Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2024 – 01:57 AM EST

PDB ID	:	9GPB
Title	:	THE ALLOSTERIC TRANSITION OF GLYCOGEN PHOSPHORYLASE
Authors	:	Barford, D.; Johnson, L.N.
Deposited on	:	1990-12-17
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 ⓘ symbol.

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

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

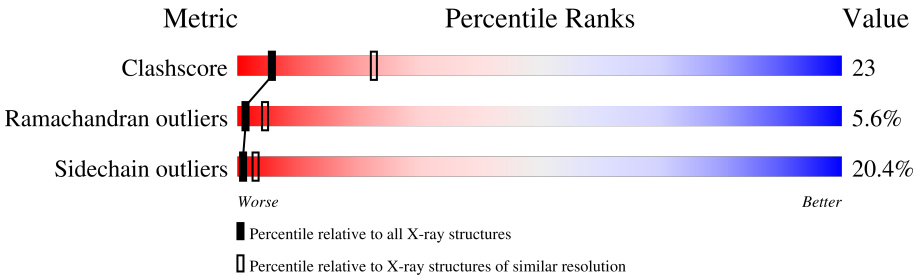
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (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	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (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	39% 38% 18% • •
1	B	842	40% 40% 14% • •
1	C	842	41% 40% 13% • •
1	D	842	32% 42% 18% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	900	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 26873 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.

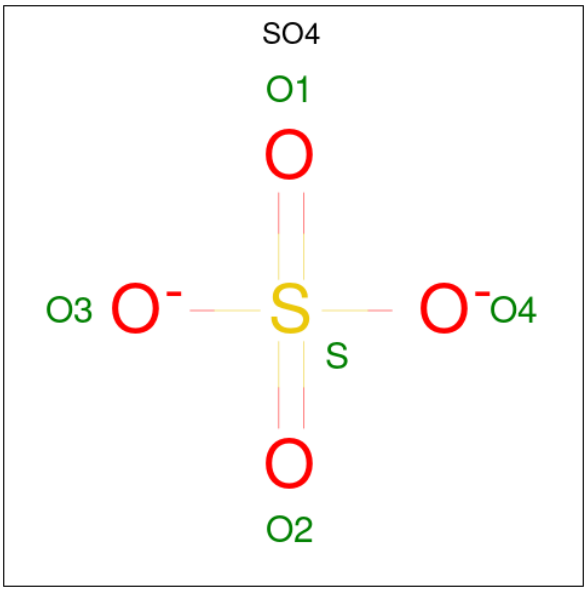
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	P	S	0	0	0
			6703	4272	1185	1215	1	30			
1	B	823	Total	C	N	O	P	S	0	0	0
			6703	4272	1185	1215	1	30			
1	C	823	Total	C	N	O	P	S	0	0	0
			6703	4271	1185	1216	1	30			
1	D	823	Total	C	N	O	P	S	0	0	0
			6704	4272	1185	1216	1	30			

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		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			
2	C	1	Total	O	S		0	0
			5	4	1			
2	C	1	Total	O	S		0	0
			5	4	1			
2	C	1	Total	O	S		0	0
			5	4	1			
2	D	1	Total	O	S		0	0
			5	4	1			
2	D	1	Total	O	S		0	0
			5	4	1			
2	D	1	Total	O	S		0	0
			5	4	1			

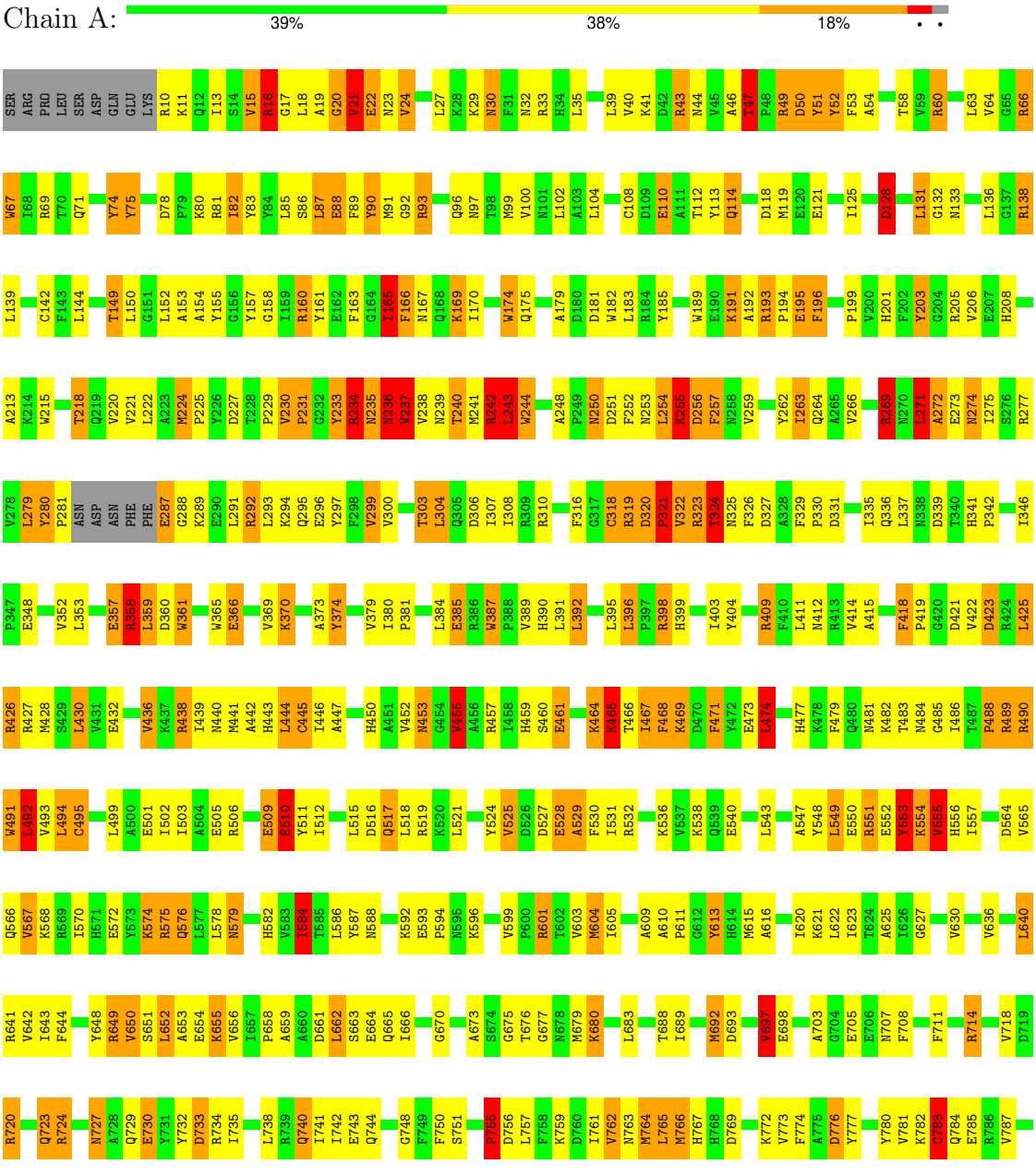
3 Residue-property plots (i)

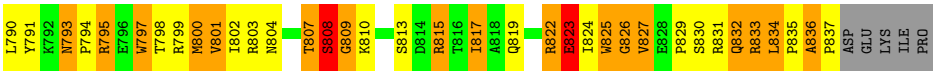
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

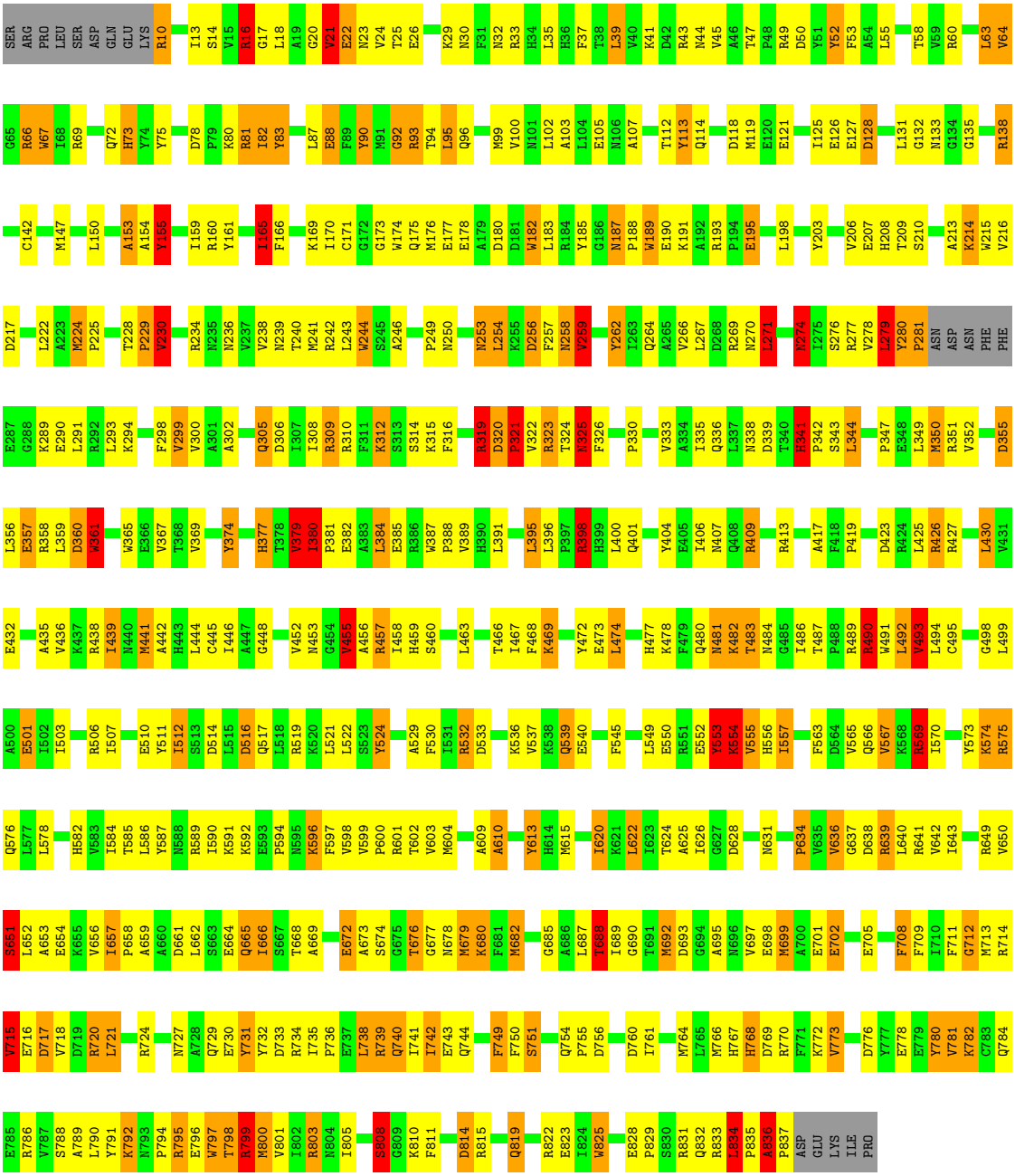
Chain A:





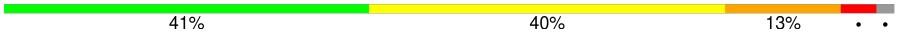
• Molecule 1: Glycogen phosphorylase, muscle form

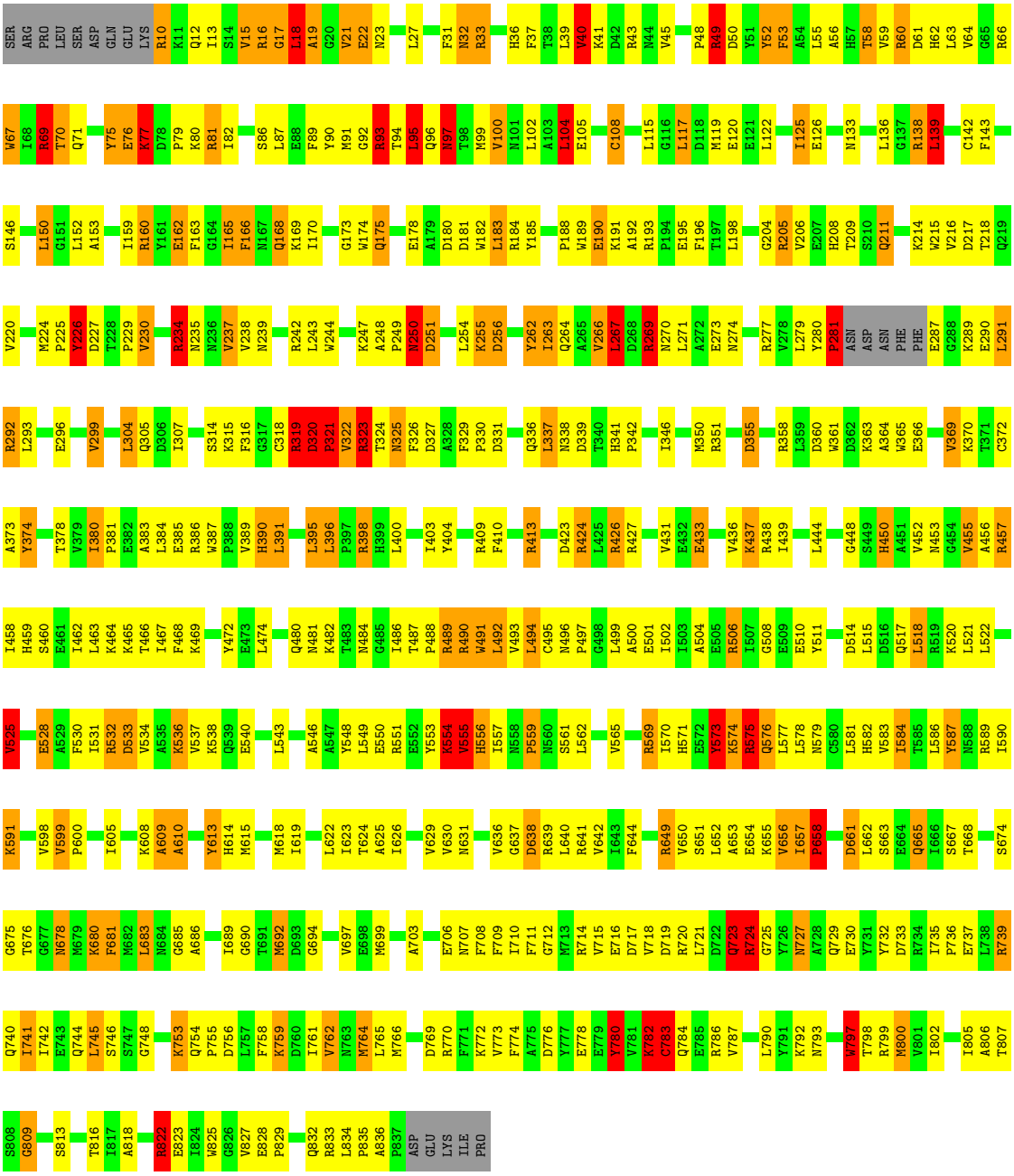
Chain B:



• Molecule 1: Glycogen phosphorylase, muscle form

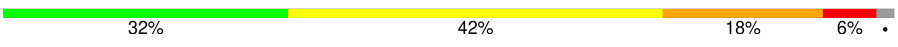
Chain C:

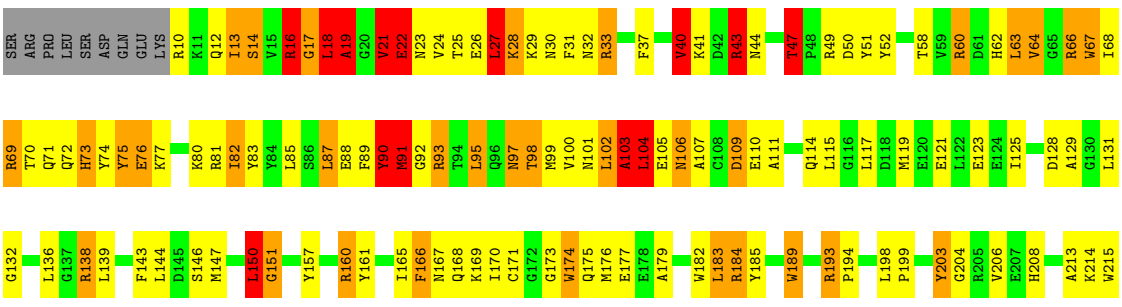


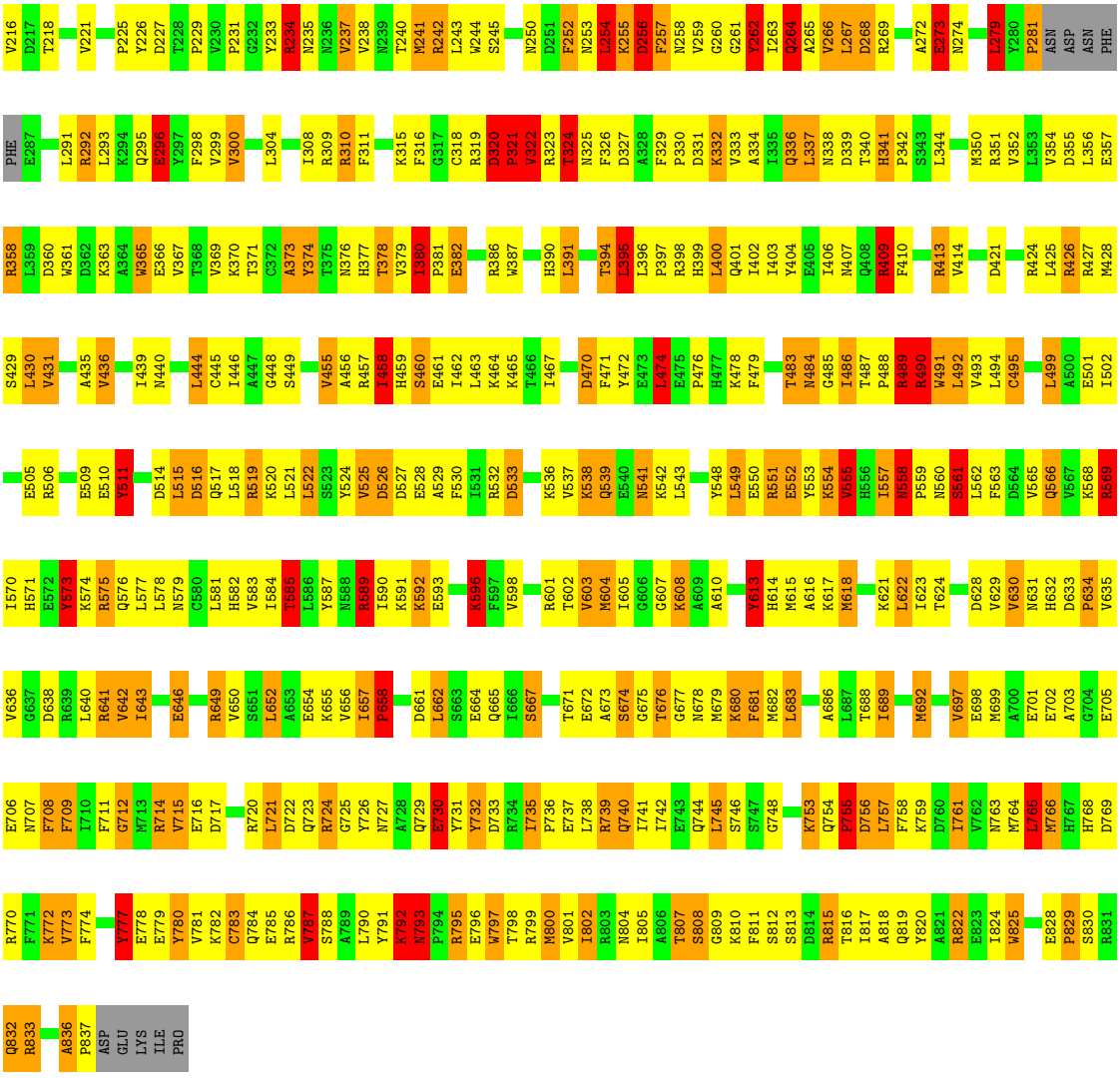


• Molecule 1: Glycogen phosphorylase, muscle form

Chain D:






V216 D217 T218 V221 P225 Y226 D227 T228 P229 V230 P231 G232 Y233 R234 M235 N236 V237 V238 N239 T240 M241 R242 L243 W244 S245 N250 D251 F252 N253 L254 K255 D256 F257 N258 V259 G260 G261 Y262 I263 Q264 A265 V266 L267 D268 R269 A272 E273 N274 L279 Y280 P281 ASN ASP ASN PHE
PHE E287 L291 R292 L293 K294 Q295 E296 Y297 F298 V299 V300 L304 I308 R309 R310 F311 K315 F316 G317 C318 R319 D320 P321 V322 R323 T324 N325 F326 D327 A328 F329 P330 D331 K332 V333 A334 I335 Q336 L337 N338 D339 T340 H341 P342 S343 L344 M350 R351 V352 L353 V354 D355 L356 E357
R358 L359 D360 W361 D362 K363 A364 W365 E366 V367 T368 V369 K370 T371 C372 A373 Y374 T375 N376 H377 T378 V379 I380 P381 E382 R386 W387 H390 L391 T394 L395 L396 P397 R398 H399 L400 Q401 I402 I403 Y404 E405 I406 N407 Q408 R409 F410 R413 V414 D421 R424 L425 R426 R427 M428
S429 L430 V431 A435 V436 I439 N440 L444 C445 I446 A447 G448 S449 V455 A456 R457 I458 H459 S460 E461 I462 L463 K464 K465 T466 I467 D470 F471 Y472 E473 L474 E475 P476 H477 K478 F479 T483 N484 G485 I486 T487 P488 R489 R490 W491 L492 V493 L494 C495 L499 A500 E501 I502
E505 R506 E509 E510 Y511 D514 L515 D516 Q517 L518 R519 K520 L521 L522 S523 Y524 V525 D526 D527 E528 A529 F530 I531 R532 D533 K536 V537 K538 Q539 E540 N541 K542 L543 Y548 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 K574 R575 Q576 L577 L578 N579 C580 L581 H582 V583 I584 T585 L586 Y587 N588 R589 I590 K591 K592 E593 K596 F597 V598 R601 T602 V603 M604 I605 G606 G607 K608 A609 A610 Y613 H614 M615 A616 K617 M618 K621 L622 I623 T624 D628 V629 V630 N631 H632 D633 P634 V635
V636 G637 D638 R639 L640 R641 V642 I643 E646 R649 V650 S651 L652 A653 E654 K655 V656 I657 P658 D661 L662 S663 E664 Q665 I666 S667 T671 E672 A673 S674 G675 T676 G677 N678 M679 K680 F681 M682 L683 A686 L687 T688 I689 M692 V697 E698 M699 A700 E701 E702 A703 G704 E705
E706 N707 F708 F709 I710 F711 G712 M713 R714 V715 E716 D717 R720 L721 D722 Q723 R724 G725 Y726 N727 A728 Q729 E730 Y731 Y732 D733 R734 I735 P736 E737 L738 R739 Q740 I741 I742 E743 Q744 L745 S746 S747 G748 K753 Q754 P755 D756 L757 F758 K759 D760 T761 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 V801 I802 R803 N804 I805 A806 T807 S808 G809 K810 F811 S812 S813 D814 R815 T816 I817 A818 Q819 Y820 A821 R822 E823 I824 W825 E828 P829 S830 R831
Q832 R833 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}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26873	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, 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	0.98	1/6827 (0.0%)	1.95	202/9236 (2.2%)
1	B	0.98	3/6827 (0.0%)	1.92	190/9236 (2.1%)
1	C	1.00	4/6827 (0.1%)	1.96	208/9237 (2.3%)
1	D	0.99	4/6829 (0.1%)	1.97	231/9240 (2.5%)
All	All	0.99	12/27310 (0.0%)	1.95	831/36949 (2.2%)

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	9
1	B	0	8
1	C	0	10
1	D	0	6
All	All	0	33

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	LEU	N-CA	-6.78	1.32	1.46
1	B	230	VAL	CA-CB	6.26	1.67	1.54
1	A	565	VAL	CA-CB	6.06	1.67	1.54
1	D	17	GLY	N-CA	-5.95	1.37	1.46
1	B	244	TRP	CG-CD2	-5.53	1.34	1.43
1	C	565	VAL	CA-CB	5.53	1.66	1.54
1	D	189	TRP	CG-CD2	-5.40	1.34	1.43
1	C	17	GLY	C-N	-5.29	1.21	1.34
1	D	16	ARG	C-N	-5.14	1.23	1.33
1	C	17	GLY	CA-C	-5.13	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	244	TRP	CD1-NE1	-5.11	1.29	1.38
1	B	182	TRP	CD1-NE1	-5.05	1.29	1.38

All (831) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	17	GLY	O-C-N	19.05	153.18	122.70
1	C	17	GLY	CA-C-N	-14.07	86.25	117.20
1	C	780	TYR	CB-CG-CD2	-13.43	112.94	121.00
1	B	780	TYR	CB-CG-CD2	-13.31	113.02	121.00
1	C	319	ARG	NE-CZ-NH2	-12.42	114.09	120.30
1	D	739	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	A	490	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	C	714	ARG	NE-CZ-NH2	-11.51	114.54	120.30
1	B	795	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	A	244	TRP	CD1-CG-CD2	11.01	115.11	106.30
1	D	409	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	A	21	VAL	CG1-CB-CG2	-10.87	93.51	110.90
1	C	613	TYR	CB-CG-CD2	-10.58	114.65	121.00
1	C	409	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	B	773	VAL	CA-CB-CG2	-10.53	95.10	110.90
1	B	780	TYR	CB-CG-CD1	10.53	127.31	121.00
1	C	49	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	D	244	TRP	CD1-CG-CD2	10.51	114.71	106.30
1	A	75	TYR	CB-CG-CD2	-10.34	114.80	121.00
1	C	799	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	D	780	TYR	CB-CG-CD2	-10.25	114.85	121.00
1	B	650	VAL	CG1-CB-CG2	-10.17	94.63	110.90
1	C	281	PRO	N-CA-C	10.13	138.43	112.10
1	D	739	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	C	60	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	D	641	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	B	575	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	C	139	LEU	CA-CB-CG	9.61	137.41	115.30
1	B	490	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	A	193	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	A	490	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	C	193	ARG	NE-CZ-NH2	-9.41	115.60	120.30
1	D	519	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	C	490	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	374	TYR	CB-CG-CD2	-9.24	115.46	121.00
1	D	244	TRP	CE2-CD2-CG	-9.21	99.93	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	491	TRP	CD1-CG-CD2	9.15	113.62	106.30
1	A	724	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	C	532	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	B	699	MET	CG-SD-CE	9.10	114.76	100.20
1	B	271	LEU	CA-CB-CG	9.09	136.21	115.30
1	D	292	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	C	189	TRP	CG-CD2-CE3	9.06	142.06	133.90
1	D	90	TYR	CB-CG-CD2	-9.06	115.57	121.00
1	A	409	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	D	489	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	404	TYR	CB-CG-CD2	-8.89	115.67	121.00
1	D	387	TRP	CD1-CG-CD2	8.87	113.40	106.30
1	B	257	PHE	CA-C-N	-8.77	97.90	117.20
1	A	244	TRP	CE2-CD2-CG	-8.76	100.29	107.30
1	D	27	LEU	CA-CB-CG	8.74	135.41	115.30
1	A	242	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	C	386	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	C	613	TYR	CB-CG-CD1	8.73	126.24	121.00
1	B	409	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	C	182	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	D	174	TRP	CD1-CG-CD2	8.66	113.23	106.30
1	D	292	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	155	TYR	CB-CG-CD1	-8.64	115.81	121.00
1	C	67	TRP	CD1-CG-CD2	8.64	113.21	106.30
1	D	361	TRP	CD1-CG-CD2	8.62	113.20	106.30
1	C	269	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	A	601	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	D	189	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	B	113	TYR	CB-CG-CD2	-8.47	115.92	121.00
1	B	83	TYR	CB-CG-CD1	-8.42	115.95	121.00
1	C	244	TRP	CD1-CG-CD2	8.42	113.04	106.30
1	A	493	VAL	CG1-CB-CG2	-8.42	97.43	110.90
1	C	160	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	128	ASP	CB-CG-OD1	8.40	125.86	118.30
1	C	358	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	D	203	TYR	CB-CG-CD2	-8.37	115.98	121.00
1	B	365	TRP	CD1-CG-CD2	8.37	113.00	106.30
1	B	724	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	B	825	TRP	CG-CD2-CE3	8.36	141.42	133.90
1	B	244	TRP	CD1-CG-CD2	8.33	112.96	106.30
1	D	793	ASN	N-CA-C	-8.30	88.58	111.00
1	A	387	TRP	CD1-CG-CD2	8.29	112.93	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	TYR	CB-CG-CD2	-8.27	116.04	121.00
1	A	613	TYR	CB-CG-CD2	-8.26	116.04	121.00
1	A	641	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	525	VAL	CG1-CB-CG2	-8.24	97.72	110.90
1	D	361	TRP	CE2-CD2-CG	-8.23	100.71	107.30
1	C	532	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	193	ARG	CG-CD-NE	-8.21	94.57	111.80
1	A	825	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	B	387	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	B	553	TYR	CB-CG-CD1	8.17	125.90	121.00
1	A	237	VAL	CG1-CB-CG2	-8.15	97.86	110.90
1	B	553	TYR	CA-CB-CG	8.14	128.86	113.40
1	C	587	TYR	CB-CG-CD1	-8.11	116.13	121.00
1	C	783	CYS	CA-CB-SG	-8.11	99.40	114.00
1	A	203	TYR	CB-CG-CD2	-8.11	116.13	121.00
1	C	255	LYS	CA-C-N	-8.10	99.38	117.20
1	D	16	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	A	75	TYR	CB-CG-CD1	8.09	125.85	121.00
1	C	491	TRP	CE2-CD2-CG	-8.07	100.84	107.30
1	A	575	ARG	N-CA-C	8.06	132.75	111.00
1	C	174	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	C	325	ASN	CA-C-N	-8.05	99.48	117.20
1	A	297	TYR	CB-CG-CD1	-8.03	116.18	121.00
1	D	795	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	A	387	TRP	CE2-CD2-CG	-8.02	100.88	107.30
1	D	511	TYR	CB-CG-CD2	-8.01	116.19	121.00
1	C	424	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	358	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	D	777	TYR	CB-CG-CD2	-7.99	116.21	121.00
1	C	320	ASP	N-CA-CB	-7.98	96.23	110.60
1	D	641	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	182	TRP	CD1-CG-CD2	7.98	112.68	106.30
1	A	67	TRP	CD1-CG-CD2	7.97	112.67	106.30
1	B	365	TRP	CE2-CD2-CG	-7.96	100.93	107.30
1	D	215	TRP	CD1-CG-CD2	7.96	112.67	106.30
1	D	387	TRP	CE2-CD2-CG	-7.94	100.95	107.30
1	D	67	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	C	491	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	D	174	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	A	491	TRP	CE2-CD2-CG	-7.87	101.01	107.30
1	C	766	MET	CG-SD-CE	-7.86	87.62	100.20
1	A	243	LEU	CA-CB-CG	7.83	133.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	189	TRP	CB-CG-CD1	-7.82	116.83	127.00
1	A	255	LYS	CA-C-N	-7.81	100.02	117.20
1	C	361	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	D	66	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	C	215	TRP	CD1-CG-CD2	7.73	112.49	106.30
1	A	182	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	D	337	LEU	CA-CB-CG	7.71	133.03	115.30
1	C	255	LYS	O-C-N	7.71	135.03	122.70
1	C	404	TYR	CA-C-N	7.70	134.14	117.20
1	A	250	ASN	O-C-N	7.69	135.00	122.70
1	C	361	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	B	825	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	C	160	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	773	VAL	CA-CB-CG1	7.63	122.35	110.90
1	D	91	MET	CA-CB-CG	-7.62	100.34	113.30
1	A	300	VAL	CA-CB-CG2	-7.62	99.47	110.90
1	A	361	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	D	19	ALA	CA-C-N	-7.61	100.97	116.20
1	B	189	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	C	67	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	C	182	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	B	182	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	D	279	LEU	CB-CG-CD1	-7.58	98.11	111.00
1	B	189	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	B	457	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	C	724	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	203	TYR	CB-CG-CD2	-7.52	116.49	121.00
1	C	33	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	D	75	TYR	CB-CG-CD2	7.51	125.50	121.00
1	C	365	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	A	649	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	D	797	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	C	174	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	A	825	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	250	ASN	CA-C-N	-7.44	100.83	117.20
1	C	189	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	C	610	ALA	N-CA-CB	7.41	120.47	110.10
1	C	18	LEU	CA-C-N	-7.40	100.92	117.20
1	B	491	TRP	CD1-CG-CD2	7.38	112.20	106.30
1	B	575	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	D	189	TRP	CE2-CD2-CG	-7.37	101.40	107.30
1	A	52	TYR	CB-CG-CD2	-7.36	116.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	490	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	D	387	TRP	CG-CD2-CE3	7.35	140.51	133.90
1	B	174	TRP	CD1-CG-CD2	7.34	112.17	106.30
1	A	509	GLU	CA-C-N	-7.34	101.05	117.20
1	D	825	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	D	431	VAL	CA-CB-CG2	-7.32	99.92	110.90
1	B	491	TRP	CE2-CD2-CG	-7.32	101.45	107.30
1	C	825	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	C	487	THR	CA-CB-CG2	7.29	122.61	112.40
1	C	319	ARG	CA-C-N	-7.28	101.18	117.20
1	C	615	MET	CG-SD-CE	-7.28	88.56	100.20
1	A	455	VAL	N-CA-CB	-7.27	95.50	111.50
1	D	394	THR	CA-CB-CG2	7.27	122.58	112.40
1	B	244	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	C	323	ARG	N-CA-C	7.27	130.62	111.00
1	D	777	TYR	CB-CG-CD1	7.26	125.36	121.00
1	D	555	VAL	N-CA-C	7.25	130.59	111.00
1	C	770	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	D	825	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	B	553	TYR	CB-CG-CD2	-7.24	116.65	121.00
1	C	189	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	D	336	GLN	CA-CB-CG	-7.23	97.50	113.40
1	D	553	TYR	CA-C-N	7.23	133.10	117.20
1	C	577	LEU	CB-CG-CD1	-7.22	98.72	111.00
1	C	244	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	D	262	TYR	CB-CG-CD2	-7.19	116.69	121.00
1	B	398	ARG	NE-CZ-NH2	7.19	123.90	120.30
1	A	724	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	74	TYR	CB-CG-CD1	7.18	125.31	121.00
1	D	281	PRO	N-CA-C	7.17	130.74	112.10
1	D	215	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	A	361	TRP	CD1-CG-CD2	7.16	112.03	106.30
1	B	438	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	D	474	LEU	CA-CB-CG	7.15	131.75	115.30
1	A	365	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	C	780	TYR	CB-CG-CD1	7.11	125.27	121.00
1	C	16	ARG	NE-CZ-NH2	7.09	123.85	120.30
1	C	489	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	A	244	TRP	CB-CG-CD1	-7.08	117.80	127.00
1	B	574	LYS	N-CA-C	-7.07	91.90	111.00
1	B	182	TRP	CD1-CG-CD2	7.07	111.95	106.30
1	C	773	VAL	CG1-CB-CG2	-7.06	99.61	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	97	ASN	CB-CG-ND2	7.05	133.63	116.70
1	A	161	TYR	CB-CG-CD1	-7.04	116.77	121.00
1	D	182	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	649	ARG	CG-CD-NE	-7.04	97.02	111.80
1	C	27	LEU	CA-CB-CG	7.03	131.48	115.30
1	C	266	VAL	CA-CB-CG2	-7.03	100.36	110.90
1	C	17	GLY	C-N-CA	7.03	139.27	121.70
1	D	409	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	182	TRP	CG-CD2-CE3	7.02	140.22	133.90
1	B	387	TRP	CE2-CD2-CG	-7.02	101.69	107.30
1	C	387	TRP	CD1-CG-CD2	7.01	111.91	106.30
1	B	799	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	D	387	TRP	CB-CG-CD1	-7.00	117.89	127.00
1	C	365	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	C	797	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	185	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	A	74	TYR	CB-CG-CD2	-6.97	116.81	121.00
1	A	66	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	A	528	GLU	CA-C-N	-6.97	101.87	117.20
1	A	831	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	C	825	TRP	CG-CD2-CE3	6.96	140.16	133.90
1	D	787	VAL	CG1-CB-CG2	-6.95	99.79	110.90
1	C	730	GLU	CA-CB-CG	6.94	128.67	113.40
1	C	825	TRP	CD1-CG-CD2	6.93	111.84	106.30
1	B	215	TRP	CD1-CG-CD2	6.92	111.83	106.30
1	D	182	TRP	CD1-CG-CD2	6.92	111.83	106.30
1	B	610	ALA	CB-CA-C	-6.91	99.73	110.10
1	B	831	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	D	822	ARG	CA-CB-CG	6.88	128.54	113.40
1	B	731	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	A	242	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	18	LEU	N-CA-C	-6.88	92.43	111.00
1	D	765	LEU	CA-CB-CG	6.88	131.12	115.30
1	B	715	VAL	CA-C-N	6.87	132.31	117.20
1	B	797	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	D	395	LEU	CA-CB-CG	6.86	131.07	115.30
1	D	67	TRP	CE2-CD2-CG	-6.85	101.82	107.30
1	B	455	VAL	N-CA-CB	-6.84	96.44	111.50
1	D	491	TRP	CD1-CG-CD2	6.84	111.78	106.30
1	B	604	MET	CG-SD-CE	-6.83	89.27	100.20
1	D	592	LYS	CA-CB-CG	6.83	128.43	113.40
1	A	808	SER	CA-C-N	6.83	129.85	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	D	797	TRP	CB-CG-CD1	-6.81	118.14	127.00
1	D	573	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	C	351	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	102	LEU	CA-CB-CG	6.80	130.94	115.30
1	B	155	TYR	CB-CG-CD2	6.78	125.07	121.00
1	D	808	SER	N-CA-C	6.77	129.28	111.00
1	B	361	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	C	216	VAL	CG1-CB-CG2	-6.75	100.09	110.90
1	B	491	TRP	CG-CD2-CE3	6.75	139.97	133.90
1	D	431	VAL	CA-CB-CG1	6.75	121.02	110.90
1	D	730	GLU	CA-CB-CG	6.74	128.23	113.40
1	D	491	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	D	160	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	D	254	LEU	CA-CB-CG	6.73	130.78	115.30
1	A	244	TRP	CG-CD1-NE1	-6.72	103.38	110.10
1	C	661	ASP	CB-CG-OD1	6.72	124.35	118.30
1	C	108	CYS	CA-CB-SG	-6.72	101.91	114.00
1	B	306	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	189	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	C	506	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	B	174	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	C	365	TRP	CG-CD2-CE3	6.69	139.92	133.90
1	A	67	TRP	CE2-CD2-CG	-6.68	101.95	107.30
1	D	676	THR	CA-CB-OG1	-6.68	94.97	109.00
1	D	613	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	B	825	TRP	CB-CG-CD1	-6.66	118.34	127.00
1	B	215	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	A	254	LEU	CA-CB-CG	6.64	130.57	115.30
1	C	58	THR	CA-CB-CG2	6.64	121.69	112.40
1	A	426	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	D	676	THR	CA-CB-CG2	6.63	121.69	112.40
1	B	379	VAL	N-CA-CB	-6.63	96.92	111.50
1	B	64	VAL	CA-CB-CG2	6.63	120.84	110.90
1	A	60	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	310	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	255	LYS	CA-C-N	-6.62	102.64	117.20
1	D	183	LEU	CA-CB-CG	6.61	130.50	115.30
1	B	430	LEU	CA-CB-CG	6.61	130.49	115.30
1	B	435	ALA	N-CA-C	-6.60	93.17	111.00
1	C	610	ALA	CB-CA-C	-6.60	100.19	110.10
1	C	797	TRP	NE1-CE2-CZ2	-6.60	123.14	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	60	ARG	CA-CB-CG	-6.60	98.88	113.40
1	B	569	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	B	601	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	D	493	VAL	CG1-CB-CG2	-6.59	100.36	110.90
1	A	780	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	B	610	ALA	N-CA-CB	6.58	119.31	110.10
1	C	650	VAL	CG1-CB-CG2	-6.58	100.37	110.90
1	A	797	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	B	487	THR	CA-CB-CG2	6.57	121.60	112.40
1	D	491	TRP	CG-CD2-CE3	6.57	139.81	133.90
1	C	168	GLN	CG-CD-NE2	6.56	132.44	116.70
1	D	365	TRP	CE2-CD2-CG	-6.56	102.06	107.30
1	C	318	CYS	CA-CB-SG	-6.54	102.22	114.00
1	B	67	TRP	CE2-CD2-CG	-6.54	102.07	107.30
1	D	373	ALA	CA-C-N	6.54	131.59	117.20
1	D	51	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	D	244	TRP	CG-CD2-CE3	6.53	139.78	133.90
1	A	436	VAL	CA-C-N	-6.52	102.85	117.20
1	B	427	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	392	LEU	CA-CB-CG	6.52	130.29	115.30
1	A	51	TYR	CB-CG-CD1	6.50	124.90	121.00
1	A	215	TRP	CD1-CG-CD2	6.50	111.50	106.30
1	A	491	TRP	CG-CD1-NE1	-6.50	103.60	110.10
1	C	474	LEU	CA-CB-CG	6.49	130.23	115.30
1	B	359	LEU	CA-C-N	-6.48	102.94	117.20
1	D	182	TRP	CA-CB-CG	6.48	126.02	113.70
1	A	102	LEU	CA-CB-CG	6.48	130.20	115.30
1	A	365	TRP	CD1-CG-CD2	6.47	111.48	106.30
1	D	797	TRP	CD1-CG-CD2	6.46	111.47	106.30
1	B	720	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	64	VAL	CA-CB-CG1	-6.44	101.25	110.90
1	B	350	MET	CA-CB-CG	6.43	124.23	113.30
1	D	585	THR	CA-CB-CG2	-6.43	103.40	112.40
1	A	21	VAL	N-CA-C	6.43	128.36	111.00
1	B	234	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	795	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	C	226	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	C	723	GLN	N-CA-C	-6.42	93.67	111.00
1	C	281	PRO	CA-N-CD	-6.41	102.53	111.50
1	D	227	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	799	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	325	ASN	CA-C-N	-6.39	103.14	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	387	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	D	583	VAL	CG1-CB-CG2	-6.39	100.68	110.90
1	A	549	LEU	CA-C-N	6.37	131.22	117.20
1	A	52	TYR	CB-CG-CD1	6.37	124.82	121.00
1	D	553	TYR	O-C-N	-6.37	112.51	122.70
1	C	182	TRP	CG-CD1-NE1	-6.37	103.73	110.10
1	D	93	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	377	HIS	CA-CB-CG	-6.36	102.78	113.60
1	B	554	LYS	N-CA-C	6.36	128.18	111.00
1	D	436	VAL	CG1-CB-CG2	-6.36	100.73	110.90
1	B	67	TRP	CD1-CG-CD2	6.36	111.39	106.30
1	B	305	GLN	CA-CB-CG	6.36	127.38	113.40
1	A	822	ARG	CA-C-N	6.35	131.18	117.20
1	B	792	LYS	CA-CB-CG	6.35	127.38	113.40
1	B	834	LEU	N-CA-C	6.35	128.15	111.00
1	A	236	ASN	N-CA-C	6.35	128.15	111.00
1	C	205	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	649	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	52	TYR	CB-CG-CD2	-6.34	117.20	121.00
1	B	688	THR	CA-C-N	-6.34	103.26	117.20
1	A	587	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	A	47	THR	CA-CB-CG2	6.33	121.26	112.40
1	A	574	LYS	CD-CE-NZ	6.33	126.25	111.70
1	D	569	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	242	ARG	CB-CG-CD	-6.32	95.16	111.60
1	D	226	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	B	242	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	255	LYS	O-C-N	6.31	132.79	122.70
1	A	387	TRP	CG-CD2-CE3	6.30	139.57	133.90
1	A	714	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	B	770	ARG	CA-CB-CG	6.29	127.25	113.40
1	C	77	LYS	CA-C-N	-6.29	103.36	117.20
1	D	673	ALA	CB-CA-C	-6.29	100.67	110.10
1	A	801	VAL	CA-CB-CG2	-6.28	101.48	110.90
1	D	658	PRO	CA-C-N	6.28	131.00	117.20
1	A	271	LEU	CA-CB-CG	6.27	129.72	115.30
1	A	128	ASP	CA-CB-CG	6.27	127.19	113.40
1	B	361	TRP	CD1-CG-CD2	6.27	111.31	106.30
1	A	825	TRP	CB-CG-CD1	-6.26	118.86	127.00
1	D	506	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	358	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	269	ARG	NE-CZ-NH2	-6.24	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	349	LEU	CA-CB-CG	6.23	129.63	115.30
1	C	762	VAL	CG1-CB-CG2	-6.23	100.93	110.90
1	A	49	ARG	CA-CB-CG	6.22	127.09	113.40
1	D	640	LEU	CA-CB-CG	6.22	129.61	115.30
1	C	450	HIS	CA-CB-CG	6.22	124.17	113.60
1	D	241	MET	CA-CB-CG	6.22	123.87	113.30
1	D	394	THR	CA-CB-OG1	-6.22	95.94	109.00
1	D	16	ARG	O-C-N	6.21	133.76	123.20
1	D	43	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	A	215	TRP	CE2-CD2-CG	-6.19	102.35	107.30
1	D	426	ARG	CA-CB-CG	6.19	127.01	113.40
1	D	551	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	182	TRP	CG-CD2-CE3	6.18	139.46	133.90
1	D	296	GLU	CA-CB-CG	6.18	127.00	113.40
1	C	81	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	825	TRP	CD1-CG-CD2	6.17	111.23	106.30
1	C	706	GLU	CB-CA-C	-6.17	98.07	110.40
1	C	69	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	D	16	ARG	CD-NE-CZ	6.15	132.21	123.60
1	D	215	TRP	CG-CD1-NE1	-6.14	103.95	110.10
1	D	18	LEU	N-CA-C	6.14	127.58	111.00
1	D	561	SER	CA-CB-OG	6.14	127.78	111.20
1	C	104	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	181	ASP	CA-C-N	-6.14	103.70	117.20
1	D	244	TRP	CG-CD1-NE1	-6.13	103.97	110.10
1	A	174	TRP	CE2-CD2-CG	-6.13	102.39	107.30
1	C	215	TRP	CE2-CD2-CG	-6.13	102.39	107.30
1	C	322	VAL	CG1-CB-CG2	6.13	120.71	110.90
1	A	427	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	D	252	PHE	O-C-N	6.13	132.50	122.70
1	B	344	LEU	CA-CB-CG	6.11	129.36	115.30
1	D	387	TRP	CG-CD1-NE1	-6.11	103.99	110.10
1	D	160	ARG	CB-CG-CD	-6.11	95.73	111.60
1	B	567	VAL	CA-C-N	-6.10	103.78	117.20
1	C	438	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	825	TRP	CG-CD2-CE3	6.08	139.37	133.90
1	D	511	TYR	CB-CG-CD1	6.07	124.64	121.00
1	A	557	ILE	CB-CG1-CD1	-6.06	96.93	113.90
1	C	299	VAL	CG1-CB-CG2	-6.06	101.21	110.90
1	C	365	TRP	CB-CG-CD1	-6.06	119.13	127.00
1	C	587	TYR	CB-CG-CD2	6.05	124.63	121.00
1	B	426	ARG	NE-CZ-NH2	-6.05	117.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	43	ARG	CA-CB-CG	6.04	126.69	113.40
1	B	477	HIS	CA-CB-CG	6.04	123.86	113.60
1	A	287	GLU	CA-CB-CG	6.04	126.68	113.40
1	B	491	TRP	CB-CG-CD1	-6.03	119.16	127.00
1	C	211	GLN	CA-CB-CG	6.02	126.65	113.40
1	C	455	VAL	CG1-CB-CG2	6.02	120.53	110.90
1	C	573	TYR	CA-CB-CG	6.02	124.84	113.40
1	B	589	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	D	731	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	D	279	LEU	CA-CB-CG	6.00	129.11	115.30
1	C	491	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	A	234	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	C	215	TRP	CG-CD1-NE1	-5.98	104.12	110.10
1	A	90	TYR	CB-CG-CD1	5.98	124.59	121.00
1	B	426	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	D	203	TYR	CA-C-N	5.97	128.14	116.20
1	D	266	VAL	CA-CB-CG2	-5.97	101.94	110.90
1	A	272	ALA	N-CA-C	-5.97	94.88	111.00
1	D	103	ALA	CB-CA-C	-5.97	101.14	110.10
1	B	312	LYS	CG-CD-CE	5.97	129.80	111.90
1	C	77	LYS	O-C-N	5.96	132.24	122.70
1	D	575	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	769	ASP	CB-CG-OD1	5.96	123.66	118.30
1	C	230	VAL	CG1-CB-CG2	-5.96	101.37	110.90
1	B	254	LEU	CA-CB-CG	5.95	128.99	115.30
1	C	324	THR	N-CA-C	-5.95	94.94	111.00
1	A	457	ARG	CA-C-N	5.95	130.28	117.20
1	D	732	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	B	355	ASP	CB-CG-OD1	5.94	123.65	118.30
1	C	583	VAL	CG1-CB-CG2	-5.94	101.40	110.90
1	D	634	PRO	CA-C-N	-5.93	104.14	117.20
1	A	553	TYR	CB-CG-CD1	5.93	124.56	121.00
1	A	374	TYR	N-CA-CB	-5.92	99.94	110.60
1	C	66	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	93	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	822	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	474	LEU	CA-CB-CG	5.92	128.91	115.30
1	C	575	ARG	N-CA-C	5.91	126.97	111.00
1	A	613	TYR	CB-CG-CD1	5.91	124.54	121.00
1	C	739	ARG	CA-CB-CG	5.90	126.39	113.40
1	C	234	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	242	ARG	CB-CG-CD	-5.89	96.28	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	655	LYS	CA-CB-CG	5.89	126.36	113.40
1	B	799	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	47	THR	N-CA-CB	-5.89	99.10	110.30
1	D	310	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	555	VAL	CB-CA-C	-5.88	100.22	111.40
1	C	589	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	413	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	611	PRO	CA-C-N	-5.87	104.45	116.20
1	A	455	VAL	O-C-N	-5.87	113.31	122.70
1	C	404	TYR	O-C-N	-5.87	113.31	122.70
1	D	490	ARG	CG-CD-NE	-5.87	99.48	111.80
1	B	676	THR	CA-C-N	5.86	127.92	116.20
1	C	319	ARG	CA-C-O	5.86	132.41	120.10
1	B	468	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	B	387	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	D	768	HIS	CA-C-N	-5.85	104.34	117.20
1	D	244	TRP	CB-CG-CD1	-5.84	119.41	127.00
1	C	455	VAL	CA-CB-CG2	-5.84	102.14	110.90
1	D	252	PHE	CA-C-N	-5.83	104.36	117.20
1	B	682	MET	CG-SD-CE	5.83	109.53	100.20
1	A	321	PRO	N-CA-C	5.83	127.25	112.10
1	D	177	GLU	CA-CB-CG	5.83	126.22	113.40
1	C	528	GLU	OE1-CD-OE2	-5.82	116.31	123.30
1	D	533	ASP	CA-CB-CG	5.82	126.21	113.40
1	B	341	HIS	CB-CG-ND1	5.82	137.76	123.20
1	B	613	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	D	716	GLU	N-CA-CB	-5.80	100.15	110.60
1	C	244	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	A	764	MET	CA-CB-CG	5.80	123.16	113.30
1	D	174	TRP	CG-CD2-CE3	5.79	139.12	133.90
1	D	256	ASP	CA-CB-CG	5.79	126.13	113.40
1	C	77	LYS	CB-CG-CD	5.79	126.65	111.60
1	A	174	TRP	CD1-CG-CD2	5.79	110.93	106.30
1	B	63	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	509	GLU	O-C-N	5.78	131.94	122.70
1	D	792	LYS	CA-CB-CG	5.78	126.11	113.40
1	D	491	TRP	CB-CG-CD1	-5.76	119.52	127.00
1	C	467	ILE	CA-C-N	5.75	129.86	117.20
1	A	20	GLY	CA-C-N	-5.75	104.54	117.20
1	C	206	VAL	CG1-CB-CG2	-5.75	101.70	110.90
1	A	205	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	D	815	ARG	NE-CZ-NH2	-5.75	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	359	LEU	CA-CB-CG	5.74	128.51	115.30
1	B	404	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	B	240	THR	CA-CB-CG2	5.74	120.43	112.40
1	A	189	TRP	CD1-CG-CD2	5.73	110.89	106.30
1	C	351	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	C	472	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	A	138	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	409	ARG	CA-CB-CG	5.73	126.00	113.40
1	D	75	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	B	715	VAL	CA-CB-CG1	-5.72	102.32	110.90
1	A	16	ARG	CA-C-N	5.71	127.62	116.20
1	A	815	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	B	472	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	C	745	LEU	CA-CB-CG	5.70	128.42	115.30
1	B	335	ILE	O-C-N	-5.70	113.59	122.70
1	C	40	VAL	CA-CB-CG1	-5.70	102.36	110.90
1	C	227	ASP	CB-CG-OD1	5.69	123.42	118.30
1	D	832	GLN	CA-CB-CG	5.69	125.92	113.40
1	A	128	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	309	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	634	PRO	N-CA-C	5.68	126.86	112.10
1	B	661	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	489	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	165	ILE	CA-C-N	-5.67	104.71	117.20
1	D	365	TRP	CD1-CG-CD2	5.67	110.84	106.30
1	C	413	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	138	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	730	GLU	N-CA-C	-5.67	95.70	111.00
1	A	169	LYS	CA-CB-CG	5.66	125.86	113.40
1	C	95	LEU	CA-C-N	5.66	129.65	117.20
1	D	598	VAL	CG1-CB-CG2	-5.66	101.84	110.90
1	A	240	THR	CA-CB-CG2	5.66	120.32	112.40
1	B	357	GLU	O-C-N	-5.66	113.65	122.70
1	D	769	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	679	MET	CA-CB-CG	5.65	122.91	113.30
1	C	390	HIS	CA-CB-CG	5.65	123.21	113.60
1	B	281	PRO	N-CA-C	5.65	126.80	112.10
1	B	797	TRP	CD1-CG-CD2	5.65	110.82	106.30
1	C	525	VAL	CA-CB-CG1	-5.65	102.42	110.90
1	A	584	ILE	CA-CB-CG2	-5.64	99.62	110.90
1	A	524	TYR	CB-CG-CD1	-5.64	117.62	121.00
1	C	797	TRP	CB-CG-CD1	-5.64	119.67	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	658	PRO	O-C-N	-5.64	113.68	122.70
1	A	474	LEU	CA-CB-CG	5.63	128.26	115.30
1	A	776	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D	344	LEU	CB-CG-CD1	-5.63	101.42	111.00
1	D	240	THR	CA-CB-CG2	5.63	120.29	112.40
1	D	67	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	D	773	VAL	CA-CB-CG2	-5.63	102.46	110.90
1	B	262	TYR	CA-CB-CG	-5.63	102.71	113.40
1	D	390	HIS	CA-CB-CG	5.62	123.16	113.60
1	A	160	ARG	CB-CG-CD	-5.62	96.99	111.60
1	D	279	LEU	CB-CG-CD2	5.62	120.55	111.00
1	D	444	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	D	74	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	D	646	GLU	CA-CB-CG	5.60	125.73	113.40
1	D	184	ARG	CA-CB-CG	5.60	125.72	113.40
1	D	765	LEU	CB-CG-CD2	-5.60	101.48	111.00
1	D	361	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	B	41	LYS	CA-CB-CG	5.59	125.70	113.40
1	A	320	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	604	MET	CG-SD-CE	-5.59	91.26	100.20
1	D	184	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	D	824	ILE	CG1-CB-CG2	-5.57	99.15	111.40
1	D	589	ARG	CA-CB-CG	5.57	125.65	113.40
1	B	493	VAL	CA-CB-CG2	-5.57	102.55	110.90
1	A	50	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	509	GLU	CA-CB-CG	5.56	125.63	113.40
1	D	322	VAL	CG1-CB-CG2	5.56	119.80	110.90
1	D	575	ARG	N-CA-C	5.56	126.01	111.00
1	C	267	LEU	CA-CB-CG	-5.56	102.52	115.30
1	D	193	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	493	VAL	CA-CB-CG2	5.55	119.23	110.90
1	C	714	ARG	CA-CB-CG	5.55	125.62	113.40
1	D	584	ILE	CG1-CB-CG2	-5.55	99.18	111.40
1	A	823	GLU	CA-CB-CG	5.55	125.61	113.40
1	B	138	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	501	GLU	CA-CB-CG	5.54	125.58	113.40
1	D	365	TRP	CB-CG-CD1	-5.53	119.81	127.00
1	A	553	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	773	VAL	CA-CB-CG2	-5.53	102.61	110.90
1	D	378	THR	CA-C-N	-5.53	105.04	117.20
1	A	825	TRP	CG-CD2-CE3	5.53	138.87	133.90
1	B	739	ARG	NE-CZ-NH2	5.53	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	515	LEU	N-CA-C	5.53	125.92	111.00
1	A	465	LYS	CB-CG-CD	5.52	125.95	111.60
1	B	740	GLN	CA-CB-CG	5.52	125.54	113.40
1	D	300	VAL	CA-CB-CG2	-5.52	102.62	110.90
1	D	174	TRP	CG-CD1-NE1	-5.51	104.58	110.10
1	B	126	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	B	203	TYR	CB-CG-CD1	5.51	124.30	121.00
1	B	185	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	B	259	VAL	N-CA-C	5.50	125.86	111.00
1	C	629	VAL	CA-CB-CG1	5.50	119.16	110.90
1	D	833	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	324	THR	CA-CB-CG2	5.50	120.10	112.40
1	A	300	VAL	CA-CB-CG1	5.49	119.14	110.90
1	B	266	VAL	N-CA-C	-5.49	96.17	111.00
1	A	575	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	D	318	CYS	CA-CB-SG	5.49	123.88	114.00
1	D	820	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	D	444	LEU	CA-CB-CG	5.48	127.90	115.30
1	D	755	PRO	CA-N-CD	-5.48	103.83	111.50
1	C	426	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	D	16	ARG	CA-C-N	-5.46	105.28	116.20
1	C	166	PHE	N-CA-C	5.46	125.75	111.00
1	A	93	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	599	VAL	CA-C-N	5.45	132.37	117.10
1	B	524	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	A	18	LEU	CA-CB-CG	5.44	127.82	115.30
1	C	238	VAL	CG1-CB-CG2	-5.44	102.20	110.90
1	B	379	VAL	CB-CA-C	5.43	121.72	111.40
1	D	97	ASN	N-CA-CB	-5.43	100.82	110.60
1	D	75	TYR	N-CA-CB	5.43	120.38	110.60
1	D	455	VAL	CG1-CB-CG2	-5.43	102.21	110.90
1	C	424	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	825	TRP	CG-CD1-NE1	-5.42	104.68	110.10
1	C	380	ILE	N-CA-C	-5.42	96.35	111.00
1	A	179	ALA	N-CA-CB	5.42	117.69	110.10
1	D	716	GLU	CA-CB-CG	5.42	125.33	113.40
1	A	720	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	325	ASN	O-C-N	5.40	131.34	122.70
1	D	772	LYS	CA-CB-CG	5.39	125.26	113.40
1	A	165	ILE	N-CA-C	-5.39	96.45	111.00
1	C	390	HIS	N-CA-CB	5.39	120.30	110.60
1	A	385	GLU	CA-CB-CG	5.38	125.24	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	650	VAL	CA-C-N	5.38	129.04	117.20
1	B	769	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	32	ASN	CA-CB-CG	-5.38	101.57	113.40
1	D	807	THR	N-CA-CB	-5.38	100.08	110.30
1	B	174	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	552	GLU	N-CA-C	-5.37	96.49	111.00
1	C	548	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	A	767	HIS	CA-C-N	5.37	129.02	117.20
1	D	81	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	24	VAL	CA-C-N	5.36	128.99	117.20
1	D	511	TYR	CA-CB-CG	5.36	123.58	113.40
1	B	257	PHE	CA-C-O	5.36	131.35	120.10
1	A	797	TRP	CD1-CG-CD2	5.35	110.58	106.30
1	C	800	MET	CA-CB-CG	-5.35	104.20	113.30
1	C	822	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	398	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	492	LEU	CA-C-N	5.34	128.96	117.20
1	B	749	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	A	308	ILE	CA-CB-CG1	-5.34	100.85	111.00
1	B	195	GLU	CA-CB-CG	5.34	125.15	113.40
1	C	782	LYS	CA-C-N	-5.34	105.45	117.20
1	C	629	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	A	179	ALA	CB-CA-C	-5.33	102.10	110.10
1	C	117	LEU	CA-CB-CG	5.33	127.57	115.30
1	C	396	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	D	60	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	269	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	374	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	D	470	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	453	ASN	CA-CB-CG	5.33	125.12	113.40
1	A	574	LYS	CB-CG-CD	5.33	125.45	111.60
1	D	73	HIS	CA-CB-CG	5.33	122.65	113.60
1	D	109	ASP	CB-CG-OD1	5.33	123.09	118.30
1	D	361	TRP	CB-CG-CD1	-5.33	120.08	127.00
1	D	548	TYR	CB-CG-CD2	-5.33	117.81	121.00
1	A	74	TYR	CA-CB-CG	5.32	123.51	113.40
1	B	64	VAL	CG1-CB-CG2	-5.32	102.38	110.90
1	B	555	VAL	N-CA-C	5.32	125.37	111.00
1	C	49	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	185	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	552	GLU	CA-C-N	-5.32	105.50	117.20
1	A	697	VAL	CA-CB-CG2	-5.32	102.92	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	797	TRP	CB-CG-CD1	-5.32	120.09	127.00
1	D	769	ASP	CA-C-N	-5.32	105.50	117.20
1	A	242	ARG	CG-CD-NE	5.31	122.95	111.80
1	A	762	VAL	CG1-CB-CG2	-5.31	102.41	110.90
1	C	374	TYR	CB-CG-CD2	-5.31	117.82	121.00
1	A	455	VAL	N-CA-C	5.30	125.32	111.00
1	C	250	ASN	N-CA-C	5.30	125.32	111.00
1	A	257	PHE	CA-C-N	-5.30	105.53	117.20
1	C	119	MET	CA-CB-CG	-5.30	104.29	113.30
1	A	510	GLU	N-CA-C	-5.30	96.70	111.00
1	C	569	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	463	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	114	GLN	CA-CB-CG	5.29	125.04	113.40
1	C	314	SER	CA-C-N	-5.29	105.56	117.20
1	C	385	GLU	CA-C-N	-5.29	105.56	117.20
1	B	489	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	189	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	B	277	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	21	VAL	O-C-N	5.27	131.13	122.70
1	B	44	ASN	CA-C-N	5.27	128.79	117.20
1	B	712	GLY	CA-C-N	-5.27	105.61	117.20
1	D	322	VAL	N-CA-CB	-5.27	99.91	111.50
1	D	658	PRO	N-CA-CB	-5.27	96.80	102.60
1	B	259	VAL	CA-C-N	-5.27	105.67	116.20
1	B	365	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	C	60	ARG	NH1-CZ-NH2	5.26	125.19	119.40
1	D	400	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	183	LEU	CA-C-N	-5.26	105.63	117.20
1	A	387	TRP	CB-CG-CD1	-5.26	120.17	127.00
1	D	553	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	182	TRP	CB-CG-CD1	-5.25	120.17	127.00
1	C	93	ARG	N-CA-C	5.25	125.18	111.00
1	B	66	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	269	ARG	CB-CG-CD	-5.25	97.95	111.60
1	C	706	GLU	N-CA-CB	5.25	120.05	110.60
1	D	16	ARG	CB-CA-C	-5.24	99.92	110.40
1	D	233	TYR	CA-C-N	-5.24	105.67	117.20
1	A	316	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	B	67	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	A	574	LYS	CA-CB-CG	5.24	124.92	113.40
1	C	266	VAL	CG1-CB-CG2	5.24	119.28	110.90
1	A	181	ASP	CA-CB-CG	5.23	124.92	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	217	ASP	CA-CB-CG	5.23	124.91	113.40
1	C	322	VAL	CA-CB-CG2	-5.23	103.06	110.90
1	D	121	GLU	CA-CB-CG	5.23	124.90	113.40
1	D	64	VAL	CG1-CB-CG2	-5.22	102.54	110.90
1	B	387	TRP	CB-CG-CD1	-5.22	120.21	127.00
1	B	178	GLU	CA-CB-CG	5.22	124.88	113.40
1	D	501	GLU	CA-CB-CG	5.22	124.88	113.40
1	D	395	LEU	CB-CA-C	-5.22	100.29	110.20
1	B	90	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	C	319	ARG	N-CA-C	-5.22	96.91	111.00
1	D	724	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	174	TRP	CB-CG-CD1	-5.21	120.22	127.00
1	A	230	VAL	CA-C-N	5.20	131.67	117.10
1	C	426	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	555	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	C	67	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	D	357	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	B	613	TYR	CB-CG-CD1	5.19	124.12	121.00
1	C	562	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	B	44	ASN	CA-C-O	-5.19	109.21	120.10
1	B	190	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	B	427	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	355	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	458	ILE	CB-CA-C	-5.17	101.25	111.60
1	D	166	PHE	N-CA-C	5.17	124.96	111.00
1	C	369	VAL	CG1-CB-CG2	-5.17	102.63	110.90
1	D	174	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	D	522	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	270	ASN	CA-C-N	-5.16	105.85	117.20
1	A	797	TRP	CG-CD2-CE3	5.15	138.54	133.90
1	A	46	ALA	CA-C-N	-5.15	105.86	117.20
1	B	750	PHE	CA-C-N	5.15	128.52	117.20
1	D	374	TYR	CA-CB-CG	5.15	123.18	113.40
1	C	18	LEU	O-C-N	5.14	130.93	122.70
1	A	324	THR	CA-CB-CG2	-5.14	105.20	112.40
1	D	592	LYS	CB-CG-CD	-5.14	98.23	111.60
1	A	803	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	380	ILE	N-CA-C	5.14	124.88	111.00
1	B	224	MET	CG-SD-CE	-5.14	91.98	100.20
1	D	321	PRO	CA-N-CD	-5.14	104.31	111.50
1	B	831	ARG	CA-CB-CG	5.13	124.70	113.40
1	C	174	TRP	CB-CG-CD1	-5.13	120.33	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	262	TYR	N-CA-C	5.13	124.86	111.00
1	C	193	ARG	CG-CD-NE	-5.13	101.03	111.80
1	A	552	GLU	O-C-N	5.13	130.91	122.70
1	A	795	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	740	GLN	CA-C-N	5.13	128.48	117.20
1	C	697	VAL	CA-C-N	5.13	128.48	117.20
1	B	279	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	A	479	PHE	N-CA-C	5.12	124.81	111.00
1	B	257	PHE	CA-CB-CG	-5.12	101.62	113.90
1	B	387	TRP	CG-CD2-CE3	5.12	138.50	133.90
1	C	195	GLU	CB-CA-C	-5.12	100.17	110.40
1	C	676	THR	CA-C-N	5.11	126.43	116.20
1	B	81	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	539	GLN	CA-CB-CG	5.11	124.64	113.40
1	D	795	ARG	CB-CG-CD	-5.11	98.32	111.60
1	C	720	ARG	CA-CB-CG	5.10	124.61	113.40
1	C	305	GLN	CB-CG-CD	5.09	124.85	111.60
1	C	365	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	C	10	ARG	CB-CG-CD	5.09	124.84	111.60
1	B	88	GLU	CB-CA-C	-5.09	100.23	110.40
1	C	528	GLU	CA-CB-CG	5.09	124.59	113.40
1	A	640	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	B	153	ALA	O-C-N	-5.08	114.57	122.70
1	D	380	ILE	CA-CB-CG2	-5.08	100.74	110.90
1	A	659	ALA	CB-CA-C	-5.08	102.48	110.10
1	C	825	TRP	CB-CG-CD1	-5.08	120.40	127.00
1	C	676	THR	CA-CB-CG2	5.08	119.51	112.40
1	A	650	VAL	N-CA-CB	-5.08	100.33	111.50
1	B	229	PRO	N-CA-C	5.08	125.30	112.10
1	C	390	HIS	CB-CA-C	-5.08	100.25	110.40
1	D	755	PRO	N-CA-C	5.08	125.30	112.10
1	A	769	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	D	486	ILE	CA-C-N	5.07	128.35	117.20
1	B	395	LEU	CA-CB-CG	5.07	126.95	115.30
1	D	714	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	218	THR	N-CA-C	5.06	124.67	111.00
1	B	620	ILE	O-C-N	-5.06	114.60	122.70
1	C	712	GLY	CA-C-N	-5.06	106.06	117.20
1	D	495	CYS	CA-CB-SG	-5.06	104.89	114.00
1	C	690	GLY	CA-C-N	-5.06	106.06	117.20
1	D	40	VAL	CA-CB-CG1	-5.06	103.31	110.90
1	A	357	GLU	OE1-CD-OE2	-5.06	117.23	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	468	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	D	676	THR	N-CA-CB	-5.06	100.69	110.30
1	C	681	PHE	CB-CA-C	-5.05	100.29	110.40
1	D	256	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	67	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	D	361	TRP	CG-CD2-CE3	5.05	138.45	133.90
1	A	572	GLU	CA-CB-CG	-5.05	102.29	113.40
1	B	319	ARG	N-CA-C	5.05	124.64	111.00
1	C	533	ASP	CB-CG-OD1	5.05	122.84	118.30
1	B	432	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	B	585	THR	CA-CB-CG2	5.04	119.46	112.40
1	D	25	THR	CA-C-N	5.04	128.29	117.20
1	B	274	ASN	N-CA-CB	-5.04	101.53	110.60
1	A	182	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	C	174	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	D	499	LEU	CA-C-N	5.04	128.28	117.20
1	D	672	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	D	445	CYS	CA-CB-SG	5.04	123.06	114.00
1	D	569	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	20	GLY	CA-C-O	5.03	129.66	120.60
1	A	308	ILE	N-CA-CB	-5.03	99.22	110.80
1	B	37	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	B	491	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	B	651	SER	CA-CB-OG	5.02	124.76	111.20
1	C	94	THR	N-CA-CB	-5.02	100.76	110.30
1	A	444	LEU	CA-CB-CG	5.02	126.84	115.30
1	A	467	ILE	CB-CA-C	-5.02	101.56	111.60
1	B	257	PHE	O-C-N	5.02	130.73	122.70
1	C	525	VAL	CB-CA-C	-5.02	101.86	111.40
1	B	640	LEU	CA-CB-CG	5.02	126.84	115.30
1	C	146	SER	CA-C-N	5.02	128.24	117.20
1	B	662	LEU	CB-CG-CD1	-5.01	102.47	111.00
1	C	613	TYR	CA-C-N	-5.01	106.18	117.20
1	C	816	THR	CA-CB-CG2	-5.01	105.39	112.40
1	D	746	SER	CA-C-N	5.01	128.23	117.20
1	B	203	TYR	CA-C-N	5.01	126.22	116.20
1	B	88	GLU	CA-CB-CG	5.01	124.42	113.40
1	D	150	LEU	CA-CB-CG	5.00	126.81	115.30
1	A	506	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	233	TYR	Sidechain
1	A	242	ARG	Sidechain
1	A	256	ASP	Mainchain
1	A	280	TYR	Peptide
1	A	418	PHE	Peptide
1	A	51	TYR	Sidechain
1	A	733	ASP	Mainchain
1	A	836	ALA	Peptide
1	B	280	TYR	Peptide
1	B	320	ASP	Peptide
1	B	341	HIS	Peptide
1	B	380	ILE	Peptide
1	B	657	ILE	Peptide
1	B	751	SER	Peptide
1	B	834	LEU	Peptide
1	B	836	ALA	Peptide
1	C	18	LEU	Mainchain
1	C	226	TYR	Sidechain
1	C	320	ASP	Peptide
1	C	52	TYR	Sidechain
1	C	613	TYR	Sidechain
1	C	657	ILE	Peptide
1	C	69	ARG	Sidechain
1	C	75	TYR	Sidechain
1	C	780	TYR	Sidechain
1	C	836	ALA	Peptide
1	D	19	ALA	Mainchain
1	D	320	ASP	Peptide
1	D	52	TYR	Sidechain
1	D	558	ASN	Peptide
1	D	657	ILE	Peptide
1	D	836	ALA	Peptide

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	6703	0	6658	305	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6703	0	6659	285	0
1	C	6703	0	6653	290	0
1	D	6704	0	6659	390	0
2	A	15	0	0	0	0
2	B	15	0	0	1	0
2	C	15	0	0	4	0
2	D	15	0	0	2	0
All	All	26873	0	26629	1223	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1223) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:PHE:CE2	1:D:18:LEU:HB3	1.46	1.51
1:C:37:PHE:HE2	1:D:18:LEU:CB	1.32	1.42
1:C:37:PHE:CE2	1:D:18:LEU:CB	2.06	1.32
1:C:15:VAL:O	1:C:17:GLY:N	1.79	1.14
2:C:900:SO4:O3	1:D:43:ARG:NH2	1.79	1.13
1:D:16:ARG:HG3	1:D:17:GLY:N	1.64	1.07
1:C:707:ASN:HA	1:C:800:MET:SD	1.97	1.03
1:C:37:PHE:CE2	1:D:18:LEU:HB2	1.95	1.02
1:D:19:ALA:HB3	1:D:62:HIS:NE2	1.77	1.00
1:D:16:ARG:CG	1:D:17:GLY:N	2.14	0.99
1:C:165:ILE:HB	1:C:279:LEU:HD13	1.43	0.99
1:D:16:ARG:HG3	1:D:17:GLY:CA	1.95	0.97
1:A:32:ASN:HD21	1:B:13:ILE:HA	1.26	0.96
1:D:19:ALA:CB	1:D:62:HIS:NE2	2.31	0.93
1:C:33:ARG:HG2	1:D:18:LEU:HG	1.52	0.92
1:D:165:ILE:HD11	1:D:281:PRO:HA	1.53	0.91
1:C:492:LEU:HG	1:C:683:LEU:HD22	1.53	0.90
1:A:550:GLU:HA	1:A:554:LYS:HA	1.53	0.90
1:C:37:PHE:CZ	1:D:18:LEU:HB2	2.07	0.90
1:C:289:LYS:CB	1:C:289:LYS:CD	2.50	0.90
1:A:21:VAL:HA	1:A:24:VAL:HB	1.53	0.89
1:D:80:LYS:HE3	1:D:334:ALA:HB2	1.55	0.88
1:A:100:VAL:HG21	1:A:494:LEU:HD22	1.56	0.86
1:D:18:LEU:O	1:D:19:ALA:HB2	1.75	0.86
1:D:171:CYS:HB2	1:D:176:MET:SD	2.15	0.86
1:D:707:ASN:HA	1:D:800:MET:SD	2.16	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:MET:SD	1:B:718:VAL:HA	2.16	0.85
1:C:15:VAL:HG23	1:C:69:ARG:HH21	1.41	0.85
1:D:766:MET:HE3	1:D:774:PHE:HE2	1.41	0.85
1:C:21:VAL:O	1:C:23:ASN:N	2.09	0.84
1:B:21:VAL:HA	1:B:24:VAL:HB	1.58	0.83
1:D:455:VAL:HG13	1:D:484:ASN:ND2	1.93	0.83
1:D:83:TYR:HE1	1:D:333:VAL:HG13	1.44	0.83
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.60	0.83
1:B:569:ARG:O	1:B:569:ARG:HG2	1.79	0.82
1:D:605:ILE:HG21	1:D:623:ILE:HD13	1.62	0.81
1:C:165:ILE:HD11	1:C:281:PRO:HA	1.61	0.81
1:B:171:CYS:SG	1:B:176:MET:SD	2.78	0.81
1:B:81:ARG:HG2	1:B:155:TYR:HE1	1.45	0.80
1:A:299:VAL:O	1:A:303:THR:HB	1.81	0.80
1:C:550:GLU:HA	1:C:554:LYS:HA	1.64	0.80
1:D:463:LEU:HD23	1:D:467:ILE:HD12	1.65	0.79
1:C:18:LEU:HG	1:D:33:ARG:HD3	1.65	0.79
1:C:173:GLY:HA2	1:C:624:THR:HG21	1.64	0.78
1:A:322:VAL:HG13	1:A:325:ASN:HB2	1.65	0.78
1:B:732:TYR:HE1	1:B:742:ILE:HG21	1.47	0.78
1:A:630:VAL:HG21	1:A:642:VAL:HG23	1.65	0.78
1:C:18:LEU:HB3	1:D:37:PHE:HE2	1.47	0.78
1:B:87:LEU:HD11	1:B:299:VAL:HG11	1.64	0.77
1:C:456:ALA:HB2	1:C:674:SER:HB2	1.66	0.77
1:C:33:ARG:CG	1:D:18:LEU:HG	2.14	0.77
1:C:37:PHE:CZ	1:D:18:LEU:CB	2.68	0.77
1:D:18:LEU:O	1:D:19:ALA:CB	2.31	0.76
1:A:511:TYR:HB2	1:A:518:LEU:HD12	1.66	0.76
1:C:15:VAL:CG2	1:C:69:ARG:HH21	1.97	0.76
1:C:96:GLN:O	1:C:100:VAL:HG13	1.85	0.76
1:A:136:LEU:HD11	1:A:339:ASP:HB2	1.68	0.76
1:D:193:ARG:HB2	1:D:225:PRO:HG2	1.67	0.76
1:C:18:LEU:HB3	1:D:37:PHE:CE2	2.22	0.75
1:C:522:LEU:HD13	1:C:806:ALA:HB3	1.67	0.75
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.68	0.74
1:C:15:VAL:C	1:C:17:GLY:H	1.87	0.74
1:B:198:LEU:HD11	1:B:302:ALA:HA	1.68	0.74
1:C:742:ILE:HD11	1:C:774:PHE:HZ	1.52	0.74
1:A:259:VAL:HG21	1:A:263:ILE:HG22	1.68	0.74
1:C:764:MET:SD	1:C:769:ASP:HA	2.27	0.74
1:D:550:GLU:HA	1:D:554:LYS:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ILE:HD13	1:A:679:MET:HB2	1.70	0.73
1:B:133:ASN:OD1	1:B:165:ILE:HG21	1.88	0.73
1:A:815:ARG:HD2	1:A:819:GLN:OE1	1.88	0.73
1:B:578:LEU:HD23	1:B:666:ILE:HD13	1.70	0.73
1:B:678:ASN:HB3	1:B:699:MET:SD	2.29	0.72
1:D:791:TYR:HA	1:D:797:TRP:CD1	2.23	0.72
1:A:195:GLU:HB2	1:A:196:PHE:HD1	1.54	0.72
1:B:343:SER:HB3	1:B:445:CYS:SG	2.30	0.72
2:C:900:SO4:O3	1:D:43:ARG:CZ	2.37	0.72
1:C:689:ILE:HA	1:C:709:PHE:HB2	1.72	0.72
1:C:326:PHE:HA	1:C:329:PHE:HB2	1.70	0.72
1:C:15:VAL:HG23	1:C:69:ARG:NH2	2.05	0.71
1:C:224:MET:SD	1:C:247:LYS:HD3	2.30	0.71
1:C:495:CYS:HB2	1:C:658:PRO:HG2	1.73	0.71
1:A:509:GLU:HG3	1:A:512:ILE:HB	1.72	0.71
1:B:336:GLN:NE2	1:B:825:TRP:HE1	1.88	0.71
1:A:784:GLN:HA	1:A:787:VAL:HB	1.71	0.71
1:A:822:ARG:HA	1:A:826:GLY:O	1.91	0.70
1:A:322:VAL:O	1:A:325:ASN:HB2	1.90	0.70
1:A:615:MET:HE1	1:A:761:ILE:HG23	1.74	0.70
1:D:804:ASN:O	1:D:807:THR:HB	1.91	0.70
1:A:326:PHE:HA	1:A:329:PHE:HB2	1.73	0.70
1:C:423:ASP:HA	1:C:426:ARG:HG2	1.74	0.69
1:C:576:GLN:H	1:C:576:GLN:HE21	1.39	0.69
1:C:53:PHE:CE2	1:C:188:PRO:HG3	2.27	0.69
1:C:783:CYS:SG	1:C:786:ARG:NH2	2.65	0.69
1:C:784:GLN:O	1:C:787:VAL:HB	1.92	0.69
1:B:482:LYS:HD2	1:B:819:GLN:HB3	1.75	0.69
1:A:81:ARG:HG2	1:A:155:TYR:HE2	1.57	0.69
1:B:81:ARG:HG2	1:B:155:TYR:CE1	2.27	0.69
1:D:783:CYS:HA	1:D:786:ARG:HE	1.58	0.69
1:D:225:PRO:HB2	1:D:242:ARG:HD2	1.75	0.69
1:D:363:LYS:O	1:D:366:GLU:HB3	1.93	0.68
1:A:348:GLU:O	1:A:352:VAL:HG23	1.94	0.68
1:D:231:PRO:HA	1:D:238:VAL:HG22	1.73	0.68
1:A:194:PRO:HA	1:A:224:MET:SD	2.34	0.68
1:A:292:ARG:HB3	1:A:387:TRP:HH2	1.59	0.68
1:A:588:ASN:HD21	1:A:744:GLN:HE22	1.41	0.68
1:D:748:GLY:HA3	1:D:755:PRO:HG3	1.75	0.68
1:A:732:TYR:HA	1:A:738:LEU:HD23	1.76	0.68
1:C:175:GLN:OE1	1:C:609:ALA:HB3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:TYR:HD2	1:D:671:THR:HB	1.58	0.68
1:D:173:GLY:HA2	1:D:624:THR:HG21	1.75	0.67
1:D:455:VAL:HG13	1:D:484:ASN:HD22	1.59	0.67
1:C:665:GLN:HG2	1:C:678:ASN:HD22	1.57	0.67
1:D:49:ARG:HA	1:D:125:ILE:HG21	1.76	0.67
1:C:37:PHE:HE2	1:D:18:LEU:HB3	0.53	0.67
1:D:350:MET:SD	1:D:365:TRP:HE3	2.18	0.67
1:D:692:MET:HB3	1:D:714:ARG:HD2	1.75	0.67
1:C:741:ILE:HG22	1:C:744:GLN:HG3	1.76	0.67
1:B:529:ALA:HA	1:B:532:ARG:NH1	2.09	0.67
1:D:160:ARG:NH2	1:D:183:LEU:HD21	2.09	0.67
1:D:604:MET:HA	1:D:643:ILE:O	1.95	0.67
1:C:711:PHE:CE1	1:C:780:TYR:HB2	2.30	0.67
1:D:652:LEU:O	1:D:656:VAL:HG23	1.95	0.67
1:A:88:GLU:HG2	1:A:132:GLY:HA2	1.77	0.66
1:B:271:LEU:HA	1:B:274:ASN:HB3	1.76	0.66
1:D:562:LEU:HD13	1:D:601:ARG:NH1	2.11	0.66
1:D:19:ALA:HB1	1:D:62:HIS:NE2	2.10	0.66
1:D:68:ILE:HG22	1:D:72:GLN:HE21	1.59	0.66
1:D:21:VAL:O	1:D:23:ASN:N	2.25	0.66
1:B:230:VAL:HG22	1:B:239:ASN:HB2	1.78	0.65
1:B:258:ASN:OD1	1:B:259:VAL:HG22	1.96	0.65
1:A:439:ILE:HG22	1:A:441:MET:SD	2.36	0.65
1:D:16:ARG:CG	1:D:17:GLY:CA	2.67	0.65
1:D:21:VAL:C	1:D:23:ASN:H	1.98	0.65
1:C:15:VAL:O	1:C:17:GLY:CA	2.45	0.65
1:D:741:ILE:HA	1:D:744:GLN:HG2	1.79	0.65
1:A:32:ASN:ND2	1:B:13:ILE:HA	2.05	0.65
1:A:138:ARG:NH1	1:A:142:CYS:SG	2.69	0.65
1:B:481:ASN:HD22	1:B:482:LYS:N	1.94	0.65
1:B:388:PRO:HD2	1:B:391:LEU:HD13	1.78	0.65
1:D:796:GLU:HA	1:D:799:ARG:HG3	1.79	0.65
1:A:336:GLN:HG3	1:A:825:TRP:HE1	1.60	0.65
1:B:557:ILE:HG13	1:B:602:THR:HG21	1.79	0.65
1:A:174:TRP:CH2	1:D:435:ALA:HB2	2.33	0.64
1:D:139:LEU:HD21	1:D:484:ASN:ND2	2.12	0.64
1:D:265:ALA:O	1:D:268:ASP:HB3	1.96	0.64
1:B:336:GLN:HE21	1:B:825:TRP:HE1	1.44	0.64
1:D:818:ALA:O	1:D:822:ARG:HG2	1.96	0.64
1:B:389:VAL:HG12	1:B:439:ILE:HD12	1.79	0.64
1:B:161:TYR:HA	1:B:276:SER:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:721:LEU:HD23	1:D:772:LYS:HE2	1.80	0.64
1:A:22:GLU:H	1:A:24:VAL:HB	1.63	0.64
1:B:536:LYS:O	1:B:540:GLU:HG2	1.98	0.64
1:C:546:ALA:HB1	1:C:557:ILE:HG21	1.78	0.64
1:B:492:LEU:HD21	1:B:499:LEU:HD23	1.79	0.64
1:A:488:PRO:HB3	1:A:515:LEU:HD13	1.80	0.64
1:B:320:ASP:HA	1:B:324:THR:HA	1.79	0.64
1:D:491:TRP:C	1:D:495:CYS:SG	2.77	0.64
1:B:395:LEU:O	1:B:396:LEU:HD12	1.98	0.63
1:D:151:GLY:HA3	1:D:830:SER:HB3	1.81	0.63
1:D:254:LEU:HA	1:D:259:VAL:HG22	1.79	0.63
1:D:766:MET:HE3	1:D:774:PHE:CE2	2.29	0.63
1:A:110:GLU:O	1:A:114:GLN:HG3	1.99	0.63
1:C:304:LEU:HD12	1:C:307:ILE:HD12	1.80	0.63
1:D:550:GLU:HG2	1:D:555:VAL:HG23	1.80	0.63
1:B:575:ARG:HH22	1:B:776:ASP:HB2	1.62	0.63
1:D:574:LYS:HA	1:D:667:SER:OG	1.98	0.63
2:C:900:SO4:S	1:D:43:ARG:NH2	2.69	0.63
1:D:414:VAL:HG11	1:D:428:MET:HG3	1.81	0.63
1:A:165:ILE:HG12	1:A:279:LEU:HB3	1.78	0.63
1:D:89:PHE:O	1:D:131:LEU:HB2	1.98	0.63
1:A:455:VAL:O	1:A:483:THR:HA	1.98	0.63
1:A:74:TYR:OH	1:A:153:ALA:HA	1.99	0.62
1:B:423:ASP:HA	1:B:426:ARG:HG2	1.80	0.62
1:D:206:VAL:HA	1:D:214:LYS:O	1.98	0.62
1:B:506:ARG:HB2	1:B:507:ILE:HG23	1.80	0.62
1:D:170:ILE:HG12	1:D:646:GLU:HB3	1.80	0.62
1:A:307:ILE:HG21	1:A:335:ILE:HD11	1.79	0.62
1:C:521:LEU:HD21	1:C:530:PHE:HZ	1.64	0.62
1:D:16:ARG:HG3	1:D:17:GLY:HA2	1.80	0.62
1:A:834:LEU:HG	1:A:835:PRO:HD2	1.81	0.62
1:C:403:ILE:HG21	1:C:439:ILE:HD13	1.80	0.62
1:A:348:GLU:HA	1:A:399:HIS:HE1	1.64	0.62
1:B:533:ASP:O	1:B:537:VAL:HG23	2.00	0.62
1:D:403:ILE:HG21	1:D:439:ILE:HD12	1.81	0.62
1:D:593:GLU:O	1:D:596:LYS:HB2	1.99	0.62
1:D:143:PHE:CG	1:D:817:ILE:HD11	2.35	0.62
1:D:165:ILE:HD11	1:D:281:PRO:CA	2.29	0.62
1:B:575:ARG:HD2	1:B:668:THR:OG1	1.98	0.61
1:D:338:ASN:OD1	1:D:377:HIS:HE1	1.82	0.61
1:D:565:VAL:HG12	1:D:604:MET:HB2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ALA:HB1	1:A:804:ASN:HD22	1.65	0.61
1:C:60:ARG:HA	1:C:63:LEU:HB2	1.83	0.61
1:A:21:VAL:HA	1:A:24:VAL:CB	2.27	0.61
1:A:149:THR:HG21	1:A:489:ARG:NH2	2.16	0.61
1:A:825:TRP:O	1:A:827:VAL:HG22	2.00	0.61
1:B:503:ILE:O	1:B:507:ILE:HG12	2.00	0.61
1:B:293:LEU:HD23	1:B:395:LEU:HD23	1.82	0.61
1:C:703:ALA:HA	1:C:807:THR:HG21	1.83	0.61
1:B:208:HIS:HA	1:B:213:ALA:HA	1.83	0.61
1:B:600:PRO:HA	1:B:639:ARG:O	2.00	0.61
1:A:157:TYR:HE1	1:A:242:ARG:HD3	1.65	0.61
1:D:252:PHE:HB2	1:D:269:ARG:NH2	2.16	0.61
1:D:322:VAL:O	1:D:325:ASN:HB2	2.01	0.61
1:A:409:ARG:O	1:A:412:ASN:HB2	2.01	0.61
1:A:426:ARG:CZ	1:D:755:PRO:HD2	2.30	0.61
1:D:235:ASN:HB2	1:D:833:ARG:HA	1.82	0.61
1:D:515:LEU:HG	1:D:518:LEU:HD12	1.82	0.61
1:A:357:GLU:O	1:A:358:ARG:HB2	2.00	0.60
1:A:381:PRO:HA	1:A:384:LEU:HD13	1.83	0.60
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.82	0.60
1:B:791:TYR:HA	1:B:797:TRP:CD1	2.36	0.60
1:D:793:ASN:HD21	1:D:796:GLU:HB3	1.66	0.60
1:A:601:ARG:HH12	1:A:787:VAL:HG12	1.67	0.60
1:D:99:MET:SD	1:D:119:MET:SD	3.00	0.60
1:D:373:ALA:HA	1:D:449:SER:HB3	1.83	0.60
1:B:511:TYR:HA	1:B:514:ASP:O	2.02	0.60
1:C:424:ARG:HA	1:C:427:ARG:NH2	2.16	0.60
1:D:175:GLN:HE21	1:D:617:LYS:HE2	1.66	0.60
1:D:351:ARG:O	1:D:355:ASP:HB2	2.00	0.60
1:C:598:VAL:HG12	1:C:639:ARG:HH21	1.67	0.60
1:D:330:PRO:HG3	1:D:367:VAL:HG13	1.83	0.60
1:A:653:ALA:HA	1:A:656:VAL:HG12	1.83	0.60
1:B:267:LEU:HD22	1:D:262:TYR:HE2	1.66	0.60
1:B:590:ILE:HG21	1:B:636:VAL:HG23	1.83	0.60
1:B:741:ILE:HA	1:B:744:GLN:HE21	1.66	0.60
1:C:675:GLY:HA3	1:C:678:ASN:OD1	2.01	0.60
1:D:19:ALA:HB1	1:D:62:HIS:CE1	2.37	0.60
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.67	0.60
1:A:432:GLU:HB3	1:A:438:ARG:HG3	1.83	0.59
1:B:495:CYS:HB3	1:B:654:GLU:HB2	1.83	0.59
1:C:322:VAL:O	1:C:325:ASN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:GLU:OE1	1:D:22:GLU:HA	2.02	0.59
1:B:187:ASN:ND2	1:B:189:TRP:H	2.01	0.59
1:B:267:LEU:HD22	1:D:262:TYR:CE2	2.37	0.59
1:B:669:ALA:HA	1:B:693:ASP:HB2	1.84	0.59
1:C:792:LYS:NZ	1:C:792:LYS:HB3	2.17	0.59
1:C:330:PRO:HG2	1:C:370:LYS:HE3	1.83	0.59
1:C:337:LEU:HG	1:C:342:PRO:HB2	1.83	0.59
1:D:269:ARG:O	1:D:273:GLU:HB3	2.03	0.59
1:A:547:ALA:O	1:A:551:ARG:HB2	2.03	0.59
1:B:173:GLY:HA2	1:B:624:THR:HG21	1.84	0.59
1:C:173:GLY:HA2	1:C:624:THR:CG2	2.32	0.59
1:B:128:ASP:OD1	1:B:651:SER:HB3	2.02	0.59
1:B:678:ASN:ND2	1:B:695:ALA:HB3	2.17	0.59
1:C:692:MET:HG2	1:C:710:ILE:HD12	1.85	0.59
1:D:521:LEU:HA	1:D:524:TYR:CD1	2.37	0.59
1:D:729:GLN:HG3	1:D:732:TYR:HB3	1.84	0.59
1:A:414:VAL:HG12	1:A:425:LEU:HD22	1.85	0.59
1:C:536:LYS:HZ2	1:C:540:GLU:CD	2.05	0.59
1:D:573:TYR:CD2	1:D:671:THR:HB	2.37	0.59
1:A:403:ILE:HG21	1:A:439:ILE:HD13	1.83	0.59
1:A:502:ILE:HD12	1:A:530:PHE:HE1	1.68	0.59
1:B:67:TRP:HA	1:B:238:VAL:HB	1.85	0.59
1:C:32:ASN:OD1	1:D:13:ILE:HG22	2.03	0.59
1:D:792:LYS:NZ	1:D:792:LYS:HB3	2.18	0.59
1:A:195:GLU:HB2	1:A:196:PHE:CD1	2.37	0.59
1:B:222:LEU:HG	1:B:249:PRO:HG3	1.85	0.59
1:B:236:ASN:HD22	1:B:836:ALA:HB3	1.68	0.58
1:B:459:HIS:CD2	1:B:673:ALA:HB1	2.38	0.58
1:D:90:TYR:HD2	1:D:138:ARG:HB2	1.68	0.58
1:A:609:ALA:HB2	1:A:620:ILE:HD11	1.83	0.58
1:B:88:GLU:HB3	1:B:132:GLY:HA2	1.85	0.58
1:D:150:LEU:HD12	1:D:829:PRO:HB3	1.85	0.58
1:A:231:PRO:HA	1:A:238:VAL:HA	1.85	0.58
1:B:161:TYR:CE2	1:B:279:LEU:HG	2.39	0.58
1:C:192:ALA:HB2	1:C:226:TYR:CE2	2.38	0.58
1:B:319:ARG:HG2	1:B:321:PRO:HD2	1.85	0.58
1:D:790:LEU:HD12	1:D:793:ASN:HD22	1.68	0.58
1:D:252:PHE:HB2	1:D:269:ARG:HH21	1.68	0.58
1:D:790:LEU:HG	1:D:797:TRP:CD1	2.39	0.58
1:A:251:ASP:HB3	1:A:255:LYS:HB2	1.84	0.58
1:B:766:MET:HA	1:B:766:MET:HE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:VAL:HG12	1:C:834:LEU:HD23	1.85	0.58
1:C:360:ASP:HB2	1:C:363:LYS:HB2	1.86	0.58
1:D:252:PHE:HD2	1:D:269:ARG:HE	1.48	0.58
1:B:10:ARG:HD2	1:B:13:ILE:HD12	1.86	0.58
1:B:738:LEU:HD12	1:B:741:ILE:HD11	1.86	0.58
1:C:584:ILE:HA	1:C:587:TYR:HB3	1.85	0.58
1:C:661:ASP:HB3	1:C:797:TRP:CH2	2.39	0.58
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.86	0.58
1:A:35:LEU:HD12	1:A:54:ALA:HB2	1.85	0.58
1:B:330:PRO:HD3	1:B:367:VAL:HG13	1.85	0.58
1:B:361:TRP:HH2	1:B:406:ILE:HA	1.68	0.58
1:D:119:MET:O	1:D:123:GLU:HG3	2.03	0.58
1:D:399:HIS:O	1:D:403:ILE:HG13	2.04	0.58
1:D:491:TRP:HA	1:D:495:CYS:SG	2.44	0.58
1:D:689:ILE:HD12	1:D:784:GLN:HE21	1.68	0.57
1:C:488:PRO:HG3	1:C:515:LEU:HD22	1.85	0.57
1:C:748:GLY:HA3	1:C:755:PRO:HA	1.87	0.57
1:D:165:ILE:HB	1:D:279:LEU:HD13	1.86	0.57
1:B:87:LEU:CD1	1:B:299:VAL:HG11	2.34	0.57
1:A:30:ASN:HB3	1:A:58:THR:HG23	1.85	0.57
1:C:582:HIS:HB2	1:C:780:TYR:HE2	1.70	0.57
1:A:203:TYR:HA	1:A:395:LEU:HA	1.87	0.57
1:B:379:VAL:HG22	1:B:380:ILE:H	1.69	0.57
1:C:790:LEU:HG	1:C:797:TRP:HD1	1.68	0.57
1:D:360:ASP:HB2	1:D:363:LYS:HB3	1.86	0.57
1:C:501:GLU:HB3	1:C:502:ILE:HD12	1.86	0.57
1:C:518:LEU:HD12	1:C:805:ILE:HG22	1.86	0.57
1:D:320:ASP:HB3	1:D:321:PRO:O	2.05	0.57
1:D:170:ILE:HA	1:D:174:TRP:O	2.05	0.57
1:D:578:LEU:HA	1:D:581:LEU:HD12	1.87	0.57
1:A:39:LEU:HD21	1:A:53:PHE:HB2	1.87	0.57
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.87	0.57
1:B:138:ARG:NH1	1:B:142:CYS:SG	2.75	0.57
1:B:615:MET:CE	1:B:761:ILE:HG12	2.35	0.57
1:D:589:ARG:HA	1:D:592:LYS:HD3	1.86	0.57
1:B:799:ARG:O	1:B:803:ARG:HD3	2.04	0.57
1:D:486:ILE:HG13	1:D:491:TRP:CD1	2.40	0.57
1:B:82:ILE:HD12	1:B:147:MET:SD	2.45	0.56
1:C:511:TYR:HA	1:C:514:ASP:O	2.05	0.56
1:D:380:ILE:HG22	1:D:382:GLU:HG3	1.87	0.56
1:D:522:LEU:O	1:D:525:VAL:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD12	1:A:817:ILE:HG22	1.86	0.56
1:C:481:ASN:O	1:C:482:LYS:HG2	2.04	0.56
1:C:758:PHE:HB3	1:C:761:ILE:HD12	1.87	0.56
1:D:311:PHE:O	1:D:316:PHE:HB2	2.05	0.56
1:A:133:ASN:OD1	1:A:165:ILE:HG21	2.04	0.56
1:D:511:TYR:HA	1:D:514:ASP:O	2.04	0.56
1:D:655:LYS:HA	1:D:658:PRO:HG2	1.87	0.56
1:C:455:VAL:HG22	1:C:484:ASN:OD1	2.05	0.56
1:C:570:ILE:HB	1:C:609:ALA:HA	1.88	0.56
1:D:569:ARG:NH2	1:D:608:LYS:HB2	2.20	0.56
1:A:199:PRO:HA	1:A:222:LEU:HD23	1.87	0.56
1:A:741:ILE:HA	1:A:744:GLN:NE2	2.21	0.56
1:B:308:ILE:HD13	1:B:352:VAL:HG11	1.86	0.56
1:D:657:ILE:HG21	1:D:680:LLP:O	2.05	0.56
1:D:515:LEU:CD2	1:D:812:SER:HB2	2.35	0.56
1:B:442:ALA:O	1:B:446:ILE:HG13	2.05	0.56
1:C:325:ASN:HB3	1:C:327:ASP:HB2	1.88	0.56
1:A:548:TYR:HD2	1:A:549:LEU:HD12	1.70	0.56
1:B:584:ILE:HG22	1:B:741:ILE:HG22	1.87	0.56
1:D:262:TYR:HB3	1:D:264:GLN:NE2	2.21	0.56
1:D:529:ALA:HA	1:D:532:ARG:NE	2.21	0.56
1:A:191:LYS:HD2	1:A:192:ALA:O	2.06	0.55
1:A:366:GLU:O	1:A:370:LYS:HB2	2.05	0.55
1:C:721:LEU:HD12	1:C:724:ARG:NE	2.21	0.55
1:D:331:ASP:HB2	1:D:332:LYS:HE2	1.86	0.55
1:C:19:ALA:HB1	1:C:21:VAL:HG22	1.89	0.55
1:B:649:ARG:HG2	1:B:649:ARG:HH11	1.71	0.55
1:C:492:LEU:HG	1:C:683:LEU:CD2	2.31	0.55
1:D:175:GLN:NE2	1:D:617:LYS:HE2	2.21	0.55
1:D:614:HIS:O	1:D:618:MET:HB2	2.06	0.55
1:B:569:ARG:CD	1:B:574:LYS:HE3	2.36	0.55
1:D:352:VAL:HA	1:D:356:LEU:HD12	1.87	0.55
1:D:603:VAL:HB	1:D:642:VAL:HG13	1.89	0.55
1:D:60:ARG:HG3	1:D:189:TRP:CZ3	2.41	0.55
1:B:169:LYS:O	1:B:176:MET:HB2	2.07	0.55
1:C:322:VAL:HG13	1:C:325:ASN:HB2	1.88	0.55
1:D:261:GLY:O	1:D:262:TYR:HB2	2.05	0.55
1:C:33:ARG:HG3	1:D:18:LEU:CD1	2.37	0.55
1:C:52:TYR:HE1	1:C:95:LEU:HD12	1.72	0.55
1:D:64:VAL:HG12	1:D:67:TRP:HE3	1.72	0.55
1:D:64:VAL:HG12	1:D:67:TRP:CE3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:MET:SD	1:D:470:ASP:HB3	2.47	0.55
1:B:22:GLU:O	1:B:25:THR:HB	2.07	0.54
1:C:13:ILE:O	1:D:43:ARG:HG2	2.07	0.54
1:D:813:SER:O	1:D:817:ILE:HG12	2.06	0.54
1:A:13:ILE:HG23	1:B:32:ASN:OD1	2.07	0.54
1:B:338:ASN:OD1	1:B:377:HIS:HE1	1.90	0.54
1:C:822:ARG:HD2	1:C:828:GLU:OE2	2.07	0.54
1:A:86:SER:HB3	1:A:89:PHE:CE1	2.42	0.54
1:A:33:ARG:HH12	1:B:18:LEU:HD22	1.71	0.54
1:B:256:ASP:HB3	1:B:258:ASN:ND2	2.23	0.54
1:D:549:LEU:HD23	1:D:557:ILE:CD1	2.37	0.54
1:B:506:ARG:HB3	1:B:524:TYR:CZ	2.43	0.54
1:D:369:VAL:HA	1:D:448:GLY:O	2.08	0.54
1:D:526:ASP:HA	1:D:799:ARG:NH1	2.23	0.54
1:A:280:TYR:HE2	1:A:291:LEU:HD22	1.72	0.54
1:A:395:LEU:HG	1:A:396:LEU:HD22	1.88	0.54
1:A:609:ALA:HB1	1:A:616:ALA:HB1	1.90	0.54
1:A:734:ARG:HG3	1:A:735:ILE:HG13	1.90	0.54
1:D:21:VAL:HG12	1:D:22:GLU:N	2.23	0.54
1:A:203:TYR:OH	1:A:294:LYS:NZ	2.41	0.54
1:A:490:ARG:O	1:A:495:CYS:HB3	2.07	0.54
1:A:509:GLU:HA	1:A:511:TYR:CD1	2.43	0.54
1:B:666:ILE:HG22	1:B:690:GLY:HA2	1.89	0.54
1:B:755:PRO:HD2	1:C:426:ARG:CZ	2.38	0.54
1:B:801:VAL:O	1:B:805:ILE:HG13	2.08	0.54
1:C:136:LEU:HD22	1:C:338:ASN:HD21	1.73	0.54
1:D:499:LEU:HB2	1:D:537:VAL:HG11	1.90	0.54
1:B:159:ILE:HG13	1:B:299:VAL:HB	1.90	0.54
1:B:666:ILE:HG22	1:B:711:PHE:HE1	1.73	0.54
1:C:678:ASN:HB2	1:C:699:MET:SD	2.48	0.54
1:A:49:ARG:HA	1:A:125:ILE:HG21	1.88	0.54
1:A:221:VAL:HG13	1:A:272:ALA:HB1	1.89	0.54
1:B:30:ASN:HA	1:B:33:ARG:HB2	1.89	0.53
1:B:698:GLU:HG2	1:B:810:LYS:HZ3	1.73	0.53
1:B:764:MET:HA	1:B:768:HIS:ND1	2.24	0.53
1:D:692:MET:HG2	1:D:697:VAL:HG22	1.89	0.53
1:A:67:TRP:CZ3	1:A:229:PRO:HD3	2.43	0.53
1:A:269:ARG:HH11	1:A:269:ARG:HG2	1.73	0.53
1:A:446:ILE:HG23	1:A:452:VAL:HG21	1.90	0.53
1:A:515:LEU:HD21	1:A:683:LEU:HD21	1.91	0.53
1:B:503:ILE:HG12	1:B:521:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:GLU:O	1:C:370:LYS:HG3	2.08	0.53
1:D:67:TRP:O	1:D:71:GLN:HB2	2.07	0.53
1:A:15:VAL:HB	1:A:69:ARG:HH21	1.73	0.53
1:A:550:GLU:HG3	1:A:554:LYS:HB2	1.91	0.53
1:B:361:TRP:CH2	1:B:406:ILE:HA	2.43	0.53
1:D:30:ASN:HB3	1:D:58:THR:HG23	1.90	0.53
1:A:322:VAL:HG13	1:A:325:ASN:CB	2.38	0.53
1:B:47:THR:HB	1:B:50:ASP:OD2	2.08	0.53
1:C:49:ARG:O	1:C:53:PHE:HB2	2.08	0.53
1:B:63:LEU:HD22	1:B:238:VAL:HG21	1.91	0.53
1:C:457:ARG:HA	1:C:481:ASN:OD1	2.09	0.53
1:D:157:TYR:CE2	1:D:242:ARG:HG2	2.44	0.53
1:B:170:ILE:HD13	1:B:175:GLN:HA	1.89	0.53
1:C:522:LEU:HD13	1:C:806:ALA:CB	2.38	0.53
1:D:527:ASP:OD2	1:D:529:ALA:HB3	2.09	0.53
1:A:652:LEU:HA	1:A:655:LYS:HE2	1.91	0.53
1:C:21:VAL:HG12	1:C:22:GLU:N	2.24	0.53
1:C:323:ARG:HB2	1:C:325:ASN:CG	2.29	0.53
1:D:309:ARG:NH2	2:D:902:SO4:O1	2.42	0.53
1:D:615:MET:SD	1:D:764:MET:HG3	2.49	0.53
1:A:666:ILE:HG22	1:A:711:PHE:CZ	2.44	0.53
1:C:556:HIS:HE1	1:C:638:ASP:HB3	1.74	0.53
1:A:670:GLY:H	1:A:693:ASP:CG	2.13	0.52
1:B:75:TYR:O	1:B:315:LYS:HD3	2.09	0.52
1:D:407:ASN:OD1	1:D:430:LEU:HB2	2.09	0.52
1:A:428:MET:HE1	1:A:474:LEU:HD11	1.90	0.52
1:C:251:ASP:OD2	1:C:255:LYS:HD2	2.09	0.52
1:D:102:LEU:HB3	1:D:104:LEU:HD22	1.90	0.52
1:D:677:GLY:O	1:D:681:PHE:HD2	1.91	0.52
1:B:688:THR:HB	1:B:708:PHE:CE2	2.44	0.52
1:C:293:LEU:HD23	1:C:395:LEU:HD11	1.91	0.52
1:D:28:LYS:HE3	1:D:114:GLN:HB3	1.91	0.52
1:D:781:VAL:O	1:D:785:GLU:HG3	2.09	0.52
1:B:455:VAL:HG12	1:B:459:HIS:HD2	1.75	0.52
1:A:60:ARG:O	1:A:64:VAL:HG22	2.09	0.52
1:B:312:LYS:HD2	1:B:326:PHE:HZ	1.73	0.52
1:B:407:ASN:HB2	1:B:430:LEU:HG	1.91	0.52
1:C:15:VAL:C	1:C:17:GLY:N	2.46	0.52
1:D:709:PHE:CD2	1:D:787:VAL:HG23	2.44	0.52
1:A:83:TYR:OH	1:A:310:ARG:HD2	2.10	0.52
1:B:64:VAL:HG12	1:B:67:TRP:HE3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:ILE:O	1:C:644:PHE:HA	2.09	0.52
1:D:250:ASN:HA	1:D:269:ARG:NH2	2.24	0.52
1:D:555:VAL:HG11	1:D:643:ILE:HG12	1.91	0.52
1:A:582:HIS:HD2	1:A:781:VAL:HG12	1.75	0.52
1:D:41:LYS:HE2	1:D:50:ASP:OD2	2.10	0.52
1:D:70:THR:OG1	1:D:237:VAL:HA	2.10	0.52
1:D:558:ASN:HB2	1:D:561:SER:OG	2.10	0.52
1:A:89:PHE:O	1:A:131:LEU:HB3	2.09	0.52
1:B:550:GLU:HG2	1:B:555:VAL:HG23	1.91	0.52
1:B:573:TYR:CE1	1:B:574:LYS:HG3	2.44	0.52
1:C:521:LEU:HD21	1:C:530:PHE:CZ	2.45	0.52
1:D:171:CYS:CB	1:D:176:MET:SD	2.95	0.52
1:D:537:VAL:O	1:D:541:ASN:HB2	2.10	0.52
1:A:568:LYS:NZ	1:A:680:LLP:OP2	2.43	0.52
1:A:85:LEU:HD21	1:A:303:THR:CG2	2.35	0.51
1:B:653:ALA:O	1:B:657:ILE:HG13	2.09	0.51
1:A:677:GLY:HA2	1:A:680:LLP:HE2	1.92	0.51
1:C:481:ASN:ND2	1:C:482:LYS:H	2.08	0.51
1:D:492:LEU:HD21	1:D:499:LEU:HD22	1.90	0.51
1:D:777:TYR:O	1:D:780:TYR:HB3	2.10	0.51
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.92	0.51
1:B:486:ILE:HG12	1:B:680:LLP:HG3	1.92	0.51
1:C:652:LEU:HD23	1:C:656:VAL:HB	1.92	0.51
1:D:735:ILE:HD13	1:D:778:GLU:HG3	1.93	0.51
1:D:737:GLU:O	1:D:740:GLN:HB3	2.10	0.51
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.93	0.51
1:A:759:LYS:NZ	1:A:763:ASN:OD1	2.43	0.51
1:A:808:SER:O	1:A:810:LYS:N	2.43	0.51
1:D:80:LYS:HE2	1:D:825:TRP:O	2.10	0.51
1:D:169:LYS:HB3	1:D:176:MET:HB2	1.93	0.51
1:D:404:TYR:CE1	1:D:431:VAL:HG21	2.46	0.51
1:A:711:PHE:HB3	1:A:783:CYS:SG	2.51	0.51
1:A:538:LYS:O	1:A:538:LYS:HG3	2.10	0.51
1:B:271:LEU:CA	1:B:274:ASN:HB3	2.40	0.51
1:D:790:LEU:HG	1:D:797:TRP:HD1	1.76	0.51
1:A:96:GLN:O	1:A:100:VAL:HG13	2.10	0.51
1:A:662:LEU:HD11	1:A:784:GLN:HE22	1.76	0.51
1:B:455:VAL:HG12	1:B:459:HIS:CD2	2.46	0.51
1:C:543:LEU:HD13	1:C:559:PRO:HG3	1.93	0.51
1:A:692:MET:SD	1:A:697:VAL:HG23	2.50	0.51
1:A:729:GLN:HB2	1:A:766:MET:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:TYR:N	1:B:155:TYR:CD1	2.79	0.51
1:B:590:ILE:HG12	1:B:598:VAL:HG11	1.93	0.51
1:C:653:ALA:HA	1:C:656:VAL:HG12	1.93	0.51
1:C:778:GLU:O	1:C:782:LYS:HD2	2.10	0.51
1:D:160:ARG:CZ	1:D:183:LEU:HD21	2.41	0.51
1:D:754:GLN:O	1:D:757:LEU:HB2	2.10	0.51
1:A:40:VAL:HG21	1:B:191:LYS:HG3	1.92	0.51
1:A:271:LEU:HA	1:A:274:ASN:ND2	2.25	0.51
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.25	0.51
1:D:459:HIS:HA	1:D:462:ILE:HG13	1.92	0.51
1:D:721:LEU:HG	1:D:726:TYR:HB2	1.92	0.51
1:D:66:ARG:CZ	1:D:837:PRO:HB3	2.41	0.50
1:D:138:ARG:HH11	1:D:650:VAL:HG11	1.76	0.50
1:A:80:LYS:HG3	1:A:331:ASP:O	2.11	0.50
1:A:795:ARG:O	1:A:799:ARG:HG3	2.11	0.50
1:A:799:ARG:HA	1:A:802:ILE:HD12	1.93	0.50
1:B:133:ASN:ND2	1:B:279:LEU:HD13	2.27	0.50
1:B:381:PRO:HG3	1:B:467:ILE:HG13	1.93	0.50
1:B:734:ARG:O	1:B:736:PRO:HD3	2.11	0.50
1:C:262:TYR:HB3	1:C:264:GLN:HE21	1.74	0.50
1:C:582:HIS:CE1	1:C:586:LEU:HD22	2.46	0.50
1:D:97:ASN:HD22	1:D:494:LEU:HD11	1.76	0.50
1:A:421:ASP:HB3	1:A:425:LEU:HD23	1.93	0.50
1:C:600:PRO:HB3	1:C:639:ARG:HA	1.93	0.50
1:C:732:TYR:HE2	1:C:742:ILE:HG21	1.76	0.50
1:D:28:LYS:CE	1:D:114:GLN:HB3	2.41	0.50
1:D:88:GLU:HG2	1:D:132:GLY:HA2	1.94	0.50
1:D:526:ASP:HA	1:D:799:ARG:HH11	1.75	0.50
1:A:766:MET:HE3	1:A:774:PHE:HE2	1.76	0.50
1:B:319:ARG:O	1:B:324:THR:HG23	2.11	0.50
1:C:97:ASN:HA	1:C:494:LEU:HD11	1.94	0.50
1:C:266:VAL:O	1:C:269:ARG:HB2	2.11	0.50
1:C:818:ALA:O	1:C:822:ARG:HB2	2.11	0.50
1:D:111:ALA:O	1:D:115:LEU:HB2	2.11	0.50
1:D:689:ILE:HG21	1:D:784:GLN:NE2	2.26	0.50
1:D:738:LEU:HA	1:D:741:ILE:HG12	1.93	0.50
1:A:235:ASN:O	1:A:237:VAL:HG12	2.12	0.50
1:B:82:ILE:HG23	1:B:154:ALA:HB2	1.94	0.50
1:C:70:THR:HG21	1:C:237:VAL:HB	1.92	0.50
1:C:614:HIS:O	1:C:618:MET:HB2	2.11	0.50
1:B:481:ASN:HD22	1:B:482:LYS:H	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LYS:HE2	1:C:331:ASP:O	2.11	0.50
1:C:159:ILE:HG13	1:C:299:VAL:CG2	2.42	0.50
1:D:19:ALA:CB	1:D:62:HIS:CE1	2.95	0.50
1:D:165:ILE:CD1	1:D:281:PRO:HA	2.35	0.50
1:B:493:VAL:HG21	1:B:512:ILE:HD12	1.93	0.50
1:B:549:LEU:HB3	1:B:555:VAL:HG21	1.94	0.50
1:B:819:GLN:O	1:B:823:GLU:HB2	2.11	0.50
1:C:52:TYR:CE1	1:C:95:LEU:HD12	2.46	0.50
1:C:100:VAL:O	1:C:234:ARG:NH1	2.44	0.50
1:D:515:LEU:HD22	1:D:812:SER:HB2	1.94	0.50
1:A:251:ASP:HB3	1:A:255:LYS:CB	2.42	0.50
1:B:49:ARG:HA	1:B:125:ILE:HG21	1.93	0.50
1:B:206:VAL:CG1	1:B:213:ALA:HB1	2.42	0.50
1:C:497:PRO:HA	1:C:500:ALA:HB3	1.94	0.50
1:D:63:LEU:HD22	1:D:238:VAL:HG11	1.93	0.50
1:D:521:LEU:HA	1:D:524:TYR:HD1	1.75	0.50
1:A:11:LYS:HA	1:B:43:ARG:NE	2.26	0.50
1:A:208:HIS:CE1	1:A:213:ALA:HB2	2.47	0.50
1:B:262:TYR:HE1	1:C:263:ILE:HG13	1.77	0.50
1:C:280:TYR:OH	1:C:291:LEU:HD13	2.12	0.50
1:C:289:LYS:CD	1:C:289:LYS:HA	2.42	0.50
1:D:63:LEU:HD21	1:D:231:PRO:HB3	1.92	0.50
1:D:424:ARG:HG2	1:D:427:ARG:NH2	2.27	0.50
1:A:666:ILE:HG22	1:A:711:PHE:HZ	1.77	0.49
1:B:456:ALA:HB2	1:B:674:SER:HB2	1.92	0.49
1:B:715:VAL:HA	1:B:718:VAL:HG23	1.94	0.49
1:C:496:ASN:HD22	1:C:658:PRO:HG3	1.77	0.49
1:D:712:GLY:H	1:D:779:GLU:HG2	1.76	0.49
1:A:395:LEU:O	1:A:396:LEU:HD13	2.13	0.49
1:B:566:GLN:HB2	1:B:664:GLU:HB2	1.93	0.49
1:C:160:ARG:HB2	1:C:243:LEU:HB3	1.94	0.49
1:C:733:ASP:HA	1:C:739:ARG:CZ	2.42	0.49
1:A:248:ALA:HB3	1:A:269:ARG:NH1	2.26	0.49
1:A:742:ILE:HD11	1:A:774:PHE:CE1	2.47	0.49
1:B:150:LEU:HD21	1:B:814:ASP:HB3	1.94	0.49
1:B:385:GLU:O	1:B:441:MET:HB2	2.12	0.49
1:C:162:GLU:OE1	1:C:277:ARG:NH1	2.46	0.49
1:D:80:LYS:NZ	1:D:330:PRO:O	2.45	0.49
1:C:267:LEU:HD22	1:C:271:LEU:HD11	1.93	0.49
1:C:480:GLN:HE22	1:C:823:GLU:HB3	1.77	0.49
1:C:619:ILE:O	1:C:622:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:THR:O	1:D:102:LEU:HB2	2.12	0.49
1:A:830:SER:OG	1:A:832:GLN:HB3	2.12	0.49
1:B:688:THR:O	1:B:709:PHE:HB2	2.13	0.49
1:C:104:LEU:HB3	1:C:108:CYS:SG	2.53	0.49
1:C:649:ARG:HG3	1:C:651:SER:HB3	1.95	0.49
1:C:93:ARG:HD3	1:C:126:GLU:HG2	1.95	0.49
1:D:60:ARG:HG3	1:D:189:TRP:CE3	2.47	0.49
1:A:16:ARG:HG3	1:A:17:GLY:H	1.78	0.49
1:A:166:PHE:HD2	1:A:167:ASN:O	1.96	0.49
1:A:623:ILE:HG21	1:A:644:PHE:HD1	1.78	0.49
1:B:732:TYR:O	1:B:739:ARG:NH1	2.46	0.49
1:A:165:ILE:HD11	1:A:281:PRO:HG3	1.93	0.49
1:A:330:PRO:HG3	1:A:370:LYS:HZ2	1.78	0.49
1:B:66:ARG:HG2	1:B:236:ASN:ND2	2.28	0.49
1:B:159:ILE:HD11	1:B:299:VAL:HG12	1.95	0.49
1:B:481:ASN:O	1:B:482:LYS:HD3	2.12	0.49
1:B:575:ARG:CZ	1:B:578:LEU:HD22	2.43	0.49
1:C:80:LYS:HD2	1:C:827:VAL:HG13	1.94	0.49
1:C:459:HIS:O	1:C:463:LEU:HG	2.13	0.49
1:D:70:THR:O	1:D:73:HIS:HB3	2.12	0.49
1:D:709:PHE:CE2	1:D:787:VAL:HG23	2.48	0.49
1:B:64:VAL:HG12	1:B:67:TRP:CE3	2.48	0.49
1:C:576:GLN:HE21	1:C:576:GLN:N	2.07	0.49
1:D:14:SER:HB2	2:D:900:SO4:O2	2.13	0.49
1:D:341:HIS:HB2	1:D:342:PRO:HD3	1.95	0.49
1:D:783:CYS:HA	1:D:786:ARG:NE	2.27	0.49
1:A:82:ILE:O	1:A:154:ALA:HA	2.12	0.49
1:C:652:LEU:O	1:C:656:VAL:HB	2.13	0.49
1:D:761:ILE:O	1:D:765:LEU:HD22	2.13	0.49
1:C:55:LEU:O	1:C:58:THR:HB	2.13	0.48
1:D:208:HIS:HA	1:D:213:ALA:HA	1.95	0.48
1:D:410:PHE:O	1:D:413:ARG:HB3	2.13	0.48
1:A:389:VAL:HG23	1:A:390:HIS:N	2.27	0.48
1:B:486:ILE:HD12	1:B:486:ILE:HA	1.59	0.48
1:D:161:TYR:CE2	1:D:279:LEU:HG	2.48	0.48
1:A:250:ASN:HB2	1:A:269:ARG:HH22	1.77	0.48
1:A:777:TYR:O	1:A:781:VAL:HG22	2.13	0.48
1:B:815:ARG:O	1:B:819:GLN:HB2	2.13	0.48
1:D:83:TYR:CE1	1:D:333:VAL:HG13	2.35	0.48
1:A:264:GLN:NE2	1:C:267:LEU:HD13	2.28	0.48
1:A:575:ARG:NH2	1:A:776:ASP:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:TYR:HE1	1:B:672:GLU:HG3	1.77	0.48
1:C:510:GLU:HB3	1:C:517:GLN:OE1	2.13	0.48
1:D:231:PRO:CA	1:D:238:VAL:HG22	2.43	0.48
1:D:316:PHE:HB3	1:D:324:THR:OG1	2.13	0.48
1:B:52:TYR:HE1	1:B:95:LEU:HD12	1.79	0.48
1:B:78:ASP:HB2	1:B:315:LYS:HG2	1.96	0.48
1:B:466:THR:OG1	1:B:467:ILE:HD12	2.13	0.48
1:B:678:ASN:HD22	1:B:695:ALA:HB3	1.76	0.48
1:C:33:ARG:CG	1:D:18:LEU:CG	2.89	0.48
1:C:55:LEU:HD22	1:C:122:LEU:HD12	1.96	0.48
1:C:571:HIS:ND1	1:C:573:TYR:HD2	2.12	0.48
1:D:90:TYR:CD2	1:D:138:ARG:HB2	2.48	0.48
1:D:801:VAL:O	1:D:805:ILE:HG13	2.14	0.48
1:A:248:ALA:HB3	1:A:269:ARG:HH11	1.79	0.48
1:B:66:ARG:O	1:B:69:ARG:HB2	2.13	0.48
1:B:133:ASN:ND2	1:B:281:PRO:HA	2.28	0.48
1:B:369:VAL:HA	1:B:448:GLY:O	2.14	0.48
1:D:241:MET:HB3	1:D:243:LEU:HD13	1.96	0.48
1:D:322:VAL:HG22	1:D:325:ASN:HB2	1.95	0.48
1:D:471:PHE:O	1:D:474:LEU:HD12	2.13	0.48
1:A:157:TYR:HE1	1:A:242:ARG:CD	2.26	0.48
1:A:158:GLY:O	1:A:243:LEU:HA	2.13	0.48
1:C:224:MET:HB2	1:C:247:LYS:HE2	1.95	0.48
1:D:21:VAL:CG1	1:D:22:GLU:N	2.71	0.48
1:D:173:GLY:HA2	1:D:624:THR:CG2	2.42	0.48
1:D:662:LEU:HD11	1:D:787:VAL:HG11	1.95	0.48
1:A:163:PHE:CE1	1:A:277:ARG:NH1	2.82	0.48
1:B:698:GLU:O	1:B:702:GLU:HB2	2.14	0.48
1:D:677:GLY:H	1:D:680:LLP:P	2.37	0.48
1:A:19:ALA:HA	1:A:21:VAL:HG22	1.96	0.48
1:A:510:GLU:HB3	1:A:517:GLN:NE2	2.29	0.48
1:C:761:ILE:O	1:C:765:LEU:HB2	2.14	0.48
1:C:491:TRP:C	1:C:495:CYS:SG	2.92	0.48
1:D:23:ASN:O	1:D:27:LEU:HG	2.13	0.48
1:D:264:GLN:O	1:D:267:LEU:HB2	2.13	0.48
1:D:657:ILE:HG23	1:D:681:PHE:CD1	2.49	0.48
1:D:810:LYS:HA	1:D:815:ARG:NE	2.29	0.48
1:A:337:LEU:HD23	1:A:445:CYS:SG	2.54	0.47
1:A:418:PHE:HE2	1:A:474:LEU:HB3	1.79	0.47
1:A:555:VAL:HG11	1:A:643:ILE:HD11	1.95	0.47
1:B:669:ALA:O	1:B:718:VAL:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:689:ILE:HG23	1:D:689:ILE:O	2.14	0.47
1:A:21:VAL:HG13	1:A:110:GLU:HG2	1.96	0.47
1:B:455:VAL:HG22	1:B:484:ASN:OD1	2.14	0.47
1:B:740:GLN:O	1:B:744:GLN:HG3	2.14	0.47
1:C:350:MET:SD	1:C:364:ALA:HB1	2.55	0.47
1:A:250:ASN:ND2	1:A:252:PHE:HB2	2.28	0.47
1:A:490:ARG:HG2	1:A:491:TRP:CE2	2.50	0.47
1:B:781:VAL:HA	1:B:784:GLN:HB2	1.95	0.47
1:C:163:PHE:O	1:C:180:ASP:HB3	2.14	0.47
1:C:741:ILE:HA	1:C:744:GLN:HG2	1.96	0.47
1:D:87:LEU:HD11	1:D:299:VAL:HG11	1.96	0.47
1:D:621:LYS:NZ	1:D:624:THR:O	2.44	0.47
1:D:759:LYS:O	1:D:759:LYS:HD3	2.14	0.47
1:A:525:VAL:O	1:A:531:ILE:HD11	2.14	0.47
1:B:727:ASN:HD21	1:C:725:GLY:HA3	1.78	0.47
1:D:536:LYS:HA	1:D:539:GLN:CD	2.35	0.47
1:B:208:HIS:CE1	1:B:213:ALA:HB2	2.49	0.47
1:C:152:LEU:HD22	1:C:827:VAL:CG2	2.45	0.47
1:D:293:LEU:HD22	1:D:391:LEU:HD23	1.97	0.47
1:D:329:PHE:HB3	1:D:330:PRO:HD3	1.95	0.47
1:B:639:ARG:HG3	1:B:639:ARG:HH11	1.79	0.47
1:C:316:PHE:CE1	1:C:319:ARG:HB3	2.50	0.47
1:A:23:ASN:O	1:A:27:LEU:HG	2.15	0.47
1:C:21:VAL:C	1:C:23:ASN:N	2.68	0.47
1:C:41:LYS:HE3	1:C:50:ASP:OD2	2.15	0.47
1:C:191:LYS:HG3	1:D:40:VAL:HG21	1.96	0.47
1:C:262:TYR:CD2	1:C:264:GLN:HB3	2.50	0.47
1:C:319:ARG:NH2	1:C:322:VAL:H	2.13	0.47
1:C:573:TYR:CZ	1:C:574:LYS:HE3	2.49	0.47
1:C:753:LYS:H	1:C:753:LYS:HD2	1.78	0.47
1:D:528:GLU:HG3	1:D:795:ARG:NH1	2.30	0.47
1:D:675:GLY:HA3	1:D:678:ASN:HD21	1.79	0.47
1:A:423:ASP:HA	1:A:426:ARG:HG2	1.97	0.47
1:A:707:ASN:HA	1:A:800:MET:SD	2.55	0.47
1:B:30:ASN:HB2	1:B:58:THR:HG23	1.97	0.47
1:B:312:LYS:HD2	1:B:326:PHE:CZ	2.50	0.47
1:B:322:VAL:HG13	1:B:325:ASN:HB2	1.96	0.47
1:B:688:THR:HG22	1:B:689:ILE:O	2.14	0.47
1:D:551:ARG:HD2	1:D:552:GLU:OE1	2.15	0.47
1:A:320:ASP:HA	1:A:324:THR:HA	1.96	0.47
1:A:336:GLN:HA	1:A:373:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PHE:N	1:A:471:PHE:CD1	2.83	0.47
1:A:486:ILE:HD13	1:A:679:MET:SD	2.55	0.47
1:A:588:ASN:ND2	1:A:744:GLN:HE22	2.10	0.47
1:C:15:VAL:O	1:C:17:GLY:HA2	2.14	0.47
1:C:181:ASP:O	1:C:184:ARG:NH2	2.48	0.47
1:C:458:ILE:O	1:C:462:ILE:HG12	2.15	0.47
1:D:742:ILE:HD11	1:D:774:PHE:HZ	1.80	0.47
1:A:81:ARG:HG2	1:A:155:TYR:CE2	2.45	0.47
1:A:99:MET:SD	1:A:108:CYS:CB	3.03	0.47
1:A:724:ARG:O	1:A:724:ARG:HG2	2.15	0.47
1:B:712:GLY:O	1:B:714:ARG:HG3	2.14	0.47
1:C:431:VAL:HG13	1:C:437:LYS:HD3	1.97	0.47
1:A:83:TYR:HD1	1:A:155:TYR:HB2	1.80	0.46
1:A:455:VAL:HA	1:A:482:LYS:O	2.15	0.46
1:A:609:ALA:CB	1:A:620:ILE:HD11	2.45	0.46
1:B:39:LEU:HD21	1:B:53:PHE:HB2	1.97	0.46
1:C:86:SER:HB3	1:C:89:PHE:CE1	2.50	0.46
1:C:515:LEU:HG	1:C:809:GLY:HA2	1.95	0.46
1:D:515:LEU:HG	1:D:515:LEU:O	2.15	0.46
1:D:566:GLN:HB2	1:D:664:GLU:O	2.15	0.46
1:A:550:GLU:CA	1:A:554:LYS:HA	2.37	0.46
1:A:698:GLU:HB3	1:A:810:LYS:NZ	2.30	0.46
1:B:711:PHE:CD2	1:B:780:TYR:HA	2.49	0.46
1:C:75:TYR:O	1:C:315:LYS:NZ	2.42	0.46
1:C:196:PHE:HB2	1:C:225:PRO:HG3	1.96	0.46
1:C:584:ILE:HG13	1:C:741:ILE:HD12	1.96	0.46
1:D:485:GLY:HA2	1:D:679:MET:SD	2.55	0.46
1:D:525:VAL:HA	1:D:802:ILE:HD12	1.96	0.46
1:D:781:VAL:HG23	1:D:782:LYS:HD3	1.96	0.46
1:A:525:VAL:O	1:A:799:ARG:HD2	2.16	0.46
1:C:511:TYR:CD2	1:C:518:LEU:HD21	2.50	0.46
1:D:632:HIS:O	1:D:634:PRO:HD3	2.15	0.46
1:D:662:LEU:HD22	1:D:689:ILE:HG22	1.97	0.46
1:A:414:VAL:HG13	1:A:428:MET:SD	2.55	0.46
1:B:175:GLN:OE1	1:B:609:ALA:HB3	2.16	0.46
1:B:587:TYR:CE1	1:B:591:LYS:HD2	2.50	0.46
1:C:168:GLN:OE1	1:C:608:LYS:HA	2.15	0.46
1:D:424:ARG:HG2	1:D:427:ARG:HH22	1.81	0.46
1:D:622:LEU:HG	1:D:758:PHE:CD1	2.51	0.46
1:D:711:PHE:CE2	1:D:780:TYR:HB2	2.51	0.46
1:D:783:CYS:HB2	1:D:786:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:O	1:A:293:LEU:HG	2.15	0.46
1:A:421:ASP:O	1:A:425:LEU:HD23	2.15	0.46
1:A:630:VAL:HG21	1:A:642:VAL:CG2	2.38	0.46
1:B:92:GLY:O	1:B:490:ARG:NH2	2.48	0.46
1:B:641:ARG:HG2	1:B:641:ARG:HH11	1.80	0.46
1:B:687:LEU:HD13	1:B:709:PHE:HE2	1.80	0.46
1:A:85:LEU:CD2	1:A:303:THR:HG21	2.37	0.46
1:B:26:GLU:OE2	1:B:29:LYS:NZ	2.48	0.46
1:B:665:GLN:HE21	1:B:678:ASN:HA	1.80	0.46
1:C:150:LEU:HD13	1:C:829:PRO:HB3	1.98	0.46
1:D:68:ILE:O	1:D:72:GLN:HG3	2.16	0.46
1:D:601:ARG:HH12	1:D:787:VAL:HG12	1.81	0.46
1:B:516:ASP:O	1:B:519:ARG:HG3	2.16	0.46
1:B:569:ARG:HD3	1:B:574:LYS:HE3	1.97	0.46
1:C:77:LYS:HG2	1:C:79:PRO:HD3	1.98	0.46
1:C:289:LYS:CD	1:C:289:LYS:CA	2.94	0.46
1:C:380:ILE:HA	1:C:381:PRO:HD3	1.70	0.46
1:D:479:PHE:CD1	1:D:479:PHE:N	2.83	0.46
1:A:422:VAL:O	1:A:426:ARG:HG2	2.16	0.46
1:A:616:ALA:O	1:A:620:ILE:HG13	2.16	0.46
1:A:797:TRP:CZ3	1:A:801:VAL:HG21	2.51	0.46
1:C:756:ASP:O	1:C:759:LYS:HB2	2.16	0.46
1:C:798:THR:O	1:C:802:ILE:HG12	2.16	0.46
1:D:27:LEU:HD11	1:D:107:ALA:O	2.16	0.46
1:D:461:GLU:HB3	1:D:465:LYS:HD2	1.97	0.46
1:A:118:ASP:HB3	1:A:121:GLU:HB2	1.97	0.46
1:A:366:GLU:HA	1:A:369:VAL:HG12	1.98	0.46
1:A:511:TYR:HB2	1:A:518:LEU:CD1	2.40	0.46
1:A:592:LYS:NZ	1:A:593:GLU:OE2	2.49	0.46
1:B:14:SER:OG	1:B:16:ARG:HG3	2.16	0.46
1:B:480:GLN:NE2	1:B:482:LYS:HE3	2.31	0.46
1:C:665:GLN:HE21	1:C:678:ASN:ND2	2.14	0.46
1:D:110:GLU:HG2	1:D:114:GLN:HE21	1.80	0.46
1:D:203:TYR:CE1	1:D:395:LEU:HD22	2.51	0.46
1:D:486:ILE:HD11	1:D:680:LLP:HE3	1.98	0.46
1:D:712:GLY:HA2	1:D:779:GLU:HG2	1.97	0.46
1:A:99:MET:SD	1:A:108:CYS:SG	3.14	0.45
1:A:509:GLU:HA	1:A:511:TYR:HD1	1.80	0.45
1:B:118:ASP:HB3	1:B:121:GLU:HB2	1.98	0.45
1:B:322:VAL:HG23	1:B:323:ARG:HH21	1.81	0.45
1:B:498:GLY:O	1:B:501:GLU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:TYR:HD2	1:C:76:GLU:OE1	1.99	0.45
1:C:322:VAL:HG13	1:C:325:ASN:HD22	1.81	0.45
1:C:528:GLU:HA	1:C:531:ILE:HB	1.98	0.45
1:C:637:GLY:O	1:C:641:ARG:NH2	2.49	0.45
1:A:489:ARG:NH1	1:A:512:ILE:O	2.49	0.45
1:A:532:ARG:O	1:A:536:LYS:HB2	2.16	0.45
1:B:100:VAL:HG21	1:B:494:LEU:HD13	1.99	0.45
1:B:582:HIS:O	1:B:586:LEU:HD13	2.16	0.45
1:B:790:LEU:HD21	1:B:800:MET:HE2	1.97	0.45
1:C:323:ARG:HE	1:C:323:ARG:HA	1.80	0.45
1:C:413:ARG:CZ	1:C:413:ARG:HB3	2.46	0.45
1:D:638:ASP:HA	1:D:641:ARG:NH2	2.32	0.45
1:A:47:THR:HB	1:A:50:ASP:OD2	2.17	0.45
1:B:573:TYR:OH	1:B:574:LYS:HE2	2.15	0.45
1:B:575:ARG:HH22	1:B:776:ASP:CB	2.28	0.45
1:B:692:MET:HE1	1:B:697:VAL:HA	1.98	0.45
1:C:138:ARG:NH1	1:C:142:CYS:SG	2.87	0.45
1:C:341:HIS:HB2	1:C:342:PRO:HD3	1.97	0.45
1:D:516:ASP:O	1:D:519:ARG:HG2	2.16	0.45
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.51	0.45
1:A:729:GLN:HA	1:A:732:TYR:HB3	1.99	0.45
1:C:369:VAL:O	1:C:450:HIS:HB3	2.16	0.45
1:D:33:ARG:HD2	1:D:37:PHE:CD2	2.52	0.45
1:D:733:ASP:O	1:D:739:ARG:NH2	2.49	0.45
1:A:323:ARG:HG2	1:A:325:ASN:HD22	1.82	0.45
1:D:379:VAL:HG11	1:D:671:THR:O	2.15	0.45
1:D:381:PRO:HB3	1:D:467:ILE:HG23	1.98	0.45
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.80	0.45
1:A:442:ALA:HB1	1:A:468:PHE:HZ	1.82	0.45
1:B:550:GLU:HG2	1:B:556:HIS:H	1.81	0.45
1:B:677:GLY:HA2	1:B:680:LLP:HD3	1.98	0.45
1:C:455:VAL:H	1:C:459:HIS:CD2	2.34	0.45
1:C:486:ILE:HG12	1:C:680:LLP:HG2	1.99	0.45
1:A:791:TYR:HD1	1:A:797:TRP:CD1	2.35	0.45
1:A:807:THR:HG22	1:A:808:SER:N	2.31	0.45
1:C:18:LEU:CB	1:D:37:PHE:HE2	2.23	0.45
1:D:214:LYS:HB3	1:D:216:VAL:HG13	1.99	0.45
1:D:568:LYS:HE2	1:D:665:GLN:NE2	2.32	0.45
1:A:160:ARG:HB2	1:A:243:LEU:HB2	1.99	0.45
1:A:230:VAL:HG23	1:A:239:ASN:HB2	1.98	0.45
1:A:235:ASN:HB2	1:A:833:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLN:HG3	1:A:825:TRP:NE1	2.31	0.45
1:A:348:GLU:HA	1:A:399:HIS:CE1	2.48	0.45
1:B:290:GLU:O	1:B:294:LYS:HB2	2.16	0.45
1:B:506:ARG:HB3	1:B:524:TYR:CE2	2.52	0.45
1:B:563:PHE:HD2	1:B:659:ALA:O	1.99	0.45
1:C:37:PHE:CE2	1:D:18:LEU:CG	2.96	0.45
1:C:37:PHE:HD1	1:D:64:VAL:HG23	1.82	0.45
1:C:190:GLU:HG3	1:C:226:TYR:HD2	1.81	0.45
1:C:191:LYS:HG3	1:D:40:VAL:CG2	2.46	0.45
1:D:329:PHE:HE2	1:D:371:THR:HG21	1.81	0.45
1:D:810:LYS:HA	1:D:815:ARG:HD3	1.98	0.45
1:A:174:TRP:CE2	1:A:621:LYS:HD3	2.52	0.45
1:A:499:LEU:HD12	1:A:502:ILE:HD11	1.99	0.45
1:C:21:VAL:C	1:C:23:ASN:H	2.14	0.45
1:D:735:ILE:HA	1:D:736:PRO:HD3	1.73	0.45
1:A:494:LEU:HD23	1:A:494:LEU:H	1.82	0.45
1:A:793:ASN:N	1:A:794:PRO:HD3	2.32	0.45
1:B:469:LYS:HE2	1:B:473:GLU:OE2	2.17	0.45
1:D:47:THR:O	1:D:50:ASP:HB2	2.17	0.45
1:D:82:ILE:HD13	1:D:82:ILE:O	2.17	0.45
1:D:587:TYR:CD1	1:D:630:VAL:HG12	2.52	0.45
1:D:699:MET:HB3	1:D:708:PHE:CZ	2.52	0.45
1:D:729:GLN:O	1:D:730:GLU:HB3	2.16	0.45
1:A:391:LEU:O	1:A:395:LEU:HD23	2.17	0.44
1:B:452:VAL:HG23	1:B:478:LYS:HD2	1.99	0.44
1:B:457:ARG:HA	1:B:481:ASN:OD1	2.17	0.44
1:B:529:ALA:O	1:B:532:ARG:HB3	2.16	0.44
1:B:636:VAL:O	1:B:639:ARG:HG3	2.16	0.44
1:C:13:ILE:HD11	1:D:31:PHE:HE1	1.82	0.44
1:D:699:MET:HB3	1:D:708:PHE:HZ	1.81	0.44
1:D:784:GLN:HA	1:D:787:VAL:HB	1.99	0.44
1:A:233:TYR:CZ	1:A:234:ARG:HD2	2.52	0.44
1:A:411:LEU:HD22	1:A:425:LEU:HD13	1.99	0.44
1:A:443:HIS:HA	1:A:446:ILE:HD12	1.99	0.44
1:A:527:ASP:OD2	1:A:529:ALA:HB3	2.16	0.44
1:B:22:GLU:HA	1:B:25:THR:HB	1.99	0.44
1:B:532:ARG:HB3	1:B:532:ARG:HH11	1.82	0.44
1:C:63:LEU:HD13	1:C:229:PRO:HG2	2.00	0.44
1:C:170:ILE:HD13	1:C:175:GLN:HA	1.98	0.44
1:C:398:ARG:HH11	1:C:398:ARG:HD3	1.57	0.44
1:D:256:ASP:OD2	1:D:258:ASN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:630:VAL:HG23	1:D:631:ASN:H	1.81	0.44
1:D:679:MET:HB3	1:D:811:PHE:HB3	1.98	0.44
1:A:33:ARG:NH1	1:B:18:LEU:HB2	2.33	0.44
1:A:446:ILE:HD11	1:A:468:PHE:CZ	2.52	0.44
1:B:721:LEU:HD12	1:B:772:LYS:HD3	1.99	0.44
1:C:266:VAL:HG22	1:C:269:ARG:HG3	1.99	0.44
1:C:410:PHE:O	1:C:413:ARG:HB2	2.16	0.44
1:D:492:LEU:HG	1:D:683:LEU:HD22	1.99	0.44
1:D:633:ASP:OD2	1:D:635:VAL:HB	2.17	0.44
1:D:741:ILE:O	1:D:745:LEU:HB2	2.17	0.44
1:B:52:TYR:CE1	1:B:95:LEU:HD12	2.52	0.44
1:B:575:ARG:NH2	1:B:578:LEU:HD22	2.33	0.44
1:B:596:LYS:HD3	1:B:597:PHE:O	2.18	0.44
1:C:162:GLU:O	1:C:183:LEU:HD11	2.17	0.44
1:C:293:LEU:HD22	1:C:391:LEU:HD22	2.00	0.44
1:D:593:GLU:HB2	1:D:596:LYS:HG3	1.99	0.44
1:B:96:GLN:HA	1:B:99:MET:HE2	1.98	0.44
1:B:727:ASN:O	1:B:730:GLU:HB3	2.18	0.44
1:B:822:ARG:NH2	1:B:829:PRO:HD2	2.33	0.44
1:C:248:ALA:HB1	1:C:250:ASN:HD22	1.82	0.44
1:D:75:TYR:HD2	1:D:76:GLU:OE2	2.00	0.44
1:D:675:GLY:HA3	1:D:678:ASN:ND2	2.32	0.44
1:D:742:ILE:HD11	1:D:774:PHE:CZ	2.53	0.44
1:B:83:TYR:HA	1:B:155:TYR:O	2.18	0.44
1:B:246:ALA:HB2	1:B:298:PHE:CZ	2.51	0.44
1:C:150:LEU:CD1	1:C:829:PRO:HB3	2.47	0.44
1:C:378:THR:O	1:C:459:HIS:CE1	2.71	0.44
1:D:138:ARG:NH1	1:D:650:VAL:HG11	2.32	0.44
1:D:398:ARG:HD2	1:D:398:ARG:HA	1.86	0.44
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.98	0.44
1:B:357:GLU:O	1:B:358:ARG:NH1	2.50	0.44
1:B:599:VAL:HG21	1:B:788:SER:HB3	1.99	0.44
1:B:733:ASP:HA	1:B:739:ARG:HH12	1.82	0.44
1:C:56:ALA:O	1:C:60:ARG:HG2	2.18	0.44
1:C:423:ASP:OD1	1:C:426:ARG:HD3	2.17	0.44
1:C:581:LEU:HD22	1:C:741:ILE:HG13	1.99	0.44
1:D:171:CYS:SG	1:D:176:MET:SD	3.16	0.44
1:D:602:THR:HA	1:D:641:ARG:O	2.17	0.44
1:D:822:ARG:NH1	1:D:828:GLU:OE1	2.50	0.44
1:A:80:LYS:HD2	1:A:827:VAL:HG13	2.00	0.44
1:A:460:SER:OG	1:A:481:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ILE:CD1	1:A:679:MET:SD	3.06	0.44
1:B:377:HIS:CD2	1:B:455:VAL:HG21	2.53	0.44
1:B:603:VAL:HG23	1:B:642:VAL:HG13	2.00	0.44
1:B:786:ARG:O	1:B:789:ALA:HB3	2.17	0.44
1:C:587:TYR:OH	1:C:591:LYS:NZ	2.48	0.44
1:D:24:VAL:O	1:D:28:LYS:HB2	2.17	0.44
1:D:70:THR:CG2	1:D:237:VAL:HG23	2.47	0.44
1:D:139:LEU:HD11	1:D:484:ASN:HB3	1.99	0.44
1:D:720:ARG:O	1:D:723:GLN:HB2	2.18	0.44
1:A:41:LYS:HE3	1:B:193:ARG:NH1	2.33	0.44
1:A:430:LEU:CD1	1:A:444:LEU:HD23	2.48	0.44
1:A:567:VAL:HB	1:A:648:TYR:CZ	2.53	0.44
1:A:579:ASN:HB2	1:A:666:ILE:HD11	2.00	0.44
1:B:80:LYS:HE3	1:B:333:VAL:O	2.18	0.44
1:C:41:LYS:HE2	1:D:193:ARG:NH1	2.33	0.44
1:C:69:ARG:NH2	2:C:900:SO4:O2	2.50	0.44
1:C:320:ASP:H	1:C:321:PRO:HD2	1.83	0.44
1:C:758:PHE:O	1:C:762:VAL:HG23	2.18	0.44
1:D:295:GLN:O	1:D:298:PHE:HB3	2.18	0.44
1:A:330:PRO:HG3	1:A:370:LYS:NZ	2.33	0.43
1:A:464:LYS:O	1:A:466:THR:N	2.51	0.43
1:A:599:VAL:HG11	1:A:791:TYR:HD2	1.83	0.43
1:B:165:ILE:HD11	1:B:281:PRO:HG3	1.98	0.43
1:D:206:VAL:HG23	1:D:397:PRO:HB2	1.99	0.43
1:D:460:SER:O	1:D:464:LYS:HG3	2.17	0.43
1:D:605:ILE:HG21	1:D:623:ILE:CD1	2.42	0.43
1:A:206:VAL:CG1	1:A:398:ARG:HD2	2.48	0.43
1:A:762:VAL:O	1:A:765:LEU:HB2	2.19	0.43
1:B:127:GLU:OE2	1:B:182:TRP:HA	2.18	0.43
1:B:417:ALA:C	1:B:419:PRO:HD3	2.38	0.43
1:B:631:ASN:HA	1:B:641:ARG:NH1	2.34	0.43
1:B:665:GLN:NE2	1:B:678:ASN:HA	2.32	0.43
1:B:731:TYR:HB3	1:B:735:ILE:HD12	2.00	0.43
1:C:230:VAL:HG23	1:C:239:ASN:HB2	1.99	0.43
1:C:575:ARG:NE	1:C:668:THR:OG1	2.51	0.43
1:D:95:LEU:O	1:D:99:MET:HG3	2.18	0.43
1:D:354:VAL:O	1:D:358:ARG:HA	2.18	0.43
1:D:650:VAL:HA	1:D:680:LLP:H2'1	2.00	0.43
1:A:163:PHE:HE1	1:A:277:ARG:NH1	2.16	0.43
1:A:575:ARG:NH2	1:A:578:LEU:HD22	2.33	0.43
1:A:604:MET:HA	1:A:643:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:ILE:HG22	1:B:711:PHE:CE1	2.51	0.43
1:C:522:LEU:O	1:C:525:VAL:HG22	2.18	0.43
1:B:207:GLU:OE1	1:B:214:LYS:NZ	2.52	0.43
1:B:380:ILE:HA	1:B:381:PRO:HD3	1.57	0.43
1:B:689:ILE:HD13	1:B:689:ILE:HG21	1.81	0.43
1:C:554:LYS:HD3	1:C:555:VAL:N	2.33	0.43
1:C:681:PHE:HB3	1:C:686:ALA:HB3	2.00	0.43
1:A:13:ILE:HB	1:B:43:ARG:HB3	2.00	0.43
1:A:27:LEU:HA	1:A:30:ASN:HB2	2.00	0.43
1:B:310:ARG:NH2	2:B:902:SO4:O1	2.51	0.43
1:B:455:VAL:H	1:B:459:HIS:CD2	2.36	0.43
1:C:13:ILE:HA	1:D:32:ASN:OD1	2.18	0.43
1:C:346:ILE:HD13	1:C:448:GLY:HA3	2.00	0.43
1:C:715:VAL:O	1:C:718:VAL:HB	2.18	0.43
1:D:542:LYS:NZ	1:D:791:TYR:OH	2.52	0.43
1:D:698:GLU:O	1:D:702:GLU:HG2	2.18	0.43
1:A:304:LEU:HA	1:A:304:LEU:HD12	1.84	0.43
1:A:576:GLN:H	1:A:576:GLN:HG2	1.57	0.43
1:A:724:ARG:HH22	1:A:727:ASN:H	1.64	0.43
1:C:32:ASN:OD1	1:C:36:HIS:HE1	2.02	0.43
1:D:486:ILE:HG12	1:D:680:LLP:HG3	2.01	0.43
1:D:489:ARG:H	1:D:489:ARG:HD3	1.83	0.43
1:A:415:ALA:HB2	1:A:425:LEU:HD11	2.01	0.43
1:A:486:ILE:HD11	1:A:676:THR:O	2.18	0.43
1:B:60:ARG:NH1	1:B:188:PRO:O	2.50	0.43
1:B:88:GLU:HG2	1:B:279:LEU:HD21	2.00	0.43
1:B:761:ILE:HG21	1:B:761:ILE:HD13	1.86	0.43
1:C:534:VAL:O	1:C:537:VAL:HB	2.19	0.43
1:D:326:PHE:HD1	1:D:329:PHE:CD1	2.36	0.43
1:D:472:TYR:O	1:D:476:PRO:HA	2.19	0.43
1:D:520:LYS:O	1:D:522:LEU:N	2.52	0.43
1:C:290:GLU:HA	1:C:391:LEU:HD21	2.01	0.43
1:D:69:ARG:O	1:D:72:GLN:HB2	2.19	0.43
1:D:406:ILE:O	1:D:409:ARG:HB2	2.19	0.43
1:D:591:LYS:NZ	1:D:633:ASP:OD2	2.52	0.43
1:A:231:PRO:HB3	1:A:238:VAL:HG22	2.01	0.43
1:C:33:ARG:HG3	1:D:18:LEU:HD11	2.01	0.43
1:C:115:LEU:HD23	1:C:115:LEU:HA	1.91	0.43
1:C:582:HIS:HB2	1:C:780:TYR:CE2	2.51	0.43
1:C:657:ILE:HD13	1:C:680:LLP:HB3	2.01	0.43
1:D:458:ILE:O	1:D:461:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:LYS:O	1:D:607:GLY:HA3	2.19	0.43
1:D:582:HIS:HA	1:D:585:THR:OG1	2.18	0.43
1:A:47:THR:O	1:A:50:ASP:HB2	2.19	0.43
1:A:724:ARG:HG2	1:A:724:ARG:HH11	1.84	0.43
1:B:764:MET:HA	1:B:768:HIS:CG	2.54	0.43
1:C:13:ILE:HD13	1:C:13:ILE:HG21	1.83	0.43
1:C:504:ALA:HB2	1:C:511:TYR:HE1	1.82	0.43
1:C:590:ILE:CG2	1:C:636:VAL:HG22	2.49	0.43
1:D:601:ARG:NH2	1:D:784:GLN:OE1	2.52	0.43
1:A:20:GLY:N	1:A:21:VAL:HG22	2.34	0.42
1:A:379:VAL:HG22	1:A:380:ILE:HD13	2.01	0.42
1:A:680:LLP:H4'1	1:A:680:LLP:H5'1	1.76	0.42
1:B:160:ARG:O	1:B:276:SER:HB3	2.19	0.42
1:B:717:ASP:HA	1:B:720:ARG:HB2	2.00	0.42
1:C:59:VAL:O	1:C:62:HIS:HB2	2.19	0.42
1:C:204:GLY:HA3	1:C:218:THR:HG22	2.02	0.42
1:C:735:ILE:HA	1:C:736:PRO:HD3	1.83	0.42
1:D:168:GLN:HG2	1:D:175:GLN:HG3	2.00	0.42
1:A:227:ASP:OD1	1:A:242:ARG:HG3	2.19	0.42
1:A:230:VAL:CG2	1:A:239:ASN:HB2	2.50	0.42
1:B:225:PRO:HB3	1:B:244:TRP:CZ3	2.53	0.42
1:B:446:ILE:O	1:B:478:LYS:HE3	2.18	0.42
1:B:569:ARG:HD2	1:B:574:LYS:HE3	2.01	0.42
1:C:13:ILE:CD1	1:D:31:PHE:HE1	2.32	0.42
1:C:224:MET:HB2	1:C:247:LYS:CE	2.49	0.42
1:D:92:GLY:H	1:D:129:ALA:HB3	1.83	0.42
1:D:204:GLY:HA3	1:D:218:THR:HG22	2.01	0.42
1:D:489:ARG:HD3	1:D:489:ARG:N	2.33	0.42
1:A:33:ARG:HH12	1:B:18:LEU:HD13	1.84	0.42
1:A:369:VAL:HG23	1:A:447:ALA:O	2.19	0.42
1:A:370:LYS:HA	1:A:450:HIS:HD2	1.84	0.42
1:A:782:LYS:HD3	1:A:785:GLU:OE2	2.18	0.42
1:B:165:ILE:HG12	1:B:279:LEU:HB3	2.01	0.42
1:C:80:LYS:NZ	1:C:330:PRO:O	2.48	0.42
1:C:355:ASP:OD1	1:C:398:ARG:NH1	2.53	0.42
1:D:446:ILE:O	1:D:478:LYS:NZ	2.52	0.42
1:A:289:LYS:HE3	1:A:289:LYS:HB2	1.80	0.42
1:C:631:ASN:OD1	1:C:641:ARG:HA	2.18	0.42
1:D:143:PHE:O	1:D:147:MET:HG3	2.20	0.42
1:D:262:TYR:HB3	1:D:264:GLN:CD	2.40	0.42
1:A:336:GLN:CG	1:A:825:TRP:HE1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:HIS:CG	1:A:673:ALA:HB1	2.54	0.42
1:A:485:GLY:C	1:A:486:ILE:HD12	2.40	0.42
1:A:791:TYR:HA	1:A:797:TRP:CD1	2.55	0.42
1:B:24:VAL:HG22	1:B:107:ALA:O	2.18	0.42
1:B:150:LEU:HB3	1:B:829:PRO:HB3	2.00	0.42
1:B:228:THR:HA	1:B:229:PRO:HD2	1.83	0.42
1:B:481:ASN:ND2	1:B:482:LYS:N	2.66	0.42
1:B:570:ILE:HG13	1:B:620:ILE:HD11	2.01	0.42
1:D:21:VAL:C	1:D:23:ASN:N	2.64	0.42
1:D:455:VAL:HG12	1:D:674:SER:CB	2.49	0.42
1:D:753:LYS:HE3	1:D:753:LYS:HB2	1.96	0.42
1:A:501:GLU:O	1:A:505:GLU:HG3	2.18	0.42
1:A:627:GLY:HA2	1:A:642:VAL:HB	2.00	0.42
1:B:159:ILE:CG1	1:B:299:VAL:HB	2.50	0.42
1:B:173:GLY:HA2	1:B:624:THR:CG2	2.49	0.42
1:B:713:MET:SD	1:B:718:VAL:CA	3.00	0.42
1:C:39:LEU:HD21	1:C:53:PHE:HB3	2.02	0.42
1:C:184:ARG:CZ	1:C:184:ARG:HB2	2.49	0.42
1:D:558:ASN:HB3	1:D:561:SER:H	1.84	0.42
1:A:201:HIS:HB2	1:A:218:THR:HB	2.01	0.42
1:B:73:HIS:NE2	1:B:834:LEU:HD11	2.35	0.42
1:C:220:VAL:O	1:C:249:PRO:HG3	2.20	0.42
1:C:626:ILE:HG22	1:C:642:VAL:HG21	2.01	0.42
1:C:689:ILE:HG23	1:C:689:ILE:O	2.19	0.42
1:A:150:LEU:HB3	1:A:829:PRO:HB2	2.01	0.42
1:A:206:VAL:HG13	1:A:398:ARG:HD2	2.01	0.42
1:C:214:LYS:HE3	1:C:214:LYS:HB2	1.73	0.42
1:C:292:ARG:O	1:C:296:GLU:HG3	2.20	0.42
1:C:741:ILE:HG22	1:C:744:GLN:CG	2.48	0.42
1:C:764:MET:SD	1:C:769:ASP:CA	3.04	0.42
1:D:490:ARG:HA	1:D:494:LEU:HD13	2.01	0.42
1:A:503:ILE:HG23	1:A:521:LEU:HD11	2.02	0.42
1:A:813:SER:O	1:A:817:ILE:HB	2.20	0.42
1:B:18:LEU:HD11	1:B:30:ASN:HD21	1.85	0.42
1:B:160:ARG:HG2	1:B:160:ARG:HH11	1.84	0.42
1:C:33:ARG:HG3	1:D:18:LEU:CG	2.50	0.42
1:C:49:ARG:HD3	1:C:185:TYR:CD2	2.55	0.42
1:D:60:ARG:O	1:D:64:VAL:HG22	2.19	0.42
1:D:515:LEU:HD23	1:D:812:SER:HB2	2.01	0.42
1:A:66:ARG:HG2	1:A:66:ARG:HH11	1.85	0.42
1:A:170:ILE:HD13	1:A:175:GLN:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LEU:HA	1:B:347:PRO:HG2	2.01	0.42
1:C:208:HIS:O	1:C:209:THR:HG23	2.19	0.42
1:C:374:TYR:CD2	1:C:452:VAL:HG13	2.55	0.42
1:C:727:ASN:ND2	1:C:729:GLN:HB3	2.35	0.42
1:C:737:GLU:O	1:C:740:GLN:HB3	2.20	0.42
1:D:88:GLU:CG	1:D:132:GLY:HA2	2.50	0.42
1:D:91:MET:HE1	1:D:144:LEU:HD12	2.02	0.42
1:D:536:LYS:O	1:D:539:GLN:N	2.53	0.42
1:D:561:SER:HB2	1:D:563:PHE:CE1	2.54	0.42
1:D:587:TYR:CE1	1:D:636:VAL:HG21	2.54	0.42
1:D:661:ASP:O	1:D:686:ALA:HA	2.20	0.42
1:A:64:VAL:HG12	1:A:67:TRP:HE3	1.84	0.41
1:A:782:LYS:HA	1:A:785:GLU:HG3	2.02	0.41
1:B:280:TYR:HA	1:B:281:PRO:HD3	1.87	0.41
1:B:381:PRO:HA	1:B:384:LEU:HD13	2.01	0.41
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.84	0.41
1:C:139:LEU:HD23	1:C:143:PHE:CE2	2.56	0.41
1:C:528:GLU:O	1:C:532:ARG:NH1	2.53	0.41
1:D:376:ASN:ND2	1:D:378:THR:H	2.18	0.41
1:D:490:ARG:HG2	1:D:491:TRP:CE2	2.54	0.41
1:A:71:GLN:O	1:A:74:TYR:N	2.54	0.41
1:A:266:VAL:O	1:A:269:ARG:HB2	2.19	0.41
1:B:165:ILE:HD13	1:B:165:ILE:HA	1.82	0.41
1:C:49:ARG:NH2	1:C:125:ILE:O	2.52	0.41
1:C:699:MET:O	1:C:708:PHE:CE1	2.73	0.41
1:D:168:GLN:HE22	1:D:170:ILE:HD11	1.85	0.41
1:D:293:LEU:CD2	1:D:391:LEU:HD23	2.51	0.41
1:D:366:GLU:HG2	1:D:370:LYS:HE3	2.02	0.41
1:D:457:ARG:HH12	1:D:698:GLU:HG2	1.85	0.41
1:A:318:CYS:O	1:A:320:ASP:N	2.53	0.41
1:A:415:ALA:O	1:A:419:PRO:HG3	2.20	0.41
1:B:592:LYS:O	1:B:594:PRO:HD3	2.20	0.41
1:C:18:LEU:HG	1:D:33:ARG:CD	2.42	0.41
1:D:404:TYR:HE1	1:D:431:VAL:HG21	1.84	0.41
1:D:810:LYS:HA	1:D:815:ARG:CD	2.50	0.41
1:A:242:ARG:HG3	1:A:242:ARG:HH11	1.85	0.41
1:A:819:GLN:O	1:A:823:GLU:HB2	2.21	0.41
1:B:180:ASP:O	1:B:182:TRP:HD1	2.03	0.41
1:B:682:MET:HB3	1:B:808:SER:OG	2.21	0.41
1:C:18:LEU:HD22	1:C:18:LEU:HA	1.95	0.41
1:C:517:GLN:HG2	1:C:520:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:753:LYS:HB2	1:C:754:GLN:OE1	2.21	0.41
1:D:103:ALA:HA	1:D:234:ARG:NH1	2.35	0.41
1:D:589:ARG:NH2	1:D:785:GLU:OE2	2.53	0.41
1:D:629:VAL:O	1:D:633:ASP:HB2	2.21	0.41
1:D:717:ASP:HA	1:D:720:ARG:CG	2.50	0.41
1:A:128:ASP:OD1	1:A:651:SER:HB3	2.21	0.41
1:A:488:PRO:HG2	1:A:489:ARG:NH1	2.35	0.41
1:A:665:GLN:HE21	1:A:688:THR:HG23	1.84	0.41
1:A:718:VAL:HG23	1:A:772:LYS:HD3	2.01	0.41
1:A:793:ASN:H	1:A:794:PRO:HD3	1.84	0.41
1:B:664:GLU:HA	1:B:689:ILE:HG23	2.01	0.41
1:C:95:LEU:HD22	1:C:99:MET:CE	2.51	0.41
1:C:746:SER:OG	1:C:762:VAL:HG11	2.21	0.41
1:A:201:HIS:HB3	1:A:220:VAL:HA	2.03	0.41
1:B:456:ALA:HA	1:B:483:THR:HG23	2.01	0.41
1:B:550:GLU:HG2	1:B:555:VAL:CG2	2.50	0.41
1:B:698:GLU:HA	1:B:701:GLU:HB3	2.02	0.41
1:C:269:ARG:O	1:C:273:GLU:HG3	2.20	0.41
1:C:571:HIS:CE1	1:C:573:TYR:HD2	2.38	0.41
1:C:575:ARG:HB3	1:C:578:LEU:HB3	2.03	0.41
1:D:146:SER:O	1:D:150:LEU:HD23	2.20	0.41
1:D:455:VAL:HG12	1:D:674:SER:OG	2.20	0.41
1:D:797:TRP:CZ3	1:D:801:VAL:HG21	2.55	0.41
1:A:414:VAL:CG1	1:A:428:MET:SD	3.09	0.41
1:A:689:ILE:HD12	1:A:784:GLN:HE21	1.84	0.41
1:A:703:ALA:HB1	1:A:804:ASN:ND2	2.34	0.41
1:A:720:ARG:HA	1:A:723:GLN:HB2	2.02	0.41
1:B:82:ILE:CD1	1:B:147:MET:SD	3.07	0.41
1:B:355:ASP:OD2	1:B:398:ARG:NH1	2.54	0.41
1:B:545:PHE:CE2	1:B:549:LEU:HD22	2.56	0.41
1:B:555:VAL:O	1:B:556:HIS:HB3	2.21	0.41
1:C:95:LEU:HD22	1:C:99:MET:HE2	2.02	0.41
1:C:504:ALA:HA	1:C:508:GLY:O	2.20	0.41
1:D:221:VAL:HG22	1:D:272:ALA:HB1	2.02	0.41
1:D:402:ILE:O	1:D:406:ILE:HG13	2.20	0.41
1:D:459:HIS:HE1	1:D:463:LEU:HD21	1.85	0.41
1:D:703:ALA:O	1:D:707:ASN:ND2	2.53	0.41
1:D:753:LYS:HE3	1:D:754:GLN:OE1	2.20	0.41
1:D:786:ARG:O	1:D:790:LEU:HB3	2.21	0.41
1:A:112:THR:OG1	1:A:119:MET:HB2	2.21	0.41
1:A:150:LEU:HD12	1:A:817:ILE:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASN:HB2	1:A:834:LEU:O	2.21	0.41
1:A:469:LYS:HE2	1:A:469:LYS:HB2	1.83	0.41
1:A:724:ARG:NH2	1:A:730:GLU:OE1	2.54	0.41
1:B:187:ASN:HD22	1:B:189:TRP:H	1.66	0.41
1:C:67:TRP:O	1:C:71:GLN:HG2	2.20	0.41
1:C:355:ASP:OD2	1:C:398:ARG:HD3	2.20	0.41
1:C:384:LEU:HD21	1:C:468:PHE:HE1	1.85	0.41
1:C:557:ILE:HG23	1:C:559:PRO:HD3	2.03	0.41
1:D:106:ASN:HA	1:D:109:ASP:HB3	2.02	0.41
1:A:21:VAL:HG12	1:A:24:VAL:HG11	2.02	0.41
1:A:170:ILE:HD13	1:A:170:ILE:HA	1.87	0.41
1:A:481:ASN:C	1:A:482:LYS:HG2	2.40	0.41
1:A:584:ILE:HG21	1:A:750:PHE:CE2	2.56	0.41
1:A:654:GLU:O	1:A:658:PRO:HD2	2.20	0.41
1:A:661:ASP:HB3	1:A:797:TRP:CZ2	2.56	0.41
1:B:102:LEU:O	1:B:103:ALA:HB3	2.21	0.41
1:B:253:ASN:O	1:B:254:LEU:HD23	2.21	0.41
1:B:271:LEU:HA	1:B:274:ASN:ND2	2.36	0.41
1:B:322:VAL:HG23	1:B:323:ARG:NH2	2.35	0.41
1:B:355:ASP:OD1	1:B:398:ARG:NH1	2.54	0.41
1:B:685:GLY:CA	1:B:801:VAL:HG13	2.51	0.41
1:B:685:GLY:HA2	1:B:801:VAL:HG13	2.03	0.41
1:B:692:MET:CE	1:B:697:VAL:HA	2.50	0.41
1:B:713:MET:HB2	1:B:776:ASP:OD1	2.21	0.41
1:C:60:ARG:O	1:C:64:VAL:HG13	2.21	0.41
1:C:322:VAL:HG13	1:C:325:ASN:CB	2.49	0.41
1:C:389:VAL:HG12	1:C:439:ILE:HG13	2.02	0.41
1:C:571:HIS:ND1	1:C:573:TYR:CD2	2.88	0.41
1:D:235:ASN:OD1	1:D:237:VAL:HG12	2.20	0.41
1:D:256:ASP:O	1:D:257:PHE:HB2	2.21	0.41
1:D:257:PHE:HD1	1:D:257:PHE:HA	1.81	0.41
1:D:304:LEU:O	1:D:308:ILE:HG13	2.21	0.41
1:D:742:ILE:HD13	1:D:742:ILE:HA	1.94	0.41
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.84	0.41
1:A:446:ILE:HD11	1:A:468:PHE:CE2	2.56	0.41
1:A:566:GLN:O	1:A:605:ILE:HA	2.21	0.41
1:B:271:LEU:HA	1:B:274:ASN:CB	2.47	0.41
1:B:738:LEU:HD12	1:B:738:LEU:HA	1.82	0.41
1:C:81:ARG:HA	1:C:153:ALA:O	2.20	0.41
1:C:336:GLN:HE22	1:C:373:ALA:HB3	1.85	0.41
1:C:462:ILE:HA	1:C:465:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:TYR:CE1	1:C:574:LYS:HE3	2.57	0.41
1:D:110:GLU:HG2	1:D:114:GLN:NE2	2.36	0.41
1:D:326:PHE:O	1:D:330:PRO:HD3	2.21	0.41
1:D:613:TYR:CD2	1:D:616:ALA:HB3	2.56	0.41
1:D:756:ASP:O	1:D:759:LYS:HB2	2.21	0.41
1:A:83:TYR:CE1	1:A:310:ARG:NH1	2.89	0.40
1:C:262:TYR:HD1	1:C:262:TYR:HA	1.71	0.40
1:D:538:LYS:O	1:D:542:LYS:HG3	2.21	0.40
1:A:353:LEU:O	1:A:357:GLU:HB2	2.21	0.40
1:A:564:ASP:HB3	1:A:603:VAL:HA	2.02	0.40
1:D:100:VAL:HG23	1:D:101:ASN:N	2.37	0.40
1:D:206:VAL:HG21	1:D:401:GLN:HE22	1.85	0.40
1:D:263:ILE:O	1:D:265:ALA:N	2.54	0.40
1:D:456:ALA:HA	1:D:483:THR:HG23	2.02	0.40
1:D:698:GLU:HA	1:D:701:GLU:HB3	2.03	0.40
1:A:461:GLU:HB3	1:A:465:LYS:HE2	2.03	0.40
1:A:761:ILE:HD13	1:A:761:ILE:HG21	1.86	0.40
1:B:279:LEU:HD22	1:B:280:TYR:H	1.86	0.40
1:B:344:LEU:HD13	1:B:396:LEU:HD21	2.02	0.40
1:B:455:VAL:H	1:B:459:HIS:HD2	1.69	0.40
1:C:10:ARG:NH2	1:D:43:ARG:O	2.55	0.40
1:C:138:ARG:HD3	1:C:138:ARG:O	2.21	0.40
1:C:205:ARG:HG3	1:C:217:ASP:HB2	2.03	0.40
1:D:386:ARG:HG2	1:D:440:ASN:HA	2.03	0.40
1:D:487:THR:HA	1:D:488:PRO:HD3	1.78	0.40
1:A:381:PRO:O	1:A:384:LEU:HB2	2.22	0.40
1:A:396:LEU:HB3	1:A:399:HIS:HB2	2.03	0.40
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.56	0.40
1:A:748:GLY:HA3	1:A:755:PRO:HA	2.03	0.40
1:B:135:GLY:HA2	1:B:138:ARG:HB3	2.03	0.40
1:B:666:ILE:H	1:B:666:ILE:HG13	1.77	0.40
1:B:810:LYS:HD3	1:B:811:PHE:CE1	2.57	0.40
1:B:822:ARG:NH1	1:B:828:GLU:OE1	2.54	0.40
1:C:336:GLN:NE2	1:C:373:ALA:HB3	2.36	0.40
1:C:665:GLN:HG2	1:C:678:ASN:ND2	2.33	0.40
1:D:69:ARG:HA	1:D:72:GLN:HB2	2.03	0.40
1:D:577:LEU:HD22	1:D:765:LEU:HD11	2.03	0.40
1:A:97:ASN:HA	1:A:100:VAL:HG22	2.04	0.40
1:A:603:VAL:HG23	1:A:642:VAL:HA	2.03	0.40
1:A:798:THR:O	1:A:802:ILE:HG13	2.21	0.40
1:B:622:LEU:HD22	1:B:626:ILE:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:GLU:O	1:B:782:LYS:HE3	2.21	0.40
1:C:133:ASN:ND2	1:C:165:ILE:HG13	2.37	0.40
1:C:262:TYR:HB3	1:C:264:GLN:HG2	2.03	0.40
1:C:433:GLU:HB3	1:C:437:LYS:HG3	2.02	0.40
1:D:296:GLU:O	1:D:299:VAL:HG12	2.21	0.40
1:D:326:PHE:CD2	1:D:326:PHE:N	2.88	0.40
1:D:382:GLU:HG3	1:D:382:GLU:H	1.64	0.40
1:D:570:ILE:HG23	1:D:576:GLN:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	816/842 (97%)	651 (80%)	112 (14%)	53 (6%)	1	3
1	B	816/842 (97%)	669 (82%)	107 (13%)	40 (5%)	2	6
1	C	818/842 (97%)	678 (83%)	102 (12%)	38 (5%)	2	8
1	D	818/842 (97%)	643 (79%)	124 (15%)	51 (6%)	1	3
All	All	3268/3368 (97%)	2641 (81%)	445 (14%)	182 (6%)	1	4

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	21	VAL
1	A	152	LEU
1	A	166	PHE
1	A	236	ASN
1	A	256	ASP
1	A	257	PHE

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Mol	Chain	Res	Type
1	A	319	ARG
1	A	321	PRO
1	A	322	VAL
1	A	342	PRO
1	A	358	ARG
1	A	465	LYS
1	A	510	GLU
1	A	555	VAL
1	A	610	ALA
1	A	793	ASN
1	A	809	GLY
1	A	836	ALA
1	B	21	VAL
1	B	166	PHE
1	B	271	LEU
1	B	321	PRO
1	B	360	ASP
1	B	380	ILE
1	B	490	ARG
1	B	553	TYR
1	B	835	PRO
1	C	16	ARG
1	C	22	GLU
1	C	166	PHE
1	C	250	ASN
1	C	323	ARG
1	C	553	TYR
1	C	555	VAL
1	C	556	HIS
1	C	599	VAL
1	C	609	ALA
1	C	610	ALA
1	C	625	ALA
1	C	658	PRO
1	C	793	ASN
1	D	22	GLU
1	D	93	ARG
1	D	166	PHE
1	D	234	ARG
1	D	253	ASN
1	D	254	LEU
1	D	256	ASP

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Mol	Chain	Res	Type
1	D	264	GLN
1	D	315	LYS
1	D	321	PRO
1	D	322	VAL
1	D	358	ARG
1	D	559	PRO
1	D	561	SER
1	D	610	ALA
1	D	658	PRO
1	D	674	SER
1	D	757	LEU
1	A	22	GLU
1	A	253	ASN
1	A	273	GLU
1	A	288	GLY
1	A	492	LEU
1	A	529	ALA
1	A	827	VAL
1	B	17	GLY
1	B	92	GLY
1	B	253	ASN
1	B	256	ASP
1	B	379	VAL
1	B	554	LYS
1	B	610	ALA
1	C	19	ALA
1	C	92	GLY
1	C	95	LEU
1	C	256	ASP
1	C	493	VAL
1	C	694	GLY
1	C	783	CYS
1	D	19	ALA
1	D	103	ALA
1	D	260	GLY
1	D	429	SER
1	D	596	LYS
1	D	712	GLY
1	D	730	GLU
1	D	836	ALA
1	A	88	GLU
1	A	91	MET

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Mol	Chain	Res	Type
1	A	318	CYS
1	A	464	LYS
1	A	473	GLU
1	A	484	ASN
1	A	556	HIS
1	A	675	GLY
1	A	730	GLU
1	A	823	GLU
1	B	153	ALA
1	B	210	SER
1	B	258	ASN
1	B	339	ASP
1	B	341	HIS
1	B	350	MET
1	B	384	LEU
1	B	517	GLN
1	B	625	ALA
1	B	808	SER
1	C	40	VAL
1	C	93	ARG
1	C	254	LEU
1	C	321	PRO
1	C	383	ALA
1	C	561	SER
1	C	723	GLN
1	C	809	GLY
1	D	21	VAL
1	D	179	ALA
1	D	262	TYR
1	D	273	GLU
1	D	715	VAL
1	D	721	LEU
1	D	725	GLY
1	D	777	TYR
1	D	783	CYS
1	D	809	GLY
1	A	625	ALA
1	A	783	CYS
1	A	808	SER
1	A	826	GLY
1	B	93	ARG
1	B	342	PRO

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Mol	Chain	Res	Type
1	B	436	VAL
1	B	638	ASP
1	B	751	SER
1	C	21	VAL
1	C	436	VAL
1	C	835	PRO
1	D	436	VAL
1	D	484	ASN
1	D	509	GLU
1	D	735	ILE
1	D	829	PRO
1	A	93	ARG
1	A	263	ILE
1	A	269	ARG
1	A	436	VAL
1	A	553	TYR
1	A	570	ILE
1	B	16	ARG
1	B	183	LEU
1	C	551	ARG
1	C	554	LYS
1	C	724	ARG
1	D	104	LEU
1	D	525	VAL
1	D	697	VAL
1	A	92	GLY
1	A	346	ILE
1	A	477	HIS
1	B	628	ASP
1	B	798	THR
1	D	91	MET
1	D	105	GLU
1	D	628	ASP
1	B	20	GLY
1	B	666	ILE
1	C	559	PRO
1	D	151	GLY
1	D	320	ASP
1	A	824	ILE
1	B	637	GLY
1	B	658	PRO
1	B	836	ALA

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Mol	Chain	Res	Type
1	C	263	ILE
1	C	685	GLY
1	D	502	ILE
1	A	594	PRO
1	A	755	PRO
1	D	40	VAL
1	A	488	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	711/730 (97%)	579 (81%)	132 (19%)	1	4
1	B	711/730 (97%)	568 (80%)	143 (20%)	1	3
1	C	710/730 (97%)	579 (82%)	131 (18%)	1	4
1	D	711/730 (97%)	537 (76%)	174 (24%)	0	1
All	All	2843/2920 (97%)	2263 (80%)	580 (20%)	1	3

All (580) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	15	VAL
1	A	16	ARG
1	A	29	LYS
1	A	30	ASN
1	A	43	ARG
1	A	44	ASN
1	A	47	THR
1	A	52	TYR
1	A	63	LEU
1	A	75	TYR
1	A	78	ASP
1	A	82	ILE
1	A	87	LEU

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Mol	Chain	Res	Type
1	A	90	TYR
1	A	104	LEU
1	A	110	GLU
1	A	128	ASP
1	A	131	LEU
1	A	139	LEU
1	A	144	LEU
1	A	149	THR
1	A	165	ILE
1	A	169	LYS
1	A	191	LYS
1	A	195	GLU
1	A	196	PHE
1	A	224	MET
1	A	231	PRO
1	A	234	ARG
1	A	235	ASN
1	A	237	VAL
1	A	240	THR
1	A	241	MET
1	A	243	LEU
1	A	254	LEU
1	A	255	LYS
1	A	262	TYR
1	A	269	ARG
1	A	271	LEU
1	A	274	ASN
1	A	279	LEU
1	A	287	GLU
1	A	292	ARG
1	A	295	GLN
1	A	296	GLU
1	A	299	VAL
1	A	303	THR
1	A	304	LEU
1	A	306	ASP
1	A	319	ARG
1	A	321	PRO
1	A	323	ARG
1	A	324	THR
1	A	327	ASP
1	A	359	LEU

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Mol	Chain	Res	Type
1	A	360	ASP
1	A	361	TRP
1	A	366	GLU
1	A	370	LYS
1	A	374	TYR
1	A	385	GLU
1	A	392	LEU
1	A	396	LEU
1	A	423	ASP
1	A	425	LEU
1	A	430	LEU
1	A	438	ARG
1	A	440	ASN
1	A	445	CYS
1	A	453	ASN
1	A	455	VAL
1	A	461	GLU
1	A	467	ILE
1	A	469	LYS
1	A	471	PHE
1	A	474	LEU
1	A	489	ARG
1	A	492	LEU
1	A	494	LEU
1	A	495	CYS
1	A	516	ASP
1	A	517	GLN
1	A	519	ARG
1	A	528	GLU
1	A	540	GLU
1	A	543	LEU
1	A	551	ARG
1	A	553	TYR
1	A	554	LYS
1	A	567	VAL
1	A	574	LYS
1	A	576	GLN
1	A	579	ASN
1	A	584	ILE
1	A	586	LEU
1	A	596	LYS
1	A	613	TYR

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Mol	Chain	Res	Type
1	A	622	LEU
1	A	636	VAL
1	A	640	LEU
1	A	649	ARG
1	A	650	VAL
1	A	652	LEU
1	A	662	LEU
1	A	663	SER
1	A	692	MET
1	A	697	VAL
1	A	705	GLU
1	A	708	PHE
1	A	714	ARG
1	A	723	GLN
1	A	727	ASN
1	A	733	ASP
1	A	740	GLN
1	A	743	GLU
1	A	751	SER
1	A	755	PRO
1	A	756	ASP
1	A	757	LEU
1	A	764	MET
1	A	765	LEU
1	A	766	MET
1	A	783	CYS
1	A	790	LEU
1	A	800	MET
1	A	807	THR
1	A	817	ILE
1	A	832	GLN
1	A	833	ARG
1	A	834	LEU
1	A	837	PRO
1	B	10	ARG
1	B	16	ARG
1	B	21	VAL
1	B	22	GLU
1	B	23	ASN
1	B	35	LEU
1	B	39	LEU
1	B	45	VAL

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Mol	Chain	Res	Type
1	B	55	LEU
1	B	72	GLN
1	B	73	HIS
1	B	82	ILE
1	B	90	TYR
1	B	94	THR
1	B	95	LEU
1	B	105	GLU
1	B	112	THR
1	B	113	TYR
1	B	114	GLN
1	B	119	MET
1	B	128	ASP
1	B	131	LEU
1	B	155	TYR
1	B	165	ILE
1	B	177	GLU
1	B	187	ASN
1	B	195	GLU
1	B	209	THR
1	B	214	LYS
1	B	216	VAL
1	B	224	MET
1	B	230	VAL
1	B	241	MET
1	B	250	ASN
1	B	259	VAL
1	B	264	GLN
1	B	274	ASN
1	B	278	VAL
1	B	279	LEU
1	B	289	LYS
1	B	291	LEU
1	B	299	VAL
1	B	300	VAL
1	B	305	GLN
1	B	309	ARG
1	B	314	SER
1	B	316	PHE
1	B	319	ARG
1	B	321	PRO
1	B	323	ARG

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Mol	Chain	Res	Type
1	B	325	ASN
1	B	341	HIS
1	B	351	ARG
1	B	356	LEU
1	B	360	ASP
1	B	361	TRP
1	B	374	TYR
1	B	382	GLU
1	B	398	ARG
1	B	400	LEU
1	B	401	GLN
1	B	409	ARG
1	B	413	ARG
1	B	425	LEU
1	B	439	ILE
1	B	441	MET
1	B	444	LEU
1	B	453	ASN
1	B	455	VAL
1	B	458	ILE
1	B	460	SER
1	B	469	LYS
1	B	474	LEU
1	B	481	ASN
1	B	482	LYS
1	B	483	THR
1	B	490	ARG
1	B	492	LEU
1	B	493	VAL
1	B	510	GLU
1	B	512	ILE
1	B	516	ASP
1	B	522	LEU
1	B	530	PHE
1	B	532	ARG
1	B	539	GLN
1	B	552	GLU
1	B	553	TYR
1	B	554	LYS
1	B	557	ILE
1	B	565	VAL
1	B	567	VAL

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Mol	Chain	Res	Type
1	B	569	ARG
1	B	596	LYS
1	B	613	TYR
1	B	622	LEU
1	B	634	PRO
1	B	636	VAL
1	B	639	ARG
1	B	643	ILE
1	B	651	SER
1	B	652	LEU
1	B	656	VAL
1	B	665	GLN
1	B	672	GLU
1	B	676	THR
1	B	679	MET
1	B	688	THR
1	B	692	MET
1	B	702	GLU
1	B	705	GLU
1	B	708	PHE
1	B	715	VAL
1	B	716	GLU
1	B	717	ASP
1	B	721	LEU
1	B	729	GLN
1	B	738	LEU
1	B	742	ILE
1	B	743	GLU
1	B	749	PHE
1	B	754	GLN
1	B	756	ASP
1	B	760	ASP
1	B	767	HIS
1	B	768	HIS
1	B	773	VAL
1	B	781	VAL
1	B	782	LYS
1	B	792	LYS
1	B	794	PRO
1	B	795	ARG
1	B	796	GLU
1	B	798	THR

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Mol	Chain	Res	Type
1	B	799	ARG
1	B	800	MET
1	B	803	ARG
1	B	808	SER
1	B	814	ASP
1	B	819	GLN
1	B	832	GLN
1	B	833	ARG
1	B	837	PRO
1	C	12	GLN
1	C	15	VAL
1	C	18	LEU
1	C	31	PHE
1	C	40	VAL
1	C	43	ARG
1	C	45	VAL
1	C	48	PRO
1	C	49	ARG
1	C	53	PHE
1	C	61	ASP
1	C	70	THR
1	C	76	GLU
1	C	77	LYS
1	C	82	ILE
1	C	87	LEU
1	C	90	TYR
1	C	91	MET
1	C	95	LEU
1	C	97	ASN
1	C	100	VAL
1	C	104	LEU
1	C	105	GLU
1	C	117	LEU
1	C	120	GLU
1	C	125	ILE
1	C	138	ARG
1	C	139	LEU
1	C	150	LEU
1	C	162	GLU
1	C	165	ILE
1	C	169	LYS
1	C	175	GLN

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Mol	Chain	Res	Type
1	C	178	GLU
1	C	183	LEU
1	C	190	GLU
1	C	198	LEU
1	C	211	GLN
1	C	234	ARG
1	C	235	ASN
1	C	237	VAL
1	C	242	ARG
1	C	251	ASP
1	C	256	ASP
1	C	262	TYR
1	C	267	LEU
1	C	269	ARG
1	C	270	ASN
1	C	274	ASN
1	C	281	PRO
1	C	287	GLU
1	C	291	LEU
1	C	292	ARG
1	C	304	LEU
1	C	319	ARG
1	C	321	PRO
1	C	337	LEU
1	C	339	ASP
1	C	372	CYS
1	C	390	HIS
1	C	391	LEU
1	C	395	LEU
1	C	396	LEU
1	C	398	ARG
1	C	400	LEU
1	C	433	GLU
1	C	437	LYS
1	C	444	LEU
1	C	453	ASN
1	C	457	ARG
1	C	460	SER
1	C	464	LYS
1	C	466	THR
1	C	469	LYS
1	C	489	ARG

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Mol	Chain	Res	Type
1	C	490	ARG
1	C	492	LEU
1	C	494	LEU
1	C	499	LEU
1	C	506	ARG
1	C	518	LEU
1	C	525	VAL
1	C	533	ASP
1	C	536	LYS
1	C	538	LYS
1	C	549	LEU
1	C	554	LYS
1	C	569	ARG
1	C	573	TYR
1	C	574	LYS
1	C	575	ARG
1	C	576	GLN
1	C	579	ASN
1	C	584	ILE
1	C	591	LYS
1	C	623	ILE
1	C	630	VAL
1	C	638	ASP
1	C	640	LEU
1	C	649	ARG
1	C	654	GLU
1	C	655	LYS
1	C	656	VAL
1	C	658	PRO
1	C	662	LEU
1	C	663	SER
1	C	665	GLN
1	C	667	SER
1	C	678	ASN
1	C	683	LEU
1	C	692	MET
1	C	716	GLU
1	C	717	ASP
1	C	719	ASP
1	C	723	GLN
1	C	724	ARG
1	C	727	ASN

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Mol	Chain	Res	Type
1	C	741	ILE
1	C	745	LEU
1	C	753	LYS
1	C	759	LYS
1	C	764	MET
1	C	772	LYS
1	C	776	ASP
1	C	782	LYS
1	C	783	CYS
1	C	797	TRP
1	C	813	SER
1	C	822	ARG
1	C	832	GLN
1	C	833	ARG
1	D	10	ARG
1	D	12	GLN
1	D	13	ILE
1	D	14	SER
1	D	16	ARG
1	D	18	LEU
1	D	22	GLU
1	D	26	GLU
1	D	27	LEU
1	D	28	LYS
1	D	29	LYS
1	D	33	ARG
1	D	40	VAL
1	D	43	ARG
1	D	44	ASN
1	D	47	THR
1	D	63	LEU
1	D	69	ARG
1	D	76	GLU
1	D	77	LYS
1	D	82	ILE
1	D	85	LEU
1	D	87	LEU
1	D	90	TYR
1	D	91	MET
1	D	95	LEU
1	D	98	THR
1	D	102	LEU

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Mol	Chain	Res	Type
1	D	104	LEU
1	D	106	ASN
1	D	117	LEU
1	D	128	ASP
1	D	136	LEU
1	D	150	LEU
1	D	167	ASN
1	D	184	ARG
1	D	194	PRO
1	D	198	LEU
1	D	199	PRO
1	D	229	PRO
1	D	234	ARG
1	D	237	VAL
1	D	242	ARG
1	D	245	SER
1	D	255	LYS
1	D	257	PHE
1	D	262	TYR
1	D	264	GLN
1	D	266	VAL
1	D	267	LEU
1	D	268	ASP
1	D	273	GLU
1	D	274	ASN
1	D	279	LEU
1	D	291	LEU
1	D	292	ARG
1	D	296	GLU
1	D	300	VAL
1	D	310	ARG
1	D	319	ARG
1	D	321	PRO
1	D	323	ARG
1	D	324	THR
1	D	327	ASP
1	D	332	LYS
1	D	336	GLN
1	D	337	LEU
1	D	339	ASP
1	D	340	THR
1	D	341	HIS

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Mol	Chain	Res	Type
1	D	374	TYR
1	D	380	ILE
1	D	382	GLU
1	D	391	LEU
1	D	394	THR
1	D	395	LEU
1	D	396	LEU
1	D	400	LEU
1	D	409	ARG
1	D	413	ARG
1	D	421	ASP
1	D	425	LEU
1	D	426	ARG
1	D	430	LEU
1	D	444	LEU
1	D	458	ILE
1	D	460	SER
1	D	474	LEU
1	D	483	THR
1	D	489	ARG
1	D	490	ARG
1	D	492	LEU
1	D	505	GLU
1	D	510	GLU
1	D	511	TYR
1	D	516	ASP
1	D	517	GLN
1	D	526	ASP
1	D	530	PHE
1	D	533	ASP
1	D	538	LYS
1	D	539	GLN
1	D	541	ASN
1	D	543	LEU
1	D	549	LEU
1	D	552	GLU
1	D	554	LYS
1	D	555	VAL
1	D	557	ILE
1	D	558	ASN
1	D	560	ASN
1	D	566	GLN

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Mol	Chain	Res	Type
1	D	569	ARG
1	D	571	HIS
1	D	573	TYR
1	D	575	ARG
1	D	579	ASN
1	D	585	THR
1	D	589	ARG
1	D	590	ILE
1	D	596	LYS
1	D	603	VAL
1	D	604	MET
1	D	608	LYS
1	D	613	TYR
1	D	618	MET
1	D	622	LEU
1	D	630	VAL
1	D	642	VAL
1	D	643	ILE
1	D	649	ARG
1	D	652	LEU
1	D	654	GLU
1	D	658	PRO
1	D	662	LEU
1	D	667	SER
1	D	676	THR
1	D	681	PHE
1	D	682	MET
1	D	683	LEU
1	D	688	THR
1	D	689	ILE
1	D	692	MET
1	D	705	GLU
1	D	706	GLU
1	D	708	PHE
1	D	709	PHE
1	D	715	VAL
1	D	722	ASP
1	D	724	ARG
1	D	727	ASN
1	D	730	GLU
1	D	740	GLN
1	D	745	LEU

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Mol	Chain	Res	Type
1	D	753	LYS
1	D	755	PRO
1	D	756	ASP
1	D	761	ILE
1	D	763	ASN
1	D	765	LEU
1	D	766	MET
1	D	770	ARG
1	D	773	VAL
1	D	787	VAL
1	D	788	SER
1	D	792	LYS
1	D	793	ASN
1	D	798	THR
1	D	800	MET
1	D	802	ILE
1	D	808	SER
1	D	816	THR
1	D	819	GLN
1	D	832	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	32	ASN
1	A	71	GLN
1	A	73	HIS
1	A	168	GLN
1	A	201	HIS
1	A	235	ASN
1	A	250	ASN
1	A	274	ASN
1	A	412	ASN
1	A	480	GLN
1	A	481	ASN
1	A	566	GLN
1	A	579	ASN
1	A	582	HIS
1	A	684	ASN
1	A	744	GLN
1	A	784	GLN

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Mol	Chain	Res	Type
1	A	804	ASN
1	B	23	ASN
1	B	44	ASN
1	B	167	ASN
1	B	187	ASN
1	B	264	GLN
1	B	274	ASN
1	B	305	GLN
1	B	336	GLN
1	B	377	HIS
1	B	390	HIS
1	B	412	ASN
1	B	453	ASN
1	B	459	HIS
1	B	480	GLN
1	B	481	ASN
1	B	582	HIS
1	B	665	GLN
1	B	678	ASN
1	B	727	ASN
1	B	744	GLN
1	B	754	GLN
1	C	36	HIS
1	C	71	GLN
1	C	264	GLN
1	C	274	ASN
1	C	336	GLN
1	C	338	ASN
1	C	377	HIS
1	C	399	HIS
1	C	459	HIS
1	C	480	GLN
1	C	481	ASN
1	C	558	ASN
1	C	566	GLN
1	C	576	GLN
1	C	579	ASN
1	C	582	HIS
1	C	665	GLN
1	C	727	ASN
1	C	784	GLN
1	D	72	GLN

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Mol	Chain	Res	Type
1	D	97	ASN
1	D	106	ASN
1	D	167	ASN
1	D	168	GLN
1	D	175	GLN
1	D	187	ASN
1	D	219	GLN
1	D	250	ASN
1	D	274	ASN
1	D	376	ASN
1	D	377	HIS
1	D	401	GLN
1	D	450	HIS
1	D	453	ASN
1	D	459	HIS
1	D	481	ASN
1	D	484	ASN
1	D	560	ASN
1	D	647	ASN
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	LLP	D	680	1	23,24,25	1.84	5 (21%)	25,32,34	1.34	2 (8%)
1	LLP	C	680	1	23,24,25	1.50	3 (13%)	25,32,34	2.12	2 (8%)
1	LLP	B	680	1	23,24,25	1.49	5 (21%)	25,32,34	1.47	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LLP	A	680	1	23,24,25	1.61	4 (17%)	25,32,34	1.21	5 (20%)

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	LLP	D	680	1	-	8/16/17/19	0/1/1/1
1	LLP	C	680	1	-	0/16/17/19	0/1/1/1
1	LLP	B	680	1	-	2/16/17/19	0/1/1/1
1	LLP	A	680	1	-	2/16/17/19	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	680	LLP	C3-C2	-5.61	1.35	1.41
1	A	680	LLP	C3-C2	-4.68	1.36	1.41
1	D	680	LLP	C4-C4'	3.43	1.53	1.46
1	A	680	LLP	C4-C5	-3.42	1.37	1.42
1	C	680	LLP	C3-C2	-3.30	1.37	1.41
1	C	680	LLP	C4-C4'	3.00	1.53	1.46
1	B	680	LLP	C4'-NZ	2.93	1.37	1.27
1	C	680	LLP	C4'-NZ	2.88	1.36	1.27
1	D	680	LLP	C4'-NZ	2.85	1.36	1.27
1	B	680	LLP	C4-C5	-2.83	1.38	1.42
1	B	680	LLP	C3-C2	-2.76	1.38	1.41
1	B	680	LLP	P-OP2	-2.46	1.45	1.54
1	A	680	LLP	P-OP3	-2.28	1.46	1.54
1	B	680	LLP	C2-N1	2.25	1.37	1.33
1	D	680	LLP	C2'-C2	-2.23	1.46	1.50
1	A	680	LLP	C4'-NZ	2.23	1.34	1.27
1	D	680	LLP	P-OP3	-2.07	1.47	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	680	LLP	OP4-C5'-C5	8.90	126.03	109.36
1	B	680	LLP	OP4-C5'-C5	5.13	118.98	109.36
1	D	680	LLP	OP4-C5'-C5	4.68	118.14	109.36
1	C	680	LLP	CD-CE-NZ	-3.23	102.28	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	680	LLP	CG-CD-CE	-2.55	104.49	113.38
1	A	680	LLP	CD-CE-NZ	-2.37	104.56	110.83
1	D	680	LLP	CG-CD-CE	-2.37	105.13	113.38
1	B	680	LLP	OP2-P-OP4	-2.10	101.19	106.67
1	A	680	LLP	C5-C6-N1	-2.07	120.47	123.83
1	A	680	LLP	OP2-P-OP4	-2.06	101.30	106.67
1	A	680	LLP	C5-C4-C4'	-2.03	118.33	121.47
1	B	680	LLP	OP3-P-OP2	2.01	115.33	107.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	680	LLP	C5'-OP4-P-OP3
1	D	680	LLP	C4-C5-C5'-OP4
1	D	680	LLP	C5'-OP4-P-OP1
1	D	680	LLP	C5'-OP4-P-OP2
1	D	680	LLP	C5'-OP4-P-OP3
1	D	680	LLP	CE-CD-CG-CB
1	B	680	LLP	C5'-OP4-P-OP2
1	D	680	LLP	C6-C5-C5'-OP4
1	D	680	LLP	CG-CD-CE-NZ
1	A	680	LLP	C4-C5-C5'-OP4
1	A	680	LLP	N-CA-CB-CG
1	D	680	LLP	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	680	LLP	5	0
1	C	680	LLP	2	0
1	B	680	LLP	2	0
1	A	680	LLP	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
2	SO4	A	901	-	4,4,4	0.58	0	6,6,6	0.37	0
2	SO4	C	901	-	4,4,4	0.40	0	6,6,6	0.32	0
2	SO4	D	900	-	4,4,4	0.54	0	6,6,6	0.41	0
2	SO4	A	902	-	4,4,4	0.53	0	6,6,6	0.35	0
2	SO4	B	901	-	4,4,4	0.69	0	6,6,6	0.25	0
2	SO4	C	900	-	4,4,4	0.63	0	6,6,6	0.33	0
2	SO4	C	902	-	4,4,4	0.29	0	6,6,6	0.67	0
2	SO4	D	902	-	4,4,4	0.45	0	6,6,6	0.30	0
2	SO4	B	902	-	4,4,4	0.28	0	6,6,6	0.51	0
2	SO4	A	900	-	4,4,4	0.31	0	6,6,6	0.47	0
2	SO4	D	901	-	4,4,4	0.61	0	6,6,6	0.52	0
2	SO4	B	900	-	4,4,4	0.35	0	6,6,6	0.52	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	SO4	1	0
2	C	900	SO4	4	0
2	D	902	SO4	1	0
2	B	902	SO4	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	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	18:LEU	C	19:ALA	N	22.68
1	B	18:LEU	C	19:ALA	N	19.70

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.