	1.88	0.75
1:C:476:GLU:O	1:C:479:VAL:HG23	1.86	0.75
1:B:470:LEU:CD1	1:B:470:LEU:H	1.98	0.75
1:C:67:MET:HB3	1:C:68:PRO:HD3	1.69	0.75
1:D:470:LEU:CD1	1:D:470:LEU:H	1.98	0.75
1:D:58:LYS:HB3	1:D:62:SER:HB3	1.68	0.75
1:B:476:GLU:O	1:B:479:VAL:HG23	1.86	0.75
1:C:119:GLN:NE2	1:C:119:GLN:H	1.84	0.75
1:D:252:ASP:HB2	1:D:253:PRO:HD3	1.69	0.75
1:D:438:ALA:C	1:D:440:ALA:H	1.88	0.75
1:C:441:ARG:HA	1:C:441:ARG:HH11	1.52	0.74
1:D:316:GLN:OE1	1:D:319:PHE:HD1	1.69	0.74
1:B:134:GLN:HE22	1:B:310:ARG:HE	1.35	0.74
1:D:535:ILE:HD13	1:D:535:ILE:O	1.86	0.74
1:A:119:GLN:H	1:A:119:GLN:NE2	1.83	0.74
1:A:26:GLY:HA2	1:A:88:CYS:SG	2.27	0.74
1:B:114:ALA:HA	1:B:117:ASP:OD1	1.88	0.74
1:B:174:LEU:HD21	1:B:261:LEU:HD22	1.70	0.74
1:B:256:GLN:HA	1:B:299:LYS:HD3	1.70	0.74
1:A:114:ALA:HA	1:A:117:ASP:OD1	1.87	0.74
1:A:16:LEU:HD12	1:A:315:CYS:SG	2.26	0.74
1:A:213:GLY:O	1:A:217:VAL:HG23	1.88	0.74
1:B:67:MET:HB3	1:B:68:PRO:HD3	1.69	0.74
1:C:83:TYR:O	1:C:87:TYR:HB3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ALA:HA	1:C:117:ASP:OD1	1.88	0.74
1:B:20:ILE:CD1	1:B:96:VAL:HG21	2.17	0.74
1:B:316:GLN:OE1	1:B:319:PHE:HD1	1.69	0.74
1:B:390:THR:HG22	1:B:419:VAL:HG11	1.70	0.74
1:C:20:ILE:CD1	1:C:96:VAL:HG21	2.17	0.74
1:C:252:ASP:HB2	1:C:253:PRO:HD3	1.69	0.74
1:D:114:ALA:HA	1:D:117:ASP:OD1	1.88	0.74
1:D:134:GLN:HE22	1:D:310:ARG:HE	1.35	0.74
1:A:390:THR:HG22	1:A:419:VAL:HG11	1.70	0.73
1:A:441:ARG:NE	1:B:221:GLY:HA3	2.03	0.73
1:B:74:LEU:HD22	1:B:75:MET:HE2	1.69	0.73
1:C:97:VAL:HB	1:C:136:ALA:HB2	1.69	0.73
1:D:20:ILE:CD1	1:D:96:VAL:HG21	2.17	0.73
1:C:221:GLY:O	1:D:441:ARG:CZ	2.37	0.73
1:B:83:TYR:O	1:B:87:TYR:HB3	1.88	0.73
1:C:441:ARG:HD3	1:D:220:PHE:O	1.87	0.73
1:B:380:SER:OG	1:B:551:VAL:HG22	1.89	0.73
1:B:97:VAL:HB	1:B:136:ALA:HB2	1.69	0.73
1:D:97:VAL:HB	1:D:136:ALA:HB2	1.69	0.73
1:D:401:LEU:N	1:D:401:LEU:HD23	2.04	0.73
1:D:83:TYR:O	1:D:87:TYR:HB3	1.88	0.73
1:A:344:PHE:CD1	1:A:400:ILE:HG12	2.22	0.73
1:A:271:SER:HB2	1:B:63:VAL:HG12	1.70	0.73
1:C:11:GLN:N	1:C:14:ARG:CB	2.52	0.73
1:C:134:GLN:HE22	1:C:310:ARG:HE	1.35	0.73
1:D:256:GLN:HA	1:D:299:LYS:HD3	1.70	0.73
1:D:390:THR:HG22	1:D:419:VAL:HG11	1.70	0.73
1:B:441:ARG:HH11	1:B:441:ARG:HA	1.52	0.73
1:A:134:GLN:HE22	1:A:310:ARG:HE	1.34	0.73
1:B:401:LEU:HD23	1:B:401:LEU:N	2.04	0.73
1:A:447:ARG:HD2	1:A:450:ILE:HD11	1.71	0.72
1:A:380:SER:OG	1:A:551:VAL:HG22	1.89	0.72
1:C:401:LEU:HD23	1:C:401:LEU:N	2.04	0.72
1:D:67:MET:HB3	1:D:68:PRO:HD3	1.69	0.72
1:A:401:LEU:H	1:A:401:LEU:HD23	1.55	0.72
1:B:213:GLY:O	1:B:217:VAL:HG23	1.89	0.72
1:C:447:ARG:HD2	1:C:450:ILE:HD11	1.71	0.72
1:D:174:LEU:HD21	1:D:261:LEU:HD22	1.70	0.72
1:B:113:VAL:HG13	1:B:114:ALA:N	2.04	0.72
1:C:213:GLY:O	1:C:217:VAL:HG23	1.89	0.72
1:C:380:SER:OG	1:C:551:VAL:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ARG:CZ	1:D:218:LEU:HD23	2.20	0.72
1:B:11:GLN:CG	1:B:12:THR:H	1.96	0.72
1:C:390:THR:HG22	1:C:419:VAL:HG11	1.70	0.72
1:D:213:GLY:O	1:D:217:VAL:HG23	1.89	0.72
1:A:174:LEU:HD21	1:A:261:LEU:HD22	1.71	0.72
1:A:441:ARG:HA	1:A:441:ARG:HH11	1.54	0.72
1:A:535:ILE:HD13	1:A:535:ILE:O	1.89	0.72
1:A:97:VAL:HB	1:A:136:ALA:HB2	1.70	0.72
1:C:416:ARG:NH1	1:D:218:LEU:HD23	2.04	0.72
1:B:447:ARG:HD2	1:B:450:ILE:HD11	1.71	0.72
1:D:113:VAL:HG13	1:D:114:ALA:N	2.04	0.72
1:D:11:GLN:N	1:D:14:ARG:CB	2.52	0.72
1:D:566:LEU:HD21	1:D:576:HIS:CD2	2.25	0.72
1:C:256:GLN:HA	1:C:299:LYS:HD3	1.70	0.71
1:D:441:ARG:HH11	1:D:441:ARG:HA	1.53	0.71
1:D:380:SER:OG	1:D:551:VAL:HG22	1.89	0.71
1:C:174:LEU:HD21	1:C:261:LEU:HD22	1.70	0.71
1:A:113:VAL:HG13	1:A:114:ALA:N	2.05	0.71
1:A:91:TRP:HA	1:B:242:MET:HE3	1.71	0.71
1:C:344:PHE:CD1	1:C:400:ILE:HG12	2.25	0.71
1:A:98:MET:SD	1:A:101:ARG:HD3	2.30	0.71
1:C:116:PHE:CE1	1:D:211:LEU:HD12	2.25	0.71
1:A:178:VAL:HA	1:A:258:ILE:HD13	1.71	0.71
1:A:566:LEU:HD21	1:A:576:HIS:CD2	2.26	0.71
1:B:103:ARG:HG2	1:B:322:LEU:HD11	1.73	0.71
1:B:344:PHE:CD1	1:B:400:ILE:HG12	2.25	0.71
1:C:103:ARG:HG2	1:C:322:LEU:HD11	1.73	0.71
1:D:447:ARG:HD2	1:D:450:ILE:HD11	1.71	0.71
1:A:103:ARG:HG2	1:A:322:LEU:HD11	1.73	0.71
1:A:221:GLY:O	1:B:441:ARG:NH1	2.24	0.71
1:B:11:GLN:N	1:B:14:ARG:CB	2.52	0.71
1:B:566:LEU:HD21	1:B:576:HIS:CD2	2.25	0.71
1:A:252:ASP:HB2	1:A:253:PRO:HD3	1.71	0.70
1:A:382:LYS:HB2	2:A:5001:ANP:O1B	1.91	0.70
1:A:68:PRO:O	1:A:72:ILE:HD13	1.90	0.70
1:A:74:LEU:HD13	1:B:260:SER:OG	1.90	0.70
1:C:354:ARG:O	1:C:355:GLU:HG3	1.91	0.70
1:C:44:MET:O	1:C:48:LEU:HD23	1.91	0.70
1:A:212:LYS:HE3	1:B:212:LYS:HE3	1.74	0.70
1:B:354:ARG:O	1:B:355:GLU:HG3	1.91	0.70
1:D:103:ARG:HG2	1:D:322:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:ARG:O	1:D:355:GLU:HG3	1.91	0.70
1:D:344:PHE:CD1	1:D:400:ILE:HG12	2.25	0.70
1:D:44:MET:O	1:D:48:LEU:HD23	1.91	0.70
1:A:381:GLY:O	1:A:385:ILE:HG22	1.91	0.70
1:A:385:ILE:O	1:A:389:ILE:HD12	1.91	0.70
1:A:67:MET:HB3	1:A:68:PRO:HD3	1.73	0.70
1:B:351:TYR:HB3	1:B:352:PRO:CD	2.20	0.70
1:D:343:GLU:HG2	1:D:365:LYS:HG3	1.72	0.70
1:A:337:ARG:HD2	1:A:338:ALA:H	1.56	0.70
1:A:89:ILE:HD12	1:A:144:ILE:HG21	1.73	0.70
1:C:113:VAL:HG13	1:C:114:ALA:N	2.04	0.70
1:C:343:GLU:HG2	1:C:365:LYS:HG3	1.72	0.70
1:A:391:ARG:O	1:A:393:TYR:N	2.24	0.70
1:A:446:SER:HB2	1:A:449:GLN:OE1	1.91	0.70
1:C:566:LEU:HD21	1:C:576:HIS:CD2	2.25	0.70
1:D:74:LEU:HD22	1:D:75:MET:HE2	1.73	0.70
1:B:98:MET:SD	1:B:101:ARG:HD3	2.32	0.70
1:B:343:GLU:HG2	1:B:365:LYS:HG3	1.72	0.70
1:C:446:SER:HB2	1:C:449:GLN:OE1	1.92	0.70
1:A:445:TYR:CD2	1:A:496:LEU:HD11	2.26	0.70
1:D:446:SER:HB2	1:D:449:GLN:OE1	1.92	0.70
1:A:223:GLN:N	1:A:223:GLN:OE1	2.21	0.70
1:A:440:ALA:HB1	1:A:497:ARG:HG3	1.72	0.70
1:A:221:GLY:O	1:B:441:ARG:CZ	2.40	0.70
1:C:58:LYS:HA	1:C:58:LYS:HZ3	1.57	0.70
1:D:98:MET:SD	1:D:101:ARG:HD3	2.32	0.70
1:B:446:SER:HB2	1:B:449:GLN:OE1	1.92	0.69
1:C:14:ARG:O	1:C:18:PRO:HD3	1.93	0.69
1:A:343:GLU:HG2	1:A:365:LYS:HG3	1.73	0.69
1:B:44:MET:O	1:B:48:LEU:HD23	1.91	0.69
1:C:188:ARG:O	1:C:192:ILE:HG12	1.93	0.69
1:C:337:ARG:HD2	1:C:338:ALA:H	1.57	0.69
1:D:316:GLN:OE1	1:D:319:PHE:CD1	2.46	0.69
1:B:188:ARG:O	1:B:192:ILE:HG12	1.93	0.69
1:C:98:MET:SD	1:C:101:ARG:HD3	2.32	0.69
1:C:91:TRP:HA	1:D:242:MET:CE	2.22	0.69
1:D:440:ALA:HB1	1:D:497:ARG:HG3	1.74	0.69
1:B:14:ARG:O	1:B:18:PRO:HD3	1.93	0.69
1:C:391:ARG:O	1:C:393:TYR:N	2.26	0.69
1:D:178:VAL:HA	1:D:258:ILE:HD13	1.75	0.69
1:A:89:ILE:O	1:A:92:VAL:HG12	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:MET:SD	1:D:109:MET:HB3	2.32	0.69
1:C:178:VAL:HA	1:C:258:ILE:HD13	1.75	0.69
1:B:337:ARG:HD2	1:B:338:ALA:H	1.57	0.69
1:D:401:LEU:H	1:D:401:LEU:HD23	1.58	0.69
1:B:97:VAL:HG13	1:B:98:MET:H	1.58	0.69
1:D:188:ARG:O	1:D:192:ILE:HG12	1.93	0.69
1:C:98:MET:HB3	1:D:238:ARG:NH2	2.08	0.69
1:D:97:VAL:HG13	1:D:98:MET:H	1.58	0.69
1:B:391:ARG:O	1:B:393:TYR:N	2.26	0.69
1:A:218:LEU:HD23	1:B:416:ARG:NH1	2.08	0.69
1:A:351:TYR:HB3	1:A:352:PRO:CD	2.21	0.69
1:C:460:MET:HE2	1:C:460:MET:HA	1.74	0.69
1:A:354:ARG:O	1:A:355:GLU:HG3	1.92	0.68
1:A:48:LEU:HD12	1:B:292:ILE:HD12	1.76	0.68
1:B:315:CYS:SG	1:B:316:GLN:NE2	2.66	0.68
1:B:316:GLN:OE1	1:B:319:PHE:CD1	2.46	0.68
1:B:401:LEU:HD23	1:B:401:LEU:H	1.58	0.68
1:B:505:ASP:HA	1:B:535:ILE:CG2	2.23	0.68
1:D:315:CYS:SG	1:D:316:GLN:NE2	2.66	0.68
1:A:256:GLN:HG2	1:A:299:LYS:CE	2.23	0.68
1:C:385:ILE:O	1:C:389:ILE:HD12	1.94	0.68
1:D:385:ILE:O	1:D:389:ILE:HD12	1.93	0.68
1:A:188:ARG:O	1:A:192:ILE:HG12	1.93	0.68
1:B:385:ILE:O	1:B:389:ILE:HD12	1.94	0.68
1:C:316:GLN:OE1	1:C:319:PHE:CD1	2.46	0.68
1:D:351:TYR:HB3	1:D:352:PRO:CD	2.20	0.68
1:A:366:ILE:HG12	1:A:372:VAL:HG21	1.75	0.68
1:B:433:VAL:HB	1:B:470:LEU:HA	1.76	0.68
1:B:467:ASP:O	1:B:468:ASN:HB2	1.94	0.68
1:C:218:LEU:HD23	1:D:416:ARG:CZ	2.23	0.68
1:C:433:VAL:HB	1:C:470:LEU:HA	1.76	0.68
1:D:391:ARG:O	1:D:393:TYR:N	2.26	0.68
1:D:433:VAL:HB	1:D:470:LEU:HA	1.76	0.68
1:A:119:GLN:N	1:A:119:GLN:HE21	1.90	0.68
1:A:316:GLN:HA	1:A:319:PHE:HB2	1.76	0.68
1:B:366:ILE:HG12	1:B:372:VAL:HG21	1.75	0.68
1:C:441:ARG:NH1	1:D:221:GLY:O	2.26	0.68
1:D:381:GLY:O	1:D:385:ILE:HG22	1.94	0.68
1:A:44:MET:O	1:A:48:LEU:HD23	1.93	0.68
1:C:467:ASP:O	1:C:468:ASN:HB2	1.93	0.68
1:D:14:ARG:O	1:D:18:PRO:HD3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CZ	1:B:429:PHE:CE1	2.76	0.68
1:C:315:CYS:SG	1:C:316:GLN:NE2	2.66	0.68
1:A:467:ASP:O	1:A:468:ASN:HB2	1.92	0.68
1:B:381:GLY:O	1:B:385:ILE:HG22	1.94	0.68
1:D:119:GLN:N	1:D:119:GLN:HE21	1.92	0.68
1:D:11:GLN:O	1:D:14:ARG:HB3	1.94	0.68
1:D:383:SER:HB2	2:D:5004:ANP:O1A	1.94	0.68
1:A:435:ASN:HA	1:A:438:ALA:HB3	1.76	0.68
1:A:460:MET:HE2	1:A:460:MET:HA	1.76	0.68
1:B:316:GLN:HA	1:B:319:PHE:HB2	1.75	0.68
1:B:440:ALA:HB1	1:B:497:ARG:HG3	1.74	0.68
1:B:89:ILE:O	1:B:92:VAL:HG12	1.94	0.68
1:C:344:PHE:CB	1:C:400:ILE:HA	2.24	0.68
1:A:433:VAL:HB	1:A:470:LEU:HA	1.76	0.68
1:C:440:ALA:HB1	1:C:497:ARG:HG3	1.74	0.68
1:D:344:PHE:CB	1:D:400:ILE:HA	2.24	0.68
1:A:11:GLN:CG	1:A:12:THR:H	1.92	0.67
1:A:505:ASP:HA	1:A:535:ILE:CG2	2.24	0.67
1:C:89:ILE:HD12	1:C:144:ILE:HG21	1.77	0.67
1:C:159:MET:O	1:C:163:TYR:HB3	1.94	0.67
1:C:366:ILE:HG12	1:C:372:VAL:HG21	1.75	0.67
1:C:67:MET:HA	1:D:267:LEU:HD22	1.76	0.67
1:A:159:MET:O	1:A:163:TYR:HB3	1.94	0.67
1:A:83:TYR:HA	1:B:249:SER:OG	1.94	0.67
1:B:178:VAL:HA	1:B:258:ILE:HD13	1.75	0.67
1:D:159:MET:O	1:D:163:TYR:HB3	1.94	0.67
1:D:316:GLN:HA	1:D:319:PHE:HB2	1.75	0.67
1:B:119:GLN:HE21	1:B:119:GLN:N	1.92	0.67
1:B:344:PHE:CB	1:B:400:ILE:HA	2.24	0.67
1:C:11:GLN:O	1:C:14:ARG:HB3	1.94	0.67
1:C:449:GLN:HB3	1:C:496:LEU:HD13	1.76	0.67
1:D:337:ARG:HD2	1:D:338:ALA:H	1.57	0.67
1:A:11:GLN:O	1:A:14:ARG:HB3	1.93	0.67
1:D:89:ILE:HD12	1:D:144:ILE:HG21	1.77	0.67
1:D:89:ILE:O	1:D:92:VAL:HG12	1.94	0.67
1:B:89:ILE:HD12	1:B:144:ILE:HG21	1.77	0.67
1:C:441:ARG:CD	1:D:221:GLY:CA	2.53	0.67
1:A:256:GLN:HG2	1:A:299:LYS:HE2	1.74	0.67
1:C:401:LEU:H	1:C:401:LEU:HD23	1.58	0.67
1:C:89:ILE:O	1:C:92:VAL:HG12	1.94	0.67
1:C:97:VAL:HG13	1:C:98:MET:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:ASP:HA	1:D:535:ILE:CG2	2.23	0.67
1:B:159:MET:O	1:B:163:TYR:HB3	1.94	0.67
1:B:165:TRP:O	1:B:169:ILE:HG13	1.95	0.67
1:C:165:TRP:O	1:C:169:ILE:HG13	1.95	0.67
1:C:505:ASP:HA	1:C:535:ILE:CG2	2.23	0.67
1:C:221:GLY:CA	1:D:441:ARG:CD	2.60	0.67
1:D:445:TYR:CD2	1:D:496:LEU:HD11	2.30	0.67
1:C:256:GLN:HG2	1:C:299:LYS:CE	2.25	0.67
1:D:366:ILE:HG12	1:D:372:VAL:HG21	1.75	0.67
1:B:11:GLN:O	1:B:14:ARG:HB3	1.94	0.67
1:C:267:LEU:HD22	1:D:67:MET:HA	1.77	0.67
1:C:382:LYS:HB2	2:C:5003:ANP:O1B	1.95	0.67
1:A:344:PHE:CB	1:A:400:ILE:HA	2.25	0.66
1:B:445:TYR:CD2	1:B:496:LEU:HD11	2.30	0.66
1:D:467:ASP:O	1:D:468:ASN:HB2	1.94	0.66
1:A:63:VAL:CG1	1:B:271:SER:HB2	2.24	0.66
1:C:119:GLN:HE21	1:C:119:GLN:N	1.92	0.66
1:C:381:GLY:O	1:C:385:ILE:HG22	1.94	0.66
1:C:109:MET:HB3	1:D:210:MET:SD	2.35	0.66
1:A:271:SER:HB2	1:B:63:VAL:CG1	2.25	0.66
1:C:238:ARG:CZ	1:D:98:MET:HB3	2.25	0.66
1:D:256:GLN:HG2	1:D:299:LYS:CE	2.25	0.66
1:D:435:ASN:HA	1:D:438:ALA:HB3	1.77	0.66
1:A:74:LEU:HD22	1:A:75:MET:CE	2.25	0.66
1:B:256:GLN:HG2	1:B:299:LYS:CE	2.25	0.66
1:A:14:ARG:O	1:A:18:PRO:HD3	1.96	0.66
1:A:269:ALA:O	1:A:273:PRO:HB2	1.96	0.66
1:A:97:VAL:HG13	1:A:98:MET:H	1.59	0.66
1:C:316:GLN:HA	1:C:319:PHE:HB2	1.75	0.66
1:C:56:PHE:HA	1:C:59:THR:CG2	2.26	0.66
1:A:439:TYR:HB3	1:B:220:PHE:CE1	2.30	0.66
1:C:223:GLN:OE1	1:C:223:GLN:N	2.25	0.66
1:C:445:TYR:CD2	1:C:496:LEU:HD11	2.29	0.66
1:D:449:GLN:HB3	1:D:496:LEU:HD13	1.76	0.66
1:A:440:ALA:HB1	1:A:497:ARG:CG	2.26	0.66
1:C:344:PHE:HB3	1:C:400:ILE:HA	1.78	0.66
1:D:223:GLN:N	1:D:223:GLN:OE1	2.25	0.66
1:C:56:PHE:CB	1:D:281:ALA:HB2	2.16	0.66
1:A:109:MET:HB3	1:B:210:MET:SD	2.36	0.66
1:B:435:ASN:HA	1:B:438:ALA:HB3	1.77	0.66
1:D:165:TRP:O	1:D:169:ILE:HG13	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ALA:O	1:C:211:LEU:HD22	1.95	0.66
1:D:256:GLN:HG2	1:D:299:LYS:HE2	1.78	0.66
1:A:165:TRP:O	1:A:169:ILE:HG13	1.97	0.65
1:A:85:SER:O	1:A:89:ILE:HG22	1.95	0.65
1:B:449:GLN:HB3	1:B:496:LEU:HD13	1.76	0.65
1:C:115:PHE:HB2	1:C:327:GLU:OE1	1.97	0.65
1:C:435:ASN:HA	1:C:438:ALA:HB3	1.77	0.65
1:A:322:LEU:O	1:A:322:LEU:HD23	1.96	0.65
1:B:141:GLY:O	1:B:144:ILE:HG12	1.97	0.65
1:D:56:PHE:HA	1:D:59:THR:CG2	2.26	0.65
1:A:242:MET:HE1	1:B:91:TRP:HA	1.78	0.65
1:A:416:ARG:NH1	1:B:218:LEU:HD23	2.11	0.65
1:C:256:GLN:HG2	1:C:299:LYS:HE2	1.78	0.65
1:D:207:ALA:O	1:D:211:LEU:HD22	1.95	0.65
1:A:58:LYS:HZ1	1:A:61:ARG:HD3	1.61	0.65
1:B:570:GLY:O	1:B:572:TYR:N	2.28	0.65
1:B:85:SER:O	1:B:89:ILE:HG22	1.96	0.65
1:D:141:GLY:O	1:D:144:ILE:HG12	1.97	0.65
1:D:216:GLU:O	1:D:220:PHE:HB2	1.97	0.65
1:A:10:TRP:C	1:A:14:ARG:CB	2.63	0.65
1:A:449:GLN:HB3	1:A:496:LEU:HD13	1.78	0.65
1:A:512:ASP:HB2	1:B:378:SER:H	1.62	0.65
1:A:115:PHE:HB2	1:A:327:GLU:OE1	1.96	0.65
1:B:216:GLU:O	1:B:220:PHE:HB2	1.97	0.65
1:A:91:TRP:HA	1:B:242:MET:HE1	1.75	0.65
1:B:115:PHE:HB2	1:B:327:GLU:OE1	1.97	0.65
1:B:56:PHE:HA	1:B:59:THR:CG2	2.26	0.65
1:D:224:GLU:OE2	1:D:225:VAL:HG23	1.97	0.65
1:A:141:GLY:O	1:A:144:ILE:HG12	1.96	0.65
1:A:207:ALA:O	1:A:211:LEU:HD22	1.96	0.65
1:C:269:ALA:O	1:C:273:PRO:HB2	1.96	0.65
1:C:351:TYR:HB3	1:C:352:PRO:CD	2.20	0.65
1:D:322:LEU:O	1:D:322:LEU:HD23	1.97	0.65
1:A:29:VAL:HG11	1:A:87:TYR:HE2	1.62	0.65
1:B:207:ALA:O	1:B:211:LEU:HD22	1.95	0.65
1:B:256:GLN:HG2	1:B:299:LYS:HE2	1.78	0.65
1:C:216:GLU:O	1:C:220:PHE:HB2	1.97	0.65
1:C:64:LEU:HB2	1:D:271:SER:OG	1.97	0.65
1:D:455:ARG:C	1:D:457:ALA:H	2.00	0.65
1:B:368:ALA:HA	1:B:531:THR:OG1	1.97	0.65
1:C:141:GLY:O	1:C:144:ILE:HG12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ALA:O	1:A:340:GLY:N	2.28	0.65
1:A:570:GLY:O	1:A:572:TYR:N	2.28	0.65
1:C:322:LEU:HD23	1:C:322:LEU:O	1.97	0.64
1:A:362:ILE:CD1	1:A:556:ILE:H	2.09	0.64
1:B:29:VAL:HG11	1:B:87:TYR:HE2	1.62	0.64
1:C:211:LEU:HD12	1:D:116:PHE:CE1	2.30	0.64
1:C:455:ARG:C	1:C:457:ALA:H	2.00	0.64
1:C:29:VAL:HG11	1:C:87:TYR:HE2	1.62	0.64
1:D:115:PHE:HB2	1:D:327:GLU:OE1	1.97	0.64
1:D:85:SER:O	1:D:89:ILE:HG22	1.96	0.64
1:A:56:PHE:HA	1:A:59:THR:CG2	2.26	0.64
1:B:269:ALA:O	1:B:273:PRO:HB2	1.96	0.64
1:C:85:SER:O	1:C:89:ILE:HG22	1.96	0.64
1:D:58:LYS:HZ1	1:D:61:ARG:HD3	1.62	0.64
1:D:74:LEU:HD22	1:D:75:MET:CE	2.27	0.64
1:C:224:GLU:OE2	1:C:225:VAL:HG23	1.97	0.64
1:C:74:LEU:HD22	1:C:75:MET:CE	2.27	0.64
1:C:97:VAL:HG13	1:C:98:MET:N	2.12	0.64
1:D:368:ALA:HA	1:D:531:THR:OG1	1.97	0.64
1:A:156:LEU:CB	1:A:294:LEU:HD13	2.27	0.64
1:A:475:GLY:N	1:A:480:LEU:CD1	2.61	0.64
1:C:138:SER:O	1:C:142:ALA:HB3	1.98	0.64
1:B:351:TYR:CB	1:B:352:PRO:CD	2.75	0.64
1:C:351:TYR:CB	1:C:352:PRO:CD	2.75	0.64
1:C:56:PHE:HB3	1:D:281:ALA:CB	2.17	0.64
1:C:570:GLY:O	1:C:572:TYR:N	2.28	0.64
1:A:185:VAL:HG11	1:A:251:SER:OG	1.97	0.64
1:C:98:MET:HB3	1:D:238:ARG:CZ	2.28	0.64
1:D:29:VAL:HG11	1:D:87:TYR:HE2	1.62	0.64
1:C:220:PHE:CE1	1:D:439:TYR:HB3	2.32	0.64
1:A:110:GLY:C	1:A:112:PRO:HD3	2.18	0.64
1:A:15:ARG:O	1:A:18:PRO:HD2	1.97	0.64
1:A:378:SER:H	1:B:512:ASP:HB2	1.63	0.64
1:A:116:PHE:CE1	1:B:211:LEU:HD12	2.27	0.64
1:B:455:ARG:C	1:B:457:ALA:H	2.00	0.64
1:B:74:LEU:HD22	1:B:75:MET:CE	2.27	0.64
1:D:344:PHE:HB3	1:D:400:ILE:HA	1.78	0.64
1:C:221:GLY:O	1:D:441:ARG:NH1	2.30	0.64
1:D:58:LYS:HZ3	1:D:58:LYS:HA	1.62	0.64
1:A:218:LEU:HD23	1:B:416:ARG:CZ	2.28	0.64
1:A:429:PHE:CE1	1:B:220:PHE:CZ	2.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:HG13	1:B:98:MET:N	2.12	0.64
1:A:10:TRP:C	1:A:14:ARG:HB3	2.18	0.64
1:A:455:ARG:C	1:A:457:ALA:H	1.99	0.64
1:B:138:SER:O	1:B:142:ALA:HB3	1.98	0.64
1:B:224:GLU:OE2	1:B:225:VAL:HG23	1.97	0.64
1:B:438:ALA:O	1:B:443:GLU:HA	1.98	0.64
1:C:368:ALA:HA	1:C:531:THR:OG1	1.97	0.64
1:D:97:VAL:HG13	1:D:98:MET:N	2.12	0.64
1:A:234:SER:O	1:A:237:MET:HB3	1.98	0.63
1:C:58:LYS:HZ1	1:C:61:ARG:HD3	1.62	0.63
1:D:269:ALA:O	1:D:273:PRO:HB2	1.96	0.63
1:A:441:ARG:CZ	1:B:221:GLY:O	2.46	0.63
1:B:110:GLY:C	1:B:112:PRO:HD3	2.19	0.63
1:D:351:TYR:CB	1:D:352:PRO:CD	2.75	0.63
1:D:440:ALA:HB1	1:D:497:ARG:CG	2.28	0.63
1:A:505:ASP:OD2	1:A:535:ILE:HD12	1.99	0.63
1:B:322:LEU:O	1:B:322:LEU:HD23	1.97	0.63
1:B:460:MET:HA	1:B:460:MET:HE2	1.80	0.63
1:C:439:TYR:HB3	1:D:220:PHE:CE1	2.33	0.63
1:A:236:LYS:O	1:A:240:GLN:HB2	1.99	0.63
1:A:374:LEU:HD23	1:A:533:LEU:HD21	1.80	0.63
1:B:344:PHE:HB3	1:B:400:ILE:HA	1.78	0.63
1:C:110:GLY:C	1:C:112:PRO:HD3	2.19	0.63
1:A:380:SER:O	2:A:5001:ANP:O2A	2.17	0.63
1:C:156:LEU:CB	1:C:294:LEU:HD13	2.29	0.63
1:D:138:SER:O	1:D:142:ALA:HB3	1.98	0.63
1:A:224:GLU:OE2	1:A:225:VAL:HG23	1.98	0.63
1:C:383:SER:HB2	2:C:5003:ANP:O1A	1.98	0.63
1:A:566:LEU:HD21	1:A:576:HIS:HD2	1.64	0.63
1:A:351:TYR:CB	1:A:352:PRO:CD	2.77	0.63
1:A:383:SER:OG	2:A:5001:ANP:O2B	2.10	0.63
1:A:20:ILE:HD13	1:A:96:VAL:CG2	2.29	0.63
1:D:110:GLY:C	1:D:112:PRO:HD3	2.19	0.63
1:A:344:PHE:HB3	1:A:400:ILE:HA	1.80	0.62
1:A:97:VAL:HG13	1:A:98:MET:N	2.13	0.62
1:D:192:ILE:CG2	1:D:244:MET:HB2	2.29	0.62
1:D:236:LYS:O	1:D:240:GLN:HB2	1.99	0.62
1:C:67:MET:HB2	1:D:267:LEU:HB3	1.81	0.62
1:D:438:ALA:O	1:D:443:GLU:HA	1.98	0.62
1:A:150:GLY:O	1:A:154:ILE:HG13	1.99	0.62
1:A:211:LEU:HD12	1:B:116:PHE:CE1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLN:C	1:B:328:LYS:H	2.03	0.62
1:B:338:ALA:O	1:B:340:GLY:N	2.32	0.62
1:B:156:LEU:CB	1:B:294:LEU:HD13	2.29	0.62
1:C:236:LYS:O	1:C:240:GLN:HB2	1.99	0.62
1:B:192:ILE:CG2	1:B:244:MET:HB2	2.29	0.62
1:C:440:ALA:HB1	1:C:497:ARG:CG	2.28	0.62
1:C:438:ALA:O	1:C:443:GLU:HA	1.99	0.62
1:A:326:GLN:C	1:A:328:LYS:H	2.02	0.62
1:A:368:ALA:HA	1:A:531:THR:OG1	1.98	0.62
1:B:374:LEU:HD23	1:B:533:LEU:HD21	1.80	0.62
1:D:156:LEU:CB	1:D:294:LEU:HD13	2.28	0.62
1:D:338:ALA:O	1:D:340:GLY:N	2.32	0.62
1:C:512:ASP:HB2	1:D:378:SER:CB	2.30	0.62
1:A:58:LYS:HZ3	1:A:58:LYS:HA	1.65	0.62
1:D:570:GLY:O	1:D:572:TYR:N	2.28	0.62
1:A:216:GLU:O	1:A:220:PHE:HB2	2.00	0.62
1:A:83:TYR:O	1:A:87:TYR:CB	2.48	0.62
1:B:185:VAL:HG11	1:B:251:SER:OG	2.00	0.62
1:A:63:VAL:HG11	1:B:271:SER:N	2.13	0.62
1:C:271:SER:OG	1:D:64:LEU:HB2	1.99	0.62
1:A:192:ILE:CG2	1:A:244:MET:HB2	2.30	0.62
1:A:291:MET:HE2	1:A:291:MET:HA	1.82	0.62
1:A:438:ALA:O	1:A:443:GLU:HA	1.99	0.62
1:C:374:LEU:HD23	1:C:533:LEU:HD21	1.80	0.62
1:D:333:ARG:HB3	1:D:333:ARG:NH1	2.15	0.62
1:B:236:LYS:O	1:B:240:GLN:HB2	1.99	0.61
1:C:338:ALA:O	1:C:340:GLY:N	2.31	0.61
1:D:460:MET:HA	1:D:460:MET:HE2	1.82	0.61
1:D:566:LEU:HD21	1:D:576:HIS:HD2	1.64	0.61
1:C:249:SER:OG	1:D:83:TYR:HA	2.00	0.61
1:B:15:ARG:O	1:B:18:PRO:HD2	2.00	0.61
1:B:440:ALA:HB1	1:B:497:ARG:CG	2.29	0.61
1:C:566:LEU:HD21	1:C:576:HIS:HD2	1.64	0.61
1:D:216:GLU:C	1:D:220:PHE:HB2	2.20	0.61
1:D:326:GLN:C	1:D:328:LYS:H	2.03	0.61
1:D:374:LEU:HD23	1:D:533:LEU:HD21	1.80	0.61
1:A:383:SER:HB2	2:A:5001:ANP:O1A	2.00	0.61
1:C:192:ILE:CG2	1:C:244:MET:HB2	2.29	0.61
1:C:267:LEU:HB3	1:D:67:MET:HB2	1.82	0.61
1:C:326:GLN:C	1:C:328:LYS:H	2.03	0.61
1:B:144:ILE:HG13	1:B:145:THR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLU:C	1:B:220:PHE:HB2	2.20	0.61
1:B:333:ARG:HB3	1:B:333:ARG:NH1	2.15	0.61
1:B:59:THR:HA	1:B:63:VAL:HG21	1.82	0.61
1:C:164:SER:OG	1:C:167:LEU:HD23	2.00	0.61
1:C:216:GLU:C	1:C:220:PHE:HB2	2.20	0.61
1:D:144:ILE:HG13	1:D:145:THR:N	2.15	0.61
1:A:213:GLY:HA2	1:B:427:HIS:HD2	1.66	0.61
1:C:185:VAL:HG11	1:C:251:SER:OG	1.99	0.61
1:A:144:ILE:HG13	1:A:145:THR:N	2.15	0.61
1:A:508:THR:HA	1:A:511:LEU:HD12	1.83	0.61
1:B:196:MET:HA	1:B:240:GLN:HG2	1.83	0.61
1:B:548:ILE:HB	1:B:565:LEU:HD11	1.82	0.61
1:C:150:GLY:O	1:C:154:ILE:HG13	2.01	0.61
1:A:138:SER:O	1:A:142:ALA:HB3	2.00	0.61
1:A:164:SER:OG	1:A:167:LEU:HD23	2.00	0.61
1:A:216:GLU:C	1:A:220:PHE:HB2	2.21	0.61
1:C:15:ARG:O	1:C:18:PRO:HD2	2.00	0.61
1:D:164:SER:OG	1:D:167:LEU:HD23	2.00	0.61
1:D:185:VAL:HG11	1:D:251:SER:OG	2.00	0.61
1:A:557:VAL:O	1:A:557:VAL:HG12	2.00	0.61
1:B:164:SER:OG	1:B:167:LEU:HD23	2.00	0.61
1:B:223:GLN:OE1	1:B:223:GLN:N	2.25	0.61
1:A:131:ASP:HB3	1:A:318:LEU:HD23	1.83	0.61
1:A:341:ASP:HB3	1:A:403:ASP:OD1	2.01	0.61
1:C:333:ARG:HB3	1:C:333:ARG:NH1	2.15	0.61
1:C:212:LYS:HE3	1:D:212:LYS:HE3	1.83	0.60
1:D:150:GLY:O	1:D:154:ILE:HG13	2.00	0.60
1:D:15:ARG:O	1:D:18:PRO:HD2	2.00	0.60
1:A:333:ARG:NH1	1:A:333:ARG:HB3	2.16	0.60
1:A:416:ARG:CZ	1:B:218:LEU:HD23	2.30	0.60
1:C:508:THR:HA	1:C:511:LEU:HD12	1.83	0.60
1:B:150:GLY:O	1:B:154:ILE:HG13	2.01	0.60
1:B:234:SER:O	1:B:237:MET:HB3	2.01	0.60
1:C:196:MET:HA	1:C:240:GLN:HG2	1.83	0.60
1:D:59:THR:HA	1:D:63:VAL:HG21	1.83	0.60
1:A:548:ILE:HB	1:A:565:LEU:HD11	1.83	0.60
1:B:482:SER:HB3	1:B:485:GLN:HG3	1.84	0.60
1:B:505:ASP:OD2	1:B:535:ILE:HD12	2.02	0.60
1:A:196:MET:HA	1:A:240:GLN:HG2	1.84	0.60
1:A:105:PHE:CZ	1:B:210:MET:HE3	2.37	0.60
1:B:566:LEU:HD21	1:B:576:HIS:HD2	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ILE:HG13	1:C:145:THR:N	2.15	0.60
1:A:284:ILE:O	1:A:284:ILE:CD1	2.49	0.60
1:B:333:ARG:HB3	1:B:333:ARG:HH11	1.67	0.60
1:C:172:VAL:O	1:C:172:VAL:HG12	2.02	0.60
1:C:548:ILE:HB	1:C:565:LEU:HD11	1.83	0.60
1:D:234:SER:O	1:D:237:MET:HB3	2.01	0.60
1:D:196:MET:HA	1:D:240:GLN:HG2	1.83	0.60
1:B:172:VAL:HG12	1:B:172:VAL:O	2.02	0.60
1:B:475:GLY:N	1:B:480:LEU:CD1	2.65	0.60
1:B:508:THR:HA	1:B:511:LEU:HD12	1.83	0.60
1:C:61:ARG:HG3	1:C:62:SER:H	1.67	0.60
1:D:172:VAL:O	1:D:172:VAL:HG12	2.02	0.60
1:A:172:VAL:HG12	1:A:172:VAL:O	2.01	0.60
1:A:438:ALA:C	1:A:440:ALA:N	2.55	0.60
1:A:558:GLU:HG3	1:A:565:LEU:HD23	1.84	0.60
1:C:475:GLY:N	1:C:480:LEU:CD1	2.65	0.60
1:D:362:ILE:HD11	1:D:555:ILE:HA	1.84	0.60
1:A:220:PHE:HZ	1:B:439:TYR:HD2	1.47	0.59
1:A:383:SER:O	1:A:386:ALA:HB3	2.02	0.59
1:B:362:ILE:HD11	1:B:555:ILE:HA	1.84	0.59
1:C:210:MET:HE3	1:D:105:PHE:CZ	2.36	0.59
1:C:436:ASN:HD21	1:C:474:ILE:HG21	1.65	0.59
1:C:59:THR:HA	1:C:63:VAL:HG21	1.83	0.59
1:D:475:GLY:N	1:D:480:LEU:CD1	2.65	0.59
1:D:508:THR:HA	1:D:511:LEU:HD12	1.83	0.59
1:D:548:ILE:HB	1:D:565:LEU:HD11	1.83	0.59
1:D:557:VAL:HG12	1:D:557:VAL:O	2.02	0.59
1:D:382:LYS:HB2	2:D:5004:ANP:O1B	2.02	0.59
1:A:393:TYR:O	1:A:395:ILE:N	2.34	0.59
1:B:175:ALA:N	1:B:176:PRO:HD2	2.18	0.59
1:C:557:VAL:O	1:C:557:VAL:HG12	2.02	0.59
1:D:333:ARG:HB3	1:D:333:ARG:HH11	1.67	0.59
1:A:475:GLY:HA3	1:A:480:LEU:H	1.67	0.59
1:C:20:ILE:HD13	1:C:96:VAL:CG2	2.33	0.59
1:B:380:SER:O	2:B:5002:ANP:O2A	2.21	0.59
1:C:234:SER:O	1:C:237:MET:HB3	2.01	0.59
1:C:558:GLU:HG3	1:C:565:LEU:HD23	1.84	0.59
1:A:105:PHE:O	1:A:108:MET:HB2	2.02	0.59
1:A:374:LEU:HB2	1:A:535:ILE:HB	1.84	0.59
1:A:58:LYS:HZ1	1:A:61:ARG:CD	2.15	0.59
1:B:83:TYR:O	1:B:87:TYR:CB	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:ALA:HB2	1:C:493:ARG:HG3	1.84	0.59
1:A:421:LEU:HD12	1:A:503:ILE:O	2.03	0.59
1:A:59:THR:HA	1:A:63:VAL:HG21	1.83	0.59
1:B:440:ALA:HB2	1:B:493:ARG:HG3	1.84	0.59
1:C:333:ARG:HH11	1:C:333:ARG:HB3	1.67	0.59
1:D:505:ASP:OD2	1:D:535:ILE:HD12	2.02	0.59
1:D:558:GLU:HG3	1:D:565:LEU:HD23	1.84	0.59
1:D:61:ARG:HG3	1:D:62:SER:H	1.67	0.59
1:C:175:ALA:N	1:C:176:PRO:HD2	2.18	0.59
1:C:505:ASP:OD2	1:C:535:ILE:HD12	2.02	0.59
1:D:482:SER:HB3	1:D:485:GLN:HG3	1.83	0.59
1:A:210:MET:SD	1:B:109:MET:HB3	2.42	0.59
1:C:131:ASP:HB3	1:C:318:LEU:HD23	1.85	0.59
1:D:167:LEU:HG	1:D:287:VAL:HG11	1.85	0.59
1:D:291:MET:HE2	1:D:291:MET:HA	1.84	0.59
1:A:482:SER:HB3	1:A:485:GLN:HG3	1.85	0.58
1:B:374:LEU:HB2	1:B:535:ILE:HB	1.85	0.58
1:B:558:GLU:HG3	1:B:565:LEU:HD23	1.84	0.58
1:C:10:TRP:C	1:C:14:ARG:HB3	2.23	0.58
1:D:342:LEU:HD13	1:D:366:ILE:HD12	1.85	0.58
1:A:440:ALA:HB1	1:A:497:ARG:CD	2.33	0.58
1:C:482:SER:HB3	1:C:485:GLN:HG3	1.84	0.58
1:C:83:TYR:O	1:C:87:TYR:CB	2.50	0.58
1:D:269:ALA:C	1:D:273:PRO:HD2	2.24	0.58
1:D:436:ASN:HD21	1:D:474:ILE:HG21	1.65	0.58
1:A:98:MET:HB3	1:B:238:ARG:NE	2.17	0.58
1:B:342:LEU:HD13	1:B:366:ILE:HD12	1.85	0.58
1:B:475:GLY:HA3	1:B:480:LEU:H	1.68	0.58
1:B:58:LYS:HB3	1:B:62:SER:CB	2.34	0.58
1:B:61:ARG:HG3	1:B:62:SER:H	1.67	0.58
1:C:105:PHE:O	1:C:108:MET:HB2	2.03	0.58
1:C:374:LEU:HB2	1:C:535:ILE:HB	1.85	0.58
1:D:341:ASP:HB3	1:D:403:ASP:OD1	2.03	0.58
1:A:362:ILE:HD11	1:A:555:ILE:HA	1.84	0.58
1:B:10:TRP:C	1:B:14:ARG:HB3	2.24	0.58
1:B:167:LEU:HG	1:B:287:VAL:HG11	1.85	0.58
1:C:341:ASP:HB3	1:C:403:ASP:OD1	2.03	0.58
1:D:475:GLY:HA3	1:D:480:LEU:H	1.68	0.58
1:D:58:LYS:HB3	1:D:62:SER:CB	2.34	0.58
1:D:83:TYR:O	1:D:87:TYR:CB	2.50	0.58
1:B:249:SER:O	1:B:253:PRO:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:LYS:NZ	2:B:5002:ANP:O1B	2.35	0.58
1:C:362:ILE:HD11	1:C:555:ILE:HA	1.84	0.58
1:C:74:LEU:HD22	1:C:75:MET:HE2	1.85	0.58
1:D:10:TRP:C	1:D:14:ARG:HB3	2.24	0.58
1:D:175:ALA:N	1:D:176:PRO:HD2	2.18	0.58
1:A:11:GLN:H	1:A:14:ARG:CB	2.14	0.58
1:A:260:SER:OG	1:B:74:LEU:HD13	2.03	0.58
1:A:503:ILE:HG23	1:A:533:LEU:HD12	1.86	0.58
1:A:56:PHE:HB3	1:B:281:ALA:HB2	1.85	0.58
1:B:291:MET:HA	1:B:291:MET:HE2	1.84	0.58
1:B:438:ALA:C	1:B:440:ALA:N	2.56	0.58
1:C:249:SER:O	1:C:253:PRO:HD2	2.04	0.58
1:D:421:LEU:HD12	1:D:503:ILE:O	2.04	0.58
1:A:10:TRP:C	1:A:14:ARG:HB2	2.22	0.58
1:A:342:LEU:HD23	1:A:342:LEU:C	2.24	0.58
1:A:31:GLY:O	1:A:35:ILE:HD13	2.03	0.58
1:A:221:GLY:CA	1:B:441:ARG:NE	2.61	0.58
1:C:167:LEU:HG	1:C:287:VAL:HG11	1.85	0.58
1:C:475:GLY:HA3	1:C:480:LEU:H	1.68	0.58
1:D:105:PHE:O	1:D:108:MET:HB2	2.03	0.58
1:A:394:ASP:O	1:A:395:ILE:HG22	2.04	0.58
1:A:84:ILE:O	1:A:87:TYR:HD2	1.87	0.58
1:B:421:LEU:HD12	1:B:503:ILE:O	2.04	0.58
1:B:557:VAL:HG12	1:B:557:VAL:O	2.02	0.58
1:C:10:TRP:C	1:C:14:ARG:CB	2.72	0.58
1:D:374:LEU:HB2	1:D:535:ILE:HB	1.85	0.58
1:A:169:ILE:HG22	1:A:169:ILE:O	2.04	0.58
1:A:440:ALA:HB2	1:A:493:ARG:HG3	1.85	0.58
1:A:442:THR:O	1:A:443:GLU:HB2	2.02	0.58
1:B:269:ALA:C	1:B:273:PRO:HD2	2.24	0.58
1:C:11:GLN:CG	1:C:12:THR:H	1.95	0.58
1:C:269:ALA:C	1:C:273:PRO:HD2	2.24	0.58
1:D:249:SER:O	1:D:253:PRO:HD2	2.04	0.58
1:D:440:ALA:HB2	1:D:493:ARG:HG3	1.84	0.58
1:A:98:MET:SD	1:A:101:ARG:NH1	2.73	0.58
1:D:10:TRP:C	1:D:14:ARG:CB	2.72	0.58
1:C:429:PHE:CE1	1:D:220:PHE:CZ	2.89	0.58
1:D:394:ASP:O	1:D:395:ILE:HG22	2.04	0.58
1:A:401:LEU:HD12	1:A:404:GLY:HA2	1.86	0.57
1:A:331:GLY:HA3	1:A:408:ARG:O	2.04	0.57
1:B:131:ASP:HB3	1:B:318:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ILE:HG23	1:B:533:LEU:HD12	1.86	0.57
1:D:393:TYR:O	1:D:395:ILE:N	2.37	0.57
1:D:503:ILE:HG23	1:D:533:LEU:HD12	1.86	0.57
1:A:210:MET:HE2	1:A:210:MET:HA	1.86	0.57
1:A:333:ARG:HB3	1:A:333:ARG:HH11	1.68	0.57
1:A:466:MET:HE2	1:A:472:THR:HG21	1.85	0.57
1:A:576:HIS:O	1:A:579:GLN:HB2	2.04	0.57
1:B:508:THR:HG21	1:B:516:GLU:OE2	2.04	0.57
1:C:393:TYR:O	1:C:395:ILE:N	2.37	0.57
1:D:131:ASP:HB3	1:D:318:LEU:HD23	1.85	0.57
1:A:167:LEU:HG	1:A:287:VAL:HG11	1.85	0.57
1:B:105:PHE:O	1:B:108:MET:HB2	2.03	0.57
1:B:238:ARG:O	1:B:242:MET:HB2	2.04	0.57
1:B:436:ASN:HD21	1:B:474:ILE:HG21	1.65	0.57
1:C:503:ILE:HG23	1:C:533:LEU:HD12	1.86	0.57
1:D:342:LEU:HD23	1:D:342:LEU:C	2.25	0.57
1:D:373:ALA:HA	1:D:534:VAL:O	2.04	0.57
1:D:541:THR:C	1:D:542:ILE:HD12	2.25	0.57
1:B:10:TRP:C	1:B:14:ARG:CB	2.72	0.57
1:B:20:ILE:HD13	1:B:96:VAL:CG2	2.33	0.57
1:B:341:ASP:HB3	1:B:403:ASP:OD1	2.03	0.57
1:B:487:GLN:HE22	1:B:510:ALA:H	1.53	0.57
1:B:58:LYS:HZ1	1:B:61:ARG:CD	2.17	0.57
1:C:342:LEU:HD13	1:C:366:ILE:HD12	1.85	0.57
1:B:98:MET:SD	1:B:101:ARG:NH1	2.77	0.57
1:B:176:PRO:O	1:B:180:ILE:HG12	2.05	0.57
1:B:393:TYR:O	1:B:395:ILE:N	2.37	0.57
1:C:238:ARG:O	1:C:242:MET:HB2	2.04	0.57
1:C:455:ARG:HB2	1:C:460:MET:HG3	1.87	0.57
1:D:49:LYS:HD2	1:D:49:LYS:O	2.05	0.57
1:A:175:ALA:N	1:A:176:PRO:HD2	2.19	0.57
1:A:541:THR:O	1:A:542:ILE:HG13	2.03	0.57
1:A:58:LYS:HB3	1:A:62:SER:CB	2.33	0.57
1:B:394:ASP:O	1:B:395:ILE:HG22	2.04	0.57
1:C:383:SER:O	1:C:386:ALA:HB3	2.05	0.57
1:C:134:GLN:HE22	1:C:310:ARG:NE	2.03	0.57
1:C:49:LYS:O	1:C:49:LYS:HD2	2.05	0.57
1:B:455:ARG:HB2	1:B:460:MET:HG3	1.87	0.57
1:B:576:HIS:O	1:B:579:GLN:HB2	2.05	0.57
1:C:576:HIS:O	1:C:579:GLN:HB2	2.05	0.57
1:D:176:PRO:O	1:D:180:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:ARG:O	1:D:242:MET:HB2	2.04	0.57
1:A:249:SER:O	1:A:253:PRO:HD2	2.05	0.57
1:A:112:PRO:HG2	1:A:328:LYS:HB3	1.87	0.57
1:A:49:LYS:O	1:A:49:LYS:HD2	2.05	0.57
1:A:58:LYS:NZ	1:A:58:LYS:HA	2.20	0.57
1:B:331:GLY:HA3	1:B:408:ARG:O	2.05	0.57
1:B:383:SER:HB2	2:B:5002:ANP:O1A	2.04	0.57
1:C:169:ILE:O	1:C:169:ILE:HG22	2.05	0.57
1:C:269:ALA:HA	1:C:273:PRO:HD2	1.87	0.57
1:C:394:ASP:O	1:C:395:ILE:HG22	2.04	0.57
1:C:373:ALA:HA	1:C:534:VAL:O	2.04	0.57
1:A:176:PRO:O	1:A:180:ILE:HG12	2.05	0.56
1:A:439:TYR:HD2	1:B:220:PHE:HZ	1.51	0.56
1:A:373:ALA:HA	1:A:534:VAL:O	2.04	0.56
1:B:344:PHE:HE2	1:B:364:LEU:HB3	1.70	0.56
1:B:373:ALA:HA	1:B:534:VAL:O	2.04	0.56
1:C:220:PHE:CZ	1:D:429:PHE:CE1	2.88	0.56
1:C:58:LYS:HB3	1:C:62:SER:CB	2.33	0.56
1:D:269:ALA:HA	1:D:273:PRO:HD2	1.87	0.56
1:D:383:SER:O	1:D:386:ALA:HB3	2.05	0.56
1:D:438:ALA:C	1:D:440:ALA:N	2.56	0.56
1:D:455:ARG:HB2	1:D:460:MET:HG3	1.87	0.56
1:D:508:THR:HG21	1:D:516:GLU:OE2	2.04	0.56
1:A:57:GLY:O	1:A:58:LYS:HD2	2.06	0.56
1:B:16:LEU:HA	1:B:319:PHE:HZ	1.70	0.56
1:B:49:LYS:HD2	1:B:49:LYS:O	2.05	0.56
1:B:374:LEU:O	1:B:535:ILE:HG12	2.05	0.56
1:C:478:GLY:HA3	1:C:486:ARG:HD2	1.88	0.56
1:C:541:THR:C	1:C:542:ILE:HD12	2.25	0.56
1:D:216:GLU:O	1:D:218:LEU:N	2.38	0.56
1:D:374:LEU:CD2	1:D:533:LEU:HD21	2.35	0.56
1:A:238:ARG:O	1:A:242:MET:HB2	2.05	0.56
1:A:455:ARG:HB2	1:A:460:MET:HG3	1.86	0.56
1:A:29:VAL:HB	1:A:88:CYS:SG	2.45	0.56
1:B:442:THR:O	1:B:443:GLU:HB2	2.04	0.56
1:C:291:MET:HA	1:C:291:MET:HE2	1.87	0.56
1:C:45:LEU:O	1:C:45:LEU:HD23	2.05	0.56
1:C:508:THR:HG21	1:C:516:GLU:OE2	2.04	0.56
1:D:284:ILE:CD1	1:D:284:ILE:O	2.52	0.56
1:D:45:LEU:O	1:D:45:LEU:HD23	2.06	0.56
1:A:216:GLU:O	1:A:218:LEU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ILE:HG22	1:B:169:ILE:O	2.05	0.56
1:B:342:LEU:C	1:B:342:LEU:HD23	2.25	0.56
1:D:20:ILE:HD13	1:D:96:VAL:CG2	2.33	0.56
1:A:214:HIS:O	1:A:218:LEU:HD13	2.06	0.56
1:B:374:LEU:CD2	1:B:533:LEU:HD21	2.35	0.56
1:A:292:ILE:HD12	1:B:48:LEU:HD12	1.88	0.56
1:C:220:PHE:O	1:D:441:ARG:CD	2.52	0.56
1:C:362:ILE:CD1	1:C:556:ILE:H	2.19	0.56
1:D:362:ILE:CD1	1:D:556:ILE:H	2.19	0.56
1:D:58:LYS:HZ1	1:D:61:ARG:CD	2.18	0.56
1:A:547:GLU:OE2	1:A:559:ARG:HB3	2.06	0.56
1:A:61:ARG:HG3	1:A:62:SER:H	1.69	0.56
1:B:134:GLN:HE22	1:B:310:ARG:NE	2.03	0.56
1:B:58:LYS:NZ	1:B:58:LYS:HA	2.21	0.56
1:C:176:PRO:O	1:C:180:ILE:HG12	2.05	0.56
1:C:442:THR:O	1:C:443:GLU:HB2	2.04	0.56
1:D:576:HIS:O	1:D:579:GLN:HB2	2.05	0.56
1:D:98:MET:SD	1:D:101:ARG:NH1	2.77	0.56
1:A:11:GLN:O	1:A:15:ARG:N	2.35	0.56
1:A:269:ALA:HA	1:A:273:PRO:HD2	1.86	0.56
1:A:45:LEU:HD23	1:A:45:LEU:O	2.06	0.56
1:A:432:THR:HA	1:A:472:THR:O	2.06	0.56
1:C:214:HIS:O	1:C:218:LEU:HD13	2.06	0.56
1:C:235:ASN:O	1:C:238:ARG:HG2	2.05	0.56
1:C:401:LEU:HD12	1:C:404:GLY:HA2	1.88	0.56
1:C:421:LEU:HD12	1:C:503:ILE:O	2.04	0.56
1:A:108:MET:CE	1:A:124:LEU:HB3	2.36	0.56
1:A:134:GLN:HE22	1:A:310:ARG:NE	2.03	0.56
1:A:16:LEU:HA	1:A:319:PHE:HZ	1.71	0.56
1:A:223:GLN:H	1:A:223:GLN:CD	2.08	0.56
1:A:441:ARG:NH1	1:B:221:GLY:O	2.39	0.56
1:A:508:THR:HG21	1:A:516:GLU:OE2	2.05	0.56
1:B:214:HIS:O	1:B:218:LEU:HD13	2.06	0.56
1:B:235:ASN:O	1:B:238:ARG:HG2	2.05	0.56
1:C:216:GLU:O	1:C:218:LEU:N	2.38	0.56
1:D:235:ASN:O	1:D:238:ARG:HG2	2.05	0.56
1:A:269:ALA:C	1:A:273:PRO:HD2	2.25	0.56
1:C:29:VAL:HB	1:C:88:CYS:SG	2.46	0.56
1:C:374:LEU:CD2	1:C:533:LEU:HD21	2.35	0.56
1:C:487:GLN:HE22	1:C:510:ALA:H	1.53	0.56
1:D:442:THR:O	1:D:443:GLU:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLY:HA3	1:A:486:ARG:HD2	1.87	0.56
1:B:210:MET:HE2	1:B:210:MET:HA	1.88	0.56
1:C:108:MET:CE	1:C:124:LEU:HB3	2.36	0.56
1:C:342:LEU:HD23	1:C:342:LEU:C	2.25	0.56
1:C:344:PHE:HE2	1:C:364:LEU:HB3	1.70	0.56
1:C:374:LEU:O	1:C:535:ILE:HG12	2.06	0.56
1:C:331:GLY:HA3	1:C:408:ARG:O	2.05	0.56
1:C:58:LYS:NZ	1:C:58:LYS:HA	2.21	0.56
1:C:97:VAL:HB	1:C:136:ALA:CB	2.36	0.56
1:D:374:LEU:O	1:D:535:ILE:HG12	2.06	0.56
1:D:382:LYS:NZ	2:D:5004:ANP:O1B	2.39	0.56
1:A:114:ALA:HA	1:A:117:ASP:CG	2.25	0.56
1:A:11:GLN:CA	1:A:14:ARG:HB3	2.36	0.56
1:A:438:ALA:O	1:A:440:ALA:N	2.39	0.56
1:B:216:GLU:O	1:B:218:LEU:N	2.38	0.56
1:C:249:SER:HG	1:D:83:TYR:HD1	1.53	0.56
1:D:487:GLN:HE22	1:D:510:ALA:H	1.53	0.56
1:A:389:ILE:O	1:A:407:LEU:HD21	2.06	0.55
1:B:269:ALA:HA	1:B:273:PRO:HD2	1.87	0.55
1:C:102:ARG:NH2	1:D:238:ARG:NH2	2.54	0.55
1:C:57:GLY:O	1:C:58:LYS:HD2	2.06	0.55
1:D:16:LEU:HA	1:D:319:PHE:HZ	1.70	0.55
1:D:214:HIS:O	1:D:218:LEU:HD13	2.06	0.55
1:D:432:THR:HA	1:D:472:THR:O	2.06	0.55
1:D:58:LYS:NZ	1:D:58:LYS:HA	2.21	0.55
1:D:57:GLY:O	1:D:58:LYS:HD2	2.06	0.55
1:A:235:ASN:O	1:A:238:ARG:HG2	2.06	0.55
1:A:368:ALA:HA	1:A:531:THR:HG1	1.71	0.55
1:B:362:ILE:CD1	1:B:556:ILE:H	2.19	0.55
1:D:344:PHE:HE2	1:D:364:LEU:HB3	1.70	0.55
1:A:220:PHE:O	1:B:441:ARG:CD	2.54	0.55
1:A:436:ASN:HD21	1:A:474:ILE:HG21	1.67	0.55
1:A:487:GLN:HE22	1:A:510:ALA:H	1.52	0.55
1:B:45:LEU:HD23	1:B:45:LEU:O	2.06	0.55
1:C:440:ALA:HB1	1:C:497:ARG:CD	2.36	0.55
1:D:114:ALA:HA	1:D:117:ASP:CG	2.26	0.55
1:A:342:LEU:HD13	1:A:366:ILE:HD12	1.87	0.55
1:A:400:ILE:O	1:A:407:LEU:HD13	2.06	0.55
1:B:114:ALA:HA	1:B:117:ASP:CG	2.26	0.55
1:B:97:VAL:HB	1:B:136:ALA:CB	2.36	0.55
1:C:114:ALA:HA	1:C:117:ASP:CG	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ARG:CD	1:D:221:GLY:O	2.54	0.55
1:D:376:GLY:HA3	1:D:551:VAL:O	2.07	0.55
1:D:29:VAL:HB	1:D:88:CYS:SG	2.46	0.55
1:A:263:LEU:HD13	1:A:263:LEU:O	2.06	0.55
1:B:440:ALA:HB1	1:B:497:ARG:CD	2.36	0.55
1:C:432:THR:HA	1:C:472:THR:O	2.07	0.55
1:C:466:MET:HE2	1:C:472:THR:HG21	1.87	0.55
1:D:331:GLY:HA3	1:D:408:ARG:O	2.05	0.55
1:D:76:ILE:O	1:D:80:ILE:HB	2.06	0.55
1:A:11:GLN:H	1:A:14:ARG:HB3	1.65	0.55
1:A:291:MET:HA	1:A:291:MET:CE	2.36	0.55
1:B:203:VAL:HG22	1:B:233:VAL:HG12	1.89	0.55
1:B:31:GLY:O	1:B:35:ILE:HD13	2.06	0.55
1:B:383:SER:O	1:B:386:ALA:HB3	2.05	0.55
1:B:432:THR:HA	1:B:472:THR:O	2.06	0.55
1:B:76:ILE:O	1:B:80:ILE:HB	2.06	0.55
1:C:196:MET:HA	1:C:240:GLN:CG	2.37	0.55
1:C:284:ILE:O	1:C:284:ILE:CD1	2.52	0.55
1:C:31:GLY:O	1:C:35:ILE:HD13	2.07	0.55
1:D:11:GLN:O	1:D:15:ARG:N	2.36	0.55
1:D:108:MET:CE	1:D:124:LEU:HB3	2.36	0.55
1:D:152:SER:O	1:D:156:LEU:HD23	2.07	0.55
1:D:169:ILE:O	1:D:169:ILE:HG22	2.05	0.55
1:C:416:ARG:HD3	1:D:218:LEU:HB3	1.88	0.55
1:D:466:MET:HE2	1:D:472:THR:HG21	1.87	0.55
1:A:374:LEU:CD2	1:A:533:LEU:HD21	2.36	0.55
1:B:101:ARG:HH21	1:B:129:THR:HA	1.72	0.55
1:B:284:ILE:CD1	1:B:284:ILE:O	2.52	0.55
1:B:401:LEU:HD12	1:B:404:GLY:HA2	1.88	0.55
1:B:376:GLY:HA3	1:B:551:VAL:O	2.07	0.55
1:C:83:TYR:HD1	1:D:249:SER:HG	1.53	0.55
1:D:31:GLY:O	1:D:35:ILE:HD13	2.06	0.55
1:D:440:ALA:HB1	1:D:497:ARG:CD	2.36	0.55
1:D:439:TYR:HA	1:D:443:GLU:HG3	1.89	0.55
1:D:97:VAL:HB	1:D:136:ALA:CB	2.36	0.55
1:A:201:GLY:O	1:A:204:THR:HB	2.07	0.55
1:A:315:CYS:SG	1:A:319:PHE:CD1	3.00	0.55
1:C:16:LEU:HA	1:C:319:PHE:HZ	1.70	0.55
1:A:166:GLN:OE1	1:A:166:GLN:HA	2.07	0.55
1:B:344:PHE:HZ	1:B:385:ILE:HD12	1.72	0.55
1:D:210:MET:HE2	1:D:210:MET:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:HIS:HD2	1:D:213:GLY:HA2	1.71	0.55
1:D:434:ALA:HB2	1:D:470:LEU:HB3	1.89	0.55
1:D:547:GLU:OE2	1:D:559:ARG:HB3	2.07	0.55
1:A:441:ARG:CD	1:B:221:GLY:CA	2.66	0.55
1:B:439:TYR:HA	1:B:443:GLU:HG3	1.89	0.55
1:C:291:MET:HA	1:C:291:MET:CE	2.37	0.55
1:D:133:GLU:O	1:D:136:ALA:HB3	2.07	0.55
1:D:478:GLY:HA3	1:D:486:ARG:HD2	1.87	0.55
1:A:152:SER:O	1:A:156:LEU:HD23	2.06	0.54
1:A:315:CYS:SG	1:A:319:PHE:CE1	3.00	0.54
1:A:362:ILE:HD11	1:A:556:ILE:H	1.72	0.54
1:A:455:ARG:HH11	1:A:456:MET:CE	2.20	0.54
1:A:97:VAL:HB	1:A:136:ALA:CB	2.37	0.54
1:B:108:MET:CE	1:B:124:LEU:HB3	2.36	0.54
1:B:402:MET:O	1:B:403:ASP:HB2	2.07	0.54
1:C:166:GLN:HA	1:C:166:GLN:OE1	2.07	0.54
1:C:441:ARG:HG2	1:D:220:PHE:O	2.07	0.54
1:D:401:LEU:HD12	1:D:404:GLY:HA2	1.88	0.54
1:A:76:ILE:O	1:A:80:ILE:HB	2.07	0.54
1:B:344:PHE:CE2	1:B:364:LEU:HB3	2.43	0.54
1:B:466:MET:HE2	1:B:472:THR:HG21	1.89	0.54
1:B:547:GLU:OE2	1:B:559:ARG:HB3	2.07	0.54
1:C:58:LYS:HZ1	1:C:61:ARG:CD	2.20	0.54
1:D:196:MET:HA	1:D:240:GLN:CG	2.37	0.54
1:D:201:GLY:O	1:D:204:THR:HB	2.07	0.54
1:D:344:PHE:HZ	1:D:385:ILE:HD12	1.72	0.54
1:A:210:MET:HE3	1:B:105:PHE:CZ	2.42	0.54
1:A:174:LEU:HD21	1:A:261:LEU:HB3	1.89	0.54
1:A:167:LEU:HD12	1:A:266:VAL:HG22	1.90	0.54
1:A:402:MET:O	1:A:403:ASP:HB2	2.06	0.54
1:A:63:VAL:CG1	1:B:267:LEU:O	2.55	0.54
1:C:112:PRO:HG2	1:C:328:LYS:HB3	1.89	0.54
1:C:438:ALA:O	1:C:440:ALA:N	2.41	0.54
1:D:111:MET:CE	1:D:326:GLN:HA	2.38	0.54
1:D:344:PHE:CE2	1:D:364:LEU:HB3	2.43	0.54
1:D:59:THR:HA	1:D:63:VAL:CG2	2.38	0.54
1:B:166:GLN:HA	1:B:166:GLN:OE1	2.07	0.54
1:B:111:MET:CE	1:B:326:GLN:HA	2.38	0.54
1:B:57:GLY:O	1:B:58:LYS:HD2	2.06	0.54
1:C:344:PHE:HZ	1:C:385:ILE:HD12	1.72	0.54
1:D:101:ARG:HH21	1:D:129:THR:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:SER:O	1:B:156:LEU:HD23	2.07	0.54
1:B:174:LEU:HD21	1:B:261:LEU:HB3	1.88	0.54
1:B:291:MET:CE	1:B:291:MET:HA	2.37	0.54
1:C:376:GLY:HA3	1:C:551:VAL:O	2.07	0.54
1:C:441:ARG:CD	1:D:220:PHE:O	2.55	0.54
1:C:460:MET:CE	1:C:460:MET:HA	2.38	0.54
1:C:76:ILE:O	1:C:80:ILE:HB	2.06	0.54
1:D:174:LEU:HD21	1:D:261:LEU:HB3	1.89	0.54
1:A:213:GLY:HA2	1:B:427:HIS:CD2	2.42	0.54
1:A:48:LEU:CD1	1:B:292:ILE:HD12	2.37	0.54
1:B:173:VAL:HG12	1:B:174:LEU:HD12	1.90	0.54
1:B:196:MET:HA	1:B:240:GLN:CG	2.37	0.54
1:A:86:SER:CB	1:B:249:SER:HB2	2.38	0.54
1:C:111:MET:CE	1:C:326:GLN:HA	2.38	0.54
1:C:101:ARG:HH21	1:C:129:THR:HA	1.72	0.54
1:C:174:LEU:HD21	1:C:261:LEU:HB3	1.89	0.54
1:C:203:VAL:HG22	1:C:233:VAL:HG12	1.89	0.54
1:C:434:ALA:HB2	1:C:470:LEU:HB3	1.89	0.54
1:D:134:GLN:HE22	1:D:310:ARG:NE	2.03	0.54
1:D:400:ILE:O	1:D:407:LEU:HD13	2.07	0.54
1:D:87:TYR:CG	1:D:88:CYS:N	2.76	0.54
1:A:196:MET:HA	1:A:240:GLN:CG	2.37	0.54
1:B:59:THR:HA	1:B:63:VAL:CG2	2.37	0.54
1:B:29:VAL:HB	1:B:88:CYS:SG	2.46	0.54
1:A:242:MET:HE3	1:B:91:TRP:HA	1.89	0.54
1:C:344:PHE:CE2	1:C:364:LEU:HB3	2.43	0.54
1:C:550:VAL:HG21	1:C:572:TYR:HB2	1.90	0.54
1:C:59:THR:HA	1:C:63:VAL:CG2	2.38	0.54
1:D:291:MET:CE	1:D:291:MET:HA	2.37	0.54
1:D:402:MET:O	1:D:403:ASP:HB2	2.07	0.54
1:A:460:MET:CE	1:A:460:MET:HA	2.38	0.54
1:B:168:SER:O	1:B:172:VAL:HG23	2.08	0.54
1:B:235:ASN:HA	1:B:238:ARG:NE	2.23	0.54
1:B:478:GLY:HA3	1:B:486:ARG:HD2	1.88	0.54
1:C:210:MET:HA	1:C:210:MET:HE2	1.89	0.54
1:C:547:GLU:OE2	1:C:559:ARG:HB3	2.07	0.54
1:C:98:MET:SD	1:C:101:ARG:NH1	2.77	0.54
1:C:441:ARG:NE	1:D:221:GLY:CA	2.68	0.54
1:D:84:ILE:O	1:D:87:TYR:HD2	1.91	0.54
1:A:10:TRP:O	1:A:11:GLN:HB3	2.08	0.54
1:A:11:GLN:O	1:A:12:THR:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:O	1:A:136:ALA:HB3	2.07	0.54
1:A:302:THR:HG23	1:A:303:ASN:N	2.23	0.54
1:A:376:GLY:HA3	1:A:551:VAL:O	2.08	0.54
1:A:493:ARG:HD3	1:A:497:ARG:NH1	2.23	0.54
1:A:542:ILE:O	1:A:544:GLN:N	2.40	0.54
1:B:112:PRO:HG2	1:B:328:LYS:HB3	1.89	0.54
1:B:434:ALA:HB2	1:B:470:LEU:HB3	1.89	0.54
1:C:389:ILE:O	1:C:407:LEU:HD21	2.08	0.54
1:C:89:ILE:HG23	1:C:90:SER:N	2.23	0.54
1:D:112:PRO:HG2	1:D:328:LYS:HB3	1.89	0.54
1:A:101:ARG:HH21	1:A:129:THR:HA	1.73	0.54
1:A:344:PHE:HE2	1:A:364:LEU:HB3	1.72	0.54
1:B:154:ILE:HA	1:B:157:PHE:CD2	2.43	0.54
1:B:295:MET:O	1:B:299:LYS:HG3	2.08	0.54
1:B:87:TYR:CG	1:B:88:CYS:N	2.76	0.54
1:C:133:GLU:O	1:C:136:ALA:HB3	2.07	0.54
1:C:152:SER:O	1:C:156:LEU:HD23	2.07	0.54
1:C:201:GLY:O	1:C:204:THR:HB	2.07	0.54
1:D:168:SER:O	1:D:172:VAL:HG23	2.08	0.54
1:A:168:SER:O	1:A:172:VAL:HG23	2.07	0.53
1:A:439:TYR:HA	1:A:443:GLU:HG3	1.90	0.53
1:C:214:HIS:CE1	1:C:218:LEU:HD11	2.43	0.53
1:C:235:ASN:HA	1:C:238:ARG:NE	2.23	0.53
1:C:400:ILE:O	1:C:407:LEU:HD13	2.07	0.53
1:C:402:MET:O	1:C:403:ASP:HB2	2.07	0.53
1:A:111:MET:CE	1:A:326:GLN:HA	2.38	0.53
1:B:11:GLN:O	1:B:15:ARG:N	2.36	0.53
1:B:133:GLU:O	1:B:136:ALA:HB3	2.07	0.53
1:C:11:GLN:O	1:C:15:ARG:N	2.36	0.53
1:C:302:THR:HG23	1:C:303:ASN:N	2.24	0.53
1:D:214:HIS:CE1	1:D:218:LEU:HD11	2.43	0.53
1:A:154:ILE:HA	1:A:157:PHE:CD2	2.42	0.53
1:A:561:THR:HG22	1:A:562:HIS:N	2.24	0.53
1:B:214:HIS:CE1	1:B:218:LEU:HD11	2.44	0.53
1:B:84:ILE:O	1:B:87:TYR:HD2	1.91	0.53
1:C:173:VAL:HG12	1:C:174:LEU:HD12	1.90	0.53
1:D:203:VAL:HG22	1:D:233:VAL:HG12	1.89	0.53
1:D:550:VAL:HG21	1:D:572:TYR:HB2	1.90	0.53
1:A:173:VAL:HG12	1:A:174:LEU:HD12	1.90	0.53
1:A:347:VAL:HG13	1:A:395:ILE:CD1	2.29	0.53
1:B:346:ASN:N	1:B:363:ASN:OD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ALA:O	1:B:440:ALA:N	2.41	0.53
1:C:439:TYR:HA	1:C:443:GLU:HG3	1.89	0.53
1:D:302:THR:HG23	1:D:303:ASN:H	1.74	0.53
1:A:203:VAL:HG22	1:A:233:VAL:HG12	1.90	0.53
1:A:263:LEU:HD13	1:A:263:LEU:C	2.29	0.53
1:A:281:ALA:HA	1:A:284:ILE:HG22	1.91	0.53
1:A:441:ARG:CD	1:B:220:PHE:O	2.54	0.53
1:A:434:ALA:HB2	1:A:470:LEU:HB3	1.91	0.53
1:A:338:ALA:CB	1:A:500:PRO:HG2	2.04	0.53
1:A:98:MET:HB3	1:B:238:ARG:HH21	1.68	0.53
1:B:302:THR:HG23	1:B:303:ASN:N	2.23	0.53
1:B:542:ILE:O	1:B:544:GLN:N	2.42	0.53
1:C:295:MET:O	1:C:299:LYS:HG3	2.09	0.53
1:C:428:LEU:HD23	1:C:493:ARG:NH2	2.24	0.53
1:C:548:ILE:N	1:C:548:ILE:HD12	2.22	0.53
1:D:16:LEU:HD23	1:D:16:LEU:O	2.08	0.53
1:D:438:ALA:O	1:D:440:ALA:N	2.41	0.53
1:D:513:THR:HG23	1:D:514:GLU:N	2.24	0.53
1:D:89:ILE:HG23	1:D:90:SER:N	2.23	0.53
1:A:296:ARG:HD3	1:A:296:ARG:C	2.29	0.53
1:A:428:LEU:HD23	1:A:493:ARG:NH2	2.24	0.53
1:A:561:THR:HG22	1:A:563:SER:H	1.73	0.53
1:B:201:GLY:O	1:B:204:THR:HB	2.07	0.53
1:B:400:ILE:O	1:B:407:LEU:HD13	2.07	0.53
1:B:89:ILE:HG23	1:B:90:SER:N	2.23	0.53
1:C:87:TYR:CG	1:C:88:CYS:N	2.76	0.53
1:D:412:LEU:HD21	1:D:416:ARG:HH11	1.73	0.53
1:D:460:MET:HA	1:D:460:MET:CE	2.38	0.53
1:D:542:ILE:O	1:D:544:GLN:N	2.42	0.53
1:A:219:ILE:HG13	1:A:220:PHE:N	2.22	0.53
1:A:220:PHE:O	1:B:441:ARG:HG2	2.07	0.53
1:A:235:ASN:HA	1:A:238:ARG:NE	2.24	0.53
1:B:389:ILE:O	1:B:407:LEU:HD21	2.08	0.53
1:C:242:MET:HE3	1:D:91:TRP:HA	1.88	0.53
1:D:166:GLN:HA	1:D:166:GLN:OE1	2.07	0.53
1:B:252:ASP:HB2	1:B:253:PRO:CD	2.38	0.53
1:B:441:ARG:HA	1:B:441:ARG:NH1	2.23	0.53
1:B:460:MET:CE	1:B:460:MET:HA	2.38	0.53
1:B:561:THR:HG22	1:B:563:SER:H	1.74	0.53
1:C:221:GLY:CA	1:D:441:ARG:NE	2.71	0.53
1:C:575:LEU:HD22	1:D:513:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:ALA:HA	1:D:531:THR:HG1	1.72	0.53
1:A:214:HIS:CE1	1:A:218:LEU:HD11	2.43	0.53
1:C:512:ASP:HB2	1:D:378:SER:N	2.20	0.53
1:D:154:ILE:HA	1:D:157:PHE:CD2	2.43	0.53
1:D:235:ASN:HA	1:D:238:ARG:NE	2.23	0.53
1:D:389:ILE:O	1:D:407:LEU:HD21	2.08	0.53
1:A:382:LYS:NZ	2:A:5001:ANP:O1B	2.42	0.53
1:C:15:ARG:C	1:C:18:PRO:HD2	2.29	0.53
1:C:383:SER:OG	2:C:5003:ANP:O2B	2.15	0.53
1:C:512:ASP:CB	1:D:378:SER:H	2.19	0.53
1:A:550:VAL:HG21	1:A:572:TYR:HB2	1.91	0.52
1:B:15:ARG:C	1:B:18:PRO:HD2	2.29	0.52
1:B:16:LEU:O	1:B:16:LEU:HD23	2.08	0.52
1:B:455:ARG:HH11	1:B:456:MET:CE	2.22	0.52
1:B:428:LEU:HD23	1:B:493:ARG:NH2	2.24	0.52
1:B:550:VAL:HG21	1:B:572:TYR:HB2	1.90	0.52
1:C:217:VAL:HA	1:C:220:PHE:CB	2.39	0.52
1:C:134:GLN:NE2	1:C:310:ARG:HE	2.06	0.52
1:C:513:THR:HG23	1:C:514:GLU:N	2.24	0.52
1:D:173:VAL:HG12	1:D:174:LEU:HD12	1.90	0.52
1:D:424:GLN:H	1:D:424:GLN:CD	2.12	0.52
1:D:47:LEU:HD13	1:D:47:LEU:O	2.10	0.52
1:A:302:THR:HG23	1:A:303:ASN:H	1.73	0.52
1:A:40:SER:O	1:A:44:MET:HG2	2.09	0.52
1:A:59:THR:HA	1:A:63:VAL:CG2	2.39	0.52
1:B:424:GLN:CD	1:B:424:GLN:H	2.12	0.52
1:B:513:THR:HG23	1:B:514:GLU:N	2.24	0.52
1:C:154:ILE:HA	1:C:157:PHE:CD2	2.43	0.52
1:C:168:SER:O	1:C:172:VAL:HG23	2.08	0.52
1:C:302:THR:HG23	1:C:303:ASN:H	1.74	0.52
1:C:346:ASN:N	1:C:363:ASN:OD1	2.38	0.52
1:C:455:ARG:HH11	1:C:456:MET:CE	2.22	0.52
1:C:83:TYR:HA	1:D:249:SER:OG	2.09	0.52
1:C:67:MET:HA	1:D:267:LEU:CD2	2.39	0.52
1:D:474:ILE:HA	1:D:480:LEU:HD11	1.91	0.52
1:A:15:ARG:C	1:A:18:PRO:HD2	2.30	0.52
1:A:346:ASN:N	1:A:363:ASN:OD1	2.38	0.52
1:A:378:SER:CB	1:B:512:ASP:HB2	2.39	0.52
1:A:388:LEU:O	1:A:388:LEU:HD23	2.08	0.52
1:A:59:THR:O	1:A:60:ASP:HB2	2.10	0.52
1:B:548:ILE:N	1:B:548:ILE:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:HB3	1:C:294:LEU:HD22	1.92	0.52
1:C:542:ILE:O	1:C:544:GLN:N	2.42	0.52
1:D:217:VAL:HA	1:D:220:PHE:CB	2.39	0.52
1:D:441:ARG:NH1	1:D:441:ARG:HA	2.24	0.52
1:A:144:ILE:HG13	1:A:145:THR:HG23	1.91	0.52
1:A:149:GLU:O	1:A:153:ILE:HD13	2.10	0.52
1:A:441:ARG:NH1	1:A:441:ARG:HA	2.23	0.52
1:A:47:LEU:HD13	1:A:47:LEU:O	2.10	0.52
1:A:513:THR:HG23	1:A:514:GLU:N	2.24	0.52
1:B:217:VAL:HA	1:B:220:PHE:CB	2.39	0.52
1:C:84:ILE:O	1:C:87:TYR:HD2	1.91	0.52
1:D:252:ASP:HB2	1:D:253:PRO:CD	2.38	0.52
1:D:428:LEU:HD23	1:D:493:ARG:NH2	2.24	0.52
1:A:127:ARG:O	1:A:131:ASP:HB2	2.10	0.52
1:A:226:GLU:HA	1:A:226:GLU:OE2	2.09	0.52
1:B:368:ALA:HA	1:B:531:THR:HG1	1.73	0.52
1:B:98:MET:HA	1:B:101:ARG:CD	2.40	0.52
1:C:167:LEU:HD12	1:C:266:VAL:HG22	1.91	0.52
1:D:219:ILE:HG13	1:D:220:PHE:N	2.25	0.52
1:D:167:LEU:HD12	1:D:266:VAL:HG22	1.91	0.52
1:C:512:ASP:HB2	1:D:378:SER:HB3	1.90	0.52
1:D:59:THR:O	1:D:60:ASP:HB2	2.09	0.52
1:A:20:ILE:HD12	1:A:139:SER:OG	2.10	0.52
1:A:219:ILE:HD13	1:B:421:LEU:HB3	1.92	0.52
1:A:427:HIS:HD2	1:B:213:GLY:HA2	1.75	0.52
1:A:87:TYR:CG	1:A:88:CYS:N	2.77	0.52
1:B:347:VAL:HG13	1:B:395:ILE:CD1	2.31	0.52
1:C:242:MET:O	1:C:245:VAL:HG22	2.10	0.52
1:D:242:MET:O	1:D:245:VAL:HG22	2.10	0.52
1:D:40:SER:O	1:D:44:MET:HG2	2.10	0.52
1:D:426:VAL:HG11	1:D:490:ALA:HB1	1.92	0.52
1:A:242:MET:O	1:A:245:VAL:HG22	2.09	0.52
1:A:562:HIS:O	1:A:566:LEU:HB2	2.10	0.52
1:B:226:GLU:HA	1:B:226:GLU:OE2	2.10	0.52
1:B:383:SER:OG	2:B:5002:ANP:O2B	2.16	0.52
1:B:541:THR:C	1:B:542:ILE:HD12	2.30	0.52
1:B:58:LYS:HZ1	1:B:61:ARG:HD3	1.74	0.52
1:C:16:LEU:O	1:C:16:LEU:HD23	2.08	0.52
1:C:279:LEU:O	1:C:283:THR:HB	2.10	0.52
1:C:388:LEU:O	1:C:388:LEU:HD23	2.10	0.52
1:C:441:ARG:NE	1:D:221:GLY:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:VAL:HG13	1:D:395:ILE:CD1	2.31	0.52
1:A:130:TYR:CD2	1:A:200:MET:HG2	2.45	0.52
1:A:238:ARG:NE	1:B:98:MET:HB3	2.25	0.52
1:A:401:LEU:CD2	1:A:401:LEU:N	2.72	0.52
1:A:87:TYR:CE2	1:A:88:CYS:SG	3.03	0.52
1:A:79:GLY:HA2	1:B:253:PRO:HB3	1.91	0.52
1:B:134:GLN:NE2	1:B:310:ARG:HE	2.06	0.52
1:B:388:LEU:HD23	1:B:388:LEU:O	2.10	0.52
1:C:474:ILE:HA	1:C:480:LEU:HD11	1.92	0.52
1:C:368:ALA:HA	1:C:531:THR:HG1	1.74	0.52
1:D:127:ARG:O	1:D:131:ASP:HB2	2.10	0.52
1:D:144:ILE:HG13	1:D:145:THR:HG23	1.92	0.52
1:D:279:LEU:O	1:D:283:THR:HB	2.10	0.52
1:D:295:MET:O	1:D:299:LYS:HG3	2.08	0.52
1:D:380:SER:O	2:D:5004:ANP:O2A	2.27	0.52
1:D:98:MET:HA	1:D:101:ARG:CD	2.40	0.52
1:A:475:GLY:N	1:A:480:LEU:HD11	2.25	0.52
1:A:548:ILE:N	1:A:548:ILE:HD12	2.25	0.52
1:A:62:SER:HA	1:A:66:TRP:CD1	2.44	0.52
1:B:144:ILE:HG13	1:B:145:THR:HG23	1.92	0.52
1:C:226:GLU:HA	1:C:226:GLU:OE2	2.10	0.52
1:C:62:SER:HA	1:C:66:TRP:CD1	2.45	0.52
1:D:108:MET:HE3	1:D:124:LEU:HB3	1.92	0.52
1:D:15:ARG:C	1:D:18:PRO:HD2	2.29	0.52
1:C:264:ALA:O	1:D:67:MET:SD	2.68	0.52
1:A:337:ARG:HD2	1:A:338:ALA:N	2.24	0.52
1:A:344:PHE:CE2	1:A:364:LEU:HB3	2.45	0.52
1:B:256:GLN:HG2	1:B:299:LYS:CD	2.40	0.52
1:B:62:SER:HA	1:B:66:TRP:CD1	2.45	0.52
1:D:388:LEU:O	1:D:388:LEU:HD23	2.10	0.52
1:D:49:LYS:O	1:D:52:LEU:HB3	2.10	0.52
1:A:167:LEU:N	1:A:167:LEU:HD22	2.25	0.51
1:A:217:VAL:HA	1:A:220:PHE:CB	2.40	0.51
1:A:284:ILE:HG23	1:A:284:ILE:O	2.10	0.51
1:A:342:LEU:HD22	1:A:366:ILE:HD12	1.91	0.51
1:A:424:GLN:H	1:A:424:GLN:CD	2.11	0.51
1:B:104:LEU:HD11	1:B:318:LEU:HD22	1.93	0.51
1:B:127:ARG:O	1:B:131:ASP:HB2	2.10	0.51
1:B:296:ARG:HD3	1:B:296:ARG:C	2.30	0.51
1:C:40:SER:O	1:C:44:MET:HG2	2.10	0.51
1:D:156:LEU:HB3	1:D:294:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:GLU:HA	1:D:226:GLU:OE2	2.10	0.51
1:D:561:THR:HG22	1:D:563:SER:H	1.74	0.51
1:A:49:LYS:O	1:A:52:LEU:HB3	2.11	0.51
1:B:315:CYS:O	1:B:319:PHE:N	2.42	0.51
1:B:40:SER:O	1:B:44:MET:HG2	2.10	0.51
1:C:47:LEU:HD13	1:C:47:LEU:O	2.09	0.51
1:C:49:LYS:O	1:C:52:LEU:HB3	2.10	0.51
1:C:98:MET:HA	1:C:101:ARG:CD	2.40	0.51
1:D:104:LEU:HD11	1:D:318:LEU:HD22	1.93	0.51
1:D:256:GLN:HG2	1:D:299:LYS:CD	2.41	0.51
1:D:302:THR:HG23	1:D:303:ASN:N	2.23	0.51
1:D:455:ARG:HH11	1:D:456:MET:CE	2.22	0.51
1:D:489:ILE:O	1:D:492:ALA:HB3	2.10	0.51
1:A:198:ASN:N	1:A:198:ASN:HD22	2.08	0.51
1:A:364:LEU:HD12	1:A:365:LYS:H	1.76	0.51
1:A:79:GLY:CA	1:B:253:PRO:HB3	2.40	0.51
1:B:149:GLU:O	1:B:153:ILE:HD13	2.11	0.51
1:B:279:LEU:O	1:B:283:THR:HB	2.10	0.51
1:C:167:LEU:N	1:C:167:LEU:HD22	2.26	0.51
1:C:424:GLN:H	1:C:424:GLN:CD	2.12	0.51
1:D:130:TYR:CD2	1:D:200:MET:HG2	2.45	0.51
1:C:513:THR:HG22	1:D:575:LEU:HD22	1.93	0.51
1:D:62:SER:HA	1:D:66:TRP:CD1	2.45	0.51
1:A:424:GLN:H	1:A:424:GLN:NE2	2.08	0.51
1:C:127:ARG:O	1:C:131:ASP:HB2	2.10	0.51
1:C:144:ILE:HG13	1:C:145:THR:HG23	1.92	0.51
1:C:256:GLN:HG2	1:C:299:LYS:CD	2.40	0.51
1:C:441:ARG:NH1	1:C:441:ARG:HA	2.23	0.51
1:A:89:ILE:HG23	1:A:90:SER:N	2.24	0.51
1:B:167:LEU:N	1:B:167:LEU:HD22	2.26	0.51
1:B:423:SER:O	1:B:424:GLN:C	2.49	0.51
1:B:59:THR:O	1:B:60:ASP:HB2	2.09	0.51
1:C:220:PHE:HZ	1:D:439:TYR:HD2	1.57	0.51
1:C:338:ALA:HB2	1:C:418:GLN:HG3	1.93	0.51
1:C:562:HIS:O	1:C:566:LEU:HB2	2.11	0.51
1:D:198:ASN:HD22	1:D:198:ASN:N	2.09	0.51
1:A:489:ILE:O	1:A:492:ALA:HB3	2.11	0.51
1:A:98:MET:HA	1:A:101:ARG:CD	2.40	0.51
1:C:281:ALA:HA	1:C:284:ILE:HG22	1.92	0.51
1:C:59:THR:O	1:C:60:ASP:HB2	2.09	0.51
1:D:346:ASN:N	1:D:363:ASN:OD1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:SER:O	1:D:424:GLN:C	2.49	0.51
1:D:424:GLN:NE2	1:D:424:GLN:H	2.09	0.51
1:B:156:LEU:HB3	1:B:294:LEU:HD22	1.92	0.51
1:B:242:MET:O	1:B:245:VAL:HG22	2.10	0.51
1:B:263:LEU:HD13	1:B:263:LEU:O	2.11	0.51
1:B:489:ILE:O	1:B:492:ALA:HB3	2.10	0.51
1:C:475:GLY:CA	1:C:480:LEU:HG	2.41	0.51
1:D:296:ARG:C	1:D:296:ARG:HD3	2.30	0.51
1:D:475:GLY:CA	1:D:480:LEU:HG	2.41	0.51
1:A:295:MET:O	1:A:299:LYS:HG3	2.10	0.51
1:A:315:CYS:O	1:A:319:PHE:N	2.43	0.51
1:A:374:LEU:O	1:A:535:ILE:HG12	2.11	0.51
1:A:63:VAL:HG13	1:B:267:LEU:O	2.10	0.51
1:B:219:ILE:HG13	1:B:220:PHE:N	2.25	0.51
1:B:47:LEU:HD13	1:B:47:LEU:O	2.10	0.51
1:D:338:ALA:HB2	1:D:418:GLN:HG3	1.93	0.51
1:A:16:LEU:HD23	1:A:16:LEU:O	2.10	0.51
1:A:252:ASP:HB2	1:A:253:PRO:CD	2.38	0.51
1:A:362:ILE:HD13	1:A:556:ILE:HG22	1.93	0.51
1:B:167:LEU:HD12	1:B:266:VAL:HG22	1.91	0.51
1:B:49:LYS:O	1:B:52:LEU:HB3	2.10	0.51
1:C:561:THR:HG22	1:C:563:SER:H	1.74	0.51
1:C:378:SER:CB	1:D:512:ASP:HB2	2.40	0.51
1:A:339:THR:HG23	1:A:403:ASP:OD2	2.11	0.51
1:A:391:ARG:C	1:A:393:TYR:H	2.13	0.51
1:B:275:VAL:O	1:B:275:VAL:HG12	2.11	0.51
1:B:302:THR:HG23	1:B:303:ASN:H	1.74	0.51
1:B:337:ARG:HD2	1:B:338:ALA:N	2.26	0.51
1:B:342:LEU:HD22	1:B:366:ILE:HD12	1.93	0.51
1:B:561:THR:HG22	1:B:562:HIS:N	2.26	0.51
1:C:198:ASN:N	1:C:198:ASN:HD22	2.09	0.51
1:C:421:LEU:HB3	1:D:219:ILE:HD13	1.92	0.51
1:C:489:ILE:O	1:C:492:ALA:HB3	2.10	0.51
1:D:167:LEU:HD22	1:D:167:LEU:N	2.26	0.51
1:A:16:LEU:HD12	1:A:315:CYS:CB	2.41	0.50
1:A:343:GLU:HB3	1:A:345:ARG:NH2	2.26	0.50
1:B:276:MET:O	1:B:276:MET:SD	2.70	0.50
1:B:401:LEU:N	1:B:401:LEU:CD2	2.74	0.50
1:B:562:HIS:O	1:B:566:LEU:HB2	2.11	0.50
1:C:219:ILE:HG13	1:C:220:PHE:N	2.25	0.50
1:C:493:ARG:HD3	1:C:497:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLU:O	1:D:153:ILE:HD13	2.11	0.50
1:D:275:VAL:HG12	1:D:275:VAL:O	2.11	0.50
1:A:156:LEU:HB3	1:A:294:LEU:HD22	1.94	0.50
1:A:193:SER:O	1:A:196:MET:HB3	2.11	0.50
1:A:279:LEU:O	1:A:283:THR:HB	2.11	0.50
1:A:541:THR:C	1:A:542:ILE:HD12	2.32	0.50
1:A:558:GLU:OE1	1:A:559:ARG:N	2.44	0.50
1:B:130:TYR:CD2	1:B:200:MET:HG2	2.45	0.50
1:C:149:GLU:O	1:C:153:ILE:HD13	2.11	0.50
1:C:174:LEU:HD23	1:C:258:ILE:O	2.11	0.50
1:D:326:GLN:C	1:D:328:LYS:N	2.64	0.50
1:D:468:ASN:O	1:D:471:ASP:HB2	2.11	0.50
1:A:35:ILE:O	1:A:38:ALA:HB3	2.11	0.50
1:B:242:MET:HA	1:B:245:VAL:HG22	1.93	0.50
1:B:474:ILE:HA	1:B:480:LEU:HD11	1.91	0.50
1:A:249:SER:OG	1:B:83:TYR:HA	2.10	0.50
1:C:276:MET:SD	1:C:276:MET:O	2.70	0.50
1:C:296:ARG:HD3	1:C:296:ARG:C	2.30	0.50
1:C:561:THR:HG22	1:C:562:HIS:N	2.26	0.50
1:D:342:LEU:HD22	1:D:366:ILE:HD12	1.93	0.50
1:D:493:ARG:HD3	1:D:497:ARG:NH1	2.26	0.50
1:A:120:SER:OG	1:A:205:THR:HG23	2.11	0.50
1:A:174:LEU:HD23	1:A:258:ILE:O	2.11	0.50
1:A:256:GLN:HA	1:A:299:LYS:CD	2.39	0.50
1:A:256:GLN:HG2	1:A:299:LYS:CD	2.41	0.50
1:A:315:CYS:SG	1:A:319:PHE:CZ	3.05	0.50
1:A:382:LYS:HB2	1:A:382:LYS:NZ	2.26	0.50
1:A:423:SER:O	1:A:424:GLN:C	2.50	0.50
1:B:343:GLU:HB3	1:B:345:ARG:NH2	2.27	0.50
1:C:423:SER:O	1:C:424:GLN:C	2.49	0.50
1:C:74:LEU:HD22	1:C:75:MET:HE1	1.93	0.50
1:D:242:MET:HA	1:D:245:VAL:HG22	1.93	0.50
1:C:242:MET:HE1	1:D:91:TRP:HA	1.91	0.50
1:D:93:SER:O	1:D:96:VAL:HG12	2.12	0.50
1:A:362:ILE:CD1	1:A:556:ILE:HG22	2.41	0.50
1:B:326:GLN:C	1:B:328:LYS:N	2.64	0.50
1:B:424:GLN:NE2	1:B:424:GLN:H	2.09	0.50
1:A:281:ALA:HB2	1:B:56:PHE:HB3	1.92	0.50
1:C:275:VAL:HG12	1:C:275:VAL:O	2.11	0.50
1:D:281:ALA:HA	1:D:284:ILE:HG22	1.92	0.50
1:D:337:ARG:HD2	1:D:338:ALA:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:SER:HB2	1:D:449:GLN:CD	2.32	0.50
1:D:562:HIS:O	1:D:566:LEU:HB2	2.11	0.50
1:A:194:LYS:O	1:A:197:GLN:HB2	2.12	0.50
1:A:474:ILE:HA	1:A:480:LEU:HD11	1.93	0.50
1:A:475:GLY:CA	1:A:480:LEU:HG	2.42	0.50
1:B:70:VAL:CG1	1:B:71:VAL:N	2.75	0.50
1:C:130:TYR:CD2	1:C:200:MET:HG2	2.45	0.50
1:C:326:GLN:HB3	1:C:328:LYS:HG2	1.94	0.50
1:C:326:GLN:C	1:C:328:LYS:N	2.64	0.50
1:C:412:LEU:HD21	1:C:416:ARG:HH11	1.74	0.50
1:C:449:GLN:HB3	1:C:496:LEU:CD1	2.41	0.50
1:C:70:VAL:CG1	1:C:71:VAL:N	2.75	0.50
1:C:93:SER:O	1:C:96:VAL:HG12	2.12	0.50
1:D:326:GLN:HB3	1:D:328:LYS:HG2	1.94	0.50
1:A:192:ILE:HG21	1:A:244:MET:HB2	1.94	0.50
1:A:33:ALA:HB2	1:A:84:ILE:CG2	2.41	0.50
1:A:446:SER:HB2	1:A:449:GLN:CD	2.31	0.50
1:A:90:SER:HB3	1:B:245:VAL:HG21	1.93	0.50
1:B:28:ILE:HG23	1:B:29:VAL:N	2.27	0.50
1:B:326:GLN:HB3	1:B:328:LYS:HG2	1.94	0.50
1:B:426:VAL:HG11	1:B:490:ALA:HB1	1.92	0.50
1:B:446:SER:HB2	1:B:449:GLN:CD	2.32	0.50
1:C:242:MET:HA	1:C:245:VAL:HG22	1.93	0.50
1:C:315:CYS:O	1:C:319:PHE:N	2.42	0.50
1:C:401:LEU:CD2	1:C:401:LEU:N	2.74	0.50
1:C:424:GLN:H	1:C:424:GLN:NE2	2.09	0.50
1:C:484:GLY:O	1:C:488:ARG:HG3	2.12	0.50
1:D:174:LEU:HD23	1:D:258:ILE:O	2.11	0.50
1:D:33:ALA:HB2	1:D:84:ILE:CG2	2.42	0.50
1:D:450:ILE:HG13	1:D:451:GLU:H	1.77	0.50
1:D:548:ILE:HD12	1:D:548:ILE:N	2.26	0.50
1:A:271:SER:N	1:B:63:VAL:HG11	2.27	0.50
1:A:315:CYS:SG	1:A:319:PHE:CG	3.05	0.50
1:B:174:LEU:CD2	1:B:261:LEU:HB3	2.42	0.50
1:B:281:ALA:HA	1:B:284:ILE:HG22	1.92	0.50
1:B:475:GLY:CA	1:B:480:LEU:HG	2.41	0.50
1:C:174:LEU:CD2	1:C:261:LEU:HB3	2.42	0.50
1:C:342:LEU:HD22	1:C:366:ILE:HD12	1.93	0.50
1:C:369:GLY:HA2	1:C:529:ASN:O	2.12	0.50
1:D:276:MET:O	1:D:276:MET:SD	2.70	0.50
1:D:315:CYS:O	1:D:319:PHE:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:THR:O	1:A:284:ILE:HG22	2.12	0.50
1:A:468:ASN:O	1:A:471:ASP:HB2	2.11	0.50
1:A:474:ILE:C	1:A:480:LEU:HD11	2.32	0.50
1:A:93:SER:O	1:A:96:VAL:HG12	2.12	0.50
1:C:20:ILE:HD12	1:C:139:SER:OG	2.12	0.50
1:C:252:ASP:HB2	1:C:253:PRO:CD	2.38	0.50
1:B:344:PHE:HZ	1:B:385:ILE:CD1	2.25	0.49
1:B:468:ASN:O	1:B:471:ASP:HB2	2.11	0.49
1:C:281:ALA:HB2	1:D:56:PHE:CB	2.16	0.49
1:C:438:ALA:C	1:C:440:ALA:N	2.56	0.49
1:C:450:ILE:HG13	1:C:451:GLU:H	1.77	0.49
1:D:120:SER:OG	1:D:205:THR:HG23	2.12	0.49
1:D:343:GLU:HB3	1:D:345:ARG:NH2	2.27	0.49
1:A:11:GLN:O	1:A:14:ARG:N	2.45	0.49
1:A:220:PHE:HZ	1:B:439:TYR:CD2	2.27	0.49
1:A:275:VAL:HG12	1:A:275:VAL:O	2.12	0.49
1:B:174:LEU:HD23	1:B:258:ILE:O	2.12	0.49
1:B:192:ILE:HG21	1:B:244:MET:HB2	1.94	0.49
1:B:369:GLY:HA2	1:B:529:ASN:O	2.12	0.49
1:B:450:ILE:HG13	1:B:451:GLU:H	1.77	0.49
1:C:104:LEU:HD11	1:C:318:LEU:HD22	1.93	0.49
1:C:446:SER:HB2	1:C:449:GLN:CD	2.32	0.49
1:C:450:ILE:HG13	1:C:451:GLU:N	2.27	0.49
1:C:218:LEU:HB3	1:D:416:ARG:HD3	1.93	0.49
1:B:198:ASN:N	1:B:198:ASN:HD22	2.09	0.49
1:B:20:ILE:HD12	1:B:139:SER:OG	2.12	0.49
1:B:280:THR:O	1:B:284:ILE:HG22	2.13	0.49
1:B:493:ARG:HD3	1:B:497:ARG:NH1	2.27	0.49
1:B:93:SER:O	1:B:96:VAL:HG12	2.12	0.49
1:C:238:ARG:NH2	1:D:102:ARG:NH2	2.60	0.49
1:D:561:THR:HG22	1:D:562:HIS:N	2.26	0.49
1:B:338:ALA:HB2	1:B:418:GLN:HG3	1.93	0.49
1:B:412:LEU:HD21	1:B:416:ARG:HH11	1.74	0.49
1:A:220:PHE:CZ	1:B:439:TYR:HD2	2.29	0.49
1:B:450:ILE:HG13	1:B:451:GLU:N	2.27	0.49
1:C:263:LEU:O	1:C:263:LEU:HD13	2.11	0.49
1:C:468:ASN:O	1:C:471:ASP:HB2	2.11	0.49
1:C:558:GLU:OE1	1:C:559:ARG:N	2.46	0.49
1:D:263:LEU:O	1:D:263:LEU:HD13	2.11	0.49
1:D:364:LEU:HD12	1:D:365:LYS:H	1.77	0.49
1:D:70:VAL:CG1	1:D:71:VAL:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HD11	1:A:318:LEU:HD22	1.94	0.49
1:A:326:GLN:HB3	1:A:328:LYS:CG	2.43	0.49
1:C:33:ALA:HB2	1:C:84:ILE:CG2	2.42	0.49
1:D:192:ILE:HG21	1:D:244:MET:HB2	1.93	0.49
1:A:16:LEU:CA	1:A:319:PHE:HZ	2.26	0.49
1:A:450:ILE:HG13	1:A:451:GLU:H	1.78	0.49
1:B:461:ASP:O	1:B:465:LYS:HG3	2.13	0.49
1:B:484:GLY:O	1:B:488:ARG:HG3	2.12	0.49
1:B:558:GLU:OE1	1:B:559:ARG:N	2.46	0.49
1:D:344:PHE:HZ	1:D:385:ILE:CD1	2.25	0.49
1:A:484:GLY:O	1:A:488:ARG:HG3	2.13	0.49
1:B:33:ALA:HB2	1:B:84:ILE:CG2	2.42	0.49
1:C:193:SER:O	1:C:196:MET:HB3	2.13	0.49
1:C:280:THR:O	1:C:284:ILE:HG22	2.13	0.49
1:D:450:ILE:HG13	1:D:451:GLU:N	2.27	0.49
1:A:242:MET:HA	1:A:245:VAL:HG22	1.94	0.49
1:A:338:ALA:HB2	1:A:418:GLN:HG3	1.94	0.49
1:A:369:GLY:HA2	1:A:529:ASN:O	2.12	0.49
1:A:377:ARG:O	1:A:379:GLY:N	2.46	0.49
1:A:548:ILE:HB	1:A:565:LEU:CD1	2.43	0.49
1:A:75:MET:HE3	1:B:257:LEU:HA	1.95	0.49
1:C:360:ARG:O	1:C:362:ILE:HG12	2.13	0.49
1:D:178:VAL:HA	1:D:258:ILE:CD1	2.43	0.49
1:D:28:ILE:HG23	1:D:29:VAL:N	2.27	0.49
1:D:326:GLN:HB3	1:D:328:LYS:CG	2.43	0.49
1:D:484:GLY:O	1:D:488:ARG:HG3	2.12	0.49
1:C:256:GLN:HE22	1:D:78:ARG:CG	2.25	0.49
1:A:141:GLY:O	1:A:144:ILE:CG1	2.61	0.49
1:B:179:SER:O	1:B:182:ILE:HG22	2.13	0.49
1:B:193:SER:O	1:B:196:MET:HB3	2.13	0.49
1:A:75:MET:SD	1:B:257:LEU:HD13	2.53	0.49
1:C:194:LYS:O	1:C:197:GLN:HB2	2.13	0.49
1:C:263:LEU:C	1:C:263:LEU:HD13	2.33	0.49
1:C:343:GLU:HB3	1:C:345:ARG:NH2	2.26	0.49
1:C:35:ILE:O	1:C:38:ALA:HB3	2.13	0.49
1:C:364:LEU:HD12	1:C:365:LYS:H	1.78	0.49
1:C:366:ILE:HG12	1:C:372:VAL:CG2	2.43	0.49
1:D:20:ILE:HD12	1:D:139:SER:OG	2.12	0.49
1:D:548:ILE:HB	1:D:565:LEU:CD1	2.43	0.49
1:D:71:VAL:O	1:D:75:MET:HG2	2.13	0.49
1:B:194:LYS:O	1:B:197:GLN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ARG:O	1:B:379:GLY:N	2.46	0.49
1:C:192:ILE:HG21	1:C:244:MET:HB2	1.94	0.49
1:C:28:ILE:HG23	1:C:29:VAL:N	2.27	0.49
1:D:194:LYS:O	1:D:197:GLN:HB2	2.13	0.49
1:C:220:PHE:C	1:D:441:ARG:HD3	2.33	0.49
1:B:360:ARG:O	1:B:362:ILE:HG12	2.13	0.48
1:C:179:SER:O	1:C:182:ILE:HG22	2.13	0.48
1:C:120:SER:OG	1:C:205:THR:HG23	2.12	0.48
1:C:326:GLN:HB3	1:C:328:LYS:CG	2.42	0.48
1:C:426:VAL:HG11	1:C:490:ALA:HB1	1.92	0.48
1:D:11:GLN:O	1:D:14:ARG:N	2.46	0.48
1:D:366:ILE:HG12	1:D:372:VAL:CG2	2.43	0.48
1:D:369:GLY:HA2	1:D:529:ASN:O	2.12	0.48
1:A:174:LEU:CD2	1:A:261:LEU:HB3	2.43	0.48
1:A:334:VAL:HG13	1:A:334:VAL:O	2.13	0.48
1:A:62:SER:HA	1:A:66:TRP:HD1	1.78	0.48
1:B:120:SER:OG	1:B:205:THR:HG23	2.12	0.48
1:C:335:ILE:HB	1:C:410:TYR:HE1	1.79	0.48
1:C:87:TYR:CE2	1:C:88:CYS:SG	3.07	0.48
1:D:174:LEU:CD2	1:D:261:LEU:HB3	2.42	0.48
1:D:335:ILE:HB	1:D:410:TYR:HE1	1.78	0.48
1:D:449:GLN:HB3	1:D:496:LEU:CD1	2.41	0.48
1:A:335:ILE:HB	1:A:410:TYR:HE1	1.78	0.48
1:A:71:VAL:O	1:A:75:MET:HG2	2.12	0.48
1:B:263:LEU:HD13	1:B:263:LEU:C	2.33	0.48
1:B:326:GLN:HB3	1:B:328:LYS:CG	2.43	0.48
1:B:449:GLN:HB3	1:B:496:LEU:CD1	2.41	0.48
1:B:548:ILE:HB	1:B:565:LEU:CD1	2.42	0.48
1:C:11:GLN:O	1:C:12:THR:C	2.52	0.48
1:C:256:GLN:HA	1:C:299:LYS:CD	2.41	0.48
1:C:344:PHE:HZ	1:C:385:ILE:CD1	2.25	0.48
1:C:377:ARG:O	1:C:379:GLY:N	2.46	0.48
1:C:390:THR:CG2	1:C:419:VAL:HG11	2.42	0.48
1:A:28:ILE:HG23	1:A:29:VAL:N	2.28	0.48
1:A:326:GLN:HB3	1:A:328:LYS:HG2	1.94	0.48
1:A:450:ILE:HG13	1:A:451:GLU:N	2.28	0.48
1:A:492:ALA:O	1:A:493:ARG:C	2.51	0.48
1:B:35:ILE:O	1:B:38:ALA:HB3	2.13	0.48
1:C:108:MET:HE3	1:C:124:LEU:HB3	1.95	0.48
1:C:441:ARG:HD3	1:D:220:PHE:C	2.34	0.48
1:C:461:ASP:O	1:C:465:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:LEU:HB3	1:D:219:ILE:CD1	2.44	0.48
1:D:377:ARG:O	1:D:379:GLY:N	2.46	0.48
1:D:390:THR:CG2	1:D:419:VAL:HG11	2.42	0.48
1:A:134:GLN:NE2	1:A:310:ARG:HE	2.06	0.48
1:A:401:LEU:HD12	1:A:404:GLY:CA	2.44	0.48
1:A:492:ALA:O	1:A:495:LEU:N	2.45	0.48
1:A:419:VAL:HG23	1:A:501:ILE:O	2.13	0.48
1:B:143:LEU:HA	1:B:146:VAL:HG12	1.96	0.48
1:C:213:GLY:HA2	1:D:427:HIS:HD2	1.79	0.48
1:C:292:ILE:HD12	1:D:48:LEU:CG	2.42	0.48
1:C:105:PHE:CZ	1:D:210:MET:HE3	2.48	0.48
1:D:263:LEU:C	1:D:263:LEU:HD13	2.33	0.48
1:D:74:LEU:HD23	1:D:78:ARG:HB3	1.96	0.48
1:A:424:GLN:N	1:A:424:GLN:CD	2.67	0.48
1:B:74:LEU:HD23	1:B:78:ARG:HB3	1.96	0.48
1:C:382:LYS:HB2	1:C:382:LYS:NZ	2.29	0.48
1:C:475:GLY:N	1:C:480:LEU:HD11	2.29	0.48
1:C:548:ILE:HB	1:C:565:LEU:CD1	2.42	0.48
1:C:74:LEU:HD23	1:C:78:ARG:HB3	1.96	0.48
1:C:71:VAL:O	1:C:75:MET:HG2	2.13	0.48
1:D:179:SER:O	1:D:182:ILE:HG22	2.13	0.48
1:D:35:ILE:O	1:D:38:ALA:HB3	2.13	0.48
1:A:269:ALA:CA	1:A:273:PRO:HD2	2.44	0.48
1:A:342:LEU:CD1	1:A:366:ILE:HD12	2.43	0.48
1:A:412:LEU:HD21	1:A:416:ARG:CZ	2.44	0.48
1:C:178:VAL:HA	1:C:258:ILE:CD1	2.43	0.48
1:C:284:ILE:HG23	1:C:284:ILE:O	2.14	0.48
1:C:419:VAL:HG23	1:C:501:ILE:O	2.14	0.48
1:D:143:LEU:HA	1:D:146:VAL:HG12	1.96	0.48
1:D:256:GLN:HA	1:D:299:LYS:CD	2.41	0.48
1:D:558:GLU:OE1	1:D:559:ARG:N	2.46	0.48
1:D:87:TYR:CE2	1:D:88:CYS:SG	3.07	0.48
1:A:110:GLY:O	1:A:112:PRO:HD3	2.14	0.48
1:A:21:ALA:HB3	1:A:22:PRO:CD	2.35	0.48
1:A:344:PHE:HZ	1:A:385:ILE:HD12	1.79	0.48
1:A:412:LEU:HD21	1:A:416:ARG:HH11	1.75	0.48
1:A:421:LEU:HD13	1:A:503:ILE:HB	1.96	0.48
1:B:11:GLN:O	1:B:14:ARG:N	2.46	0.48
1:B:364:LEU:HD12	1:B:365:LYS:H	1.77	0.48
1:A:220:PHE:C	1:B:441:ARG:HD3	2.33	0.48
1:B:76:ILE:HG22	1:B:77:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:GLY:O	1:D:112:PRO:HD3	2.14	0.48
1:D:269:ALA:CA	1:D:273:PRO:HD2	2.44	0.48
1:D:360:ARG:O	1:D:362:ILE:HG12	2.13	0.48
1:D:461:ASP:O	1:D:465:LYS:HG3	2.13	0.48
1:A:475:GLY:H	1:A:480:LEU:HD12	1.78	0.48
1:A:70:VAL:CG1	1:A:71:VAL:N	2.76	0.48
1:B:269:ALA:CA	1:B:273:PRO:HD2	2.44	0.48
1:C:11:GLN:O	1:C:14:ARG:N	2.46	0.48
1:C:165:TRP:CH2	1:C:166:GLN:HG2	2.49	0.48
1:C:220:PHE:O	1:D:441:ARG:HG2	2.13	0.48
1:C:298:LEU:HD23	1:C:298:LEU:C	2.34	0.48
1:D:280:THR:O	1:D:284:ILE:HG22	2.13	0.48
1:D:134:GLN:NE2	1:D:310:ARG:HE	2.06	0.48
1:D:523:LEU:O	1:D:527:GLN:HG2	2.14	0.48
1:A:273:PRO:O	1:A:277:ASP:O	2.32	0.48
1:A:437:ILE:HG23	1:A:493:ARG:HA	1.96	0.48
1:A:475:GLY:O	1:A:478:GLY:N	2.47	0.48
1:A:74:LEU:HD23	1:A:78:ARG:HB3	1.96	0.48
1:B:366:ILE:HG12	1:B:372:VAL:CG2	2.43	0.48
1:B:71:VAL:O	1:B:75:MET:HG2	2.13	0.48
1:C:76:ILE:HG22	1:C:77:LEU:N	2.28	0.48
1:D:193:SER:O	1:D:196:MET:HB3	2.13	0.48
1:D:76:ILE:HG22	1:D:77:LEU:N	2.28	0.48
1:B:254:ILE:O	1:B:257:LEU:HB3	2.14	0.47
1:B:87:TYR:CE2	1:B:88:CYS:SG	3.07	0.47
1:C:110:GLY:O	1:C:112:PRO:HD3	2.14	0.47
1:C:475:GLY:O	1:C:476:GLU:C	2.52	0.47
1:A:165:TRP:CH2	1:A:166:GLN:HG2	2.49	0.47
1:B:169:ILE:C	1:B:170:ILE:HD13	2.34	0.47
1:B:335:ILE:HB	1:B:410:TYR:HE1	1.78	0.47
1:C:342:LEU:C	1:C:343:GLU:HG3	2.34	0.47
1:C:432:THR:HB	1:C:470:LEU:O	2.15	0.47
1:C:467:ASP:O	1:C:468:ASN:CB	2.62	0.47
1:D:467:ASP:O	1:D:468:ASN:CB	2.62	0.47
1:A:276:MET:SD	1:A:276:MET:O	2.72	0.47
1:A:348:THR:HG23	1:A:360:ARG:HA	1.96	0.47
1:B:21:ALA:HB3	1:B:22:PRO:CD	2.36	0.47
1:B:70:VAL:HG13	1:B:71:VAL:N	2.29	0.47
1:C:254:ILE:O	1:C:257:LEU:HB3	2.14	0.47
1:C:111:MET:HE2	1:C:326:GLN:HA	1.96	0.47
1:D:165:TRP:CH2	1:D:166:GLN:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:VAL:HG13	1:D:334:VAL:O	2.14	0.47
1:D:342:LEU:C	1:D:343:GLU:HG3	2.34	0.47
1:A:342:LEU:C	1:A:343:GLU:HG3	2.34	0.47
1:A:461:ASP:O	1:A:465:LYS:HG3	2.14	0.47
1:A:52:LEU:HD11	1:B:289:SER:HB2	1.96	0.47
1:B:541:THR:O	1:B:542:ILE:HG13	2.13	0.47
1:C:252:ASP:CB	1:C:253:PRO:HD3	2.42	0.47
1:C:412:LEU:HD21	1:C:416:ARG:CZ	2.44	0.47
1:D:10:TRP:C	1:D:14:ARG:HB2	2.35	0.47
1:D:475:GLY:O	1:D:476:GLU:C	2.52	0.47
1:A:179:SER:O	1:A:182:ILE:HG22	2.14	0.47
1:A:326:GLN:C	1:A:328:LYS:N	2.64	0.47
1:B:110:GLY:O	1:B:112:PRO:HD3	2.14	0.47
1:B:178:VAL:HA	1:B:258:ILE:CD1	2.43	0.47
1:B:334:VAL:HG13	1:B:334:VAL:O	2.15	0.47
1:C:185:VAL:HG12	1:C:189:PHE:CE2	2.50	0.47
1:C:475:GLY:O	1:C:478:GLY:N	2.47	0.47
1:C:62:SER:HA	1:C:66:TRP:HD1	1.80	0.47
1:D:284:ILE:HG23	1:D:284:ILE:O	2.14	0.47
1:D:298:LEU:HD23	1:D:298:LEU:C	2.34	0.47
1:D:372:VAL:O	1:D:533:LEU:HD22	2.15	0.47
1:D:382:LYS:NZ	1:D:382:LYS:HB2	2.29	0.47
1:C:482:SER:HB2	2:D:5004:ANP:H5'1	1.96	0.47
1:A:143:LEU:HA	1:A:146:VAL:HG12	1.96	0.47
1:A:298:LEU:HD23	1:A:298:LEU:C	2.34	0.47
1:A:475:GLY:N	1:A:480:LEU:HD12	2.30	0.47
1:B:192:ILE:HG22	1:B:244:MET:HB2	1.97	0.47
1:B:273:PRO:O	1:B:276:MET:HB3	2.15	0.47
1:B:424:GLN:N	1:B:424:GLN:CD	2.68	0.47
1:C:339:THR:HG23	1:C:403:ASP:OD2	2.15	0.47
1:C:342:LEU:CD1	1:C:366:ILE:HD12	2.44	0.47
1:C:523:LEU:O	1:C:527:GLN:HG2	2.14	0.47
1:D:21:ALA:HB3	1:D:22:PRO:CD	2.36	0.47
1:D:339:THR:HG23	1:D:403:ASP:OD2	2.15	0.47
1:D:342:LEU:CD1	1:D:366:ILE:HD12	2.44	0.47
1:D:419:VAL:HG23	1:D:501:ILE:O	2.14	0.47
1:B:89:ILE:CD1	1:B:144:ILE:HD13	2.45	0.47
1:B:391:ARG:C	1:B:393:TYR:H	2.18	0.47
1:C:348:THR:HG23	1:C:360:ARG:HA	1.97	0.47
1:C:372:VAL:O	1:C:533:LEU:HD22	2.15	0.47
1:C:98:MET:HA	1:C:101:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:VAL:HG12	1:D:189:PHE:CE2	2.50	0.47
1:D:348:THR:HG23	1:D:360:ARG:HA	1.97	0.47
1:D:475:GLY:N	1:D:480:LEU:HD11	2.29	0.47
1:A:221:GLY:O	1:B:441:ARG:CD	2.63	0.47
1:A:441:ARG:HA	1:A:441:ARG:HD2	1.69	0.47
1:A:70:VAL:HG13	1:A:71:VAL:N	2.30	0.47
1:B:141:GLY:O	1:B:144:ILE:CG1	2.63	0.47
1:B:185:VAL:HG12	1:B:189:PHE:CE2	2.50	0.47
1:B:256:GLN:HA	1:B:299:LYS:CD	2.41	0.47
1:B:298:LEU:HD23	1:B:298:LEU:C	2.34	0.47
1:B:492:ALA:O	1:B:493:ARG:C	2.53	0.47
1:B:506:GLU:N	1:B:535:ILE:O	2.48	0.47
1:C:269:ALA:CA	1:C:273:PRO:HD2	2.44	0.47
1:C:427:HIS:CD2	1:D:213:GLY:HA2	2.49	0.47
1:D:273:PRO:O	1:D:276:MET:HB3	2.15	0.47
1:D:391:ARG:C	1:D:393:TYR:H	2.18	0.47
1:D:492:ALA:O	1:D:495:LEU:N	2.47	0.47
1:A:512:ASP:HB3	1:A:515:SER:OG	2.15	0.47
1:B:16:LEU:CA	1:B:319:PHE:HZ	2.27	0.47
1:B:284:ILE:HG23	1:B:284:ILE:O	2.14	0.47
1:B:475:GLY:O	1:B:476:GLU:C	2.52	0.47
1:B:475:GLY:N	1:B:480:LEU:HD11	2.29	0.47
1:B:98:MET:HA	1:B:101:ARG:HD3	1.96	0.47
1:C:421:LEU:HD13	1:C:503:ILE:HB	1.97	0.47
1:D:254:ILE:O	1:D:257:LEU:HB3	2.14	0.47
1:D:274:SER:C	1:D:276:MET:H	2.18	0.47
1:D:98:MET:HA	1:D:101:ARG:HD3	1.97	0.47
1:A:449:GLN:HB3	1:A:496:LEU:CD1	2.44	0.47
1:B:475:GLY:O	1:B:478:GLY:N	2.47	0.47
1:C:21:ALA:HB3	1:C:22:PRO:CD	2.36	0.47
1:C:273:PRO:O	1:C:276:MET:HB3	2.15	0.47
1:C:274:SER:C	1:C:276:MET:H	2.18	0.47
1:C:283:THR:C	1:C:285:THR:H	2.18	0.47
1:C:512:ASP:HB3	1:C:515:SER:OG	2.14	0.47
1:C:543:GLU:HG2	1:C:562:HIS:CE1	2.50	0.47
1:C:89:ILE:CD1	1:C:144:ILE:HD13	2.45	0.47
1:D:11:GLN:O	1:D:12:THR:C	2.52	0.47
1:D:169:ILE:C	1:D:170:ILE:HD13	2.35	0.47
1:D:424:GLN:N	1:D:424:GLN:CD	2.68	0.47
1:D:512:ASP:HB3	1:D:515:SER:OG	2.14	0.47
1:A:11:GLN:CG	1:A:12:THR:N	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:TRP:CH2	1:B:166:GLN:HG2	2.49	0.47
1:B:372:VAL:O	1:B:533:LEU:HD22	2.15	0.47
1:C:132:SER:O	1:C:135:VAL:HG12	2.15	0.47
1:C:334:VAL:O	1:C:334:VAL:HG13	2.15	0.47
1:C:391:ARG:C	1:C:393:TYR:H	2.18	0.47
1:D:192:ILE:HG22	1:D:244:MET:HB2	1.97	0.47
1:D:283:THR:C	1:D:285:THR:H	2.18	0.47
1:C:221:GLY:O	1:D:441:ARG:NE	2.48	0.47
1:A:475:GLY:O	1:A:476:GLU:C	2.52	0.46
1:A:96:VAL:O	1:A:99:THR:HG22	2.15	0.46
1:B:17:TRP:N	1:B:18:PRO:CD	2.79	0.46
1:B:348:THR:HG23	1:B:360:ARG:HA	1.97	0.46
1:B:342:LEU:CD1	1:B:366:ILE:HD12	2.44	0.46
1:B:419:VAL:HG23	1:B:501:ILE:O	2.14	0.46
1:B:455:ARG:HD2	1:B:456:MET:CE	2.46	0.46
1:B:467:ASP:O	1:B:468:ASN:CB	2.63	0.46
1:B:523:LEU:O	1:B:527:GLN:HG2	2.14	0.46
1:C:169:ILE:C	1:C:170:ILE:HD13	2.35	0.46
1:C:424:GLN:N	1:C:424:GLN:CD	2.68	0.46
1:D:89:ILE:CD1	1:D:144:ILE:HD13	2.45	0.46
1:D:401:LEU:HD12	1:D:404:GLY:CA	2.45	0.46
1:D:475:GLY:O	1:D:478:GLY:N	2.47	0.46
1:D:565:LEU:HD13	1:D:572:TYR:CD2	2.50	0.46
1:D:70:VAL:HG13	1:D:71:VAL:N	2.29	0.46
1:A:390:THR:CG2	1:A:419:VAL:HG11	2.43	0.46
1:A:496:LEU:HD12	1:A:496:LEU:O	2.15	0.46
1:A:523:LEU:O	1:A:527:GLN:HG2	2.16	0.46
1:A:557:VAL:O	1:A:557:VAL:CG1	2.64	0.46
1:B:274:SER:C	1:B:276:MET:H	2.18	0.46
1:B:565:LEU:HD13	1:B:572:TYR:CD2	2.50	0.46
1:C:221:GLY:O	1:D:441:ARG:CD	2.63	0.46
1:C:401:LEU:HD12	1:C:404:GLY:CA	2.45	0.46
1:C:520:GLN:HA	1:C:520:GLN:NE2	2.30	0.46
1:C:70:VAL:HG13	1:C:71:VAL:N	2.29	0.46
1:D:17:TRP:N	1:D:18:PRO:CD	2.79	0.46
1:A:296:ARG:HD3	1:A:297:PRO:N	2.31	0.46
1:A:316:GLN:NE2	1:A:319:PHE:CD1	2.83	0.46
1:A:372:VAL:O	1:A:533:LEU:HD22	2.15	0.46
1:B:132:SER:O	1:B:135:VAL:HG12	2.15	0.46
1:B:256:GLN:HG2	1:B:299:LYS:HD2	1.98	0.46
1:B:339:THR:HG23	1:B:403:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:PHE:HB2	1:B:400:ILE:HA	1.97	0.46
1:B:520:GLN:NE2	1:B:520:GLN:HA	2.30	0.46
1:C:267:LEU:CD2	1:D:67:MET:HA	2.44	0.46
1:D:455:ARG:C	1:D:457:ALA:N	2.69	0.46
1:D:421:LEU:HD13	1:D:503:ILE:HB	1.97	0.46
1:D:543:GLU:HG2	1:D:562:HIS:CE1	2.50	0.46
1:A:89:ILE:CD1	1:A:144:ILE:HD13	2.46	0.46
1:A:274:SER:C	1:A:276:MET:H	2.18	0.46
1:A:309:GLN:O	1:A:310:ARG:C	2.53	0.46
1:A:344:PHE:HB2	1:A:400:ILE:HA	1.96	0.46
1:A:426:VAL:HG11	1:A:490:ALA:HB1	1.94	0.46
1:A:64:LEU:HB2	1:B:271:SER:OG	2.15	0.46
1:A:76:ILE:HG22	1:A:77:LEU:N	2.29	0.46
1:B:252:ASP:CB	1:B:253:PRO:HD3	2.43	0.46
1:B:342:LEU:C	1:B:343:GLU:HG3	2.34	0.46
1:B:421:LEU:HD13	1:B:503:ILE:HB	1.97	0.46
1:B:512:ASP:HB3	1:B:515:SER:OG	2.14	0.46
1:C:17:TRP:N	1:C:18:PRO:CD	2.79	0.46
1:C:91:TRP:HA	1:D:242:MET:HE1	1.95	0.46
1:D:132:SER:O	1:D:135:VAL:HG12	2.15	0.46
1:D:16:LEU:CA	1:D:319:PHE:HZ	2.28	0.46
1:D:455:ARG:HD2	1:D:456:MET:HE1	1.98	0.46
1:D:432:THR:HB	1:D:470:LEU:O	2.15	0.46
1:A:108:MET:HE3	1:A:124:LEU:HB3	1.97	0.46
1:C:192:ILE:HG22	1:C:244:MET:HB2	1.97	0.46
1:C:344:PHE:HB2	1:C:400:ILE:HA	1.97	0.46
1:C:535:ILE:O	1:C:535:ILE:CD1	2.62	0.46
1:D:541:THR:O	1:D:542:ILE:HG13	2.15	0.46
1:A:185:VAL:HG12	1:A:189:PHE:CE2	2.50	0.46
1:A:506:GLU:N	1:A:535:ILE:O	2.48	0.46
1:A:543:GLU:HG2	1:A:562:HIS:CE1	2.51	0.46
1:B:10:TRP:C	1:B:14:ARG:HB2	2.35	0.46
1:B:543:GLU:HG2	1:B:562:HIS:CE1	2.50	0.46
1:C:143:LEU:HA	1:C:146:VAL:HG12	1.96	0.46
1:C:441:ARG:CD	1:D:221:GLY:C	2.83	0.46
1:D:412:LEU:HD21	1:D:416:ARG:CZ	2.44	0.46
1:A:217:VAL:O	1:A:217:VAL:HG12	2.16	0.46
1:A:535:ILE:CD1	1:A:535:ILE:O	2.61	0.46
1:B:432:THR:HB	1:B:470:LEU:O	2.15	0.46
1:C:16:LEU:CA	1:C:319:PHE:HZ	2.27	0.46
1:C:455:ARG:HD2	1:C:456:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:ALA:O	1:C:495:LEU:N	2.47	0.46
1:C:541:THR:O	1:C:542:ILE:HG13	2.15	0.46
1:D:256:GLN:HG2	1:D:299:LYS:HD2	1.98	0.46
1:D:326:GLN:O	1:D:328:LYS:N	2.49	0.46
1:D:437:ILE:HG23	1:D:493:ARG:HA	1.98	0.46
1:D:520:GLN:NE2	1:D:520:GLN:HA	2.30	0.46
1:A:112:PRO:O	1:A:113:VAL:CG1	2.60	0.46
1:A:132:SER:O	1:A:135:VAL:HG12	2.16	0.46
1:A:283:THR:C	1:A:285:THR:H	2.19	0.46
1:A:131:ASP:CB	1:A:318:LEU:HD23	2.46	0.46
1:A:366:ILE:HG12	1:A:372:VAL:CG2	2.42	0.46
1:A:520:GLN:HA	1:A:520:GLN:NE2	2.29	0.46
1:A:63:VAL:HG11	1:B:271:SER:CA	2.46	0.46
1:A:98:MET:HA	1:A:101:ARG:HD3	1.97	0.46
1:B:157:PHE:C	1:B:157:PHE:CD1	2.89	0.46
1:B:16:LEU:HD12	1:B:315:CYS:CB	2.46	0.46
1:A:427:HIS:CD2	1:B:213:GLY:HA2	2.50	0.46
1:C:141:GLY:O	1:C:144:ILE:CG1	2.63	0.46
1:C:492:ALA:O	1:C:493:ARG:C	2.53	0.46
1:D:112:PRO:O	1:D:113:VAL:CG1	2.62	0.46
1:A:326:GLN:O	1:A:328:LYS:N	2.49	0.46
1:A:455:ARG:HD2	1:A:456:MET:CE	2.45	0.46
1:B:382:LYS:HB2	1:B:382:LYS:NZ	2.30	0.46
1:B:437:ILE:HG23	1:B:493:ARG:HA	1.98	0.46
1:C:437:ILE:HG23	1:C:493:ARG:HA	1.98	0.46
1:C:67:MET:SD	1:D:264:ALA:O	2.73	0.46
1:D:344:PHE:HB2	1:D:400:ILE:HA	1.97	0.46
1:D:455:ARG:HD2	1:D:456:MET:CE	2.46	0.46
1:D:62:SER:HA	1:D:66:TRP:HD1	1.80	0.46
1:C:256:GLN:HE22	1:D:78:ARG:HG2	1.80	0.46
1:A:108:MET:O	1:A:111:MET:HB2	2.16	0.46
1:A:218:LEU:N	1:A:218:LEU:HD12	2.31	0.46
1:A:223:GLN:O	1:A:226:GLU:HB2	2.16	0.46
1:A:459:ALA:HB1	1:A:462:PHE:CE1	2.51	0.46
1:A:432:THR:HB	1:A:470:LEU:O	2.16	0.46
1:B:111:MET:HE2	1:B:326:GLN:HA	1.98	0.46
1:C:10:TRP:C	1:C:14:ARG:HB2	2.35	0.46
1:C:96:VAL:O	1:C:99:THR:HG22	2.16	0.46
1:D:492:ALA:O	1:D:493:ARG:C	2.53	0.46
1:D:506:GLU:N	1:D:535:ILE:O	2.48	0.46
1:A:344:PHE:HZ	1:A:385:ILE:CD1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLN:O	1:B:12:THR:C	2.52	0.45
1:B:401:LEU:HD12	1:B:404:GLY:CA	2.45	0.45
1:B:62:SER:HA	1:B:66:TRP:HD1	1.79	0.45
1:C:10:TRP:O	1:C:11:GLN:HB3	2.16	0.45
1:C:145:THR:HA	1:C:148:ARG:HB3	1.98	0.45
1:C:565:LEU:HD13	1:C:572:TYR:CD2	2.50	0.45
1:D:401:LEU:CD2	1:D:401:LEU:N	2.74	0.45
1:A:100:MET:CE	1:A:100:MET:HA	2.46	0.45
1:A:254:ILE:O	1:A:257:LEU:HB3	2.16	0.45
1:A:273:PRO:O	1:A:276:MET:HB3	2.17	0.45
1:A:474:ILE:CG1	1:A:475:GLY:N	2.80	0.45
1:A:63:VAL:HG12	1:A:64:LEU:N	2.30	0.45
1:B:11:GLN:CA	1:B:14:ARG:HB3	2.46	0.45
1:B:296:ARG:HD3	1:B:297:PRO:N	2.31	0.45
1:C:326:GLN:O	1:C:328:LYS:N	2.49	0.45
1:C:349:PHE:HA	1:C:396:ASP:HB3	1.97	0.45
1:D:100:MET:CE	1:D:100:MET:HA	2.46	0.45
1:A:343:GLU:HB3	1:A:345:ARG:HH21	1.81	0.45
1:A:437:ILE:O	1:A:440:ALA:HB3	2.16	0.45
1:B:10:TRP:O	1:B:11:GLN:HB3	2.16	0.45
1:B:326:GLN:O	1:B:328:LYS:N	2.49	0.45
1:B:412:LEU:HD21	1:B:416:ARG:CZ	2.44	0.45
1:B:441:ARG:HA	1:B:441:ARG:HD2	1.60	0.45
1:C:100:MET:CE	1:C:100:MET:HA	2.46	0.45
1:C:157:PHE:CD1	1:C:157:PHE:C	2.89	0.45
1:C:463:ILE:O	1:C:466:MET:HG2	2.17	0.45
1:A:118:LYS:NZ	1:A:352:PRO:HG3	2.32	0.45
1:A:169:ILE:C	1:A:170:ILE:HD13	2.37	0.45
1:A:174:LEU:HD22	1:A:262:ALA:CB	2.40	0.45
1:A:192:ILE:HG22	1:A:244:MET:HB2	1.98	0.45
1:A:111:MET:HE2	1:A:326:GLN:HA	1.98	0.45
1:B:190:ARG:HA	1:B:313:ALA:HB2	1.98	0.45
1:B:508:THR:O	1:B:510:ALA:N	2.50	0.45
1:C:296:ARG:HD3	1:C:297:PRO:N	2.31	0.45
1:C:439:TYR:HD2	1:D:220:PHE:HZ	1.63	0.45
1:D:157:PHE:C	1:D:157:PHE:CD1	2.90	0.45
1:D:207:ALA:O	1:D:210:MET:HB3	2.17	0.45
1:D:366:ILE:HG23	1:D:372:VAL:HG23	1.99	0.45
1:A:112:PRO:O	1:A:327:GLU:OE1	2.34	0.45
1:A:467:ASP:O	1:A:468:ASN:CB	2.61	0.45
1:A:565:LEU:HD13	1:A:572:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:GLU:HB3	1:C:345:ARG:HH21	1.81	0.45
1:D:441:ARG:HD2	1:D:441:ARG:HA	1.62	0.45
1:D:96:VAL:O	1:D:99:THR:HG22	2.16	0.45
1:A:190:ARG:HA	1:A:313:ALA:HB2	1.97	0.45
1:A:315:CYS:SG	1:A:319:PHE:CE2	3.10	0.45
1:A:455:ARG:C	1:A:457:ALA:N	2.69	0.45
1:B:207:ALA:O	1:B:210:MET:HB3	2.17	0.45
1:C:175:ALA:N	1:C:176:PRO:CD	2.80	0.45
1:C:253:PRO:HG3	1:D:79:GLY:HA2	1.99	0.45
1:A:252:ASP:CB	1:A:253:PRO:HD3	2.44	0.45
1:A:75:MET:CE	1:B:257:LEU:HA	2.46	0.45
1:B:104:LEU:O	1:B:105:PHE:C	2.55	0.45
1:B:431:ASP:HB3	1:B:435:ASN:HB2	1.99	0.45
1:B:463:ILE:O	1:B:466:MET:HG2	2.17	0.45
1:B:492:ALA:O	1:B:495:LEU:N	2.47	0.45
1:B:535:ILE:CD1	1:B:535:ILE:O	2.62	0.45
1:C:273:PRO:O	1:C:277:ASP:O	2.35	0.45
1:C:16:LEU:HD12	1:C:315:CYS:CB	2.46	0.45
1:C:347:VAL:HG13	1:C:395:ILE:CD1	2.31	0.45
1:C:439:TYR:O	1:D:220:PHE:CE1	2.69	0.45
1:D:339:THR:HG23	1:D:339:THR:O	2.17	0.45
1:D:431:ASP:HB3	1:D:435:ASN:HB2	1.99	0.45
1:D:459:ALA:HB1	1:D:462:PHE:CE1	2.52	0.45
1:A:178:VAL:CA	1:A:258:ILE:HD13	2.45	0.45
1:B:223:GLN:H	1:B:223:GLN:CD	2.12	0.45
1:B:273:PRO:O	1:B:277:ASP:O	2.35	0.45
1:B:343:GLU:HB3	1:B:345:ARG:HH21	1.81	0.45
1:D:10:TRP:O	1:D:11:GLN:HB3	2.16	0.45
1:D:11:GLN:CA	1:D:14:ARG:HB3	2.46	0.45
1:D:273:PRO:O	1:D:277:ASP:O	2.35	0.45
1:D:296:ARG:HD3	1:D:297:PRO:N	2.31	0.45
1:D:190:ARG:HA	1:D:313:ALA:HB2	1.98	0.45
1:D:474:ILE:C	1:D:480:LEU:HD11	2.37	0.45
1:D:74:LEU:O	1:D:78:ARG:HB3	2.17	0.45
1:A:437:ILE:HA	1:A:493:ARG:HB2	1.99	0.45
1:A:508:THR:O	1:A:510:ALA:N	2.50	0.45
1:A:535:ILE:HG23	1:A:535:ILE:O	2.16	0.45
1:B:283:THR:C	1:B:285:THR:H	2.18	0.45
1:B:474:ILE:C	1:B:480:LEU:HD11	2.37	0.45
1:B:96:VAL:O	1:B:99:THR:HG22	2.16	0.45
1:C:100:MET:HA	1:C:100:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LEU:O	1:C:105:PHE:C	2.55	0.45
1:C:337:ARG:HD2	1:C:338:ALA:N	2.26	0.45
1:C:508:THR:O	1:C:510:ALA:N	2.50	0.45
1:C:512:ASP:HB3	1:C:515:SER:CB	2.47	0.45
1:A:145:THR:HA	1:A:148:ARG:HB3	1.99	0.45
1:A:197:GLN:O	1:A:200:MET:N	2.50	0.45
1:B:217:VAL:O	1:B:217:VAL:HG12	2.17	0.45
1:B:223:GLN:O	1:B:226:GLU:HB2	2.17	0.45
1:B:382:LYS:HB2	1:B:382:LYS:HZ2	1.81	0.45
1:C:207:ALA:O	1:C:210:MET:HB3	2.17	0.45
1:C:439:TYR:HB3	1:D:220:PHE:HZ	1.75	0.45
1:D:16:LEU:HD12	1:D:315:CYS:CB	2.46	0.45
1:D:175:ALA:N	1:D:176:PRO:CD	2.80	0.45
1:D:468:ASN:HB2	1:D:472:THR:OG1	2.17	0.45
1:A:157:PHE:C	1:A:157:PHE:CD1	2.90	0.44
1:A:249:SER:HB2	1:B:86:SER:CB	2.47	0.44
1:A:316:GLN:HA	1:A:316:GLN:OE1	2.17	0.44
1:A:445:TYR:HD2	1:A:496:LEU:HD21	1.83	0.44
1:A:468:ASN:HB2	1:A:472:THR:OG1	2.17	0.44
1:A:93:SER:OG	1:A:94:GLY:N	2.50	0.44
1:B:339:THR:O	1:B:339:THR:HG23	2.17	0.44
1:B:431:ASP:HB3	1:B:432:THR:H	1.46	0.44
1:B:459:ALA:HB1	1:B:462:PHE:CE1	2.52	0.44
1:B:468:ASN:HB2	1:B:472:THR:OG1	2.17	0.44
1:C:256:GLN:HG2	1:C:299:LYS:HD2	1.98	0.44
1:C:260:SER:OG	1:D:74:LEU:HD13	2.17	0.44
1:C:395:ILE:CG1	1:C:396:ASP:H	2.14	0.44
1:C:474:ILE:C	1:C:480:LEU:HD11	2.37	0.44
1:D:316:GLN:HA	1:D:316:GLN:OE1	2.17	0.44
1:B:390:THR:CG2	1:B:419:VAL:HG11	2.42	0.44
1:C:455:ARG:C	1:C:457:ALA:N	2.69	0.44
1:D:108:MET:O	1:D:111:MET:HB2	2.17	0.44
1:D:111:MET:HE2	1:D:326:GLN:HA	1.98	0.44
1:D:343:GLU:HB3	1:D:345:ARG:HH21	1.81	0.44
1:A:178:VAL:HA	1:A:258:ILE:CD1	2.42	0.44
1:A:37:ASN:HA	1:A:37:ASN:HD22	1.53	0.44
1:C:10:TRP:CG	1:C:11:GLN:N	2.85	0.44
1:C:108:MET:O	1:C:111:MET:HB2	2.17	0.44
1:C:437:ILE:O	1:C:440:ALA:HB3	2.18	0.44
1:C:506:GLU:N	1:C:535:ILE:O	2.48	0.44
1:D:463:ILE:O	1:D:466:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLN:HA	1:A:520:GLN:HE21	1.82	0.44
1:A:539:LEU:HA	1:A:542:ILE:CD1	2.31	0.44
1:B:100:MET:CE	1:B:100:MET:HA	2.46	0.44
1:B:10:TRP:CG	1:B:11:GLN:N	2.85	0.44
1:B:309:GLN:O	1:B:310:ARG:C	2.56	0.44
1:C:223:GLN:O	1:C:226:GLU:HB2	2.18	0.44
1:C:468:ASN:HB2	1:C:472:THR:OG1	2.17	0.44
1:D:10:TRP:CG	1:D:11:GLN:N	2.85	0.44
1:A:512:ASP:HB3	1:A:515:SER:CB	2.47	0.44
1:A:74:LEU:O	1:A:75:MET:C	2.55	0.44
1:B:145:THR:HA	1:B:148:ARG:HB3	1.98	0.44
1:B:142:ALA:HB1	1:B:308:PHE:HD2	1.83	0.44
1:A:512:ASP:HB2	1:B:378:SER:CB	2.48	0.44
1:B:74:LEU:O	1:B:78:ARG:HB3	2.17	0.44
1:C:11:GLN:CA	1:C:14:ARG:HB3	2.46	0.44
1:C:63:VAL:HG12	1:C:64:LEU:N	2.32	0.44
1:C:74:LEU:O	1:C:78:ARG:HB3	2.17	0.44
1:C:97:VAL:CG1	1:C:98:MET:N	2.81	0.44
1:D:141:GLY:O	1:D:144:ILE:CG1	2.63	0.44
1:D:145:THR:HA	1:D:148:ARG:HB3	1.98	0.44
1:D:218:LEU:HD12	1:D:218:LEU:N	2.32	0.44
1:D:223:GLN:CD	1:D:223:GLN:H	2.12	0.44
1:D:380:SER:O	1:D:382:LYS:N	2.49	0.44
1:A:104:LEU:O	1:A:105:PHE:C	2.54	0.44
1:A:256:GLN:HG2	1:A:299:LYS:HD2	1.99	0.44
1:A:366:ILE:HG23	1:A:372:VAL:HG23	2.00	0.44
1:B:437:ILE:O	1:B:440:ALA:HB3	2.17	0.44
1:B:512:ASP:HB3	1:B:515:SER:CB	2.47	0.44
1:B:557:VAL:CG1	1:B:557:VAL:O	2.66	0.44
1:C:217:VAL:HG12	1:C:217:VAL:O	2.17	0.44
1:C:238:ARG:HG3	1:D:95:LYS:NZ	2.33	0.44
1:C:339:THR:O	1:C:339:THR:HG23	2.17	0.44
1:D:508:THR:HG22	1:D:538:ARG:NH2	2.33	0.44
1:A:315:CYS:SG	1:A:319:PHE:CD2	3.10	0.44
1:A:431:ASP:HB3	1:A:435:ASN:HB2	1.98	0.44
1:A:450:ILE:O	1:A:451:GLU:C	2.56	0.44
1:A:512:ASP:HB3	1:A:515:SER:HB2	2.00	0.44
1:B:108:MET:O	1:B:111:MET:HB2	2.17	0.44
1:B:520:GLN:HE21	1:B:520:GLN:HA	1.82	0.44
1:B:508:THR:HG22	1:B:538:ARG:NH2	2.33	0.44
1:C:21:ALA:CB	1:C:22:PRO:HD3	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ALA:HB1	1:D:308:PHE:HD2	1.83	0.44
1:D:520:GLN:HE21	1:D:520:GLN:HA	1.82	0.44
1:A:113:VAL:HG12	1:A:327:GLU:CD	2.38	0.44
1:A:29:VAL:CG1	1:A:87:TYR:HE2	2.28	0.44
1:B:170:ILE:N	1:B:170:ILE:HD13	2.33	0.44
1:B:218:LEU:HD12	1:B:218:LEU:N	2.32	0.44
1:C:190:ARG:HA	1:C:313:ALA:HB2	1.98	0.44
1:C:459:ALA:HB1	1:C:462:PHE:CE1	2.52	0.44
1:D:252:ASP:CB	1:D:253:PRO:HD3	2.43	0.44
1:D:445:TYR:HD2	1:D:496:LEU:HD21	1.83	0.44
1:D:466:MET:CE	1:D:472:THR:HG21	2.48	0.44
1:D:474:ILE:CG1	1:D:475:GLY:N	2.81	0.44
1:A:342:LEU:CD2	1:A:366:ILE:HD12	2.48	0.44
1:A:441:ARG:HD3	1:B:220:PHE:C	2.38	0.44
1:A:97:VAL:CG1	1:A:98:MET:H	2.30	0.44
1:B:49:LYS:HB3	1:B:50:PRO:HD3	2.00	0.44
1:B:67:MET:CB	1:B:68:PRO:HD3	2.45	0.44
1:C:170:ILE:N	1:C:170:ILE:HD13	2.33	0.44
1:C:475:GLY:O	1:C:477:ASN:N	2.51	0.44
1:C:508:THR:HG22	1:C:538:ARG:NH2	2.33	0.44
1:C:102:ARG:NH2	1:D:238:ARG:CZ	2.81	0.44
1:D:37:ASN:HD22	1:D:37:ASN:HA	1.54	0.44
1:D:475:GLY:O	1:D:477:ASN:N	2.51	0.44
1:C:378:SER:N	1:D:512:ASP:HB2	2.23	0.44
1:A:338:ALA:O	1:A:339:THR:O	2.32	0.43
1:A:95:LYS:NZ	1:B:239:LEU:HD21	2.33	0.43
1:B:316:GLN:OE1	1:B:316:GLN:HA	2.17	0.43
1:B:475:GLY:O	1:B:477:ASN:N	2.51	0.43
1:B:496:LEU:O	1:B:496:LEU:HD12	2.18	0.43
1:B:580:PHE:HB2	1:B:581:GLY:H	1.68	0.43
1:C:218:LEU:HD12	1:C:218:LEU:N	2.32	0.43
1:C:380:SER:O	1:C:382:LYS:N	2.50	0.43
1:C:520:GLN:HE21	1:C:520:GLN:HA	1.82	0.43
1:C:557:VAL:O	1:C:557:VAL:CG1	2.66	0.43
1:D:203:VAL:HA	1:D:233:VAL:HG11	2.00	0.43
1:A:218:LEU:HB3	1:B:416:ARG:HD3	2.00	0.43
1:A:463:ILE:O	1:A:466:MET:HG2	2.17	0.43
1:B:445:TYR:HD2	1:B:496:LEU:HD21	1.83	0.43
1:C:112:PRO:O	1:C:113:VAL:CG1	2.62	0.43
1:D:104:LEU:O	1:D:105:PHE:C	2.56	0.43
1:A:10:TRP:CG	1:A:11:GLN:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:THR:O	1:A:388:LEU:HB2	2.18	0.43
1:A:488:ARG:O	1:A:491:ILE:HB	2.18	0.43
1:A:416:ARG:HD3	1:B:218:LEU:HB3	2.00	0.43
1:A:439:TYR:CD2	1:B:220:PHE:HZ	2.33	0.43
1:B:333:ARG:CB	1:B:333:ARG:HH11	2.30	0.43
1:B:72:ILE:N	1:B:72:ILE:CD1	2.81	0.43
1:C:416:ARG:NH1	1:D:218:LEU:CD2	2.78	0.43
1:C:474:ILE:CG1	1:C:475:GLY:N	2.81	0.43
1:C:72:ILE:CD1	1:C:72:ILE:N	2.81	0.43
1:D:183:ARG:HD2	1:D:183:ARG:HA	1.84	0.43
1:D:178:VAL:CA	1:D:258:ILE:HD13	2.47	0.43
1:D:508:THR:O	1:D:510:ALA:N	2.50	0.43
1:D:512:ASP:HB3	1:D:515:SER:CB	2.47	0.43
1:B:466:MET:CE	1:B:472:THR:HG21	2.48	0.43
1:C:309:GLN:O	1:C:310:ARG:C	2.56	0.43
1:C:131:ASP:CB	1:C:318:LEU:HD23	2.48	0.43
1:C:365:LYS:HE2	1:C:367:PRO:HG3	2.01	0.43
1:C:513:THR:CG2	1:D:575:LEU:HD22	2.49	0.43
1:C:96:VAL:HA	1:C:99:THR:HG22	2.01	0.43
1:D:309:GLN:O	1:D:310:ARG:C	2.56	0.43
1:D:437:ILE:O	1:D:440:ALA:HB3	2.18	0.43
1:D:475:GLY:H	1:D:480:LEU:HD12	1.83	0.43
1:D:577:LYS:C	1:D:579:GLN:N	2.72	0.43
1:A:17:TRP:N	1:A:18:PRO:CD	2.81	0.43
1:A:480:LEU:O	1:A:481:LEU:HB3	2.17	0.43
1:A:84:ILE:O	1:A:87:TYR:CD2	2.69	0.43
1:B:175:ALA:N	1:B:176:PRO:CD	2.80	0.43
1:B:131:ASP:CB	1:B:318:LEU:HD23	2.48	0.43
1:B:366:ILE:HG23	1:B:372:VAL:HG23	1.99	0.43
1:B:474:ILE:CG1	1:B:475:GLY:N	2.81	0.43
1:B:96:VAL:HA	1:B:99:THR:HG22	2.01	0.43
1:C:174:LEU:HD22	1:C:262:ALA:CB	2.39	0.43
1:C:466:MET:CE	1:C:472:THR:HG21	2.48	0.43
1:C:512:ASP:HB3	1:C:515:SER:HB2	2.01	0.43
1:D:496:LEU:HD12	1:D:496:LEU:O	2.18	0.43
1:D:63:VAL:HG12	1:D:64:LEU:N	2.32	0.43
1:A:175:ALA:N	1:A:176:PRO:CD	2.82	0.43
1:A:473:ILE:O	1:A:473:ILE:HG23	2.19	0.43
1:A:49:LYS:HB3	1:A:50:PRO:HD3	2.01	0.43
1:B:58:LYS:HZ1	1:B:61:ARG:CG	2.31	0.43
1:C:214:HIS:O	1:C:215:LYS:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ILE:HG23	1:C:372:VAL:HG23	1.99	0.43
1:C:378:SER:HB3	1:D:512:ASP:HB2	2.01	0.43
1:C:441:ARG:CG	1:D:220:PHE:O	2.66	0.43
1:C:49:LYS:HB3	1:C:50:PRO:HD3	2.00	0.43
1:C:74:LEU:O	1:C:75:MET:C	2.57	0.43
1:D:217:VAL:O	1:D:217:VAL:HG12	2.17	0.43
1:D:223:GLN:O	1:D:226:GLU:HB2	2.18	0.43
1:D:74:LEU:O	1:D:75:MET:C	2.57	0.43
1:A:113:VAL:CG1	1:A:114:ALA:N	2.73	0.43
1:A:333:ARG:CB	1:A:333:ARG:HH11	2.32	0.43
1:A:475:GLY:O	1:A:477:ASN:N	2.52	0.43
1:A:97:VAL:CG1	1:A:98:MET:N	2.81	0.43
1:B:561:THR:O	1:B:562:HIS:C	2.57	0.43
1:C:437:ILE:HA	1:C:493:ARG:HB2	2.01	0.43
1:C:78:ARG:CG	1:D:256:GLN:HE22	2.31	0.43
1:D:412:LEU:HD21	1:D:416:ARG:HD2	2.01	0.43
1:D:72:ILE:CD1	1:D:72:ILE:N	2.81	0.43
1:A:203:VAL:HA	1:A:233:VAL:HG11	2.00	0.43
1:A:445:TYR:HB3	1:A:446:SER:H	1.73	0.43
1:A:561:THR:O	1:A:562:HIS:C	2.57	0.43
1:B:512:ASP:HB3	1:B:515:SER:HB2	2.01	0.43
1:B:63:VAL:HG12	1:B:64:LEU:N	2.32	0.43
1:C:316:GLN:OE1	1:C:316:GLN:HA	2.17	0.43
1:C:475:GLY:H	1:C:480:LEU:HD12	1.83	0.43
1:C:218:LEU:CD2	1:D:416:ARG:NH1	2.79	0.43
1:D:97:VAL:CG1	1:D:98:MET:H	2.30	0.43
1:A:339:THR:O	1:A:339:THR:HG23	2.18	0.43
1:A:74:LEU:O	1:A:78:ARG:HB3	2.18	0.43
1:B:113:VAL:CG2	1:B:114:ALA:H	2.15	0.43
1:B:437:ILE:HA	1:B:493:ARG:HB2	2.01	0.43
1:C:112:PRO:O	1:C:327:GLU:OE1	2.37	0.43
1:C:333:ARG:CB	1:C:333:ARG:HH11	2.30	0.43
1:C:431:ASP:HB3	1:C:435:ASN:HB2	1.99	0.43
1:C:513:THR:O	1:C:516:GLU:HB3	2.19	0.43
1:D:100:MET:HE3	1:D:100:MET:HA	2.00	0.43
1:D:131:ASP:CB	1:D:318:LEU:HD23	2.48	0.43
1:D:112:PRO:O	1:D:327:GLU:OE1	2.37	0.43
1:D:557:VAL:O	1:D:557:VAL:CG1	2.66	0.43
1:A:16:LEU:HD11	1:A:135:VAL:CG2	2.48	0.43
1:A:235:ASN:C	1:A:237:MET:N	2.73	0.43
1:A:33:ALA:O	1:A:81:THR:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:THR:O	1:A:412:LEU:C	2.57	0.43
1:A:412:LEU:HD21	1:A:416:ARG:HD2	2.01	0.43
1:B:178:VAL:HB	1:B:258:ILE:HG21	2.01	0.43
1:B:315:CYS:SG	1:B:319:PHE:CD1	3.12	0.43
1:B:113:VAL:HG12	1:B:327:GLU:CD	2.39	0.43
1:B:513:THR:O	1:B:516:GLU:HB3	2.19	0.43
1:C:496:LEU:O	1:C:496:LEU:HD12	2.18	0.43
1:D:113:VAL:HG12	1:D:327:GLU:CD	2.39	0.43
1:D:49:LYS:HB3	1:D:50:PRO:HD3	2.00	0.43
1:D:29:VAL:CG1	1:D:87:TYR:HE2	2.30	0.43
1:D:93:SER:OG	1:D:94:GLY:N	2.52	0.43
1:A:142:ALA:HB1	1:A:308:PHE:HD2	1.84	0.42
1:A:197:GLN:O	1:A:198:ASN:C	2.57	0.42
1:A:371:THR:HA	1:A:532:SER:O	2.19	0.42
1:B:475:GLY:H	1:B:480:LEU:HD12	1.83	0.42
1:B:93:SER:OG	1:B:94:GLY:N	2.52	0.42
1:C:315:CYS:SG	1:C:319:PHE:CD1	3.12	0.42
1:C:441:ARG:HD2	1:C:441:ARG:HA	1.61	0.42
1:C:445:TYR:HD2	1:C:496:LEU:HD21	1.83	0.42
1:A:220:PHE:O	1:B:441:ARG:CG	2.67	0.42
1:A:280:THR:O	1:A:284:ILE:CG2	2.67	0.42
1:B:112:PRO:O	1:B:327:GLU:OE1	2.37	0.42
1:B:299:LYS:HZ2	1:B:299:LYS:CB	2.32	0.42
1:C:580:PHE:HB2	1:C:581:GLY:H	1.68	0.42
1:C:29:VAL:CG1	1:C:87:TYR:HE2	2.30	0.42
1:C:125:LEU:HD21	1:D:125:LEU:HD23	2.01	0.42
1:D:178:VAL:HB	1:D:258:ILE:HG21	2.01	0.42
1:D:315:CYS:SG	1:D:319:PHE:CD1	3.12	0.42
1:A:95:LYS:NZ	1:B:238:ARG:HG3	2.34	0.42
1:B:74:LEU:O	1:B:75:MET:C	2.57	0.42
1:C:203:VAL:HA	1:C:233:VAL:HG11	2.00	0.42
1:C:220:PHE:CE1	1:D:439:TYR:O	2.71	0.42
1:C:412:LEU:HD21	1:C:416:ARG:HD2	2.01	0.42
1:C:93:SER:HA	1:C:96:VAL:HG12	2.01	0.42
1:D:170:ILE:HD13	1:D:170:ILE:N	2.33	0.42
1:D:197:GLN:O	1:D:200:MET:N	2.52	0.42
1:C:102:ARG:HH21	1:D:238:ARG:NH2	2.17	0.42
1:D:315:CYS:SG	1:D:319:PHE:CE1	3.13	0.42
1:D:488:ARG:O	1:D:491:ILE:HB	2.20	0.42
1:D:513:THR:O	1:D:516:GLU:HB3	2.19	0.42
1:A:508:THR:HG22	1:A:538:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:SER:HA	1:A:96:VAL:HG12	2.01	0.42
1:B:197:GLN:O	1:B:200:MET:N	2.52	0.42
1:B:203:VAL:HA	1:B:233:VAL:HG11	2.00	0.42
1:B:315:CYS:SG	1:B:319:PHE:CE1	3.13	0.42
1:B:97:VAL:CG1	1:B:98:MET:H	2.30	0.42
1:D:349:PHE:CD2	1:D:388:LEU:HD11	2.55	0.42
1:D:515:SER:O	1:D:518:ALA:HB3	2.20	0.42
1:A:111:MET:HE3	1:A:326:GLN:OE1	2.19	0.42
1:A:183:ARG:HA	1:A:183:ARG:HD2	1.85	0.42
1:A:360:ARG:O	1:A:362:ILE:HG12	2.20	0.42
1:A:378:SER:HB3	1:B:512:ASP:HB2	2.02	0.42
1:A:577:LYS:C	1:A:579:GLN:N	2.72	0.42
1:A:96:VAL:HA	1:A:99:THR:HG22	2.01	0.42
1:B:349:PHE:CD2	1:B:388:LEU:HD11	2.55	0.42
1:B:365:LYS:HE2	1:B:367:PRO:HG3	2.01	0.42
1:B:412:LEU:HD21	1:B:416:ARG:HD2	2.01	0.42
1:B:93:SER:HA	1:B:96:VAL:HG12	2.01	0.42
1:C:235:ASN:C	1:C:237:MET:N	2.73	0.42
1:C:308:PHE:C	1:C:308:PHE:CD1	2.93	0.42
1:C:482:SER:HB3	1:C:485:GLN:CG	2.50	0.42
1:C:488:ARG:O	1:C:491:ILE:HB	2.20	0.42
1:C:48:LEU:CG	1:D:292:ILE:HD12	2.48	0.42
1:D:308:PHE:C	1:D:308:PHE:CD1	2.93	0.42
1:D:107:HIS:CD2	1:D:322:LEU:HA	2.54	0.42
1:D:535:ILE:O	1:D:535:ILE:HG23	2.20	0.42
1:B:167:LEU:O	1:B:170:ILE:HB	2.20	0.42
1:B:354:ARG:C	1:B:355:GLU:HG3	2.39	0.42
1:A:271:SER:CA	1:B:63:VAL:HG11	2.49	0.42
1:A:441:ARG:NE	1:B:221:GLY:CA	2.79	0.42
1:A:542:ILE:C	1:A:544:GLN:N	2.73	0.42
1:B:214:HIS:O	1:B:215:LYS:C	2.57	0.42
1:B:308:PHE:C	1:B:308:PHE:CD1	2.93	0.42
1:B:15:ARG:HH21	1:B:319:PHE:HD1	1.68	0.42
1:B:384:THR:N	2:B:5002:ANP:O1A	2.53	0.42
1:C:113:VAL:HG12	1:C:327:GLU:CD	2.39	0.42
1:C:476:GLU:O	1:C:477:ASN:HB3	2.20	0.42
1:D:354:ARG:C	1:D:355:GLU:HG3	2.39	0.42
1:A:140:SER:OG	1:A:141:GLY:N	2.53	0.42
1:A:163:TYR:OH	1:A:286:VAL:HB	2.20	0.42
1:A:349:PHE:CD2	1:A:388:LEU:HD11	2.55	0.42
1:A:433:VAL:O	1:A:434:ALA:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:ILE:O	1:B:535:ILE:HG23	2.20	0.42
1:B:29:VAL:CG1	1:B:87:TYR:HE2	2.30	0.42
1:C:577:LYS:C	1:C:579:GLN:N	2.72	0.42
1:C:20:ILE:HD11	1:C:96:VAL:HG21	1.99	0.42
1:D:421:LEU:HD12	1:D:422:VAL:H	1.85	0.42
1:D:93:SER:HA	1:D:96:VAL:HG12	2.01	0.42
1:A:219:ILE:O	1:A:220:PHE:C	2.58	0.42
1:A:391:ARG:O	1:A:394:ASP:OD1	2.38	0.42
1:A:97:VAL:O	1:A:100:MET:HB3	2.20	0.42
1:B:107:HIS:CD2	1:B:322:LEU:HA	2.54	0.42
1:B:349:PHE:HA	1:B:396:ASP:HB3	1.97	0.42
1:A:221:GLY:C	1:B:441:ARG:CD	2.87	0.42
1:C:15:ARG:HH21	1:C:319:PHE:HD1	1.68	0.42
1:C:197:GLN:O	1:C:200:MET:N	2.52	0.42
1:C:354:ARG:C	1:C:355:GLU:HG3	2.39	0.42
1:C:93:SER:OG	1:C:94:GLY:N	2.52	0.42
1:D:478:GLY:HA3	1:D:486:ARG:CD	2.50	0.42
1:A:107:HIS:CD2	1:A:322:LEU:HA	2.55	0.42
1:A:421:LEU:HD12	1:A:422:VAL:H	1.85	0.42
1:B:16:LEU:HD11	1:B:135:VAL:CG2	2.50	0.42
1:B:235:ASN:C	1:B:237:MET:N	2.73	0.42
1:B:163:TYR:OH	1:B:286:VAL:HB	2.20	0.42
1:B:421:LEU:HD12	1:B:422:VAL:H	1.85	0.42
1:B:450:ILE:O	1:B:451:GLU:C	2.58	0.42
1:B:488:ARG:O	1:B:491:ILE:HB	2.20	0.42
1:C:142:ALA:HB1	1:C:308:PHE:HD2	1.83	0.42
1:C:167:LEU:O	1:C:170:ILE:HB	2.20	0.42
1:C:269:ALA:HA	1:C:273:PRO:CD	2.50	0.42
1:C:391:ARG:O	1:C:394:ASP:OD1	2.38	0.42
1:C:511:LEU:H	1:C:538:ARG:HH22	1.68	0.42
1:D:113:VAL:CG2	1:D:114:ALA:H	2.15	0.42
1:D:214:HIS:O	1:D:215:LYS:C	2.57	0.42
1:D:365:LYS:HE2	1:D:367:PRO:HG3	2.01	0.42
1:D:33:ALA:HB2	1:D:84:ILE:HG22	2.02	0.42
1:A:316:GLN:CD	1:A:319:PHE:CD1	2.93	0.41
1:A:446:SER:HB2	1:A:449:GLN:NE2	2.35	0.41
1:B:338:ALA:O	1:B:339:THR:O	2.37	0.41
1:B:577:LYS:C	1:B:579:GLN:N	2.72	0.41
1:C:338:ALA:HB3	1:C:500:PRO:CB	2.50	0.41
1:D:16:LEU:HD11	1:D:135:VAL:CG2	2.50	0.41
1:D:338:ALA:O	1:D:339:THR:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:TYR:HB3	1:D:446:SER:H	1.76	0.41
1:D:512:ASP:HB3	1:D:515:SER:HB2	2.01	0.41
1:A:214:HIS:O	1:A:215:LYS:C	2.58	0.41
1:A:426:VAL:O	1:A:486:ARG:NH2	2.53	0.41
1:B:371:THR:HA	1:B:532:SER:O	2.21	0.41
1:B:561:THR:C	1:B:563:SER:N	2.73	0.41
1:C:101:ARG:HB2	1:C:128:ILE:HG23	2.03	0.41
1:C:16:LEU:HD11	1:C:135:VAL:CG2	2.50	0.41
1:C:280:THR:O	1:C:284:ILE:CG2	2.68	0.41
1:C:299:LYS:CB	1:C:299:LYS:HZ2	2.33	0.41
1:C:315:CYS:SG	1:C:319:PHE:CE1	3.13	0.41
1:C:349:PHE:CD2	1:C:388:LEU:HD11	2.55	0.41
1:C:480:LEU:O	1:C:481:LEU:HB3	2.20	0.41
1:D:167:LEU:O	1:D:170:ILE:HB	2.20	0.41
1:D:197:GLN:O	1:D:198:ASN:C	2.59	0.41
1:D:28:ILE:O	1:D:32:ILE:HG12	2.21	0.41
1:C:219:ILE:HD13	1:D:421:LEU:HB3	2.02	0.41
1:D:480:LEU:O	1:D:481:LEU:HB3	2.20	0.41
1:D:97:VAL:O	1:D:100:MET:HB3	2.20	0.41
1:A:15:ARG:HH21	1:A:319:PHE:HD1	1.68	0.41
1:A:308:PHE:CD1	1:A:308:PHE:C	2.93	0.41
1:B:28:ILE:CG2	1:B:29:VAL:N	2.83	0.41
1:C:107:HIS:CD2	1:C:322:LEU:HA	2.54	0.41
1:C:28:ILE:O	1:C:32:ILE:HG12	2.20	0.41
1:C:33:ALA:HB2	1:C:84:ILE:HG22	2.02	0.41
1:C:421:LEU:HD12	1:C:422:VAL:H	1.85	0.41
1:C:542:ILE:C	1:C:544:GLN:N	2.74	0.41
1:D:101:ARG:HB2	1:D:128:ILE:HG23	2.03	0.41
1:D:476:GLU:O	1:D:477:ASN:HB3	2.20	0.41
1:D:437:ILE:HA	1:D:493:ARG:HB2	2.01	0.41
1:D:511:LEU:H	1:D:538:ARG:HH22	1.68	0.41
1:D:96:VAL:HA	1:D:99:THR:HG22	2.00	0.41
1:A:33:ALA:HB2	1:A:84:ILE:HG22	2.03	0.41
1:A:365:LYS:HE2	1:A:367:PRO:HG3	2.01	0.41
1:B:294:LEU:O	1:B:297:PRO:HD2	2.20	0.41
1:B:380:SER:O	1:B:382:LYS:N	2.49	0.41
1:A:225:VAL:HG21	1:B:443:GLU:HG2	2.02	0.41
1:C:163:TYR:OH	1:C:286:VAL:HB	2.20	0.41
1:C:535:ILE:O	1:C:535:ILE:HG23	2.20	0.41
1:D:391:ARG:O	1:D:394:ASP:OD1	2.38	0.41
1:A:157:PHE:HB2	1:A:171:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:O	1:B:63:VAL:CG1	2.68	0.41
1:A:331:GLY:C	1:A:332:LYS:HG3	2.41	0.41
1:A:488:ARG:O	1:A:492:ALA:N	2.51	0.41
1:B:542:ILE:C	1:B:544:GLN:N	2.74	0.41
1:C:178:VAL:HB	1:C:258:ILE:HG21	2.01	0.41
1:D:280:THR:O	1:D:284:ILE:CG2	2.69	0.41
1:D:28:ILE:CG2	1:D:29:VAL:N	2.83	0.41
1:D:333:ARG:CB	1:D:333:ARG:HH11	2.30	0.41
1:D:33:ALA:O	1:D:81:THR:CG2	2.69	0.41
1:D:20:ILE:HD11	1:D:96:VAL:HG21	1.99	0.41
1:A:415:LEU:O	1:A:418:GLN:HB2	2.20	0.41
1:A:513:THR:O	1:A:516:GLU:HB3	2.21	0.41
1:B:192:ILE:O	1:B:196:MET:HB2	2.21	0.41
1:C:164:SER:HG	1:C:167:LEU:HD23	1.85	0.41
1:C:296:ARG:N	1:C:297:PRO:HD2	2.36	0.41
1:C:33:ALA:O	1:C:81:THR:CG2	2.69	0.41
1:C:371:THR:HA	1:C:532:SER:O	2.21	0.41
1:C:478:GLY:HA3	1:C:486:ARG:CD	2.50	0.41
1:D:561:THR:C	1:D:563:SER:N	2.73	0.41
1:A:23:PHE:CZ	1:A:95:LYS:HB3	2.55	0.41
1:A:28:ILE:CG2	1:A:29:VAL:N	2.83	0.41
1:A:549:VAL:HG13	1:A:556:ILE:CD1	2.50	0.41
1:B:33:ALA:O	1:B:81:THR:CG2	2.69	0.41
1:B:480:LEU:O	1:B:481:LEU:HB3	2.20	0.41
1:C:450:ILE:O	1:C:451:GLU:C	2.58	0.41
1:C:515:SER:O	1:C:518:ALA:HB3	2.20	0.41
1:C:575:LEU:HD22	1:D:513:THR:CG2	2.50	0.41
1:D:118:LYS:NZ	1:D:352:PRO:HG3	2.36	0.41
1:D:343:GLU:OE2	1:D:365:LYS:HE3	2.21	0.41
1:C:512:ASP:H	1:D:378:SER:HB2	1.85	0.41
1:D:84:ILE:O	1:D:87:TYR:CD2	2.72	0.41
1:A:192:ILE:O	1:A:196:MET:HB2	2.20	0.41
1:A:292:ILE:HD12	1:B:48:LEU:CD1	2.49	0.41
1:A:47:LEU:CD1	1:A:51:LEU:HD12	2.50	0.41
1:A:558:GLU:CD	1:A:559:ARG:N	2.74	0.41
1:B:280:THR:O	1:B:284:ILE:CG2	2.68	0.41
1:B:411:THR:O	1:B:411:THR:HG23	2.21	0.41
1:B:455:ARG:C	1:B:457:ALA:N	2.69	0.41
1:C:192:ILE:O	1:C:196:MET:HB2	2.21	0.41
1:C:220:PHE:HZ	1:D:439:TYR:CD2	2.38	0.41
1:C:28:ILE:CG2	1:C:29:VAL:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:VAL:HA	1:C:398:GLY:HA3	2.03	0.41
1:C:561:THR:O	1:C:562:HIS:C	2.57	0.41
1:C:97:VAL:O	1:C:100:MET:HB3	2.20	0.41
1:D:15:ARG:HH21	1:D:319:PHE:HD1	1.68	0.41
1:D:269:ALA:HA	1:D:273:PRO:CD	2.50	0.41
1:A:167:LEU:O	1:A:170:ILE:HB	2.20	0.41
1:A:354:ARG:C	1:A:355:GLU:HG3	2.41	0.41
1:A:411:THR:O	1:A:411:THR:HG23	2.21	0.41
1:A:511:LEU:H	1:A:538:ARG:HH22	1.69	0.41
1:A:87:TYR:CD2	1:A:88:CYS:N	2.89	0.41
1:A:20:ILE:HD11	1:A:96:VAL:HG21	2.00	0.41
1:B:515:SER:O	1:B:518:ALA:HB3	2.20	0.41
1:C:362:ILE:HD11	1:C:556:ILE:H	1.86	0.41
1:D:219:ILE:O	1:D:220:PHE:C	2.59	0.41
1:D:248:SER:O	1:D:251:SER:HB3	2.21	0.41
1:D:450:ILE:O	1:D:451:GLU:C	2.58	0.41
1:D:87:TYR:CD2	1:D:88:CYS:N	2.89	0.41
1:A:391:ARG:NH2	1:A:408:ARG:HA	2.36	0.41
1:A:445:TYR:CE2	1:A:496:LEU:HD11	2.55	0.41
1:A:515:SER:O	1:A:518:ALA:HB3	2.21	0.41
1:A:550:VAL:HB	1:A:558:GLU:HB3	2.03	0.41
1:A:87:TYR:CZ	1:A:88:CYS:SG	3.04	0.41
1:A:96:VAL:C	1:A:99:THR:HG22	2.41	0.41
1:B:33:ALA:HB2	1:B:84:ILE:HG22	2.02	0.41
1:B:478:GLY:HA3	1:B:486:ARG:CD	2.50	0.41
1:B:535:ILE:C	1:B:535:ILE:HD13	2.41	0.41
1:B:87:TYR:CD2	1:B:88:CYS:N	2.89	0.41
1:B:97:VAL:CG1	1:B:98:MET:N	2.81	0.41
1:C:213:GLY:HA2	1:D:427:HIS:CD2	2.55	0.41
1:C:220:PHE:O	1:D:441:ARG:CG	2.69	0.41
1:C:343:GLU:OE2	1:C:365:LYS:HE3	2.21	0.41
1:C:572:TYR:CD1	1:C:572:TYR:C	2.94	0.41
1:D:360:ARG:HB3	1:D:361:ASN:H	1.73	0.41
1:D:535:ILE:CD1	1:D:535:ILE:O	2.62	0.41
1:D:93:SER:HB3	1:D:140:SER:CB	2.44	0.41
1:A:198:ASN:N	1:A:198:ASN:ND2	2.69	0.41
1:A:269:ALA:HA	1:A:273:PRO:CD	2.49	0.41
1:A:347:VAL:HA	1:A:398:GLY:HA3	2.03	0.41
1:A:98:MET:CB	1:B:238:ARG:NE	2.82	0.41
1:B:343:GLU:OE2	1:B:365:LYS:HE3	2.21	0.41
1:B:342:LEU:CD2	1:B:366:ILE:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:SER:OG	1:C:141:GLY:N	2.53	0.41
1:C:384:THR:O	1:C:388:LEU:HB2	2.21	0.41
1:D:235:ASN:C	1:D:237:MET:N	2.73	0.41
1:D:294:LEU:O	1:D:297:PRO:HD2	2.20	0.41
1:A:146:VAL:O	1:A:150:GLY:HA3	2.21	0.40
1:A:235:ASN:OD1	1:A:238:ARG:HD2	2.21	0.40
1:A:439:TYR:O	1:A:443:GLU:OE2	2.39	0.40
1:A:474:ILE:CA	1:A:480:LEU:HD11	2.51	0.40
1:B:101:ARG:HB2	1:B:128:ILE:HG23	2.03	0.40
1:B:174:LEU:HD22	1:B:262:ALA:CB	2.40	0.40
1:B:296:ARG:N	1:B:297:PRO:HD2	2.36	0.40
1:B:391:ARG:O	1:B:394:ASP:OD1	2.38	0.40
1:B:473:ILE:O	1:B:473:ILE:HG23	2.22	0.40
1:C:197:GLN:O	1:C:198:ASN:C	2.59	0.40
1:C:342:LEU:CD2	1:C:366:ILE:HD12	2.51	0.40
1:C:441:ARG:HD3	1:D:221:GLY:C	2.37	0.40
1:C:491:ILE:O	1:C:495:LEU:HB2	2.21	0.40
1:C:67:MET:CB	1:C:68:PRO:HD3	2.45	0.40
1:C:87:TYR:CD2	1:C:88:CYS:N	2.89	0.40
1:D:163:TYR:OH	1:D:286:VAL:HB	2.20	0.40
1:D:495:LEU:HA	1:D:495:LEU:HD12	1.95	0.40
1:D:97:VAL:CG1	1:D:98:MET:N	2.81	0.40
1:A:277:ASP:C	1:A:279:LEU:H	2.25	0.40
1:A:317:THR:O	1:A:320:ALA:HB3	2.22	0.40
1:A:558:GLU:OE2	1:A:565:LEU:CD2	2.69	0.40
1:A:572:TYR:CD1	1:A:572:TYR:C	2.94	0.40
1:B:111:MET:HE3	1:B:326:GLN:OE1	2.21	0.40
1:B:193:SER:O	1:B:197:GLN:HG3	2.21	0.40
1:B:118:LYS:NZ	1:B:352:PRO:HG3	2.36	0.40
1:B:446:SER:HB2	1:B:449:GLN:NE2	2.36	0.40
1:B:476:GLU:O	1:B:477:ASN:HB3	2.20	0.40
1:B:84:ILE:O	1:B:87:TYR:CD2	2.73	0.40
1:C:219:ILE:O	1:C:220:PHE:C	2.59	0.40
1:C:445:TYR:HB3	1:C:446:SER:H	1.76	0.40
1:C:446:SER:HB2	1:C:449:GLN:NE2	2.36	0.40
1:D:296:ARG:N	1:D:297:PRO:HD2	2.36	0.40
1:D:371:THR:HA	1:D:532:SER:O	2.21	0.40
1:D:384:THR:O	1:D:388:LEU:HB2	2.21	0.40
1:D:561:THR:O	1:D:562:HIS:C	2.57	0.40
1:A:236:LYS:O	1:A:236:LYS:HG2	2.22	0.40
1:A:401:LEU:HD12	1:A:404:GLY:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ARG:HH11	1:A:456:MET:HE2	1.86	0.40
1:A:466:MET:CE	1:A:472:THR:HG21	2.49	0.40
1:A:93:SER:HB3	1:A:140:SER:CB	2.44	0.40
1:B:146:VAL:O	1:B:150:GLY:HA3	2.22	0.40
1:B:219:ILE:O	1:B:220:PHE:C	2.59	0.40
1:B:384:THR:O	1:B:388:LEU:HB2	2.21	0.40
1:A:221:GLY:N	1:B:441:ARG:HD3	2.28	0.40
1:B:558:GLU:CD	1:B:559:ARG:N	2.75	0.40
1:C:171:LEU:C	1:C:171:LEU:HD23	2.41	0.40
1:C:272:PHE:HB2	1:C:273:PRO:CD	2.37	0.40
1:C:118:LYS:NZ	1:C:352:PRO:HG3	2.36	0.40
1:C:378:SER:H	1:D:512:ASP:CB	2.24	0.40
1:C:444:GLU:HA	1:C:444:GLU:OE1	2.21	0.40
1:C:473:ILE:O	1:C:473:ILE:HG23	2.21	0.40
1:C:550:VAL:HB	1:C:558:GLU:HB3	2.03	0.40
1:C:74:LEU:HD23	1:C:74:LEU:C	2.42	0.40
1:C:84:ILE:O	1:C:87:TYR:CD2	2.73	0.40
1:D:171:LEU:HD23	1:D:171:LEU:C	2.41	0.40
1:D:319:PHE:HA	1:D:319:PHE:HD2	1.82	0.40
1:D:491:ILE:O	1:D:495:LEU:HB2	2.21	0.40
1:A:101:ARG:HB2	1:A:128:ILE:HG23	2.03	0.40
1:B:97:VAL:O	1:B:100:MET:HB3	2.20	0.40
1:B:248:SER:O	1:B:251:SER:HB3	2.21	0.40
1:B:28:ILE:O	1:B:32:ILE:HG12	2.20	0.40
1:B:315:CYS:O	1:B:319:PHE:HB2	2.22	0.40
1:B:74:LEU:HD23	1:B:74:LEU:C	2.42	0.40
1:C:178:VAL:CA	1:C:258:ILE:HD13	2.48	0.40
1:C:391:ARG:NH2	1:C:408:ARG:HA	2.36	0.40
1:D:277:ASP:C	1:D:279:LEU:H	2.24	0.40
1:D:342:LEU:CD2	1:D:366:ILE:HD12	2.51	0.40
1:D:347:VAL:HA	1:D:398:GLY:HA3	2.03	0.40
1:D:446:SER:HB2	1:D:449:GLN:NE2	2.36	0.40
1:D:440:ALA:HB1	1:D:497:ARG:NE	2.37	0.40
1:D:542:ILE:C	1:D:544:GLN:N	2.74	0.40
1:A:102:ARG:CD	1:B:231:ASP:OD1	2.69	0.40
1:A:141:GLY:C	1:A:144:ILE:HG12	2.42	0.40
1:A:248:SER:O	1:A:251:SER:HB3	2.22	0.40
1:A:338:ALA:HB3	1:A:500:PRO:CB	2.48	0.40
1:A:400:ILE:HG22	1:A:407:LEU:HD11	2.03	0.40
1:B:338:ALA:HB3	1:B:500:PRO:CB	2.50	0.40
1:B:444:GLU:OE1	1:B:444:GLU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ILE:O	1:B:495:LEU:HB2	2.21	0.40
1:B:572:TYR:CD1	1:B:572:TYR:C	2.94	0.40
1:C:11:GLN:CG	1:C:12:THR:N	2.63	0.40
1:C:143:LEU:HD23	1:C:143:LEU:HA	1.96	0.40
1:C:248:SER:O	1:C:251:SER:HB3	2.21	0.40
1:C:411:THR:HG23	1:C:411:THR:O	2.21	0.40
1:C:125:LEU:HD23	1:D:125:LEU:HD21	2.03	0.40
1:D:11:GLN:CG	1:D:12:THR:N	2.63	0.40
1:D:192:ILE:O	1:D:196:MET:HB2	2.21	0.40
1:D:111:MET:HE3	1:D:326:GLN:OE1	2.21	0.40
1:D:411:THR:HG23	1:D:411:THR:O	2.21	0.40
1:D:415:LEU:O	1:D:418:GLN:HB2	2.22	0.40
1:D:572:TYR:C	1:D:572:TYR:CD1	2.94	0.40
1:D:74:LEU:HD23	1:D:74:LEU:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	570/582 (98%)	414 (73%)	102 (18%)	54 (10%)	0 8
1	B	570/582 (98%)	413 (72%)	107 (19%)	50 (9%)	1 10
1	C	570/582 (98%)	413 (72%)	107 (19%)	50 (9%)	1 10
1	D	570/582 (98%)	414 (73%)	106 (19%)	50 (9%)	1 10
All	All	2280/2328 (98%)	1654 (72%)	422 (18%)	204 (9%)	1 10

All (204) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP

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Mol	Chain	Res	Type
1	A	113	VAL
1	A	161	PHE
1	A	217	VAL
1	A	351	TYR
1	A	392	PHE
1	A	394	ASP
1	A	395	ILE
1	A	509	SER
1	A	571	VAL
1	B	60	ASP
1	B	113	VAL
1	B	161	PHE
1	B	217	VAL
1	B	351	TYR
1	B	392	PHE
1	B	394	ASP
1	B	395	ILE
1	B	509	SER
1	B	571	VAL
1	C	60	ASP
1	C	113	VAL
1	C	161	PHE
1	C	217	VAL
1	C	351	TYR
1	C	392	PHE
1	C	394	ASP
1	C	395	ILE
1	C	509	SER
1	C	571	VAL
1	D	60	ASP
1	D	113	VAL
1	D	161	PHE
1	D	217	VAL
1	D	351	TYR
1	D	392	PHE
1	D	394	ASP
1	D	395	ILE
1	D	509	SER
1	D	571	VAL
1	A	63	VAL
1	A	76	ILE
1	A	114	ALA

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Mol	Chain	Res	Type
1	A	140	SER
1	A	339	THR
1	A	353	GLY
1	A	361	ASN
1	A	378	SER
1	A	381	GLY
1	A	382	LYS
1	A	439	TYR
1	A	539	LEU
1	A	543	GLU
1	B	63	VAL
1	B	76	ILE
1	B	114	ALA
1	B	140	SER
1	B	353	GLY
1	B	361	ASN
1	B	378	SER
1	B	381	GLY
1	B	382	LYS
1	B	439	TYR
1	B	442	THR
1	B	539	LEU
1	B	543	GLU
1	C	63	VAL
1	C	114	ALA
1	C	140	SER
1	C	353	GLY
1	C	361	ASN
1	C	378	SER
1	C	381	GLY
1	C	382	LYS
1	C	439	TYR
1	C	442	THR
1	C	539	LEU
1	C	543	GLU
1	D	63	VAL
1	D	76	ILE
1	D	114	ALA
1	D	140	SER
1	D	353	GLY
1	D	361	ASN
1	D	378	SER

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Mol	Chain	Res	Type
1	D	381	GLY
1	D	382	LYS
1	D	439	TYR
1	D	442	THR
1	D	539	LEU
1	D	543	GLU
1	A	52	LEU
1	A	57	GLY
1	A	59	THR
1	A	118	LYS
1	A	129	THR
1	A	276	MET
1	A	327	GLU
1	A	346	ASN
1	A	413	ALA
1	A	492	ALA
1	B	52	LEU
1	B	57	GLY
1	B	59	THR
1	B	118	LYS
1	B	129	THR
1	B	276	MET
1	B	280	THR
1	B	327	GLU
1	B	339	THR
1	B	346	ASN
1	B	413	ALA
1	B	476	GLU
1	B	492	ALA
1	C	52	LEU
1	C	57	GLY
1	C	59	THR
1	C	76	ILE
1	C	118	LYS
1	C	129	THR
1	C	276	MET
1	C	280	THR
1	C	327	GLU
1	C	339	THR
1	C	346	ASN
1	C	413	ALA
1	C	492	ALA

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Mol	Chain	Res	Type
1	D	52	LEU
1	D	57	GLY
1	D	59	THR
1	D	118	LYS
1	D	129	THR
1	D	276	MET
1	D	280	THR
1	D	327	GLU
1	D	339	THR
1	D	346	ASN
1	D	413	ALA
1	D	476	GLU
1	D	492	ALA
1	A	11	GLN
1	A	216	GLU
1	A	280	THR
1	A	324	SER
1	A	424	GLN
1	A	442	THR
1	A	456	MET
1	A	459	ALA
1	A	476	GLU
1	A	527	GLN
1	B	216	GLU
1	B	424	GLN
1	B	456	MET
1	B	459	ALA
1	C	216	GLU
1	C	424	GLN
1	C	456	MET
1	C	459	ALA
1	C	476	GLU
1	D	216	GLU
1	D	424	GLN
1	D	456	MET
1	D	459	ALA
1	A	47	LEU
1	A	272	PHE
1	A	391	ARG
1	A	441	ARG
1	A	458	TYR
1	B	47	LEU

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Mol	Chain	Res	Type
1	B	272	PHE
1	B	324	SER
1	B	458	TYR
1	B	527	GLN
1	C	47	LEU
1	C	272	PHE
1	C	324	SER
1	C	458	TYR
1	C	527	GLN
1	D	47	LEU
1	D	272	PHE
1	D	324	SER
1	D	458	TYR
1	D	527	GLN
1	A	87	TYR
1	B	391	ARG
1	C	391	ARG
1	D	391	ARG
1	A	111	MET
1	B	111	MET
1	C	111	MET
1	D	111	MET
1	A	112	PRO
1	A	542	ILE
1	B	542	ILE
1	C	542	ILE
1	D	542	ILE
1	A	275	VAL
1	B	128	ILE
1	B	275	VAL
1	C	128	ILE
1	C	275	VAL
1	D	128	ILE
1	D	275	VAL
1	A	128	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	483/493 (98%)	441 (91%)	42 (9%)	10	38
1	B	483/493 (98%)	443 (92%)	40 (8%)	11	40
1	C	483/493 (98%)	443 (92%)	40 (8%)	11	40
1	D	483/493 (98%)	443 (92%)	40 (8%)	11	40
All	All	1932/1972 (98%)	1770 (92%)	162 (8%)	11	40

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	37	ASN
1	A	49	LYS
1	A	72	ILE
1	A	87	TYR
1	A	88	CYS
1	A	98	MET
1	A	113	VAL
1	A	117	ASP
1	A	119	GLN
1	A	127	ARG
1	A	157	PHE
1	A	165	TRP
1	A	170	ILE
1	A	187	LYS
1	A	211	LEU
1	A	224	GLU
1	A	253	PRO
1	A	284	ILE
1	A	291	MET
1	A	292	ILE
1	A	312	MET
1	A	315	CYS
1	A	319	PHE
1	A	329	ASP
1	A	342	LEU
1	A	344	PHE
1	A	345	ARG
1	A	385	ILE
1	A	391	ARG
1	A	394	ASP

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Mol	Chain	Res	Type
1	A	401	LEU
1	A	408	ARG
1	A	424	GLN
1	A	431	ASP
1	A	470	LEU
1	A	480	LEU
1	A	535	ILE
1	A	537	HIS
1	A	558	GLU
1	A	566	LEU
1	A	579	GLN
1	B	34	LEU
1	B	37	ASN
1	B	49	LYS
1	B	72	ILE
1	B	87	TYR
1	B	88	CYS
1	B	98	MET
1	B	113	VAL
1	B	117	ASP
1	B	119	GLN
1	B	127	ARG
1	B	157	PHE
1	B	165	TRP
1	B	187	LYS
1	B	211	LEU
1	B	224	GLU
1	B	253	PRO
1	B	284	ILE
1	B	291	MET
1	B	292	ILE
1	B	312	MET
1	B	315	CYS
1	B	319	PHE
1	B	329	ASP
1	B	339	THR
1	B	344	PHE
1	B	345	ARG
1	B	385	ILE
1	B	391	ARG
1	B	394	ASP
1	B	401	LEU

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Mol	Chain	Res	Type
1	B	408	ARG
1	B	424	GLN
1	B	431	ASP
1	B	470	LEU
1	B	480	LEU
1	B	535	ILE
1	B	558	GLU
1	B	566	LEU
1	B	579	GLN
1	C	34	LEU
1	C	37	ASN
1	C	49	LYS
1	C	72	ILE
1	C	87	TYR
1	C	88	CYS
1	C	98	MET
1	C	113	VAL
1	C	117	ASP
1	C	119	GLN
1	C	127	ARG
1	C	157	PHE
1	C	165	TRP
1	C	187	LYS
1	C	211	LEU
1	C	224	GLU
1	C	253	PRO
1	C	284	ILE
1	C	291	MET
1	C	292	ILE
1	C	312	MET
1	C	315	CYS
1	C	319	PHE
1	C	329	ASP
1	C	339	THR
1	C	344	PHE
1	C	345	ARG
1	C	385	ILE
1	C	391	ARG
1	C	394	ASP
1	C	401	LEU
1	C	408	ARG
1	C	424	GLN

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Mol	Chain	Res	Type
1	C	431	ASP
1	C	470	LEU
1	C	480	LEU
1	C	535	ILE
1	C	558	GLU
1	C	566	LEU
1	C	579	GLN
1	D	34	LEU
1	D	37	ASN
1	D	49	LYS
1	D	72	ILE
1	D	87	TYR
1	D	88	CYS
1	D	98	MET
1	D	113	VAL
1	D	117	ASP
1	D	119	GLN
1	D	127	ARG
1	D	157	PHE
1	D	165	TRP
1	D	187	LYS
1	D	211	LEU
1	D	224	GLU
1	D	253	PRO
1	D	284	ILE
1	D	291	MET
1	D	292	ILE
1	D	312	MET
1	D	315	CYS
1	D	319	PHE
1	D	329	ASP
1	D	339	THR
1	D	344	PHE
1	D	345	ARG
1	D	385	ILE
1	D	391	ARG
1	D	394	ASP
1	D	401	LEU
1	D	408	ARG
1	D	424	GLN
1	D	431	ASP
1	D	470	LEU

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Mol	Chain	Res	Type
1	D	480	LEU
1	D	535	ILE
1	D	558	GLU
1	D	566	LEU
1	D	579	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	107	HIS
1	A	119	GLN
1	A	134	GLN
1	A	198	ASN
1	A	256	GLN
1	A	316	GLN
1	A	427	HIS
1	A	435	ASN
1	A	464	ASN
1	A	468	ASN
1	A	520	GLN
1	A	537	HIS
1	A	576	HIS
1	B	37	ASN
1	B	107	HIS
1	B	119	GLN
1	B	134	GLN
1	B	198	ASN
1	B	316	GLN
1	B	427	HIS
1	B	435	ASN
1	B	464	ASN
1	B	468	ASN
1	B	520	GLN
1	B	537	HIS
1	B	576	HIS
1	C	37	ASN
1	C	107	HIS
1	C	119	GLN
1	C	134	GLN
1	C	198	ASN
1	C	256	GLN

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Mol	Chain	Res	Type
1	C	316	GLN
1	C	427	HIS
1	C	435	ASN
1	C	464	ASN
1	C	468	ASN
1	C	520	GLN
1	C	537	HIS
1	C	576	HIS
1	D	37	ASN
1	D	107	HIS
1	D	119	GLN
1	D	134	GLN
1	D	198	ASN
1	D	256	GLN
1	D	316	GLN
1	D	435	ASN
1	D	464	ASN
1	D	468	ASN
1	D	520	GLN
1	D	537	HIS
1	D	576	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	ANP	A	5001	-	29,33,33	2.23	11 (37%)	31,52,52	2.10	8 (25%)
2	ANP	C	5003	-	29,33,33	2.01	12 (41%)	31,52,52	1.99	7 (22%)
2	ANP	D	5004	-	29,33,33	1.96	9 (31%)	31,52,52	1.95	8 (25%)
2	ANP	B	5002	-	29,33,33	2.16	11 (37%)	31,52,52	1.95	8 (25%)

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
2	ANP	A	5001	-	-	4/14/38/38	0/3/3/3
2	ANP	C	5003	-	-	4/14/38/38	0/3/3/3
2	ANP	D	5004	-	-	4/14/38/38	0/3/3/3
2	ANP	B	5002	-	-	4/14/38/38	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5002	ANP	PB-O3A	-6.64	1.50	1.59
2	A	5001	ANP	PB-O3A	-6.61	1.50	1.59
2	C	5003	ANP	PB-O3A	-5.64	1.52	1.59
2	D	5004	ANP	PB-O3A	-5.40	1.52	1.59
2	B	5002	ANP	PB-O2B	-3.81	1.46	1.56
2	A	5001	ANP	PB-O2B	-3.77	1.46	1.56
2	D	5004	ANP	PG-O2G	-3.45	1.47	1.56
2	B	5002	ANP	PG-O2G	-3.36	1.47	1.56
2	A	5001	ANP	PG-O2G	-3.33	1.47	1.56
2	A	5001	ANP	PG-N3B	-3.12	1.55	1.63
2	A	5001	ANP	C2'-C1'	3.11	1.58	1.53
2	C	5003	ANP	PG-O2G	-3.08	1.48	1.56
2	D	5004	ANP	PB-O2B	-3.02	1.48	1.56
2	C	5003	ANP	PB-O2B	-3.00	1.48	1.56
2	A	5001	ANP	C4-N3	2.83	1.39	1.35
2	B	5002	ANP	C2'-C1'	2.67	1.57	1.53
2	D	5004	ANP	C2'-C1'	2.60	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5002	ANP	C8-N7	-2.59	1.30	1.34
2	D	5004	ANP	C8-N7	-2.57	1.30	1.34
2	D	5004	ANP	PG-O3G	-2.52	1.50	1.56
2	A	5001	ANP	PB-N3B	-2.51	1.56	1.63
2	A	5001	ANP	O4'-C1'	2.49	1.44	1.41
2	C	5003	ANP	PA-O5'	-2.47	1.49	1.59
2	B	5002	ANP	O4'-C1'	2.46	1.44	1.41
2	C	5003	ANP	PG-O3G	-2.46	1.50	1.56
2	B	5002	ANP	PG-O3G	-2.44	1.50	1.56
2	C	5003	ANP	C8-N7	-2.43	1.30	1.34
2	A	5001	ANP	C8-N7	-2.41	1.30	1.34
2	C	5003	ANP	C4-N3	2.39	1.39	1.35
2	A	5001	ANP	PG-O3G	-2.38	1.50	1.56
2	B	5002	ANP	PG-O1G	2.33	1.49	1.46
2	D	5004	ANP	C4-N3	2.33	1.38	1.35
2	D	5004	ANP	O4'-C1'	2.32	1.44	1.41
2	C	5003	ANP	O4'-C1'	2.29	1.44	1.41
2	D	5004	ANP	PG-N3B	-2.21	1.57	1.63
2	A	5001	ANP	PA-O5'	-2.21	1.50	1.59
2	C	5003	ANP	PB-N3B	-2.17	1.57	1.63
2	C	5003	ANP	PA-O1A	-2.12	1.43	1.50
2	C	5003	ANP	PG-N3B	-2.11	1.57	1.63
2	B	5002	ANP	C3'-C4'	-2.09	1.47	1.53
2	C	5003	ANP	C2'-C1'	2.07	1.56	1.53
2	B	5002	ANP	PA-O5'	-2.05	1.51	1.59
2	B	5002	ANP	PG-N3B	-2.00	1.58	1.63

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5001	ANP	O1G-PG-N3B	-6.08	102.82	111.77
2	B	5002	ANP	O1G-PG-N3B	-5.81	103.22	111.77
2	D	5004	ANP	O1G-PG-N3B	-5.58	103.56	111.77
2	C	5003	ANP	O1G-PG-N3B	-5.39	103.84	111.77
2	A	5001	ANP	O2B-PB-O1B	4.70	119.77	109.92
2	C	5003	ANP	O2B-PB-O1B	4.68	119.73	109.92
2	D	5004	ANP	O2B-PB-O1B	4.57	119.49	109.92
2	B	5002	ANP	O2B-PB-O1B	4.53	119.42	109.92
2	A	5001	ANP	O1B-PB-N3B	-4.30	105.44	111.77
2	C	5003	ANP	O1B-PB-N3B	-4.24	105.53	111.77
2	C	5003	ANP	O3G-PG-O2G	3.82	117.81	107.64
2	A	5001	ANP	O3G-PG-O2G	3.73	117.57	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	5004	ANP	O3G-PG-O2G	3.50	116.97	107.64
2	B	5002	ANP	O3G-PG-O2G	3.24	116.27	107.64
2	B	5002	ANP	O4'-C1'-C2'	-3.10	102.39	106.93
2	D	5004	ANP	O2B-PB-O3A	3.09	114.96	104.64
2	A	5001	ANP	C4-C5-N7	3.06	112.59	109.40
2	C	5003	ANP	O2B-PB-O3A	3.03	114.76	104.64
2	A	5001	ANP	O2B-PB-O3A	3.00	114.64	104.64
2	D	5004	ANP	C4-C5-N7	2.95	112.47	109.40
2	B	5002	ANP	O2B-PB-O3A	2.94	114.46	104.64
2	B	5002	ANP	O1B-PB-N3B	-2.94	107.44	111.77
2	B	5002	ANP	C4-C5-N7	2.92	112.44	109.40
2	D	5004	ANP	O4'-C1'-C2'	-2.84	102.77	106.93
2	A	5001	ANP	O4'-C1'-C2'	-2.84	102.78	106.93
2	D	5004	ANP	O1B-PB-N3B	-2.77	107.69	111.77
2	C	5003	ANP	O4'-C1'-C2'	-2.77	102.89	106.93
2	C	5003	ANP	C4-C5-N7	2.58	112.09	109.40
2	D	5004	ANP	O3A-PB-N3B	-2.42	99.87	106.59
2	B	5002	ANP	O3A-PB-N3B	-2.17	100.58	106.59
2	A	5001	ANP	O3A-PB-N3B	-2.09	100.78	106.59

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5001	ANP	PB-N3B-PG-O1G
2	A	5001	ANP	PG-N3B-PB-O1B
2	C	5003	ANP	PB-N3B-PG-O1G
2	C	5003	ANP	PG-N3B-PB-O1B
2	D	5004	ANP	PB-N3B-PG-O1G
2	D	5004	ANP	PG-N3B-PB-O1B
2	B	5002	ANP	PB-N3B-PG-O1G
2	B	5002	ANP	PG-N3B-PB-O1B
2	B	5002	ANP	C4'-C5'-O5'-PA
2	A	5001	ANP	C4'-C5'-O5'-PA
2	C	5003	ANP	C4'-C5'-O5'-PA
2	D	5004	ANP	C4'-C5'-O5'-PA
2	A	5001	ANP	PA-O3A-PB-O2B
2	C	5003	ANP	PA-O3A-PB-O2B
2	D	5004	ANP	PA-O3A-PB-O2B
2	B	5002	ANP	PA-O3A-PB-O2B

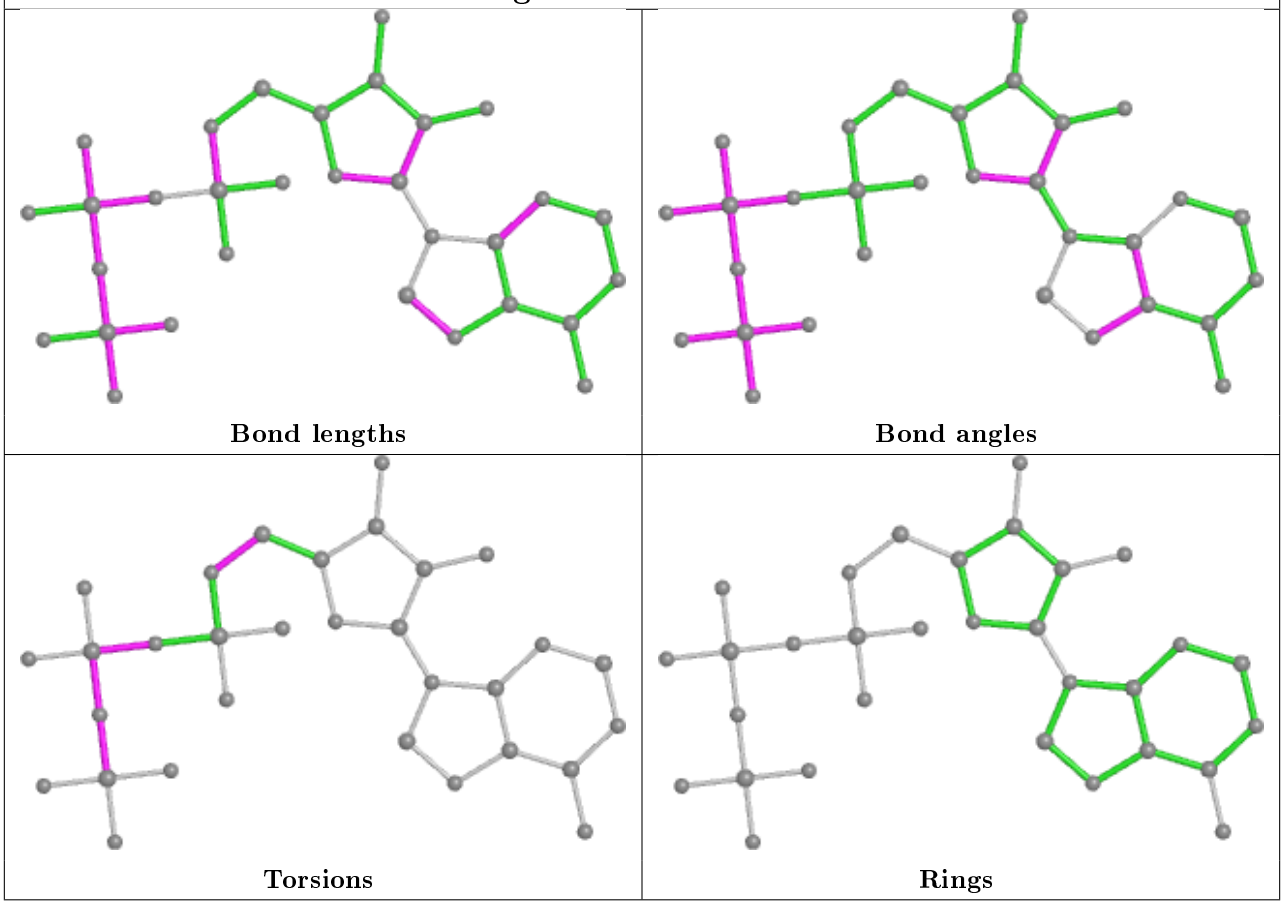
There are no ring outliers.

4 monomers are involved in 19 short contacts:

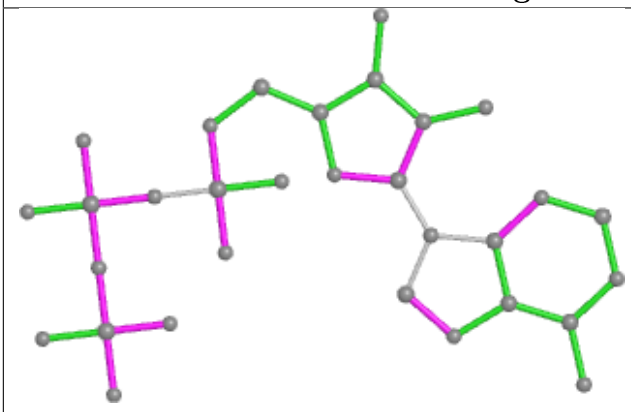
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	ANP	5	0
2	C	5003	ANP	3	0
2	D	5004	ANP	5	0
2	B	5002	ANP	6	0

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.

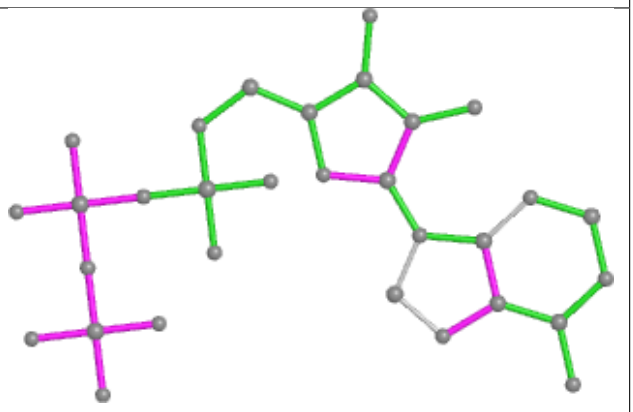
Ligand ANP A 5001



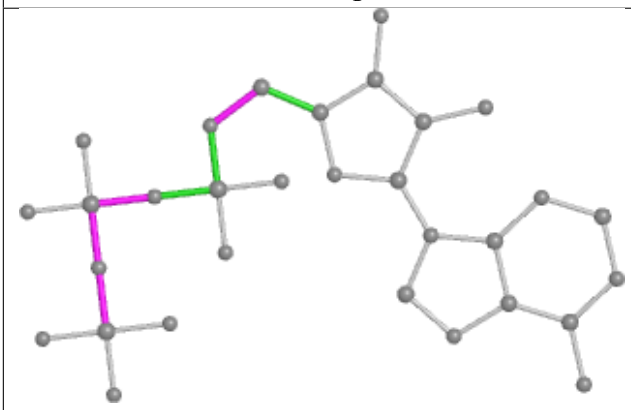
Ligand ANP C 5003



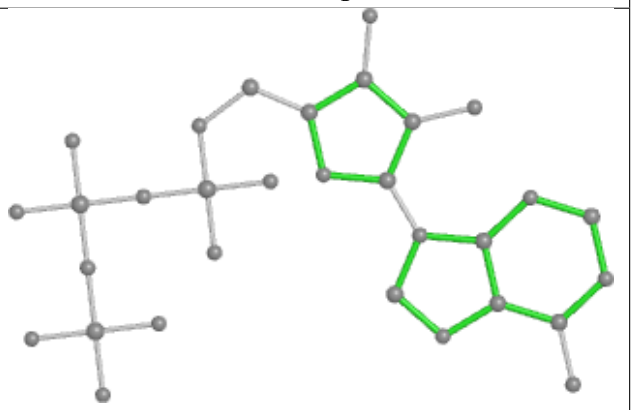
Bond lengths



Bond angles

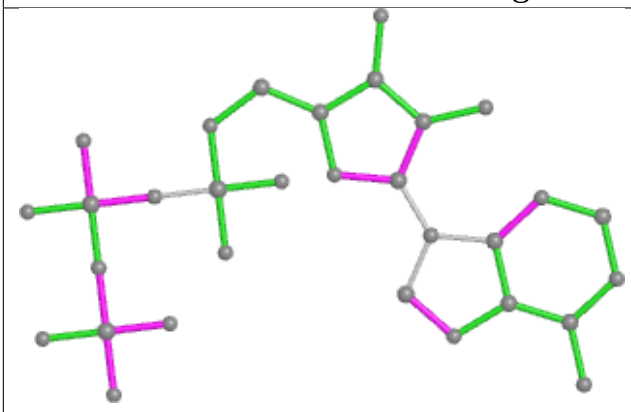


Torsions

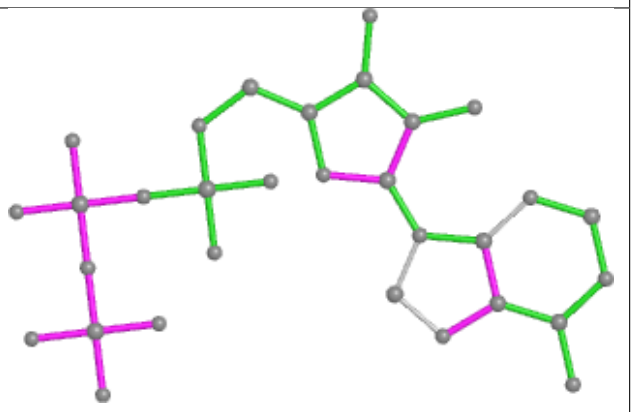


Rings

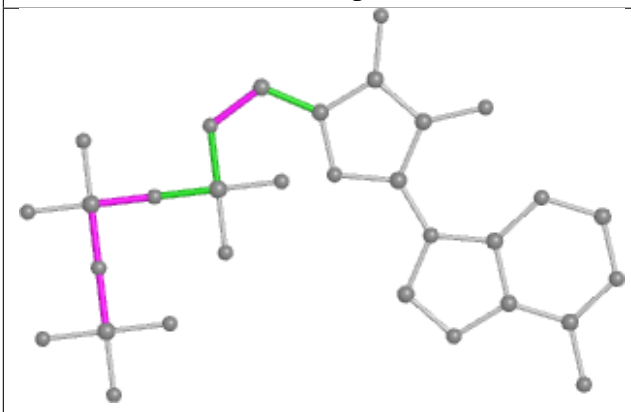
Ligand ANP D 5004



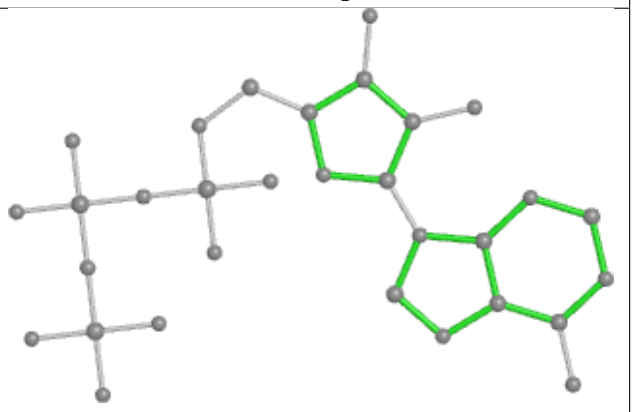
Bond lengths



Bond angles

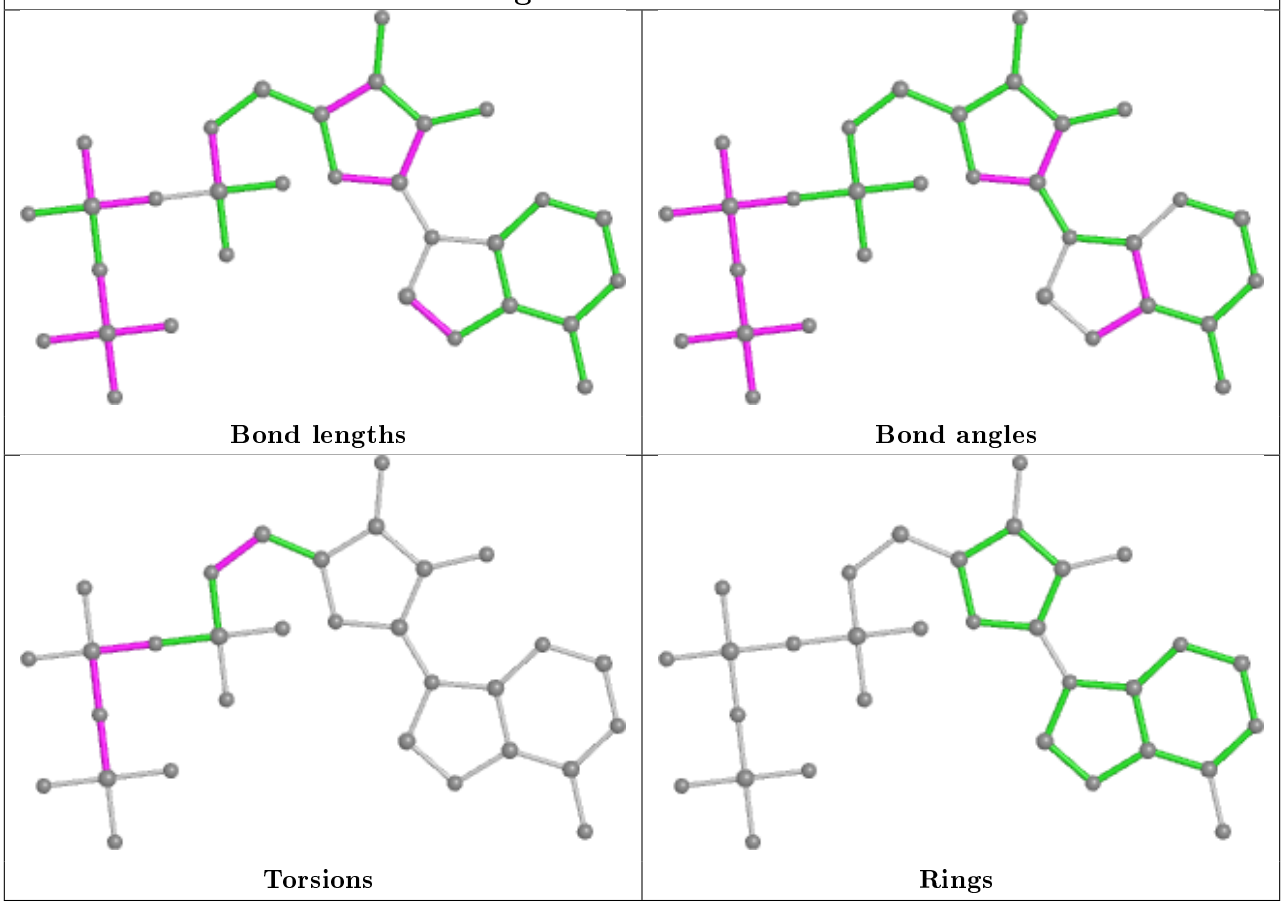


Torsions



Rings

Ligand ANP B 5002



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	572/582 (98%)	-0.12	28 (4%)	29	22	61, 154, 203, 205	0
1	B	572/582 (98%)	-0.27	19 (3%)	46	35	55, 135, 200, 205	0
1	C	572/582 (98%)	-0.32	16 (2%)	53	40	66, 137, 197, 205	0
1	D	572/582 (98%)	-0.30	12 (2%)	63	52	59, 146, 201, 205	0
All	All	2288/2328 (98%)	-0.26	75 (3%)	46	35	55, 143, 201, 205	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	ASP	6.0
1	A	61	ARG	5.6
1	B	163	TYR	4.6
1	D	60	ASP	4.3
1	B	353	GLY	4.1
1	C	442	THR	4.0
1	A	581	GLY	4.0
1	A	10	TRP	4.0
1	A	336	ASP	3.8
1	A	163	TYR	3.7
1	B	10	TRP	3.7
1	B	59	THR	3.6
1	D	162	TYR	3.5
1	C	162	TYR	3.5
1	B	162	TYR	3.4
1	A	65	LEU	3.4
1	B	50	PRO	3.4
1	D	163	TYR	3.3
1	C	56	PHE	3.3
1	A	282	GLY	3.2
1	B	60	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	441	ARG	3.2
1	D	56	PHE	3.1
1	D	10	TRP	3.0
1	C	163	TYR	3.0
1	C	274	SER	3.0
1	A	277	ASP	2.9
1	C	60	ASP	2.9
1	D	356	VAL	2.9
1	C	448	GLU	2.8
1	A	448	GLU	2.7
1	A	354	ARG	2.7
1	A	162	TYR	2.7
1	B	56	PHE	2.7
1	D	353	GLY	2.7
1	B	336	ASP	2.7
1	C	59	THR	2.7
1	A	281	ALA	2.6
1	D	54	ASP	2.6
1	A	286	VAL	2.6
1	A	137	SER	2.6
1	A	334	VAL	2.5
1	B	169	ILE	2.5
1	A	333	ARG	2.5
1	C	10	TRP	2.5
1	B	354	ARG	2.5
1	C	337	ARG	2.5
1	D	399	HIS	2.4
1	B	57	GLY	2.4
1	A	276	MET	2.4
1	A	353	GLY	2.4
1	B	55	GLY	2.4
1	A	580	PHE	2.4
1	A	59	THR	2.3
1	A	268	TYR	2.3
1	B	286	VAL	2.3
1	B	272	PHE	2.2
1	A	446	SER	2.2
1	A	58	LYS	2.2
1	D	137	SER	2.2
1	C	354	ARG	2.2
1	B	11	GLN	2.2
1	C	61	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	440	ALA	2.1
1	B	356	VAL	2.1
1	A	68	PRO	2.1
1	A	184	VAL	2.1
1	A	295	MET	2.1
1	D	441	ARG	2.1
1	C	273	PRO	2.1
1	B	72	ILE	2.0
1	C	332	LYS	2.0
1	D	337	ARG	2.0
1	B	333	ARG	2.0
1	A	14	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

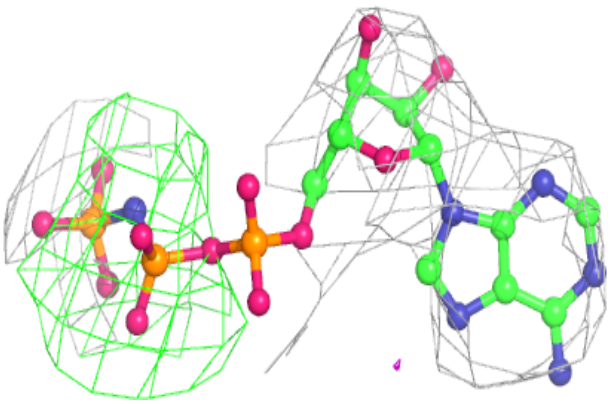
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

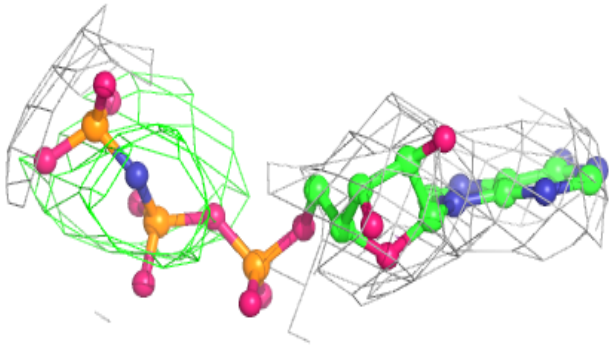
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ANP	A	5001	31/31	0.91	0.24	121,121,121,121	0
2	ANP	C	5003	31/31	0.92	0.26	111,111,111,111	0
2	ANP	D	5004	31/31	0.92	0.22	139,139,139,139	0
2	ANP	B	5002	31/31	0.93	0.22	124,124,124,124	0

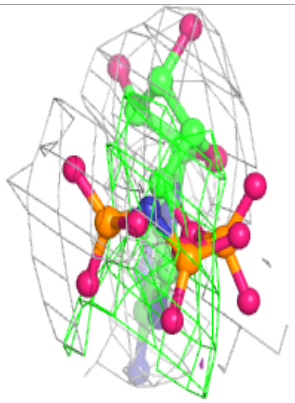
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 5001:

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

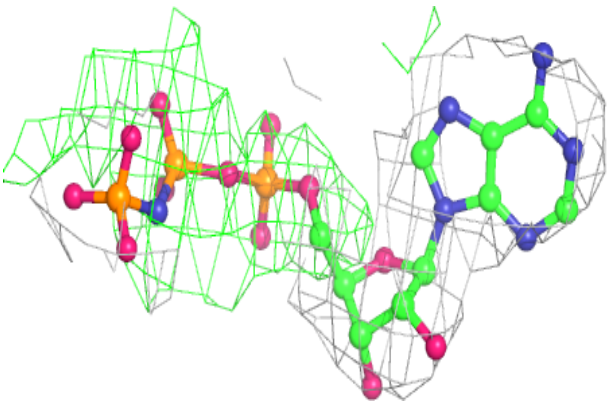


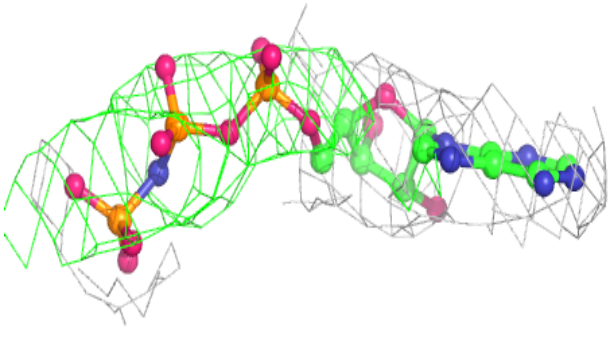


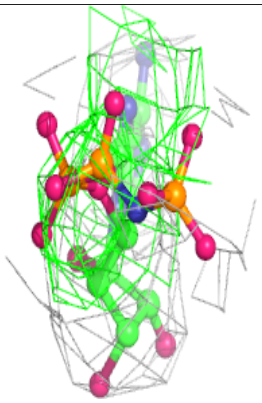


Electron density around ANP C 5003:

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

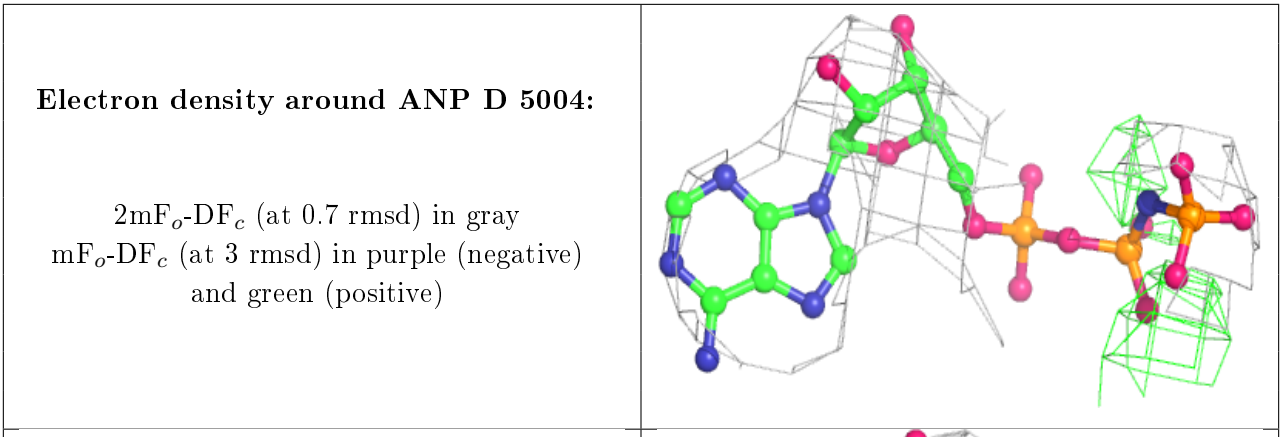


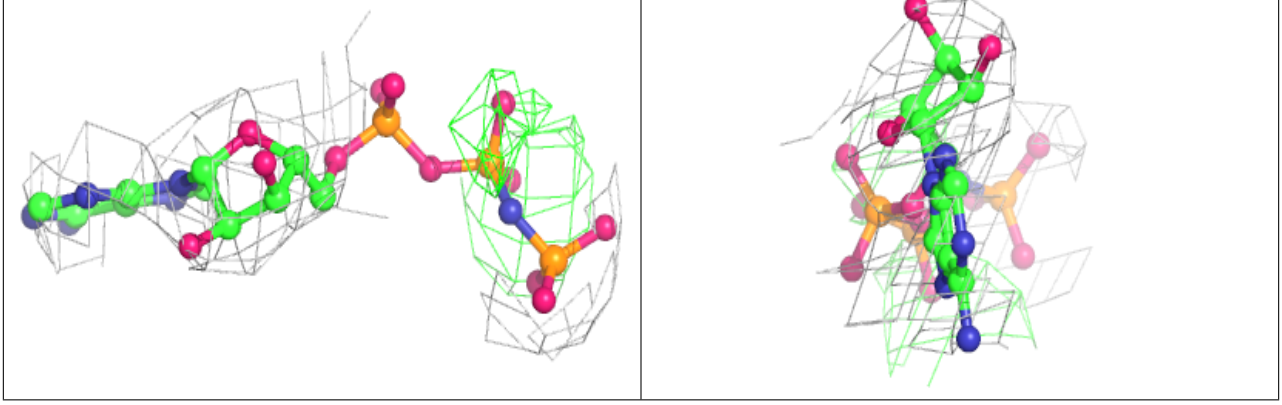




Electron density around ANP D 5004:

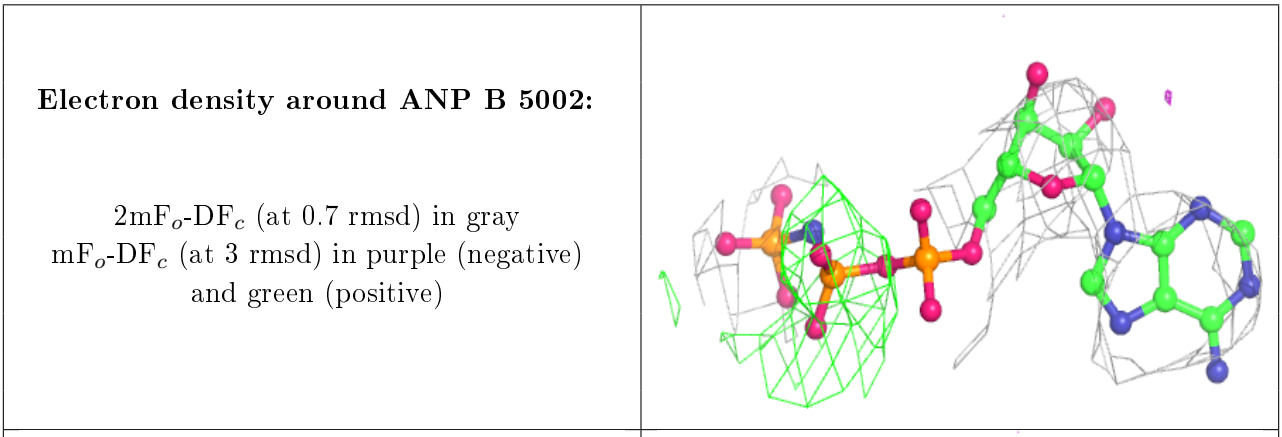
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

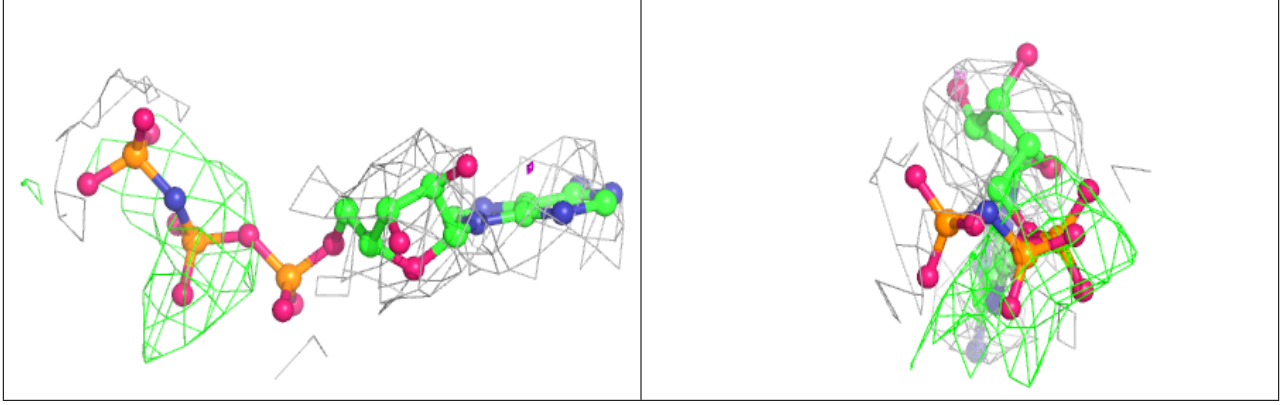




Electron density around ANP B 5002:

$2mF_o$-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.