Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:33 PM EDT

PDB ID	:	1GPA
Title	:	STRUCTURAL MECHANISM FOR GLYCOGEN PHOSPHORYLASE CONTROL BY PHOSPHORYLATION AND AMP
Authors	:	Barford, D.; Hu, S.-H.; Johnson, L.N.
Deposited on	:	1990-11-13
Resolution	:	2.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

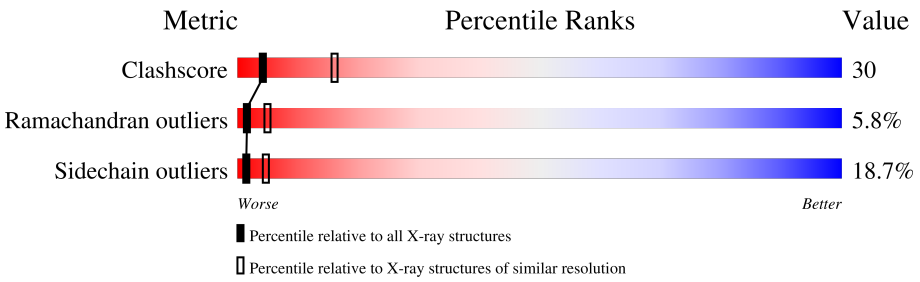
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	35% 42% 16% 5% •
1	B	842	37% 41% 16% • •
1	C	842	35% 40% 18% 6% •
1	D	842	31% 42% 20% 6% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27029 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.

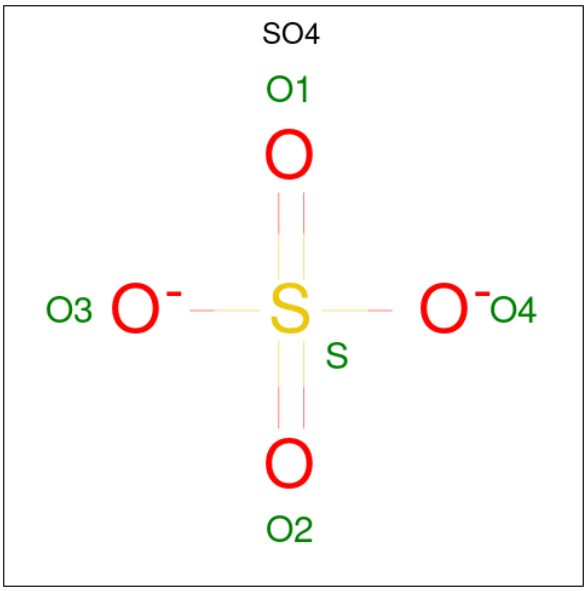
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	828	6732	4287	1190	1224	1	30	44	0	0
1	B	827	6733	4286	1189	1227	1	30	24	0	0
1	C	828	6732	4287	1190	1224	1	30	0	0	0
1	D	828	6732	4287	1190	1224	1	30	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

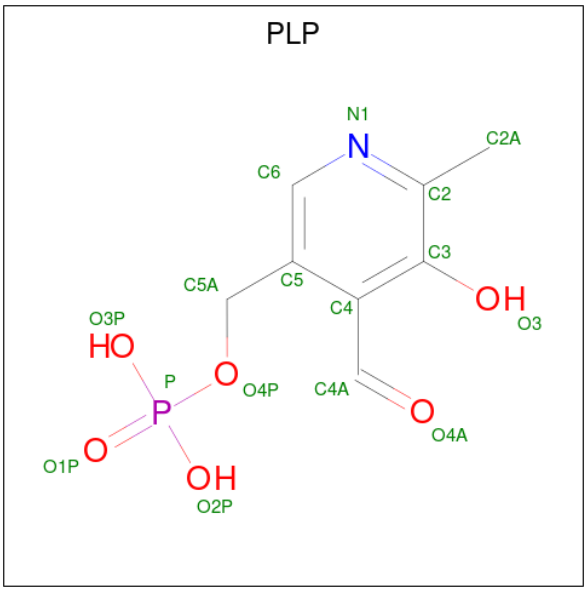
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489
B	380	ILE	LEU	CONFLICT	UNP P00489
C	380	ILE	LEU	CONFLICT	UNP P00489
D	380	ILE	LEU	CONFLICT	UNP P00489

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

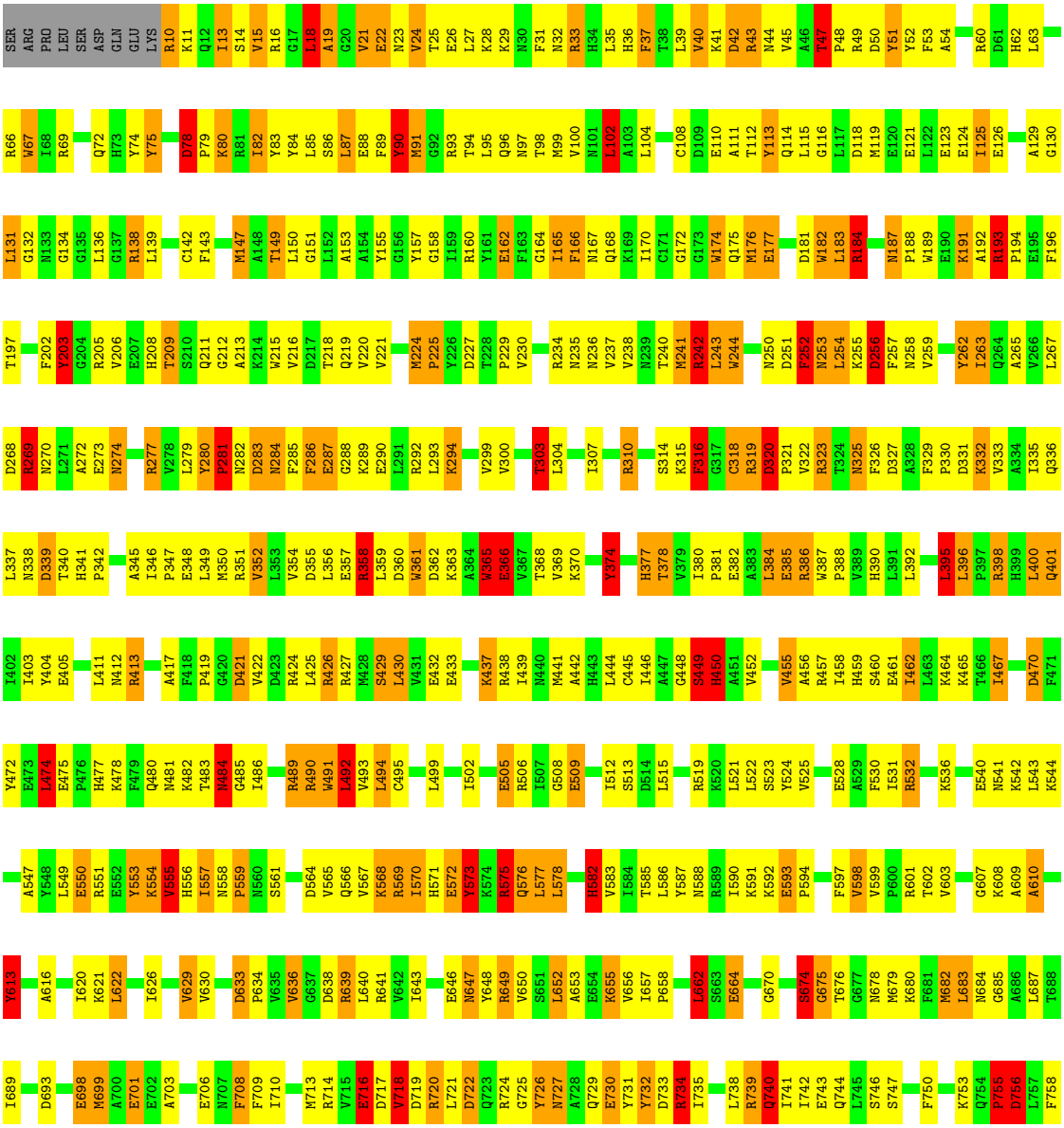
3 Residue-property plots (i)

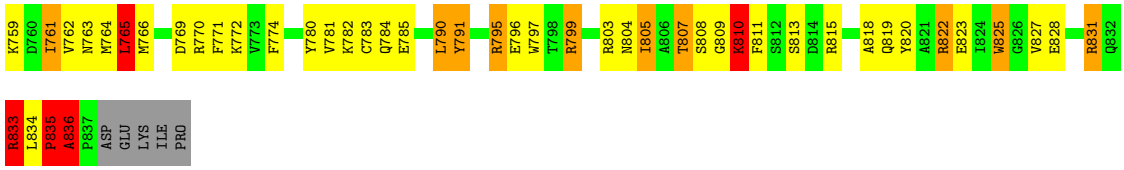
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: GLYCOGEN PHOSPHORYLASE A

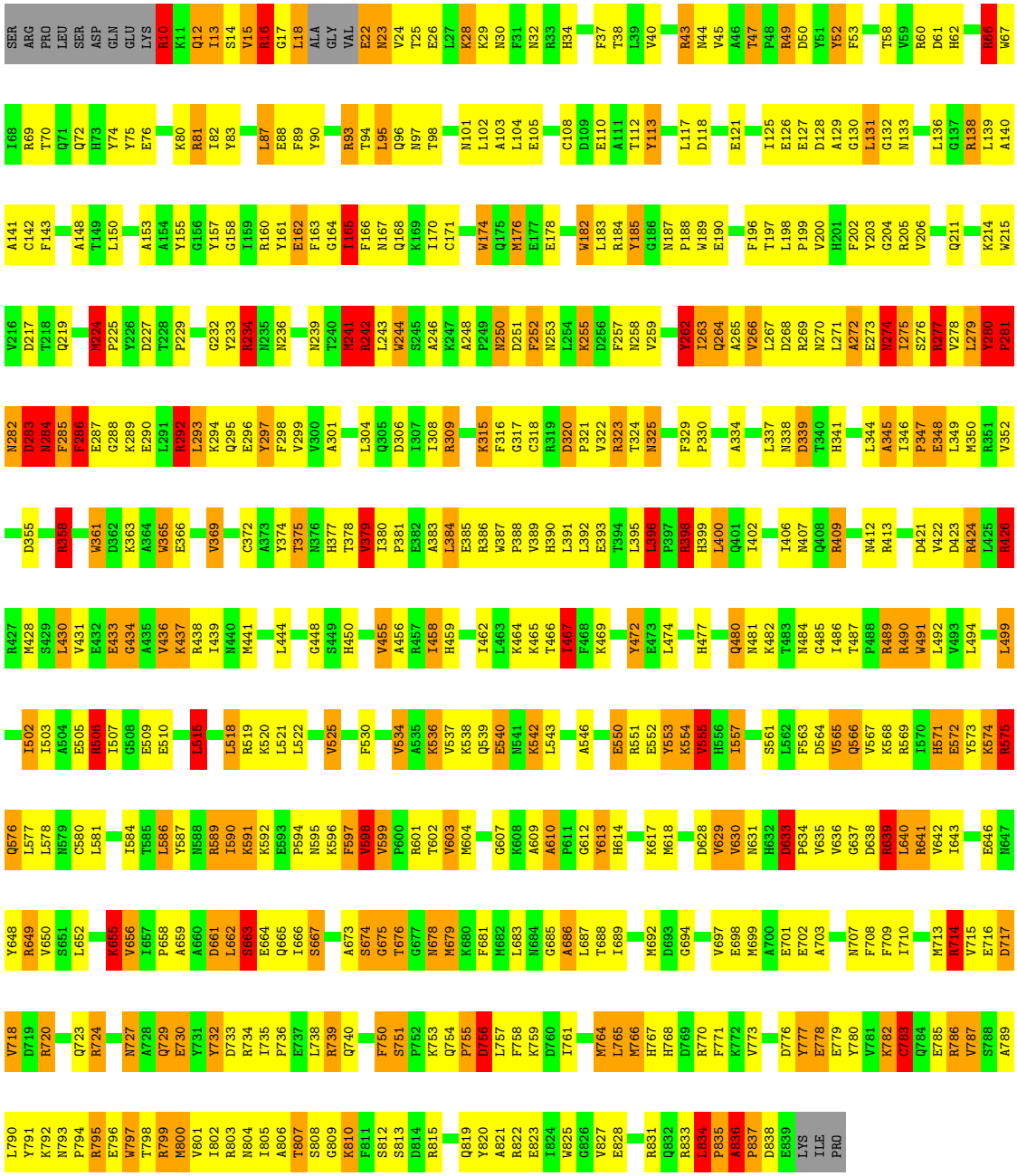
Chain A: 35% 42% 16% 5% •





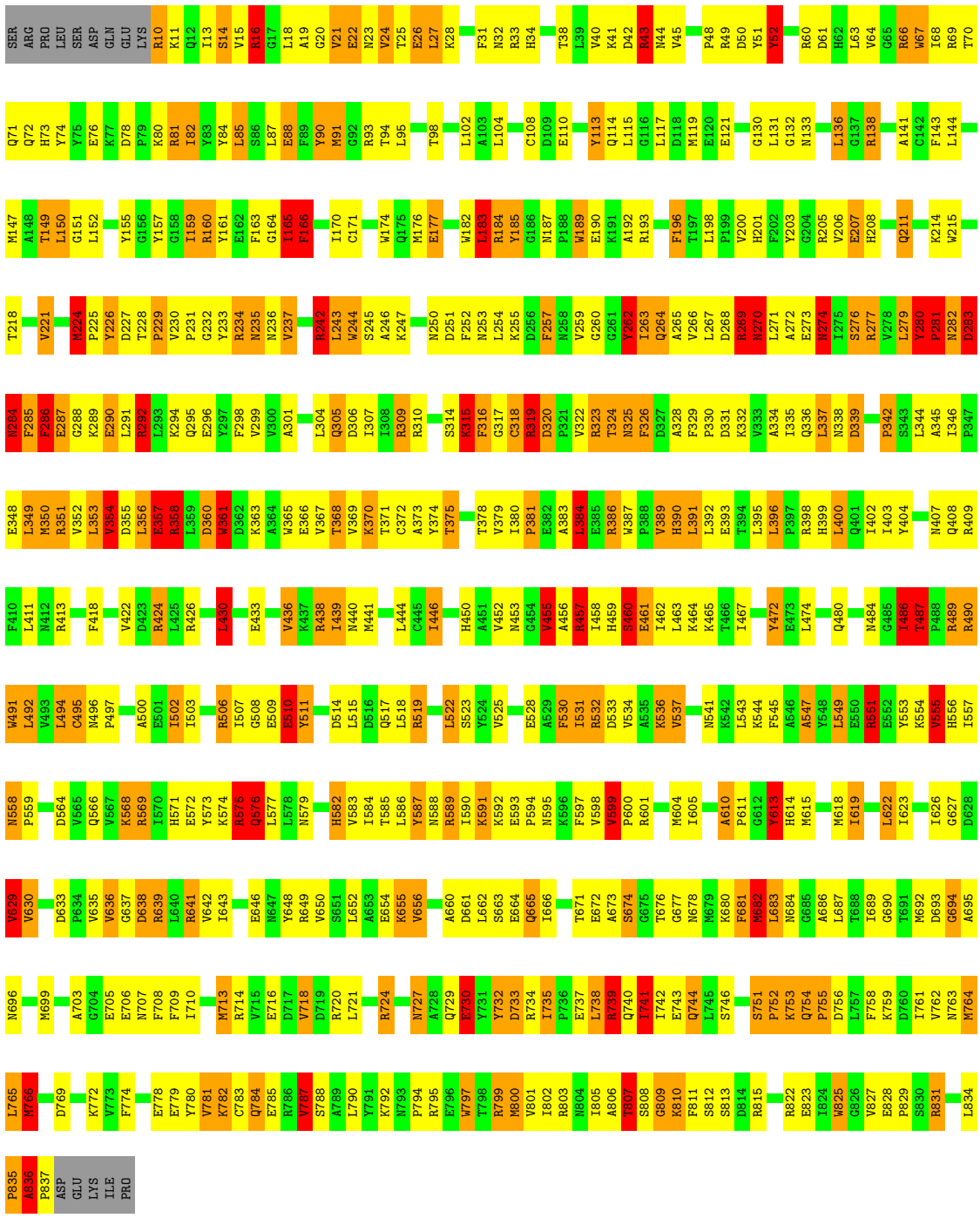
• Molecule 1: GLYCOGEN PHOSPHORYLASE A

Chain B: 37% 41% 16%



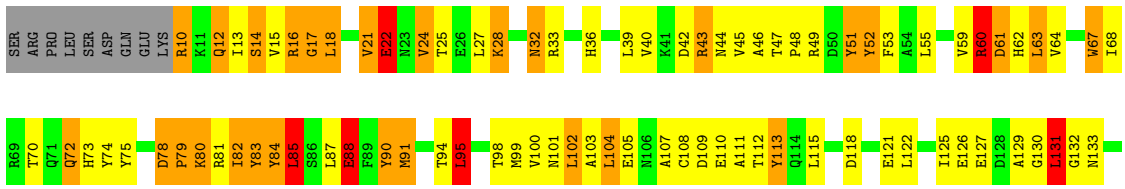
• Molecule 1: GLYCOGEN PHOSPHORYLASE A

Chain C: 35% 40% 18% 6%



• Molecule 1: GLYCOGEN PHOSPHORYLASE A

Chain D: 31% 42% 20% 6% •



L136 G137 R138 L139 A140 A141 C142 F143 L144 D145 S146 M147 L152 A153 A154 Y155 I159 R160 G164 I165 F166 N167 Q168 K169 I170 G173 W174 Q175 M176 E177 E178 D181 W182 L183 R184 Y185 G186 N187 P188 W189 E190 K191 A192 R193 P194 E195 L198 Y203 G204 R205 V206 E207 H208
T209 S210 Q211 K214 W215 V216 D217 T218 Q219 L222 A223 M224 P225 Y226 D227 T228 P229 V230 P231 G232 Y233 R234 N235 N236 V237 V238 N239 T240 M241 R242 L243 W244 S245 A246 K247 A248 P249 N250 D251 F252 N253 L254 K255 D256 F257 N258 V259 G260 G261 Y262 I263 Q264 A265 D268 R269 A272
E273 N274 R277 V278 L279 Y280 P281 N282 D283 N284 F285 F286 E287 G288 K289 E290 L291 R292 L293 K294 Y297 F298 V299 A302 T303 D306 I307 I308 R309 R310 F311 K312 S313 S314 K315 F316 G317 C318 R319 D320 P321 V322 R323 T324 N325 F326 D327 A328 F329 P330 D331 K332 I335 Q336 L337
N338 D339 T340 H341 P342 S343 L344 E348 L349 M350 R351 V352 L353 V354 D355 L356 E357 R358 L359 D360 W361 A364 W365 T368 V369 K370 T371 C372 A373 Y374 H377 T378 V379 I380 L384 E385 R386 W387 P388 V389 H390 L391 L392 L395 L396 P397 R398 H399 L400 Q401 I402 I403 Y404 E405
I406 N407 Q408 R409 F410 R413 V414 R424 L425 R426 R427 M428 S429 L430 G434 A435 V436 K437 R438 I439 N440 L444 C445 S449 H450 A451 V452 V455 A456 R457 I458 H459 S460 E461 I462 L463 K464 K465 T466 I467 F468 K469 Y472 E473 L474 H477 K478 T483 N484 G485 I486
T487 P488 R489 R490 W491 L492 V493 L494 C495 N496 P497 G498 L499 A500 E501 I502 I503 A504 E505 R506 I507 G508 E509 E510 Y511 I512 S513 D514 L515 D516 Q517 L518 R519 K520 L521 L522 S523 Y524 V525 D526 D527 F530 I531 R532 D533 V534 A535 K536 V537 K538 Q539 E540 N541 K542 L543 K544 F545 L549
E550 R551 E552 Y553 K554 V555 H556 I557 N558 P559 N560 S561 L562 F563 D564 V565 Q566 V567 K568 R569 I570 H571 E572 Y573 R574 R575 Q576 L577 L578 N579 C580 L581 H582 V583 I584 T585 L586 Y587 N588 R589 I590 K591 K592 E593 P594 N595 V598 V599 P600 R601 T602 V603 M604 I605 A610 F611 G612 Y613
H614 K617 M618 I619 I620 K621 L622 I623 T624 A625 K626 G627 D628 V629 V630 N631 H632 D633 P634 V635 V636 G637 D638 R639 L640 R641 V642 I643 F644 L645 E646 N647 Y648 R649 L652 K655 V656 I657 P658 A659 A660 D661 L662 S663 E664 Q665 I666 S674 G675 T676 G677 N678 M679 K680 F681 M682
L683 N684 L687 T688 I689 G690 T691 M692 D693 G694 A695 N696 V697 E698 M699 A700 E701 E702 A703 G704 E705 E706 N707 F708 F709 I710 F711 G712 M713 R714 V715 E716 D717 V718 D719 R720 L721 D722 Q723 R724 G725 Y726 N727 E730 Y731 Y732 D733 R734 I735 P736 E737 L738 R739 Q740 I741 I742 E743 Q744
L745 S746 F750 P752 K753 Q754 P755 D756 L757 F758 K759 D760 I761 V762 N763 M764 L765 M766 H767 H768 D769 R770 F771 K772 V773 F774 Y777 E778 E779 Y780 V781 K782 C783 Q784 E785 R786 V787 S788 A789 L790 Y791 K792 N793 P794 R795 E796 W797 T798 R799 M800 W801 I802 R803 N804 I805 A806 T807
S808 G809 K810 F811 S812 S813 D814 R815 A818 A821 R822 E823 Y824 W825 E828 R831 Q832 R833 L834 P835 A836 P837 ASP GLU LYS ILE PRO

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.00Å 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27029	wwPDB-VP
Average B, all atoms ($Å^2$)	22.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, PLP, SO4

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	1.12	5/6873 (0.1%)	2.11	267/9300 (2.9%)
1	B	1.07	5/6873 (0.1%)	2.08	259/9298 (2.8%)
1	C	1.11	5/6873 (0.1%)	2.10	264/9300 (2.8%)
1	D	1.09	7/6873 (0.1%)	2.19	266/9300 (2.9%)
All	All	1.10	22/27492 (0.1%)	2.12	1056/37198 (2.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	11
1	C	0	9
1	D	0	15
All	All	0	46

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	VAL	C-N	26.58	1.95	1.34
1	A	756	ASP	N-CA	15.44	1.77	1.46
1	A	47	THR	N-CA	-11.92	1.22	1.46
1	D	22	GLU	CD-OE2	6.78	1.33	1.25
1	A	543	LEU	N-CA	6.35	1.59	1.46
1	D	281	PRO	CA-C	-6.26	1.40	1.52
1	A	262	TYR	CB-CG	6.20	1.60	1.51
1	B	837	PRO	CA-C	-6.11	1.40	1.52
1	B	837	PRO	N-CA	-5.84	1.37	1.47
1	D	189	TRP	CG-CD2	-5.74	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	245	SER	CA-CB	-5.72	1.44	1.52
1	D	501	GLU	CB-CG	5.68	1.62	1.52
1	C	460	SER	CA-CB	-5.54	1.44	1.52
1	B	490	ARG	CZ-NH1	5.35	1.40	1.33
1	D	525	VAL	CA-CB	5.33	1.66	1.54
1	C	67	TRP	CD1-NE1	-5.28	1.28	1.38
1	D	501	GLU	CG-CD	5.26	1.59	1.51
1	B	244	TRP	CG-CD2	-5.25	1.34	1.43
1	D	507	ILE	CA-CB	5.11	1.66	1.54
1	B	182	TRP	CG-CD2	-5.08	1.35	1.43
1	C	393	GLU	CA-CB	-5.05	1.42	1.53
1	A	797	TRP	CG-CD2	-5.03	1.35	1.43

All (1056) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	24	VAL	O-C-N	26.50	165.09	122.70
1	D	251	ASP	CA-CB-CG	25.67	169.87	113.40
1	D	24	VAL	CA-C-N	-20.73	71.59	117.20
1	D	575	ARG	NE-CZ-NH1	18.09	129.35	120.30
1	D	281	PRO	O-C-N	17.08	150.02	122.70
1	D	24	VAL	C-N-CA	-16.78	79.76	121.70
1	C	24	VAL	O-C-N	16.03	148.35	122.70
1	A	490	ARG	NE-CZ-NH1	14.31	127.45	120.30
1	D	641	ARG	NE-CZ-NH1	13.93	127.27	120.30
1	D	292	ARG	NE-CZ-NH2	-13.40	113.60	120.30
1	D	780	TYR	CB-CG-CD2	-13.37	112.98	121.00
1	C	358	ARG	NE-CZ-NH2	-13.24	113.68	120.30
1	A	358	ARG	NE-CZ-NH2	-13.06	113.77	120.30
1	D	575	ARG	NE-CZ-NH2	-13.03	113.79	120.30
1	C	160	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	D	142	CYS	CA-CB-SG	-12.52	91.47	114.00
1	B	409	ARG	NE-CZ-NH2	-12.27	114.17	120.30
1	C	24	VAL	CA-C-N	-12.07	90.64	117.20
1	A	90	TYR	CB-CG-CD2	-11.76	113.94	121.00
1	A	374	TYR	CB-CG-CD2	-11.53	114.08	121.00
1	A	234	ARG	NE-CZ-NH2	-11.47	114.57	120.30
1	D	250	ASN	CA-CB-CG	11.43	138.55	113.40
1	B	292	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	B	386	ARG	NE-CZ-NH2	-11.17	114.71	120.30
1	B	601	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	D	799	ARG	NE-CZ-NH2	-11.15	114.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	783	CYS	CA-CB-SG	-10.93	94.33	114.00
1	D	286	PHE	O-C-N	10.93	140.18	122.70
1	A	286	PHE	O-C-N	10.91	140.16	122.70
1	A	739	ARG	NE-CZ-NH2	10.91	125.76	120.30
1	D	641	ARG	NE-CZ-NH2	-10.87	114.86	120.30
1	C	286	PHE	O-C-N	10.82	140.01	122.70
1	D	292	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	A	242	ARG	NE-CZ-NH2	-10.75	114.92	120.30
1	C	783	CYS	CA-CB-SG	-10.75	94.66	114.00
1	A	551	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	D	281	PRO	CA-C-N	-10.57	93.95	117.20
1	D	244	TRP	CD1-CG-CD2	10.53	114.72	106.30
1	C	386	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	A	182	TRP	CD1-CG-CD2	10.42	114.64	106.30
1	A	281	PRO	O-C-N	10.39	139.33	122.70
1	A	262	TYR	CB-CA-C	10.28	130.97	110.40
1	B	786	ARG	NE-CZ-NH1	10.25	125.43	120.30
1	C	281	PRO	O-C-N	10.24	139.09	122.70
1	B	297	TYR	CB-CG-CD2	-10.24	114.86	121.00
1	A	421	ASP	CA-C-N	-10.12	94.94	117.20
1	D	244	TRP	CG-CD2-CE3	10.12	143.01	133.90
1	C	51	TYR	CB-CG-CD2	-10.11	114.93	121.00
1	A	262	TYR	CA-C-N	-10.06	95.07	117.20
1	C	93	ARG	NE-CZ-NH2	-9.99	115.31	120.30
1	D	319	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	C	292	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	A	815	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	B	649	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	A	489	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	D	358	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	C	490	ARG	NE-CZ-NH2	-9.87	115.37	120.30
1	B	426	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	B	386	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	C	799	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	A	386	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	D	782	LYS	CA-CB-CG	9.60	134.51	113.40
1	C	67	TRP	CD1-CG-CD2	9.59	113.97	106.30
1	C	676	THR	CA-CB-CG2	9.57	125.80	112.40
1	C	365	TRP	CD1-CG-CD2	9.46	113.87	106.30
1	B	50	ASP	CB-CG-OD1	9.39	126.75	118.30
1	B	292	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	C	491	TRP	CD1-CG-CD2	9.36	113.79	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	244	TRP	CE2-CD2-CG	-9.36	99.81	107.30
1	A	490	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	D	91	MET	CA-CB-CG	-9.34	97.42	113.30
1	B	509	GLU	CA-C-N	-9.33	96.68	117.20
1	B	424	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	A	491	TRP	CD1-CG-CD2	9.31	113.75	106.30
1	A	649	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	B	714	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	B	387	TRP	CD1-CG-CD2	9.27	113.71	106.30
1	A	639	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	D	365	TRP	CD1-CG-CD2	9.21	113.67	106.30
1	D	831	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	C	292	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	B	361	TRP	CD1-CG-CD2	9.16	113.63	106.30
1	A	365	TRP	CD1-CG-CD2	9.16	113.63	106.30
1	B	641	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	495	CYS	CA-CB-SG	9.14	130.45	114.00
1	C	676	THR	CA-CB-OG1	-9.13	89.82	109.00
1	B	203	TYR	CB-CG-CD2	-9.11	115.53	121.00
1	D	720	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	A	193	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	B	409	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	C	553	TYR	CB-CG-CD1	9.09	126.46	121.00
1	C	350	MET	CG-SD-CE	-9.04	85.73	100.20
1	D	310	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	C	205	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	D	438	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	C	489	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	B	491	TRP	CD1-CG-CD2	8.96	113.47	106.30
1	D	365	TRP	CE2-CD2-CG	-8.94	100.15	107.30
1	D	365	TRP	CG-CD2-CE3	8.92	141.93	133.90
1	B	490	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	C	491	TRP	CE2-CD2-CG	-8.89	100.19	107.30
1	A	613	TYR	CB-CG-CD2	-8.83	115.70	121.00
1	B	309	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	A	244	TRP	CD1-CG-CD2	8.82	113.35	106.30
1	C	825	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	D	244	TRP	CB-CG-CD1	-8.80	115.55	127.00
1	A	404	TYR	CB-CG-CD2	-8.78	115.73	121.00
1	A	365	TRP	CE2-CD2-CG	-8.78	100.28	107.30
1	B	224	MET	CA-CB-CG	8.77	128.21	113.30
1	A	262	TYR	CA-C-O	8.74	138.45	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	93	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	277	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	C	160	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	B	66	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	374	TYR	CB-CG-CD1	8.66	126.20	121.00
1	C	656	VAL	CA-CB-CG2	-8.65	97.93	110.90
1	C	351	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	C	610	ALA	N-CA-CB	8.61	122.15	110.10
1	D	262	TYR	N-CA-C	8.58	134.17	111.00
1	C	630	VAL	CG1-CB-CG2	-8.56	97.20	110.90
1	D	457	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	D	490	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	C	374	TYR	CB-CG-CD2	-8.54	115.88	121.00
1	A	799	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	C	43	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	D	303	THR	CA-CB-CG2	8.48	124.27	112.40
1	B	491	TRP	CE2-CD2-CG	-8.45	100.54	107.30
1	B	286	PHE	O-C-N	8.44	136.21	122.70
1	A	174	TRP	CD1-CG-CD2	8.42	113.04	106.30
1	C	182	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	D	557	ILE	CG1-CB-CG2	-8.39	92.94	111.40
1	A	575	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	D	427	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	A	491	TRP	CE2-CD2-CG	-8.34	100.63	107.30
1	D	780	TYR	CB-CG-CD1	8.34	126.00	121.00
1	C	113	TYR	CB-CG-CD2	-8.34	116.00	121.00
1	B	67	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	D	739	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	C	52	TYR	CB-CG-CD2	-8.28	116.03	121.00
1	D	67	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	A	257	PHE	CA-C-N	-8.26	99.03	117.20
1	D	51	TYR	CB-CG-CD2	-8.26	116.05	121.00
1	C	629	VAL	CA-CB-CG2	-8.24	98.53	110.90
1	A	66	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	D	138	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	D	263	ILE	CA-C-N	-8.20	99.15	117.20
1	C	263	ILE	CA-C-N	-8.15	99.26	117.20
1	A	182	TRP	CE2-CD2-CG	-8.14	100.78	107.30
1	C	365	TRP	CE2-CD2-CG	-8.13	100.80	107.30
1	C	205	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	C	424	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	244	TRP	CE2-CD2-CG	-8.11	100.81	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	745	LEU	CA-CB-CG	8.11	133.96	115.30
1	A	45	VAL	CA-CB-CG2	-8.11	98.74	110.90
1	B	365	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	C	244	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	C	457	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	472	TYR	CB-CG-CD1	-8.05	116.17	121.00
1	C	553	TYR	CB-CG-CD2	-8.06	116.17	121.00
1	B	472	TYR	CB-CG-CD2	-8.01	116.20	121.00
1	D	639	ARG	CA-CB-CG	-8.00	95.79	113.40
1	D	262	TYR	CB-CG-CD1	-7.99	116.20	121.00
1	D	315	LYS	CA-CB-CG	-7.96	95.89	113.40
1	C	138	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	B	131	LEU	CA-CB-CG	7.92	133.51	115.30
1	D	286	PHE	CA-C-N	-7.91	99.81	117.20
1	B	365	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	A	325	ASN	CA-C-N	-7.90	99.83	117.20
1	D	215	TRP	CD1-CG-CD2	7.89	112.62	106.30
1	C	325	ASN	CA-C-N	-7.88	99.87	117.20
1	A	583	VAL	CG1-CB-CG2	-7.88	98.30	110.90
1	D	679	MET	CG-SD-CE	-7.86	87.62	100.20
1	B	325	ASN	CA-C-N	-7.86	99.90	117.20
1	A	795	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	676	THR	CA-CB-CG2	7.85	123.39	112.40
1	A	831	ARG	CA-CB-CG	7.85	130.67	113.40
1	D	720	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	D	682	MET	CG-SD-CE	7.84	112.75	100.20
1	D	601	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	B	506	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	286	PHE	CA-C-N	-7.81	100.03	117.20
1	A	351	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	C	90	TYR	CB-CG-CD1	7.78	125.67	121.00
1	A	541	ASN	CB-CG-ND2	7.78	135.37	116.70
1	C	286	PHE	CA-C-N	-7.77	100.10	117.20
1	D	184	ARG	N-CA-C	-7.77	90.01	111.00
1	B	825	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	D	90	TYR	CB-CG-CD2	-7.74	116.36	121.00
1	D	424	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	B	281	PRO	O-C-N	7.73	135.07	122.70
1	C	174	TRP	CE2-CD2-CG	-7.71	101.14	107.30
1	B	81	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	555	VAL	CA-CB-CG1	-7.70	99.36	110.90
1	D	398	ARG	NE-CZ-NH2	7.69	124.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	533	ASP	CA-CB-CG	7.68	130.29	113.40
1	C	455	VAL	N-CA-CB	-7.67	94.63	111.50
1	C	441	MET	CG-SD-CE	7.64	112.43	100.20
1	B	189	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	A	724	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	B	825	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	C	613	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	B	387	TRP	CE2-CD2-CG	-7.62	101.21	107.30
1	A	633	ASP	CB-CG-OD1	7.61	125.15	118.30
1	B	174	TRP	CD1-CG-CD2	7.61	112.38	106.30
1	B	365	TRP	CG-CD2-CE3	7.59	140.73	133.90
1	B	662	LEU	CA-CB-CG	7.59	132.76	115.30
1	A	51	TYR	CB-CG-CD2	-7.58	116.45	121.00
1	C	67	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	B	800	MET	CA-CB-CG	7.57	126.16	113.30
1	C	374	TYR	CB-CG-CD1	7.57	125.54	121.00
1	D	365	TRP	CB-CG-CD1	-7.56	117.17	127.00
1	B	241	MET	CG-SD-CE	7.54	112.27	100.20
1	C	825	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	D	283	ASP	O-C-N	7.53	134.75	122.70
1	A	10	ARG	CA-C-N	7.53	133.76	117.20
1	B	83	TYR	CB-CG-CD1	-7.52	116.49	121.00
1	C	244	TRP	CG-CD2-CE3	7.52	140.67	133.90
1	D	189	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	B	490	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	C	551	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	D	303	THR	CA-CB-OG1	-7.49	93.28	109.00
1	C	174	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	A	726	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	B	10	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	174	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	300	VAL	CA-CB-CG2	-7.44	99.74	110.90
1	C	555	VAL	CA-CB-CG1	-7.42	99.77	110.90
1	D	551	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	491	TRP	CG-CD2-CE3	7.41	140.57	133.90
1	C	724	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	D	81	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	B	234	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	90	TYR	CB-CG-CD1	7.39	125.43	121.00
1	B	81	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	413	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	B	799	ARG	NE-CZ-NH2	-7.37	116.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	598	VAL	N-CA-CB	-7.36	95.30	111.50
1	B	61	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	791	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	D	714	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	D	569	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	127	GLU	CA-CB-CG	7.33	129.54	113.40
1	C	354	VAL	CG1-CB-CG2	-7.32	99.18	110.90
1	B	553	TYR	CA-CB-CG	7.32	127.31	113.40
1	C	237	VAL	CA-CB-CG1	-7.32	99.93	110.90
1	C	587	TYR	CB-CG-CD1	-7.31	116.61	121.00
1	C	67	TRP	CG-CD1-NE1	-7.28	102.82	110.10
1	C	358	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	D	583	VAL	CA-CB-CG2	-7.27	100.00	110.90
1	B	436	VAL	CA-CB-CG2	-7.27	100.00	110.90
1	C	795	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	D	565	VAL	CB-CA-C	-7.26	97.61	111.40
1	A	532	ARG	CA-CB-CG	7.25	129.34	113.40
1	D	208	HIS	CA-CB-CG	7.24	125.91	113.60
1	B	639	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	754	GLN	N-CA-C	-7.22	91.50	111.00
1	D	769	ASP	CB-CG-OD1	7.22	124.80	118.30
1	D	745	LEU	CB-CG-CD1	-7.21	98.74	111.00
1	B	597	PHE	O-C-N	7.21	134.24	122.70
1	C	244	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	B	509	GLU	O-C-N	7.20	134.22	122.70
1	D	159	ILE	CG1-CB-CG2	-7.20	95.56	111.40
1	C	84	TYR	CB-CG-CD2	-7.19	116.68	121.00
1	A	267	LEU	CA-CB-CG	-7.17	98.82	115.30
1	D	797	TRP	CE2-CD2-CG	-7.16	101.58	107.30
1	C	639	ARG	CA-CB-CG	-7.14	97.69	113.40
1	B	597	PHE	CA-C-N	-7.14	101.49	117.20
1	A	269	ARG	CA-CB-CG	7.12	129.07	113.40
1	C	277	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	252	PHE	N-CA-C	7.12	130.22	111.00
1	C	45	VAL	CA-CB-CG2	-7.12	100.23	110.90
1	C	184	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	244	TRP	CD1-CG-CD2	7.07	111.96	106.30
1	B	679	MET	CG-SD-CE	-7.07	88.89	100.20
1	C	81	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	361	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	B	75	TYR	CB-CG-CD1	-7.04	116.78	121.00
1	B	491	TRP	CB-CG-CD1	-7.04	117.85	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	766	MET	CG-SD-CE	7.04	111.45	100.20
1	B	836	ALA	N-CA-C	7.02	129.97	111.00
1	D	745	LEU	CB-CA-C	-7.02	96.86	110.20
1	A	182	TRP	CG-CD1-NE1	-7.01	103.09	110.10
1	D	361	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	B	242	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	455	VAL	CG1-CB-CG2	6.98	122.07	110.90
1	C	108	CYS	CA-CB-SG	-6.97	101.45	114.00
1	A	610	ALA	N-CA-CB	6.97	119.85	110.10
1	A	505	GLU	CA-CB-CG	6.96	128.72	113.40
1	D	457	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	662	LEU	CA-CB-CG	6.96	131.30	115.30
1	C	182	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	B	174	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	C	591	LYS	O-C-N	6.95	133.81	122.70
1	D	281	PRO	CA-N-CD	-6.93	101.79	111.50
1	D	506	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	C	283	ASP	O-C-N	6.92	133.77	122.70
1	B	489	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	822	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	B	732	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	A	24	VAL	O-C-N	6.90	133.74	122.70
1	B	262	TYR	N-CA-C	6.90	129.63	111.00
1	A	243	LEU	CA-CB-CG	6.89	131.15	115.30
1	A	138	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	C	189	TRP	NE1-CE2-CZ2	-6.89	122.83	130.40
1	B	16	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	D	444	LEU	CB-CG-CD1	-6.87	99.31	111.00
1	B	534	VAL	CG1-CB-CG2	-6.87	99.90	110.90
1	B	836	ALA	O-C-N	6.87	134.15	121.10
1	C	610	ALA	CB-CA-C	-6.87	99.80	110.10
1	D	699	MET	CG-SD-CE	-6.87	89.21	100.20
1	B	66	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	491	TRP	CE2-CD2-CG	-6.85	101.82	107.30
1	B	131	LEU	N-CA-CB	-6.84	96.72	110.40
1	C	491	TRP	CG-CD1-NE1	-6.84	103.26	110.10
1	A	358	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	427	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	540	GLU	CA-CB-CG	6.83	128.43	113.40
1	A	810	LYS	CA-CB-CG	6.83	128.43	113.40
1	C	16	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	387	TRP	CD1-CG-CD2	6.81	111.75	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	699	MET	CG-SD-CE	-6.81	89.31	100.20
1	D	299	VAL	CA-CB-CG2	-6.80	100.69	110.90
1	D	193	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	263	ILE	CA-C-N	-6.80	102.25	117.20
1	A	457	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	D	182	TRP	CE2-CD2-CG	-6.79	101.87	107.30
1	A	323	ARG	CA-CB-CG	6.79	128.33	113.40
1	D	808	SER	CA-C-N	6.79	129.77	116.20
1	C	90	TYR	CB-CG-CD2	-6.78	116.93	121.00
1	D	610	ALA	N-CA-CB	6.78	119.59	110.10
1	D	109	ASP	CB-CG-OD1	6.78	124.40	118.30
1	C	361	TRP	CD1-CG-CD2	6.77	111.72	106.30
1	A	598	VAL	CG1-CB-CG2	-6.77	100.07	110.90
1	C	797	TRP	NE1-CE2-CZ2	-6.77	122.96	130.40
1	B	714	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	365	TRP	CB-CG-CD1	-6.76	118.21	127.00
1	C	318	CYS	CA-CB-SG	6.76	126.17	114.00
1	C	629	VAL	CA-CB-CG1	6.73	121.00	110.90
1	A	361	TRP	CD1-CG-CD2	6.73	111.69	106.30
1	B	339	ASP	CA-C-N	6.72	131.99	117.20
1	D	282	ASN	O-C-N	6.72	133.45	122.70
1	A	835	PRO	N-CA-C	6.71	129.55	112.10
1	B	754	GLN	CA-CB-CG	6.71	128.16	113.40
1	D	807	THR	N-CA-CB	-6.70	97.57	110.30
1	D	533	ASP	CB-CA-C	-6.69	97.01	110.40
1	A	37	PHE	CB-CG-CD2	-6.69	116.12	120.80
1	C	553	TYR	CA-CB-CG	6.67	126.07	113.40
1	D	189	TRP	CD1-CG-CD2	6.67	111.64	106.30
1	A	387	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	A	551	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	569	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	B	663	SER	CA-CB-OG	6.66	129.19	111.20
1	A	676	THR	CA-CB-OG1	-6.65	95.03	109.00
1	D	833	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	D	16	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	D	405	GLU	CA-CB-CG	6.64	128.01	113.40
1	A	575	ARG	O-C-N	-6.63	112.09	122.70
1	B	387	TRP	CG-CD1-NE1	-6.62	103.48	110.10
1	C	224	MET	CA-CB-CG	6.62	124.55	113.30
1	C	766	MET	CG-SD-CE	6.62	110.79	100.20
1	B	339	ASP	O-C-N	-6.61	112.12	122.70
1	B	396	LEU	CA-CB-CG	6.61	130.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	182	TRP	CD1-CG-CD2	6.61	111.59	106.30
1	A	649	ARG	CG-CD-NE	-6.60	97.94	111.80
1	C	769	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	649	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	B	661	ASP	CB-CG-OD1	6.59	124.23	118.30
1	C	810	LYS	CA-CB-CG	6.58	127.89	113.40
1	A	610	ALA	CB-CA-C	-6.58	100.22	110.10
1	A	310	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	49	ARG	CA-CB-CG	6.57	127.86	113.40
1	B	67	TRP	CG-CD1-NE1	-6.57	103.53	110.10
1	D	269	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	358	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	587	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	C	361	TRP	CE2-CD2-CG	-6.55	102.06	107.30
1	B	203	TYR	CB-CG-CD1	6.54	124.93	121.00
1	A	795	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	427	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	D	361	TRP	CD1-CG-CD2	6.54	111.53	106.30
1	D	572	GLU	CA-CB-CG	-6.54	99.02	113.40
1	C	398	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	45	VAL	CA-CB-CG1	6.53	120.69	110.90
1	C	171	CYS	CA-CB-SG	-6.53	102.26	114.00
1	C	189	TRP	CE2-CD2-CG	-6.52	102.08	107.30
1	A	676	THR	N-CA-CB	-6.52	97.91	110.30
1	C	211	GLN	CB-CG-CD	6.51	128.53	111.60
1	B	797	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	A	384	LEU	CA-CB-CG	6.51	130.26	115.30
1	A	234	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	D	215	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	A	124	GLU	OE1-CD-OE2	-6.49	115.51	123.30
1	C	325	ASN	O-C-N	6.49	133.09	122.70
1	B	723	GLN	CA-CB-CG	-6.49	99.12	113.40
1	C	489	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	803	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	C	472	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	D	766	MET	CG-SD-CE	6.47	110.56	100.20
1	C	724	ARG	CA-CB-CG	6.47	127.64	113.40
1	D	494	LEU	CA-CB-CG	6.46	130.16	115.30
1	A	67	TRP	CD1-CG-CD2	6.46	111.47	106.30
1	B	491	TRP	NE1-CE2-CZ2	-6.45	123.30	130.40
1	A	281	PRO	CA-C-N	-6.44	103.03	117.20
1	B	189	TRP	CD1-CG-CD2	6.44	111.45	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	505	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	A	822	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	269	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	C	739	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	D	90	TYR	CB-CG-CD1	6.43	124.86	121.00
1	C	316	PHE	CA-C-N	6.43	129.06	116.20
1	C	314	SER	CA-C-N	-6.43	103.06	117.20
1	D	782	LYS	N-CA-CB	-6.43	99.03	110.60
1	D	306	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	553	TYR	CB-CG-CD1	6.42	124.85	121.00
1	A	565	VAL	CG1-CB-CG2	-6.41	100.64	110.90
1	C	45	VAL	N-CA-CB	-6.41	97.41	111.50
1	A	791	TYR	CB-CG-CD1	6.40	124.84	121.00
1	B	433	GLU	CA-CB-CG	6.40	127.49	113.40
1	B	720	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	815	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	C	24	VAL	C-N-CA	-6.39	105.73	121.70
1	D	825	TRP	CG-CD2-CE3	6.39	139.65	133.90
1	C	337	LEU	CA-CB-CG	6.38	129.98	115.30
1	C	365	TRP	CG-CD1-NE1	-6.38	103.72	110.10
1	A	176	MET	CA-CB-CG	-6.38	102.45	113.30
1	C	281	PRO	CA-C-N	-6.38	103.17	117.20
1	D	138	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	684	ASN	CA-C-N	-6.38	103.45	116.20
1	B	244	TRP	CE2-CD2-CG	-6.37	102.20	107.30
1	D	491	TRP	CD1-CG-CD2	6.37	111.40	106.30
1	B	205	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	C	177	GLU	CA-CB-CG	6.36	127.39	113.40
1	D	712	GLY	CA-C-N	-6.35	103.23	117.20
1	A	238	VAL	CG1-CB-CG2	-6.34	100.75	110.90
1	C	807	THR	N-CA-CB	-6.34	98.25	110.30
1	D	800	MET	CG-SD-CE	-6.34	90.06	100.20
1	A	361	TRP	CE2-CD2-CG	-6.34	102.23	107.30
1	A	836	ALA	CA-C-O	6.34	133.41	120.10
1	B	398	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	C	438	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	60	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	D	174	TRP	CE2-CD2-CG	-6.33	102.23	107.30
1	D	639	ARG	CB-CG-CD	6.33	128.05	111.60
1	A	316	PHE	N-CA-C	6.33	128.08	111.00
1	D	83	TYR	CB-CG-CD1	-6.32	117.21	121.00
1	B	215	TRP	CD1-CG-CD2	6.32	111.36	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	61	ASP	CA-C-N	-6.32	103.30	117.20
1	B	675	GLY	CA-C-N	-6.31	103.31	117.20
1	A	396	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	189	TRP	CE2-CD2-CG	-6.30	102.26	107.30
1	D	67	TRP	CE2-CD2-CG	-6.30	102.26	107.30
1	C	575	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	D	323	ARG	CA-CB-CG	6.29	127.25	113.40
1	B	506	ARG	CB-CG-CD	6.29	127.94	111.60
1	A	491	TRP	CB-CG-CD1	-6.28	118.83	127.00
1	C	532	ARG	CA-CB-CG	6.28	127.22	113.40
1	A	52	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	B	676	THR	N-CA-CB	-6.27	98.39	110.30
1	A	405	GLU	CA-CB-CG	6.27	127.18	113.40
1	B	374	TYR	CB-CG-CD2	-6.26	117.24	121.00
1	A	477	HIS	CA-CB-CG	6.26	124.24	113.60
1	A	582	HIS	CA-C-N	6.26	130.97	117.20
1	C	660	ALA	O-C-N	6.25	132.71	122.70
1	C	48	PRO	CA-N-CD	-6.25	102.75	111.50
1	B	67	TRP	CE2-CD2-CG	-6.25	102.30	107.30
1	D	287	GLU	CB-CA-C	6.25	122.89	110.40
1	A	734	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	455	VAL	N-CA-CB	-6.23	97.79	111.50
1	C	787	VAL	CA-CB-CG2	-6.23	101.55	110.90
1	B	267	LEU	CA-C-N	6.23	130.91	117.20
1	A	825	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	D	786	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	770	ARG	CA-CB-CG	6.22	127.09	113.40
1	C	553	TYR	O-C-N	-6.22	112.74	122.70
1	A	277	ARG	CD-NE-CZ	6.22	132.31	123.60
1	A	803	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	C	323	ARG	CA-CB-CG	6.22	127.08	113.40
1	A	91	MET	CG-SD-CE	-6.21	90.26	100.20
1	D	387	TRP	CE2-CD2-CG	-6.21	102.33	107.30
1	A	682	MET	CA-CB-CG	6.21	123.85	113.30
1	D	824	ILE	CA-CB-CG2	-6.20	98.49	110.90
1	D	512	ILE	CG1-CB-CG2	-6.20	97.76	111.40
1	C	491	TRP	CB-CG-CD1	-6.20	118.94	127.00
1	D	613	TYR	CB-CG-CD2	-6.19	117.29	121.00
1	C	165	ILE	N-CA-C	-6.19	94.30	111.00
1	B	264	GLN	N-CA-C	-6.18	94.31	111.00
1	D	365	TRP	CG-CD1-NE1	-6.18	103.92	110.10
1	C	365	TRP	CG-CD2-CE3	6.18	139.46	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	656	VAL	CA-CB-CG1	6.18	120.17	110.90
1	D	437	LYS	CB-CG-CD	-6.18	95.54	111.60
1	A	457	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	489	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	167	ASN	CB-CG-ND2	6.18	131.52	116.70
1	C	149	THR	O-C-N	-6.18	112.82	122.70
1	C	601	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	720	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	270	ASN	CA-C-N	6.17	130.78	117.20
1	C	650	VAL	CG1-CB-CG2	-6.17	101.03	110.90
1	A	241	MET	CA-CB-CG	-6.17	102.82	113.30
1	B	215	TRP	CE2-CD2-CG	-6.16	102.38	107.30
1	B	426	ARG	CA-CB-CG	6.16	126.94	113.40
1	B	515	LEU	CA-C-N	6.15	130.73	117.20
1	B	28	LYS	CB-CG-CD	-6.15	95.62	111.60
1	A	45	VAL	N-CA-CB	-6.14	97.98	111.50
1	A	102	LEU	CA-CB-CG	6.14	129.43	115.30
1	B	286	PHE	CA-C-N	-6.14	103.70	117.20
1	A	244	TRP	CB-CG-CD1	-6.13	119.03	127.00
1	B	777	TYR	CA-C-N	6.13	130.69	117.20
1	D	208	HIS	CB-CA-C	-6.13	98.13	110.40
1	A	568	LYS	CB-CG-CD	6.13	127.54	111.60
1	D	215	TRP	N-CA-C	-6.13	94.45	111.00
1	D	138	ARG	CG-CD-NE	6.13	124.67	111.80
1	B	428	MET	CA-CB-CG	-6.12	102.89	113.30
1	D	622	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	205	ARG	CA-CB-CG	6.12	126.86	113.40
1	A	382	GLU	CA-CB-CG	6.11	126.85	113.40
1	D	379	VAL	CA-CB-CG2	-6.11	101.73	110.90
1	D	386	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	43	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	C	387	TRP	CE2-CD2-CG	-6.10	102.42	107.30
1	C	390	HIS	CA-CB-CG	6.09	123.96	113.60
1	D	534	VAL	CA-CB-CG2	-6.08	101.77	110.90
1	B	739	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	67	TRP	CE2-CD2-CG	-6.08	102.44	107.30
1	C	831	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	751	SER	CA-CB-OG	6.08	127.61	111.20
1	C	244	TRP	CB-CG-CD1	-6.07	119.11	127.00
1	C	315	LYS	CA-CB-CG	-6.07	100.05	113.40
1	A	716	GLU	CA-CB-CG	6.06	126.74	113.40
1	B	72	GLN	CA-CB-CG	6.06	126.74	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	274	ASN	CA-CB-CG	6.06	126.73	113.40
1	C	744	GLN	CA-CB-CG	-6.06	100.07	113.40
1	B	639	ARG	N-CA-CB	-6.06	99.70	110.60
1	D	95	LEU	CB-CG-CD1	-6.05	100.72	111.00
1	B	306	ASP	CB-CG-OD1	6.04	123.74	118.30
1	D	174	TRP	CD1-CG-CD2	6.04	111.13	106.30
1	D	506	ARG	NH1-CZ-NH2	-6.04	112.75	119.40
1	A	722	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	277	ARG	CB-CG-CD	6.03	127.28	111.60
1	C	370	LYS	CB-CG-CD	-6.03	95.92	111.60
1	A	238	VAL	N-CA-C	-6.03	94.73	111.00
1	C	597	PHE	CA-CB-CG	-6.03	99.44	113.90
1	C	784	GLN	CG-CD-NE2	6.02	131.14	116.70
1	D	648	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	A	770	ARG	CG-CD-NE	6.01	124.43	111.80
1	D	589	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	640	LEU	CB-CG-CD1	-6.01	100.79	111.00
1	A	351	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	C	490	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	D	424	ARG	CA-CB-CG	6.00	126.61	113.40
1	A	263	ILE	CA-CB-CG1	6.00	122.40	111.00
1	A	47	THR	CA-C-O	-6.00	107.50	120.10
1	C	69	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	486	ILE	CA-CB-CG1	-6.00	99.60	111.00
1	A	184	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	474	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	646	GLU	CA-C-N	-5.99	104.02	117.20
1	B	537	VAL	CG1-CB-CG2	-5.99	101.32	110.90
1	D	438	ARG	CG-CD-NE	-5.99	99.22	111.80
1	D	309	ARG	CA-CB-CG	5.99	126.58	113.40
1	C	455	VAL	CB-CA-C	5.98	122.76	111.40
1	A	43	ARG	CG-CD-NE	5.97	124.34	111.80
1	A	263	ILE	CA-CB-CG2	-5.97	98.96	110.90
1	A	674	SER	CA-C-N	5.97	128.13	116.20
1	C	263	ILE	CA-CB-CG2	-5.97	98.97	110.90
1	C	532	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	613	TYR	CB-CG-CD1	5.96	124.58	121.00
1	D	657	ILE	CA-CB-CG1	-5.96	99.68	111.00
1	A	400	LEU	CA-CB-CG	5.95	128.99	115.30
1	C	641	ARG	N-CA-CB	5.95	121.32	110.60
1	C	553	TYR	CA-C-N	5.95	130.29	117.20
1	C	166	PHE	N-CA-C	5.95	127.07	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	430	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	A	641	ARG	CG-CD-NE	-5.95	99.31	111.80
1	D	84	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	D	88	GLU	OE1-CD-OE2	-5.94	116.17	123.30
1	A	825	TRP	CG-CD2-CE3	5.93	139.24	133.90
1	D	506	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	47	THR	CA-C-N	5.92	133.67	117.10
1	B	182	TRP	CD1-CG-CD2	5.91	111.03	106.30
1	D	581	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	A	256	ASP	CA-CB-CG	5.91	126.40	113.40
1	C	815	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	C	781	VAL	O-C-N	-5.91	113.25	122.70
1	A	825	TRP	CD1-CG-CD2	5.91	111.03	106.30
1	D	400	LEU	CA-CB-CG	5.91	128.88	115.30
1	C	733	ASP	CA-CB-CG	-5.90	100.41	113.40
1	D	519	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	B	16	ARG	CB-CA-C	-5.90	98.61	110.40
1	A	15	VAL	CB-CA-C	-5.90	100.20	111.40
1	A	350	MET	CG-SD-CE	-5.90	90.77	100.20
1	B	275	ILE	CG1-CB-CG2	-5.89	98.43	111.40
1	A	556	HIS	N-CA-C	-5.89	95.09	111.00
1	B	750	PHE	O-C-N	-5.89	113.27	122.70
1	C	45	VAL	CB-CA-C	5.89	122.58	111.40
1	B	642	VAL	CA-C-N	5.88	130.14	117.20
1	C	365	TRP	CB-CG-CD1	-5.88	119.36	127.00
1	D	428	MET	CA-CB-CG	-5.88	103.30	113.30
1	A	215	TRP	CD1-CG-CD2	5.88	111.00	106.30
1	C	189	TRP	CB-CG-CD1	-5.88	119.36	127.00
1	C	221	VAL	O-C-N	-5.88	113.30	122.70
1	D	325	ASN	N-CA-CB	5.88	121.18	110.60
1	D	387	TRP	CD1-CG-CD2	5.87	111.00	106.30
1	C	114	GLN	CA-CB-CG	-5.87	100.48	113.40
1	C	182	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	A	243	LEU	N-CA-CB	-5.86	98.67	110.40
1	C	422	VAL	CA-CB-CG2	-5.86	102.11	110.90
1	D	523	SER	CA-CB-OG	5.86	127.03	111.20
1	D	455	VAL	N-CA-CB	-5.86	98.61	111.50
1	C	648	TYR	CB-CG-CD2	-5.86	117.49	121.00
1	D	745	LEU	N-CA-CB	5.85	122.11	110.40
1	C	591	LYS	CA-C-N	-5.85	104.33	117.20
1	A	352	VAL	CA-C-N	5.85	130.06	117.20
1	B	561	SER	N-CA-CB	-5.85	101.73	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	804	ASN	CB-CA-C	-5.85	98.71	110.40
1	B	598	VAL	CB-CA-C	5.84	122.50	111.40
1	B	182	TRP	CE2-CD2-CG	-5.84	102.63	107.30
1	D	808	SER	O-C-N	-5.84	113.27	123.20
1	B	361	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	D	676	THR	CA-CB-CG2	5.83	120.57	112.40
1	C	161	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	A	740	GLN	CA-CB-CG	5.83	126.22	113.40
1	C	262	TYR	N-CA-C	5.83	126.73	111.00
1	C	509	GLU	CA-C-N	-5.82	104.40	117.20
1	C	85	LEU	CA-CB-CG	5.82	128.68	115.30
1	D	493	VAL	CA-CB-CG1	-5.82	102.17	110.90
1	D	283	ASP	CA-C-N	-5.82	104.40	117.20
1	A	575	ARG	CA-C-N	5.81	129.99	117.20
1	B	771	PHE	CA-CB-CG	-5.81	99.95	113.90
1	C	283	ASP	CA-C-N	-5.81	104.41	117.20
1	D	274	ASN	N-CA-CB	-5.81	100.14	110.60
1	D	257	PHE	CA-C-N	-5.80	104.43	117.20
1	C	797	TRP	CE2-CD2-CG	-5.79	102.67	107.30
1	B	551	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	613	TYR	CA-C-N	5.79	129.94	117.20
1	B	474	LEU	CA-CB-CG	5.79	128.61	115.30
1	D	527	ASP	CA-C-N	-5.79	104.47	117.20
1	B	347	PRO	CA-C-N	5.79	129.93	117.20
1	A	303	THR	CA-C-N	5.78	129.92	117.20
1	D	491	TRP	NE1-CE2-CZ2	-5.78	124.04	130.40
1	D	825	TRP	CE2-CD2-CG	-5.77	102.68	107.30
1	B	797	TRP	CD1-CG-CD2	5.77	110.92	106.30
1	B	350	MET	CG-SD-CE	-5.77	90.97	100.20
1	A	365	TRP	CB-CG-CD1	-5.76	119.51	127.00
1	D	263	ILE	CA-CB-CG2	-5.76	99.38	110.90
1	D	351	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	300	VAL	CA-CB-CG1	5.76	119.53	110.90
1	D	384	LEU	CA-CB-CG	5.75	128.53	115.30
1	D	434	GLY	O-C-N	5.75	131.90	122.70
1	C	780	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	D	474	LEU	CA-CB-CG	5.75	128.52	115.30
1	D	649	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	C	797	TRP	CB-CG-CD1	-5.75	119.53	127.00
1	B	324	THR	CA-CB-CG2	-5.74	104.36	112.40
1	D	810	LYS	CA-CB-CG	5.74	126.03	113.40
1	B	372	CYS	CA-CB-SG	-5.74	103.67	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	724	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	C	228	THR	CA-C-N	5.74	133.17	117.10
1	D	676	THR	CA-CB-OG1	-5.74	96.95	109.00
1	C	349	LEU	CA-CB-CG	5.73	128.48	115.30
1	C	292	ARG	CA-CB-CG	-5.73	100.80	113.40
1	D	226	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	B	430	LEU	CA-CB-CG	5.72	128.46	115.30
1	B	477	HIS	CA-CB-CG	5.72	123.33	113.60
1	B	755	PRO	CA-C-N	-5.72	104.61	117.20
1	D	424	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	D	244	TRP	CG-CD1-NE1	-5.72	104.38	110.10
1	A	646	GLU	OE1-CD-OE2	-5.72	116.44	123.30
1	C	730	GLU	N-CA-C	-5.72	95.56	111.00
1	D	184	ARG	CA-CB-CG	5.71	125.96	113.40
1	A	421	ASP	O-C-N	5.71	131.83	122.70
1	A	242	ARG	N-CA-C	-5.71	95.59	111.00
1	A	254	LEU	CA-CB-CG	5.71	128.43	115.30
1	B	90	TYR	CA-CB-CG	5.71	124.24	113.40
1	B	566	GLN	N-CA-C	-5.71	95.59	111.00
1	D	292	ARG	CA-CB-CG	-5.71	100.85	113.40
1	D	836	ALA	N-CA-C	5.71	126.40	111.00
1	A	570	ILE	O-C-N	-5.70	113.58	122.70
1	C	346	ILE	CA-C-N	5.70	133.06	117.10
1	D	283	ASP	CB-CA-C	5.70	121.79	110.40
1	A	15	VAL	CA-CB-CG1	-5.69	102.36	110.90
1	A	698	GLU	CA-CB-CG	-5.69	100.87	113.40
1	C	661	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	250	ASN	CA-C-N	-5.69	104.68	117.20
1	D	349	LEU	CA-CB-CG	5.69	128.39	115.30
1	C	389	VAL	CG1-CB-CG2	-5.69	101.80	110.90
1	C	183	LEU	N-CA-C	-5.69	95.65	111.00
1	A	206	VAL	CG1-CB-CG2	-5.68	101.81	110.90
1	A	215	TRP	CE2-CD2-CG	-5.68	102.75	107.30
1	C	825	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	A	639	ARG	N-CA-CB	-5.68	100.38	110.60
1	B	375	THR	CA-CB-CG2	5.68	120.35	112.40
1	D	254	LEU	CA-CB-CG	5.68	128.36	115.30
1	D	272	ALA	N-CA-C	-5.68	95.67	111.00
1	D	425	LEU	CA-CB-CG	5.67	128.33	115.30
1	C	260	GLY	N-CA-C	-5.66	98.94	113.10
1	D	215	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	C	494	LEU	N-CA-CB	-5.65	99.09	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	739	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	D	505	GLU	N-CA-CB	5.65	120.77	110.60
1	D	203	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	244	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	D	815	ARG	NE-CZ-NH1	-5.65	117.48	120.30
1	C	262	TYR	CA-C-N	-5.64	104.78	117.20
1	D	506	ARG	CB-CG-CD	5.64	126.27	111.60
1	B	491	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	C	319	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	583	VAL	CG1-CB-CG2	-5.64	101.87	110.90
1	D	511	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	D	781	VAL	CG1-CB-CG2	-5.63	101.89	110.90
1	B	639	ARG	CB-CA-C	5.63	121.66	110.40
1	C	787	VAL	CA-CB-CG1	5.63	119.34	110.90
1	A	33	ARG	CA-CB-CG	5.63	125.78	113.40
1	C	189	TRP	CG-CD2-CE3	5.63	138.96	133.90
1	C	357	GLU	CA-C-N	5.63	129.58	117.20
1	B	638	ASP	CA-C-N	-5.62	104.83	117.20
1	D	80	LYS	O-C-N	5.62	131.70	122.70
1	B	44	ASN	CB-CA-C	-5.62	99.16	110.40
1	B	275	ILE	CA-CB-CG2	-5.62	99.66	110.90
1	D	176	MET	CG-SD-CE	-5.62	91.21	100.20
1	B	770	ARG	CA-CB-CG	5.62	125.76	113.40
1	C	387	TRP	CD1-CG-CD2	5.62	110.79	106.30
1	A	559	PRO	CA-CB-CG	-5.61	93.34	104.00
1	A	541	ASN	OD1-CG-ND2	-5.61	109.00	121.90
1	A	191	LYS	CA-C-N	-5.61	104.86	117.20
1	C	615	MET	CG-SD-CE	-5.61	91.23	100.20
1	B	160	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	431	VAL	CB-CA-C	-5.60	100.76	111.40
1	C	349	LEU	CB-CG-CD2	-5.59	101.49	111.00
1	A	395	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	B	16	ARG	C-N-CA	-5.59	110.56	122.30
1	D	166	PHE	N-CA-C	5.59	126.09	111.00
1	C	575	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	216	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	C	713	MET	CA-CB-CG	5.58	122.78	113.30
1	C	754	GLN	CA-CB-CG	5.58	125.67	113.40
1	A	780	TYR	CB-CG-CD2	-5.58	117.66	121.00
1	C	161	TYR	CB-CG-CD2	5.57	124.34	121.00
1	A	149	THR	N-CA-CB	-5.57	99.71	110.30
1	A	553	TYR	CA-CB-CG	5.57	123.98	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	831	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	464	LYS	CB-CG-CD	5.57	126.07	111.60
1	B	718	VAL	CA-CB-CG1	5.57	119.25	110.90
1	A	60	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	183	LEU	N-CA-C	-5.56	95.98	111.00
1	A	283	ASP	O-C-N	5.56	131.60	122.70
1	A	597	PHE	CA-C-N	-5.56	104.97	117.20
1	C	355	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	270	ASN	O-C-N	-5.56	113.81	122.70
1	C	714	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	780	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	B	283	ASP	O-C-N	5.55	131.58	122.70
1	D	573	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	C	16	ARG	N-CA-C	5.55	125.98	111.00
1	A	578	LEU	CB-CG-CD2	-5.55	101.57	111.00
1	A	413	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	647	ASN	CA-C-N	-5.55	105.00	117.20
1	A	765	LEU	CA-CB-CG	5.54	128.05	115.30
1	C	638	ASP	CA-C-N	-5.54	105.01	117.20
1	D	182	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	C	270	ASN	CA-CB-CG	-5.54	101.22	113.40
1	C	224	MET	CG-SD-CE	5.54	109.06	100.20
1	C	610	ALA	N-CA-C	-5.53	96.06	111.00
1	D	46	ALA	CB-CA-C	-5.53	101.81	110.10
1	A	78	ASP	N-CA-CB	-5.53	100.65	110.60
1	A	225	PRO	CA-N-CD	-5.53	103.77	111.50
1	B	825	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	C	510	GLU	N-CA-C	-5.52	96.09	111.00
1	B	277	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	C	732	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	C	94	THR	CA-CB-OG1	-5.51	97.42	109.00
1	D	713	MET	CA-CB-CG	5.51	122.67	113.30
1	A	797	TRP	CE2-CD2-CG	-5.51	102.89	107.30
1	A	16	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	A	160	ARG	CB-CG-CD	-5.51	97.28	111.60
1	B	467	ILE	CB-CG1-CD1	5.51	129.32	113.90
1	A	655	LYS	CA-CB-CG	5.50	125.51	113.40
1	D	299	VAL	CA-CB-CG1	5.50	119.14	110.90
1	A	532	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	583	VAL	CB-CA-C	-5.49	100.97	111.40
1	D	28	LYS	CA-CB-CG	-5.49	101.33	113.40
1	D	335	ILE	O-C-N	-5.49	113.92	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	424	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	575	ARG	N-CA-C	5.48	125.81	111.00
1	B	739	ARG	CG-CD-NE	5.48	123.32	111.80
1	A	401	GLN	CA-CB-CG	5.48	125.46	113.40
1	B	266	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	A	782	LYS	CA-C-O	-5.48	108.59	120.10
1	C	185	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	C	597	PHE	O-C-N	5.47	131.46	122.70
1	D	67	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	D	319	ARG	CA-CB-CG	5.47	125.43	113.40
1	A	339	ASP	CA-C-N	5.46	129.22	117.20
1	B	424	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	781	VAL	CA-C-N	-5.46	105.19	117.20
1	C	487	THR	CA-CB-CG2	5.46	120.04	112.40
1	B	686	ALA	N-CA-C	-5.45	96.28	111.00
1	A	192	ALA	N-CA-CB	-5.45	102.47	110.10
1	D	27	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	D	91	MET	CG-SD-CE	-5.45	91.49	100.20
1	A	438	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	51	TYR	CD1-CG-CD2	5.44	123.89	117.90
1	D	292	ARG	CG-CD-NE	-5.44	100.38	111.80
1	C	446	ILE	CB-CA-C	-5.44	100.72	111.60
1	B	553	TYR	CA-C-N	5.43	129.16	117.20
1	D	635	VAL	CG1-CB-CG2	-5.43	102.20	110.90
1	A	24	VAL	CA-C-N	-5.43	105.25	117.20
1	B	542	LYS	CB-CG-CD	5.43	125.71	111.60
1	B	274	ASN	CB-CG-ND2	5.43	129.72	116.70
1	C	517	GLN	CA-CB-CG	-5.42	101.47	113.40
1	D	78	ASP	N-CA-C	5.42	125.63	111.00
1	D	457	ARG	CA-CB-CG	-5.41	101.49	113.40
1	C	721	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	B	575	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	B	167	ASN	CB-CG-OD1	-5.40	110.80	121.60
1	C	174	TRP	NE1-CE2-CD2	5.40	112.70	107.30
1	C	326	PHE	N-CA-CB	-5.40	100.88	110.60
1	D	733	ASP	CA-CB-CG	-5.40	101.52	113.40
1	B	268	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	765	LEU	CA-CB-CG	5.40	127.71	115.30
1	A	449	SER	CA-CB-OG	-5.40	96.63	111.20
1	B	387	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	A	413	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	D	95	LEU	CA-C-N	5.39	129.06	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	509	GLU	O-C-N	5.39	131.32	122.70
1	A	678	ASN	CB-CG-ND2	5.39	129.63	116.70
1	B	205	ARG	N-CA-CB	-5.38	100.91	110.60
1	B	334	ALA	N-CA-CB	5.38	117.63	110.10
1	A	675	GLY	N-CA-C	-5.38	99.66	113.10
1	C	654	GLU	OE1-CD-OE2	-5.37	116.85	123.30
1	D	530	PHE	CA-CB-CG	-5.37	101.00	113.90
1	C	316	PHE	O-C-N	-5.37	114.07	123.20
1	D	785	GLU	CB-CG-CD	5.37	128.70	114.20
1	B	168	GLN	CA-CB-CG	5.37	125.21	113.40
1	B	465	LYS	CA-C-N	5.37	129.01	117.20
1	D	699	MET	CA-CB-CG	5.37	122.42	113.30
1	A	577	LEU	CA-C-N	5.37	129.01	117.20
1	C	779	GLU	CA-CB-CG	-5.37	101.60	113.40
1	B	47	THR	N-CA-CB	-5.36	100.11	110.30
1	C	430	LEU	CA-CB-CG	5.36	127.64	115.30
1	D	91	MET	N-CA-C	5.36	125.47	111.00
1	A	350	MET	CA-CB-CG	-5.36	104.20	113.30
1	A	664	GLU	N-CA-CB	-5.36	100.96	110.60
1	B	165	ILE	N-CA-C	-5.36	96.54	111.00
1	D	715	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	A	761	ILE	CB-CG1-CD1	-5.35	98.91	113.90
1	D	427	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	281	PRO	CA-N-CD	-5.35	104.01	111.50
1	A	54	ALA	CA-C-N	5.35	128.96	117.20
1	D	649	ARG	CB-CG-CD	5.34	125.49	111.60
1	A	131	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	555	VAL	O-C-N	-5.34	114.15	122.70
1	B	178	GLU	CA-C-N	5.34	128.95	117.20
1	B	718	VAL	CA-CB-CG2	-5.34	102.89	110.90
1	A	254	LEU	CB-CA-C	-5.34	100.06	110.20
1	D	810	LYS	O-C-N	-5.33	114.16	122.70
1	C	368	THR	CA-CB-CG2	5.33	119.87	112.40
1	D	792	LYS	CB-CA-C	-5.33	99.73	110.40
1	A	197	THR	N-CA-CB	-5.33	100.17	110.30
1	B	770	ARG	CG-CD-NE	5.33	122.99	111.80
1	B	184	ARG	CA-CB-CG	5.33	125.12	113.40
1	C	98	THR	CA-CB-OG1	-5.33	97.81	109.00
1	D	520	LYS	CA-CB-CG	5.32	125.11	113.40
1	D	332	LYS	CB-CG-CD	5.32	125.44	111.60
1	D	583	VAL	CA-CB-CG1	5.32	118.88	110.90
1	C	307	ILE	CA-C-N	5.32	128.90	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	622	LEU	CA-CB-CG	5.32	127.53	115.30
1	D	325	ASN	CA-C-N	-5.32	105.50	117.20
1	D	581	LEU	CB-CG-CD2	5.32	120.04	111.00
1	B	434	GLY	CA-C-N	-5.32	105.51	117.20
1	D	695	ALA	CA-C-N	5.32	128.90	117.20
1	D	764	MET	CA-CB-CG	5.32	122.34	113.30
1	C	237	VAL	CA-CB-CG2	5.31	118.87	110.90
1	B	720	ARG	CB-CG-CD	5.31	125.41	111.60
1	B	649	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	831	ARG	CA-CB-CG	5.31	125.08	113.40
1	D	514	ASP	CA-CB-CG	5.31	125.08	113.40
1	B	348	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	D	280	TYR	CB-CG-CD1	-5.31	117.82	121.00
1	A	339	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	174	TRP	CG-CD2-CE3	5.30	138.67	133.90
1	B	334	ALA	CB-CA-C	-5.30	102.15	110.10
1	B	257	PHE	CA-C-N	-5.30	105.55	117.20
1	A	586	LEU	CB-CA-C	-5.29	100.14	110.20
1	A	805	ILE	CA-C-N	5.29	128.85	117.20
1	D	189	TRP	NE1-CE2-CD2	5.29	112.59	107.30
1	D	561	SER	N-CA-C	5.29	125.29	111.00
1	B	553	TYR	N-CA-CB	5.29	120.12	110.60
1	B	379	VAL	CA-CB-CG2	-5.29	102.97	110.90
1	B	160	ARG	CB-CG-CD	-5.29	97.86	111.60
1	A	553	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	366	GLU	CA-CB-CG	5.28	125.01	113.40
1	A	255	LYS	O-C-N	5.28	131.15	122.70
1	C	436	VAL	CA-CB-CG2	-5.27	102.99	110.90
1	A	699	MET	CA-CB-CG	5.27	122.27	113.30
1	B	609	ALA	N-CA-C	5.27	125.23	111.00
1	A	718	VAL	CA-CB-CG1	5.27	118.81	110.90
1	C	536	LYS	CA-CB-CG	5.27	125.00	113.40
1	D	792	LYS	N-CA-CB	5.27	120.08	110.60
1	B	597	PHE	CB-CA-C	-5.26	99.87	110.40
1	B	317	GLY	N-CA-C	-5.26	99.95	113.10
1	C	555	VAL	CA-CB-CG2	5.26	118.78	110.90
1	A	243	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	B	836	ALA	CB-CA-C	-5.25	102.22	110.10
1	C	136	LEU	CA-C-N	5.25	126.71	116.20
1	C	255	LYS	CA-C-N	-5.25	105.64	117.20
1	B	795	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	267	LEU	CA-C-N	5.25	128.74	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	509	GLU	CA-C-N	-5.25	105.66	117.20
1	B	45	VAL	CA-CB-CG2	-5.24	103.04	110.90
1	C	264	GLN	N-CA-C	-5.24	96.85	111.00
1	D	178	GLU	CA-CB-CG	5.24	124.93	113.40
1	A	39	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	A	732	TYR	CA-CB-CG	5.24	123.35	113.40
1	B	610	ALA	N-CA-C	-5.24	96.86	111.00
1	C	765	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	18	LEU	O-C-N	5.23	131.07	122.70
1	A	602	THR	N-CA-C	-5.23	96.88	111.00
1	A	833	ARG	CA-CB-CG	5.23	124.91	113.40
1	B	345	ALA	CB-CA-C	-5.23	102.25	110.10
1	A	593	GLU	CA-CB-CG	5.23	124.90	113.40
1	C	244	TRP	CG-CD1-NE1	-5.23	104.87	110.10
1	B	597	PHE	N-CA-CB	5.22	120.00	110.60
1	B	205	ARG	CA-C-N	5.21	128.67	117.20
1	C	88	GLU	N-CA-CB	-5.21	101.21	110.60
1	B	574	LYS	CA-CB-CG	5.21	124.86	113.40
1	A	333	VAL	O-C-N	-5.21	114.36	122.70
1	C	159	ILE	CG1-CB-CG2	-5.21	99.94	111.40
1	D	797	TRP	CD1-CG-CD2	5.21	110.46	106.30
1	A	252	PHE	N-CA-CB	-5.20	101.23	110.60
1	B	555	VAL	CA-CB-CG2	5.20	118.71	110.90
1	B	189	TRP	NE1-CE2-CD2	5.20	112.50	107.30
1	A	333	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	B	185	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	C	274	ASN	N-CA-C	5.20	125.03	111.00
1	C	269	ARG	CA-CB-CG	5.20	124.83	113.40
1	A	543	LEU	CA-C-O	-5.19	109.19	120.10
1	B	69	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	205	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	437	LYS	N-CA-CB	-5.19	101.25	110.60
1	D	189	TRP	CE2-CD2-CE3	5.19	124.93	118.70
1	D	769	ASP	CB-CG-OD2	-5.19	113.62	118.30
1	C	384	LEU	CA-CB-CG	5.19	127.23	115.30
1	B	301	ALA	CB-CA-C	-5.18	102.32	110.10
1	D	233	TYR	O-C-N	5.18	131.00	122.70
1	C	138	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	531	ILE	N-CA-CB	-5.18	98.89	110.80
1	B	293	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	C	26	GLU	CA-C-N	5.17	128.58	117.20
1	A	429	SER	CA-CB-OG	5.17	125.16	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	342	PRO	N-CD-CG	-5.17	95.45	103.20
1	B	316	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	B	433	GLU	CB-CA-C	-5.16	100.07	110.40
1	B	552	GLU	C-N-CA	5.16	134.61	121.70
1	B	795	ARG	CB-CG-CD	5.16	125.03	111.60
1	D	704	GLY	CA-C-N	-5.16	105.84	117.20
1	B	834	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	D	522	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	569	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	573	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	B	641	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	787	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	B	525	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	D	16	ARG	C-N-CA	-5.15	111.48	122.30
1	D	302	ALA	N-CA-CB	-5.15	102.90	110.10
1	D	358	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	242	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	543	LEU	CA-C-N	5.14	128.51	117.20
1	C	226	TYR	CA-C-N	5.14	128.51	117.20
1	D	626	ILE	O-C-N	5.14	131.94	123.20
1	C	85	LEU	CB-CA-C	-5.14	100.43	110.20
1	C	641	ARG	CB-CA-C	-5.14	100.12	110.40
1	B	740	GLN	CA-CB-CG	5.14	124.70	113.40
1	B	777	TYR	O-C-N	-5.13	114.49	122.70
1	A	450	HIS	CA-CB-CG	5.12	122.31	113.60
1	C	211	GLN	CG-CD-NE2	5.12	129.00	116.70
1	D	533	ASP	N-CA-CB	5.12	119.82	110.60
1	B	633	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	797	TRP	NE1-CE2-CD2	5.12	112.42	107.30
1	C	686	ALA	CA-C-N	-5.12	105.94	117.20
1	C	433	GLU	CB-CA-C	-5.12	100.17	110.40
1	D	492	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	D	268	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	730	GLU	N-CA-C	-5.11	97.20	111.00
1	A	572	GLU	CA-C-N	5.11	128.44	117.20
1	A	718	VAL	CA-CB-CG2	-5.11	103.24	110.90
1	A	833	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	B	275	ILE	CA-CB-CG1	5.11	120.70	111.00
1	C	290	GLU	O-C-N	-5.11	114.53	122.70
1	C	681	PHE	CB-CG-CD1	-5.11	117.23	120.80
1	D	631	ASN	CA-CB-CG	5.11	124.63	113.40
1	B	422	VAL	CA-CB-CG2	-5.10	103.25	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	438	ARG	CB-CA-C	-5.10	100.19	110.40
1	D	658	PRO	CA-C-N	5.10	128.43	117.20
1	B	487	THR	N-CA-C	-5.10	97.23	111.00
1	D	181	ASP	N-CA-CB	5.10	119.78	110.60
1	B	764	MET	CA-CB-CG	5.10	121.97	113.30
1	B	393	GLU	CA-CB-CG	5.09	124.61	113.40
1	D	618	MET	CB-CG-SD	-5.09	97.12	112.40
1	A	303	THR	CA-C-O	-5.09	109.41	120.10
1	D	554	LYS	CA-CB-CG	5.09	124.60	113.40
1	C	547	ALA	CB-CA-C	-5.09	102.47	110.10
1	D	233	TYR	CA-C-N	-5.09	106.01	117.20
1	D	177	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	C	242	ARG	CA-CB-CG	5.08	124.58	113.40
1	B	804	ASN	CA-CB-CG	-5.08	102.23	113.40
1	C	655	LYS	CA-CB-CG	5.08	124.57	113.40
1	B	113	TYR	CA-CB-CG	5.08	123.04	113.40
1	C	764	MET	CA-CB-CG	5.07	121.92	113.30
1	A	484	ASN	CA-C-N	5.07	126.34	116.20
1	C	375	THR	O-C-N	-5.07	114.58	122.70
1	B	764	MET	CG-SD-CE	5.07	108.31	100.20
1	C	532	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	437	LYS	CA-CB-CG	5.07	124.55	113.40
1	B	200	VAL	N-CA-C	-5.07	97.32	111.00
1	D	131	LEU	CA-CB-CG	5.06	126.95	115.30
1	C	718	VAL	CA-CB-CG2	-5.06	103.31	110.90
1	A	724	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	688	THR	N-CA-CB	-5.06	100.69	110.30
1	B	43	ARG	CA-CB-CG	5.05	124.52	113.40
1	C	636	VAL	CG1-CB-CG2	-5.05	102.81	110.90
1	A	718	VAL	CG1-CB-CG2	-5.05	102.81	110.90
1	B	602	THR	N-CA-C	-5.05	97.36	111.00
1	B	604	MET	CA-CB-CG	5.05	121.89	113.30
1	A	470	ASP	CB-CG-OD2	5.05	122.84	118.30
1	C	674	SER	CA-C-N	5.05	126.29	116.20
1	D	610	ALA	N-CA-C	-5.04	97.38	111.00
1	D	630	VAL	CB-CA-C	-5.04	101.82	111.40
1	B	105	GLU	N-CA-C	5.04	124.60	111.00
1	C	597	PHE	CA-C-N	-5.04	106.12	117.20
1	A	378	THR	CA-CB-CG2	5.03	119.45	112.40
1	B	148	ALA	CB-CA-C	-5.03	102.55	110.10
1	C	274	ASN	N-CA-CB	-5.03	101.54	110.60
1	C	514	ASP	N-CA-CB	5.03	119.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	741	ILE	CA-CB-CG2	-5.03	100.84	110.90
1	A	113	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	C	257	PHE	CA-C-N	-5.02	106.15	117.20
1	D	90	TYR	CA-CB-CG	5.02	122.94	113.40
1	C	104	LEU	CA-C-N	5.02	128.25	117.20
1	B	16	ARG	N-CA-C	5.02	124.56	111.00
1	A	94	THR	CA-C-N	5.02	128.24	117.20
1	A	639	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	131	LEU	CB-CA-C	5.01	119.73	110.20
1	C	799	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	C	280	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	C	381	PRO	N-CA-C	5.01	125.13	112.10
1	D	767	HIS	N-CA-C	5.01	124.53	111.00
1	D	812	SER	CA-CB-OG	-5.01	97.67	111.20
1	A	22	GLU	CA-C-N	-5.01	106.18	117.20
1	C	795	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	D	378	THR	CA-C-N	-5.01	106.18	117.20
1	A	449	SER	CA-C-N	-5.00	106.19	117.20
1	A	255	LYS	CA-C-N	-5.00	106.20	117.20
1	B	87	LEU	CA-CB-CG	5.00	126.80	115.30
1	B	352	VAL	CG1-CB-CG2	-5.00	102.90	110.90
1	D	664	GLU	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	203	TYR	Sidechain
1	A	320	ASP	Peptide
1	A	380	ILE	Peptide
1	A	421	ASP	Mainchain
1	A	51	TYR	Sidechain
1	A	569	ARG	Sidechain
1	A	573	TYR	Sidechain
1	A	820	TYR	Sidechain
1	A	833	ARG	Sidechain
1	A	836	ALA	Peptide
1	B	277	ARG	Sidechain
1	B	292	ARG	Sidechain
1	B	320	ASP	Peptide
1	B	52	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	573	TYR	Sidechain
1	B	599	VAL	Peptide
1	B	639	ARG	Sidechain
1	B	777	TYR	Sidechain
1	B	820	TYR	Sidechain
1	B	834	LEU	Peptide
1	B	836	ALA	Peptide
1	C	309	ARG	Sidechain
1	C	320	ASP	Peptide
1	C	33	ARG	Sidechain
1	C	358	ARG	Sidechain
1	C	52	TYR	Sidechain
1	C	569	ARG	Sidechain
1	C	599	VAL	Peptide
1	C	751	SER	Peptide
1	C	836	ALA	Peptide
1	D	155	TYR	Sidechain
1	D	185	TYR	Sidechain
1	D	226	TYR	Sidechain
1	D	320	ASP	Peptide
1	D	51	TYR	Sidechain
1	D	52	TYR	Sidechain
1	D	524	TYR	Sidechain
1	D	60	ARG	Sidechain
1	D	648	TYR	Sidechain
1	D	649	ARG	Sidechain
1	D	777	TYR	Sidechain
1	D	791	TYR	Sidechain
1	D	795	ARG	Sidechain
1	D	836	ALA	Peptide
1	D	84	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6732	0	6675	411	1
1	B	6733	0	6667	363	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6732	0	6674	391	0
1	D	6732	0	6674	454	1
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
3	A	15	0	7	1	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
3	D	15	0	6	1	0
All	All	27029	0	26717	1582	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1582) 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:756:ASP:N	1:A:756:ASP:CA	1.77	1.46
1:C:279:LEU:HD22	1:C:281:PRO:CD	1.62	1.28
1:C:279:LEU:HD22	1:C:281:PRO:CG	1.70	1.22
1:B:283:ASP:OD2	1:B:383:ALA:HB1	1.39	1.21
1:C:283:ASP:OD2	1:C:383:ALA:HB1	1.37	1.19
1:C:24:VAL:C	1:C:25:THR:N	1.95	1.19
1:A:555:VAL:HG21	1:A:643:ILE:CD1	1.71	1.19
1:D:279:LEU:HD22	1:D:281:PRO:CD	1.71	1.18
1:A:157:TYR:CD2	1:A:303:THR:CG2	2.26	1.18
1:B:283:ASP:OD2	1:B:383:ALA:CB	1.92	1.18
1:D:279:LEU:CD2	1:D:281:PRO:HD2	1.72	1.17
1:D:251:ASP:OD1	1:D:255:LYS:HE2	1.40	1.17
1:D:251:ASP:OD1	1:D:255:LYS:HG3	1.46	1.15
1:C:279:LEU:CD2	1:C:281:PRO:CD	2.24	1.15
1:C:196:PHE:HB3	1:C:309:ARG:HH12	1.09	1.15
1:A:42:ASP:OD1	1:A:43:ARG:N	1.82	1.11
1:A:299:VAL:O	1:A:303:THR:OG1	1.69	1.09
1:D:502:ILE:HG22	1:D:506:ARG:HH21	1.13	1.09
1:B:402:ILE:O	1:B:406:ILE:HG13	1.52	1.09
1:C:280:TYR:N	1:C:281:PRO:HD2	1.62	1.09
1:C:24:VAL:HG12	1:C:28:LYS:HE2	1.29	1.08
1:C:279:LEU:CD2	1:C:281:PRO:HD3	1.88	1.04
1:D:509:GLU:OE1	1:D:510:GLU:N	1.91	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:VAL:HG21	1:A:643:ILE:HD11	1.41	1.02
1:C:283:ASP:OD2	1:C:383:ALA:CB	2.05	1.02
1:A:21:VAL:HG11	1:A:23:ASN:ND2	1.74	1.02
1:A:157:TYR:CD2	1:A:303:THR:HG22	1.91	1.02
1:D:692:MET:SD	1:D:710:ILE:HD13	2.01	1.00
1:A:274:ASN:HA	1:A:277:ARG:HG3	1.44	1.00
1:C:196:PHE:HB3	1:C:309:ARG:NH1	1.77	0.99
1:D:274:ASN:HA	1:D:277:ARG:HG3	1.43	0.98
1:A:316:PHE:CE2	1:A:332:LYS:NZ	2.32	0.98
1:B:280:TYR:N	1:B:281:PRO:HD2	1.77	0.98
1:D:279:LEU:HD22	1:D:281:PRO:HD2	0.99	0.97
1:D:251:ASP:OD1	1:D:255:LYS:CE	2.14	0.95
1:B:280:TYR:CE2	1:B:289:LYS:HE3	2.02	0.95
1:B:280:TYR:HE2	1:B:289:LYS:HE3	1.30	0.94
1:C:198:LEU:HD22	1:C:305:GLN:OE1	1.67	0.94
1:D:279:LEU:CD2	1:D:281:PRO:CD	2.40	0.94
1:B:363:LYS:NZ	1:B:366:GLU:OE1	2.01	0.93
1:D:315:LYS:HG2	1:D:318:CYS:SG	2.10	0.92
1:D:502:ILE:HG22	1:D:506:ARG:NH2	1.82	0.92
1:D:251:ASP:OD1	1:D:255:LYS:CG	2.18	0.92
1:C:692:MET:SD	1:C:710:ILE:HD13	2.10	0.91
1:C:279:LEU:HD22	1:C:281:PRO:HG3	1.51	0.91
1:A:386:ARG:NE	1:A:432:GLU:OE2	2.02	0.90
1:C:15:VAL:O	1:C:18:LEU:CD2	2.20	0.90
1:A:316:PHE:CZ	1:A:332:LYS:HE2	2.07	0.90
1:A:555:VAL:HG21	1:A:643:ILE:HD12	1.53	0.90
1:B:566:GLN:HB2	1:B:664:GLU:HB2	1.53	0.90
1:B:18:LEU:N	1:B:18:LEU:HD22	1.87	0.89
1:A:549:LEU:HD23	1:A:557:ILE:HG12	1.54	0.88
1:C:115:LEU:HD23	1:D:12:GLN:HB3	1.53	0.88
1:C:350:MET:O	1:C:354:VAL:HG23	1.74	0.88
1:D:424:ARG:HH22	1:D:473:GLU:CD	1.77	0.88
1:D:720:ARG:HG3	1:D:720:ARG:HH11	1.39	0.88
1:C:284:ASN:ND2	1:C:285:PHE:H	1.70	0.88
1:D:754:GLN:NE2	1:D:757:LEU:CD1	2.36	0.87
1:B:283:ASP:OD2	1:B:383:ALA:HB2	1.76	0.86
1:C:322:VAL:O	1:C:325:ASN:HB2	1.75	0.86
1:C:15:VAL:O	1:C:18:LEU:HD23	1.75	0.86
1:D:112:THR:HA	1:D:115:LEU:HD12	1.55	0.85
1:A:21:VAL:CG1	1:A:23:ASN:ND2	2.39	0.85
1:A:21:VAL:CB	1:A:23:ASN:HD22	1.88	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:TYR:H	1:C:281:PRO:HD2	1.37	0.85
1:D:577:LEU:HD13	1:D:765:LEU:HD11	1.58	0.85
1:C:224:MET:HG2	1:C:247:LYS:HD2	1.57	0.84
1:D:558:ASN:HD21	1:D:560:ASN:HB2	1.39	0.84
1:A:75:TYR:HE1	1:A:315:LYS:HG3	1.41	0.84
1:A:316:PHE:HE2	1:A:332:LYS:NZ	1.74	0.84
1:C:280:TYR:N	1:C:281:PRO:CD	2.39	0.84
1:D:21:VAL:HG12	1:D:22:GLU:H	1.42	0.84
1:C:160:ARG:HB2	1:C:243:LEU:HB3	1.59	0.84
1:A:433:GLU:OE2	1:A:437:LYS:NZ	2.11	0.83
1:A:446:ILE:HG23	1:A:452:VAL:HG21	1.59	0.83
1:A:24:VAL:HG13	1:A:111:ALA:HA	1.60	0.83
1:B:18:LEU:HD22	1:B:18:LEU:H	1.43	0.82
1:B:402:ILE:HG22	1:B:406:ILE:HD11	1.62	0.82
1:D:734:ARG:HB2	1:D:735:ILE:HD12	1.61	0.82
1:C:491:TRP:HA	1:C:495:CYS:SG	2.19	0.82
1:B:284:ASN:ND2	1:B:285:PHE:H	1.77	0.81
1:C:21:VAL:HG12	1:C:22:GLU:HG2	1.62	0.81
1:C:279:LEU:HD22	1:C:281:PRO:HD3	1.53	0.81
1:C:24:VAL:N	1:C:25:THR:N	2.29	0.81
1:D:225:PRO:HB2	1:D:242:ARG:HD2	1.62	0.81
1:C:400:LEU:HD22	1:C:404:TYR:CE2	2.16	0.81
1:D:707:ASN:HA	1:D:800:MET:SD	2.20	0.81
1:D:510:GLU:HB3	1:D:517:GLN:HE22	1.45	0.80
1:A:157:TYR:HD2	1:A:303:THR:CG2	1.86	0.80
1:A:274:ASN:CA	1:A:277:ARG:HG3	2.12	0.79
1:D:491:TRP:HA	1:D:495:CYS:SG	2.22	0.79
1:C:284:ASN:ND2	1:C:285:PHE:N	2.30	0.79
1:A:555:VAL:HB	1:A:557:ILE:HD13	1.64	0.79
1:A:42:ASP:OD1	1:A:42:ASP:C	2.21	0.79
1:D:21:VAL:HG12	1:D:22:GLU:N	1.98	0.79
1:B:280:TYR:OH	1:B:289:LYS:NZ	2.14	0.78
1:D:279:LEU:HD22	1:D:281:PRO:CG	2.13	0.78
1:D:754:GLN:NE2	1:D:757:LEU:HD13	1.98	0.78
1:D:661:ASP:HB3	1:D:797:TRP:HH2	1.48	0.78
1:D:690:GLY:O	1:D:710:ILE:HA	1.83	0.78
1:A:256:ASP:HB3	1:A:258:ASN:ND2	1.97	0.78
1:A:326:PHE:HA	1:A:329:PHE:HB2	1.65	0.78
1:A:398:ARG:HA	1:A:401:GLN:HG3	1.64	0.78
1:A:102:LEU:HD23	1:A:104:LEU:HD21	1.65	0.78
1:B:88:GLU:HG3	1:B:132:GLY:HA2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:HE2	1:A:395:LEU:HD21	1.63	0.77
1:A:157:TYR:CD2	1:A:303:THR:HG23	2.20	0.77
1:B:456:ALA:HB2	1:B:674:SER:HB2	1.67	0.77
1:C:279:LEU:HD23	1:C:281:PRO:CD	2.11	0.77
1:D:645:LEU:HD11	1:D:656:VAL:HG21	1.66	0.77
1:C:235:ASN:H	1:C:235:ASN:HD22	1.32	0.77
1:C:349:LEU:O	1:C:353:LEU:HG	1.83	0.77
1:B:283:ASP:CG	1:B:383:ALA:HB1	2.04	0.77
1:C:196:PHE:CB	1:C:309:ARG:HH12	1.93	0.77
1:D:491:TRP:HA	1:D:495:CYS:HG	1.49	0.77
1:A:21:VAL:HB	1:A:23:ASN:HD22	1.50	0.77
1:C:284:ASN:O	1:C:285:PHE:CB	2.32	0.77
1:C:282:ASN:O	1:C:284:ASN:N	2.17	0.77
1:D:284:ASN:ND2	1:D:285:PHE:H	1.81	0.77
1:D:510:GLU:HB3	1:D:517:GLN:NE2	2.00	0.77
1:A:319:ARG:HD3	1:A:332:LYS:NZ	2.00	0.76
1:C:279:LEU:HD23	1:C:281:PRO:HD3	1.65	0.76
1:C:279:LEU:CD2	1:C:281:PRO:HD2	2.14	0.76
1:D:455:VAL:H	1:D:459:HIS:HD2	1.33	0.76
1:C:547:ALA:O	1:C:551:ARG:HB2	1.85	0.75
1:D:280:TYR:N	1:D:281:PRO:HD2	2.01	0.75
1:A:555:VAL:HB	1:A:557:ILE:CD1	2.15	0.75
1:D:219:GLN:NE2	1:D:268:ASP:CG	2.39	0.75
1:D:612:GLY:H	1:D:617:LYS:HE2	1.51	0.75
1:A:685:GLY:HA2	1:A:805:ILE:HD11	1.68	0.75
1:A:718:VAL:HG22	1:A:772:LYS:HE2	1.68	0.75
1:A:765:LEU:HG	1:A:774:PHE:HE1	1.51	0.75
1:C:24:VAL:CA	1:C:25:THR:N	2.49	0.75
1:D:519:ARG:HA	1:D:806:ALA:HB1	1.68	0.75
1:B:284:ASN:ND2	1:B:285:PHE:N	2.33	0.75
1:A:557:ILE:HD11	1:A:643:ILE:HD11	1.68	0.75
1:A:703:ALA:HB2	1:A:807:THR:HG21	1.68	0.75
1:D:692:MET:HB2	1:D:714:ARG:HD2	1.67	0.75
1:B:486:ILE:HD13	1:B:679:MET:HB2	1.69	0.75
1:D:284:ASN:O	1:D:285:PHE:CB	2.35	0.74
1:B:282:ASN:O	1:B:284:ASN:N	2.19	0.74
1:A:221:VAL:HG13	1:A:272:ALA:HB1	1.67	0.74
1:D:373:ALA:HA	1:D:449:SER:HB3	1.69	0.74
1:C:357:GLU:O	1:C:358:ARG:HD3	1.87	0.74
1:B:22:GLU:OE1	1:B:62:HIS:CD2	2.41	0.74
1:C:319:ARG:HD3	1:C:332:LYS:HE2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:LEU:CD2	1:D:281:PRO:CG	2.66	0.74
1:C:284:ASN:CG	1:C:285:PHE:H	1.91	0.74
1:A:74:TYR:OH	1:A:153:ALA:HA	1.88	0.73
1:A:316:PHE:HZ	1:A:332:LYS:HE2	1.53	0.73
1:A:648:TYR:HA	1:A:652:LEU:HD12	1.68	0.73
1:A:756:ASP:O	1:A:759:LYS:HB2	1.88	0.73
1:C:32:ASN:HD21	1:D:13:ILE:HA	1.53	0.73
1:D:64:VAL:HG12	1:D:67:TRP:CE3	2.23	0.73
1:D:279:LEU:HD13	1:D:281:PRO:HG2	1.69	0.73
1:D:565:VAL:HG21	1:D:681:PHE:HE1	1.54	0.73
1:B:379:VAL:HG12	1:B:380:ILE:HG23	1.71	0.72
1:C:677:GLY:HA2	1:C:680:LYS:HE2	1.70	0.72
1:D:129:ALA:HB1	1:D:131:LEU:HD23	1.71	0.72
1:A:139:LEU:HD11	1:A:484:ASN:ND2	2.04	0.72
1:D:183:LEU:HD23	1:D:187:ASN:HB3	1.71	0.72
1:A:316:PHE:CZ	1:A:332:LYS:CE	2.73	0.72
1:A:482:LYS:HE3	1:A:819:GLN:O	1.89	0.72
1:B:369:VAL:O	1:B:450:HIS:HB3	1.89	0.72
1:A:316:PHE:CE2	1:A:332:LYS:CE	2.72	0.72
1:A:413:ARG:NH2	1:A:475:GLU:HG3	2.05	0.71
1:D:98:THR:O	1:D:102:LEU:HB2	1.90	0.71
1:D:251:ASP:OD1	1:D:255:LYS:CD	2.37	0.71
1:B:506:ARG:HG2	1:B:530:PHE:CE1	2.25	0.71
1:D:713:MET:HG2	1:D:718:VAL:HG23	1.70	0.71
1:A:555:VAL:CG2	1:A:643:ILE:CD1	2.63	0.71
1:C:530:PHE:HE1	1:C:802:ILE:HG12	1.56	0.71
1:D:64:VAL:HG12	1:D:67:TRP:HE3	1.56	0.71
1:A:157:TYR:HD2	1:A:303:THR:HG23	1.53	0.71
1:A:157:TYR:CE2	1:A:303:THR:HG22	2.25	0.71
1:D:280:TYR:H	1:D:281:PRO:HD2	1.56	0.71
1:D:279:LEU:CD1	1:D:281:PRO:HG2	2.21	0.71
1:D:350:MET:O	1:D:354:VAL:HG23	1.90	0.71
1:C:336:GLN:NE2	1:C:825:TRP:HE1	1.89	0.71
1:B:81:ARG:HD3	1:B:155:TYR:CE1	2.26	0.71
1:B:164:GLY:O	1:B:279:LEU:HB2	1.90	0.71
1:A:88:GLU:HG2	1:A:132:GLY:HA2	1.72	0.70
1:C:225:PRO:HB2	1:C:242:ARG:HD2	1.73	0.70
1:C:280:TYR:H	1:C:281:PRO:CD	2.03	0.70
1:B:81:ARG:HG2	1:B:153:ALA:HB1	1.74	0.70
1:B:284:ASN:O	1:B:285:PHE:CB	2.37	0.70
1:A:422:VAL:HA	1:A:425:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASN:CG	1:B:285:PHE:H	1.94	0.70
1:C:19:ALA:C	1:C:21:VAL:H	1.89	0.70
1:D:251:ASP:CG	1:D:255:LYS:HE2	2.12	0.70
1:A:653:ALA:HA	1:A:656:VAL:HG12	1.73	0.70
1:A:168:GLN:OE1	1:A:608:LYS:HA	1.92	0.70
1:A:319:ARG:HD3	1:A:332:LYS:HZ2	1.54	0.70
1:A:601:ARG:HH22	1:A:784:GLN:HE22	1.40	0.70
1:C:729:GLN:HA	1:C:732:TYR:HB3	1.72	0.69
1:D:341:HIS:HB2	1:D:342:PRO:HD3	1.74	0.69
1:D:386:ARG:HG3	1:D:440:ASN:HA	1.73	0.69
1:A:162:GLU:OE2	1:A:277:ARG:NH2	2.25	0.69
1:C:70:THR:HG22	1:C:74:TYR:CZ	2.28	0.69
1:D:204:GLY:HA2	1:D:217:ASP:O	1.93	0.69
1:D:219:GLN:HE21	1:D:268:ASP:CG	1.95	0.69
1:A:698:GLU:HA	1:A:701:GLU:HG3	1.74	0.69
1:B:17:GLY:H	1:B:18:LEU:HD22	1.56	0.69
1:C:315:LYS:HE2	1:C:318:CYS:SG	2.33	0.69
1:D:284:ASN:ND2	1:D:285:PHE:N	2.40	0.69
1:D:758:PHE:HD1	1:D:761:ILE:HD11	1.56	0.69
1:C:23:ASN:C	1:C:25:THR:N	2.46	0.69
1:A:316:PHE:CZ	1:A:332:LYS:NZ	2.57	0.69
1:B:18:LEU:H	1:B:18:LEU:CD2	2.06	0.68
1:B:518:LEU:O	1:B:521:LEU:HB3	1.92	0.68
1:A:42:ASP:OD1	1:A:44:ASN:N	2.26	0.68
1:A:27:LEU:HD21	1:A:62:HIS:HE1	1.58	0.68
1:A:86:SER:HB3	1:A:89:PHE:HE1	1.58	0.68
1:D:235:ASN:HB2	1:D:833:ARG:HA	1.75	0.68
1:C:360:ASP:N	1:C:360:ASP:OD1	2.25	0.68
1:D:24:VAL:HG12	1:D:28:LYS:HE2	1.76	0.68
1:D:661:ASP:HB3	1:D:797:TRP:CH2	2.29	0.68
1:B:102:LEU:HB3	1:B:104:LEU:HD13	1.74	0.68
1:D:713:MET:HG3	1:D:717:ASP:HB2	1.75	0.68
1:B:515:LEU:HB3	1:B:809:GLY:HA2	1.74	0.68
1:D:688:THR:HB	1:D:708:PHE:CE1	2.28	0.68
1:B:280:TYR:N	1:B:281:PRO:CD	2.53	0.68
1:B:286:PHE:O	1:B:287:GLU:HG2	1.94	0.68
1:D:766:MET:HE3	1:D:774:PHE:HE2	1.58	0.68
1:A:27:LEU:HD21	1:A:62:HIS:CE1	2.29	0.67
1:A:307:ILE:HD13	1:A:335:ILE:HD11	1.77	0.67
1:A:732:TYR:CE1	1:A:739:ARG:HG2	2.29	0.67
1:B:459:HIS:HB2	1:B:673:ALA:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:ILE:HA	1:B:505:GLU:HB2	1.74	0.67
1:C:320:ASP:HA	1:C:324:THR:HA	1.77	0.67
1:A:522:LEU:O	1:A:525:VAL:HG23	1.93	0.67
1:A:629:VAL:HG11	1:A:750:PHE:HE1	1.59	0.67
1:B:22:GLU:OE2	1:B:104:LEU:HD11	1.93	0.67
1:B:70:THR:HG22	1:B:74:TYR:CE2	2.29	0.67
1:B:273:GLU:HG2	1:B:277:ARG:HH21	1.58	0.67
1:D:88:GLU:OE1	1:D:133:ASN:N	2.27	0.67
1:D:322:VAL:O	1:D:325:ASN:HB2	1.95	0.67
1:A:110:GLU:HG3	1:A:114:GLN:NE2	2.10	0.67
1:C:136:LEU:HD11	1:C:338:ASN:OD1	1.94	0.67
1:B:93:ARG:HG2	1:B:126:GLU:HB3	1.77	0.67
1:C:737:GLU:O	1:C:740:GLN:HB3	1.95	0.67
1:A:550:GLU:HA	1:A:554:LYS:HA	1.77	0.67
1:D:571:HIS:ND1	1:D:573:TYR:HD1	1.91	0.67
1:A:194:PRO:HA	1:A:224:MET:SD	2.35	0.66
1:C:592:LYS:HG3	1:C:593:GLU:HG3	1.77	0.66
1:D:688:THR:HB	1:D:708:PHE:HE1	1.60	0.66
1:C:525:VAL:HG12	1:C:799:ARG:HD2	1.77	0.66
1:D:138:ARG:HH11	1:D:138:ARG:HG3	1.60	0.66
1:C:131:LEU:HD21	1:C:243:LEU:HD21	1.76	0.66
1:C:678:ASN:ND2	1:C:695:ALA:HB3	2.10	0.66
1:D:284:ASN:CG	1:D:285:PHE:H	1.99	0.66
1:A:347:PRO:HD3	1:A:444:LEU:HD21	1.77	0.66
1:C:252:PHE:CZ	1:C:269:ARG:HB3	2.30	0.66
1:C:323:ARG:CZ	1:C:323:ARG:HB3	2.26	0.66
1:D:138:ARG:NH1	1:D:142:CYS:SG	2.68	0.66
1:C:663:SER:HB3	1:C:681:PHE:CD1	2.30	0.66
1:D:88:GLU:HG2	1:D:132:GLY:HA2	1.76	0.66
1:B:522:LEU:HD13	1:B:806:ALA:HB3	1.77	0.66
1:C:742:ILE:HD11	1:C:774:PHE:HZ	1.60	0.66
1:D:74:TYR:HD1	1:D:79:PRO:HG3	1.60	0.66
1:D:68:ILE:HG22	1:D:72:GLN:OE1	1.96	0.65
1:A:115:LEU:HD22	1:B:13:ILE:HG13	1.78	0.65
1:A:381:PRO:HB3	1:A:467:ILE:HD12	1.77	0.65
1:B:263:ILE:HG21	1:B:266:VAL:HG23	1.79	0.65
1:D:738:LEU:HA	1:D:741:ILE:HG12	1.78	0.65
1:D:756:ASP:O	1:D:759:LYS:HB2	1.96	0.65
1:D:395:LEU:HD23	1:D:396:LEU:HD22	1.78	0.65
1:B:455:VAL:HG12	1:B:674:SER:HB3	1.79	0.65
1:C:534:VAL:O	1:C:537:VAL:HB	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:796:GLU:HA	1:D:799:ARG:HG3	1.78	0.65
1:A:136:LEU:HG	1:A:338:ASN:HD21	1.61	0.65
1:A:102:LEU:HD23	1:A:104:LEU:CD2	2.26	0.65
1:D:721:LEU:HG	1:D:726:TYR:HB2	1.79	0.65
1:C:459:HIS:CE1	1:C:463:LEU:HD21	2.32	0.64
1:C:480:GLN:HE22	1:C:823:GLU:HB3	1.62	0.64
1:D:351:ARG:O	1:D:355:ASP:HB2	1.97	0.64
1:A:23:ASN:HB3	1:A:25:THR:HB	1.79	0.64
1:D:410:PHE:O	1:D:414:VAL:HG23	1.96	0.64
1:A:337:LEU:HG	1:A:342:PRO:HB2	1.78	0.64
1:B:229:PRO:HA	1:B:239:ASN:O	1.98	0.64
1:B:455:VAL:H	1:B:459:HIS:HD2	1.44	0.64
1:C:21:VAL:CG1	1:C:22:GLU:HG2	2.27	0.64
1:B:139:LEU:HD11	1:B:143:PHE:CE1	2.33	0.64
1:D:103:ALA:HA	1:D:234:ARG:HH21	1.62	0.64
1:A:505:GLU:OE1	1:A:506:ARG:NH2	2.27	0.64
1:B:34:HIS:HA	1:B:38:THR:HB	1.78	0.64
1:A:87:LEU:HD22	1:A:341:HIS:HB3	1.80	0.64
1:B:138:ARG:NH1	1:B:491:TRP:HE1	1.96	0.64
1:B:793:ASN:ND2	1:B:796:GLU:HB2	2.12	0.64
1:D:21:VAL:CG1	1:D:22:GLU:H	1.93	0.64
1:D:290:GLU:O	1:D:294:LYS:HB2	1.98	0.64
1:B:24:VAL:HG21	1:B:110:GLU:HG2	1.79	0.63
1:B:133:ASN:ND2	1:B:281:PRO:HB3	2.14	0.63
1:B:630:VAL:HG23	1:B:636:VAL:HG11	1.79	0.63
1:D:502:ILE:HG13	1:D:503:ILE:H	1.62	0.63
1:D:603:VAL:HG23	1:D:641:ARG:O	1.98	0.63
1:C:326:PHE:HA	1:C:329:PHE:HB2	1.80	0.63
1:B:81:ARG:HD3	1:B:155:TYR:HE1	1.63	0.63
1:C:133:ASN:OD1	1:C:165:ILE:HG21	1.97	0.63
1:D:682:MET:HG2	1:D:808:SER:OG	1.99	0.63
1:A:209:THR:HG23	1:A:212:GLY:H	1.63	0.63
1:C:20:GLY:HA3	1:C:26:GLU:HG3	1.80	0.63
1:C:316:PHE:HA	1:C:319:ARG:HB2	1.80	0.63
1:C:718:VAL:HG13	1:C:772:LYS:HE2	1.81	0.63
1:D:735:ILE:HG22	1:D:738:LEU:H	1.63	0.63
1:A:269:ARG:NH2	1:A:273:GLU:OE1	2.31	0.63
1:D:502:ILE:HG13	1:D:503:ILE:N	2.14	0.63
1:B:793:ASN:HD21	1:B:796:GLU:HB2	1.62	0.63
1:C:24:VAL:CG1	1:C:28:LYS:HE2	2.17	0.63
1:C:91:MET:HE1	1:C:144:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:ASN:HD21	1:C:744:GLN:HE22	1.44	0.63
1:D:390:HIS:CE1	1:D:391:LEU:HD12	2.33	0.63
1:A:78:ASP:OD2	1:A:332:LYS:NZ	2.31	0.63
1:D:555:VAL:HB	1:D:557:ILE:HD13	1.79	0.63
1:D:558:ASN:ND2	1:D:560:ASN:HB2	2.13	0.63
1:A:74:TYR:HD1	1:A:79:PRO:HG3	1.63	0.62
1:B:133:ASN:ND2	1:B:281:PRO:CG	2.62	0.62
1:B:170:ILE:HG12	1:B:646:GLU:HG3	1.82	0.62
1:D:281:PRO:HD3	1:D:292:ARG:HH12	1.64	0.62
1:D:629:VAL:HG12	1:D:630:VAL:N	2.12	0.62
1:D:631:ASN:HD21	1:D:642:VAL:H	1.45	0.62
1:A:21:VAL:HG11	1:A:23:ASN:HD21	1.62	0.62
1:B:12:GLN:HA	1:B:16:ARG:NH2	2.14	0.62
1:C:70:THR:HG22	1:C:74:TYR:CE2	2.34	0.62
1:D:74:TYR:CD1	1:D:79:PRO:HG3	2.33	0.62
1:A:32:ASN:ND2	1:B:13:ILE:HA	2.14	0.62
1:D:582:HIS:HA	1:D:585:THR:OG1	1.99	0.62
1:D:284:ASN:OD1	1:D:610:ALA:HB1	1.99	0.62
1:D:396:LEU:O	1:D:399:HIS:HB2	1.99	0.62
1:B:515:LEU:HD22	1:B:812:SER:HB2	1.81	0.62
1:C:130:GLY:O	1:C:164:GLY:HA2	2.00	0.62
1:C:317:GLY:HA2	1:C:320:ASP:HB2	1.82	0.62
1:B:729:GLN:HA	1:B:732:TYR:HB3	1.81	0.62
1:C:687:LEU:HD12	1:C:797:TRP:CZ2	2.35	0.62
1:B:204:GLY:HA2	1:B:217:ASP:O	2.00	0.62
1:C:64:VAL:HG12	1:C:67:TRP:HE3	1.64	0.62
1:C:283:ASP:CG	1:C:383:ALA:HB1	2.20	0.62
1:A:115:LEU:HD22	1:B:13:ILE:CG1	2.29	0.62
1:A:721:LEU:HD21	1:A:726:TYR:CD1	2.35	0.62
1:B:590:ILE:HG22	1:B:636:VAL:HG22	1.81	0.62
1:D:75:TYR:OH	1:D:315:LYS:HG3	2.00	0.62
1:D:662:LEU:HD22	1:D:689:ILE:HG22	1.81	0.62
1:C:284:ASN:HD22	1:C:285:PHE:N	1.96	0.62
1:C:335:ILE:HG13	1:C:371:THR:HG22	1.82	0.62
1:D:486:ILE:HG12	1:D:680:LYS:HG3	1.83	0.61
1:B:133:ASN:ND2	1:B:281:PRO:CB	2.64	0.61
1:B:685:GLY:HA2	1:B:801:VAL:HG13	1.81	0.61
1:C:196:PHE:HB3	1:C:309:ARG:CZ	2.29	0.61
1:A:430:LEU:N	1:A:430:LEU:CD2	2.62	0.61
1:B:739:ARG:HG3	1:B:739:ARG:HH11	1.64	0.61
1:C:133:ASN:OD1	1:C:165:ILE:CG2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:GLN:NE2	1:D:268:ASP:OD1	2.33	0.61
1:A:67:TRP:CZ3	1:A:229:PRO:HG3	2.36	0.61
1:A:316:PHE:CE2	1:A:332:LYS:HE2	2.34	0.61
1:C:379:VAL:HG11	1:C:671:THR:O	1.99	0.61
1:A:568:LYS:O	1:A:607:GLY:HA3	2.01	0.61
1:B:251:ASP:HB3	1:B:255:LYS:HB2	1.82	0.61
1:C:235:ASN:OD1	1:C:237:VAL:HG22	2.00	0.61
1:D:326:PHE:O	1:D:330:PRO:HD3	1.99	0.61
1:A:181:ASP:O	1:A:184:ARG:HB2	2.00	0.61
1:A:459:HIS:O	1:A:462:ILE:HG12	2.00	0.61
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.83	0.61
1:B:506:ARG:HG2	1:B:530:PHE:HE1	1.65	0.61
1:C:193:ARG:HD2	1:C:196:PHE:HE2	1.65	0.61
1:D:17:GLY:C	1:D:18:LEU:HD13	2.20	0.61
1:B:17:GLY:N	1:B:18:LEU:HD22	2.16	0.61
1:C:492:LEU:HG	1:C:683:LEU:HD22	1.83	0.61
1:C:522:LEU:O	1:C:525:VAL:HG23	2.01	0.61
1:B:251:ASP:HB3	1:B:255:LYS:HG3	1.83	0.61
1:C:689:ILE:HA	1:C:709:PHE:HB2	1.82	0.61
1:C:588:ASN:HD21	1:C:744:GLN:NE2	1.99	0.61
1:C:678:ASN:O	1:C:681:PHE:HB2	2.01	0.61
1:A:119:MET:O	1:A:123:GLU:HG3	2.01	0.60
1:B:233:TYR:CZ	1:B:234:ARG:HD3	2.36	0.60
1:C:486:ILE:O	1:C:812:SER:HA	2.01	0.60
1:D:711:PHE:CE2	1:D:780:TYR:HB2	2.36	0.60
1:A:18:LEU:HD22	1:A:18:LEU:N	2.15	0.60
1:A:157:TYR:CD2	1:A:303:THR:HG21	2.33	0.60
1:C:456:ALA:O	1:C:460:SER:HB2	2.00	0.60
1:D:280:TYR:HE2	1:D:289:LYS:CE	2.15	0.60
1:D:552:GLU:O	1:D:553:TYR:CD1	2.54	0.60
1:D:575:ARG:HB3	1:D:578:LEU:HB2	1.82	0.60
1:D:583:VAL:HG21	1:D:603:VAL:HG21	1.82	0.60
1:A:21:VAL:CG1	1:A:23:ASN:HD22	2.09	0.60
1:C:70:THR:O	1:C:73:HIS:HB3	2.02	0.60
1:D:458:ILE:HD11	1:D:694:GLY:HA2	1.84	0.60
1:A:322:VAL:O	1:A:325:ASN:HB2	2.01	0.60
1:A:336:GLN:NE2	1:A:825:TRP:HE1	2.00	0.60
1:B:280:TYR:H	1:B:281:PRO:HD2	1.60	0.60
1:A:765:LEU:HG	1:A:774:PHE:CE1	2.33	0.60
1:B:284:ASN:HD22	1:B:285:PHE:N	2.00	0.60
1:B:761:ILE:HG22	1:B:765:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:ILE:HD13	1:C:639:ARG:HB3	1.84	0.60
1:C:280:TYR:HE2	1:C:289:LYS:CE	2.15	0.60
1:D:504:ALA:HA	1:D:508:GLY:H	1.66	0.60
1:A:721:LEU:HD21	1:A:726:TYR:HD1	1.66	0.60
1:B:138:ARG:NH1	1:B:142:CYS:SG	2.75	0.60
1:B:262:TYR:HB3	1:B:264:GLN:OE1	2.02	0.60
1:D:256:ASP:HB3	1:D:258:ASN:ND2	2.16	0.60
1:D:716:GLU:O	1:D:720:ARG:HG2	2.02	0.60
1:C:262:TYR:HB3	1:C:264:GLN:OE1	2.02	0.59
1:B:581:LEU:HD13	1:B:738:LEU:HD11	1.84	0.59
1:C:682:MET:SD	1:C:699:MET:HG2	2.42	0.59
1:B:161:TYR:HE1	1:B:295:GLN:HE22	1.50	0.59
1:B:227:ASP:OD1	1:B:242:ARG:HD3	2.01	0.59
1:B:103:ALA:HB2	1:B:234:ARG:HE	1.66	0.59
1:B:294:LYS:HG3	1:B:395:LEU:HD21	1.84	0.59
1:B:499:LEU:O	1:B:503:ILE:HG13	2.02	0.59
1:D:24:VAL:HG13	1:D:111:ALA:HA	1.84	0.59
1:D:754:GLN:NE2	1:D:757:LEU:HD11	2.15	0.59
1:C:555:VAL:HG21	1:C:643:ILE:HD12	1.83	0.59
1:C:687:LEU:HD12	1:C:797:TRP:CE2	2.38	0.59
1:C:699:MET:HB3	1:C:708:PHE:HE2	1.67	0.59
1:D:227:ASP:OD1	1:D:242:ARG:HD3	2.02	0.59
1:A:203:TYR:O	1:A:218:THR:HG22	2.03	0.59
1:B:12:GLN:HA	1:B:16:ARG:HH22	1.68	0.59
1:B:49:ARG:O	1:B:52:TYR:HB3	2.02	0.59
1:A:110:GLU:HG3	1:A:114:GLN:HE21	1.66	0.59
1:A:730:GLU:O	1:A:734:ARG:CD	2.50	0.59
1:C:389:VAL:HG12	1:C:439:ILE:HG13	1.84	0.59
1:A:23:ASN:HB3	1:A:26:GLU:H	1.67	0.59
1:B:507:ILE:HD13	1:B:521:LEU:HB2	1.85	0.59
1:D:348:GLU:O	1:D:352:VAL:HG23	2.03	0.59
1:A:322:VAL:HG21	1:A:327:ASP:OD2	2.02	0.59
1:B:171:CYS:O	1:B:174:TRP:HB2	2.03	0.59
1:C:152:LEU:HD22	1:C:827:VAL:HG21	1.85	0.59
1:C:19:ALA:C	1:C:21:VAL:N	2.50	0.58
1:C:761:ILE:O	1:C:765:LEU:HB2	2.02	0.58
1:B:196:PHE:HB3	1:B:309:ARG:NH2	2.17	0.58
1:B:258:ASN:OD1	1:B:259:VAL:HG22	2.02	0.58
1:C:730:GLU:O	1:C:734:ARG:HG3	2.01	0.58
1:B:687:LEU:HD21	1:B:800:MET:HB3	1.83	0.58
1:C:381:PRO:HD3	1:C:467:ILE:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:751:SER:N	1:C:752:PRO:HD2	2.18	0.58
1:A:158:GLY:O	1:A:243:LEU:HA	2.03	0.58
1:D:18:LEU:HD13	1:D:18:LEU:N	2.18	0.58
1:D:636:VAL:O	1:D:639:ARG:HB2	2.02	0.58
1:D:665:GLN:NE2	1:D:678:ASN:HA	2.18	0.58
1:A:746:SER:HB3	1:A:762:VAL:HG21	1.85	0.58
1:B:685:GLY:HA2	1:B:801:VAL:CG1	2.34	0.58
1:B:833:ARG:HB2	1:B:833:ARG:CZ	2.33	0.58
1:C:280:TYR:HE2	1:C:289:LYS:HE3	1.67	0.58
1:D:22:GLU:OE1	1:D:22:GLU:HA	2.03	0.58
1:A:24:VAL:O	1:A:28:LYS:N	2.30	0.58
1:C:519:ARG:HG3	1:C:806:ALA:O	2.03	0.58
1:D:53:PHE:HE1	1:D:188:PRO:HD3	1.69	0.58
1:D:594:PRO:O	1:D:639:ARG:NH2	2.36	0.58
1:D:810:LYS:HG3	1:D:811:PHE:CE1	2.39	0.58
1:A:430:LEU:N	1:A:430:LEU:HD23	2.18	0.58
1:C:573:TYR:CE2	1:C:672:GLU:OE1	2.57	0.58
1:B:96:GLN:HG2	1:B:494:LEU:HD11	1.84	0.58
1:B:136:LEU:HD11	1:B:338:ASN:HD21	1.69	0.58
1:C:23:ASN:HB2	1:C:26:GLU:H	1.68	0.58
1:D:110:GLU:HA	1:D:113:TYR:HD2	1.68	0.58
1:A:48:PRO:HB2	1:A:125:ILE:HD12	1.85	0.58
1:D:430:LEU:O	1:D:439:ILE:HA	2.01	0.58
1:A:366:GLU:HG2	1:A:370:LYS:HD2	1.86	0.58
1:C:742:ILE:HD11	1:C:774:PHE:CZ	2.38	0.58
1:C:336:GLN:HE22	1:C:373:ALA:HB3	1.68	0.57
1:C:10:ARG:N	1:C:13:ILE:HD12	2.20	0.57
1:D:279:LEU:HD22	1:D:281:PRO:HG2	1.87	0.57
1:D:700:ALA:HB2	1:D:710:ILE:HD11	1.86	0.57
1:A:486:ILE:HD13	1:A:679:MET:HB2	1.86	0.57
1:C:15:VAL:O	1:C:18:LEU:HD22	2.03	0.57
1:A:326:PHE:CD1	1:A:359:LEU:HD11	2.39	0.57
1:D:280:TYR:O	1:D:281:PRO:O	2.22	0.57
1:D:645:LEU:CD1	1:D:656:VAL:HG21	2.34	0.57
1:A:136:LEU:HG	1:A:338:ASN:ND2	2.19	0.57
1:B:555:VAL:HG11	1:B:643:ILE:CD1	2.34	0.57
1:B:703:ALA:HB2	1:B:807:THR:HG21	1.87	0.57
1:D:225:PRO:HB3	1:D:244:TRP:CZ3	2.40	0.57
1:A:18:LEU:HD22	1:A:18:LEU:H	1.68	0.57
1:A:86:SER:HB3	1:A:89:PHE:CE1	2.39	0.57
1:A:236:ASN:HB2	1:A:834:LEU:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:GLU:O	1:A:352:VAL:HG23	2.05	0.57
1:C:196:PHE:HB3	1:C:309:ARG:HH22	1.70	0.57
1:D:60:ARG:HD2	1:D:189:TRP:HA	1.86	0.57
1:D:235:ASN:HA	1:D:833:ARG:HG3	1.87	0.57
1:A:13:ILE:HD11	1:B:117:LEU:HD11	1.87	0.57
1:A:292:ARG:HG3	1:A:292:ARG:HH11	1.69	0.57
1:A:590:ILE:HG21	1:A:636:VAL:HG13	1.87	0.57
1:C:279:LEU:O	1:C:280:TYR:HD1	1.88	0.57
1:D:778:GLU:HB3	1:D:782:LYS:NZ	2.20	0.57
1:D:102:LEU:HB3	1:D:104:LEU:HD22	1.87	0.57
1:A:590:ILE:HD11	1:A:598:VAL:HG21	1.87	0.56
1:A:727:ASN:O	1:A:730:GLU:HG2	2.05	0.56
1:B:133:ASN:HD22	1:B:281:PRO:HB3	1.68	0.56
1:D:662:LEU:HD11	1:D:784:GLN:HE22	1.69	0.56
1:D:575:ARG:HG2	1:D:578:LEU:HD22	1.87	0.56
1:A:21:VAL:C	1:A:22:GLU:HG2	2.26	0.56
1:A:274:ASN:HA	1:A:277:ARG:CG	2.27	0.56
1:B:233:TYR:CE2	1:B:234:ARG:HD3	2.39	0.56
1:B:323:ARG:HG2	1:B:325:ASN:HB2	1.87	0.56
1:B:566:GLN:HB2	1:B:664:GLU:CB	2.30	0.56
1:B:592:LYS:O	1:B:594:PRO:HD3	2.04	0.56
1:B:612:GLY:H	1:B:617:LYS:HE2	1.69	0.56
1:B:716:GLU:O	1:B:720:ARG:HG2	2.05	0.56
1:C:21:VAL:HG12	1:C:22:GLU:CG	2.33	0.56
1:C:351:ARG:HD3	1:C:399:HIS:CE1	2.40	0.56
1:C:574:LYS:HB2	1:C:576:GLN:NE2	2.20	0.56
1:D:549:LEU:HD23	1:D:557:ILE:HG12	1.86	0.56
1:D:781:VAL:O	1:D:784:GLN:HB2	2.06	0.56
1:B:280:TYR:HE2	1:B:289:LYS:CE	2.11	0.56
1:C:515:LEU:HB3	1:C:809:GLY:HA2	1.86	0.56
1:C:636:VAL:O	1:C:639:ARG:HD3	2.05	0.56
1:A:744:GLN:HA	1:A:747:SER:HG	1.71	0.56
1:C:801:VAL:O	1:C:805:ILE:HG13	2.06	0.56
1:B:10:ARG:N	1:B:13:ILE:HD12	2.21	0.56
1:B:365:TRP:O	1:B:369:VAL:HG12	2.06	0.56
1:C:390:HIS:CD2	1:C:436:VAL:HG21	2.40	0.56
1:C:407:ASN:O	1:C:411:LEU:HG	2.06	0.56
1:A:357:GLU:O	1:A:358:ARG:HB2	2.06	0.56
1:A:629:VAL:HG12	1:A:630:VAL:N	2.21	0.56
1:D:563:PHE:HD2	1:D:659:ALA:O	1.87	0.56
1:D:707:ASN:OD1	1:D:800:MET:SD	2.64	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ARG:CZ	1:B:142:CYS:SG	2.94	0.56
1:C:21:VAL:HG12	1:C:22:GLU:N	2.20	0.56
1:C:455:VAL:HG22	1:C:484:ASN:OD1	2.06	0.56
1:B:689:ILE:HA	1:B:709:PHE:O	2.06	0.56
1:C:196:PHE:HB3	1:C:309:ARG:NH2	2.20	0.56
1:D:370:LYS:HA	1:D:450:HIS:HD2	1.70	0.56
1:D:542:LYS:HE3	1:D:563:PHE:CE2	2.41	0.56
1:A:155:TYR:CE1	1:A:240:THR:HB	2.41	0.56
1:B:293:LEU:HD21	1:B:392:LEU:HD12	1.88	0.56
1:C:43:ARG:HG3	1:D:13:ILE:O	2.05	0.56
1:D:279:LEU:CD2	1:D:281:PRO:HG2	2.35	0.56
1:D:587:TYR:HB2	1:D:640:LEU:HD12	1.88	0.56
1:D:587:TYR:O	1:D:591:LYS:HG2	2.06	0.56
1:A:88:GLU:HG2	1:A:132:GLY:CA	2.36	0.55
1:B:390:HIS:CE1	1:B:391:LEU:HD12	2.41	0.55
1:B:550:GLU:HA	1:B:554:LYS:HA	1.88	0.55
1:A:521:LEU:HD21	1:A:530:PHE:HZ	1.70	0.55
1:A:636:VAL:O	1:A:639:ARG:HB2	2.07	0.55
1:C:32:ASN:ND2	1:D:13:ILE:HA	2.19	0.55
1:C:192:ALA:HA	1:C:226:TYR:HA	1.88	0.55
1:C:399:HIS:O	1:C:403:ILE:HG13	2.07	0.55
1:D:85:LEU:HD22	1:D:342:PRO:HB3	1.89	0.55
1:D:739:ARG:HH11	1:D:739:ARG:HG3	1.71	0.55
1:A:235:ASN:OD1	1:A:237:VAL:HG22	2.07	0.55
1:A:609:ALA:HB2	1:A:620:ILE:CD1	2.36	0.55
1:C:280:TYR:O	1:C:281:PRO:O	2.25	0.55
1:D:489:ARG:HD3	1:D:489:ARG:N	2.22	0.55
1:D:509:GLU:OE1	1:D:510:GLU:CA	2.54	0.55
1:B:766:MET:CE	1:B:766:MET:HA	2.36	0.55
1:C:263:ILE:HB	1:C:266:VAL:HG23	1.88	0.55
1:C:573:TYR:HE2	1:C:672:GLU:OE1	1.88	0.55
1:D:499:LEU:O	1:D:503:ILE:HD12	2.07	0.55
1:D:545:PHE:CZ	1:D:656:VAL:HG23	2.41	0.55
1:B:171:CYS:SG	1:B:176:MET:HG2	2.46	0.55
1:B:322:VAL:HG22	1:B:323:ARG:NH1	2.22	0.55
1:C:24:VAL:C	1:C:25:THR:CA	2.73	0.55
1:A:129:ALA:HA	1:A:182:TRP:CZ3	2.42	0.55
1:A:720:ARG:HG3	1:A:720:ARG:HH11	1.72	0.55
1:A:83:TYR:OH	1:A:310:ARG:HD2	2.06	0.55
1:A:731:TYR:HA	1:A:734:ARG:HD3	1.89	0.55
1:B:30:ASN:HB2	1:B:58:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:VAL:HG22	1:D:484:ASN:OD1	2.06	0.55
1:A:139:LEU:HD21	1:A:484:ASN:HD21	1.72	0.54
1:A:388:PRO:HB2	1:A:390:HIS:CD2	2.43	0.54
1:B:466:THR:OG1	1:B:467:ILE:HD13	2.07	0.54
1:B:530:PHE:CE2	1:B:534:VAL:HG23	2.41	0.54
1:D:24:VAL:O	1:D:25:THR:O	2.24	0.54
1:A:461:GLU:HB3	1:A:465:LYS:NZ	2.23	0.54
1:B:15:VAL:O	1:B:17:GLY:N	2.38	0.54
1:D:279:LEU:HD22	1:D:280:TYR:N	2.22	0.54
1:D:562:LEU:HB3	1:D:601:ARG:HB3	1.90	0.54
1:A:340:THR:OG1	1:A:385:GLU:HB2	2.07	0.54
1:A:459:HIS:HA	1:A:462:ILE:HD11	1.89	0.54
1:A:613:TYR:CD2	1:A:616:ALA:HB2	2.43	0.54
1:C:23:ASN:O	1:C:26:GLU:N	2.40	0.54
1:C:378:THR:O	1:C:459:HIS:HE1	1.91	0.54
1:D:237:VAL:HG12	1:D:834:LEU:HD13	1.88	0.54
1:A:165:ILE:HD12	1:A:166:PHE:CD1	2.43	0.54
1:B:665:GLN:CD	1:B:678:ASN:OD1	2.46	0.54
1:C:366:GLU:HG2	1:C:370:LYS:HE2	1.88	0.54
1:C:605:ILE:HG21	1:C:623:ILE:HD13	1.89	0.54
1:B:555:VAL:HG11	1:B:643:ILE:HD11	1.88	0.54
1:B:756:ASP:O	1:B:759:LYS:HB2	2.06	0.54
1:D:390:HIS:CE1	1:D:391:LEU:CD1	2.90	0.54
1:D:489:ARG:HD3	1:D:489:ARG:H	1.71	0.54
1:D:713:MET:HG3	1:D:717:ASP:CB	2.38	0.54
1:C:584:ILE:HD11	1:C:626:ILE:HD11	1.89	0.54
1:C:766:MET:HE3	1:C:766:MET:HA	1.89	0.54
1:A:740:GLN:O	1:A:744:GLN:HG3	2.07	0.54
1:A:336:GLN:HE21	1:A:825:TRP:HE1	1.56	0.54
1:A:761:ILE:HG22	1:A:765:LEU:HD22	1.89	0.54
1:C:177:GLU:OE2	1:C:611:PRO:HB3	2.08	0.54
1:D:322:VAL:HG13	1:D:325:ASN:HB3	1.90	0.54
1:D:626:ILE:HG22	1:D:642:VAL:HG11	1.90	0.54
1:D:804:ASN:O	1:D:807:THR:HB	2.07	0.54
1:A:682:MET:SD	1:A:699:MET:HG2	2.48	0.54
1:B:97:ASN:HD22	1:B:494:LEU:HD22	1.72	0.54
1:B:118:ASP:HB3	1:B:121:GLU:HB2	1.90	0.54
1:B:381:PRO:HB3	1:B:467:ILE:HG23	1.90	0.54
1:C:519:ARG:O	1:C:522:LEU:N	2.41	0.54
1:D:10:ARG:N	1:D:13:ILE:HD12	2.22	0.54
1:D:477:HIS:CD2	1:D:477:HIS:O	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:PHE:HD1	1:D:549:LEU:HD22	1.73	0.54
1:A:174:TRP:CH2	1:D:435:ALA:HA	2.43	0.54
1:A:316:PHE:CE1	1:A:319:ARG:HB3	2.43	0.54
1:A:385:GLU:O	1:A:386:ARG:HG3	2.08	0.54
1:B:578:LEU:O	1:B:581:LEU:N	2.41	0.54
1:B:707:ASN:HA	1:B:800:MET:SD	2.48	0.54
1:C:487:THR:HG23	1:C:489:ARG:HB2	1.89	0.54
1:D:565:VAL:CG2	1:D:660:ALA:HB1	2.38	0.54
1:A:13:ILE:HA	1:B:32:ASN:OD1	2.08	0.53
1:A:732:TYR:O	1:A:739:ARG:NH1	2.42	0.53
1:C:592:LYS:O	1:C:594:PRO:HD3	2.08	0.53
1:D:67:TRP:CE3	1:D:229:PRO:HB3	2.43	0.53
1:B:631:ASN:OD1	1:B:641:ARG:HA	2.08	0.53
1:C:369:VAL:O	1:C:450:HIS:HB3	2.07	0.53
1:A:555:VAL:HG21	1:A:557:ILE:HD11	1.89	0.53
1:A:687:LEU:HD13	1:A:709:PHE:HE1	1.73	0.53
1:B:196:PHE:HB3	1:B:309:ARG:HH22	1.73	0.53
1:B:698:GLU:O	1:B:702:GLU:HG2	2.08	0.53
1:C:716:GLU:O	1:C:720:ARG:HG2	2.08	0.53
1:A:37:PHE:CZ	1:B:18:LEU:HB2	2.44	0.53
1:B:287:GLU:O	1:B:289:LYS:N	2.41	0.53
1:C:42:ASP:OD1	1:C:44:ASN:HB2	2.08	0.53
1:C:568:LYS:HE2	3:C:999:PLP:O3P	2.08	0.53
1:D:173:GLY:O	1:D:624:THR:HG21	2.08	0.53
1:A:48:PRO:HB2	1:A:125:ILE:CD1	2.38	0.53
1:D:455:VAL:H	1:D:459:HIS:CD2	2.22	0.53
1:D:793:ASN:ND2	1:D:796:GLU:HB2	2.24	0.53
1:A:253:ASN:O	1:A:259:VAL:HG23	2.08	0.53
1:C:511:TYR:CD2	1:C:518:LEU:HD11	2.44	0.53
1:D:424:ARG:HA	1:D:427:ARG:HB2	1.90	0.53
1:D:515:LEU:HB3	1:D:809:GLY:HA2	1.91	0.53
1:B:296:GLU:O	1:B:299:VAL:HG12	2.08	0.53
1:B:640:LEU:HD23	1:B:641:ARG:H	1.74	0.53
1:C:13:ILE:HG23	1:D:32:ASN:ND2	2.23	0.53
1:C:319:ARG:NH2	1:C:328:ALA:HB1	2.23	0.53
1:C:323:ARG:HH21	1:C:325:ASN:ND2	2.06	0.53
1:D:164:GLY:O	1:D:279:LEU:HB2	2.09	0.53
1:A:11:LYS:HA	1:B:43:ARG:NH1	2.23	0.53
1:B:661:ASP:O	1:B:686:ALA:HA	2.08	0.53
1:D:555:VAL:HG12	1:D:556:HIS:H	1.74	0.53
1:D:621:LYS:HG3	1:D:758:PHE:HZ	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLU:O	1:A:289:LYS:N	2.42	0.53
1:A:374:TYR:CD2	1:A:445:CYS:HB3	2.44	0.53
1:B:133:ASN:OD1	1:B:165:ILE:HG21	2.09	0.53
1:C:746:SER:HB3	1:C:762:VAL:HG21	1.91	0.53
1:D:10:ARG:N	1:D:10:ARG:HD2	2.24	0.53
1:D:36:HIS:O	1:D:40:VAL:HA	2.08	0.53
1:D:450:HIS:HE1	1:D:824:ILE:HG22	1.74	0.53
1:D:720:ARG:HG3	1:D:720:ARG:NH1	2.12	0.53
1:A:525:VAL:O	1:A:531:ILE:HD11	2.09	0.52
1:C:316:PHE:CD1	1:C:319:ARG:HB3	2.44	0.52
1:C:720:ARG:HG3	1:C:720:ARG:NH1	2.24	0.52
1:D:198:LEU:HD11	1:D:309:ARG:NH2	2.24	0.52
1:D:338:ASN:OD1	1:D:377:HIS:HE1	1.93	0.52
1:B:133:ASN:ND2	1:B:281:PRO:HG3	2.24	0.52
1:B:423:ASP:O	1:B:426:ARG:HG3	2.09	0.52
1:C:591:LYS:HD3	1:C:635:VAL:HB	1.91	0.52
1:A:75:TYR:CE1	1:A:315:LYS:HG3	2.32	0.52
1:A:456:ALA:HA	1:A:483:THR:OG1	2.10	0.52
1:A:459:HIS:HA	1:A:462:ILE:CD1	2.39	0.52
1:B:381:PRO:HD3	1:B:467:ILE:HD12	1.91	0.52
1:B:396:LEU:HB3	1:B:399:HIS:CD2	2.45	0.52
1:B:503:ILE:HG23	1:B:507:ILE:HD11	1.90	0.52
1:B:703:ALA:CA	1:B:807:THR:HG21	2.39	0.52
1:B:707:ASN:HB3	1:B:800:MET:SD	2.50	0.52
1:C:24:VAL:O	1:C:28:LYS:N	2.32	0.52
1:D:284:ASN:HD22	1:D:285:PHE:N	2.05	0.52
1:A:316:PHE:CZ	1:A:319:ARG:HB3	2.44	0.52
1:A:601:ARG:HH22	1:A:784:GLN:NE2	2.06	0.52
1:B:52:TYR:HE1	1:B:95:LEU:HD12	1.74	0.52
1:C:10:ARG:O	1:C:13:ILE:HB	2.09	0.52
1:C:286:PHE:O	1:C:287:GLU:HG2	2.09	0.52
1:C:496:ASN:ND2	1:C:541:ASN:OD1	2.42	0.52
1:C:587:TYR:CD1	1:C:630:VAL:HG12	2.45	0.52
1:D:47:THR:HG22	1:D:48:PRO:HD2	1.92	0.52
1:D:740:GLN:O	1:D:744:GLN:HG3	2.08	0.52
1:B:586:LEU:HD23	1:B:640:LEU:HD11	1.91	0.52
1:D:379:VAL:HG12	1:D:380:ILE:HG12	1.91	0.52
1:B:732:TYR:O	1:B:739:ARG:NH1	2.42	0.52
1:C:11:LYS:HA	1:D:43:ARG:NH1	2.24	0.52
1:C:196:PHE:CB	1:C:309:ARG:HH22	2.23	0.52
1:D:160:ARG:HB2	1:D:243:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:590:ILE:HD11	1:D:598:VAL:HG21	1.92	0.52
1:D:718:VAL:HG13	1:D:772:LYS:HE2	1.92	0.52
1:A:588:ASN:HD21	1:A:741:ILE:HG22	1.75	0.52
1:A:742:ILE:HD11	1:A:774:PHE:HZ	1.74	0.52
1:B:346:ILE:HB	1:B:347:PRO:HD2	1.91	0.52
1:B:131:LEU:HD11	1:B:243:LEU:HD23	1.91	0.52
1:C:138:ARG:O	1:C:138:ARG:HG3	2.10	0.52
1:C:599:VAL:HG11	1:C:788:SER:O	2.10	0.52
1:C:614:HIS:O	1:C:618:MET:HB2	2.10	0.52
1:D:224:MET:HG2	1:D:247:LYS:HD2	1.92	0.52
1:D:486:ILE:HD11	1:D:680:LYS:HE3	1.92	0.52
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.10	0.52
1:C:279:LEU:HD23	1:C:281:PRO:HD2	1.85	0.52
1:C:361:TRP:CZ3	1:C:409:ARG:HD2	2.44	0.52
1:A:411:LEU:HD21	1:A:429:SER:HA	1.91	0.52
1:A:11:LYS:HA	1:B:43:ARG:HH11	1.75	0.51
1:A:398:ARG:O	1:A:401:GLN:HB2	2.10	0.51
1:A:708:PHE:HB3	1:A:710:ILE:CD1	2.40	0.51
1:B:24:VAL:O	1:B:28:LYS:HG3	2.10	0.51
1:B:586:LEU:H	1:B:586:LEU:HD22	1.75	0.51
1:D:498:GLY:O	1:D:501:GLU:N	2.43	0.51
1:D:567:VAL:HG23	1:D:567:VAL:O	2.10	0.51
1:D:732:TYR:O	1:D:739:ARG:NH1	2.43	0.51
1:A:270:ASN:OD1	1:B:269:ARG:HD3	2.10	0.51
1:B:727:ASN:O	1:B:730:GLU:HB3	2.11	0.51
1:C:203:TYR:O	1:C:215:TRP:CZ2	2.62	0.51
1:D:328:ALA:O	1:D:331:ASP:HB2	2.09	0.51
1:D:533:ASP:O	1:D:537:VAL:HG23	2.11	0.51
1:D:571:HIS:ND1	1:D:572:GLU:N	2.58	0.51
1:A:96:GLN:O	1:A:100:VAL:HG13	2.10	0.51
1:A:609:ALA:HB2	1:A:620:ILE:HD11	1.92	0.51
1:C:283:ASP:OD2	1:C:383:ALA:HB2	2.03	0.51
1:D:70:THR:HG21	1:D:238:VAL:H	1.74	0.51
1:D:549:LEU:HB3	1:D:557:ILE:HG12	1.92	0.51
1:A:790:LEU:O	1:A:790:LEU:HG	2.11	0.51
1:B:274:ASN:HA	1:B:277:ARG:HG3	1.91	0.51
1:C:80:LYS:HE2	1:C:825:TRP:O	2.11	0.51
1:C:200:VAL:HG22	1:C:301:ALA:HB3	1.92	0.51
1:D:627:GLY:O	1:D:631:ASN:HB2	2.10	0.51
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.76	0.51
1:B:481:ASN:O	1:B:482:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:ARG:HG3	1:B:714:ARG:HH11	1.75	0.51
1:B:766:MET:HA	1:B:766:MET:HE2	1.93	0.51
1:B:834:LEU:HD23	1:B:835:PRO:HD2	1.92	0.51
1:D:138:ARG:HD3	1:D:491:TRP:HZ2	1.75	0.51
1:D:495:CYS:O	1:D:658:PRO:HG2	2.11	0.51
1:D:822:ARG:NH1	1:D:828:GLU:HG3	2.26	0.51
1:A:378:THR:O	1:A:459:HIS:HE1	1.94	0.51
1:A:502:ILE:HA	1:A:505:GLU:HB2	1.91	0.51
1:B:161:TYR:CE2	1:B:279:LEU:HG	2.46	0.51
1:B:161:TYR:O	1:B:182:TRP:HZ2	1.93	0.51
1:C:67:TRP:O	1:C:71:GLN:HG2	2.10	0.51
1:C:144:LEU:HD13	1:C:230:VAL:HG11	1.91	0.51
1:C:379:VAL:HG13	1:C:380:ILE:HG12	1.93	0.51
1:D:138:ARG:NH2	1:D:490:ARG:HD3	2.26	0.51
1:C:13:ILE:HG23	1:D:32:ASN:HD21	1.74	0.51
1:D:631:ASN:ND2	1:D:642:VAL:H	2.08	0.51
1:D:735:ILE:HD12	1:D:735:ILE:H	1.75	0.51
1:A:719:ASP:O	1:A:722:ASP:HB2	2.11	0.51
1:B:280:TYR:H	1:B:281:PRO:CD	2.20	0.51
1:B:767:HIS:HB2	1:B:768:HIS:CE1	2.45	0.51
1:C:184:ARG:HD2	1:C:185:TYR:CE2	2.46	0.51
1:C:665:GLN:HB3	1:C:696:ASN:HD21	1.75	0.51
1:A:316:PHE:HE2	1:A:332:LYS:CE	2.16	0.51
1:A:354:VAL:O	1:A:358:ARG:HA	2.10	0.51
1:B:161:TYR:HA	1:B:276:SER:O	2.10	0.51
1:C:34:HIS:HD2	1:C:38:THR:OG1	1.94	0.51
1:D:741:ILE:HG22	1:D:744:GLN:NE2	2.26	0.51
1:B:480:GLN:HG2	1:B:482:LYS:HE2	1.92	0.50
1:B:567:VAL:HB	1:B:648:TYR:CE1	2.46	0.50
1:B:790:LEU:HG	1:B:797:TRP:HD1	1.76	0.50
1:D:281:PRO:HD3	1:D:292:ARG:NH1	2.25	0.50
1:D:513:SER:C	1:D:831:ARG:HH21	2.14	0.50
1:D:698:GLU:HA	1:D:701:GLU:CG	2.41	0.50
1:A:384:LEU:HB2	1:A:386:ARG:HH12	1.76	0.50
1:A:492:LEU:HG	1:A:683:LEU:HD22	1.92	0.50
1:A:519:ARG:O	1:A:522:LEU:HB2	2.10	0.50
1:A:588:ASN:ND2	1:A:741:ILE:HG22	2.26	0.50
1:C:13:ILE:HA	1:D:32:ASN:OD1	2.11	0.50
1:C:735:ILE:HG22	1:C:738:LEU:H	1.75	0.50
1:D:108:CYS:O	1:D:112:THR:HG23	2.11	0.50
1:D:601:ARG:NH2	1:D:784:GLN:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:THR:HG23	1:C:453:ASN:ND2	2.27	0.50
1:D:59:VAL:O	1:D:62:HIS:HB2	2.12	0.50
1:D:489:ARG:HA	1:D:493:VAL:HG23	1.93	0.50
1:D:536:LYS:O	1:D:540:GLU:N	2.45	0.50
1:D:662:LEU:CD1	1:D:784:GLN:HE22	2.24	0.50
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.93	0.50
1:B:789:ALA:O	1:B:792:LYS:NZ	2.41	0.50
1:A:656:VAL:HG13	1:A:657:ILE:N	2.26	0.50
1:B:584:ILE:HD13	1:B:750:PHE:CE2	2.46	0.50
1:C:291:LEU:O	1:C:295:GLN:HG3	2.12	0.50
1:C:349:LEU:O	1:C:353:LEU:CG	2.58	0.50
1:D:168:GLN:HE21	1:D:647:ASN:H	1.59	0.50
1:D:504:ALA:HA	1:D:508:GLY:N	2.27	0.50
1:D:754:GLN:HE22	1:D:757:LEU:HD11	1.77	0.50
1:A:33:ARG:HH22	1:B:30:ASN:HD21	1.60	0.50
1:A:202:PHE:O	1:A:218:THR:HB	2.12	0.50
1:A:480:GLN:NE2	1:A:823:GLU:HB3	2.27	0.50
1:A:708:PHE:HB3	1:A:710:ILE:HD12	1.94	0.50
1:D:24:VAL:O	1:D:28:LYS:HG3	2.11	0.50
1:D:450:HIS:O	1:D:478:LYS:HG3	2.12	0.50
1:D:721:LEU:HD21	1:D:726:TYR:CD1	2.47	0.50
1:D:754:GLN:HE21	1:D:757:LEU:CD1	2.24	0.50
1:A:509:GLU:CG	1:A:512:ILE:HD12	2.42	0.50
1:C:193:ARG:HD2	1:C:196:PHE:CE2	2.47	0.50
1:C:206:VAL:HA	1:C:214:LYS:O	2.11	0.50
1:C:207:GLU:HB3	1:C:214:LYS:HB2	1.93	0.50
1:C:221:VAL:HG13	1:C:272:ALA:HB1	1.94	0.50
1:C:233:TYR:OH	1:C:234:ARG:NH1	2.44	0.50
1:D:147:MET:O	1:D:152:LEU:HB2	2.11	0.50
1:D:505:GLU:OE1	1:D:506:ARG:NH2	2.45	0.50
1:D:784:GLN:O	1:D:787:VAL:HG12	2.12	0.50
1:A:21:VAL:O	1:A:22:GLU:CB	2.59	0.50
1:B:93:ARG:O	1:B:490:ARG:NH2	2.45	0.50
1:B:378:THR:HG21	1:B:384:LEU:HD13	1.92	0.50
1:C:391:LEU:O	1:C:391:LEU:HD23	2.12	0.50
1:C:458:ILE:HD11	1:C:694:GLY:HA2	1.93	0.50
1:C:790:LEU:HB3	1:C:797:TRP:CD1	2.47	0.50
1:D:491:TRP:CA	1:D:495:CYS:HG	2.22	0.50
1:D:502:ILE:HA	1:D:505:GLU:HB2	1.93	0.50
1:D:538:LYS:NZ	1:D:660:ALA:O	2.45	0.50
1:D:549:LEU:HD23	1:D:557:ILE:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:599:VAL:HG21	1:D:788:SER:O	2.11	0.50
1:A:352:VAL:HA	1:A:356:LEU:HD23	1.93	0.50
1:C:491:TRP:CA	1:C:495:CYS:SG	2.98	0.50
1:C:741:ILE:HA	1:C:744:GLN:HB2	1.93	0.50
1:A:716:GLU:O	1:A:719:ASP:HB2	2.11	0.49
1:C:599:VAL:HG21	1:C:788:SER:HB3	1.93	0.49
1:C:626:ILE:HG22	1:C:642:VAL:HG21	1.94	0.49
1:D:565:VAL:HG21	1:D:681:PHE:CE1	2.42	0.49
1:A:74:TYR:CZ	1:A:153:ALA:HA	2.46	0.49
1:A:168:GLN:HB3	1:A:647:ASN:HA	1.93	0.49
1:B:280:TYR:CE2	1:B:289:LYS:CE	2.87	0.49
1:B:783:CYS:SG	1:B:786:ARG:NH2	2.85	0.49
1:C:784:GLN:O	1:C:787:VAL:HG12	2.12	0.49
1:D:279:LEU:HD21	1:D:281:PRO:CG	2.41	0.49
1:A:74:TYR:CD1	1:A:79:PRO:HG3	2.47	0.49
1:B:687:LEU:HD13	1:B:709:PHE:HE1	1.77	0.49
1:D:80:LYS:HG2	1:D:332:LYS:O	2.12	0.49
1:D:280:TYR:O	1:D:281:PRO:C	2.50	0.49
1:D:588:ASN:HD21	1:D:744:GLN:NE2	2.10	0.49
1:D:759:LYS:NZ	1:D:763:ASN:OD1	2.40	0.49
1:A:349:LEU:HD23	1:A:368:THR:HG23	1.93	0.49
1:B:101:ASN:HB3	1:B:232:GLY:O	2.12	0.49
1:B:284:ASN:CG	1:B:285:PHE:N	2.64	0.49
1:C:23:ASN:O	1:C:27:LEU:N	2.46	0.49
1:C:315:LYS:O	1:C:319:ARG:HB2	2.12	0.49
1:C:720:ARG:HG3	1:C:720:ARG:HH11	1.76	0.49
1:D:287:GLU:O	1:D:289:LYS:N	2.45	0.49
1:A:411:LEU:HD11	1:A:429:SER:HB2	1.93	0.49
1:B:546:ALA:O	1:B:550:GLU:HB2	2.12	0.49
1:B:835:PRO:O	1:B:836:ALA:HB3	2.12	0.49
1:C:329:PHE:HB3	1:C:330:PRO:HD3	1.95	0.49
1:C:363:LYS:O	1:C:367:VAL:HG23	2.12	0.49
1:C:464:LYS:HG2	1:C:472:TYR:CD2	2.47	0.49
1:C:545:PHE:HE2	1:C:604:MET:SD	2.35	0.49
1:A:742:ILE:CD1	1:A:774:PHE:HZ	2.26	0.49
1:B:252:PHE:CZ	1:B:269:ARG:HB3	2.48	0.49
1:B:522:LEU:HD13	1:B:806:ALA:CB	2.42	0.49
1:B:629:VAL:HG12	1:B:630:VAL:N	2.28	0.49
1:C:591:LYS:CD	1:C:635:VAL:HB	2.43	0.49
1:D:424:ARG:NH2	1:D:473:GLU:CD	2.58	0.49
1:D:766:MET:HE3	1:D:774:PHE:CE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:VAL:H	1:C:459:HIS:HD2	1.60	0.49
1:D:70:THR:O	1:D:73:HIS:HB3	2.11	0.49
1:D:742:ILE:HD11	1:D:774:PHE:CE1	2.48	0.49
1:A:42:ASP:OD1	1:A:43:ARG:CA	2.60	0.49
1:A:322:VAL:O	1:A:322:VAL:HG22	2.12	0.49
1:C:733:ASP:HA	1:C:739:ARG:HH12	1.77	0.49
1:A:481:ASN:O	1:A:482:LYS:HG2	2.13	0.49
1:A:834:LEU:HD23	1:A:835:PRO:HD2	1.95	0.49
1:B:23:ASN:OD1	1:B:25:THR:N	2.46	0.49
1:D:170:ILE:HD13	1:D:175:GLN:HA	1.95	0.49
1:D:565:VAL:HG21	1:D:660:ALA:HB1	1.95	0.49
1:D:736:PRO:O	1:D:740:GLN:HB3	2.13	0.49
1:C:279:LEU:C	1:C:281:PRO:HD2	2.31	0.49
1:D:73:HIS:ND1	1:D:834:LEU:HD11	2.28	0.49
1:D:703:ALA:CA	1:D:807:THR:HG21	2.43	0.49
1:A:319:ARG:HD3	1:A:332:LYS:HZ3	1.78	0.48
1:A:680:LYS:O	1:A:684:ASN:HB2	2.13	0.48
1:B:269:ARG:O	1:B:273:GLU:HB2	2.12	0.48
1:B:574:LYS:HA	1:B:667:SER:OG	2.12	0.48
1:C:91:MET:CE	1:C:144:LEU:HD12	2.42	0.48
1:D:319:ARG:O	1:D:321:PRO:HD3	2.13	0.48
1:D:338:ASN:OD1	1:D:377:HIS:CE1	2.66	0.48
1:D:522:LEU:O	1:D:525:VAL:HG23	2.13	0.48
1:B:89:PHE:CE1	1:B:140:ALA:HB1	2.48	0.48
1:C:280:TYR:O	1:C:281:PRO:C	2.51	0.48
1:C:352:VAL:HG13	1:C:356:LEU:HD23	1.95	0.48
1:D:458:ILE:O	1:D:462:ILE:HG12	2.14	0.48
1:A:403:ILE:CG2	1:A:439:ILE:HD13	2.42	0.48
1:D:140:ALA:O	1:D:144:LEU:HG	2.13	0.48
1:D:630:VAL:HG23	1:D:631:ASN:N	2.28	0.48
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.63	0.48
1:A:564:ASP:HB3	1:A:603:VAL:HA	1.94	0.48
1:B:94:THR:HG22	1:B:98:THR:OG1	2.13	0.48
1:B:503:ILE:O	1:B:507:ILE:HG12	2.13	0.48
1:C:284:ASN:CG	1:C:285:PHE:N	2.62	0.48
1:C:732:TYR:HE1	1:C:739:ARG:HA	1.77	0.48
1:D:483:THR:HB	1:D:815:ARG:HH22	1.78	0.48
1:A:139:LEU:HD11	1:A:484:ASN:HD21	1.78	0.48
1:B:246:ALA:HB2	1:B:298:PHE:CZ	2.48	0.48
1:C:23:ASN:HB3	1:C:25:THR:HB	1.95	0.48
1:C:68:ILE:O	1:C:72:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:HA	1:C:334:ALA:HB3	1.94	0.48
1:C:352:VAL:HG13	1:C:356:LEU:CD2	2.42	0.48
1:C:589:ARG:O	1:C:592:LYS:HB3	2.13	0.48
1:C:709:PHE:CZ	1:C:787:VAL:HG23	2.49	0.48
1:D:21:VAL:HA	1:D:62:HIS:NE2	2.28	0.48
1:A:622:LEU:HA	1:A:758:PHE:CE1	2.49	0.48
1:C:528:GLU:OE1	1:C:532:ARG:NH2	2.39	0.48
1:D:42:ASP:OD1	1:D:45:VAL:HG23	2.14	0.48
1:D:665:GLN:HE22	1:D:678:ASN:HA	1.77	0.48
1:A:138:ARG:HG3	1:A:138:ARG:HH11	1.78	0.48
1:A:327:ASP:OD1	1:A:363:LYS:NZ	2.45	0.48
1:B:574:LYS:HB2	1:B:576:GLN:NE2	2.29	0.48
1:C:41:LYS:HG3	1:C:50:ASP:OD2	2.13	0.48
1:C:316:PHE:O	1:C:324:THR:HG22	2.14	0.48
1:A:143:PHE:HB3	1:A:147:MET:HE2	1.96	0.48
1:A:166:PHE:CD2	1:A:177:GLU:HB3	2.49	0.48
1:A:196:PHE:HB2	1:A:225:PRO:HG3	1.94	0.48
1:A:592:LYS:NZ	1:A:593:GLU:OE2	2.45	0.48
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.13	0.48
1:B:797:TRP:O	1:B:800:MET:HB2	2.14	0.48
1:C:64:VAL:HG12	1:C:67:TRP:CE3	2.46	0.48
1:C:292:ARG:O	1:C:296:GLU:HG3	2.13	0.48
1:A:80:LYS:HD3	1:A:825:TRP:O	2.13	0.48
1:C:16:ARG:HG3	1:C:16:ARG:O	2.14	0.48
1:C:262:TYR:HD1	1:C:263:ILE:H	1.62	0.48
1:C:759:LYS:HG2	1:C:763:ASN:OD1	2.14	0.48
1:D:49:ARG:HA	1:D:125:ILE:HG21	1.96	0.48
1:D:311:PHE:O	1:D:316:PHE:HB2	2.13	0.48
1:D:789:ALA:HA	1:D:792:LYS:NZ	2.29	0.48
1:A:326:PHE:HD1	1:A:359:LEU:HD11	1.79	0.48
1:C:23:ASN:CB	1:C:26:GLU:H	2.25	0.48
1:C:85:LEU:HD22	1:C:342:PRO:HB3	1.96	0.48
1:C:703:ALA:HB3	1:C:708:PHE:CE1	2.49	0.48
1:A:252:PHE:CZ	1:A:269:ARG:HB3	2.49	0.47
1:A:499:LEU:HD23	1:A:499:LEU:O	2.13	0.47
1:A:742:ILE:CD1	1:A:765:LEU:HD23	2.44	0.47
1:B:158:GLY:O	1:B:243:LEU:HA	2.14	0.47
1:B:225:PRO:HB2	1:B:242:ARG:HD2	1.96	0.47
1:B:389:VAL:HG12	1:B:439:ILE:CD1	2.44	0.47
1:C:232:GLY:HA3	1:C:235:ASN:HD21	1.79	0.47
1:D:509:GLU:HA	1:D:511:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:H	1:A:356:LEU:HD22	1.78	0.47
1:B:571:HIS:ND1	1:B:572:GLU:N	2.61	0.47
1:B:640:LEU:HD23	1:B:641:ARG:N	2.29	0.47
1:D:193:ARG:HB2	1:D:225:PRO:HG2	1.96	0.47
1:D:515:LEU:O	1:D:518:LEU:HB2	2.14	0.47
1:A:756:ASP:OD1	1:D:426:ARG:NH2	2.48	0.47
1:A:759:LYS:HE3	1:A:759:LYS:HB3	1.73	0.47
1:D:53:PHE:CE1	1:D:188:PRO:HD3	2.49	0.47
1:D:374:TYR:HD2	1:D:452:VAL:HG22	1.77	0.47
1:D:521:LEU:HD11	1:D:530:PHE:CE1	2.48	0.47
1:D:802:ILE:HA	1:D:805:ILE:HD12	1.96	0.47
1:A:13:ILE:HG22	1:B:43:ARG:HB2	1.95	0.47
1:A:411:LEU:HD21	1:A:429:SER:CA	2.45	0.47
1:B:163:PHE:HB2	1:B:277:ARG:O	2.15	0.47
1:B:251:ASP:HB3	1:B:255:LYS:CG	2.44	0.47
1:D:754:GLN:HA	1:D:755:PRO:HD3	1.64	0.47
1:A:32:ASN:ND2	1:B:13:ILE:HG23	2.29	0.47
1:B:713:MET:SD	1:B:718:VAL:HA	2.55	0.47
1:C:235:ASN:H	1:C:235:ASN:ND2	2.06	0.47
1:C:703:ALA:HB2	1:C:807:THR:HG21	1.96	0.47
1:B:568:LYS:O	1:B:607:GLY:HA3	2.14	0.47
1:B:709:PHE:CD2	1:B:787:VAL:HG23	2.49	0.47
1:A:167:ASN:O	1:A:177:GLU:HA	2.15	0.47
1:A:316:PHE:HE2	1:A:332:LYS:HZ1	1.57	0.47
1:B:569:ARG:O	1:B:574:LYS:HG3	2.15	0.47
1:B:575:ARG:O	1:B:578:LEU:N	2.47	0.47
1:B:590:ILE:CG2	1:B:636:VAL:HG22	2.45	0.47
1:C:23:ASN:O	1:C:24:VAL:C	2.51	0.47
1:C:133:ASN:CG	1:C:165:ILE:HG21	2.35	0.47
1:C:143:PHE:HB3	1:C:147:MET:HE2	1.97	0.47
1:C:183:LEU:HD23	1:C:187:ASN:HB2	1.96	0.47
1:C:201:HIS:HB3	1:C:218:THR:HG21	1.97	0.47
1:C:446:ILE:HD12	1:C:452:VAL:HG21	1.96	0.47
1:D:24:VAL:O	1:D:25:THR:C	2.44	0.47
1:D:315:LYS:O	1:D:319:ARG:HB2	2.15	0.47
1:D:538:LYS:O	1:D:542:LYS:HG3	2.15	0.47
1:D:645:LEU:HD22	1:D:652:LEU:HD13	1.95	0.47
1:D:789:ALA:HA	1:D:792:LYS:HZ1	1.79	0.47
1:A:155:TYR:CD1	1:A:240:THR:HB	2.50	0.47
1:C:348:GLU:OE1	1:C:399:HIS:HE1	1.98	0.47
1:B:22:GLU:OE2	1:B:104:LEU:CD1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:798:THR:O	1:B:802:ILE:HG13	2.15	0.47
1:C:271:LEU:HA	1:C:274:ASN:HD22	1.79	0.47
1:C:519:ARG:O	1:C:522:LEU:HB2	2.15	0.47
1:D:297:TYR:HB2	1:D:396:LEU:HD21	1.97	0.47
1:A:513:SER:C	1:A:831:ARG:HH21	2.18	0.47
1:A:759:LYS:NZ	1:A:763:ASN:OD1	2.43	0.47
1:B:88:GLU:HG3	1:B:132:GLY:CA	2.42	0.47
1:C:323:ARG:C	1:C:325:ASN:N	2.68	0.47
1:C:571:HIS:HB3	1:C:574:LYS:HG2	1.96	0.47
1:D:741:ILE:HG22	1:D:744:GLN:HE21	1.80	0.47
1:A:89:PHE:CD2	1:A:241:MET:SD	3.08	0.46
1:A:235:ASN:O	1:A:236:ASN:HB2	2.16	0.46
1:A:493:VAL:HG21	1:A:512:ILE:HD13	1.96	0.46
1:B:603:VAL:HB	1:B:641:ARG:O	2.15	0.46
1:C:585:THR:O	1:C:588:ASN:HB2	2.15	0.46
1:D:577:LEU:HD13	1:D:765:LEU:CD1	2.39	0.46
1:A:422:VAL:HA	1:A:425:LEU:CD1	2.44	0.46
1:C:14:SEP:HB2	1:C:16:ARG:HG2	1.96	0.46
1:D:64:VAL:O	1:D:68:ILE:HD12	2.15	0.46
1:D:192:ALA:HB2	1:D:226:TYR:CE2	2.50	0.46
1:D:662:LEU:HD23	1:D:687:LEU:O	2.15	0.46
1:A:322:VAL:HG13	1:A:325:ASN:CB	2.45	0.46
1:B:163:PHE:HD2	1:B:277:ARG:HB3	1.81	0.46
1:B:251:ASP:HB3	1:B:255:LYS:CB	2.45	0.46
1:B:369:VAL:HA	1:B:448:GLY:O	2.15	0.46
1:B:575:ARG:NH1	1:B:666:ILE:O	2.46	0.46
1:B:819:GLN:O	1:B:823:GLU:HB2	2.14	0.46
1:C:157:TYR:CE1	1:C:242:ARG:HG2	2.50	0.46
1:D:147:MET:SD	1:D:154:ALA:CB	3.03	0.46
1:D:766:MET:CE	1:D:774:PHE:HE2	2.26	0.46
1:A:203:TYR:CZ	1:A:395:LEU:HD13	2.51	0.46
1:A:531:ILE:HD13	1:A:799:ARG:HG2	1.98	0.46
1:A:629:VAL:HG11	1:A:750:PHE:CE1	2.44	0.46
1:A:744:GLN:HA	1:A:747:SER:OG	2.15	0.46
1:B:241:MET:SD	1:B:243:LEU:HD11	2.55	0.46
1:B:821:ALA:HB1	1:B:827:VAL:O	2.14	0.46
1:C:28:LYS:HG2	1:C:115:LEU:HD11	1.98	0.46
1:C:254:LEU:HD22	1:C:257:PHE:CZ	2.51	0.46
1:C:491:TRP:C	1:C:495:CYS:SG	2.94	0.46
1:A:326:PHE:O	1:A:330:PRO:HD3	2.16	0.46
1:A:557:ILE:HD11	1:A:643:ILE:CD1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ARG:NH2	1:A:784:GLN:HE22	2.12	0.46
1:B:103:ALA:HB2	1:B:234:ARG:NE	2.31	0.46
1:B:252:PHE:O	1:B:259:VAL:HG11	2.16	0.46
1:D:496:ASN:ND2	1:D:658:PRO:HB3	2.31	0.46
1:D:786:ARG:O	1:D:789:ALA:HB3	2.15	0.46
1:A:486:ILE:HG23	1:A:491:TRP:CD1	2.50	0.46
1:C:456:ALA:HB3	1:C:459:HIS:HB3	1.96	0.46
1:C:574:LYS:HB2	1:C:576:GLN:HE21	1.80	0.46
1:D:169:LYS:HA	1:D:169:LYS:HD2	1.82	0.46
1:D:257:PHE:CD1	1:D:257:PHE:N	2.84	0.46
1:D:486:ILE:HD12	1:D:486:ILE:HA	1.51	0.46
1:D:643:ILE:HD13	1:D:643:ILE:HA	1.72	0.46
1:A:191:LYS:HD2	1:A:191:LYS:HA	1.79	0.46
1:A:331:ASP:CB	1:A:332:LYS:HG2	2.45	0.46
1:A:528:GLU:OE2	1:A:795:ARG:HD2	2.15	0.46
1:B:81:ARG:HH11	1:B:81:ARG:HG3	1.79	0.46
1:B:297:TYR:HE1	1:B:348:GLU:OE1	1.99	0.46
1:B:815:ARG:NH1	1:B:819:GLN:OE1	2.48	0.46
1:C:642:VAL:O	1:C:643:ILE:HD13	2.16	0.46
1:D:222:LEU:HD23	1:D:222:LEU:HA	1.75	0.46
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.98	0.46
1:A:426:ARG:NH1	1:D:755:PRO:HG2	2.30	0.46
1:A:698:GLU:HB3	1:A:810:LYS:NZ	2.30	0.46
1:B:87:LEU:HD13	1:B:299:VAL:HG11	1.98	0.46
1:B:563:PHE:HD2	1:B:659:ALA:O	1.98	0.46
1:C:386:ARG:HD3	1:C:438:ARG:HD2	1.98	0.46
1:D:335:ILE:HG13	1:D:371:THR:HG22	1.96	0.46
1:D:818:ALA:O	1:D:821:ALA:HB3	2.15	0.46
1:A:49:ARG:O	1:A:53:PHE:HD2	1.99	0.46
1:A:90:TYR:HE2	1:A:134:GLY:HA2	1.81	0.46
1:B:455:VAL:HG13	1:B:484:ASN:CG	2.36	0.46
1:C:372:CYS:O	1:C:450:HIS:HD2	1.99	0.46
1:C:678:ASN:CB	1:C:699:MET:HE1	2.46	0.46
1:C:792:LYS:O	1:C:794:PRO:HD3	2.16	0.46
1:A:116:GLY:O	1:B:10:ARG:HD3	2.16	0.46
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.50	0.46
1:C:590:ILE:O	1:C:594:PRO:HA	2.15	0.46
1:D:83:TYR:CE2	1:D:307:ILE:HG12	2.51	0.46
1:D:378:THR:O	1:D:459:HIS:HE1	1.99	0.46
1:A:102:LEU:HB3	1:A:104:LEU:HD22	1.98	0.45
1:A:170:ILE:HD13	1:A:175:GLN:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:TYR:CE2	3:D:999:PLP:H2A3	2.51	0.45
1:D:206:VAL:HA	1:D:214:LYS:O	2.16	0.45
1:D:790:LEU:HD21	1:D:800:MET:HG3	1.98	0.45
1:A:582:HIS:HA	1:A:585:THR:HB	1.98	0.45
1:B:304:LEU:HD21	1:B:349:LEU:CA	2.46	0.45
1:D:754:GLN:HB3	1:D:757:LEU:HD13	1.97	0.45
1:D:836:ALA:HA	1:D:837:PRO:HD2	1.78	0.45
1:A:41:LYS:HA	1:A:41:LYS:HD3	1.71	0.45
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.72	0.45
1:A:455:VAL:H	1:A:459:HIS:CD2	2.33	0.45
1:A:599:VAL:HG11	1:A:791:TYR:HD2	1.81	0.45
1:A:730:GLU:O	1:A:734:ARG:HD2	2.16	0.45
1:A:730:GLU:O	1:A:734:ARG:HD3	2.17	0.45
1:B:17:GLY:CA	1:B:18:LEU:HD22	2.46	0.45
1:B:455:VAL:HG13	1:B:484:ASN:ND2	2.31	0.45
1:C:337:LEU:HD11	1:C:345:ALA:HB3	1.99	0.45
1:C:753:LYS:HD2	1:C:753:LYS:N	2.30	0.45
1:D:582:HIS:O	1:D:586:LEU:HD13	2.16	0.45
1:A:18:LEU:HB2	1:B:37:PHE:CZ	2.51	0.45
1:A:304:LEU:HD11	1:A:345:ALA:HB1	1.99	0.45
1:A:490:ARG:HG3	1:A:494:LEU:HD11	1.98	0.45
1:A:544:LYS:O	1:A:547:ALA:HB3	2.16	0.45
1:B:49:ARG:HH11	1:B:125:ILE:HG22	1.82	0.45
1:C:19:ALA:HB1	1:C:21:VAL:H	1.81	0.45
1:C:78:ASP:O	1:C:332:LYS:NZ	2.50	0.45
1:C:543:LEU:HD12	1:C:559:PRO:CB	2.46	0.45
1:D:118:ASP:HB3	1:D:121:GLU:HB3	1.97	0.45
1:D:542:LYS:NZ	1:D:661:ASP:OD2	2.50	0.45
1:D:698:GLU:HA	1:D:701:GLU:HG2	1.99	0.45
1:A:18:LEU:O	1:A:19:ALA:CB	2.65	0.45
1:B:648:TYR:CE2	3:B:999:PLP:H2A2	2.52	0.45
1:B:733:ASP:O	1:B:739:ARG:NH1	2.50	0.45
1:C:155:TYR:N	1:C:155:TYR:CD1	2.84	0.45
1:C:541:ASN:O	1:C:544:LYS:N	2.49	0.45
1:D:244:TRP:CE2	1:D:302:ALA:HB1	2.51	0.45
1:D:279:LEU:HD21	1:D:281:PRO:CD	2.38	0.45
1:D:549:LEU:O	1:D:555:VAL:N	2.50	0.45
1:D:687:LEU:HD12	1:D:797:TRP:CE2	2.51	0.45
1:A:524:TYR:CD1	1:A:524:TYR:N	2.85	0.45
1:A:571:HIS:ND1	1:A:572:GLU:N	2.64	0.45
1:A:834:LEU:HD23	1:A:835:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ASP:OD2	1:B:398:ARG:NH1	2.49	0.45
1:C:160:ARG:NH2	1:C:190:GLU:OE2	2.49	0.45
1:D:545:PHE:HD1	1:D:549:LEU:CD2	2.29	0.45
1:D:758:PHE:CD1	1:D:761:ILE:HD11	2.44	0.45
1:A:455:VAL:H	1:A:459:HIS:HD2	1.65	0.45
1:A:571:HIS:CE1	1:A:613:TYR:OH	2.70	0.45
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.98	0.45
1:C:317:GLY:CA	1:C:320:ASP:HB2	2.46	0.45
1:C:682:MET:CE	1:C:807:THR:HG22	2.46	0.45
1:C:727:ASN:C	1:C:727:ASN:HD22	2.20	0.45
1:D:424:ARG:NH2	1:D:473:GLU:OE1	2.46	0.45
1:D:486:ILE:HD11	1:D:680:LYS:CE	2.47	0.45
1:A:24:VAL:CG1	1:A:111:ALA:HA	2.39	0.45
1:A:93:ARG:O	1:A:490:ARG:NH2	2.49	0.45
1:A:157:TYR:CE2	1:A:242:ARG:HG2	2.52	0.45
1:A:460:SER:CB	1:A:481:ASN:HB2	2.46	0.45
1:B:49:ARG:HE	1:B:185:TYR:HD2	1.65	0.45
1:B:575:ARG:HB3	1:B:666:ILE:CD1	2.46	0.45
1:C:19:ALA:HB1	1:C:21:VAL:HA	1.99	0.45
1:C:52:TYR:HH	1:C:189:TRP:HZ2	1.58	0.45
1:C:569:ARG:O	1:C:574:LYS:HG3	2.17	0.45
1:D:60:ARG:O	1:D:64:VAL:HG22	2.16	0.45
1:D:159:ILE:HG21	1:D:159:ILE:HD13	1.78	0.45
1:D:297:TYR:CG	1:D:396:LEU:HD21	2.52	0.45
1:D:410:PHE:O	1:D:413:ARG:HB2	2.17	0.45
1:A:24:VAL:HG13	1:A:111:ALA:CA	2.40	0.45
1:A:461:GLU:HB3	1:A:465:LYS:HZ2	1.81	0.45
1:A:542:LYS:NZ	1:A:561:SER:O	2.50	0.45
1:A:725:GLY:HA3	1:D:727:ASN:HD21	1.81	0.45
1:B:138:ARG:HH21	1:B:141:ALA:CB	2.30	0.45
1:C:336:GLN:NE2	1:C:373:ALA:HB3	2.32	0.45
1:C:379:VAL:HB	1:C:673:ALA:HB2	1.98	0.45
1:C:566:GLN:HB2	1:C:664:GLU:HB2	1.98	0.45
1:C:573:TYR:CD2	1:C:671:THR:HB	2.52	0.45
1:D:280:TYR:HE2	1:D:289:LYS:HE3	1.82	0.45
1:D:496:ASN:HB2	1:D:684:ASN:OD1	2.17	0.45
1:D:518:LEU:HD12	1:D:518:LEU:HA	1.72	0.45
1:A:97:ASN:HA	1:A:494:LEU:HD22	1.99	0.45
1:A:369:VAL:HA	1:A:448:GLY:O	2.17	0.45
1:B:24:VAL:HG12	1:B:28:LYS:HE2	1.97	0.45
1:B:505:GLU:HB3	1:B:506:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:TYR:CE2	1:C:289:LYS:CE	2.99	0.45
1:C:379:VAL:HG13	1:C:380:ILE:CD1	2.47	0.45
1:C:571:HIS:ND1	1:C:572:GLU:N	2.65	0.45
1:C:604:MET:HA	1:C:643:ILE:O	2.17	0.45
1:C:727:ASN:HD22	1:C:729:GLN:N	2.15	0.45
1:D:55:LEU:HD23	1:D:95:LEU:HD11	1.98	0.45
1:D:104:LEU:HB3	1:D:108:CYS:SG	2.57	0.45
1:D:191:LYS:HD2	1:D:191:LYS:HA	1.77	0.45
1:D:350:MET:SD	1:D:365:TRP:HE3	2.40	0.45
1:D:361:TRP:CZ3	1:D:409:ARG:HD2	2.51	0.45
1:D:389:VAL:HG22	1:D:437:LYS:O	2.17	0.45
1:D:455:VAL:CG1	1:D:674:SER:HB2	2.47	0.45
1:A:703:ALA:CB	1:A:807:THR:HG21	2.43	0.44
1:A:746:SER:CB	1:A:762:VAL:HG21	2.47	0.44
1:B:396:LEU:O	1:B:399:HIS:HB2	2.16	0.44
1:B:400:LEU:HD23	1:B:400:LEU:HA	1.78	0.44
1:B:538:LYS:HG3	1:B:542:LYS:HD3	1.99	0.44
1:B:739:ARG:HH11	1:B:739:ARG:CG	2.29	0.44
1:C:13:ILE:O	1:D:43:ARG:NH1	2.50	0.44
1:C:268:ASP:O	1:C:270:ASN:N	2.50	0.44
1:C:543:LEU:HD12	1:C:559:PRO:HB3	1.98	0.44
1:C:682:MET:O	1:C:684:ASN:N	2.51	0.44
1:D:192:ALA:HA	1:D:226:TYR:HA	1.98	0.44
1:D:575:ARG:HD3	1:D:666:ILE:O	2.17	0.44
1:D:746:SER:HB3	1:D:762:VAL:HG21	1.98	0.44
1:A:36:HIS:O	1:A:40:VAL:HA	2.16	0.44
1:A:244:TRP:HE1	1:A:303:THR:HG23	1.82	0.44
1:A:413:ARG:HH21	1:A:474:LEU:HD13	1.83	0.44
1:A:706:GLU:H	1:A:706:GLU:CD	2.20	0.44
1:B:40:VAL:HG12	1:B:40:VAL:O	2.17	0.44
1:B:282:ASN:C	1:B:284:ASN:N	2.66	0.44
1:B:283:ASP:OD1	1:B:383:ALA:HB1	2.17	0.44
1:B:687:LEU:CD1	1:B:709:PHE:HE1	2.30	0.44
1:C:193:ARG:HB2	1:C:225:PRO:HG2	1.99	0.44
1:C:290:GLU:HG2	1:C:294:LYS:HE2	1.98	0.44
1:C:588:ASN:ND2	1:C:744:GLN:HE22	2.10	0.44
1:D:326:PHE:HD2	1:D:329:PHE:CD2	2.35	0.44
1:D:457:ARG:HB2	1:D:698:GLU:OE1	2.17	0.44
1:A:230:VAL:HG23	1:A:230:VAL:O	2.17	0.44
1:A:320:ASP:HB3	1:A:321:PRO:HA	1.98	0.44
1:A:485:GLY:O	1:A:486:ILE:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:GLN:HA	1:B:211:GLN:NE2	2.32	0.44
1:C:19:ALA:CB	1:C:21:VAL:H	2.30	0.44
1:C:822:ARG:HD3	1:C:828:GLU:OE2	2.16	0.44
1:D:28:LYS:HD2	1:D:115:LEU:HG	2.00	0.44
1:D:63:LEU:HD23	1:D:238:VAL:HG21	1.99	0.44
1:D:122:LEU:O	1:D:125:ILE:HB	2.17	0.44
1:A:316:PHE:HZ	1:A:332:LYS:CE	2.18	0.44
1:A:566:GLN:HB2	1:A:664:GLU:HB2	2.00	0.44
1:A:626:ILE:O	1:A:630:VAL:HG13	2.17	0.44
1:A:735:ILE:H	1:A:735:ILE:HG13	1.41	0.44
1:A:796:GLU:HA	1:A:799:ARG:HB2	2.00	0.44
1:B:292:ARG:NH2	1:B:341:HIS:CD2	2.86	0.44
1:B:565:VAL:HG11	1:B:656:VAL:HG21	1.99	0.44
1:C:80:LYS:HG3	1:C:331:ASP:O	2.18	0.44
1:C:163:PHE:HE2	1:C:277:ARG:HH11	1.65	0.44
1:C:418:PHE:CE2	1:C:424:ARG:NE	2.86	0.44
1:D:14:SEP:P	1:D:15:VAL:H	2.40	0.44
1:D:231:PRO:HA	1:D:238:VAL:HA	1.99	0.44
1:D:297:TYR:CD2	1:D:396:LEU:HD11	2.52	0.44
1:D:329:PHE:HB3	1:D:330:PRO:HD3	1.98	0.44
1:D:584:ILE:HG12	1:D:750:PHE:CZ	2.52	0.44
1:A:99:MET:SD	1:A:108:CYS:SG	3.15	0.44
1:A:573:TYR:HB3	1:A:771:PHE:CE1	2.51	0.44
1:A:585:THR:OG1	1:A:741:ILE:HD13	2.17	0.44
1:A:685:GLY:CA	1:A:805:ILE:HD11	2.43	0.44
1:A:721:LEU:HG	1:A:726:TYR:HB2	1.98	0.44
1:A:733:ASP:C	1:A:739:ARG:HH12	2.20	0.44
1:B:596:LYS:NZ	1:B:597:PHE:O	2.51	0.44
1:C:836:ALA:HA	1:C:837:PRO:HD2	1.76	0.44
1:D:647:ASN:O	1:D:649:ARG:HG2	2.18	0.44
1:A:23:ASN:C	1:A:25:THR:N	2.64	0.44
1:A:69:ARG:HA	1:A:72:GLN:HG2	2.00	0.44
1:A:575:ARG:HG2	1:A:578:LEU:HD22	1.99	0.44
1:A:648:TYR:CE2	3:A:999:PLP:H2A2	2.52	0.44
1:A:810:LYS:HG3	1:A:811:PHE:CE1	2.53	0.44
1:B:280:TYR:O	1:B:281:PRO:O	2.36	0.44
1:C:71:GLN:HA	1:C:74:TYR:CD2	2.52	0.44
1:C:558:ASN:HA	1:C:559:PRO:HD3	1.85	0.44
1:D:337:LEU:HB2	1:D:373:ALA:O	2.17	0.44
1:D:589:ARG:NH2	1:D:785:GLU:OE2	2.51	0.44
1:A:403:ILE:HG22	1:A:439:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:HIS:O	1:A:478:LYS:HA	2.18	0.44
1:C:336:GLN:HG2	1:C:825:TRP:HZ2	1.82	0.44
1:D:36:HIS:CD2	1:D:42:ASP:HA	2.52	0.44
1:D:263:ILE:HG22	1:D:265:ALA:HB3	1.99	0.44
1:D:530:PHE:CE2	1:D:802:ILE:HG12	2.52	0.44
1:D:834:LEU:HA	1:D:835:PRO:HD2	1.69	0.44
1:A:67:TRP:CE3	1:A:229:PRO:HG3	2.53	0.44
1:A:90:TYR:CE1	1:A:650:VAL:HG23	2.52	0.44
1:A:403:ILE:HG21	1:A:439:ILE:HG21	2.00	0.44
1:A:442:ALA:O	1:A:446:ILE:HG13	2.18	0.44
1:A:450:HIS:O	1:A:478:LYS:HG3	2.18	0.44
1:B:320:ASP:HB3	1:B:321:PRO:HA	2.00	0.44
1:B:614:HIS:O	1:B:618:MET:HB2	2.17	0.44
1:B:636:VAL:O	1:B:639:ARG:HD3	2.17	0.44
1:C:19:ALA:HB3	1:C:21:VAL:HG22	1.99	0.44
1:C:461:GLU:HG3	1:C:465:LYS:NZ	2.33	0.44
1:C:571:HIS:CG	1:C:613:TYR:HH	2.35	0.44
1:D:502:ILE:CG2	1:D:506:ARG:NH2	2.69	0.44
1:D:626:ILE:CG2	1:D:642:VAL:HG11	2.47	0.44
1:A:102:LEU:HB3	1:A:104:LEU:CD2	2.48	0.44
1:A:555:VAL:CG2	1:A:643:ILE:HD11	2.29	0.44
1:C:18:LEU:O	1:D:33:ARG:NH1	2.50	0.44
1:C:230:VAL:HA	1:C:231:PRO:HD2	1.80	0.44
1:C:348:GLU:OE1	1:C:399:HIS:CE1	2.71	0.44
1:C:591:LYS:HD2	1:C:591:LYS:HA	1.82	0.44
1:D:211:GLN:HE21	1:D:211:GLN:HA	1.83	0.44
1:A:82:ILE:HG13	1:A:825:TRP:CD2	2.53	0.43
1:A:172:GLY:O	1:A:621:LYS:NZ	2.47	0.43
1:A:555:VAL:CG2	1:A:557:ILE:HD11	2.48	0.43
1:A:756:ASP:N	1:A:756:ASP:CB	2.70	0.43
1:B:197:THR:HG23	1:B:224:MET:CB	2.48	0.43
1:B:337:LEU:HD11	1:B:345:ALA:HB3	1.99	0.43
1:C:246:ALA:HB3	1:C:276:SER:OG	2.18	0.43
1:C:290:GLU:O	1:C:294:LYS:HB2	2.17	0.43
1:C:577:LEU:HD11	1:C:619:ILE:HD11	1.99	0.43
1:C:699:MET:HB3	1:C:708:PHE:CE2	2.49	0.43
1:D:280:TYR:N	1:D:281:PRO:CD	2.78	0.43
1:D:390:HIS:ND1	1:D:391:LEU:HD12	2.32	0.43
1:D:590:ILE:HG22	1:D:590:ILE:O	2.18	0.43
1:D:619:ILE:O	1:D:623:ILE:HG13	2.18	0.43
1:A:515:LEU:HD12	1:A:515:LEU:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ILE:HG21	1:A:620:ILE:HG13	2.01	0.43
1:B:53:PHE:CE1	1:B:188:PRO:HD3	2.53	0.43
1:B:338:ASN:OD1	1:B:377:HIS:HE1	2.01	0.43
1:B:339:ASP:HB2	1:B:377:HIS:CE1	2.53	0.43
1:B:407:ASN:HB2	1:B:430:LEU:HG	2.00	0.43
1:C:375:THR:HG23	1:C:453:ASN:HD21	1.83	0.43
1:D:387:TRP:O	1:D:438:ARG:HB3	2.18	0.43
1:A:689:ILE:HD12	1:A:784:GLN:HE21	1.83	0.43
1:B:296:GLU:HA	1:B:299:VAL:HG12	1.99	0.43
1:B:455:VAL:HG12	1:B:674:SER:CB	2.45	0.43
1:B:655:LYS:O	1:B:658:PRO:HD2	2.18	0.43
1:D:490:ARG:HA	1:D:494:LEU:HG	2.00	0.43
1:D:498:GLY:O	1:D:500:ALA:N	2.52	0.43
1:D:521:LEU:HA	1:D:524:TYR:CD1	2.53	0.43
1:D:758:PHE:HD1	1:D:761:ILE:CD1	2.26	0.43
1:D:810:LYS:O	1:D:815:ARG:NE	2.47	0.43
1:A:164:GLY:O	1:A:279:LEU:HB2	2.19	0.43
1:A:480:GLN:HE22	1:A:823:GLU:HB3	1.84	0.43
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.59	0.43
1:A:733:ASP:HA	1:A:739:ARG:HH12	1.83	0.43
1:B:263:ILE:CG2	1:B:266:VAL:HG23	2.48	0.43
1:B:421:ASP:OD2	1:B:424:ARG:HB2	2.19	0.43
1:B:590:ILE:HG22	1:B:590:ILE:O	2.19	0.43
1:C:203:TYR:O	1:C:215:TRP:NE1	2.51	0.43
1:C:746:SER:HB3	1:C:762:VAL:HG11	2.01	0.43
1:D:80:LYS:O	1:D:153:ALA:HB3	2.18	0.43
1:A:24:VAL:HG11	1:A:114:GLN:HE22	1.84	0.43
1:A:445:CYS:O	1:A:449:SER:HB2	2.18	0.43
1:A:509:GLU:HG2	1:A:512:ILE:HD12	1.98	0.43
1:A:633:ASP:HA	1:A:634:PRO:HD3	1.79	0.43
1:B:161:TYR:CE1	1:B:279:LEU:HA	2.53	0.43
1:C:71:GLN:HA	1:C:74:TYR:HD2	1.83	0.43
1:C:138:ARG:NH2	1:C:141:ALA:HB3	2.34	0.43
1:C:159:ILE:HD13	1:C:159:ILE:HG21	1.80	0.43
1:C:252:PHE:HZ	1:C:269:ARG:HB3	1.79	0.43
1:C:386:ARG:HG2	1:C:440:ASN:HA	2.00	0.43
1:D:272:ALA:O	1:D:274:ASN:N	2.52	0.43
1:D:589:ARG:O	1:D:592:LYS:N	2.51	0.43
1:D:665:GLN:HB3	1:D:696:ASN:HD21	1.83	0.43
1:A:93:ARG:HG2	1:A:126:GLU:HG2	2.00	0.43
1:A:338:ASN:OD1	1:A:377:HIS:CE1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:CD	1:B:29:LYS:HZ1	2.21	0.43
1:B:434:GLY:HA2	1:C:754:GLN:HE22	1.84	0.43
1:B:703:ALA:CB	1:B:807:THR:HG21	2.48	0.43
1:C:13:ILE:HD11	1:D:115:LEU:HB3	1.99	0.43
1:C:198:LEU:HD13	1:C:305:GLN:HB3	2.01	0.43
1:D:70:THR:HG21	1:D:238:VAL:O	2.19	0.43
1:D:464:LYS:HD2	1:D:472:TYR:CZ	2.54	0.43
1:D:587:TYR:CD1	1:D:630:VAL:HG12	2.53	0.43
1:D:588:ASN:HD21	1:D:744:GLN:HE22	1.67	0.43
1:D:689:ILE:HD12	1:D:784:GLN:HE21	1.83	0.43
1:A:131:LEU:HD21	1:A:243:LEU:HD21	2.00	0.43
1:A:322:VAL:HG13	1:A:325:ASN:HB3	2.01	0.43
1:A:355:ASP:OD1	1:A:398:ARG:NH1	2.51	0.43
1:A:449:SER:O	1:A:478:LYS:HE2	2.18	0.43
1:A:575:ARG:HG2	1:A:578:LEU:HB2	2.01	0.43
1:A:591:LYS:HA	1:A:591:LYS:HD2	1.78	0.43
1:B:26:GLU:O	1:B:29:LYS:HB3	2.19	0.43
1:B:692:MET:SD	1:B:697:VAL:HG22	2.57	0.43
1:B:734:ARG:O	1:B:736:PRO:HD3	2.18	0.43
1:B:792:LYS:O	1:B:794:PRO:HD3	2.18	0.43
1:C:133:ASN:HB2	1:C:165:ILE:HG21	1.99	0.43
1:C:270:ASN:HD21	1:D:269:ARG:HD3	1.84	0.43
1:C:322:VAL:HG13	1:C:325:ASN:CB	2.48	0.43
1:D:21:VAL:CG1	1:D:22:GLU:N	2.59	0.43
1:A:662:LEU:HD21	1:A:689:ILE:HB	2.01	0.43
1:A:733:ASP:HA	1:A:739:ARG:NH1	2.33	0.43
1:B:735:ILE:HA	1:B:736:PRO:HD2	1.90	0.43
1:C:60:ARG:O	1:C:64:VAL:HG22	2.19	0.43
1:C:88:GLU:CG	1:C:132:GLY:HA2	2.49	0.43
1:D:203:TYR:CE1	1:D:395:LEU:HD12	2.54	0.43
1:A:63:LEU:HD12	1:A:98:THR:HG21	1.99	0.43
1:A:354:VAL:HG21	1:A:361:TRP:CD1	2.53	0.43
1:B:485:GLY:HA3	1:B:813:SER:HA	2.01	0.43
1:B:518:LEU:HD12	1:B:518:LEU:HA	1.82	0.43
1:B:587:TYR:CD1	1:B:636:VAL:HG21	2.54	0.43
1:B:698:GLU:HA	1:B:701:GLU:HG2	2.00	0.43
1:C:263:ILE:HG22	1:C:265:ALA:HB3	2.01	0.43
1:C:480:GLN:NE2	1:C:823:GLU:HB3	2.30	0.43
1:D:583:VAL:CG2	1:D:603:VAL:HG21	2.48	0.43
1:B:375:THR:HG22	1:B:377:HIS:CE1	2.53	0.43
1:C:203:TYR:O	1:C:215:TRP:HZ2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:PRO:HA	1:C:500:ALA:HB3	2.01	0.43
1:D:352:VAL:O	1:D:356:LEU:HB2	2.18	0.43
1:D:407:ASN:HB2	1:D:430:LEU:HD12	2.00	0.43
1:A:21:VAL:O	1:A:22:GLU:CG	2.67	0.42
1:A:417:ALA:O	1:A:419:PRO:HD3	2.19	0.42
1:B:80:LYS:O	1:B:153:ALA:HB3	2.19	0.42
1:C:133:ASN:OD1	1:C:165:ILE:HD12	2.19	0.42
1:D:22:GLU:OE1	1:D:107:ALA:HB2	2.19	0.42
1:D:168:GLN:O	1:D:647:ASN:HB2	2.19	0.42
1:D:570:ILE:HD13	1:D:620:ILE:HG12	2.00	0.42
1:A:118:ASP:O	1:A:121:GLU:HB3	2.20	0.42
1:B:138:ARG:NH2	1:B:142:CYS:SG	2.92	0.42
1:B:304:LEU:O	1:B:308:ILE:HG13	2.19	0.42
1:B:315:LYS:O	1:B:318:CYS:HB2	2.19	0.42
1:B:338:ASN:OD1	1:B:377:HIS:CE1	2.72	0.42
1:B:361:TRP:CZ3	1:B:409:ARG:HD3	2.54	0.42
1:B:663:SER:HB2	1:B:681:PHE:CD2	2.54	0.42
1:C:396:LEU:HG	1:C:399:HIS:CD2	2.53	0.42
1:C:627:GLY:O	1:C:629:VAL:N	2.52	0.42
1:C:810:LYS:HB3	1:C:811:PHE:CE1	2.54	0.42
1:D:297:TYR:CE1	1:D:399:HIS:CE1	3.07	0.42
1:D:735:ILE:H	1:D:735:ILE:CD1	2.31	0.42
1:A:18:LEU:CB	1:B:37:PHE:CZ	3.03	0.42
1:A:165:ILE:HD12	1:A:166:PHE:HD1	1.82	0.42
1:A:225:PRO:HD3	1:A:244:TRP:HZ3	1.84	0.42
1:B:458:ILE:HD11	1:B:694:GLY:H	1.83	0.42
1:C:407:ASN:OD1	1:C:430:LEU:HG	2.20	0.42
1:D:563:PHE:CD2	1:D:659:ALA:O	2.70	0.42
1:A:90:TYR:HB3	1:A:138:ARG:HA	2.02	0.42
1:A:582:HIS:NE2	1:A:784:GLN:OE1	2.52	0.42
1:B:66:ARG:HB3	1:B:236:ASN:O	2.20	0.42
1:B:157:TYR:HA	1:B:242:ARG:O	2.19	0.42
1:B:515:LEU:HG	1:B:518:LEU:HD22	2.02	0.42
1:B:557:ILE:HD12	1:B:557:ILE:HA	1.79	0.42
1:C:515:LEU:HD22	1:C:812:SER:HB2	2.02	0.42
1:D:146:SER:OG	1:D:813:SER:HB2	2.19	0.42
1:A:193:ARG:HB2	1:A:225:PRO:HG2	2.02	0.42
1:A:208:HIS:CE1	1:A:213:ALA:HB2	2.54	0.42
1:B:225:PRO:HB3	1:B:244:TRP:CE3	2.54	0.42
1:B:782:LYS:O	1:B:785:GLU:N	2.53	0.42
1:C:206:VAL:HG12	1:C:208:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PRO:HD3	1:C:244:TRP:CZ3	2.54	0.42
1:C:310:ARG:HH11	1:C:310:ARG:HD2	1.69	0.42
1:C:457:ARG:O	1:C:461:GLU:HB2	2.19	0.42
1:D:492:LEU:HG	1:D:683:LEU:HD22	2.01	0.42
1:D:792:LYS:HE2	1:D:792:LYS:HB2	1.76	0.42
1:A:165:ILE:HB	1:A:279:LEU:HD13	2.00	0.42
1:B:202:PHE:CE1	1:B:297:TYR:HD2	2.36	0.42
1:B:635:VAL:O	1:B:639:ARG:NH1	2.52	0.42
1:C:66:ARG:NH1	1:C:236:ASN:OD1	2.50	0.42
1:C:344:LEU:HD23	1:C:344:LEU:HA	1.86	0.42
1:C:492:LEU:CG	1:C:683:LEU:HD22	2.48	0.42
1:C:582:HIS:CD2	1:C:781:VAL:HG22	2.54	0.42
1:D:349:LEU:HD23	1:D:368:THR:HG23	2.01	0.42
1:B:10:ARG:N	1:B:13:ILE:HB	2.34	0.42
1:B:17:GLY:H	1:B:18:LEU:CD2	2.29	0.42
1:B:206:VAL:CG2	1:B:398:ARG:HD2	2.50	0.42
1:B:395:LEU:HA	1:B:395:LEU:HD12	1.84	0.42
1:B:589:ARG:O	1:B:591:LYS:N	2.52	0.42
1:B:790:LEU:HG	1:B:797:TRP:CD1	2.55	0.42
1:C:295:GLN:O	1:C:298:PHE:HB3	2.20	0.42
1:D:100:VAL:HG23	1:D:101:ASN:N	2.34	0.42
1:B:138:ARG:HH21	1:B:141:ALA:HB3	1.85	0.42
1:B:139:LEU:HA	1:B:139:LEU:HD12	1.74	0.42
1:C:304:LEU:CD2	1:C:349:LEU:HB2	2.50	0.42
1:C:316:PHE:HA	1:C:319:ARG:CB	2.46	0.42
1:C:322:VAL:HG13	1:C:325:ASN:HB3	2.01	0.42
1:C:464:LYS:HB2	1:C:464:LYS:HE3	1.64	0.42
1:D:99:MET:O	1:D:103:ALA:N	2.52	0.42
1:D:536:LYS:HE2	1:D:536:LYS:HB2	1.85	0.42
1:D:567:VAL:HB	1:D:648:TYR:CZ	2.55	0.42
1:A:365:TRP:O	1:A:369:VAL:HG12	2.20	0.42
1:A:385:GLU:HB3	1:A:441:MET:HB2	2.02	0.42
1:A:528:GLU:OE1	1:A:532:ARG:NH2	2.53	0.42
1:C:242:ARG:NH2	2:C:902:SO4:O1	2.50	0.42
1:A:781:VAL:O	1:A:785:GLU:HG3	2.20	0.42
1:B:138:ARG:HH11	1:B:491:TRP:HE1	1.64	0.42
1:B:433:GLU:OE2	1:B:437:LYS:NZ	2.53	0.42
1:C:117:LEU:HA	1:C:117:LEU:HD23	1.75	0.42
1:C:149:THR:HG21	1:C:489:ARG:NH2	2.35	0.42
1:C:707:ASN:HA	1:C:800:MET:SD	2.59	0.42
1:C:781:VAL:O	1:C:785:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:792:LYS:C	1:C:794:PRO:HD3	2.40	0.42
1:D:206:VAL:HG11	1:D:401:GLN:HE22	1.85	0.42
1:D:515:LEU:CD2	1:D:683:LEU:HD11	2.50	0.42
1:D:566:GLN:O	1:D:605:ILE:HA	2.20	0.42
1:D:682:MET:SD	1:D:699:MET:HG2	2.60	0.42
1:D:778:GLU:HB3	1:D:782:LYS:HZ2	1.84	0.42
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.83	0.41
1:A:157:TYR:CE2	1:A:303:THR:CG2	2.89	0.41
1:A:521:LEU:HD12	1:A:521:LEU:HA	1.61	0.41
1:A:594:PRO:O	1:A:639:ARG:NH2	2.51	0.41
1:A:699:MET:HB2	1:A:699:MET:HE3	1.76	0.41
1:B:554:LYS:HD2	1:B:554:LYS:C	2.40	0.41
1:C:133:ASN:OD1	1:C:165:ILE:HG23	2.19	0.41
1:C:282:ASN:C	1:C:284:ASN:N	2.65	0.41
1:D:374:TYR:CG	1:D:445:CYS:HB3	2.54	0.41
1:D:530:PHE:HB3	1:D:531:ILE:HG13	2.02	0.41
1:D:614:HIS:HE1	1:D:760:ASP:OD2	2.02	0.41
1:D:703:ALA:HA	1:D:807:THR:HG21	2.02	0.41
1:D:707:ASN:CA	1:D:800:MET:SD	3.02	0.41
1:A:32:ASN:HD21	1:B:13:ILE:HG12	1.85	0.41
1:A:413:ARG:NH2	1:A:474:LEU:O	2.53	0.41
1:B:182:TRP:CE2	1:B:183:LEU:HG	2.55	0.41
1:B:338:ASN:O	1:B:339:ASP:HB3	2.20	0.41
1:B:388:PRO:HA	1:B:438:ARG:HG2	2.02	0.41
1:B:564:ASP:HB2	1:B:603:VAL:HA	2.01	0.41
1:B:565:VAL:HG11	1:B:656:VAL:CG2	2.50	0.41
1:B:715:VAL:O	1:B:718:VAL:HG12	2.20	0.41
1:B:778:GLU:HB3	1:B:782:LYS:NZ	2.35	0.41
1:C:81:ARG:HD3	1:C:155:TYR:CE1	2.55	0.41
1:C:304:LEU:N	1:C:304:LEU:HD12	2.35	0.41
1:C:549:LEU:HD23	1:C:557:ILE:HG12	2.02	0.41
1:C:690:GLY:O	1:C:710:ILE:HA	2.20	0.41
1:D:284:ASN:CG	1:D:285:PHE:N	2.70	0.41
1:D:689:ILE:HG23	1:D:689:ILE:O	2.19	0.41
1:A:47:THR:OG1	1:A:50:ASP:OD2	2.38	0.41
1:A:84:TYR:N	1:A:155:TYR:O	2.52	0.41
1:A:575:ARG:O	1:A:577:LEU:N	2.53	0.41
1:B:402:ILE:CG2	1:B:406:ILE:HD11	2.42	0.41
1:B:580:CYS:O	1:B:584:ILE:HG13	2.20	0.41
1:C:591:LYS:HZ2	1:C:633:ASP:CG	2.20	0.41
1:C:790:LEU:HD21	1:C:800:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:ILE:HG21	1:D:620:ILE:HG13	2.01	0.41
1:A:80:LYS:NZ	1:A:330:PRO:O	2.50	0.41
1:A:532:ARG:HE	1:A:532:ARG:HB3	1.58	0.41
1:A:670:GLY:H	1:A:693:ASP:CG	2.24	0.41
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.79	0.41
1:D:565:VAL:HG22	1:D:660:ALA:HB1	2.02	0.41
1:D:761:ILE:O	1:D:765:LEU:HD22	2.20	0.41
1:A:294:LYS:HE3	1:A:294:LYS:HB2	1.88	0.41
1:A:555:VAL:CG2	1:A:557:ILE:CD1	2.99	0.41
1:A:674:SER:OG	1:A:675:GLY:N	2.54	0.41
1:B:233:TYR:OH	1:B:234:ARG:NH1	2.54	0.41
1:B:385:GLU:O	1:B:441:MET:HB2	2.20	0.41
1:C:519:ARG:HA	1:C:806:ALA:O	2.21	0.41
1:C:522:LEU:HD13	1:C:522:LEU:HA	1.80	0.41
1:D:564:ASP:HB3	1:D:603:VAL:HA	2.01	0.41
1:A:356:LEU:HD22	1:A:356:LEU:N	2.35	0.41
1:A:588:ASN:HD21	1:A:744:GLN:NE2	2.19	0.41
1:B:190:GLU:HA	1:B:227:ASP:O	2.19	0.41
1:B:795:ARG:O	1:B:799:ARG:HG3	2.21	0.41
1:C:31:PHE:O	1:C:31:PHE:CD1	2.74	0.41
1:C:502:ILE:HG13	1:C:503:ILE:N	2.35	0.41
1:D:661:ASP:CB	1:D:797:TRP:HH2	2.26	0.41
1:A:262:TYR:OH	1:D:263:ILE:HD11	2.20	0.41
1:A:293:LEU:HD21	1:A:392:LEU:HD12	2.02	0.41
1:B:13:ILE:HD13	1:B:13:ILE:HG21	1.89	0.41
1:B:329:PHE:HB3	1:B:330:PRO:HD3	2.03	0.41
1:B:520:LYS:O	1:B:522:LEU:N	2.54	0.41
1:C:530:PHE:O	1:C:533:ASP:N	2.54	0.41
1:C:678:ASN:HD22	1:C:695:ALA:HB3	1.85	0.41
1:D:388:PRO:HD2	1:D:391:LEU:HB2	2.02	0.41
1:D:549:LEU:CB	1:D:557:ILE:HG12	2.50	0.41
1:D:790:LEU:C	1:D:797:TRP:HD1	2.24	0.41
1:A:115:LEU:HD22	1:B:13:ILE:HG12	2.02	0.41
1:B:379:VAL:HG22	1:B:462:ILE:HD11	2.03	0.41
1:A:74:TYR:HE1	1:A:153:ALA:HB2	1.86	0.41
1:A:268:ASP:O	1:A:270:ASN:N	2.53	0.41
1:A:318:CYS:C	1:A:320:ASP:H	2.24	0.41
1:A:755:PRO:C	1:A:756:ASP:CA	2.72	0.41
1:A:822:ARG:HH11	1:A:822:ARG:HG2	1.86	0.41
1:B:322:VAL:O	1:B:323:ARG:HG2	2.21	0.41
1:B:381:PRO:HG3	1:B:467:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:LEU:O	1:B:395:LEU:N	2.54	0.41
1:B:402:ILE:C	1:B:406:ILE:HG13	2.30	0.41
1:B:633:ASP:HA	1:B:634:PRO:HD3	1.88	0.41
1:C:110:GLU:O	1:C:113:TYR:HB3	2.20	0.41
1:C:381:PRO:O	1:C:384:LEU:HB2	2.20	0.41
1:C:557:ILE:HD11	1:C:643:ILE:HD11	2.02	0.41
1:D:578:LEU:HB3	1:D:666:ILE:HD12	2.02	0.41
1:D:633:ASP:HA	1:D:634:PRO:HD3	1.82	0.41
1:A:32:ASN:HD22	1:B:13:ILE:HG23	1.86	0.41
1:A:63:LEU:HD21	1:A:229:PRO:HB2	2.03	0.41
1:A:74:TYR:CE1	1:A:153:ALA:HB2	2.55	0.41
1:B:182:TRP:CD1	1:B:182:TRP:N	2.88	0.41
1:C:166:PHE:CD2	1:C:177:GLU:HB3	2.55	0.41
1:C:587:TYR:CZ	1:C:591:LYS:HG3	2.56	0.41
1:C:834:LEU:HD23	1:C:835:PRO:HD2	2.03	0.41
1:D:82:ILE:HD11	1:D:147:MET:SD	2.61	0.41
1:D:279:LEU:CD2	1:D:280:TYR:N	2.84	0.41
1:A:35:LEU:HD12	1:A:35:LEU:HA	1.85	0.40
1:A:49:ARG:HH11	1:A:125:ILE:HG22	1.85	0.40
1:A:492:LEU:HD12	1:A:683:LEU:HD21	2.03	0.40
1:A:698:GLU:HA	1:A:701:GLU:CG	2.47	0.40
1:B:674:SER:OG	1:B:675:GLY:N	2.54	0.40
1:B:810:LYS:O	1:B:815:ARG:NH2	2.50	0.40
1:C:402:ILE:HG21	1:C:402:ILE:HD13	1.90	0.40
1:D:505:GLU:HB2	1:D:506:ARG:HE	1.86	0.40
1:D:542:LYS:HE3	1:D:563:PHE:CD2	2.56	0.40
1:D:699:MET:HB3	1:D:708:PHE:CZ	2.56	0.40
1:D:706:GLU:CD	1:D:706:GLU:H	2.24	0.40
1:B:155:TYR:N	1:B:155:TYR:CD1	2.89	0.40
1:B:751:SER:HB3	1:B:758:PHE:HE2	1.86	0.40
1:C:143:PHE:HB3	1:C:147:MET:CE	2.50	0.40
1:C:150:LEU:H	1:C:150:LEU:HG	1.58	0.40
1:D:159:ILE:HG22	1:D:160:ARG:N	2.36	0.40
1:D:165:ILE:HG12	1:D:279:LEU:HB3	2.02	0.40
1:D:455:VAL:HG13	1:D:674:SER:HB2	2.03	0.40
1:D:531:ILE:HG21	1:D:795:ARG:HG3	2.04	0.40
1:D:835:PRO:HB2	1:D:836:ALA:H	1.70	0.40
1:A:818:ALA:O	1:A:822:ARG:HG3	2.21	0.40
1:B:26:GLU:OE1	1:B:29:LYS:NZ	2.54	0.40
1:B:162:GLU:HB2	1:B:277:ARG:HA	2.03	0.40
1:B:248:ALA:HB2	1:B:269:ARG:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:LYS:O	1:B:472:TYR:HB3	2.21	0.40
1:B:521:LEU:HD11	1:B:530:PHE:CZ	2.56	0.40
1:B:530:PHE:CE2	1:B:534:VAL:CG2	3.04	0.40
1:B:539:GLN:O	1:B:543:LEU:HD13	2.22	0.40
1:B:581:LEU:HD13	1:B:738:LEU:CD1	2.50	0.40
1:B:590:ILE:HG12	1:B:598:VAL:HG21	2.02	0.40
1:B:665:GLN:NE2	1:B:678:ASN:OD1	2.54	0.40
1:B:713:MET:HG2	1:B:717:ASP:OD2	2.22	0.40
1:B:714:ARG:HH11	1:B:714:ARG:CG	2.34	0.40
1:B:792:LYS:HE2	1:B:792:LYS:HB2	1.74	0.40
1:C:822:ARG:HD3	1:C:822:ARG:HH11	1.75	0.40
1:D:236:ASN:HB2	1:D:834:LEU:O	2.20	0.40
1:D:631:ASN:HD21	1:D:642:VAL:N	2.17	0.40
1:D:692:MET:SD	1:D:710:ILE:HG21	2.60	0.40
1:D:697:VAL:H	1:D:697:VAL:HG23	1.37	0.40
1:D:778:GLU:HB3	1:D:782:LYS:HZ3	1.84	0.40
1:A:187:ASN:HA	1:A:188:PRO:HD2	1.99	0.40
1:A:365:TRP:CE3	1:A:365:TRP:HA	2.56	0.40
1:A:413:ARG:HH21	1:A:475:GLU:HG3	1.83	0.40
1:A:729:GLN:HA	1:A:732:TYR:HB3	2.03	0.40
1:B:272:ALA:HA	1:B:275:ILE:HG13	2.04	0.40
1:B:515:LEU:HD21	1:B:683:LEU:HD11	2.03	0.40
1:C:88:GLU:HG3	1:C:132:GLY:HA2	2.03	0.40
1:C:598:VAL:O	1:C:600:PRO:HD3	2.22	0.40
1:C:766:MET:HE3	1:C:774:PHE:HE2	1.87	0.40
1:C:766:MET:HA	1:C:766:MET:CE	2.49	0.40
1:C:782:LYS:HA	1:C:782:LYS:HZ2	1.87	0.40
1:D:231:PRO:HA	1:D:238:VAL:HG22	2.03	0.40
1:D:359:LEU:HD12	1:D:364:ALA:HB2	2.04	0.40
1:D:662:LEU:HA	1:D:687:LEU:O	2.21	0.40
1:A:733:ASP:OD1	1:A:733:ASP:N	2.54	0.40
1:B:198:LEU:HA	1:B:199:PRO:HD2	1.96	0.40
1:B:290:GLU:O	1:B:294:LYS:HD3	2.22	0.40
1:B:426:ARG:NH2	1:C:756:ASP:OD2	2.54	0.40
1:B:536:LYS:O	1:B:540:GLU:HB2	2.20	0.40
1:B:575:ARG:NH2	1:B:776:ASP:OD2	2.53	0.40
1:D:94:THR:H	1:D:126:GLU:CD	2.25	0.40
1:D:112:THR:CA	1:D:115:LEU:HD12	2.40	0.40
1:D:136:LEU:HD11	1:D:338:ASN:ND2	2.37	0.40
1:D:214:LYS:HB3	1:D:216:VAL:HG13	2.04	0.40
1:D:233:TYR:OH	1:D:234:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:620:ILE:O	1:D:624:THR:HG23	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:O	1:D:370:LYS:NZ[2_646]	1.97	0.23

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	825/842 (98%)	656 (80%)	130 (16%)	39 (5%)	2 8
1	B	822/842 (98%)	674 (82%)	105 (13%)	43 (5%)	2 6
1	C	825/842 (98%)	673 (82%)	100 (12%)	52 (6%)	1 4
1	D	825/842 (98%)	635 (77%)	133 (16%)	57 (7%)	1 3
All	All	3297/3368 (98%)	2638 (80%)	468 (14%)	191 (6%)	1 5

All (191) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	166	PHE
1	A	252	PHE
1	A	256	ASP
1	A	265	ALA
1	A	281	PRO
1	A	282	ASN
1	A	283	ASP
1	A	284	ASN

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Mol	Chain	Res	Type
1	A	358	ARG
1	A	553	TYR
1	A	555	VAL
1	A	610	ALA
1	A	730	GLU
1	B	13	ILE
1	B	16	ARG
1	B	166	PHE
1	B	234	ARG
1	B	252	PHE
1	B	265	ALA
1	B	281	PRO
1	B	282	ASN
1	B	283	ASP
1	B	284	ASN
1	B	315	LYS
1	B	436	VAL
1	B	553	TYR
1	B	555	VAL
1	B	590	ILE
1	B	599	VAL
1	B	610	ALA
1	B	637	GLY
1	B	808	SER
1	B	835	PRO
1	B	837	PRO
1	C	16	ARG
1	C	166	PHE
1	C	234	ARG
1	C	281	PRO
1	C	282	ASN
1	C	283	ASP
1	C	284	ASN
1	C	285	PHE
1	C	315	LYS
1	C	555	VAL
1	C	575	ARG
1	C	599	VAL
1	C	610	ALA
1	C	683	LEU
1	C	752	PRO
1	C	836	ALA

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Mol	Chain	Res	Type
1	D	22	GLU
1	D	78	ASP
1	D	281	PRO
1	D	284	ASN
1	D	337	LEU
1	D	358	ARG
1	D	467	ILE
1	D	555	VAL
1	D	610	ALA
1	D	674	SER
1	D	697	VAL
1	D	730	GLU
1	D	751	SER
1	D	835	PRO
1	A	130	GLY
1	A	149	THR
1	A	285	PHE
1	A	288	GLY
1	A	508	GLY
1	A	576	GLN
1	A	769	ASP
1	A	836	ALA
1	B	129	ALA
1	B	272	ALA
1	B	285	PHE
1	B	288	GLY
1	B	510	GLU
1	B	572	GLU
1	B	655	LYS
1	B	730	GLU
1	B	836	ALA
1	C	27	LEU
1	C	324	THR
1	C	506	ARG
1	C	508	GLY
1	C	511	TYR
1	C	531	ILE
1	C	576	GLN
1	C	674	SER
1	C	682	MET
1	C	730	GLU
1	C	809	GLY

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Mol	Chain	Res	Type
1	D	130	GLY
1	D	234	ARG
1	D	273	GLU
1	D	285	PHE
1	D	288	GLY
1	D	313	SER
1	D	314	SER
1	D	315	LYS
1	D	429	SER
1	D	477	HIS
1	D	508	GLY
1	D	509	GLU
1	D	510	GLU
1	D	525	VAL
1	D	599	VAL
1	D	683	LEU
1	D	694	GLY
1	D	725	GLY
1	D	808	SER
1	A	21	VAL
1	A	147	MET
1	A	203	TYR
1	A	755	PRO
1	A	835	PRO
1	B	515	LEU
1	B	656	VAL
1	B	756	ASP
1	C	151	GLY
1	C	269	ARG
1	C	357	GLU
1	C	530	PHE
1	D	17	GLY
1	D	319	ARG
1	D	323	ARG
1	D	499	LEU
1	D	515	LEU
1	D	836	ALA
1	A	78	ASP
1	A	184	ARG
1	A	464	LYS
1	A	492	LEU
1	A	734	ARG

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Mol	Chain	Res	Type
1	C	384	LEU
1	C	510	GLU
1	C	637	GLY
1	C	755	PRO
1	C	758	PHE
1	D	21	VAL
1	D	85	LEU
1	D	166	PHE
1	D	254	LEU
1	D	260	GLY
1	D	466	THR
1	D	629	VAL
1	D	789	ALA
1	A	287	GLU
1	A	320	ASP
1	B	280	TYR
1	B	678	ASN
1	B	729	GLN
1	C	21	VAL
1	C	339	ASP
1	C	694	GLY
1	D	253	ASN
1	D	269	ARG
1	D	282	ASN
1	D	287	GLU
1	D	457	ARG
1	D	723	GLN
1	D	734	ARG
1	A	467	ILE
1	B	358	ARG
1	B	755	PRO
1	C	165	ILE
1	C	280	TYR
1	C	287	GLU
1	C	629	VAL
1	C	735	ILE
1	C	829	PRO
1	D	339	ASP
1	D	755	PRO
1	A	280	TYR
1	B	629	VAL
1	B	773	VAL

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Mol	Chain	Res	Type
1	C	40	VAL
1	A	151	GLY
1	B	130	GLY
1	B	805	ILE
1	C	507	ILE
1	C	537	VAL
1	C	835	PRO
1	D	186	GLY
1	A	193	ARG
1	C	288	GLY
1	C	666	ILE
1	A	40	VAL
1	B	525	VAL
1	C	229	PRO

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	714/730 (98%)	585 (82%)	129 (18%)	1 5
1	B	715/730 (98%)	600 (84%)	115 (16%)	2 7
1	C	714/730 (98%)	574 (80%)	140 (20%)	1 4
1	D	714/730 (98%)	563 (79%)	151 (21%)	1 3
All	All	2857/2920 (98%)	2322 (81%)	535 (19%)	1 5

All (535) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	13	ILE
1	A	15	VAL
1	A	18	LEU
1	A	29	LYS
1	A	31	PHE
1	A	42	ASP

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Mol	Chain	Res	Type
1	A	47	THR
1	A	75	TYR
1	A	80	LYS
1	A	82	ILE
1	A	85	LEU
1	A	87	LEU
1	A	90	TYR
1	A	91	MET
1	A	95	LEU
1	A	102	LEU
1	A	112	THR
1	A	125	ILE
1	A	142	CYS
1	A	162	GLU
1	A	165	ILE
1	A	176	MET
1	A	177	GLU
1	A	187	ASN
1	A	209	THR
1	A	211	GLN
1	A	219	GLN
1	A	220	VAL
1	A	224	MET
1	A	242	ARG
1	A	250	ASN
1	A	251	ASP
1	A	253	ASN
1	A	254	LEU
1	A	263	ILE
1	A	269	ARG
1	A	274	ASN
1	A	280	TYR
1	A	281	PRO
1	A	284	ASN
1	A	286	PHE
1	A	290	GLU
1	A	294	LYS
1	A	303	THR
1	A	314	SER
1	A	316	PHE
1	A	318	CYS
1	A	319	ARG

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Mol	Chain	Res	Type
1	A	323	ARG
1	A	332	LYS
1	A	339	ASP
1	A	358	ARG
1	A	360	ASP
1	A	362	ASP
1	A	365	TRP
1	A	366	GLU
1	A	374	TYR
1	A	377	HIS
1	A	385	GLU
1	A	395	LEU
1	A	396	LEU
1	A	398	ARG
1	A	400	LEU
1	A	412	ASN
1	A	426	ARG
1	A	430	LEU
1	A	449	SER
1	A	450	HIS
1	A	455	VAL
1	A	458	ILE
1	A	462	ILE
1	A	470	ASP
1	A	474	LEU
1	A	484	ASN
1	A	489	ARG
1	A	492	LEU
1	A	494	LEU
1	A	509	GLU
1	A	523	SER
1	A	536	LYS
1	A	540	GLU
1	A	550	GLU
1	A	554	LYS
1	A	555	VAL
1	A	557	ILE
1	A	558	ASN
1	A	559	PRO
1	A	567	VAL
1	A	575	ARG
1	A	576	GLN

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Mol	Chain	Res	Type
1	A	582	HIS
1	A	613	TYR
1	A	622	LEU
1	A	629	VAL
1	A	636	VAL
1	A	638	ASP
1	A	649	ARG
1	A	652	LEU
1	A	655	LYS
1	A	662	LEU
1	A	674	SER
1	A	683	LEU
1	A	701	GLU
1	A	708	PHE
1	A	713	MET
1	A	714	ARG
1	A	716	GLU
1	A	717	ASP
1	A	718	VAL
1	A	720	ARG
1	A	727	ASN
1	A	738	LEU
1	A	740	GLN
1	A	743	GLU
1	A	753	LYS
1	A	755	PRO
1	A	756	ASP
1	A	764	MET
1	A	765	LEU
1	A	766	MET
1	A	790	LEU
1	A	807	THR
1	A	808	SER
1	A	810	LYS
1	A	813	SER
1	A	827	VAL
1	A	828	GLU
1	A	833	ARG
1	B	10	ARG
1	B	12	GLN
1	B	15	VAL
1	B	18	LEU

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Mol	Chain	Res	Type
1	B	22	GLU
1	B	23	ASN
1	B	47	THR
1	B	66	ARG
1	B	76	GLU
1	B	82	ILE
1	B	95	LEU
1	B	108	CYS
1	B	112	THR
1	B	113	TYR
1	B	128	ASP
1	B	138	ARG
1	B	150	LEU
1	B	162	GLU
1	B	165	ILE
1	B	176	MET
1	B	187	ASN
1	B	214	LYS
1	B	219	GLN
1	B	224	MET
1	B	241	MET
1	B	242	ARG
1	B	250	ASN
1	B	253	ASN
1	B	255	LYS
1	B	262	TYR
1	B	263	ILE
1	B	271	LEU
1	B	274	ASN
1	B	278	VAL
1	B	279	LEU
1	B	280	TYR
1	B	281	PRO
1	B	283	ASP
1	B	284	ASN
1	B	286	PHE
1	B	292	ARG
1	B	323	ARG
1	B	358	ARG
1	B	369	VAL
1	B	379	VAL
1	B	384	LEU

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Mol	Chain	Res	Type
1	B	396	LEU
1	B	398	ARG
1	B	400	LEU
1	B	412	ASN
1	B	426	ARG
1	B	444	LEU
1	B	458	ILE
1	B	467	ILE
1	B	480	GLN
1	B	489	ARG
1	B	492	LEU
1	B	499	LEU
1	B	502	ILE
1	B	506	ARG
1	B	518	LEU
1	B	519	ARG
1	B	536	LYS
1	B	550	GLU
1	B	554	LYS
1	B	555	VAL
1	B	557	ILE
1	B	565	VAL
1	B	571	HIS
1	B	575	ARG
1	B	576	GLN
1	B	577	LEU
1	B	586	LEU
1	B	589	ARG
1	B	591	LYS
1	B	595	ASN
1	B	598	VAL
1	B	603	VAL
1	B	613	TYR
1	B	628	ASP
1	B	630	VAL
1	B	633	ASP
1	B	640	LEU
1	B	649	ARG
1	B	650	VAL
1	B	652	LEU
1	B	655	LYS
1	B	662	LEU

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Mol	Chain	Res	Type
1	B	663	SER
1	B	667	SER
1	B	674	SER
1	B	676	THR
1	B	688	THR
1	B	708	PHE
1	B	710	ILE
1	B	714	ARG
1	B	717	ASP
1	B	724	ARG
1	B	727	ASN
1	B	753	LYS
1	B	756	ASP
1	B	757	LEU
1	B	764	MET
1	B	765	LEU
1	B	778	GLU
1	B	779	GLU
1	B	782	LYS
1	B	783	CYS
1	B	791	TYR
1	B	807	THR
1	B	810	LYS
1	B	828	GLU
1	B	831	ARG
1	B	834	LEU
1	B	838	ASP
1	C	10	ARG
1	C	22	GLU
1	C	43	ARG
1	C	49	ARG
1	C	61	ASP
1	C	63	LEU
1	C	66	ARG
1	C	76	GLU
1	C	82	ILE
1	C	87	LEU
1	C	90	TYR
1	C	91	MET
1	C	95	LEU
1	C	102	LEU
1	C	119	MET

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Mol	Chain	Res	Type
1	C	121	GLU
1	C	150	LEU
1	C	165	ILE
1	C	170	ILE
1	C	176	MET
1	C	183	LEU
1	C	196	PHE
1	C	207	GLU
1	C	211	GLN
1	C	224	MET
1	C	227	ASP
1	C	229	PRO
1	C	235	ASN
1	C	242	ARG
1	C	243	LEU
1	C	250	ASN
1	C	251	ASP
1	C	253	ASN
1	C	259	VAL
1	C	262	TYR
1	C	269	ARG
1	C	270	ASN
1	C	273	GLU
1	C	274	ASN
1	C	276	SER
1	C	279	LEU
1	C	280	TYR
1	C	281	PRO
1	C	284	ASN
1	C	286	PHE
1	C	292	ARG
1	C	299	VAL
1	C	305	GLN
1	C	306	ASP
1	C	319	ARG
1	C	339	ASP
1	C	353	LEU
1	C	354	VAL
1	C	356	LEU
1	C	358	ARG
1	C	360	ASP
1	C	361	TRP

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Mol	Chain	Res	Type
1	C	368	THR
1	C	391	LEU
1	C	392	LEU
1	C	395	LEU
1	C	396	LEU
1	C	400	LEU
1	C	408	GLN
1	C	413	ARG
1	C	426	ARG
1	C	430	LEU
1	C	439	ILE
1	C	444	LEU
1	C	455	VAL
1	C	457	ARG
1	C	460	SER
1	C	461	GLU
1	C	462	ILE
1	C	474	LEU
1	C	486	ILE
1	C	487	THR
1	C	490	ARG
1	C	492	LEU
1	C	494	LEU
1	C	495	CYS
1	C	502	ILE
1	C	506	ARG
1	C	510	GLU
1	C	519	ARG
1	C	522	LEU
1	C	523	SER
1	C	531	ILE
1	C	536	LYS
1	C	549	LEU
1	C	551	ARG
1	C	554	LYS
1	C	555	VAL
1	C	556	HIS
1	C	558	ASN
1	C	564	ASP
1	C	568	LYS
1	C	575	ARG
1	C	576	GLN

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Mol	Chain	Res	Type
1	C	579	ASN
1	C	582	HIS
1	C	586	LEU
1	C	589	ARG
1	C	595	ASN
1	C	613	TYR
1	C	619	ILE
1	C	622	LEU
1	C	638	ASP
1	C	641	ARG
1	C	646	GLU
1	C	649	ARG
1	C	652	LEU
1	C	655	LYS
1	C	656	VAL
1	C	662	LEU
1	C	665	GLN
1	C	682	MET
1	C	693	ASP
1	C	705	GLU
1	C	706	GLU
1	C	713	MET
1	C	724	ARG
1	C	727	ASN
1	C	738	LEU
1	C	739	ARG
1	C	741	ILE
1	C	743	GLU
1	C	753	LYS
1	C	755	PRO
1	C	764	MET
1	C	766	MET
1	C	778	GLU
1	C	782	LYS
1	C	787	VAL
1	C	800	MET
1	C	803	ARG
1	C	807	THR
1	C	808	SER
1	C	813	SER
1	C	831	ARG
1	D	10	ARG

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Mol	Chain	Res	Type
1	D	12	GLN
1	D	16	ARG
1	D	18	LEU
1	D	22	GLU
1	D	32	ASN
1	D	39	LEU
1	D	43	ARG
1	D	44	ASN
1	D	52	TYR
1	D	60	ARG
1	D	61	ASP
1	D	63	LEU
1	D	72	GLN
1	D	79	PRO
1	D	82	ILE
1	D	85	LEU
1	D	87	LEU
1	D	88	GLU
1	D	91	MET
1	D	95	LEU
1	D	102	LEU
1	D	104	LEU
1	D	105	GLU
1	D	113	TYR
1	D	127	GLU
1	D	131	LEU
1	D	138	ARG
1	D	147	MET
1	D	165	ILE
1	D	167	ASN
1	D	169	LYS
1	D	181	ASP
1	D	183	LEU
1	D	187	ASN
1	D	195	GLU
1	D	209	THR
1	D	211	GLN
1	D	219	GLN
1	D	224	MET
1	D	229	PRO
1	D	240	THR
1	D	242	ARG

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Mol	Chain	Res	Type
1	D	243	LEU
1	D	245	SER
1	D	249	PRO
1	D	250	ASN
1	D	251	ASP
1	D	253	ASN
1	D	255	LYS
1	D	263	ILE
1	D	269	ARG
1	D	277	ARG
1	D	279	LEU
1	D	280	TYR
1	D	281	PRO
1	D	283	ASP
1	D	284	ASN
1	D	286	PHE
1	D	291	LEU
1	D	294	LYS
1	D	299	VAL
1	D	306	ASP
1	D	309	ARG
1	D	314	SER
1	D	319	ARG
1	D	323	ARG
1	D	324	THR
1	D	337	LEU
1	D	339	ASP
1	D	340	THR
1	D	344	LEU
1	D	356	LEU
1	D	358	ARG
1	D	374	TYR
1	D	380	ILE
1	D	392	LEU
1	D	396	LEU
1	D	398	ARG
1	D	400	LEU
1	D	403	ILE
1	D	408	GLN
1	D	426	ARG
1	D	436	VAL
1	D	444	LEU

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Mol	Chain	Res	Type
1	D	455	VAL
1	D	457	ARG
1	D	461	GLU
1	D	469	LYS
1	D	474	LEU
1	D	487	THR
1	D	489	ARG
1	D	490	ARG
1	D	492	LEU
1	D	494	LEU
1	D	499	LEU
1	D	506	ARG
1	D	507	ILE
1	D	509	GLU
1	D	511	TYR
1	D	533	ASP
1	D	534	VAL
1	D	536	LYS
1	D	543	LEU
1	D	549	LEU
1	D	550	GLU
1	D	554	LYS
1	D	555	VAL
1	D	557	ILE
1	D	561	SER
1	D	562	LEU
1	D	565	VAL
1	D	575	ARG
1	D	579	ASN
1	D	582	HIS
1	D	589	ARG
1	D	594	PRO
1	D	595	ASN
1	D	598	VAL
1	D	600	PRO
1	D	601	ARG
1	D	603	VAL
1	D	613	TYR
1	D	622	LEU
1	D	626	ILE
1	D	628	ASP
1	D	638	ASP

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Mol	Chain	Res	Type
1	D	652	LEU
1	D	655	LYS
1	D	662	LEU
1	D	665	GLN
1	D	691	THR
1	D	708	PHE
1	D	714	ARG
1	D	720	ARG
1	D	724	ARG
1	D	727	ASN
1	D	739	ARG
1	D	740	GLN
1	D	743	GLU
1	D	753	LYS
1	D	756	ASP
1	D	757	LEU
1	D	764	MET
1	D	766	MET
1	D	770	ARG
1	D	779	GLU
1	D	782	LYS
1	D	797	TRP
1	D	824	ILE
1	D	831	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	32	ASN
1	A	62	HIS
1	A	96	GLN
1	A	97	ASN
1	A	167	ASN
1	A	208	HIS
1	A	219	GLN
1	A	239	ASN
1	A	253	ASN
1	A	336	GLN
1	A	453	ASN
1	A	459	HIS
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	484	ASN
1	A	566	GLN
1	A	579	ASN
1	A	588	ASN
1	A	614	HIS
1	A	678	ASN
1	A	744	GLN
1	A	784	GLN
1	B	34	HIS
1	B	96	GLN
1	B	97	ASN
1	B	211	GLN
1	B	274	ASN
1	B	284	ASN
1	B	295	GLN
1	B	336	GLN
1	B	341	HIS
1	B	377	HIS
1	B	390	HIS
1	B	453	ASN
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN
1	B	576	GLN
1	B	614	HIS
1	B	740	GLN
1	B	804	ASN
1	C	32	ASN
1	C	34	HIS
1	C	167	ASN
1	C	208	HIS
1	C	235	ASN
1	C	270	ASN
1	C	274	ASN
1	C	284	ASN
1	C	336	GLN
1	C	341	HIS
1	C	399	HIS
1	C	412	ASN
1	C	450	HIS
1	C	453	ASN
1	C	459	HIS

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Mol	Chain	Res	Type
1	C	480	GLN
1	C	481	ASN
1	C	556	HIS
1	C	576	GLN
1	C	727	ASN
1	C	740	GLN
1	C	744	GLN
1	C	754	GLN
1	C	804	ASN
1	D	23	ASN
1	D	34	HIS
1	D	167	ASN
1	D	219	GLN
1	D	284	ASN
1	D	336	GLN
1	D	377	HIS
1	D	390	HIS
1	D	399	HIS
1	D	401	GLN
1	D	450	HIS
1	D	453	ASN
1	D	459	HIS
1	D	477	HIS
1	D	480	GLN
1	D	481	ASN
1	D	556	HIS
1	D	614	HIS
1	D	631	ASN
1	D	665	GLN
1	D	727	ASN
1	D	744	GLN
1	D	754	GLN
1	D	793	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SEP	D	14	1	8,9,10	1.22	0	8,12,14	13.73	1 (12%)
1	SEP	C	14	1	8,9,10	1.30	1 (12%)	8,12,14	4.09	2 (25%)
1	SEP	A	14	1	8,9,10	1.17	0	8,12,14	2.86	2 (25%)
1	SEP	B	14	1	8,9,10	1.09	0	8,12,14	2.49	2 (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
1	SEP	D	14	1	-	4/5/8/10	-
1	SEP	C	14	1	-	2/5/8/10	-
1	SEP	A	14	1	-	5/5/8/10	-
1	SEP	B	14	1	-	5/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	SEP	CA-N	-2.11	1.41	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	14	SEP	OG-CB-CA	-38.78	70.41	108.14
1	C	14	SEP	OG-CB-CA	11.01	118.86	108.14
1	A	14	SEP	OG-CB-CA	7.29	115.24	108.14
1	B	14	SEP	OG-CB-CA	6.21	114.19	108.14
1	A	14	SEP	O2P-P-OG	2.87	114.38	106.73
1	B	14	SEP	OG-P-O1P	2.50	113.48	106.47
1	C	14	SEP	O2P-P-OG	2.43	113.19	106.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	14	SEP	N-CA-CB-OG
1	A	14	SEP	CA-CB-OG-P
1	A	14	SEP	CB-OG-P-O2P
1	A	14	SEP	CB-OG-P-O3P
1	B	14	SEP	CA-CB-OG-P
1	B	14	SEP	CB-OG-P-O2P
1	B	14	SEP	CB-OG-P-O3P
1	C	14	SEP	N-CA-CB-OG
1	C	14	SEP	CA-CB-OG-P
1	D	14	SEP	N-CA-CB-OG
1	D	14	SEP	CB-OG-P-O2P
1	A	14	SEP	CB-OG-P-O1P
1	B	14	SEP	CB-OG-P-O1P
1	D	14	SEP	CB-OG-P-O1P
1	D	14	SEP	CB-OG-P-O3P
1	B	14	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	14	SEP	1	0
1	C	14	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
3	PLP	B	999	1	15,15,16	1.30	2 (13%)	20,22,23	1.71	2 (10%)
2	SO4	D	902	-	4,4,4	0.52	0	6,6,6	0.34	0
3	PLP	C	999	1	15,15,16	1.36	1 (6%)	20,22,23	1.22	2 (10%)
2	SO4	A	901	-	4,4,4	0.39	0	6,6,6	0.46	0
3	PLP	A	999	1	15,15,16	2.20	4 (26%)	20,22,23	1.48	4 (20%)
2	SO4	A	902	-	4,4,4	0.36	0	6,6,6	0.33	0
2	SO4	B	901	-	4,4,4	0.31	0	6,6,6	0.40	0
2	SO4	C	901	-	4,4,4	0.25	0	6,6,6	0.43	0
2	SO4	C	902	-	4,4,4	0.41	0	6,6,6	0.46	0
2	SO4	D	901	-	4,4,4	0.26	0	6,6,6	0.71	0
2	SO4	B	902	-	4,4,4	0.45	0	6,6,6	0.39	0
3	PLP	D	999	1	15,15,16	1.46	2 (13%)	20,22,23	1.14	2 (10%)

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
3	PLP	C	999	1	-	1/6/6/8	0/1/1/1
3	PLP	D	999	1	-	2/6/6/8	0/1/1/1
3	PLP	A	999	1	-	3/6/6/8	0/1/1/1
3	PLP	B	999	1	-	2/6/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C5-C4	-5.49	1.34	1.40
3	C	999	PLP	C3-C2	-3.93	1.37	1.40
3	A	999	PLP	C3-C2	-3.58	1.37	1.40
3	D	999	PLP	C3-C2	-3.45	1.37	1.40
3	A	999	PLP	C2A-C2	-3.11	1.45	1.50
3	B	999	PLP	C3-C2	-2.58	1.38	1.40
3	A	999	PLP	C4A-C4	-2.46	1.46	1.51
3	D	999	PLP	C4A-C4	-2.08	1.47	1.51
3	B	999	PLP	C2-N1	2.01	1.37	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	999	PLP	O4P-C5A-C5	5.39	119.62	109.35
3	A	999	PLP	C4A-C4-C5	-4.17	116.64	120.94
3	C	999	PLP	O4P-C5A-C5	3.53	116.08	109.35
3	D	999	PLP	O4P-C5A-C5	2.69	114.47	109.35
3	C	999	PLP	O3P-P-O4P	2.64	113.75	106.73
3	B	999	PLP	O2P-P-O4P	2.57	113.56	106.73
3	A	999	PLP	O4P-C5A-C5	2.47	114.06	109.35
3	D	999	PLP	O2P-P-O4P	2.33	112.94	106.73
3	A	999	PLP	O3P-P-O4P	2.07	112.25	106.73
3	A	999	PLP	C4A-C4-C3	2.05	123.97	120.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PLP	C5A-O4P-P-O2P
3	A	999	PLP	C5A-O4P-P-O3P
3	B	999	PLP	C5A-O4P-P-O2P
3	B	999	PLP	C5A-O4P-P-O3P
3	D	999	PLP	C5A-O4P-P-O2P
3	D	999	PLP	C5A-O4P-P-O3P
3	A	999	PLP	C5A-O4P-P-O1P
3	C	999	PLP	C5A-O4P-P-O3P

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	999	PLP	1	0
3	C	999	PLP	1	0
3	A	999	PLP	1	0
2	C	902	SO4	1	0
3	D	999	PLP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	24:VAL	C	25:THR	N	1.95

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.