Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 02:07 PM EDT

PDB ID	:	1ABB
Title	:	CONTROL OF PHOSPHORYLASE B CONFORMATION BY A MODIFIED COFACTOR: CRYSTALLOGRAPHIC STUDIES ON R-STATE GLYCOGEN PHOSPHORYLASE RECONSTITUTED WITH PYRIDOXAL 5'-DIPHOSPHATE
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Deposited on	:	1992-04-09
Resolution	:	2.80 Å(reported)

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

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

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

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

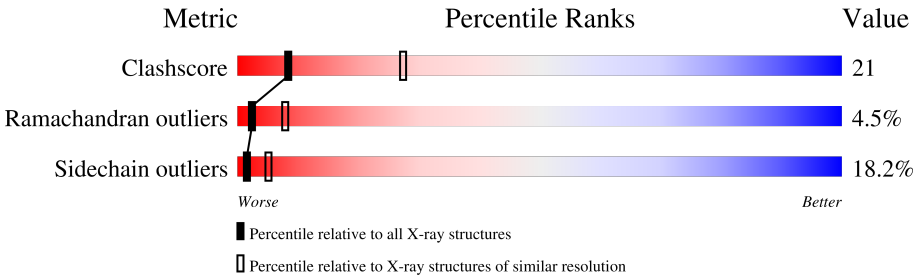
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	828	45% 36% 14% .
1	B	828	40% 39% 15% 5%
1	C	828	43% 39% 14% .
1	D	828	36% 42% 16% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26960 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.

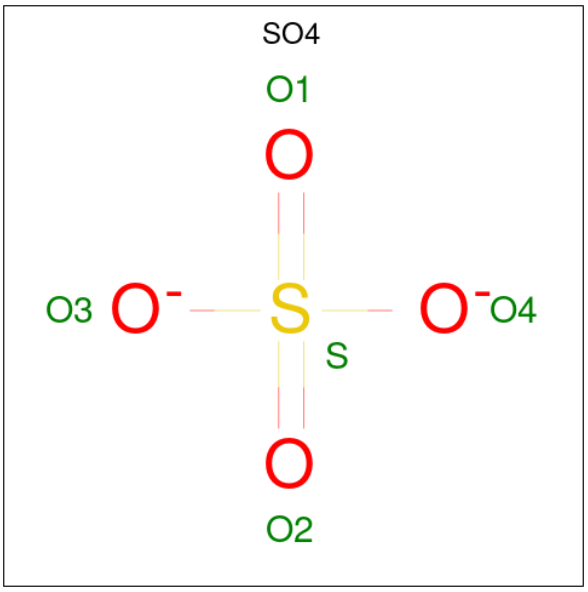
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	824	Total	C	N	O	S	0	0	1
			6693	4264	1185	1214	30			
1	B	824	Total	C	N	O	S	0	0	1
			6693	4264	1185	1214	30			
1	C	824	Total	C	N	O	S	0	0	1
			6693	4264	1185	1214	30			
1	D	824	Total	C	N	O	S	0	0	1
			6693	4264	1185	1214	30			

There are 4 discrepancies between the modelled and reference sequences:

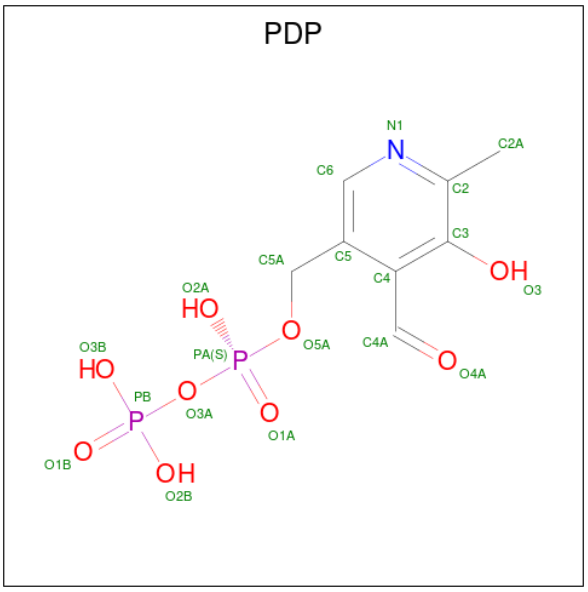
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

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



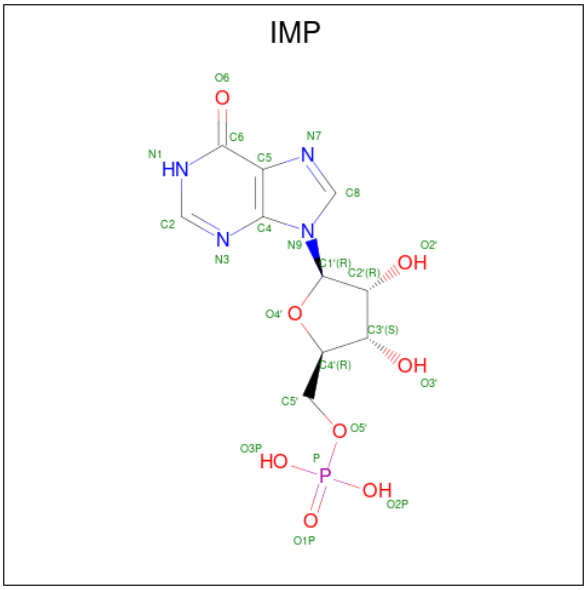
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is PYRIDOXAL-5'-DIPHOSPHATE (three-letter code: PDP) (formula: $C_8H_{11}NO_9P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			19	8	1	8	2		
3	B	1	Total	C	N	O	P	0	0
			19	8	1	8	2		
3	C	1	Total	C	N	O	P	0	0
			19	8	1	8	2		
3	D	1	Total	C	N	O	P	0	0
			19	8	1	8	2		

- Molecule 4 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

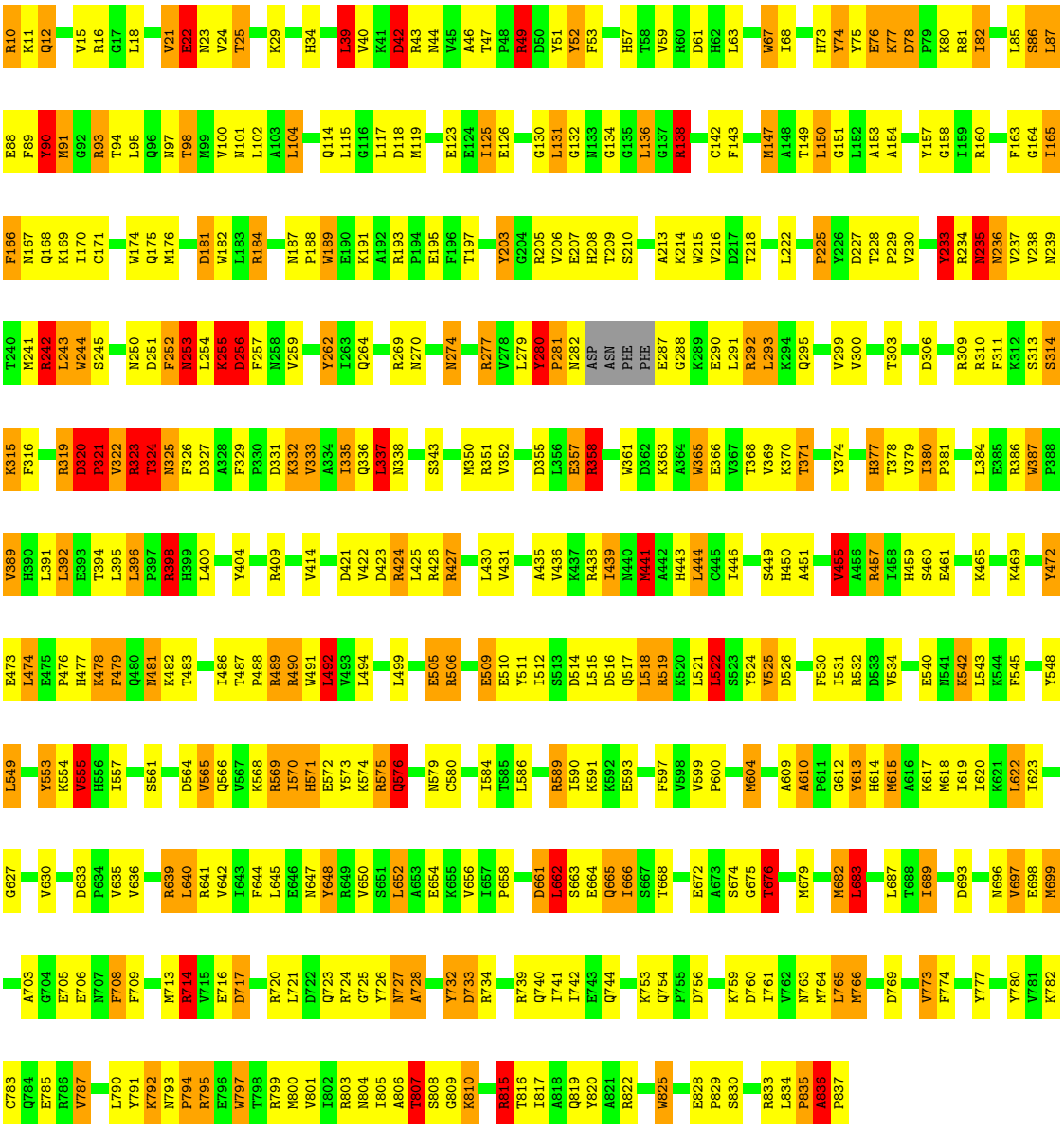
3 Residue-property plots (i)

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.

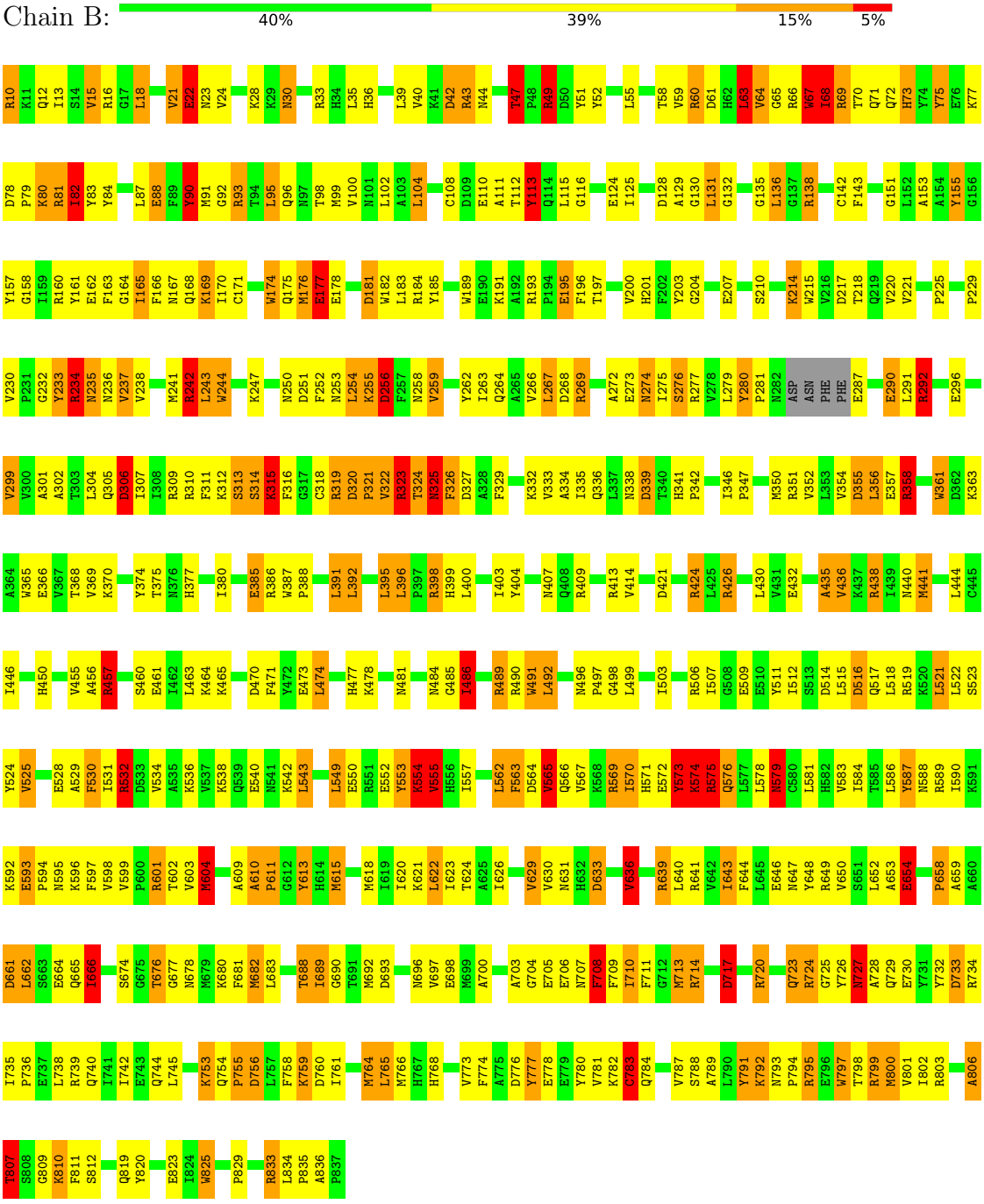
• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain A:



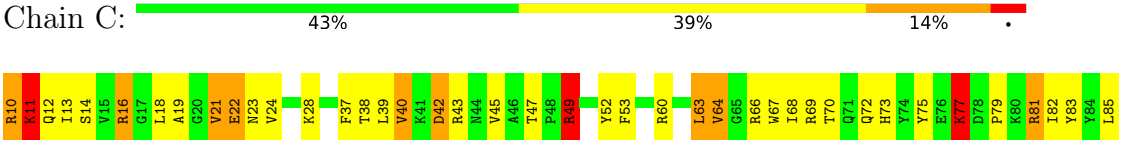
• Molecule 1: GLYCOGEN PHOSPHORYLASE B

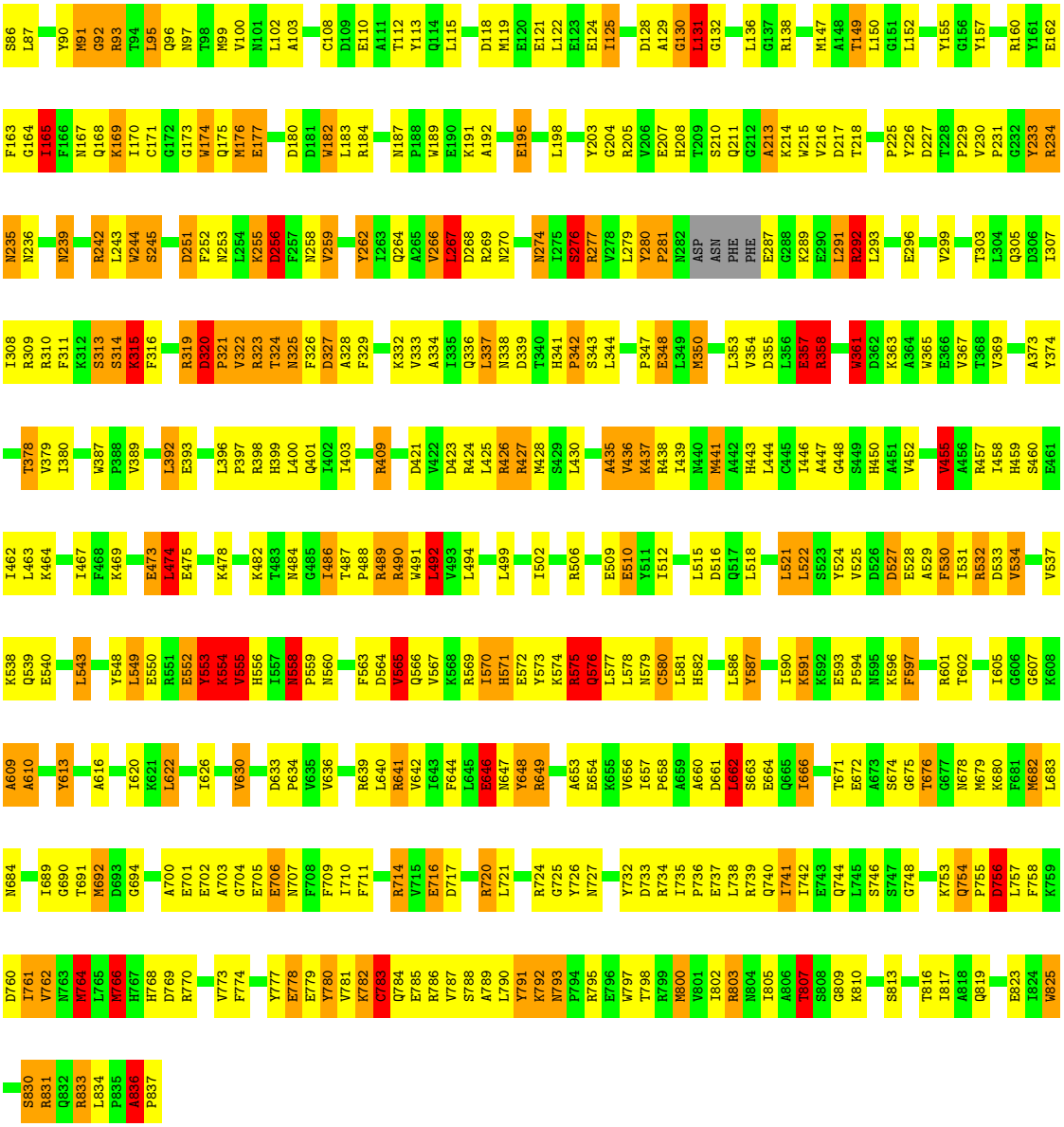
Chain B:



• Molecule 1: GLYCOGEN PHOSPHORYLASE B

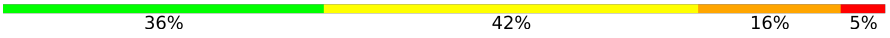
Chain C:

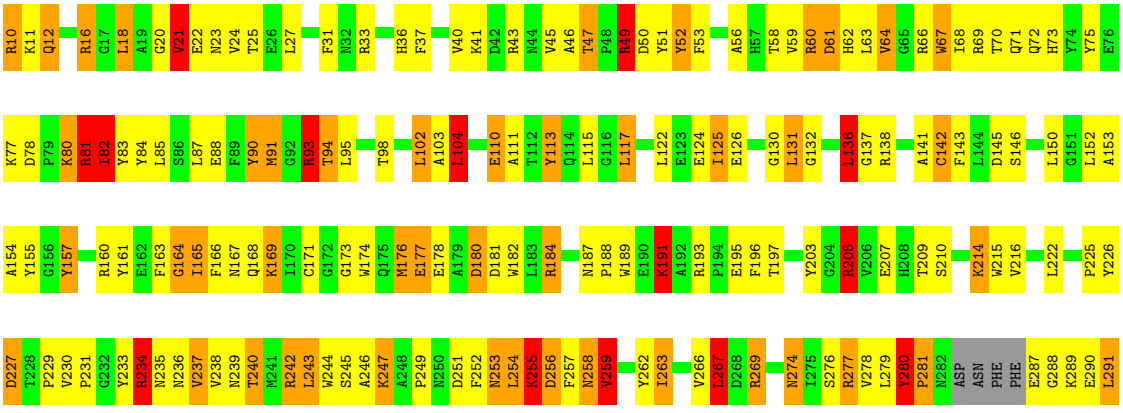


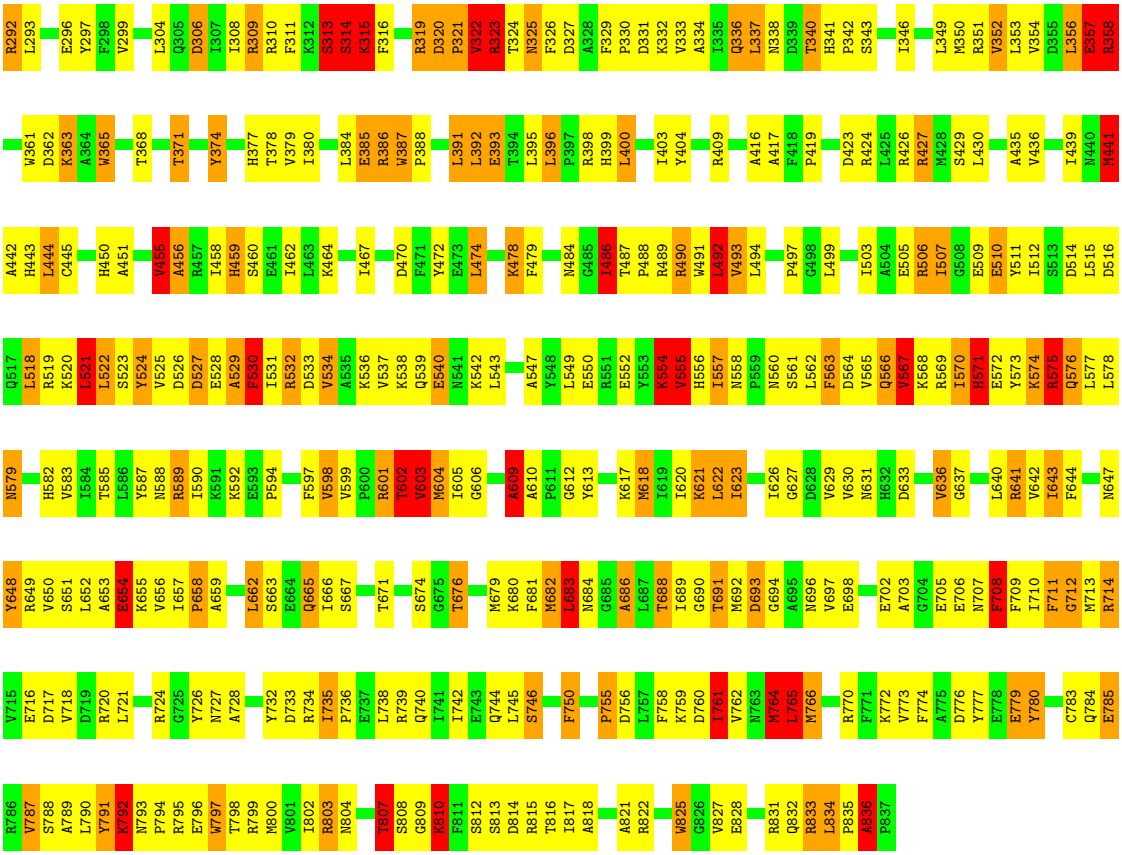


• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain D:






R292 L293 E296 Y297 F298 V299 L304 Q305 D306 I307 I308 R309 R310 F311 K312 S313 S314 K315 F316 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 I346 L349 M350 R351 V352 L353 V354 D355 L356 E357 R358
W361 D362 K363 A364 W365 T368 T371 Y374 H377 T378 V379 I380 L384 E385 R386 W387 P388 L391 L392 E393 T394 L395 L396 P397 R398 H399 L400 I403 Y404 R409 A416 A417 F418 P419 D423 R424 L425 R426 R427 M428 S429 L430 A435 V436 I439 N440 M441
A442 H443 L444 C445 H450 A451 V455 A456 R457 I458 H459 S460 E461 I462 L463 K464 I467 D470 F471 Y472 E473 L474 K478 F479 N484 G485 I486 T487 P488 R489 R490 W491 L492 V493 L494 P497 G498 L499 I503 A504 E505 R506 I507 G508 E509 E510 Y511 I512 S513 D514 L515 D516
Q517 L518 R519 K520 L521 L522 S523 Y524 V525 D526 D527 E528 A529 F530 I531 R532 D533 V534 A535 K536 V537 K538 Q539 E540 N541 K542 L543 A547 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 H582 V583 I584 T585 L586 Y587 N588 R589 I590 K591 K592 E593 P594 F597 V598 V599 P600 R601 T602 V603 M604 I605 G606 A609 A610 P611 G612 Y613 K617 M618 I619 I620 K621 L622 I623 I626 G627 D628 V629 V630 N631 H632 D633 V636 G637 L640 R641 V642 I643 F644 M647
Y648 R649 V650 S651 L652 A653 E654 K655 V656 I657 P658 A659 L662 S663 E664 Q665 I666 S667 T671 S674 G675 T676 M679 K680 F681 M682 L683 N684 G685 A686 L687 T688 I689 G690 T691 M692 D693 G694 A695 N696 V697 E698 E702 A703 G704 E705 E706 N707 F708 F709 I710 F711 G712 M713 R714
V715 E716 D717 V718 D719 R720 L721 R724 G725 Y726 N727 A728 Y732 D733 R734 I735 P736 E737 L738 R739 Q740 I741 I742 E743 Q744 L745 S746 F750 P755 D756 L757 F758 K759 D760 I761 V762 N763 M764 L765 M766 R770 F771 K772 V773 F774 A775 D776 Y777 E778 E779 Y780 C783 Q784 E785
R786 V787 S788 A789 L790 Y791 K792 N793 P794 R795 E796 W797 T798 R799 M800 V801 I802 R803 N804 T807 S808 G809 K810 F811 S812 S813 D814 R815 T816 I817 A818 A821 R822 W825 G826 V827 E828 R831 Q832 R833 L834 P835 A836 P837

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 188.10Å 88.10Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26960	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	1.06	2/6843 (0.0%)	2.09	248/9258 (2.7%)
1	B	1.12	7/6843 (0.1%)	2.08	261/9258 (2.8%)
1	C	1.04	3/6843 (0.0%)	2.05	229/9258 (2.5%)
1	D	1.07	6/6843 (0.1%)	2.10	260/9258 (2.8%)
All	All	1.07	18/27372 (0.1%)	2.08	998/37032 (2.7%)

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	6
1	B	0	10
1	C	0	4
1	D	0	7
All	All	0	27

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	ILE	N-CA	-23.27	0.99	1.46
1	B	69	ARG	CB-CG	11.74	1.84	1.52
1	B	80	LYS	CA-CB	-10.47	1.30	1.53
1	B	68	ILE	CB-CG1	9.71	1.81	1.54
1	A	586	LEU	CA-CB	-6.57	1.38	1.53
1	D	21	VAL	CA-CB	6.32	1.68	1.54
1	D	750	PHE	CA-CB	-6.07	1.40	1.53
1	D	393	GLU	CA-CB	-5.87	1.41	1.53
1	C	460	SER	CA-CB	-5.81	1.44	1.52
1	B	182	TRP	CG-CD2	-5.77	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	565	VAL	CA-CB	5.44	1.66	1.54
1	D	227	ASP	CA-CB	-5.44	1.42	1.53
1	C	215	TRP	CD2-CE2	-5.43	1.34	1.41
1	C	387	TRP	CD2-CE2	-5.30	1.34	1.41
1	D	82	ILE	CA-CB	5.20	1.66	1.54
1	B	797	TRP	CG-CD2	-5.14	1.34	1.43
1	B	82	ILE	CA-CB	5.09	1.66	1.54
1	D	361	TRP	CG-CD2	-5.03	1.35	1.43

All (998) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	490	ARG	NE-CZ-NH2	-18.76	110.92	120.30
1	C	160	ARG	NE-CZ-NH2	-18.13	111.23	120.30
1	A	490	ARG	NE-CZ-NH1	17.65	129.13	120.30
1	B	73	HIS	CA-CB-CG	14.99	139.08	113.60
1	C	160	ARG	NE-CZ-NH1	14.81	127.71	120.30
1	B	426	ARG	NE-CZ-NH1	14.64	127.62	120.30
1	C	203	TYR	CB-CG-CD2	-14.42	112.35	121.00
1	D	780	TYR	CB-CG-CD2	-13.68	112.79	121.00
1	C	184	ARG	NE-CZ-NH2	-13.19	113.70	120.30
1	A	90	TYR	CB-CG-CD2	-12.81	113.32	121.00
1	B	68	ILE	CB-CG1-CD1	12.05	147.63	113.90
1	A	203	TYR	CB-CG-CD1	-12.04	113.78	121.00
1	D	160	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	B	310	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	C	182	TRP	CD1-CG-CD2	11.91	115.83	106.30
1	B	69	ARG	CA-CB-CG	-11.84	87.35	113.40
1	A	548	TYR	CB-CG-CD2	-11.36	114.19	121.00
1	A	76	GLU	CA-CB-CG	11.22	138.08	113.40
1	D	60	ARG	NE-CZ-NH2	-11.19	114.70	120.30
1	B	409	ARG	NE-CZ-NH2	-11.19	114.71	120.30
1	B	426	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	D	81	ARG	NE-CZ-NH2	-11.11	114.74	120.30
1	C	490	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	B	613	TYR	CB-CG-CD2	-10.98	114.41	121.00
1	C	766	MET	CG-SD-CE	10.73	117.37	100.20
1	D	157	TYR	CB-CG-CD1	-10.71	114.58	121.00
1	B	519	ARG	NE-CZ-NH1	10.67	125.63	120.30
1	B	573	TYR	CB-CG-CD2	-10.57	114.66	121.00
1	C	81	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	A	93	ARG	NE-CZ-NH1	10.45	125.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	292	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	D	409	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	D	713	MET	CG-SD-CE	-10.32	83.69	100.20
1	A	676	THR	CA-CB-CG2	10.32	126.84	112.40
1	B	184	ARG	NE-CZ-NH2	-10.27	115.17	120.30
1	D	325	ASN	CA-C-N	-10.19	94.78	117.20
1	B	490	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	B	81	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	C	490	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	B	587	TYR	CB-CG-CD1	-10.08	114.95	121.00
1	A	491	TRP	CD1-CG-CD2	10.01	114.31	106.30
1	A	491	TRP	CE2-CD2-CG	-9.90	99.38	107.30
1	B	455	VAL	N-CA-CB	-9.88	89.75	111.50
1	A	780	TYR	CB-CG-CD2	-9.86	115.09	121.00
1	C	491	TRP	CD1-CG-CD2	9.81	114.15	106.30
1	B	325	ASN	CA-C-N	-9.80	95.65	117.20
1	B	639	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	C	325	ASN	CA-C-N	-9.73	95.80	117.20
1	D	650	VAL	CG1-CB-CG2	-9.71	95.36	110.90
1	A	398	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	D	184	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	B	67	TRP	CD1-CG-CD2	9.61	113.99	106.30
1	C	455	VAL	N-CA-CB	-9.56	90.47	111.50
1	B	395	LEU	CA-CB-CG	9.54	137.25	115.30
1	D	676	THR	CA-CB-CG2	9.50	125.71	112.40
1	A	174	TRP	CD1-CG-CD2	9.50	113.90	106.30
1	A	699	MET	CA-CB-CG	9.48	129.42	113.30
1	D	49	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	B	80	LYS	N-CA-CB	9.46	127.62	110.60
1	C	795	ARG	NE-CZ-NH2	-9.45	115.57	120.30
1	B	650	VAL	CG1-CB-CG2	-9.43	95.82	110.90
1	B	49	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	C	649	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	B	174	TRP	CD1-CG-CD2	9.39	113.81	106.30
1	C	244	TRP	CG-CD2-CE3	9.37	142.34	133.90
1	B	720	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	C	67	TRP	CD1-CG-CD2	9.30	113.74	106.30
1	B	365	TRP	CD1-CG-CD2	9.30	113.74	106.30
1	D	398	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	C	365	TRP	CG-CD2-CE3	9.27	142.24	133.90
1	B	67	TRP	NE1-CE2-CZ2	-9.23	120.25	130.40
1	C	409	ARG	NE-CZ-NH2	-9.17	115.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	491	TRP	CE2-CD2-CG	-9.14	99.98	107.30
1	B	81	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	491	TRP	CG-CD2-CE3	9.13	142.12	133.90
1	C	387	TRP	CD1-CG-CD2	9.12	113.60	106.30
1	A	477	HIS	CA-CB-CG	9.12	129.10	113.60
1	B	81	ARG	CA-C-N	-9.11	97.15	117.20
1	B	81	ARG	CB-CA-C	-9.10	92.20	110.40
1	D	724	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	138	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	D	365	TRP	CG-CD2-CE3	9.06	142.06	133.90
1	A	825	TRP	CG-CD2-CE3	9.05	142.05	133.90
1	B	67	TRP	CE2-CD2-CG	-9.04	100.07	107.30
1	D	365	TRP	CD1-CG-CD2	9.04	113.53	106.30
1	A	575	ARG	N-CA-C	9.02	135.35	111.00
1	A	374	TYR	CB-CG-CD2	-9.00	115.60	121.00
1	B	47	THR	CA-CB-CG2	8.99	124.99	112.40
1	C	613	TYR	CB-CG-CD2	-8.99	115.61	121.00
1	A	184	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	679	MET	CG-SD-CE	-8.97	85.85	100.20
1	D	815	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	D	292	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	D	361	TRP	CD1-CG-CD2	8.86	113.39	106.30
1	A	238	VAL	CG1-CB-CG2	-8.86	96.73	110.90
1	B	438	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	B	68	ILE	CG1-CB-CG2	-8.81	92.01	111.40
1	D	613	TYR	CB-CG-CD2	-8.81	115.71	121.00
1	C	825	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	B	365	TRP	CE2-CD2-CG	-8.80	100.26	107.30
1	D	323	ARG	CA-CB-CG	8.80	132.76	113.40
1	C	649	ARG	CG-CD-NE	-8.79	93.33	111.80
1	B	215	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	D	426	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	C	610	ALA	N-CA-CB	8.78	122.39	110.10
1	A	51	TYR	CB-CG-CD2	-8.78	115.73	121.00
1	C	292	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	C	764	MET	CA-CB-CG	8.73	128.15	113.30
1	A	427	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	B	610	ALA	N-CA-CB	8.71	122.29	110.10
1	B	613	TYR	CB-CG-CD1	8.70	126.22	121.00
1	C	325	ASN	O-C-N	8.70	136.61	122.70
1	A	474	LEU	CA-CB-CG	8.69	135.30	115.30
1	D	67	TRP	CD1-CG-CD2	8.69	113.25	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	226	TYR	CB-CG-CD2	-8.68	115.80	121.00
1	B	365	TRP	CG-CD2-CE3	8.66	141.70	133.90
1	D	244	TRP	CG-CD2-CE3	8.65	141.68	133.90
1	A	203	TYR	CB-CG-CD2	8.63	126.18	121.00
1	D	489	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	D	174	TRP	CE2-CD2-CG	-8.61	100.41	107.30
1	D	676	THR	CA-CB-OG1	-8.58	90.98	109.00
1	C	215	TRP	CD1-CG-CD2	8.56	113.15	106.30
1	B	182	TRP	CD1-CG-CD2	8.56	113.14	106.30
1	C	93	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	D	244	TRP	CE2-CD2-CG	-8.55	100.46	107.30
1	A	16	ARG	CA-C-N	8.54	133.28	116.20
1	B	639	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	61	ASP	CB-CG-OD1	8.52	125.97	118.30
1	C	244	TRP	CE2-CD2-CG	-8.52	100.48	107.30
1	C	534	VAL	CG1-CB-CG2	-8.50	97.31	110.90
1	B	489	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	365	TRP	CE2-CD2-CG	-8.44	100.55	107.30
1	D	90	TYR	CB-CG-CD2	-8.43	115.94	121.00
1	A	193	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	B	242	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	A	424	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	C	365	TRP	CB-CG-CD1	-8.38	116.10	127.00
1	A	182	TRP	CD1-CG-CD2	8.36	112.99	106.30
1	C	455	VAL	CB-CA-C	8.34	127.24	111.40
1	D	297	TYR	CB-CG-CD1	-8.32	116.01	121.00
1	B	174	TRP	CE2-CD2-CG	-8.29	100.67	107.30
1	A	243	LEU	CA-CB-CG	8.29	134.36	115.30
1	C	773	VAL	CA-CB-CG2	-8.29	98.47	110.90
1	C	807	THR	N-CA-CB	-8.27	94.58	110.30
1	D	215	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	C	67	TRP	CE2-CD2-CG	-8.27	100.68	107.30
1	B	93	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	325	ASN	CA-C-N	-8.25	99.05	117.20
1	A	720	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	D	365	TRP	CE2-CD2-CG	-8.23	100.71	107.30
1	C	182	TRP	CE2-CD2-CG	-8.23	100.72	107.30
1	C	365	TRP	CE2-CD2-CG	-8.23	100.72	107.30
1	D	45	VAL	CG1-CB-CG2	-8.22	97.75	110.90
1	A	640	LEU	CB-CG-CD1	-8.21	97.05	111.00
1	B	182	TRP	CE2-CD2-CG	-8.20	100.74	107.30
1	C	365	TRP	CD1-CG-CD2	8.19	112.85	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	676	THR	CA-CB-OG1	-8.18	91.82	109.00
1	B	648	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	C	387	TRP	CE2-CD2-CG	-8.16	100.77	107.30
1	D	641	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	B	113	TYR	CB-CG-CD2	-8.14	116.11	121.00
1	A	233	TYR	CB-CG-CD1	-8.13	116.12	121.00
1	C	491	TRP	CG-CD2-CE3	8.11	141.20	133.90
1	B	365	TRP	CB-CG-CD1	-8.10	116.47	127.00
1	D	43	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	D	361	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	A	174	TRP	CE2-CD2-CG	-8.06	100.85	107.30
1	B	61	ASP	CB-CG-OD1	8.04	125.53	118.30
1	D	385	GLU	CA-CB-CG	8.03	131.06	113.40
1	A	491	TRP	CB-CG-CD1	-8.02	116.58	127.00
1	B	491	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	D	113	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	A	586	LEU	CB-CG-CD2	-7.98	97.44	111.00
1	D	807	THR	N-CA-CB	-7.96	95.17	110.30
1	D	69	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	396	LEU	CA-CB-CG	7.93	133.54	115.30
1	D	16	ARG	CA-C-N	7.92	132.05	116.20
1	A	332	LYS	CA-CB-CG	-7.92	95.97	113.40
1	B	242	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	714	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	C	387	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	B	60	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	D	803	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	322	VAL	CA-C-N	7.88	134.53	117.20
1	D	365	TRP	CB-CG-CD1	-7.87	116.77	127.00
1	D	81	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	C	374	TYR	CB-CG-CD2	-7.85	116.29	121.00
1	D	395	LEU	CA-CB-CG	7.83	133.32	115.30
1	D	708	PHE	CB-CG-CD2	-7.83	115.32	120.80
1	D	351	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	B	610	ALA	CB-CA-C	-7.81	98.39	110.10
1	C	244	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	D	780	TYR	CB-CG-CD1	7.79	125.67	121.00
1	C	816	THR	CA-CB-CG2	-7.78	101.51	112.40
1	A	365	TRP	NE1-CE2-CZ2	-7.78	121.84	130.40
1	C	244	TRP	CB-CG-CD1	-7.78	116.89	127.00
1	A	639	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	B	491	TRP	CE2-CD2-CG	-7.76	101.09	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	64	VAL	CG1-CB-CG2	-7.76	98.48	110.90
1	D	191	LYS	CA-CB-CG	-7.76	96.33	113.40
1	A	46	ALA	O-C-N	7.74	135.08	122.70
1	D	720	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	C	457	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	16	ARG	N-CA-C	7.73	131.87	111.00
1	D	67	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	D	182	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	D	613	TYR	CB-CG-CD1	7.68	125.61	121.00
1	B	825	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	D	233	TYR	CB-CG-CD1	-7.65	116.41	121.00
1	A	74	TYR	CB-CG-CD2	-7.63	116.42	121.00
1	C	215	TRP	CG-CD1-NE1	-7.61	102.49	110.10
1	A	803	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	409	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	438	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	389	VAL	CA-CB-CG2	7.59	122.29	110.90
1	D	693	ASP	CB-CG-OD1	7.56	125.10	118.30
1	A	59	VAL	CA-CB-CG2	-7.55	99.57	110.90
1	B	267	LEU	CA-CB-CG	-7.55	97.92	115.30
1	A	509	GLU	CB-CA-C	-7.55	95.30	110.40
1	D	810	LYS	CA-CB-CG	7.51	129.91	113.40
1	D	554	LYS	CA-CB-CG	7.50	129.91	113.40
1	A	49	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	555	VAL	N-CA-C	7.49	131.22	111.00
1	A	610	ALA	N-CA-CB	7.49	120.58	110.10
1	A	215	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	A	138	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	D	604	MET	CG-SD-CE	7.47	112.16	100.20
1	C	93	ARG	N-CA-C	7.47	131.18	111.00
1	B	254	LEU	CA-CB-CG	7.46	132.47	115.30
1	B	47	THR	CA-CB-OG1	-7.45	93.35	109.00
1	D	787	VAL	CG1-CB-CG2	-7.45	98.98	110.90
1	B	358	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	C	800	MET	CA-CB-CG	-7.43	100.67	113.30
1	D	244	TRP	CB-CG-CD1	-7.43	117.34	127.00
1	B	825	TRP	CE2-CD2-CG	-7.42	101.37	107.30
1	B	553	TYR	CA-C-N	7.41	133.51	117.20
1	A	160	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	716	GLU	CA-CB-CG	7.37	129.62	113.40
1	D	325	ASN	O-C-N	7.36	134.47	122.70
1	D	773	VAL	CA-CB-CG2	-7.36	99.86	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	241	MET	CG-SD-CE	7.36	111.97	100.20
1	D	492	LEU	CA-CB-CG	7.34	132.19	115.30
1	B	575	ARG	CB-CG-CD	-7.33	92.54	111.60
1	B	361	TRP	CD1-CG-CD2	7.32	112.16	106.30
1	B	649	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	280	TYR	CB-CG-CD1	-7.32	116.61	121.00
1	D	351	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	A	389	VAL	CA-CB-CG1	-7.31	99.94	110.90
1	C	182	TRP	CG-CD1-NE1	-7.31	102.79	110.10
1	C	654	GLU	CA-CB-CG	7.30	129.46	113.40
1	B	174	TRP	CB-CG-CD1	-7.30	117.52	127.00
1	D	398	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	D	566	GLN	CA-CB-CG	7.29	129.44	113.40
1	A	160	ARG	CB-CG-CD	-7.27	92.70	111.60
1	C	532	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	D	189	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	D	243	LEU	CA-CB-CG	7.24	131.96	115.30
1	C	267	LEU	CA-C-N	7.24	133.13	117.20
1	C	102	LEU	CA-CB-CG	7.24	131.95	115.30
1	A	42	ASP	N-CA-CB	-7.24	97.57	110.60
1	D	84	TYR	CB-CG-CD1	-7.23	116.66	121.00
1	A	455	VAL	CG1-CB-CG2	7.23	122.47	110.90
1	D	244	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	B	174	TRP	CG-CD2-CE3	7.22	140.40	133.90
1	C	189	TRP	CD1-CG-CD2	7.20	112.06	106.30
1	D	770	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	C	277	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	825	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	A	244	TRP	CD1-CG-CD2	7.17	112.03	106.30
1	D	567	VAL	CA-CB-CG1	-7.17	100.15	110.90
1	D	773	VAL	CA-CB-CG1	7.17	121.65	110.90
1	C	803	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	386	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	277	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	661	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	90	TYR	CB-CG-CD1	7.13	125.28	121.00
1	B	355	ASP	CB-CG-OD1	7.13	124.71	118.30
1	B	234	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	D	641	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	A	387	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	A	351	ARG	CA-C-N	7.10	132.82	117.20
1	C	387	TRP	CB-CG-CD1	-7.09	117.78	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	473	GLU	CA-CB-CG	-7.09	97.81	113.40
1	A	61	ASP	CA-CB-CG	7.08	128.99	113.40
1	A	229	PRO	N-CA-CB	-7.07	94.81	103.30
1	A	610	ALA	CB-CA-C	-7.07	99.49	110.10
1	B	575	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	242	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	795	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	387	TRP	CD1-CG-CD2	7.05	111.94	106.30
1	D	490	ARG	CG-CD-NE	-7.05	96.99	111.80
1	A	807	THR	N-CA-CB	-7.05	96.91	110.30
1	A	157	TYR	CB-CG-CD1	-7.02	116.79	121.00
1	D	491	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	C	676	THR	N-CA-CB	-7.01	96.97	110.30
1	C	575	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	D	189	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	A	67	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	B	178	GLU	CA-C-N	6.98	132.56	117.20
1	B	244	TRP	CD1-CG-CD2	6.98	111.89	106.30
1	B	22	GLU	CA-C-N	-6.96	101.89	117.20
1	B	398	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	555	VAL	CB-CA-C	-6.95	98.19	111.40
1	A	455	VAL	N-CA-CB	-6.95	96.21	111.50
1	D	52	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	A	215	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	A	472	TYR	CB-CG-CD1	-6.94	116.83	121.00
1	D	682	MET	CA-CB-CG	6.94	125.10	113.30
1	D	777	TYR	CB-CG-CD1	-6.93	116.84	121.00
1	A	59	VAL	CA-CB-CG1	6.93	121.30	110.90
1	C	610	ALA	CB-CA-C	-6.91	99.73	110.10
1	C	491	TRP	CB-CG-CD1	-6.91	118.02	127.00
1	B	215	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	D	827	VAL	CG1-CB-CG2	-6.91	99.85	110.90
1	D	493	VAL	CA-CB-CG1	-6.91	100.54	110.90
1	B	555	VAL	CB-CA-C	-6.90	98.29	111.40
1	B	193	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	519	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	D	244	TRP	NE1-CE2-CZ2	-6.88	122.84	130.40
1	A	509	GLU	N-CA-CB	6.86	122.95	110.60
1	B	489	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	543	LEU	CA-CB-CG	6.85	131.06	115.30
1	D	676	THR	N-CA-CB	-6.85	97.28	110.30
1	A	94	THR	CA-C-N	6.85	132.27	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	756	ASP	CB-CG-OD2	6.85	124.46	118.30
1	B	310	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	532	ARG	CA-CB-CG	6.83	128.42	113.40
1	D	306	ASP	CB-CG-OD2	6.83	124.44	118.30
1	C	113	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	B	470	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	780	TYR	CB-CG-CD1	6.80	125.08	121.00
1	A	668	THR	CA-C-N	6.79	132.15	117.20
1	C	720	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	D	18	LEU	CA-CB-CG	6.79	130.91	115.30
1	C	428	MET	CA-CB-CG	-6.78	101.77	113.30
1	D	322	VAL	CA-C-N	6.77	132.10	117.20
1	B	81	ARG	CA-C-O	6.77	134.31	120.10
1	D	215	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	C	387	TRP	CG-CD1-NE1	-6.76	103.34	110.10
1	A	230	VAL	CG1-CB-CG2	-6.75	100.10	110.90
1	D	277	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	D	648	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	B	569	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	B	155	TYR	CB-CG-CD2	-6.74	116.96	121.00
1	D	184	ARG	CB-CG-CD	-6.74	94.08	111.60
1	C	591	LYS	CB-CG-CD	-6.73	94.10	111.60
1	A	435	ALA	N-CA-C	-6.73	92.84	111.00
1	D	174	TRP	NE1-CE2-CZ2	-6.73	123.00	130.40
1	D	499	LEU	N-CA-CB	6.73	123.85	110.40
1	C	174	TRP	CD1-CG-CD2	6.72	111.68	106.30
1	C	587	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	C	387	TRP	NE1-CE2-CZ2	-6.72	123.01	130.40
1	D	182	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	C	280	TYR	CA-CB-CG	-6.71	100.64	113.40
1	B	601	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	D	136	LEU	CA-CB-CG	6.71	130.74	115.30
1	A	189	TRP	CD1-CG-CD2	6.71	111.67	106.30
1	B	791	TYR	CB-CG-CD1	-6.70	116.98	121.00
1	C	825	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	D	424	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	D	174	TRP	CB-CG-CD1	-6.68	118.31	127.00
1	C	310	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	C	641	ARG	CA-CB-CG	-6.67	98.73	113.40
1	A	518	LEU	CA-CB-CG	6.66	130.62	115.30
1	D	455	VAL	N-CA-CB	-6.66	96.85	111.50
1	C	427	ARG	NE-CZ-NH2	-6.66	116.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	75	TYR	CB-CA-C	6.65	123.70	110.40
1	A	825	TRP	CB-CG-CD1	-6.64	118.36	127.00
1	C	565	VAL	CG1-CB-CG2	-6.64	100.28	110.90
1	B	463	LEU	CA-CB-CG	6.61	130.51	115.30
1	A	358	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	D	444	LEU	CB-CG-CD1	-6.60	99.78	111.00
1	A	662	LEU	CA-CB-CG	6.60	130.48	115.30
1	C	40	VAL	CG1-CB-CG2	-6.60	100.34	110.90
1	C	49	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	D	247	LYS	CA-CB-CG	-6.59	98.90	113.40
1	C	646	GLU	CA-CB-CG	6.59	127.90	113.40
1	A	693	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	215	TRP	CG-CD1-NE1	-6.58	103.52	110.10
1	D	174	TRP	CD1-CG-CD2	6.57	111.56	106.30
1	C	791	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	D	177	GLU	CA-CB-CG	6.57	127.85	113.40
1	A	716	GLU	CB-CG-CD	6.56	131.91	114.20
1	B	361	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	B	602	THR	N-CA-C	-6.56	93.29	111.00
1	A	306	ASP	CB-CG-OD2	6.55	124.20	118.30
1	B	455	VAL	CB-CA-C	6.55	123.84	111.40
1	C	613	TYR	CB-CG-CD1	6.55	124.93	121.00
1	A	40	VAL	CA-C-N	-6.54	102.81	117.20
1	A	216	VAL	CG1-CB-CG2	-6.54	100.43	110.90
1	D	459	HIS	CA-C-N	6.54	131.58	117.20
1	B	682	MET	CB-CG-SD	-6.53	92.81	112.40
1	A	803	ARG	CA-CB-CG	-6.52	99.05	113.40
1	A	293	LEU	CB-CG-CD2	-6.52	99.91	111.00
1	B	491	TRP	CB-CG-CD1	-6.52	118.53	127.00
1	C	831	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	174	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	C	527	ASP	CB-CG-OD1	6.48	124.14	118.30
1	D	764	MET	CA-CB-CG	6.48	124.31	113.30
1	D	269	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	42	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	108	CYS	CA-CB-SG	-6.46	102.38	114.00
1	B	189	TRP	NE1-CE2-CZ2	-6.45	123.31	130.40
1	D	816	THR	CA-CB-CG2	-6.44	103.38	112.40
1	A	181	ASP	CA-C-N	-6.43	103.05	117.20
1	A	740	GLN	CA-CB-CG	6.43	127.54	113.40
1	D	365	TRP	CG-CD1-NE1	-6.43	103.67	110.10
1	A	46	ALA	CA-C-N	-6.43	103.06	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	435	ALA	N-CA-C	-6.43	93.65	111.00
1	C	555	VAL	CB-CA-C	-6.42	99.19	111.40
1	D	507	ILE	CB-CA-C	-6.42	98.75	111.60
1	C	19	ALA	N-CA-C	6.42	128.34	111.00
1	B	200	VAL	CG1-CB-CG2	-6.41	100.64	110.90
1	B	174	TRP	CG-CD1-NE1	-6.40	103.70	110.10
1	D	825	TRP	CE2-CD2-CG	-6.40	102.18	107.30
1	B	181	ASP	CA-CB-CG	6.39	127.47	113.40
1	A	361	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	A	94	THR	O-C-N	-6.38	112.49	122.70
1	C	189	TRP	CE2-CD2-CG	-6.38	102.20	107.30
1	B	354	VAL	CG1-CB-CG2	-6.37	100.71	110.90
1	B	615	MET	CG-SD-CE	-6.36	90.02	100.20
1	B	553	TYR	O-C-N	-6.36	112.53	122.70
1	B	335	ILE	CA-C-N	6.36	131.19	117.20
1	B	776	ASP	CB-CG-OD2	6.35	124.01	118.30
1	B	435	ALA	N-CA-C	-6.34	93.88	111.00
1	C	389	VAL	CG1-CB-CG2	-6.33	100.77	110.90
1	A	769	ASP	CB-CG-OD1	6.33	123.99	118.30
1	A	682	MET	CG-SD-CE	-6.32	90.09	100.20
1	B	676	THR	CA-C-N	6.31	128.82	116.20
1	B	67	TRP	CB-CG-CD1	-6.31	118.80	127.00
1	D	563	PHE	CA-C-N	-6.31	103.32	117.20
1	A	792	LYS	CA-CB-CG	6.30	127.26	113.40
1	B	292	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	387	TRP	CE2-CD2-CG	-6.29	102.27	107.30
1	D	575	ARG	N-CA-C	6.29	127.98	111.00
1	A	492	LEU	CA-C-N	6.29	131.03	117.20
1	A	424	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	573	TYR	CB-CG-CD1	6.28	124.77	121.00
1	A	182	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	D	323	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	12	GLN	CA-CB-CG	6.26	127.17	113.40
1	C	795	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	D	791	TYR	CB-CG-CD1	6.25	124.75	121.00
1	C	350	MET	CG-SD-CE	-6.25	90.20	100.20
1	C	553	TYR	CA-C-N	6.25	130.95	117.20
1	A	505	GLU	CA-CB-CG	6.25	127.14	113.40
1	B	604	MET	CA-CB-CG	6.25	123.92	113.30
1	C	69	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	D	563	PHE	O-C-N	6.24	132.68	122.70
1	B	51	TYR	CB-CG-CD2	-6.23	117.26	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	633	ASP	CB-CG-OD2	6.23	123.91	118.30
1	D	776	ASP	CB-CG-OD2	6.23	123.91	118.30
1	D	49	ARG	CA-CB-CG	6.23	127.10	113.40
1	A	280	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	A	300	VAL	CA-CB-CG2	-6.22	101.56	110.90
1	D	450	HIS	CA-C-N	6.22	130.89	117.20
1	D	825	TRP	CD1-CG-CD2	6.22	111.28	106.30
1	A	365	TRP	CD1-CG-CD2	6.22	111.28	106.30
1	D	499	LEU	CB-CA-C	-6.21	98.40	110.20
1	C	389	VAL	CA-C-N	6.21	130.86	117.20
1	D	773	VAL	CG1-CB-CG2	-6.21	100.97	110.90
1	D	233	TYR	CB-CG-CD2	6.20	124.72	121.00
1	D	67	TRP	CG-CD2-CE3	6.20	139.47	133.90
1	A	648	TYR	CB-CG-CD2	-6.19	117.29	121.00
1	B	708	PHE	CA-C-N	6.19	130.82	117.20
1	D	491	TRP	CE2-CD2-CG	-6.19	102.35	107.30
1	A	150	LEU	CD1-CG-CD2	-6.18	91.96	110.50
1	B	490	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	149	THR	OG1-CB-CG2	-6.18	95.79	110.00
1	B	765	LEU	CA-CB-CG	6.18	129.51	115.30
1	C	676	THR	CA-CB-CG2	6.17	121.04	112.40
1	D	836	ALA	CA-C-N	6.17	134.37	117.10
1	B	241	MET	CA-CB-CG	-6.17	102.81	113.30
1	D	603	VAL	CG1-CB-CG2	6.16	120.76	110.90
1	C	770	ARG	CA-CB-CG	6.16	126.95	113.40
1	B	666	ILE	N-CA-C	6.16	127.63	111.00
1	A	337	LEU	CA-CB-CG	6.16	129.46	115.30
1	D	309	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	A	325	ASN	O-C-N	6.15	132.53	122.70
1	A	335	ILE	CG1-CB-CG2	-6.15	97.88	111.40
1	A	815	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	124	GLU	OE1-CD-OE2	-6.14	115.93	123.30
1	C	215	TRP	CE2-CD2-CG	-6.14	102.39	107.30
1	C	216	VAL	CG1-CB-CG2	-6.13	101.08	110.90
1	C	95	LEU	CA-C-N	6.13	130.69	117.20
1	A	499	LEU	CA-CB-CG	6.12	129.38	115.30
1	C	324	THR	N-CA-C	-6.12	94.47	111.00
1	C	552	GLU	N-CA-C	-6.12	94.48	111.00
1	A	800	MET	CG-SD-CE	6.12	109.98	100.20
1	A	708	PHE	O-C-N	-6.11	112.92	122.70
1	B	723	GLN	CA-CB-CG	6.11	126.85	113.40
1	A	125	ILE	CG1-CB-CG2	-6.11	97.95	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	778	GLU	CA-CB-CG	6.11	126.84	113.40
1	B	84	TYR	CB-CG-CD2	6.10	124.66	121.00
1	B	67	TRP	CG-CD1-NE1	-6.10	104.00	110.10
1	B	170	ILE	O-C-N	-6.10	112.94	122.70
1	A	661	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	247	LYS	CA-CB-CG	-6.10	99.98	113.40
1	B	244	TRP	CE2-CD2-CG	-6.09	102.43	107.30
1	C	77	LYS	CA-CB-CG	6.09	126.80	113.40
1	B	68	ILE	N-CA-C	6.09	127.43	111.00
1	B	157	TYR	CA-C-N	6.08	128.37	116.20
1	D	337	LEU	O-C-N	-6.08	112.97	122.70
1	B	708	PHE	CB-CG-CD2	-6.07	116.55	120.80
1	C	233	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	C	267	LEU	CA-C-O	-6.06	107.37	120.10
1	B	396	LEU	CB-CG-CD2	-6.06	100.70	111.00
1	A	441	MET	CG-SD-CE	-6.05	90.51	100.20
1	C	93	ARG	N-CA-CB	-6.05	99.70	110.60
1	C	464	LYS	CB-CG-CD	-6.03	95.91	111.60
1	D	426	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	C	348	GLU	CA-C-N	6.03	130.47	117.20
1	C	491	TRP	CG-CD1-NE1	-6.03	104.07	110.10
1	C	702	GLU	CB-CA-C	-6.03	98.34	110.40
1	A	665	GLN	CA-C-N	6.02	130.44	117.20
1	C	788	SER	CA-C-N	-6.01	103.98	117.20
1	B	81	ARG	CB-CG-CD	-6.00	95.99	111.60
1	D	623	ILE	CA-CB-CG2	-6.00	98.89	110.90
1	B	351	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	193	ARG	CG-CD-NE	-5.99	99.23	111.80
1	B	602	THR	CA-C-N	-5.98	104.04	117.20
1	D	255	LYS	CA-C-N	-5.98	104.04	117.20
1	B	689	ILE	CA-C-N	5.97	128.15	116.20
1	A	394	THR	CA-C-N	5.97	130.34	117.20
1	A	67	TRP	CE2-CD2-CG	-5.97	102.52	107.30
1	C	762	VAL	CG1-CB-CG2	-5.97	101.35	110.90
1	D	362	ASP	N-CA-CB	-5.97	99.86	110.60
1	B	33	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	B	740	GLN	CA-CB-CG	5.97	126.53	113.40
1	B	10	ARG	CA-C-N	5.96	130.32	117.20
1	D	552	GLU	N-CA-C	-5.96	94.90	111.00
1	D	374	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	B	659	ALA	CB-CA-C	-5.96	101.17	110.10
1	D	47	THR	CA-CB-CG2	5.95	120.73	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	666	ILE	O-C-N	-5.95	113.18	122.70
1	D	233	TYR	N-CA-CB	5.95	121.31	110.60
1	D	745	LEU	CA-CB-CG	5.95	128.98	115.30
1	D	521	LEU	CA-CB-CG	5.95	128.98	115.30
1	B	714	ARG	O-C-N	-5.94	113.20	122.70
1	C	825	TRP	CG-CD1-NE1	-5.94	104.16	110.10
1	B	322	VAL	CA-C-N	5.94	130.26	117.20
1	B	385	GLU	CA-CB-CG	5.93	126.44	113.40
1	C	189	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	C	554	LYS	CB-CA-C	-5.92	98.56	110.40
1	D	746	SER	CA-CB-OG	-5.92	95.22	111.20
1	A	321	PRO	N-CA-C	5.91	127.47	112.10
1	B	365	TRP	CG-CD1-NE1	-5.91	104.19	110.10
1	B	477	HIS	CA-CB-CG	5.91	123.64	113.60
1	A	16	ARG	O-C-N	-5.90	113.17	123.20
1	C	176	MET	CG-SD-CE	5.89	109.63	100.20
1	B	486	ILE	CB-CG1-CD1	-5.89	97.40	113.90
1	C	118	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	603	VAL	CB-CA-C	-5.89	100.20	111.40
1	A	182	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	C	160	ARG	CB-CG-CD	-5.89	96.28	111.60
1	A	683	LEU	CA-CB-CG	5.89	128.85	115.30
1	C	773	VAL	CA-CB-CG1	5.89	119.73	110.90
1	C	706	GLU	CB-CA-C	-5.89	98.63	110.40
1	A	641	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	371	THR	O-C-N	-5.87	113.30	122.70
1	A	244	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	C	10	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	D	427	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	D	456	ALA	CA-C-N	5.85	130.07	117.20
1	A	184	ARG	CA-C-N	5.85	130.06	117.20
1	A	238	VAL	O-C-N	-5.84	113.35	122.70
1	B	90	TYR	CB-CG-CD2	-5.84	117.49	121.00
1	B	290	GLU	CB-CA-C	-5.84	98.71	110.40
1	C	575	ARG	CA-C-N	5.84	130.04	117.20
1	A	93	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	302	ALA	N-CA-CB	-5.84	101.93	110.10
1	D	322	VAL	O-C-N	-5.83	113.36	122.70
1	B	275	ILE	N-CA-C	-5.83	95.25	111.00
1	C	783	CYS	CA-CB-SG	-5.83	103.50	114.00
1	B	323	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	D	716	GLU	CA-CB-CG	5.82	126.21	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	567	VAL	CA-C-N	-5.82	104.39	117.20
1	C	788	SER	O-C-N	5.82	132.01	122.70
1	B	555	VAL	N-CA-C	5.81	126.70	111.00
1	B	799	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	640	LEU	CB-CG-CD2	5.81	120.88	111.00
1	A	777	TYR	CB-CG-CD1	-5.81	117.51	121.00
1	D	765	LEU	CA-CB-CG	5.81	128.66	115.30
1	D	371	THR	CA-C-N	5.81	129.97	117.20
1	B	88	GLU	CA-CB-CG	5.80	126.16	113.40
1	B	490	ARG	CG-CD-NE	-5.80	99.62	111.80
1	D	164	GLY	CA-C-N	-5.79	104.45	117.20
1	B	424	ARG	CB-CG-CD	-5.79	96.55	111.60
1	D	486	ILE	N-CA-CB	-5.79	97.49	110.80
1	A	244	TRP	CE2-CD2-CG	-5.79	102.67	107.30
1	C	791	TYR	CB-CG-CD1	5.79	124.47	121.00
1	B	404	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	B	457	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	404	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	C	182	TRP	CH2-CZ2-CE2	5.77	123.17	117.40
1	A	825	TRP	NE1-CE2-CZ2	-5.77	124.05	130.40
1	B	554	LYS	CA-CB-CG	5.77	126.09	113.40
1	D	618	MET	CA-CB-CG	-5.77	103.49	113.30
1	B	704	GLY	CA-C-N	-5.77	104.51	117.20
1	A	430	LEU	O-C-N	-5.76	113.48	122.70
1	D	233	TYR	CB-CA-C	-5.76	98.88	110.40
1	C	239	ASN	O-C-N	-5.75	113.50	122.70
1	D	493	VAL	CB-CA-C	-5.75	100.48	111.40
1	B	220	VAL	CG1-CB-CG2	-5.74	101.72	110.90
1	D	91	MET	CG-SD-CE	-5.74	91.02	100.20
1	B	306	ASP	CB-CG-OD1	5.73	123.46	118.30
1	C	597	PHE	CA-C-N	-5.73	104.60	117.20
1	C	203	TYR	CD1-CG-CD2	5.72	124.20	117.90
1	A	697	VAL	CA-C-N	5.72	129.79	117.20
1	D	679	MET	CG-SD-CE	-5.72	91.04	100.20
1	A	457	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	822	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	791	TYR	CB-CG-CD2	5.69	124.41	121.00
1	D	93	ARG	N-CA-C	5.69	126.36	111.00
1	D	392	LEU	CA-CB-CG	5.69	128.38	115.30
1	B	177	GLU	CA-CB-CG	5.68	125.91	113.40
1	C	92	GLY	O-C-N	-5.68	113.61	122.70
1	C	610	ALA	N-CA-C	-5.68	95.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	TYR	CG-CD2-CE2	-5.68	116.75	121.30
1	A	365	TRP	NE1-CE2-CD2	5.68	112.98	107.30
1	C	119	MET	CA-CB-CG	-5.68	103.65	113.30
1	C	268	ASP	CB-CG-OD1	5.67	123.41	118.30
1	D	16	ARG	O-C-N	-5.67	113.56	123.20
1	C	554	LYS	CA-CB-CG	5.67	125.87	113.40
1	D	404	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	D	337	LEU	CA-C-N	5.66	129.66	117.20
1	C	203	TYR	CG-CD2-CE2	-5.66	116.77	121.30
1	D	37	PHE	CB-CG-CD2	-5.66	116.84	120.80
1	A	42	ASP	CB-CA-C	5.66	121.72	110.40
1	C	280	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	B	648	TYR	CB-CG-CD1	5.64	124.39	121.00
1	D	470	ASP	CB-CG-OD1	5.64	123.38	118.30
1	D	160	ARG	N-CA-C	-5.64	95.77	111.00
1	D	393	GLU	CB-CA-C	-5.64	99.12	110.40
1	A	575	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	558	ASN	N-CA-C	-5.63	95.78	111.00
1	A	361	TRP	CD1-CG-CD2	5.63	110.81	106.30
1	A	77	LYS	CA-CB-CG	5.63	125.79	113.40
1	A	825	TRP	CD1-CG-CD2	5.63	110.81	106.30
1	B	93	ARG	NH1-CZ-NH2	5.63	125.59	119.40
1	B	777	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	C	830	SER	N-CA-CB	-5.63	102.06	110.50
1	D	142	CYS	CA-CB-SG	-5.62	103.88	114.00
1	A	773	VAL	CA-CB-CG2	-5.62	102.47	110.90
1	B	189	TRP	CE2-CD2-CG	-5.62	102.80	107.30
1	C	266	VAL	CA-CB-CG2	-5.62	102.46	110.90
1	A	597	PHE	CA-C-N	-5.62	104.83	117.20
1	B	543	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	250	ASN	CA-C-N	-5.62	104.84	117.20
1	A	365	TRP	CB-CG-CD1	-5.62	119.69	127.00
1	C	552	GLU	CB-CG-CD	5.62	129.37	114.20
1	C	825	TRP	CB-CG-CD1	-5.62	119.70	127.00
1	C	91	MET	CG-SD-CE	-5.62	91.22	100.20
1	C	455	VAL	CA-CB-CG2	-5.62	102.48	110.90
1	C	467	ILE	CG1-CB-CG2	-5.62	99.05	111.40
1	A	682	MET	CA-CB-CG	5.61	122.84	113.30
1	A	782	LYS	CB-CG-CD	5.61	126.20	111.60
1	D	352	VAL	CG1-CB-CG2	-5.61	101.92	110.90
1	D	67	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	D	589	ARG	CA-CB-CG	-5.61	101.07	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	MET	CG-SD-CE	5.60	109.17	100.20
1	B	710	ILE	CA-C-N	5.60	129.52	117.20
1	D	117	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	47	THR	CA-CB-CG2	5.60	120.24	112.40
1	D	180	ASP	CA-C-N	5.60	129.52	117.20
1	D	574	LYS	CG-CD-CE	-5.60	95.11	111.90
1	B	280	TYR	CB-CG-CD1	-5.59	117.64	121.00
1	D	174	TRP	NE1-CE2-CD2	5.59	112.89	107.30
1	A	189	TRP	CE2-CD2-CG	-5.59	102.83	107.30
1	B	589	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	482	LYS	N-CA-C	-5.59	95.92	111.00
1	C	565	VAL	CA-CB-CG2	5.59	119.28	110.90
1	A	39	LEU	CA-CB-CG	5.57	128.12	115.30
1	A	324	THR	N-CA-C	-5.57	95.95	111.00
1	C	276	SER	N-CA-CB	-5.57	102.15	110.50
1	D	815	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	B	523	SER	O-C-N	-5.55	113.82	122.70
1	D	735	ILE	N-CA-CB	-5.54	98.05	110.80
1	A	490	ARG	CG-CD-NE	-5.54	100.16	111.80
1	B	290	GLU	CA-CB-CG	5.54	125.59	113.40
1	D	797	TRP	CE2-CD2-CG	-5.53	102.87	107.30
1	B	697	VAL	CA-CB-CG2	-5.53	102.60	110.90
1	C	357	GLU	OE1-CD-OE2	-5.53	116.66	123.30
1	B	609	ALA	CB-CA-C	-5.53	101.81	110.10
1	B	221	VAL	N-CA-C	-5.53	96.08	111.00
1	C	292	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	806	ALA	CB-CA-C	-5.52	101.82	110.10
1	D	255	LYS	O-C-N	5.52	131.53	122.70
1	A	589	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	30	ASN	CB-CA-C	-5.51	99.38	110.40
1	C	464	LYS	CA-CB-CG	5.50	125.51	113.40
1	A	805	ILE	CA-C-N	5.50	129.31	117.20
1	B	565	VAL	CG1-CB-CG2	-5.50	102.10	110.90
1	A	22	GLU	CA-C-N	-5.50	105.11	117.20
1	C	556	HIS	N-CA-CB	5.50	120.49	110.60
1	B	491	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	C	11	LYS	CA-CB-CG	5.49	125.49	113.40
1	A	187	ASN	N-CA-C	-5.49	96.17	111.00
1	A	238	VAL	CA-C-N	5.49	129.28	117.20
1	D	104	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	C	426	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	430	LEU	CA-C-N	5.48	129.25	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	491	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	D	667	SER	CB-CA-C	-5.48	99.70	110.10
1	A	676	THR	N-CA-CB	-5.47	99.90	110.30
1	B	563	PHE	CA-C-N	-5.47	105.16	117.20
1	A	374	TYR	CB-CG-CD1	5.47	124.28	121.00
1	B	203	TYR	CG-CD2-CE2	-5.47	116.92	121.30
1	B	267	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	B	602	THR	CA-CB-CG2	-5.46	104.76	112.40
1	C	189	TRP	CG-CD2-CE3	5.46	138.81	133.90
1	B	658	PRO	CA-N-CD	-5.46	103.86	111.50
1	C	95	LEU	O-C-N	-5.46	113.97	122.70
1	C	124	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	B	69	ARG	CB-CG-CD	5.45	125.78	111.60
1	B	361	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	D	507	ILE	N-CA-C	5.45	125.71	111.00
1	A	78	ASP	CB-CG-OD1	5.45	123.20	118.30
1	C	473	GLU	CA-CB-CG	-5.45	101.42	113.40
1	D	246	ALA	CB-CA-C	-5.45	101.93	110.10
1	B	64	VAL	CG1-CB-CG2	-5.44	102.19	110.90
1	A	174	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	B	485	GLY	C-N-CA	5.44	135.30	121.70
1	C	320	ASP	CB-CG-OD1	5.44	123.20	118.30
1	B	664	GLU	N-CA-CB	-5.44	100.81	110.60
1	C	724	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	176	MET	CG-SD-CE	-5.44	91.50	100.20
1	D	491	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	B	574	LYS	CG-CD-CE	-5.43	95.60	111.90
1	B	131	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	323	ARG	CA-CB-CG	5.42	125.33	113.40
1	A	633	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	728	ALA	N-CA-C	5.42	125.64	111.00
1	B	387	TRP	CG-CD1-NE1	-5.42	104.68	110.10
1	A	534	VAL	CG1-CB-CG2	-5.42	102.22	110.90
1	B	157	TYR	O-C-N	-5.42	113.98	123.20
1	D	506	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	B	636	VAL	CA-CB-CG1	-5.42	102.77	110.90
1	D	442	ALA	CA-C-N	5.42	129.13	117.20
1	D	567	VAL	CA-CB-CG2	5.42	119.03	110.90
1	B	374	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	643	ILE	CA-CB-CG1	-5.42	100.71	111.00
1	B	413	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	825	TRP	CG-CD2-CE3	5.41	138.77	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	713	MET	CG-SD-CE	-5.41	91.55	100.20
1	B	93	ARG	N-CA-C	5.41	125.60	111.00
1	A	491	TRP	NE1-CE2-CZ2	-5.40	124.46	130.40
1	B	350	MET	CB-CA-C	-5.40	99.59	110.40
1	D	547	ALA	CB-CA-C	-5.40	102.00	110.10
1	A	689	ILE	CA-C-N	5.40	126.99	116.20
1	A	650	VAL	CG1-CB-CG2	-5.39	102.27	110.90
1	A	787	VAL	CA-CB-CG2	-5.39	102.81	110.90
1	D	577	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	A	351	ARG	CA-C-O	-5.38	108.79	120.10
1	B	234	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	602	THR	N-CA-C	-5.38	96.46	111.00
1	B	388	PRO	CA-C-N	5.38	129.04	117.20
1	C	215	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	C	447	ALA	CA-C-N	5.38	126.95	116.20
1	D	266	VAL	CA-CB-CG2	-5.38	102.84	110.90
1	B	803	ARG	CA-CB-CG	-5.37	101.58	113.40
1	C	692	MET	CG-SD-CE	-5.37	91.60	100.20
1	D	708	PHE	CA-C-N	5.37	129.02	117.20
1	B	272	ALA	N-CA-C	-5.37	96.50	111.00
1	B	745	LEU	CA-CB-CG	5.37	127.66	115.30
1	C	435	ALA	N-CA-C	-5.37	96.50	111.00
1	C	792	LYS	CA-CB-CG	5.37	125.22	113.40
1	A	352	VAL	CB-CA-C	-5.37	101.20	111.40
1	B	387	TRP	CE2-CD2-CG	-5.37	103.00	107.30
1	A	117	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	280	TYR	CA-CB-CG	-5.37	103.20	113.40
1	B	299	VAL	CA-CB-CG2	-5.37	102.85	110.90
1	D	145	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	240	THR	CA-C-N	5.37	129.01	117.20
1	B	759	LYS	CB-CA-C	-5.36	99.67	110.40
1	B	713	MET	CA-CB-CG	5.36	122.41	113.30
1	C	213	ALA	N-CA-C	-5.36	96.53	111.00
1	B	724	ARG	CA-CB-CG	5.36	125.19	113.40
1	C	339	ASP	O-C-N	-5.36	114.13	122.70
1	D	258	ASN	N-CA-C	-5.36	96.53	111.00
1	D	792	LYS	CA-CB-CG	5.36	125.18	113.40
1	C	437	LYS	CB-CG-CD	-5.35	97.69	111.60
1	A	293	LEU	CB-CG-CD1	5.35	120.09	111.00
1	C	524	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	D	643	ILE	O-C-N	5.35	131.26	122.70
1	A	136	LEU	CA-CB-CG	5.35	127.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	525	VAL	CG1-CB-CG2	-5.35	102.35	110.90
1	A	427	ARG	CA-C-N	5.34	128.96	117.20
1	C	131	LEU	CA-CB-CG	5.34	127.59	115.30
1	B	268	ASP	CB-CG-OD1	5.34	123.10	118.30
1	D	205	ARG	N-CA-CB	-5.33	101.00	110.60
1	D	455	VAL	CB-CA-C	5.33	121.54	111.40
1	B	783	CYS	CA-CB-SG	-5.33	104.40	114.00
1	C	447	ALA	O-C-N	-5.33	114.14	123.20
1	B	633	ASP	CB-CG-OD1	5.33	123.09	118.30
1	B	579	ASN	N-CA-CB	-5.33	101.01	110.60
1	A	804	ASN	CB-CA-C	-5.32	99.75	110.40
1	D	142	CYS	CB-CA-C	-5.32	99.75	110.40
1	B	565	VAL	CA-CB-CG2	5.32	118.88	110.90
1	D	358	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	519	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	755	PRO	CA-C-N	-5.32	105.50	117.20
1	C	389	VAL	O-C-N	-5.32	114.19	122.70
1	C	132	GLY	CA-C-N	-5.31	105.51	117.20
1	D	189	TRP	NE1-CE2-CZ2	-5.31	124.56	130.40
1	D	386	ARG	CB-CG-CD	-5.31	97.79	111.60
1	D	667	SER	N-CA-CB	5.31	118.47	110.50
1	A	622	LEU	CA-CB-CG	5.31	127.52	115.30
1	C	112	THR	CA-CB-CG2	-5.31	104.96	112.40
1	B	797	TRP	CE2-CD2-CG	-5.31	103.05	107.30
1	B	233	TYR	CA-CB-CG	-5.30	103.32	113.40
1	D	164	GLY	O-C-N	5.30	131.19	122.70
1	C	367	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	A	49	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	233	TYR	CA-CB-CG	-5.30	103.33	113.40
1	B	636	VAL	CB-CA-C	-5.30	101.33	111.40
1	D	530	PHE	N-CA-CB	5.30	120.14	110.60
1	B	764	MET	CG-SD-CE	5.30	108.67	100.20
1	B	63	LEU	CA-CB-CG	5.29	127.47	115.30
1	C	430	LEU	CA-CB-CG	5.29	127.47	115.30
1	D	160	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	534	VAL	CA-C-N	5.29	128.83	117.20
1	B	717	ASP	CB-CG-OD1	5.28	123.06	118.30
1	B	116	GLY	CA-C-N	-5.28	105.58	117.20
1	C	81	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	203	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	D	761	ILE	CA-CB-CG2	-5.28	100.34	110.90
1	A	522	LEU	CA-CB-CG	5.28	127.44	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	689	ILE	O-C-N	-5.28	114.23	123.20
1	D	575	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	255	LYS	CA-C-N	-5.27	105.61	117.20
1	B	803	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	C	778	GLU	CA-CB-CG	5.27	124.99	113.40
1	C	679	MET	CG-SD-CE	5.26	108.62	100.20
1	A	797	TRP	NE1-CE2-CD2	5.26	112.56	107.30
1	D	157	TYR	CG-CD2-CE2	-5.26	117.09	121.30
1	D	505	GLU	CA-CB-CG	5.26	124.97	113.40
1	C	165	ILE	N-CA-C	-5.25	96.81	111.00
1	C	674	SER	CA-C-N	5.25	126.71	116.20
1	B	727	ASN	CB-CG-ND2	5.25	129.31	116.70
1	B	143	PHE	CB-CG-CD2	-5.25	117.13	120.80
1	A	320	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	326	PHE	N-CA-CB	-5.24	101.16	110.60
1	D	575	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	D	94	THR	CA-CB-OG1	-5.24	97.99	109.00
1	A	262	TYR	CA-C-N	-5.24	105.67	117.20
1	D	555	VAL	C-N-CA	5.24	134.80	121.70
1	A	427	ARG	O-C-N	-5.24	114.32	122.70
1	D	362	ASP	CB-CA-C	5.23	120.87	110.40
1	A	525	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	D	61	ASP	CA-CB-CG	5.23	124.90	113.40
1	B	184	ARG	CB-CG-CD	-5.22	98.03	111.60
1	A	377	HIS	CA-CB-CG	5.21	122.47	113.60
1	B	42	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	249	PRO	O-C-N	-5.21	114.36	122.70
1	C	662	LEU	N-CA-C	-5.21	96.94	111.00
1	D	441	MET	N-CA-CB	-5.21	101.23	110.60
1	A	666	ILE	N-CA-C	5.20	125.04	111.00
1	A	553	TYR	CA-CB-CG	5.20	123.28	113.40
1	D	555	VAL	CB-CA-C	-5.20	101.52	111.40
1	C	448	GLY	CA-C-N	5.20	128.63	117.20
1	D	94	THR	CA-CB-CG2	5.20	119.68	112.40
1	A	517	GLN	N-CA-CB	-5.19	101.25	110.60
1	A	564	ASP	N-CA-CB	-5.19	101.25	110.60
1	A	714	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	C	45	VAL	N-CA-CB	-5.19	100.07	111.50
1	A	615	MET	CG-SD-CE	5.19	108.51	100.20
1	C	702	GLU	N-CA-CB	5.19	119.95	110.60
1	D	636	VAL	CA-CB-CG1	-5.19	103.11	110.90
1	A	253	ASN	CA-CB-CG	5.19	124.82	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	602	THR	O-C-N	5.19	131.01	122.70
1	C	239	ASN	CA-C-N	5.19	128.62	117.20
1	B	323	ARG	CA-CB-CG	5.19	124.81	113.40
1	B	323	ARG	CB-CA-C	-5.19	100.02	110.40
1	A	131	LEU	CA-CB-CG	5.19	127.23	115.30
1	D	361	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	D	467	ILE	O-C-N	-5.18	114.41	122.70
1	D	124	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	D	177	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	D	649	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	98	THR	N-CA-CB	-5.17	100.47	110.30
1	A	654	GLU	CA-CB-CG	5.17	124.78	113.40
1	B	93	ARG	CG-CD-NE	-5.17	100.94	111.80
1	D	267	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	A	73	HIS	CA-C-N	5.17	128.57	117.20
1	C	189	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	D	49	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	A	734	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	654	GLU	CA-C-N	5.17	128.57	117.20
1	A	236	ASN	N-CA-C	5.17	124.95	111.00
1	C	266	VAL	CA-CB-CG1	5.16	118.65	110.90
1	C	809	GLY	CA-C-N	5.16	128.56	117.20
1	D	601	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	604	MET	CA-C-N	5.16	128.56	117.20
1	C	215	TRP	CA-CB-CG	5.16	123.51	113.70
1	C	187	ASN	CA-C-N	5.16	131.54	117.10
1	B	611	PRO	N-CD-CG	-5.15	95.47	103.20
1	A	229	PRO	O-C-N	-5.15	114.46	122.70
1	D	310	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	D	506	ARG	CA-C-N	5.15	128.53	117.20
1	A	86	SER	CB-CA-C	-5.14	100.33	110.10
1	D	472	TYR	CB-CG-CD1	-5.14	117.91	121.00
1	A	542	LYS	CA-CB-CG	-5.14	102.09	113.40
1	D	340	THR	CA-CB-CG2	-5.14	105.20	112.40
1	D	346	ILE	CA-C-N	5.14	131.49	117.10
1	C	280	TYR	CD1-CG-CD2	5.14	123.55	117.90
1	B	84	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	B	325	ASN	N-CA-C	5.14	124.87	111.00
1	B	438	ARG	CG-CD-NE	-5.14	101.01	111.80
1	B	538	LYS	CB-CA-C	-5.14	100.13	110.40
1	C	361	TRP	CE2-CD2-CG	-5.14	103.19	107.30
1	D	555	VAL	N-CA-C	5.13	124.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	563	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	C	443	HIS	CA-CB-CG	5.13	122.32	113.60
1	D	474	LEU	CA-CB-CG	5.12	127.09	115.30
1	D	797	TRP	NE1-CE2-CZ2	-5.12	124.76	130.40
1	A	91	MET	CB-CG-SD	-5.12	97.03	112.40
1	A	174	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	C	13	ILE	N-CA-C	-5.12	97.17	111.00
1	C	64	VAL	CG1-CB-CG2	-5.12	102.70	110.90
1	D	215	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	A	727	ASN	CB-CG-ND2	5.12	128.99	116.70
1	B	598	VAL	CB-CA-C	5.12	121.12	111.40
1	A	644	PHE	CA-C-N	5.11	128.44	117.20
1	D	357	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	C	754	GLN	N-CA-CB	5.11	119.80	110.60
1	A	723	GLN	CA-CB-CG	5.11	124.63	113.40
1	C	706	GLU	CA-CB-CG	5.11	124.64	113.40
1	D	609	ALA	N-CA-CB	-5.11	102.95	110.10
1	A	724	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	D	174	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	D	267	LEU	CA-CB-CG	-5.11	103.56	115.30
1	B	326	PHE	CB-CA-C	5.10	120.61	110.40
1	C	792	LYS	N-CA-CB	-5.10	101.42	110.60
1	C	800	MET	CG-SD-CE	5.10	108.36	100.20
1	D	69	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	197	THR	N-CA-CB	-5.10	100.61	110.30
1	B	396	LEU	CB-CG-CD1	5.10	119.67	111.00
1	B	755	PRO	CA-C-N	-5.10	105.99	117.20
1	A	455	VAL	CB-CA-C	5.09	121.08	111.40
1	B	398	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	177	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	C	279	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	548	TYR	CG-CD2-CE2	-5.09	117.23	121.30
1	B	269	ARG	CA-CB-CG	5.09	124.59	113.40
1	A	531	ILE	CA-C-N	5.09	128.39	117.20
1	C	353	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	387	TRP	CE2-CD2-CG	-5.09	103.23	107.30
1	D	450	HIS	O-C-N	-5.09	114.56	122.70
1	C	293	LEU	CA-CB-CG	5.08	127.00	115.30
1	D	602	THR	N-CA-C	-5.08	97.27	111.00
1	C	22	GLU	CA-C-N	-5.08	106.01	117.20
1	A	676	THR	O-C-N	-5.08	114.56	123.20
1	B	230	VAL	CA-CB-CG1	-5.08	103.28	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	80	LYS	CG-CD-CE	-5.08	96.68	111.90
1	B	563	PHE	CB-CG-CD1	5.08	124.35	120.80
1	C	365	TRP	CG-CD1-NE1	-5.08	105.03	110.10
1	A	519	ARG	CG-CD-NE	-5.07	101.14	111.80
1	B	244	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	D	810	LYS	CD-CE-NZ	5.07	123.35	111.70
1	C	13	ILE	CA-CB-CG2	-5.06	100.77	110.90
1	D	571	HIS	CB-CG-ND1	5.06	135.86	123.20
1	C	47	THR	CA-CB-CG2	5.06	119.49	112.40
1	C	714	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	656	VAL	CA-CB-CG2	-5.06	103.31	110.90
1	C	701	GLU	CA-C-N	5.06	128.33	117.20
1	A	439	ILE	N-CA-C	-5.06	97.34	111.00
1	B	10	ARG	CB-CG-CD	5.05	124.74	111.60
1	C	67	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	D	263	ILE	CA-C-N	5.05	128.32	117.20
1	C	63	LEU	CA-CB-CG	5.05	126.92	115.30
1	B	365	TRP	NE1-CE2-CZ2	-5.05	124.84	130.40
1	A	575	ARG	O-C-N	-5.05	114.62	122.70
1	A	189	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	C	52	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	C	474	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	269	ARG	CA-C-N	5.04	128.29	117.20
1	C	150	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	D	203	TYR	CG-CD2-CE2	-5.04	117.27	121.30
1	C	182	TRP	CG-CD2-CE3	5.04	138.43	133.90
1	B	10	ARG	O-C-N	-5.03	114.65	122.70
1	C	478	LYS	CA-CB-CG	-5.03	102.33	113.40
1	B	706	GLU	CB-CA-C	-5.03	100.34	110.40
1	C	308	ILE	CG1-CB-CG2	-5.03	100.34	111.40
1	D	184	ARG	NH1-CZ-NH2	5.03	124.93	119.40
1	B	90	TYR	CA-CB-CG	5.03	122.95	113.40
1	C	279	LEU	CB-CG-CD1	-5.03	102.46	111.00
1	C	293	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	C	339	ASP	CA-C-N	5.02	128.25	117.20
1	D	180	ASP	O-C-N	-5.02	114.67	122.70
1	A	235	ASN	CB-CG-ND2	5.02	128.74	116.70
1	C	648	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	A	732	TYR	CB-CG-CD1	5.02	124.01	121.00
1	D	686	ALA	CB-CA-C	5.01	117.62	110.10
1	B	807	THR	N-CA-CB	-5.01	100.78	110.30
1	D	314	SER	CA-CB-OG	5.01	124.72	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	654	GLU	CA-C-N	5.00	128.21	117.20
1	B	552	GLU	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ARG	Sidechain
1	A	280	TYR	Peptide
1	A	320	ASP	Peptide
1	A	52	TYR	Sidechain
1	A	836	ALA	Peptide
1	A	90	TYR	Sidechain
1	B	113	TYR	Sidechain
1	B	280	TYR	Peptide
1	B	320	ASP	Peptide
1	B	325	ASN	Mainchain
1	B	52	TYR	Sidechain
1	B	573	TYR	Sidechain
1	B	613	TYR	Sidechain
1	B	67	TRP	Peptide
1	B	820	TYR	Sidechain
1	B	90	TYR	Sidechain
1	C	280	TYR	Peptide
1	C	320	ASP	Peptide
1	C	780	TYR	Sidechain
1	C	836	ALA	Peptide
1	D	280	TYR	Peptide
1	D	320	ASP	Peptide
1	D	52	TYR	Sidechain
1	D	524	TYR	Sidechain
1	D	648	TYR	Sidechain
1	D	750	PHE	Sidechain
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	6693	0	6653	239	3
1	B	6693	0	6653	289	3
1	C	6693	0	6653	273	0
1	D	6693	0	6653	342	6
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
3	A	19	0	7	2	0
3	B	19	0	7	2	0
3	C	19	0	6	1	0
3	D	19	0	6	0	0
4	A	23	0	11	2	0
4	B	23	0	11	4	0
4	C	23	0	11	1	0
4	D	23	0	11	2	0
All	All	26960	0	26682	1123	6

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 21.

All (1123) 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:B:68:ILE:CB	1:B:68:ILE:CG1	1.81	1.57
1:B:69:ARG:CG	1:B:69:ARG:CB	1.84	1.54
1:B:73:HIS:CD2	1:B:834:LEU:HD21	1.61	1.30
1:B:69:ARG:CG	1:B:69:ARG:CA	2.33	1.06
1:B:73:HIS:CD2	1:B:834:LEU:CD2	2.32	1.01
1:D:88:GLU:HG2	1:D:132:GLY:HA2	1.45	0.98
1:B:68:ILE:CG1	1:B:68:ILE:CG2	2.41	0.96
1:D:322:VAL:HG13	1:D:325:ASN:HB2	1.46	0.96
1:D:791:TYR:HA	1:D:797:TRP:CD1	2.02	0.95
1:B:88:GLU:HG2	1:B:132:GLY:HA2	1.46	0.94
1:D:766:MET:HE3	1:D:774:PHE:HE2	1.36	0.91
1:D:235:ASN:ND2	1:D:237:VAL:HG13	1.88	0.88
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.56	0.87
1:D:707:ASN:HA	1:D:800:MET:SD	2.14	0.87
1:B:70:THR:OG1	1:B:237:VAL:HA	1.73	0.87
1:B:73:HIS:HD2	1:B:834:LEU:HD21	1.22	0.87
1:D:456:ALA:HB3	1:D:459:HIS:HB3	1.57	0.86
1:A:509:GLU:HG3	1:A:512:ILE:HD12	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:LEU:HD21	1:D:231:PRO:HB3	1.58	0.85
1:D:235:ASN:HD22	1:D:237:VAL:HG13	1.42	0.83
1:B:290:GLU:HG2	1:B:391:LEU:HD21	1.57	0.83
1:B:49:ARG:HH21	1:B:125:ILE:HG22	1.46	0.81
1:B:574:LYS:HB3	1:B:576:GLN:HE22	1.46	0.81
1:A:88:GLU:HG2	1:A:132:GLY:HA2	1.63	0.79
1:C:509:GLU:HG3	1:C:512:ILE:HD12	1.65	0.78
1:D:235:ASN:HA	1:D:833:ARG:HG3	1.66	0.77
1:A:75:TYR:OH	1:A:310:ARG:HG2	1.84	0.77
1:C:738:LEU:HD12	1:C:741:ILE:HD11	1.67	0.77
1:D:703:ALA:HA	1:D:807:THR:HG21	1.66	0.77
1:D:193:ARG:HB2	1:D:225:PRO:HG2	1.68	0.77
1:A:630:VAL:HG21	1:A:642:VAL:HG23	1.66	0.76
1:A:322:VAL:HG13	1:A:325:ASN:HB2	1.67	0.76
1:B:81:ARG:HD3	1:B:155:TYR:HE2	1.49	0.76
1:B:67:TRP:O	1:B:71:GLN:HG2	1.86	0.76
1:B:322:VAL:HG13	1:B:325:ASN:HB2	1.68	0.75
1:C:68:ILE:O	1:C:72:GLN:HG3	1.86	0.75
1:D:304:LEU:O	1:D:308:ILE:HG13	1.87	0.75
1:C:225:PRO:HB2	1:C:242:ARG:HD2	1.66	0.75
1:D:486:ILE:HG12	1:D:680:LYS:HG3	1.68	0.74
1:B:171:CYS:SG	1:B:176:MET:HG3	2.27	0.74
1:C:529:ALA:O	1:C:532:ARG:HG2	1.87	0.74
1:D:326:PHE:HA	1:D:329:PHE:HB2	1.67	0.74
1:D:49:ARG:HH21	1:D:125:ILE:HG22	1.52	0.73
1:D:343:SER:HB3	1:D:445:CYS:SG	2.28	0.73
1:C:707:ASN:HA	1:C:800:MET:SD	2.27	0.73
1:C:766:MET:HE3	1:C:766:MET:HA	1.69	0.73
1:B:503:ILE:HG23	1:B:521:LEU:HD11	1.71	0.73
1:D:795:ARG:O	1:D:799:ARG:HG3	1.87	0.72
1:D:81:ARG:HG3	1:D:81:ARG:HH11	1.54	0.72
1:D:562:LEU:HG	1:D:791:TYR:CD2	2.24	0.72
1:B:486:ILE:HD11	1:B:676:THR:HG23	1.71	0.72
1:B:707:ASN:HA	1:B:800:MET:SD	2.30	0.72
1:B:130:GLY:O	1:B:164:GLY:HA2	1.90	0.71
1:D:341:HIS:HB2	1:D:342:PRO:HD3	1.72	0.71
1:C:528:GLU:HB3	1:C:532:ARG:NH2	2.05	0.71
1:B:168:GLN:NE2	1:B:647:ASN:H	1.88	0.71
1:A:689:ILE:HA	1:A:709:PHE:HB2	1.73	0.71
1:B:73:HIS:HD2	1:B:834:LEU:CD2	1.88	0.71
1:D:574:LYS:HB3	1:D:576:GLN:HE22	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:766:MET:HE3	1:D:774:PHE:CE2	2.23	0.70
1:B:165:ILE:HD13	1:B:166:PHE:HD1	1.56	0.70
1:D:569:ARG:HH21	1:D:573:TYR:HE1	1.39	0.70
1:C:682:MET:HE3	1:C:807:THR:HG22	1.74	0.70
1:B:69:ARG:CG	1:B:69:ARG:HA	2.21	0.69
1:C:781:VAL:HG23	1:C:782:LYS:HE3	1.74	0.69
1:D:587:TYR:CD1	1:D:630:VAL:HG12	2.26	0.69
1:D:68:ILE:O	1:D:72:GLN:HG3	1.92	0.69
1:A:206:VAL:HG21	1:A:398:ARG:HB2	1.75	0.69
1:C:168:GLN:HE21	1:C:647:ASN:H	1.40	0.69
1:C:369:VAL:O	1:C:450:HIS:HB3	1.92	0.69
1:A:574:LYS:HZ2	1:A:672:GLU:CD	1.95	0.69
1:B:565:VAL:HG23	1:B:567:VAL:HG13	1.74	0.69
1:B:733:ASP:HA	1:B:739:ARG:NH1	2.08	0.69
1:B:47:THR:HG22	1:B:49:ARG:H	1.57	0.69
1:B:163:PHE:HD2	1:B:277:ARG:HG2	1.58	0.69
1:D:98:THR:O	1:D:102:LEU:HB2	1.94	0.68
1:D:460:SER:O	1:D:464:LYS:HG3	1.93	0.68
1:C:522:LEU:O	1:C:525:VAL:HG23	1.92	0.68
1:C:553:TYR:CE2	1:C:646:GLU:HB3	2.28	0.68
1:D:487:THR:HG23	1:D:490:ARG:H	1.59	0.68
1:D:516:ASP:HA	1:D:809:GLY:HA3	1.76	0.68
1:C:168:GLN:NE2	1:C:647:ASN:H	1.90	0.68
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.75	0.68
1:C:601:ARG:NH2	1:C:662:LEU:HD12	2.09	0.68
1:B:82:ILE:HB	1:B:334:ALA:HB3	1.75	0.67
1:D:231:PRO:HA	1:D:238:VAL:HG22	1.75	0.67
1:B:688:THR:HB	1:B:708:PHE:CE1	2.29	0.67
1:D:103:ALA:HA	1:D:234:ARG:HH11	1.58	0.67
1:C:533:ASP:O	1:C:537:VAL:HG23	1.94	0.67
1:A:449:SER:O	1:A:478:LYS:HD3	1.95	0.67
1:C:421:ASP:O	1:C:425:LEU:HD23	1.95	0.67
1:D:87:LEU:HD22	1:D:341:HIS:HB3	1.75	0.67
1:B:499:LEU:HD21	1:B:503:ILE:HD11	1.77	0.67
1:A:311:PHE:O	1:A:316:PHE:HB3	1.95	0.67
1:A:369:VAL:O	1:A:450:HIS:HB3	1.94	0.67
1:D:143:PHE:CG	1:D:817:ILE:HD11	2.29	0.66
1:B:511:TYR:HA	1:B:514:ASP:O	1.95	0.66
1:A:721:LEU:HD21	1:A:726:TYR:HD1	1.59	0.66
1:B:791:TYR:HA	1:B:797:TRP:CD1	2.30	0.66
1:C:574:LYS:HB3	1:C:576:GLN:HE22	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:726:TYR:CD1	1:D:772:LYS:HG2	2.30	0.66
1:C:49:ARG:HH21	1:C:125:ILE:HG22	1.61	0.66
1:D:563:PHE:HD2	1:D:659:ALA:O	1.79	0.66
1:A:130:GLY:O	1:A:164:GLY:HA2	1.95	0.66
1:A:168:GLN:HE21	1:A:647:ASN:H	1.43	0.66
1:C:37:PHE:CD2	1:D:61:ASP:HB3	2.31	0.66
1:D:709:PHE:HB3	1:D:783:CYS:SG	2.36	0.66
1:D:138:ARG:NH1	1:D:142:CYS:SG	2.69	0.66
1:B:738:LEU:HD13	1:B:777:TYR:CD2	2.30	0.66
1:D:458:ILE:HD11	1:D:694:GLY:HA2	1.76	0.66
1:B:166:PHE:CD2	1:B:177:GLU:HB3	2.31	0.65
1:B:201:HIS:HB3	1:B:218:THR:HB	1.78	0.65
1:C:521:LEU:HG	1:C:530:PHE:CZ	2.30	0.65
1:B:70:THR:HG23	1:B:237:VAL:HB	1.78	0.65
1:C:162:GLU:HA	1:C:183:LEU:HD12	1.77	0.65
1:B:795:ARG:O	1:B:799:ARG:HG3	1.97	0.65
1:C:474:LEU:HD13	1:C:475:GLU:HG3	1.79	0.65
1:B:168:GLN:HE21	1:B:647:ASN:H	1.43	0.65
1:B:726:TYR:OH	1:B:774:PHE:HB2	1.96	0.65
1:D:464:LYS:HE3	1:D:479:PHE:HB3	1.79	0.65
1:B:742:ILE:HD11	1:B:774:PHE:HZ	1.61	0.65
1:A:80:LYS:HE2	1:A:331:ASP:O	1.96	0.64
1:B:24:VAL:O	1:B:28:LYS:HG3	1.98	0.64
1:D:709:PHE:CE2	1:D:787:VAL:HG23	2.31	0.64
1:A:522:LEU:HA	1:A:525:VAL:HG23	1.78	0.64
1:C:322:VAL:HG13	1:C:325:ASN:HB2	1.80	0.64
1:C:636:VAL:O	1:C:639:ARG:HD3	1.97	0.64
1:A:662:LEU:HG	1:A:787:VAL:HG11	1.80	0.64
1:D:712:GLY:H	1:D:779:GLU:HG2	1.62	0.64
1:D:798:THR:O	1:D:802:ILE:HG13	1.97	0.64
1:B:766:MET:HA	1:B:766:MET:HE2	1.79	0.64
1:D:630:VAL:HG21	1:D:642:VAL:HG23	1.80	0.64
1:B:366:GLU:HG2	1:B:370:LYS:HE2	1.79	0.64
1:A:309:ARG:NH2	4:A:920:IMP:O3P	2.31	0.64
1:B:486:ILE:CD1	1:B:676:THR:HG23	2.28	0.64
1:D:130:GLY:O	1:D:164:GLY:HA2	1.98	0.64
1:C:662:LEU:HD21	1:C:689:ILE:HB	1.81	0.63
1:D:692:MET:SD	1:D:710:ILE:HD12	2.37	0.63
1:C:83:TYR:CE2	1:C:307:ILE:HG12	2.33	0.63
1:A:549:LEU:HD23	1:A:557:ILE:HG13	1.80	0.63
1:D:63:LEU:HD13	1:D:229:PRO:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:HIS:CD2	1:D:834:LEU:HD21	2.34	0.63
1:A:460:SER:OG	1:A:481:ASN:HB2	1.99	0.63
1:B:68:ILE:CG1	1:B:68:ILE:CA	2.75	0.63
1:B:68:ILE:CB	1:B:68:ILE:HG12	2.19	0.62
1:B:529:ALA:O	1:B:532:ARG:HG2	1.99	0.62
1:B:68:ILE:CB	1:B:68:ILE:HG13	2.19	0.62
1:B:274:ASN:HA	1:B:277:ARG:HB2	1.82	0.62
1:D:455:VAL:H	1:D:459:HIS:HD2	1.46	0.62
1:C:630:VAL:HG21	1:C:642:VAL:HG23	1.81	0.62
1:A:149:THR:HA	1:A:235:ASN:OD1	1.98	0.62
1:D:557:ILE:HG22	1:D:558:ASN:H	1.63	0.62
1:D:193:ARG:HB3	1:D:196:PHE:HD2	1.64	0.62
1:D:612:GLY:H	1:D:617:LYS:HE3	1.64	0.62
1:A:326:PHE:HA	1:A:329:PHE:HB2	1.82	0.62
1:B:158:GLY:HA2	1:B:299:VAL:HG21	1.80	0.62
1:C:171:CYS:SG	1:C:176:MET:HG3	2.40	0.62
1:D:803:ARG:O	1:D:807:THR:HB	1.99	0.62
1:A:426:ARG:CZ	1:D:755:PRO:HD2	2.30	0.61
1:C:596:LYS:HD3	1:C:597:PHE:N	2.15	0.61
1:B:562:LEU:HD23	1:B:661:ASP:HB2	1.82	0.61
1:A:426:ARG:NH1	1:D:755:PRO:HD2	2.16	0.61
1:B:69:ARG:CA	1:B:69:ARG:HG2	2.30	0.61
1:C:525:VAL:O	1:C:531:ILE:HD11	2.00	0.61
1:D:522:LEU:O	1:D:525:VAL:HG23	1.99	0.61
1:A:102:LEU:HD23	1:A:104:LEU:HD11	1.82	0.61
1:A:574:LYS:CE	3:A:931:PDP:O1B	2.48	0.61
1:B:171:CYS:HB2	1:B:176:MET:SD	2.41	0.61
1:C:235:ASN:HA	1:C:833:ARG:HG3	1.83	0.61
1:B:81:ARG:HG2	1:B:153:ALA:CB	2.31	0.61
1:A:74:TYR:CE2	1:A:153:ALA:HA	2.36	0.61
1:C:620:ILE:HG12	1:C:644:PHE:CZ	2.35	0.61
1:C:211:GLN:HG3	1:C:358:ARG:HE	1.64	0.60
1:A:82:ILE:HG23	1:A:154:ALA:HB2	1.82	0.60
1:D:163:PHE:CE1	1:D:181:ASP:HB3	2.36	0.60
1:D:582:HIS:CE1	1:D:784:GLN:HG3	2.37	0.60
1:B:692:MET:SD	1:B:710:ILE:HD12	2.40	0.60
1:D:721:LEU:HD21	1:D:726:TYR:HD1	1.66	0.60
1:A:355:ASP:OD2	1:A:398:ARG:HD3	2.01	0.60
1:B:590:ILE:HG21	1:B:636:VAL:HG13	1.84	0.60
1:D:601:ARG:NH2	1:D:662:LEU:HD12	2.16	0.60
1:D:682:MET:HE1	1:D:808:SER:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:THR:CG2	1:B:237:VAL:HB	2.31	0.60
1:D:564:ASP:HB3	1:D:603:VAL:HA	1.83	0.60
1:B:63:LEU:HD22	1:B:229:PRO:HB2	1.83	0.60
1:B:542:LYS:HG2	1:B:563:PHE:CD2	2.37	0.60
1:C:204:GLY:HA2	1:C:217:ASP:O	2.02	0.60
1:B:81:ARG:HG2	1:B:153:ALA:HB1	1.84	0.60
1:B:357:GLU:O	1:B:358:ARG:HB2	2.02	0.60
1:D:590:ILE:HG12	1:D:598:VAL:HG11	1.84	0.60
1:C:499:LEU:HD12	1:C:537:VAL:HG11	1.84	0.60
1:C:766:MET:HA	1:C:766:MET:CE	2.31	0.60
1:D:102:LEU:O	1:D:104:LEU:HD12	2.01	0.60
1:D:735:ILE:HG22	1:D:738:LEU:HB2	1.83	0.60
1:C:601:ARG:HH22	1:C:662:LEU:HD12	1.66	0.59
1:A:569:ARG:HH21	1:A:573:TYR:HE1	1.51	0.59
1:B:764:MET:HA	1:B:768:HIS:CE1	2.38	0.59
1:D:259:VAL:HG12	1:D:263:ILE:HA	1.82	0.59
1:D:605:ILE:HG21	1:D:623:ILE:HD13	1.84	0.59
1:A:181:ASP:O	1:A:184:ARG:HB2	2.01	0.59
1:B:163:PHE:CD2	1:B:277:ARG:HG2	2.37	0.59
1:D:681:PHE:HB3	1:D:686:ALA:HB3	1.84	0.59
1:A:86:SER:HB3	1:A:89:PHE:CE1	2.36	0.59
1:B:615:MET:CE	1:B:761:ILE:HG12	2.32	0.59
1:C:21:VAL:HG22	1:C:22:GLU:N	2.17	0.59
1:C:163:PHE:O	1:C:180:ASP:HB3	2.01	0.59
1:B:165:ILE:HD13	1:B:166:PHE:CD1	2.37	0.59
1:C:455:VAL:H	1:C:459:HIS:HD2	1.51	0.59
1:D:533:ASP:O	1:D:536:LYS:HB3	2.02	0.59
1:A:21:VAL:HG13	1:A:22:GLU:H	1.68	0.59
1:A:357:GLU:O	1:A:358:ARG:HB2	2.03	0.59
1:B:703:ALA:HA	1:B:807:THR:HG21	1.83	0.59
1:D:602:THR:HG23	1:D:641:ARG:HB2	1.84	0.59
1:D:519:ARG:O	1:D:522:LEU:HB2	2.02	0.59
1:C:326:PHE:HA	1:C:329:PHE:HB2	1.83	0.59
1:C:626:ILE:O	1:C:630:VAL:HG13	2.01	0.59
1:A:288:GLY:HA2	1:A:387:TRP:HZ3	1.68	0.58
1:D:622:LEU:HA	1:D:758:PHE:CZ	2.38	0.58
1:A:721:LEU:HD21	1:A:726:TYR:CD1	2.38	0.58
1:D:227:ASP:OD1	1:D:242:ARG:HD3	2.03	0.58
1:B:326:PHE:HA	1:B:329:PHE:HB2	1.85	0.58
1:D:529:ALA:O	1:D:532:ARG:HG2	2.03	0.58
1:D:582:HIS:NE2	1:D:784:GLN:HG3	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLY:O	1:A:243:LEU:HA	2.04	0.58
1:B:204:GLY:HA2	1:B:217:ASP:O	2.04	0.58
1:B:499:LEU:O	1:B:503:ILE:HG13	2.03	0.58
1:C:791:TYR:HA	1:C:797:TRP:CD1	2.39	0.58
1:D:235:ASN:HD22	1:D:237:VAL:H	1.51	0.58
1:D:451:ALA:HA	1:D:478:LYS:HG2	1.85	0.58
1:D:818:ALA:O	1:D:821:ALA:HB3	2.02	0.58
1:D:122:LEU:O	1:D:125:ILE:HG12	2.04	0.58
1:A:100:VAL:HG23	1:A:101:ASN:OD1	2.03	0.58
1:D:81:ARG:HD3	1:D:155:TYR:HE1	1.69	0.58
1:A:336:GLN:HE21	1:A:825:TRP:HE1	1.52	0.58
1:C:738:LEU:HD13	1:C:777:TYR:CD2	2.38	0.58
1:D:690:GLY:O	1:D:710:ILE:HA	2.04	0.58
1:A:274:ASN:HA	1:A:277:ARG:HB2	1.85	0.58
1:C:534:VAL:O	1:C:537:VAL:HB	2.03	0.58
1:C:703:ALA:HA	1:C:807:THR:HG21	1.86	0.58
1:D:166:PHE:CD2	1:D:177:GLU:HB3	2.39	0.58
1:B:73:HIS:CG	1:B:834:LEU:HD21	2.33	0.57
1:B:264:GLN:HE22	1:D:267:LEU:HD22	1.68	0.57
1:B:522:LEU:HD13	1:B:806:ALA:HB3	1.86	0.57
1:C:613:TYR:CD2	1:C:616:ALA:HB2	2.39	0.57
1:C:323:ARG:N	1:C:323:ARG:HE	2.02	0.57
1:D:601:ARG:HH12	1:D:787:VAL:HG12	1.68	0.57
1:A:138:ARG:HG3	1:A:138:ARG:HH11	1.70	0.57
1:A:208:HIS:HA	1:A:213:ALA:HA	1.86	0.57
1:A:682:MET:CE	1:A:808:SER:HA	2.35	0.57
1:A:834:LEU:HG	1:A:835:PRO:HD2	1.86	0.57
1:B:700:ALA:HA	1:B:708:PHE:CD2	2.40	0.57
1:B:264:GLN:NE2	1:D:267:LEU:HD22	2.19	0.57
1:D:70:THR:O	1:D:73:HIS:HB3	2.03	0.57
1:D:169:LYS:CG	1:D:171:CYS:SG	2.93	0.57
1:D:574:LYS:HB3	1:D:576:GLN:NE2	2.19	0.57
1:C:63:LEU:HD13	1:C:229:PRO:HG2	1.87	0.57
1:C:605:ILE:O	1:C:644:PHE:HA	2.04	0.57
1:A:645:LEU:HD11	1:A:656:VAL:HG21	1.86	0.57
1:D:169:LYS:HG2	1:D:171:CYS:SG	2.44	0.57
1:D:528:GLU:HB3	1:D:532:ARG:NH2	2.19	0.57
1:A:423:ASP:HA	1:A:426:ARG:HG2	1.87	0.57
1:C:726:TYR:OH	1:C:774:PHE:HB2	2.04	0.56
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.87	0.56
1:A:150:LEU:HB3	1:A:829:PRO:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:MET:SD	1:A:699:MET:HG2	2.45	0.56
1:B:522:LEU:HD13	1:B:806:ALA:CB	2.36	0.56
1:D:80:LYS:HE3	1:D:825:TRP:O	2.05	0.56
1:D:567:VAL:HA	1:D:606:GLY:O	2.05	0.56
1:B:316:PHE:HA	1:B:319:ARG:HB3	1.86	0.56
1:D:258:ASN:OD1	1:D:259:VAL:HG22	2.04	0.56
1:D:349:LEU:HD23	1:D:368:THR:HG23	1.86	0.56
1:D:458:ILE:HD11	1:D:694:GLY:CA	2.34	0.56
1:B:21:VAL:HG13	1:B:22:GLU:H	1.70	0.56
1:B:111:ALA:O	1:B:115:LEU:HG	2.06	0.56
1:B:742:ILE:HD11	1:B:774:PHE:CZ	2.40	0.56
1:D:315:LYS:N	1:D:315:LYS:HD2	2.21	0.56
1:D:601:ARG:HH22	1:D:662:LEU:HD12	1.71	0.56
1:A:580:CYS:O	1:A:584:ILE:HG13	2.06	0.56
1:A:618:MET:HB3	1:A:761:ILE:HD11	1.88	0.56
1:B:235:ASN:HA	1:B:833:ARG:HG3	1.87	0.56
1:D:514:ASP:HB2	1:D:831:ARG:NH1	2.20	0.56
1:B:564:ASP:OD1	1:B:662:LEU:HD12	2.06	0.56
1:C:336:GLN:NE2	1:C:373:ALA:HB3	2.21	0.56
1:C:421:ASP:CG	1:C:424:ARG:HB2	2.26	0.56
1:A:311:PHE:CE1	1:A:329:PHE:HA	2.41	0.56
1:A:615:MET:CE	1:A:761:ILE:HG12	2.35	0.56
1:B:15:VAL:O	1:B:18:LEU:HD22	2.05	0.56
1:D:102:LEU:HB3	1:D:104:LEU:HD12	1.85	0.56
1:A:97:ASN:HA	1:A:100:VAL:HG22	1.87	0.56
1:A:143:PHE:O	1:A:147:MET:HG3	2.06	0.56
1:A:333:VAL:HG12	1:A:371:THR:HG23	1.87	0.56
1:B:138:ARG:NH1	1:B:142:CYS:SG	2.78	0.55
1:B:160:ARG:HG2	1:B:160:ARG:HH11	1.71	0.55
1:C:83:TYR:HE2	1:C:333:VAL:HG13	1.71	0.55
1:B:709:PHE:CD2	1:B:787:VAL:HG23	2.41	0.55
1:C:573:TYR:CD2	1:C:671:THR:HB	2.41	0.55
1:D:578:LEU:HB3	1:D:666:ILE:HD12	1.89	0.55
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.72	0.55
1:B:375:THR:HG22	1:B:377:HIS:CE1	2.42	0.55
1:D:707:ASN:CA	1:D:800:MET:SD	2.92	0.55
1:A:486:ILE:HD11	1:A:676:THR:HG23	1.88	0.55
1:B:69:ARG:HG2	1:B:69:ARG:N	2.21	0.55
1:B:311:PHE:O	1:B:316:PHE:HB3	2.07	0.55
1:C:314:SER:O	1:C:316:PHE:N	2.40	0.55
1:D:703:ALA:O	1:D:707:ASN:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.42	0.55
1:A:661:ASP:HB3	1:A:797:TRP:CH2	2.41	0.55
1:B:169:LYS:HA	1:B:646:GLU:OE2	2.07	0.55
1:B:819:GLN:O	1:B:823:GLU:HB2	2.07	0.55
1:A:759:LYS:NZ	1:A:763:ASN:OD1	2.38	0.55
1:C:21:VAL:HG22	1:C:22:GLU:H	1.71	0.55
1:D:458:ILE:O	1:D:462:ILE:HG23	2.07	0.55
1:A:170:ILE:HD13	1:A:175:GLN:HA	1.89	0.54
1:D:569:ARG:NH2	1:D:573:TYR:HE1	2.05	0.54
1:B:255:LYS:O	1:B:256:ASP:HB2	2.07	0.54
1:C:130:GLY:O	1:C:164:GLY:HA2	2.07	0.54
1:C:521:LEU:HG	1:C:530:PHE:HZ	1.72	0.54
1:D:379:VAL:HG23	1:D:462:ILE:HD11	1.90	0.54
1:B:524:TYR:CD1	1:B:524:TYR:N	2.74	0.54
1:B:312:LYS:HE3	1:B:326:PHE:HZ	1.71	0.54
1:B:703:ALA:CA	1:B:807:THR:HG21	2.38	0.54
1:B:755:PRO:HD2	1:C:426:ARG:CZ	2.38	0.54
1:D:521:LEU:HG	1:D:530:PHE:CZ	2.42	0.54
1:D:583:VAL:HG21	1:D:603:VAL:HG21	1.89	0.54
1:C:336:GLN:HE22	1:C:373:ALA:HB3	1.73	0.54
1:A:165:ILE:HD13	1:A:166:PHE:CD1	2.43	0.54
1:A:795:ARG:O	1:A:799:ARG:HG3	2.07	0.54
1:B:69:ARG:HD3	1:B:72:GLN:OE1	2.07	0.54
1:B:81:ARG:HA	1:B:153:ALA:O	2.08	0.54
1:D:230:VAL:HG22	1:D:239:ASN:O	2.07	0.54
1:A:165:ILE:HD11	1:A:282:ASN:N	2.22	0.54
1:D:403:ILE:HG21	1:D:439:ILE:HD12	1.89	0.54
1:A:22:GLU:OE1	1:A:104:LEU:HD23	2.08	0.54
1:C:786:ARG:O	1:C:789:ALA:HB3	2.08	0.54
1:D:309:ARG:NH2	4:D:920:IMP:O3P	2.40	0.54
1:A:732:TYR:O	1:A:739:ARG:HG3	2.08	0.54
1:B:292:ARG:O	1:B:296:GLU:HG3	2.07	0.54
1:B:565:VAL:HB	1:B:604:MET:CE	2.37	0.54
1:D:81:ARG:HG3	1:D:81:ARG:NH1	2.22	0.54
1:D:393:GLU:HG3	1:D:400:LEU:HD12	1.89	0.54
1:D:698:GLU:HG2	1:D:810:LYS:NZ	2.23	0.54
1:A:455:VAL:HA	1:A:482:LYS:O	2.08	0.53
1:C:316:PHE:CZ	1:C:328:ALA:HB3	2.44	0.53
1:C:732:TYR:CE2	1:C:739:ARG:HA	2.44	0.53
1:D:280:TYR:HE2	1:D:291:LEU:HD13	1.72	0.53
1:D:742:ILE:HD11	1:D:774:PHE:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:790:LEU:HG	1:D:790:LEU:O	2.07	0.53
1:B:304:LEU:HD12	1:B:307:ILE:HD12	1.89	0.53
1:C:836:ALA:HB1	1:C:837:PRO:HA	1.91	0.53
1:A:363:LYS:HZ2	1:A:366:GLU:CD	2.12	0.53
1:D:732:TYR:CE1	1:D:739:ARG:HA	2.43	0.53
1:A:441:MET:HE2	1:A:444:LEU:HD12	1.90	0.53
1:A:545:PHE:HE2	1:A:604:MET:SD	2.32	0.53
1:B:492:LEU:HG	1:B:683:LEU:HD22	1.89	0.53
1:C:309:ARG:NH2	4:C:920:IMP:O3P	2.42	0.53
1:C:548:TYR:CE1	1:C:552:GLU:HB2	2.43	0.53
1:B:336:GLN:HG2	1:B:825:TRP:HE1	1.73	0.53
1:B:460:SER:O	1:B:464:LYS:HG3	2.08	0.53
1:C:329:PHE:CE1	1:C:333:VAL:HG21	2.43	0.53
1:D:689:ILE:HA	1:D:709:PHE:HB2	1.91	0.53
1:A:455:VAL:H	1:A:459:HIS:HD2	1.57	0.53
1:B:720:ARG:O	1:B:723:GLN:HB3	2.09	0.53
1:A:87:LEU:HD12	1:A:299:VAL:HG11	1.91	0.53
1:B:104:LEU:HB3	1:B:108:CYS:SG	2.48	0.53
1:D:75:TYR:CE2	1:D:314:SER:HA	2.44	0.53
1:D:626:ILE:O	1:D:629:VAL:HB	2.09	0.53
1:A:21:VAL:O	1:A:23:ASN:N	2.42	0.53
1:A:255:LYS:O	1:A:256:ASP:HB2	2.07	0.53
1:B:574:LYS:HB3	1:B:576:GLN:NE2	2.22	0.53
1:D:536:LYS:O	1:D:539:GLN:HB3	2.09	0.53
1:A:661:ASP:HB3	1:A:797:TRP:CZ2	2.44	0.53
1:A:761:ILE:O	1:A:765:LEU:HD22	2.09	0.53
1:C:175:GLN:NE2	1:C:609:ALA:HB3	2.23	0.53
1:C:192:ALA:HB2	1:C:226:TYR:CE2	2.44	0.53
1:D:163:PHE:HA	1:D:180:ASP:O	2.08	0.53
1:A:421:ASP:O	1:A:425:LEU:HD23	2.08	0.53
1:C:781:VAL:HG23	1:C:782:LYS:CE	2.37	0.53
1:A:482:LYS:HE3	1:A:819:GLN:O	2.09	0.52
1:D:618:MET:O	1:D:621:LYS:HB3	2.09	0.52
1:A:492:LEU:HG	1:A:683:LEU:HD22	1.91	0.52
1:B:578:LEU:HD13	1:B:773:VAL:HG13	1.92	0.52
1:B:584:ILE:O	1:B:587:TYR:HB3	2.09	0.52
1:C:38:THR:HG22	1:C:39:LEU:HD12	1.90	0.52
1:A:703:ALA:HA	1:A:807:THR:HG21	1.91	0.52
1:C:692:MET:SD	1:C:710:ILE:HD12	2.49	0.52
1:D:293:LEU:HD23	1:D:391:LEU:HD13	1.91	0.52
1:D:599:VAL:HG21	1:D:788:SER:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:663:SER:HB2	1:D:681:PHE:CD2	2.44	0.52
1:D:688:THR:HB	1:D:708:PHE:CE1	2.44	0.52
1:A:441:MET:CE	1:A:444:LEU:HD12	2.40	0.52
1:C:782:LYS:HA	1:C:785:GLU:OE1	2.09	0.52
1:D:385:GLU:HG2	1:D:441:MET:HG2	1.91	0.52
1:A:203:TYR:O	1:A:218:THR:HG22	2.10	0.52
1:C:492:LEU:HD21	1:C:499:LEU:HD23	1.91	0.52
1:C:577:LEU:HA	1:C:580:CYS:HB2	1.90	0.52
1:A:319:ARG:NH2	1:A:320:ASP:O	2.43	0.52
1:B:352:VAL:HA	1:B:356:LEU:HD22	1.91	0.52
1:C:96:GLN:O	1:C:100:VAL:HG13	2.10	0.52
1:D:63:LEU:CD2	1:D:231:PRO:HB3	2.36	0.52
1:D:399:HIS:O	1:D:403:ILE:HG13	2.09	0.52
1:B:631:ASN:HB3	1:B:641:ARG:HH11	1.74	0.52
1:C:245:SER:HA	1:C:276:SER:OG	2.10	0.52
1:D:93:ARG:HG2	1:D:126:GLU:HB3	1.92	0.52
1:A:698:GLU:HB3	1:A:810:LYS:NZ	2.24	0.52
1:B:516:ASP:HA	1:B:809:GLY:HA3	1.92	0.52
1:B:579:ASN:O	1:B:583:VAL:HG23	2.10	0.52
1:C:255:LYS:O	1:C:256:ASP:HB2	2.10	0.52
1:C:737:GLU:O	1:C:740:GLN:HB3	2.09	0.52
1:C:357:GLU:O	1:C:358:ARG:HB2	2.10	0.52
1:D:49:ARG:NH2	1:D:125:ILE:O	2.43	0.52
1:D:222:LEU:HB2	1:D:247:LYS:O	2.10	0.52
1:D:319:ARG:NH2	1:D:320:ASP:O	2.42	0.52
1:D:455:VAL:HG22	1:D:484:ASN:OD1	2.10	0.52
1:D:620:ILE:HG23	1:D:644:PHE:CE2	2.45	0.52
1:A:310:ARG:O	1:A:314:SER:HB2	2.10	0.52
1:A:630:VAL:CG2	1:A:642:VAL:HG23	2.37	0.52
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.75	0.52
1:C:115:LEU:O	1:D:10:ARG:N	2.43	0.52
1:C:204:GLY:HA3	1:C:218:THR:HG22	1.92	0.52
1:D:11:LYS:NZ	2:D:900:SO4:O4	2.43	0.52
1:D:60:ARG:O	1:D:64:VAL:HG22	2.10	0.52
1:A:189:TRP:O	1:A:228:THR:HG23	2.10	0.51
1:C:81:ARG:HD3	1:C:155:TYR:HE2	1.73	0.51
1:C:319:ARG:NH2	1:C:320:ASP:O	2.43	0.51
1:D:592:LYS:C	1:D:594:PRO:HD3	2.31	0.51
1:A:609:ALA:HB2	1:A:620:ILE:HD12	1.91	0.51
1:C:566:GLN:HB2	1:C:664:GLU:HB2	1.91	0.51
1:D:278:VAL:HG22	1:D:279:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:665:GLN:HB3	1:D:696:ASN:HD21	1.75	0.51
1:A:323:ARG:N	1:A:323:ARG:HE	2.08	0.51
1:B:322:VAL:O	1:B:325:ASN:HB2	2.11	0.51
1:D:793:ASN:N	1:D:794:PRO:HD3	2.26	0.51
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.91	0.51
1:B:369:VAL:O	1:B:450:HIS:HB3	2.10	0.51
1:B:570:ILE:O	1:B:570:ILE:HG22	2.11	0.51
1:A:460:SER:CB	1:A:481:ASN:HB2	2.40	0.51
1:B:49:ARG:NH2	1:B:125:ILE:O	2.44	0.51
1:B:599:VAL:HG21	1:B:788:SER:O	2.09	0.51
1:C:40:VAL:CG2	1:D:191:LYS:HG3	2.41	0.51
1:C:754:GLN:O	1:C:757:LEU:HB2	2.11	0.51
1:C:764:MET:HA	1:C:768:HIS:CE1	2.45	0.51
1:D:601:ARG:HH12	1:D:787:VAL:CG1	2.23	0.51
1:A:488:PRO:HB3	1:A:515:LEU:HD22	1.92	0.51
1:C:564:ASP:CG	1:C:601:ARG:HH21	2.13	0.51
1:D:604:MET:HG2	1:D:643:ILE:CG2	2.39	0.51
1:A:197:THR:CG2	1:A:222:LEU:HD13	2.41	0.51
1:B:28:LYS:HG2	1:B:115:LEU:HD11	1.93	0.51
1:B:456:ALA:C	1:B:481:ASN:HD21	2.14	0.51
1:D:575:ARG:HB3	1:D:666:ILE:HG13	1.92	0.51
1:D:36:HIS:O	1:D:40:VAL:HA	2.11	0.51
1:C:521:LEU:HG	1:C:530:PHE:CE2	2.45	0.51
1:B:571:HIS:ND1	1:B:572:GLU:N	2.59	0.51
1:B:755:PRO:HD2	1:C:426:ARG:NH1	2.26	0.51
1:A:39:LEU:HD21	1:A:53:PHE:HB2	1.94	0.50
1:A:574:LYS:HE3	3:A:931:PDP:O1B	2.11	0.50
1:B:64:VAL:O	1:B:68:ILE:HG12	2.11	0.50
1:C:63:LEU:HD21	1:C:231:PRO:HD3	1.93	0.50
1:C:73:HIS:CD2	1:C:834:LEU:HD11	2.46	0.50
1:C:573:TYR:HD2	1:C:671:THR:HB	1.76	0.50
1:D:59:VAL:O	1:D:62:HIS:HB2	2.11	0.50
1:C:766:MET:HE3	1:C:774:PHE:HE2	1.77	0.50
1:D:81:ARG:HD3	1:D:155:TYR:CE1	2.46	0.50
1:D:734:ARG:O	1:D:739:ARG:NH2	2.44	0.50
1:A:350:MET:SD	1:A:368:THR:OG1	2.62	0.50
1:A:488:PRO:HG2	1:A:489:ARG:NH1	2.26	0.50
1:B:569:ARG:NH2	3:B:932:PDP:O3B	2.45	0.50
1:C:738:LEU:O	1:C:741:ILE:HG12	2.11	0.50
1:D:73:HIS:O	1:D:77:LYS:HB3	2.12	0.50
1:D:417:ALA:O	1:D:419:PRO:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:VAL:HG22	1:D:512:ILE:HD13	1.94	0.50
1:B:258:ASN:OD1	1:B:259:VAL:HG13	2.12	0.50
1:C:49:ARG:NH2	1:C:125:ILE:O	2.44	0.50
1:C:60:ARG:O	1:C:64:VAL:HG13	2.12	0.50
1:C:733:ASP:HA	1:C:739:ARG:NH1	2.26	0.50
1:A:570:ILE:HG22	1:A:570:ILE:O	2.11	0.50
1:D:761:ILE:O	1:D:764:MET:HB3	2.12	0.50
1:A:42:ASP:OD2	1:A:44:ASN:HB2	2.12	0.50
1:A:209:THR:OG1	1:A:214:LYS:HE3	2.12	0.50
1:A:293:LEU:HD21	1:A:392:LEU:CD1	2.42	0.50
1:B:136:LEU:HD13	1:B:338:ASN:HD21	1.75	0.50
1:B:263:ILE:O	1:B:266:VAL:HG23	2.12	0.50
1:B:338:ASN:OD1	1:B:377:HIS:HE1	1.95	0.50
1:C:575:ARG:HG2	1:C:578:LEU:HD23	1.92	0.50
1:C:748:GLY:HA3	1:C:755:PRO:HB3	1.93	0.50
1:D:169:LYS:HG3	1:D:171:CYS:SG	2.51	0.50
1:C:83:TYR:CE2	1:C:333:VAL:HG13	2.47	0.50
1:D:311:PHE:O	1:D:316:PHE:HB3	2.10	0.50
1:A:34:HIS:CD2	1:A:57:HIS:HB3	2.47	0.50
1:A:483:THR:HB	1:A:815:ARG:HH22	1.77	0.50
1:B:83:TYR:CE2	1:B:333:VAL:HG13	2.47	0.50
1:C:21:VAL:O	1:C:23:ASN:N	2.45	0.50
1:C:40:VAL:HG21	1:D:191:LYS:HG3	1.94	0.50
1:D:796:GLU:HA	1:D:799:ARG:HB2	1.94	0.50
1:A:228:THR:HB	1:A:241:MET:HE3	1.94	0.49
1:B:457:ARG:HA	1:B:481:ASN:ND2	2.27	0.49
1:C:691:THR:HG23	1:C:711:PHE:CE1	2.47	0.49
1:C:746:SER:OG	1:C:762:VAL:HG11	2.12	0.49
1:C:813:SER:O	1:C:817:ILE:HG12	2.12	0.49
1:A:24:VAL:HG11	1:A:114:GLN:NE2	2.27	0.49
1:A:39:LEU:HD11	1:A:53:PHE:HB3	1.94	0.49
1:A:52:TYR:OH	1:A:126:GLU:HG3	2.12	0.49
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.47	0.49
1:A:836:ALA:HB1	1:A:837:PRO:HA	1.92	0.49
1:C:169:LYS:HA	1:C:646:GLU:OE2	2.11	0.49
1:D:255:LYS:O	1:D:256:ASP:HB2	2.12	0.49
1:B:55:LEU:O	1:B:59:VAL:HG23	2.11	0.49
1:C:732:TYR:O	1:C:739:ARG:HG3	2.12	0.49
1:D:80:LYS:HG3	1:D:331:ASP:O	2.12	0.49
1:D:288:GLY:HA2	1:D:387:TRP:CZ3	2.47	0.49
1:D:605:ILE:HD12	1:D:623:ILE:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:709:PHE:CD2	1:D:787:VAL:HG23	2.47	0.49
1:B:96:GLN:O	1:B:100:VAL:HG22	2.12	0.49
1:C:764:MET:SD	1:C:769:ASP:HA	2.52	0.49
1:D:322:VAL:O	1:D:325:ASN:N	2.45	0.49
1:A:49:ARG:HH21	1:A:125:ILE:HG22	1.77	0.49
1:A:163:PHE:CE1	1:A:181:ASP:HB3	2.48	0.49
1:B:65:GLY:O	1:B:68:ILE:HB	2.12	0.49
1:B:71:GLN:NE2	1:B:238:VAL:O	2.46	0.49
1:B:386:ARG:HD3	1:B:432:GLU:OE2	2.12	0.49
1:B:497:PRO:HG2	1:B:498:GLY:H	1.77	0.49
1:C:531:ILE:O	1:C:798:THR:HG21	2.13	0.49
1:C:601:ARG:NH2	1:C:784:GLN:OE1	2.43	0.49
1:D:242:ARG:O	1:D:242:ARG:HG3	2.12	0.49
1:D:274:ASN:HA	1:D:277:ARG:HB2	1.94	0.49
1:A:366:GLU:HG2	1:A:370:LYS:HE2	1.94	0.49
1:A:733:ASP:HA	1:A:739:ARG:NH1	2.27	0.49
1:B:665:GLN:NE2	1:B:678:ASN:HA	2.28	0.49
1:C:83:TYR:CD2	1:C:307:ILE:HG12	2.47	0.49
1:C:489:ARG:HD3	1:C:489:ARG:N	2.27	0.49
1:C:550:GLU:HA	1:C:554:LYS:HA	1.94	0.49
1:D:759:LYS:O	1:D:762:VAL:HB	2.12	0.49
1:D:173:GLY:O	1:D:621:LYS:HD2	2.12	0.49
1:D:525:VAL:O	1:D:531:ILE:HD11	2.13	0.49
1:D:538:LYS:O	1:D:542:LYS:HG3	2.13	0.49
1:A:82:ILE:HG22	1:A:153:ALA:O	2.13	0.49
1:A:338:ASN:OD1	1:A:377:HIS:CE1	2.65	0.49
1:A:343:SER:OG	1:A:441:MET:HG3	2.12	0.49
1:B:81:ARG:HD3	1:B:155:TYR:CE2	2.37	0.49
1:D:21:VAL:HG22	1:D:22:GLU:N	2.26	0.49
1:D:64:VAL:O	1:D:68:ILE:HG12	2.11	0.49
1:C:49:ARG:HG3	1:C:53:PHE:HE2	1.78	0.49
1:C:582:HIS:HD2	1:C:781:VAL:HG12	1.77	0.49
1:D:357:GLU:O	1:D:358:ARG:HB2	2.11	0.49
1:D:488:PRO:O	1:D:492:LEU:HB3	2.12	0.49
1:D:627:GLY:HA2	1:D:630:VAL:HG22	1.93	0.49
1:C:66:ARG:NH1	1:C:236:ASN:OD1	2.44	0.49
1:C:574:LYS:HZ1	1:C:672:GLU:CD	2.16	0.49
1:C:741:ILE:HA	1:C:744:GLN:HE21	1.76	0.49
1:D:503:ILE:HG23	1:D:521:LEU:HD11	1.95	0.49
1:D:693:ASP:O	1:D:696:ASN:HB2	2.12	0.49
1:B:69:ARG:CG	1:B:69:ARG:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:ILE:O	1:B:624:THR:HG23	2.13	0.48
1:C:87:LEU:HD11	1:C:299:VAL:HG11	1.94	0.48
1:C:115:LEU:HD23	1:D:12:GLN:HB3	1.95	0.48
1:C:122:LEU:O	1:C:125:ILE:HG12	2.13	0.48
1:D:67:TRP:O	1:D:71:GLN:HG2	2.13	0.48
1:D:313:SER:O	1:D:315:LYS:N	2.46	0.48
1:A:648:TYR:HA	1:A:652:LEU:HD12	1.95	0.48
1:B:35:LEU:HA	1:B:39:LEU:HD22	1.94	0.48
1:B:320:ASP:HA	1:B:324:THR:HA	1.94	0.48
1:B:528:GLU:HB3	1:B:532:ARG:NH2	2.28	0.48
1:B:601:ARG:NH2	1:B:784:GLN:OE1	2.46	0.48
1:C:97:ASN:HB2	1:C:494:LEU:HD11	1.94	0.48
1:C:661:ASP:HB3	1:C:797:TRP:CZ2	2.47	0.48
1:A:455:VAL:H	1:A:459:HIS:CD2	2.31	0.48
1:B:315:LYS:NZ	4:B:920:IMP:HN1	2.11	0.48
1:B:336:GLN:HE21	1:B:825:TRP:HE1	1.61	0.48
1:B:549:LEU:HD23	1:B:557:ILE:HG13	1.95	0.48
1:C:70:THR:O	1:C:73:HIS:HB3	2.13	0.48
1:D:522:LEU:HD11	1:D:803:ARG:HG2	1.95	0.48
1:D:537:VAL:O	1:D:540:GLU:HB2	2.13	0.48
1:A:168:GLN:NE2	1:A:647:ASN:H	2.10	0.48
1:A:793:ASN:N	1:A:794:PRO:HD3	2.28	0.48
1:B:386:ARG:HG3	1:B:440:ASN:HA	1.95	0.48
1:B:689:ILE:HA	1:B:709:PHE:HB2	1.95	0.48
1:D:308:ILE:HD12	1:D:352:VAL:HG11	1.94	0.48
1:D:507:ILE:HG21	1:D:520:LYS:HB2	1.95	0.48
1:D:530:PHE:HD1	1:D:534:VAL:HG23	1.79	0.48
1:B:174:TRP:CE3	1:C:435:ALA:HB2	2.48	0.48
1:B:385:GLU:O	1:B:441:MET:HB2	2.12	0.48
1:B:499:LEU:CD2	1:B:503:ILE:HD11	2.42	0.48
1:C:325:ASN:HB3	1:C:327:ASP:HB2	1.94	0.48
1:A:138:ARG:NH1	1:A:142:CYS:SG	2.87	0.48
1:A:766:MET:HE3	1:A:774:PHE:CE2	2.48	0.48
1:B:78:ASP:OD2	1:B:332:LYS:NZ	2.34	0.48
1:B:225:PRO:HB2	1:B:242:ARG:HD2	1.95	0.48
1:C:803:ARG:O	1:C:807:THR:HB	2.13	0.48
1:B:461:GLU:OE1	1:B:465:LYS:NZ	2.45	0.48
1:C:175:GLN:HE22	1:C:609:ALA:HB3	1.79	0.48
1:D:493:VAL:HG12	1:D:493:VAL:O	2.12	0.48
1:A:316:PHE:HA	1:A:319:ARG:HB3	1.96	0.48
1:A:630:VAL:HG21	1:A:642:VAL:CG2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.77	0.48
1:D:205:ARG:HG2	1:D:216:VAL:HG23	1.95	0.48
1:A:320:ASP:HA	1:A:324:THR:HA	1.95	0.48
1:B:195:GLU:HB2	1:B:196:PHE:CD1	2.49	0.48
1:B:507:ILE:HD13	1:B:521:LEU:HD13	1.95	0.48
1:D:82:ILE:HD13	1:D:82:ILE:O	2.14	0.48
1:A:389:VAL:CG1	1:A:439:ILE:HG12	2.44	0.48
1:B:313:SER:O	1:B:315:LYS:N	2.47	0.48
1:C:103:ALA:HA	1:C:234:ARG:HH11	1.79	0.48
1:C:147:MET:O	1:C:152:LEU:HB2	2.14	0.48
1:D:110:GLU:O	1:D:113:TYR:HB3	2.14	0.48
1:D:338:ASN:OD1	1:D:377:HIS:HE1	1.97	0.48
1:B:733:ASP:HA	1:B:739:ARG:HH12	1.74	0.47
1:B:753:LYS:O	1:B:754:GLN:HG3	2.14	0.47
1:A:293:LEU:HD21	1:A:392:LEU:HD12	1.95	0.47
1:B:136:LEU:HD13	1:B:338:ASN:ND2	2.30	0.47
1:B:414:VAL:HG22	1:B:474:LEU:HG	1.96	0.47
1:C:732:TYR:HE2	1:C:742:ILE:HB	1.80	0.47
1:B:323:ARG:HE	1:B:323:ARG:N	2.12	0.47
1:B:491:TRP:HZ3	1:B:654:GLU:N	2.12	0.47
1:B:518:LEU:O	1:B:521:LEU:HB2	2.15	0.47
1:C:83:TYR:HD1	1:C:155:TYR:HB2	1.79	0.47
1:D:479:PHE:CD1	1:D:479:PHE:N	2.82	0.47
1:A:233:TYR:OH	1:A:234:ARG:NH2	2.47	0.47
1:B:338:ASN:OD1	1:B:377:HIS:CE1	2.67	0.47
1:B:436:VAL:HB	1:B:438:ARG:NH2	2.29	0.47
1:C:378:THR:O	1:C:459:HIS:CE1	2.67	0.47
1:D:656:VAL:HG13	1:D:657:ILE:N	2.29	0.47
1:A:310:ARG:HA	1:A:313:SER:OG	2.14	0.47
1:A:355:ASP:OD1	1:A:398:ARG:NH1	2.48	0.47
1:C:208:HIS:HA	1:C:213:ALA:HA	1.95	0.47
1:C:558:ASN:OD1	1:C:560:ASN:HB2	2.15	0.47
1:D:82:ILE:HB	1:D:334:ALA:HB3	1.97	0.47
1:D:88:GLU:OE2	1:D:137:GLY:HA3	2.14	0.47
1:D:350:MET:SD	1:D:365:TRP:HE3	2.38	0.47
1:D:761:ILE:O	1:D:765:LEU:HD22	2.15	0.47
1:A:817:ILE:HD13	1:A:817:ILE:HA	1.81	0.47
1:B:158:GLY:O	1:B:243:LEU:HA	2.14	0.47
1:A:171:CYS:SG	1:A:176:MET:HG3	2.55	0.47
1:A:422:VAL:O	1:A:425:LEU:HB2	2.15	0.47
1:A:571:HIS:ND1	1:A:572:GLU:N	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:VAL:O	1:B:23:ASN:N	2.48	0.47
1:B:698:GLU:HB3	1:B:810:LYS:HZ3	1.80	0.47
1:B:730:GLU:O	1:B:734:ARG:HG3	2.15	0.47
1:C:149:THR:HG23	1:C:233:TYR:H	1.79	0.47
1:C:311:PHE:O	1:C:316:PHE:HB3	2.14	0.47
1:C:379:VAL:HG23	1:C:462:ILE:CD1	2.45	0.47
1:D:230:VAL:O	1:D:238:VAL:HA	2.14	0.47
1:D:352:VAL:HA	1:D:356:LEU:HD22	1.97	0.47
1:D:589:ARG:NH2	1:D:785:GLU:OE2	2.47	0.47
1:A:154:ALA:O	1:A:239:ASN:HB3	2.15	0.47
1:B:69:ARG:NH1	1:B:72:GLN:OE1	2.37	0.47
1:B:341:HIS:HB2	1:B:342:PRO:HD3	1.97	0.47
1:C:251:ASP:HB3	1:C:255:LYS:HB3	1.97	0.47
1:C:337:LEU:HG	1:C:342:PRO:HB2	1.96	0.47
1:C:721:LEU:HD21	1:C:726:TYR:CD1	2.50	0.47
1:D:515:LEU:HD21	1:D:683:LEU:HD11	1.95	0.47
1:A:790:LEU:HD23	1:A:797:TRP:CD1	2.50	0.47
1:B:590:ILE:HG23	1:B:639:ARG:CZ	2.45	0.47
1:B:592:LYS:NZ	1:B:593:GLU:CD	2.68	0.47
1:C:333:VAL:HG12	1:C:334:ALA:N	2.30	0.47
1:D:253:ASN:H	1:D:259:VAL:HG21	1.80	0.47
1:D:691:THR:HG23	1:D:711:PHE:CE1	2.49	0.47
1:C:499:LEU:HD21	1:C:805:ILE:HD13	1.96	0.47
1:C:502:ILE:HD13	1:C:537:VAL:HG21	1.97	0.47
1:C:662:LEU:HD22	1:C:689:ILE:HG22	1.97	0.47
1:D:31:PHE:CZ	1:D:117:LEU:HD11	2.50	0.47
1:D:515:LEU:O	1:D:518:LEU:HD23	2.15	0.47
1:B:530:PHE:O	1:B:534:VAL:HG23	2.14	0.46
1:C:274:ASN:HB2	1:C:277:ARG:HB2	1.96	0.46
1:D:157:TYR:CE1	1:D:242:ARG:HG2	2.50	0.46
1:A:635:VAL:O	1:A:639:ARG:NH1	2.48	0.46
1:A:733:ASP:O	1:A:739:ARG:NH2	2.46	0.46
1:B:81:ARG:HA	1:B:153:ALA:HB3	1.98	0.46
1:B:83:TYR:CE1	1:B:155:TYR:CD2	3.03	0.46
1:D:136:LEU:CD1	1:D:338:ASN:ND2	2.78	0.46
1:D:168:GLN:NE2	1:D:647:ASN:H	2.13	0.46
1:D:550:GLU:HA	1:D:554:LYS:HA	1.96	0.46
1:B:421:ASP:OD2	1:B:424:ARG:HB2	2.14	0.46
1:C:341:HIS:HB2	1:C:342:PRO:HD3	1.98	0.46
1:D:169:LYS:HD2	1:D:178:GLU:OE2	2.15	0.46
1:A:662:LEU:HA	1:A:687:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASN:HB2	1:B:58:THR:HG23	1.96	0.46
1:C:73:HIS:NE2	1:C:834:LEU:HD11	2.30	0.46
1:C:262:TYR:HD1	1:C:264:GLN:H	1.62	0.46
1:C:721:LEU:HD21	1:C:726:TYR:HD1	1.80	0.46
1:A:280:TYR:HD1	1:A:281:PRO:HD3	1.80	0.46
1:B:36:HIS:O	1:B:40:VAL:HA	2.15	0.46
1:B:689:ILE:HD11	1:B:783:CYS:HB3	1.97	0.46
1:C:198:LEU:HD13	1:C:305:GLN:CD	2.36	0.46
1:C:350:MET:O	1:C:354:VAL:HG23	2.16	0.46
1:C:398:ARG:O	1:C:401:GLN:HB2	2.15	0.46
1:C:778:GLU:O	1:C:782:LYS:HG2	2.16	0.46
1:D:522:LEU:O	1:D:524:TYR:N	2.49	0.46
1:B:784:GLN:O	1:B:787:VAL:HB	2.16	0.46
1:C:313:SER:O	1:C:315:LYS:N	2.49	0.46
1:A:506:ARG:HB3	1:A:524:TYR:CZ	2.50	0.46
1:B:232:GLY:HA3	1:B:235:ASN:HD21	1.80	0.46
1:C:96:GLN:HA	1:C:99:MET:CE	2.45	0.46
1:C:403:ILE:HG21	1:C:439:ILE:HD12	1.98	0.46
1:D:597:PHE:HE2	1:D:792:LYS:HD2	1.81	0.46
1:A:21:VAL:HG23	1:A:104:LEU:HD21	1.98	0.46
1:B:711:PHE:CD2	1:B:780:TYR:HA	2.51	0.46
1:C:86:SER:HB2	1:C:338:ASN:HD22	1.81	0.46
1:C:235:ASN:H	1:C:235:ASN:HD22	1.63	0.46
1:C:361:TRP:CZ3	1:C:409:ARG:HD2	2.51	0.46
1:C:423:ASP:OD1	1:C:426:ARG:HD3	2.15	0.46
1:C:781:VAL:HG23	1:C:782:LYS:NZ	2.31	0.46
1:A:115:LEU:HD22	1:B:13:ILE:HG12	1.98	0.46
1:A:380:ILE:HA	1:A:381:PRO:HD3	1.86	0.46
1:B:102:LEU:HB3	1:B:104:LEU:HD12	1.98	0.46
1:B:690:GLY:O	1:B:710:ILE:HA	2.16	0.46
1:B:798:THR:O	1:B:802:ILE:HG13	2.16	0.46
1:C:81:ARG:HD3	1:C:155:TYR:CE2	2.51	0.46
1:A:732:TYR:HB2	1:A:766:MET:HE1	1.98	0.45
1:B:766:MET:CE	1:B:774:PHE:HE2	2.29	0.45
1:D:542:LYS:HA	1:D:659:ALA:HB1	1.98	0.45
1:D:558:ASN:OD1	1:D:560:ASN:HB2	2.16	0.45
1:B:138:ARG:HG3	1:B:138:ARG:HH11	1.81	0.45
1:C:486:ILE:HG12	1:C:680:LYS:HG3	1.98	0.45
1:C:182:TRP:CE2	1:C:183:LEU:HG	2.52	0.45
1:D:56:ALA:O	1:D:60:ARG:HB2	2.16	0.45
1:D:152:LEU:O	1:D:154:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:721:LEU:HD21	1:D:726:TYR:CD1	2.48	0.45
1:B:588:ASN:HD21	1:B:744:GLN:NE2	2.14	0.45
1:C:398:ARG:HH11	1:C:398:ARG:HD3	1.60	0.45
1:D:626:ILE:HG22	1:D:642:VAL:HG21	1.98	0.45
1:A:492:LEU:HG	1:A:683:LEU:CD2	2.47	0.45
1:B:575:ARG:HG2	1:B:773:VAL:HG22	1.98	0.45
1:B:724:ARG:HD2	1:B:725:GLY:O	2.16	0.45
1:D:458:ILE:HG13	1:D:459:HIS:N	2.32	0.45
1:D:631:ASN:OD1	1:D:641:ARG:HA	2.15	0.45
1:A:424:ARG:NH2	1:A:473:GLU:OE1	2.50	0.45
1:A:672:GLU:HA	1:A:672:GLU:OE1	2.17	0.45
1:A:766:MET:HA	1:A:766:MET:CE	2.47	0.45
1:B:169:LYS:HG2	1:B:171:CYS:SG	2.56	0.45
1:B:492:LEU:HD21	1:B:499:LEU:HD23	1.98	0.45
1:B:511:TYR:CE1	1:B:512:ILE:HG12	2.51	0.45
1:A:314:SER:C	1:A:316:PHE:H	2.20	0.45
1:A:457:ARG:HA	1:A:481:ASN:ND2	2.32	0.45
1:A:570:ILE:HB	1:A:609:ALA:HA	1.99	0.45
1:A:627:GLY:HA2	1:A:642:VAL:HB	1.99	0.45
1:B:496:ASN:HA	1:B:497:PRO:HD2	1.66	0.45
1:B:742:ILE:CD1	1:B:774:PHE:HZ	2.27	0.45
1:B:764:MET:HG2	1:B:768:HIS:CE1	2.52	0.45
1:D:165:ILE:HD13	1:D:166:PHE:CD1	2.51	0.45
1:D:626:ILE:CG2	1:D:642:VAL:HG21	2.47	0.45
1:D:728:ALA:HB3	1:D:766:MET:O	2.16	0.45
1:A:469:LYS:O	1:A:472:TYR:HB3	2.17	0.45
1:C:205:ARG:HH21	1:C:217:ASP:CG	2.20	0.45
1:C:539:GLN:O	1:C:543:LEU:HD23	2.17	0.45
1:C:590:ILE:O	1:C:594:PRO:HA	2.16	0.45
1:D:235:ASN:HD22	1:D:237:VAL:CG1	2.23	0.45
1:D:521:LEU:HG	1:D:530:PHE:HZ	1.82	0.45
1:D:582:HIS:CD2	1:D:784:GLN:HG3	2.52	0.45
1:A:619:ILE:O	1:A:623:ILE:HG13	2.16	0.45
1:B:162:GLU:HA	1:B:183:LEU:HD12	1.98	0.45
1:B:426:ARG:NH2	1:C:756:ASP:OD1	2.50	0.45
1:C:129:ALA:HB1	1:C:131:LEU:HD22	1.98	0.45
1:C:348:GLU:OE1	1:C:399:HIS:HE1	2.00	0.45
1:C:653:ALA:HB1	1:C:657:ILE:HD12	1.99	0.45
1:D:36:HIS:HA	1:D:41:LYS:O	2.17	0.45
1:D:604:MET:HA	1:D:643:ILE:O	2.15	0.45
1:B:21:VAL:HG22	1:B:22:GLU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PRO:HB3	1:B:244:TRP:CE3	2.52	0.45
1:C:37:PHE:CG	1:D:61:ASP:HB3	2.52	0.45
1:C:591:LYS:HZ2	1:C:633:ASP:CG	2.20	0.45
1:C:690:GLY:HA2	1:C:711:PHE:HE1	1.82	0.45
1:D:53:PHE:HE1	1:D:188:PRO:HD3	1.82	0.45
1:D:94:THR:HG22	1:D:98:THR:OG1	2.17	0.45
1:D:528:GLU:O	1:D:532:ARG:NE	2.50	0.45
1:A:759:LYS:HD2	1:A:759:LYS:HA	1.78	0.44
1:B:161:TYR:HA	1:B:276:SER:O	2.18	0.44
1:B:588:ASN:HD21	1:B:744:GLN:HE22	1.65	0.44
1:C:225:PRO:CB	1:C:242:ARG:HD2	2.42	0.44
1:C:289:LYS:HG2	1:C:291:LEU:H	1.82	0.44
1:D:66:ARG:NH1	1:D:236:ASN:OD1	2.50	0.44
1:D:207:GLU:OE2	1:D:214:LYS:NZ	2.49	0.44
1:D:579:ASN:HB2	1:D:666:ILE:CD1	2.47	0.44
1:A:22:GLU:OE2	1:A:104:LEU:HA	2.17	0.44
1:A:98:THR:O	1:A:102:LEU:HB2	2.17	0.44
1:A:119:MET:O	1:A:123:GLU:HG3	2.16	0.44
1:A:572:GLU:H	1:A:613:TYR:HH	1.65	0.44
1:A:766:MET:HE3	1:A:774:PHE:HE2	1.81	0.44
1:B:207:GLU:OE1	1:B:214:LYS:NZ	2.51	0.44
1:B:528:GLU:OE2	1:B:795:ARG:HD2	2.17	0.44
1:B:622:LEU:HA	1:B:758:PHE:CZ	2.52	0.44
1:C:138:ARG:O	1:C:138:ARG:HG3	2.15	0.44
1:C:165:ILE:HD11	1:C:281:PRO:C	2.37	0.44
1:C:575:ARG:HG2	1:C:578:LEU:CD2	2.47	0.44
1:D:322:VAL:HG13	1:D:325:ASN:CB	2.32	0.44
1:D:522:LEU:CD1	1:D:803:ARG:HG2	2.47	0.44
1:A:522:LEU:HD13	1:A:806:ALA:HB3	1.99	0.44
1:B:68:ILE:CG1	1:B:68:ILE:HG23	2.41	0.44
1:B:195:GLU:HB2	1:B:196:PHE:HD1	1.83	0.44
1:B:536:LYS:HA	1:B:536:LYS:HD2	1.85	0.44
1:B:596:LYS:HD3	1:B:597:PHE:N	2.31	0.44
1:C:567:VAL:HB	1:C:648:TYR:CZ	2.52	0.44
1:D:597:PHE:CE2	1:D:792:LYS:HD2	2.53	0.44
1:B:110:GLU:O	1:B:113:TYR:HB3	2.17	0.44
1:B:680:LYS:NZ	3:B:932:PDP:O3	2.50	0.44
1:D:259:VAL:CG1	1:D:263:ILE:HA	2.48	0.44
1:B:590:ILE:HG21	1:B:636:VAL:CG1	2.46	0.44
1:C:322:VAL:HG22	1:C:325:ASN:ND2	2.32	0.44
1:C:393:GLU:O	1:C:397:PRO:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:734:ARG:O	1:C:739:ARG:NH2	2.50	0.44
1:C:779:GLU:O	1:C:782:LYS:HB2	2.17	0.44
1:D:87:LEU:HD11	1:D:299:VAL:HG11	2.00	0.44
1:A:253:ASN:C	1:A:254:LEU:HD12	2.38	0.44
1:A:264:GLN:NE2	1:C:267:LEU:HD22	2.33	0.44
1:A:714:ARG:H	1:A:717:ASP:CG	2.21	0.44
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.18	0.44
1:B:799:ARG:HA	1:B:802:ILE:HD12	2.00	0.44
1:D:804:ASN:O	1:D:807:THR:HG22	2.18	0.44
1:D:822:ARG:NH1	1:D:828:GLU:OE1	2.51	0.44
1:B:49:ARG:HH11	1:B:185:TYR:HD2	1.65	0.44
1:B:79:PRO:HG2	1:B:153:ALA:HB2	2.00	0.44
1:C:355:ASP:OD2	1:C:398:ARG:HD3	2.18	0.44
1:C:423:ASP:O	1:C:427:ARG:HG3	2.18	0.44
1:D:138:ARG:HH11	1:D:138:ARG:HG3	1.83	0.44
1:A:509:GLU:O	1:A:511:TYR:N	2.51	0.44
1:B:233:TYR:OH	1:B:234:ARG:NH2	2.50	0.44
1:C:207:GLU:OE1	1:C:214:LYS:NZ	2.50	0.44
1:C:379:VAL:HG23	1:C:462:ILE:HD12	1.99	0.44
1:C:582:HIS:NE2	1:C:586:LEU:HD13	2.33	0.44
1:D:78:ASP:CG	1:D:332:LYS:HZ1	2.21	0.44
1:D:423:ASP:O	1:D:427:ARG:HG3	2.18	0.44
1:D:430:LEU:HD23	1:D:430:LEU:HA	1.79	0.44
1:A:207:GLU:OE1	1:A:214:LYS:NZ	2.49	0.44
1:A:335:ILE:HG21	1:A:335:ILE:HD13	1.74	0.44
1:A:336:GLN:NE2	1:A:825:TRP:HE1	2.16	0.44
1:A:600:PRO:HB3	1:A:639:ARG:HA	2.00	0.44
1:A:817:ILE:O	1:A:820:TYR:N	2.50	0.44
1:B:596:LYS:HD3	1:B:596:LYS:C	2.38	0.44
1:B:682:MET:HE1	1:B:811:PHE:CE2	2.53	0.44
1:C:738:LEU:HD13	1:C:777:TYR:CE2	2.53	0.44
1:D:570:ILE:HB	1:D:609:ALA:HA	2.00	0.44
1:D:735:ILE:HA	1:D:736:PRO:HD3	1.65	0.44
1:D:789:ALA:O	1:D:792:LYS:NZ	2.49	0.44
1:B:135:GLY:H	1:B:569:ARG:NH2	2.15	0.43
1:C:392:LEU:HD12	1:C:392:LEU:HA	1.90	0.43
1:C:437:LYS:HE2	1:C:437:LYS:HB2	1.68	0.43
1:C:446:ILE:HG12	1:C:452:VAL:HG21	2.00	0.43
1:C:689:ILE:HA	1:C:709:PHE:HB2	2.00	0.43
1:C:690:GLY:HA2	1:C:711:PHE:CE1	2.52	0.43
1:D:87:LEU:HD21	1:D:296:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:HD2	1:B:115:LEU:HD21	2.00	0.43
1:B:251:ASP:HB3	1:B:255:LYS:HB3	2.00	0.43
1:B:329:PHE:CE1	1:B:333:VAL:HG21	2.53	0.43
1:C:77:LYS:HG3	1:C:79:PRO:HD3	2.00	0.43
1:C:258:ASN:OD1	1:C:259:VAL:HG22	2.17	0.43
1:D:155:TYR:HD2	1:D:240:THR:HB	1.83	0.43
1:A:687:LEU:HD13	1:A:709:PHE:HE2	1.83	0.43
4:A:920:IMP:H2	1:B:44:ASN:ND2	2.34	0.43
1:B:532:ARG:HE	1:B:532:ARG:HB3	1.63	0.43
1:C:11:LYS:HB3	1:C:11:LYS:HE3	1.84	0.43
1:D:536:LYS:HA	1:D:536:LYS:HD2	1.94	0.43
1:D:733:ASP:OD1	1:D:739:ARG:NH1	2.51	0.43
1:B:75:TYR:OH	4:B:920:IMP:O1P	2.24	0.43
1:B:486:ILE:HG12	1:B:680:LYS:HG3	1.99	0.43
1:B:525:VAL:O	1:B:531:ILE:HD11	2.18	0.43
1:C:567:VAL:HG23	1:C:567:VAL:O	2.18	0.43
1:D:138:ARG:O	1:D:141:ALA:HB3	2.19	0.43
1:D:509:GLU:O	1:D:511:TYR:CD1	2.71	0.43
1:B:315:LYS:HZ1	4:B:920:IMP:HN1	1.66	0.43
1:C:587:TYR:OH	1:C:591:LYS:NZ	2.52	0.43
1:C:738:LEU:HD21	1:C:774:PHE:CD1	2.53	0.43
1:D:327:ASP:OD1	1:D:363:LYS:NZ	2.49	0.43
1:A:490:ARG:HA	1:A:494:LEU:HD13	1.99	0.43
1:A:574:LYS:NZ	1:A:672:GLU:OE1	2.51	0.43
1:A:732:TYR:CE1	1:A:739:ARG:HA	2.54	0.43
1:A:764:MET:C	1:A:764:MET:SD	2.97	0.43
1:B:177:GLU:OE1	1:B:611:PRO:HB3	2.18	0.43
1:D:455:VAL:H	1:D:459:HIS:CD2	2.30	0.43
1:D:592:LYS:O	1:D:594:PRO:HD3	2.17	0.43
1:A:53:PHE:HD1	1:A:188:PRO:HG3	1.83	0.43
1:D:567:VAL:HG12	1:D:606:GLY:HA3	2.01	0.43
1:A:797:TRP:CZ3	1:A:801:VAL:HG21	2.53	0.43
1:B:301:ALA:O	1:B:305:GLN:HG3	2.19	0.43
1:B:604:MET:HE2	1:B:604:MET:HB2	1.76	0.43
1:C:322:VAL:O	1:C:325:ASN:N	2.52	0.43
1:C:633:ASP:HA	1:C:634:PRO:HD3	1.78	0.43
1:D:571:HIS:ND1	1:D:572:GLU:N	2.66	0.43
1:A:252:PHE:O	1:A:253:ASN:HB3	2.17	0.43
1:B:370:LYS:HB2	1:B:370:LYS:HE3	1.81	0.43
1:B:766:MET:HE3	1:B:774:PHE:HE2	1.82	0.43
1:C:195:GLU:H	1:C:195:GLU:HG3	1.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:VAL:CG2	1:C:239:ASN:HB2	2.48	0.43
1:C:738:LEU:O	1:C:742:ILE:HG12	2.19	0.43
1:A:557:ILE:HG23	1:A:557:ILE:HD12	1.81	0.43
1:B:516:ASP:OD1	1:B:809:GLY:HA3	2.19	0.43
1:C:343:SER:OG	1:C:441:MET:HG3	2.19	0.43
1:D:187:ASN:HA	1:D:188:PRO:HD2	1.94	0.43
1:D:766:MET:HA	1:D:766:MET:HE2	2.01	0.43
1:A:387:TRP:HA	1:A:387:TRP:CE3	2.54	0.42
1:A:698:GLU:HB3	1:A:810:LYS:HZ3	1.84	0.42
1:B:104:LEU:HB3	1:B:108:CYS:HG	1.84	0.42
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.99	0.42
1:C:227:ASP:OD1	1:C:242:ARG:HD3	2.19	0.42
1:C:510:GLU:OE2	1:C:831:ARG:NH2	2.51	0.42
1:D:350:MET:O	1:D:354:VAL:HB	2.18	0.42
1:D:492:LEU:HD11	1:D:511:TYR:HE2	1.84	0.42
1:D:566:GLN:HE22	1:D:576:GLN:HA	1.84	0.42
1:D:758:PHE:O	1:D:762:VAL:HG23	2.19	0.42
1:A:10:ARG:O	1:B:43:ARG:HD3	2.19	0.42
1:A:90:TYR:HD2	1:A:134:GLY:O	2.02	0.42
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.19	0.42
1:A:589:ARG:NH2	1:A:785:GLU:OE2	2.53	0.42
1:C:316:PHE:HZ	1:C:328:ALA:HB3	1.83	0.42
1:D:280:TYR:CE2	1:D:291:LEU:HD13	2.54	0.42
1:D:511:TYR:HD2	1:D:518:LEU:HD21	1.84	0.42
1:D:527:ASP:OD2	1:D:529:ALA:HB3	2.20	0.42
1:B:274:ASN:HB3	1:B:277:ARG:HE	1.84	0.42
1:B:309:ARG:NH2	4:B:920:IMP:O3P	2.51	0.42
1:B:336:GLN:HG3	1:B:825:TRP:HZ2	1.84	0.42
1:B:363:LYS:HZ2	1:B:366:GLU:CD	2.22	0.42
1:B:446:ILE:HG21	1:B:471:PHE:CD1	2.54	0.42
1:B:594:PRO:O	1:B:639:ARG:NH2	2.52	0.42
1:B:735:ILE:HA	1:B:736:PRO:HD3	1.81	0.42
1:D:570:ILE:O	1:D:570:ILE:HG22	2.20	0.42
1:D:709:PHE:HD2	1:D:783:CYS:SG	2.42	0.42
1:D:742:ILE:HD11	1:D:774:PHE:HZ	1.83	0.42
1:A:473:GLU:O	1:A:476:PRO:HD3	2.19	0.42
1:A:505:GLU:CD	1:A:506:ARG:HH21	2.22	0.42
1:A:519:ARG:HA	1:A:806:ALA:O	2.19	0.42
1:B:96:GLN:HA	1:B:99:MET:HE2	2.02	0.42
1:C:85:LEU:O	1:C:342:PRO:HG2	2.20	0.42
1:C:573:TYR:HD2	1:C:671:THR:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:758:PHE:HB3	1:C:761:ILE:HG13	2.02	0.42
1:D:184:ARG:HH11	1:D:184:ARG:HD2	1.70	0.42
1:D:333:VAL:HG12	1:D:334:ALA:N	2.35	0.42
1:D:515:LEU:CD2	1:D:812:SER:HB2	2.48	0.42
1:D:567:VAL:HG12	1:D:606:GLY:CA	2.49	0.42
1:D:575:ARG:HD3	1:D:666:ILE:O	2.18	0.42
1:B:314:SER:O	1:B:316:PHE:N	2.53	0.42
1:C:157:TYR:CD2	1:C:303:THR:HG23	2.55	0.42
1:C:436:VAL:HB	1:C:438:ARG:NH2	2.35	0.42
1:D:698:GLU:OE2	1:D:810:LYS:HE2	2.20	0.42
1:D:732:TYR:O	1:D:739:ARG:HG3	2.19	0.42
1:A:67:TRP:HE3	1:A:68:ILE:HD13	1.85	0.42
1:A:322:VAL:HG13	1:A:325:ASN:CB	2.46	0.42
1:A:526:ASP:OD2	1:A:799:ARG:NH1	2.52	0.42
1:A:542:LYS:NZ	1:A:661:ASP:OD2	2.51	0.42
1:A:599:VAL:HG11	1:A:791:TYR:HD2	1.84	0.42
1:B:60:ARG:O	1:B:63:LEU:HB2	2.19	0.42
1:B:550:GLU:HA	1:B:554:LYS:HA	2.01	0.42
1:B:564:ASP:HB3	1:B:603:VAL:HA	2.02	0.42
1:B:677:GLY:O	1:B:681:PHE:HD2	2.02	0.42
1:C:207:GLU:N	1:C:214:LYS:O	2.53	0.42
1:C:225:PRO:HD3	1:C:244:TRP:CZ3	2.55	0.42
1:C:738:LEU:HD12	1:C:738:LEU:HA	1.88	0.42
1:C:790:LEU:O	1:C:793:ASN:HB3	2.19	0.42
1:D:46:ALA:HB3	1:D:51:TYR:CZ	2.55	0.42
1:D:315:LYS:HZ1	4:D:920:IMP:HN1	1.68	0.42
1:D:487:THR:HA	1:D:488:PRO:HD2	1.76	0.42
1:D:557:ILE:HG23	1:D:602:THR:HG21	2.01	0.42
1:D:726:TYR:CE1	1:D:772:LYS:HG2	2.54	0.42
1:B:392:LEU:HD12	1:B:392:LEU:HA	1.82	0.42
1:C:168:GLN:HE21	1:C:647:ASN:N	2.11	0.42
1:C:344:LEU:HD23	1:C:347:PRO:HG2	2.02	0.42
1:C:518:LEU:O	1:C:521:LEU:HB2	2.20	0.42
1:C:798:THR:O	1:C:802:ILE:HG13	2.20	0.42
1:D:714:ARG:O	1:D:718:VAL:HG23	2.19	0.42
1:A:90:TYR:HB3	1:A:138:ARG:HA	2.01	0.42
1:A:461:GLU:HB3	1:A:465:LYS:NZ	2.35	0.42
1:B:256:ASP:HB3	1:B:258:ASN:OD1	2.19	0.42
1:B:623:ILE:HG21	1:B:644:PHE:HD1	1.85	0.42
1:B:693:ASP:O	1:B:696:ASN:HB2	2.20	0.42
1:C:591:LYS:NZ	1:C:633:ASP:CG	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:TYR:HD2	1:D:157:TYR:CE2	2.37	0.42
1:D:280:TYR:HD1	1:D:281:PRO:HD3	1.85	0.42
1:D:536:LYS:O	1:D:539:GLN:N	2.53	0.42
1:D:746:SER:OG	1:D:762:VAL:HG21	2.19	0.42
1:A:225:PRO:HB3	1:A:244:TRP:CE3	2.55	0.42
1:A:532:ARG:HE	1:A:532:ARG:HB3	1.78	0.42
1:C:14:SER:OG	1:C:16:ARG:NH1	2.52	0.42
1:C:327:ASP:OD1	1:C:363:LYS:NZ	2.52	0.42
1:C:575:ARG:HB3	1:C:666:ILE:HG13	2.02	0.42
1:D:24:VAL:HG13	1:D:111:ALA:N	2.34	0.42
1:D:75:TYR:CD2	1:D:314:SER:HA	2.55	0.42
1:D:253:ASN:C	1:D:254:LEU:HD12	2.39	0.42
1:A:256:ASP:O	1:A:257:PHE:HB2	2.20	0.42
1:A:519:ARG:HA	1:A:806:ALA:HB1	2.01	0.42
1:A:623:ILE:HG13	1:A:623:ILE:H	1.74	0.42
1:B:407:ASN:OD1	1:B:430:LEU:HG	2.20	0.42
1:B:615:MET:O	1:B:618:MET:N	2.53	0.42
1:B:727:ASN:HD21	1:C:725:GLY:HA3	1.85	0.42
1:C:578:LEU:HD11	1:C:780:TYR:CD2	2.55	0.42
1:C:735:ILE:CD1	1:C:778:GLU:HB2	2.50	0.42
1:C:817:ILE:HD13	1:C:817:ILE:HA	1.84	0.42
1:D:682:MET:O	1:D:684:ASN:N	2.53	0.42
1:D:682:MET:CE	1:D:808:SER:HA	2.49	0.42
1:D:734:ARG:HB2	1:D:735:ILE:HG13	2.01	0.42
1:A:815:ARG:HD2	1:A:816:THR:N	2.35	0.41
1:B:68:ILE:CG2	1:B:68:ILE:HG13	2.40	0.41
1:B:319:ARG:O	1:B:319:ARG:NE	2.51	0.41
1:C:198:LEU:HD13	1:C:305:GLN:OE1	2.20	0.41
1:C:292:ARG:O	1:C:296:GLU:HG3	2.19	0.41
1:C:455:VAL:HG22	1:C:484:ASN:OD1	2.19	0.41
1:C:735:ILE:HA	1:C:736:PRO:HD3	1.72	0.41
1:D:146:SER:O	1:D:150:LEU:HG	2.20	0.41
1:D:253:ASN:N	1:D:259:VAL:HG21	2.35	0.41
1:D:525:VAL:O	1:D:799:ARG:HD2	2.20	0.41
1:D:630:VAL:HG23	1:D:631:ASN:N	2.36	0.41
1:A:292:ARG:O	1:A:295:GLN:HB2	2.21	0.41
1:A:518:LEU:O	1:A:521:LEU:HB2	2.20	0.41
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.59	0.41
1:C:682:MET:CE	1:C:807:THR:HG22	2.47	0.41
1:D:322:VAL:HG22	1:D:325:ASN:ND2	2.36	0.41
1:D:651:SER:HA	1:D:654:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:VAL:HG22	1:A:474:LEU:HG	2.02	0.41
1:A:479:PHE:CD1	1:A:479:PHE:N	2.88	0.41
1:A:636:VAL:O	1:A:639:ARG:HD3	2.21	0.41
1:B:67:TRP:O	1:B:71:GLN:CG	2.61	0.41
1:B:251:ASP:HB3	1:B:255:LYS:HD3	2.02	0.41
1:B:590:ILE:CG2	1:B:636:VAL:HG13	2.49	0.41
1:B:622:LEU:HA	1:B:622:LEU:HD23	1.82	0.41
1:B:727:ASN:O	1:B:729:GLN:N	2.53	0.41
1:C:170:ILE:HG23	1:C:173:GLY:HA2	2.02	0.41
1:D:336:GLN:HE21	1:D:825:TRP:HE1	1.68	0.41
1:D:582:HIS:O	1:D:585:THR:HB	2.20	0.41
1:D:698:GLU:O	1:D:702:GLU:HG2	2.20	0.41
1:A:81:ARG:O	1:A:333:VAL:HA	2.20	0.41
1:A:665:GLN:HB3	1:A:696:ASN:HD21	1.84	0.41
1:B:626:ILE:O	1:B:629:VAL:HB	2.20	0.41
1:C:458:ILE:HD11	1:C:694:GLY:N	2.35	0.41
1:C:716:GLU:O	1:C:720:ARG:HG2	2.20	0.41
1:D:341:HIS:HB2	1:D:342:PRO:CD	2.45	0.41
1:D:601:ARG:NH1	1:D:787:VAL:HG12	2.35	0.41
1:D:656:VAL:CG1	1:D:657:ILE:N	2.83	0.41
1:A:163:PHE:HE1	1:A:181:ASP:HB3	1.85	0.41
1:A:379:VAL:HG13	1:A:380:ILE:N	2.36	0.41
1:B:732:TYR:HE2	1:B:742:ILE:HG21	1.85	0.41
1:D:70:THR:OG1	1:D:237:VAL:HA	2.21	0.41
1:D:620:ILE:HG23	1:D:644:PHE:CZ	2.55	0.41
1:A:423:ASP:OD2	1:A:427:ARG:NH1	2.54	0.41
1:B:515:LEU:CD2	1:B:812:SER:HB2	2.50	0.41
1:B:688:THR:CB	1:B:708:PHE:CE1	3.02	0.41
1:D:306:ASP:OD1	1:D:309:ARG:NH1	2.54	0.41
1:D:314:SER:O	1:D:316:PHE:N	2.54	0.41
1:D:573:TYR:CD2	1:D:671:THR:HB	2.55	0.41
1:A:125:ILE:HD12	1:A:125:ILE:HG23	1.76	0.41
1:A:455:VAL:O	1:A:483:THR:HA	2.20	0.41
1:A:472:TYR:CD1	1:A:476:PRO:HA	2.55	0.41
1:A:721:LEU:O	1:A:725:GLY:N	2.53	0.41
1:B:346:ILE:HB	1:B:347:PRO:CD	2.51	0.41
1:B:565:VAL:HB	1:B:604:MET:HE2	2.02	0.41
1:C:72:GLN:O	1:C:75:TYR:N	2.52	0.41
1:C:488:PRO:HB3	1:C:515:LEU:HD13	2.01	0.41
1:C:700:ALA:O	1:C:704:GLY:N	2.54	0.41
1:D:47:THR:H	1:D:50:ASP:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:LYS:HD2	1:D:315:LYS:H	1.85	0.41
1:D:353:LEU:HD23	1:D:353:LEU:HA	1.79	0.41
1:D:707:ASN:OD1	1:D:800:MET:SD	2.79	0.41
1:C:571:HIS:ND1	1:C:572:GLU:N	2.69	0.41
1:D:27:LEU:HD23	1:D:58:THR:HG22	2.03	0.41
1:D:371:THR:O	1:D:371:THR:HG22	2.20	0.41
1:D:735:ILE:HG22	1:D:738:LEU:CB	2.49	0.41
1:A:22:GLU:CD	1:A:104:LEU:HA	2.41	0.41
1:A:49:ARG:NH2	1:A:125:ILE:O	2.54	0.41
1:A:288:GLY:HA2	1:A:387:TRP:CZ3	2.53	0.41
1:A:322:VAL:O	1:A:325:ASN:HB2	2.21	0.41
1:A:443:HIS:HA	1:A:446:ILE:HD12	2.03	0.41
1:B:66:ARG:NH1	1:B:236:ASN:OD1	2.54	0.41
1:B:110:GLU:OE1	1:B:113:TYR:HD2	2.04	0.41
1:B:355:ASP:OD1	1:B:398:ARG:NH1	2.54	0.41
1:B:399:HIS:O	1:B:403:ILE:HD12	2.21	0.41
1:B:562:LEU:HB3	1:B:601:ARG:HG2	2.02	0.41
1:B:581:LEU:HD11	1:B:774:PHE:HE1	1.86	0.41
1:B:789:ALA:O	1:B:792:LYS:NZ	2.54	0.41
1:C:115:LEU:HD23	1:C:115:LEU:HA	1.99	0.41
1:C:211:GLN:HG3	1:C:358:ARG:NE	2.32	0.41
1:C:309:ARG:HH11	1:C:309:ARG:HD3	1.69	0.41
1:C:336:GLN:HG2	1:C:825:TRP:HE1	1.85	0.41
1:C:458:ILE:HD11	1:C:694:GLY:CA	2.51	0.41
1:C:538:LYS:NZ	1:C:684:ASN:O	2.52	0.41
1:C:553:TYR:CZ	1:C:646:GLU:HB3	2.56	0.41
1:C:676:THR:HG22	3:C:933:PDP:C4A	2.51	0.41
1:D:396:LEU:O	1:D:399:HIS:HB2	2.20	0.41
1:D:510:GLU:OE2	1:D:831:ARG:NH2	2.54	0.41
1:D:576:GLN:O	1:D:579:ASN:HB3	2.21	0.41
1:D:588:ASN:HD21	1:D:744:GLN:NE2	2.19	0.41
1:D:597:PHE:HE2	1:D:792:LYS:CD	2.34	0.41
1:D:711:PHE:HE2	1:D:780:TYR:HB2	1.86	0.41
1:D:733:ASP:HA	1:D:739:ARG:NH1	2.35	0.41
1:A:235:ASN:C	1:A:235:ASN:HD22	2.24	0.41
1:A:431:VAL:HG22	1:A:439:ILE:HD13	2.03	0.41
1:A:457:ARG:HE	1:A:457:ARG:HB2	1.75	0.41
1:B:435:ALA:HB2	1:C:174:TRP:CE3	2.56	0.41
1:C:459:HIS:O	1:C:463:LEU:HG	2.21	0.41
1:C:565:VAL:HG11	1:C:660:ALA:HB2	2.02	0.41
1:C:783:CYS:SG	1:C:786:ARG:NH2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:819:GLN:O	1:C:823:GLU:HB2	2.21	0.41
1:D:338:ASN:OD1	1:D:377:HIS:CE1	2.74	0.41
1:D:430:LEU:HD23	1:D:443:HIS:HB2	2.03	0.41
1:A:206:VAL:CG1	1:A:213:ALA:HB1	2.51	0.40
1:A:612:GLY:H	1:A:617:LYS:HE3	1.86	0.40
1:A:682:MET:HE2	1:A:808:SER:HA	2.03	0.40
1:B:68:ILE:CG1	1:B:68:ILE:H	2.33	0.40
1:C:24:VAL:O	1:C:28:LYS:HG3	2.21	0.40
1:C:548:TYR:O	1:C:550:GLU:N	2.54	0.40
1:C:622:LEU:HD23	1:C:758:PHE:CZ	2.56	0.40
1:D:235:ASN:ND2	1:D:237:VAL:H	2.18	0.40
1:D:458:ILE:HG13	1:D:459:HIS:H	1.85	0.40
1:A:335:ILE:HG22	1:A:337:LEU:CD1	2.51	0.40
1:A:742:ILE:HD11	1:A:774:PHE:CE1	2.56	0.40
1:C:570:ILE:HG12	1:C:607:GLY:HA3	2.03	0.40
1:C:692:MET:CE	1:C:710:ILE:HG21	2.52	0.40
1:D:131:LEU:HD12	1:D:161:TYR:H	1.85	0.40
1:D:509:GLU:O	1:D:511:TYR:N	2.54	0.40
1:D:529:ALA:O	1:D:530:PHE:C	2.60	0.40
1:D:568:LYS:HB3	1:D:574:LYS:HG2	2.03	0.40
1:A:338:ASN:OD1	1:A:377:HIS:HE1	2.04	0.40
1:A:568:LYS:HA	1:A:568:LYS:HD3	1.90	0.40
1:B:306:ASP:OD1	1:B:309:ARG:NH1	2.54	0.40
1:B:604:MET:HA	1:B:643:ILE:O	2.22	0.40
1:C:322:VAL:O	1:C:325:ASN:CB	2.70	0.40
1:C:576:GLN:H	1:C:576:GLN:NE2	2.19	0.40
1:D:47:THR:HG22	1:D:49:ARG:H	1.86	0.40
1:D:655:LYS:O	1:D:658:PRO:HD2	2.22	0.40
1:A:168:GLN:HB3	1:A:647:ASN:HA	2.03	0.40
1:A:197:THR:HG21	1:A:222:LEU:HD13	2.04	0.40
1:A:264:GLN:HE22	1:C:267:LEU:HD22	1.86	0.40
1:B:98:THR:O	1:B:102:LEU:HB2	2.22	0.40
1:C:581:LEU:HD22	1:C:741:ILE:HG13	2.03	0.40
1:D:146:SER:HB3	1:D:814:ASP:HA	2.02	0.40
1:D:503:ILE:HD13	1:D:503:ILE:HG21	1.80	0.40
1:B:661:ASP:HB3	1:B:797:TRP:CZ2	2.57	0.40
1:D:20:GLY:O	1:D:23:ASN:HB2	2.22	0.40
1:D:21:VAL:O	1:D:23:ASN:N	2.54	0.40
1:D:326:PHE:O	1:D:330:PRO:HD2	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:GLU:N	1:D:323:ARG:NH2[2_646]	1.85	0.35
1:B:595:ASN:O	1:D:22:GLU:O[2_746]	1.87	0.33
1:A:25:THR:OG1	1:D:822:ARG:O[2_646]	1.98	0.22
1:B:595:ASN:OD1	1:D:21:VAL:N[2_746]	2.04	0.16
1:B:595:ASN:OD1	1:D:20:GLY:C[2_746]	2.10	0.10
1:A:11:LYS:NZ	1:D:416:ALA:O[2_646]	2.19	0.01

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	820/828 (99%)	676 (82%)	104 (13%)	40 (5%)	2	7
1	B	820/828 (99%)	699 (85%)	83 (10%)	38 (5%)	2	7
1	C	820/828 (99%)	680 (83%)	107 (13%)	33 (4%)	3	9
1	D	820/828 (99%)	665 (81%)	117 (14%)	38 (5%)	2	7
All	All	3280/3312 (99%)	2720 (83%)	411 (12%)	149 (4%)	2	8

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	ARG
1	A	151	GLY
1	A	233	TYR
1	A	236	ASN
1	A	321	PRO
1	A	358	ARG
1	A	576	GLN
1	A	610	ALA
1	A	697	VAL
1	A	728	ALA
1	B	21	VAL
1	B	68	ILE

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Mol	Chain	Res	Type
1	B	93	ARG
1	B	281	PRO
1	B	314	SER
1	B	321	PRO
1	B	358	ARG
1	B	570	ILE
1	B	610	ALA
1	B	674	SER
1	B	728	ALA
1	B	793	ASN
1	C	93	ARG
1	C	314	SER
1	C	315	LYS
1	C	321	PRO
1	C	358	ARG
1	C	609	ALA
1	C	610	ALA
1	C	836	ALA
1	D	21	VAL
1	D	314	SER
1	D	321	PRO
1	D	358	ARG
1	D	556	HIS
1	D	609	ALA
1	A	22	GLU
1	A	210	SER
1	A	252	PHE
1	A	256	ASP
1	A	555	VAL
1	A	664	GLU
1	A	809	GLY
1	A	836	ALA
1	B	92	GLY
1	B	129	ALA
1	B	151	GLY
1	B	210	SER
1	B	252	PHE
1	B	256	ASP
1	B	315	LYS
1	B	555	VAL
1	B	629	VAL
1	B	654	GLU

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Mol	Chain	Res	Type
1	B	666	ILE
1	B	836	ALA
1	C	21	VAL
1	C	92	GLY
1	C	210	SER
1	C	253	ASN
1	C	256	ASP
1	C	281	PRO
1	C	549	LEU
1	C	553	TYR
1	C	563	PHE
1	C	576	GLN
1	D	115	LEU
1	D	210	SER
1	D	252	PHE
1	D	256	ASP
1	D	259	VAL
1	D	281	PRO
1	D	315	LYS
1	D	429	SER
1	D	510	GLU
1	D	555	VAL
1	D	557	ILE
1	D	654	GLU
1	D	674	SER
1	D	683	LEU
1	D	712	GLY
1	D	836	ALA
1	A	21	VAL
1	A	253	ASN
1	A	281	PRO
1	A	514	ASP
1	A	553	TYR
1	A	835	PRO
1	B	22	GLU
1	B	253	ASN
1	B	339	ASP
1	B	484	ASN
1	B	553	TYR
1	B	653	ALA
1	B	756	ASP
1	B	829	PRO

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Mol	Chain	Res	Type
1	C	11	LYS
1	C	252	PHE
1	C	357	GLU
1	C	675	GLY
1	C	683	LEU
1	D	93	ARG
1	D	234	ARG
1	D	313	SER
1	D	610	ALA
1	D	653	ALA
1	D	835	PRO
1	A	315	LYS
1	A	357	GLU
1	A	675	GLY
1	B	794	PRO
1	B	835	PRO
1	C	436	VAL
1	C	555	VAL
1	C	559	PRO
1	D	104	LEU
1	D	153	ALA
1	D	357	GLU
1	D	523	SER
1	D	529	ALA
1	A	314	SER
1	A	436	VAL
1	A	451	ALA
1	A	479	PHE
1	A	570	ILE
1	A	590	ILE
1	A	674	SER
1	B	436	VAL
1	C	492	LEU
1	C	787	VAL
1	D	253	ASN
1	D	436	VAL
1	A	166	PHE
1	B	95	LEU
1	B	273	GLU
1	C	570	ILE
1	C	793	ASN
1	D	570	ILE

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Mol	Chain	Res	Type
1	A	259	VAL
1	D	637	GLY
1	D	697	VAL
1	A	773	VAL
1	C	130	GLY
1	A	78	ASP
1	C	666	ILE
1	C	342	PRO
1	A	322	VAL
1	A	666	ILE
1	B	259	VAL

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	712/717 (99%)	589 (83%)	123 (17%)	2 6
1	B	712/717 (99%)	578 (81%)	134 (19%)	1 5
1	C	712/717 (99%)	591 (83%)	121 (17%)	2 6
1	D	712/717 (99%)	572 (80%)	140 (20%)	1 4
All	All	2848/2868 (99%)	2330 (82%)	518 (18%)	1 5

All (518) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	12	GLN
1	A	15	VAL
1	A	18	LEU
1	A	25	THR
1	A	29	LYS
1	A	39	LEU
1	A	42	ASP
1	A	43	ARG
1	A	49	ARG

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Mol	Chain	Res	Type
1	A	63	LEU
1	A	76	GLU
1	A	77	LYS
1	A	82	ILE
1	A	87	LEU
1	A	90	TYR
1	A	91	MET
1	A	95	LEU
1	A	104	LEU
1	A	118	ASP
1	A	131	LEU
1	A	136	LEU
1	A	138	ARG
1	A	165	ILE
1	A	167	ASN
1	A	169	LYS
1	A	191	LYS
1	A	195	GLU
1	A	205	ARG
1	A	225	PRO
1	A	235	ASN
1	A	237	VAL
1	A	242	ARG
1	A	245	SER
1	A	251	ASP
1	A	255	LYS
1	A	256	ASP
1	A	262	TYR
1	A	269	ARG
1	A	270	ASN
1	A	274	ASN
1	A	279	LEU
1	A	287	GLU
1	A	290	GLU
1	A	291	LEU
1	A	292	ARG
1	A	315	LYS
1	A	319	ARG
1	A	321	PRO
1	A	323	ARG
1	A	324	THR
1	A	327	ASP

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Mol	Chain	Res	Type
1	A	332	LYS
1	A	333	VAL
1	A	337	LEU
1	A	358	ARG
1	A	365	TRP
1	A	378	THR
1	A	380	ILE
1	A	384	LEU
1	A	391	LEU
1	A	392	LEU
1	A	395	LEU
1	A	396	LEU
1	A	398	ARG
1	A	400	LEU
1	A	441	MET
1	A	444	LEU
1	A	455	VAL
1	A	478	LYS
1	A	481	ASN
1	A	487	THR
1	A	489	ARG
1	A	492	LEU
1	A	506	ARG
1	A	516	ASP
1	A	522	LEU
1	A	530	PHE
1	A	540	GLU
1	A	543	LEU
1	A	549	LEU
1	A	554	LYS
1	A	555	VAL
1	A	561	SER
1	A	565	VAL
1	A	569	ARG
1	A	571	HIS
1	A	575	ARG
1	A	576	GLN
1	A	579	ASN
1	A	591	LYS
1	A	593	GLU
1	A	613	TYR
1	A	614	HIS

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Mol	Chain	Res	Type
1	A	622	LEU
1	A	640	LEU
1	A	652	LEU
1	A	658	PRO
1	A	662	LEU
1	A	663	SER
1	A	676	THR
1	A	683	LEU
1	A	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	714	ARG
1	A	717	ASP
1	A	727	ASN
1	A	733	ASP
1	A	753	LYS
1	A	754	GLN
1	A	756	ASP
1	A	760	ASP
1	A	765	LEU
1	A	766	MET
1	A	792	LYS
1	A	794	PRO
1	A	807	THR
1	A	810	LYS
1	A	815	ARG
1	A	828	GLU
1	A	830	SER
1	A	833	ARG
1	B	10	ARG
1	B	12	GLN
1	B	15	VAL
1	B	16	ARG
1	B	18	LEU
1	B	42	ASP
1	B	43	ARG
1	B	47	THR
1	B	49	ARG
1	B	63	LEU
1	B	77	LYS
1	B	80	LYS
1	B	82	ILE

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Mol	Chain	Res	Type
1	B	87	LEU
1	B	90	TYR
1	B	91	MET
1	B	95	LEU
1	B	104	LEU
1	B	112	THR
1	B	113	TYR
1	B	128	ASP
1	B	131	LEU
1	B	136	LEU
1	B	138	ARG
1	B	165	ILE
1	B	167	ASN
1	B	169	LYS
1	B	176	MET
1	B	177	GLU
1	B	181	ASP
1	B	191	LYS
1	B	195	GLU
1	B	214	LYS
1	B	234	ARG
1	B	235	ASN
1	B	237	VAL
1	B	242	ARG
1	B	243	LEU
1	B	250	ASN
1	B	254	LEU
1	B	255	LYS
1	B	256	ASP
1	B	262	TYR
1	B	267	LEU
1	B	269	ARG
1	B	274	ASN
1	B	276	SER
1	B	279	LEU
1	B	287	GLU
1	B	291	LEU
1	B	292	ARG
1	B	306	ASP
1	B	313	SER
1	B	315	LYS
1	B	318	CYS

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Mol	Chain	Res	Type
1	B	319	ARG
1	B	321	PRO
1	B	323	ARG
1	B	324	THR
1	B	327	ASP
1	B	339	ASP
1	B	356	LEU
1	B	358	ARG
1	B	361	TRP
1	B	368	THR
1	B	380	ILE
1	B	391	LEU
1	B	392	LEU
1	B	395	LEU
1	B	396	LEU
1	B	400	LEU
1	B	441	MET
1	B	444	LEU
1	B	457	ARG
1	B	474	LEU
1	B	478	LYS
1	B	486	ILE
1	B	489	ARG
1	B	492	LEU
1	B	506	ARG
1	B	509	GLU
1	B	516	ASP
1	B	517	GLN
1	B	521	LEU
1	B	530	PHE
1	B	532	ARG
1	B	540	GLU
1	B	543	LEU
1	B	549	LEU
1	B	554	LYS
1	B	555	VAL
1	B	562	LEU
1	B	565	VAL
1	B	573	TYR
1	B	574	LYS
1	B	575	ARG
1	B	576	GLN

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Mol	Chain	Res	Type
1	B	579	ASN
1	B	586	LEU
1	B	593	GLU
1	B	604	MET
1	B	621	LYS
1	B	622	LEU
1	B	630	VAL
1	B	633	ASP
1	B	636	VAL
1	B	640	LEU
1	B	652	LEU
1	B	654	GLU
1	B	658	PRO
1	B	662	LEU
1	B	666	ILE
1	B	688	THR
1	B	705	GLU
1	B	708	PHE
1	B	714	ARG
1	B	717	ASP
1	B	727	ASN
1	B	733	ASP
1	B	753	LYS
1	B	756	ASP
1	B	759	LYS
1	B	760	ASP
1	B	765	LEU
1	B	781	VAL
1	B	782	LYS
1	B	783	CYS
1	B	792	LYS
1	B	795	ARG
1	B	800	MET
1	B	801	VAL
1	B	807	THR
1	B	810	LYS
1	B	833	ARG
1	C	10	ARG
1	C	12	GLN
1	C	16	ARG
1	C	18	LEU
1	C	42	ASP

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Mol	Chain	Res	Type
1	C	43	ARG
1	C	49	ARG
1	C	77	LYS
1	C	82	ILE
1	C	90	TYR
1	C	91	MET
1	C	95	LEU
1	C	110	GLU
1	C	121	GLU
1	C	125	ILE
1	C	128	ASP
1	C	131	LEU
1	C	136	LEU
1	C	165	ILE
1	C	167	ASN
1	C	169	LYS
1	C	177	GLU
1	C	191	LYS
1	C	195	GLU
1	C	234	ARG
1	C	235	ASN
1	C	242	ARG
1	C	243	LEU
1	C	245	SER
1	C	251	ASP
1	C	255	LYS
1	C	256	ASP
1	C	259	VAL
1	C	262	TYR
1	C	266	VAL
1	C	267	LEU
1	C	269	ARG
1	C	270	ASN
1	C	274	ASN
1	C	276	SER
1	C	287	GLU
1	C	291	LEU
1	C	292	ARG
1	C	313	SER
1	C	315	LYS
1	C	319	ARG
1	C	321	PRO

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Mol	Chain	Res	Type
1	C	323	ARG
1	C	324	THR
1	C	327	ASP
1	C	332	LYS
1	C	337	LEU
1	C	358	ARG
1	C	361	TRP
1	C	378	THR
1	C	380	ILE
1	C	392	LEU
1	C	396	LEU
1	C	400	LEU
1	C	441	MET
1	C	444	LEU
1	C	455	VAL
1	C	469	LYS
1	C	473	GLU
1	C	474	LEU
1	C	486	ILE
1	C	487	THR
1	C	489	ARG
1	C	490	ARG
1	C	492	LEU
1	C	506	ARG
1	C	510	GLU
1	C	516	ASP
1	C	521	LEU
1	C	522	LEU
1	C	527	ASP
1	C	530	PHE
1	C	540	GLU
1	C	549	LEU
1	C	554	LYS
1	C	555	VAL
1	C	558	ASN
1	C	565	VAL
1	C	569	ARG
1	C	571	HIS
1	C	575	ARG
1	C	576	GLN
1	C	579	ASN
1	C	580	CYS

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Mol	Chain	Res	Type
1	C	593	GLU
1	C	622	LEU
1	C	630	VAL
1	C	640	LEU
1	C	641	ARG
1	C	646	GLU
1	C	649	ARG
1	C	658	PRO
1	C	662	LEU
1	C	663	SER
1	C	678	ASN
1	C	682	MET
1	C	705	GLU
1	C	706	GLU
1	C	714	ARG
1	C	716	GLU
1	C	717	ASP
1	C	727	ASN
1	C	741	ILE
1	C	753	LYS
1	C	756	ASP
1	C	760	ASP
1	C	761	ILE
1	C	764	MET
1	C	766	MET
1	C	782	LYS
1	C	783	CYS
1	C	792	LYS
1	C	807	THR
1	C	810	LYS
1	C	830	SER
1	C	833	ARG
1	D	10	ARG
1	D	12	GLN
1	D	16	ARG
1	D	18	LEU
1	D	25	THR
1	D	33	ARG
1	D	49	ARG
1	D	80	LYS
1	D	81	ARG
1	D	82	ILE

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Mol	Chain	Res	Type
1	D	85	LEU
1	D	90	TYR
1	D	91	MET
1	D	95	LEU
1	D	102	LEU
1	D	104	LEU
1	D	110	GLU
1	D	125	ILE
1	D	131	LEU
1	D	136	LEU
1	D	165	ILE
1	D	167	ASN
1	D	169	LYS
1	D	176	MET
1	D	191	LYS
1	D	195	GLU
1	D	197	THR
1	D	205	ARG
1	D	209	THR
1	D	214	LYS
1	D	234	ARG
1	D	237	VAL
1	D	242	ARG
1	D	243	LEU
1	D	245	SER
1	D	251	ASP
1	D	254	LEU
1	D	255	LYS
1	D	257	PHE
1	D	259	VAL
1	D	262	TYR
1	D	267	LEU
1	D	269	ARG
1	D	274	ASN
1	D	276	SER
1	D	287	GLU
1	D	289	LYS
1	D	290	GLU
1	D	291	LEU
1	D	292	ARG
1	D	313	SER
1	D	315	LYS

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Mol	Chain	Res	Type
1	D	319	ARG
1	D	321	PRO
1	D	322	VAL
1	D	323	ARG
1	D	324	THR
1	D	336	GLN
1	D	337	LEU
1	D	340	THR
1	D	356	LEU
1	D	358	ARG
1	D	363	LYS
1	D	374	TYR
1	D	378	THR
1	D	380	ILE
1	D	384	LEU
1	D	386	ARG
1	D	388	PRO
1	D	391	LEU
1	D	392	LEU
1	D	396	LEU
1	D	400	LEU
1	D	441	MET
1	D	444	LEU
1	D	455	VAL
1	D	474	LEU
1	D	478	LYS
1	D	486	ILE
1	D	492	LEU
1	D	494	LEU
1	D	497	PRO
1	D	506	ARG
1	D	518	LEU
1	D	521	LEU
1	D	522	LEU
1	D	526	ASP
1	D	527	ASP
1	D	530	PHE
1	D	532	ARG
1	D	540	GLU
1	D	543	LEU
1	D	549	LEU
1	D	554	LYS

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Mol	Chain	Res	Type
1	D	555	VAL
1	D	561	SER
1	D	565	VAL
1	D	567	VAL
1	D	571	HIS
1	D	575	ARG
1	D	576	GLN
1	D	579	ASN
1	D	598	VAL
1	D	602	THR
1	D	603	VAL
1	D	621	LYS
1	D	622	LEU
1	D	636	VAL
1	D	640	LEU
1	D	652	LEU
1	D	658	PRO
1	D	662	LEU
1	D	665	GLN
1	D	676	THR
1	D	683	LEU
1	D	688	THR
1	D	691	THR
1	D	705	GLU
1	D	706	GLU
1	D	708	PHE
1	D	711	PHE
1	D	714	ARG
1	D	717	ASP
1	D	727	ASN
1	D	740	GLN
1	D	756	ASP
1	D	760	ASP
1	D	761	ILE
1	D	764	MET
1	D	765	LEU
1	D	766	MET
1	D	779	GLU
1	D	785	GLU
1	D	792	LYS
1	D	807	THR
1	D	810	LYS

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Mol	Chain	Res	Type
1	D	813	SER
1	D	832	GLN
1	D	833	ARG
1	D	834	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	97	ASN
1	A	167	ASN
1	A	168	GLN
1	A	211	GLN
1	A	235	ASN
1	A	264	GLN
1	A	336	GLN
1	A	377	HIS
1	A	399	HIS
1	A	453	ASN
1	A	459	HIS
1	A	481	ASN
1	A	566	GLN
1	A	579	ASN
1	A	744	GLN
1	B	44	ASN
1	B	168	GLN
1	B	211	GLN
1	B	235	ASN
1	B	264	GLN
1	B	336	GLN
1	B	377	HIS
1	B	399	HIS
1	B	453	ASN
1	B	459	HIS
1	B	481	ASN
1	B	566	GLN
1	B	576	GLN
1	B	579	ASN
1	B	665	GLN
1	B	707	ASN
1	B	744	GLN
1	C	34	HIS

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Mol	Chain	Res	Type
1	C	97	ASN
1	C	167	ASN
1	C	168	GLN
1	C	211	GLN
1	C	235	ASN
1	C	336	GLN
1	C	338	ASN
1	C	377	HIS
1	C	399	HIS
1	C	450	HIS
1	C	459	HIS
1	C	481	ASN
1	C	566	GLN
1	C	576	GLN
1	C	665	GLN
1	C	744	GLN
1	D	71	GLN
1	D	168	GLN
1	D	235	ASN
1	D	336	GLN
1	D	377	HIS
1	D	453	ASN
1	D	459	HIS
1	D	481	ASN
1	D	576	GLN
1	D	665	GLN
1	D	678	ASN
1	D	744	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (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	$\#\|Z\| > 2$
4	IMP	D	920	-	21,25,25	1.85	6 (28%)	24,38,38	1.34	3 (12%)
3	PDP	B	932	1	17,19,20	1.82	3 (17%)	24,29,30	1.54	5 (20%)
2	SO4	B	900	-	4,4,4	0.24	0	6,6,6	0.54	0
2	SO4	C	900	-	4,4,4	0.15	0	6,6,6	0.54	0
3	PDP	C	933	1	17,19,20	1.23	2 (11%)	24,29,30	1.19	3 (12%)
4	IMP	C	920	-	21,25,25	2.05	9 (42%)	24,38,38	1.53	7 (29%)
3	PDP	D	934	1	17,19,20	1.73	3 (17%)	24,29,30	1.21	3 (12%)
4	IMP	B	920	-	21,25,25	2.15	7 (33%)	24,38,38	1.66	7 (29%)
2	SO4	D	900	-	4,4,4	0.08	0	6,6,6	0.40	0
4	IMP	A	920	-	21,25,25	2.21	9 (42%)	24,38,38	1.46	5 (20%)
3	PDP	A	931	1	17,19,20	1.25	1 (5%)	24,29,30	1.28	4 (16%)
2	SO4	A	900	-	4,4,4	0.25	0	6,6,6	0.45	0

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
4	IMP	D	920	-	-	1/6/26/26	0/3/3/3
3	PDP	B	932	1	-	4/12/12/14	0/1/1/1
3	PDP	C	933	1	-	5/12/12/14	0/1/1/1
4	IMP	C	920	-	-	0/6/26/26	0/3/3/3
3	PDP	D	934	1	-	5/12/12/14	0/1/1/1
4	IMP	B	920	-	-	1/6/26/26	0/3/3/3
4	IMP	A	920	-	-	0/6/26/26	0/3/3/3
3	PDP	A	931	1	-	5/12/12/14	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	934	PDP	C3-C2	-5.17	1.35	1.40
4	B	920	IMP	C5-C6	-4.98	1.37	1.47
3	B	932	PDP	C3-C2	-4.77	1.36	1.40
4	D	920	IMP	C5-C6	-4.46	1.38	1.47
4	A	920	IMP	O6-C6	4.32	1.32	1.23
4	C	920	IMP	O6-C6	4.23	1.31	1.23
4	A	920	IMP	O4'-C4'	-3.76	1.36	1.45
4	D	920	IMP	O6-C6	3.74	1.30	1.23
4	A	920	IMP	O4'-C1'	3.70	1.46	1.41
4	C	920	IMP	C5-C6	-3.63	1.40	1.47
4	C	920	IMP	C2'-C1'	-3.56	1.48	1.53
4	B	920	IMP	O4'-C4'	-3.55	1.37	1.45
3	B	932	PDP	C2-N1	3.35	1.40	1.33
4	B	920	IMP	O6-C6	3.33	1.30	1.23
4	B	920	IMP	C5'-C4'	3.26	1.61	1.51
4	A	920	IMP	C5-C6	-3.20	1.40	1.47
4	B	920	IMP	C6-N1	-3.17	1.32	1.38
3	C	933	PDP	C3-C2	-3.00	1.37	1.40
4	C	920	IMP	C5-C4	-2.93	1.35	1.43
4	A	920	IMP	C8-N7	-2.87	1.30	1.35
4	B	920	IMP	C5-C4	-2.76	1.36	1.43
4	C	920	IMP	C2-N3	2.64	1.34	1.29
4	A	920	IMP	P-O3P	-2.62	1.44	1.54
4	A	920	IMP	C2'-C1'	-2.56	1.49	1.53
4	C	920	IMP	C8-N7	-2.53	1.30	1.35
4	D	920	IMP	O4'-C4'	-2.51	1.39	1.45
3	C	933	PDP	C2-N1	2.44	1.38	1.33
4	C	920	IMP	C5'-C4'	2.44	1.59	1.51
4	D	920	IMP	C6-N1	-2.43	1.33	1.38
4	B	920	IMP	C8-N7	-2.21	1.31	1.35
3	B	932	PDP	C2A-C2	2.20	1.54	1.50
4	A	920	IMP	C2-N3	2.19	1.33	1.29
4	C	920	IMP	O4'-C1'	2.16	1.44	1.41
4	D	920	IMP	C8-N7	-2.15	1.31	1.35
3	D	934	PDP	C4A-C4	-2.14	1.47	1.51
3	D	934	PDP	C2A-C2	-2.13	1.46	1.50
4	C	920	IMP	P-O3P	-2.11	1.46	1.54
3	A	931	PDP	C3-C2	-2.10	1.38	1.40
4	D	920	IMP	C2'-C1'	-2.02	1.50	1.53
4	A	920	IMP	P-O5'	2.02	1.66	1.60

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	920	IMP	O5'-C5'-C4'	3.80	122.06	108.99
4	A	920	IMP	P-O5'-C5'	3.70	128.50	118.30
3	B	932	PDP	PA-O3A-PB	-3.70	120.14	132.83
3	B	932	PDP	O5A-C5A-C5	3.23	115.51	109.35
4	C	920	IMP	O3P-P-O5'	-3.07	98.57	106.73
4	C	920	IMP	O2P-P-O5'	2.85	114.31	106.73
3	C	933	PDP	PA-O3A-PB	-2.83	123.11	132.83
4	A	920	IMP	O5'-C5'-C4'	2.71	118.30	108.99
3	D	934	PDP	O3B-PB-O2B	2.66	117.79	107.64
4	B	920	IMP	P-O5'-C5'	2.65	125.59	118.30
3	B	932	PDP	C5-C6-N1	-2.65	119.41	123.82
4	D	920	IMP	O4'-C4'-C5'	-2.58	100.89	109.37
4	D	920	IMP	O4'-C1'-C2'	2.52	110.61	106.93
3	B	932	PDP	C6-C5-C4	2.49	120.12	118.16
3	A	931	PDP	C4A-C4-C5	-2.46	118.40	120.94
3	D	934	PDP	C5-C6-N1	-2.39	119.83	123.82
3	A	931	PDP	PA-O3A-PB	-2.31	124.88	132.83
4	C	920	IMP	C4-N3-C2	-2.30	106.21	115.55
4	B	920	IMP	C5-C6-N1	2.29	118.00	113.95
3	D	934	PDP	PA-O3A-PB	-2.29	124.98	132.83
4	B	920	IMP	O4'-C1'-C2'	2.23	110.19	106.93
4	B	920	IMP	O6-C6-N1	-2.23	117.61	120.32
4	C	920	IMP	O5'-C5'-C4'	2.22	116.64	108.99
4	C	920	IMP	P-O5'-C5'	2.15	124.22	118.30
3	A	931	PDP	C5-C6-N1	-2.14	120.25	123.82
3	C	933	PDP	O3B-PB-O2B	2.14	115.81	107.64
4	A	920	IMP	O2P-P-O5'	2.10	112.33	106.73
4	D	920	IMP	C5-C6-N1	2.10	117.66	113.95
4	B	920	IMP	O2'-C2'-C1'	-2.09	103.14	110.85
4	B	920	IMP	O2P-P-O5'	2.07	112.24	106.73
3	C	933	PDP	O3A-PB-O1B	-2.05	99.79	111.19
3	A	931	PDP	O3B-PB-O2B	2.03	115.41	107.64
3	B	932	PDP	O3B-PB-O2B	2.03	115.40	107.64
4	A	920	IMP	C5-C6-N1	2.03	117.54	113.95
4	C	920	IMP	O4'-C1'-C2'	2.01	109.86	106.93
4	C	920	IMP	O2'-C2'-C1'	-2.00	103.47	110.85
4	A	920	IMP	O3P-P-O5'	-2.00	101.41	106.73

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	931	PDP	C5A-O5A-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	931	PDP	C5A-O5A-PA-O2A
3	B	932	PDP	C5A-O5A-PA-O3A
3	C	933	PDP	C5A-O5A-PA-O2A
3	D	934	PDP	C5A-O5A-PA-O1A
3	D	934	PDP	C5A-O5A-PA-O2A
3	D	934	PDP	PB-O3A-PA-O1A
3	A	931	PDP	PB-O3A-PA-O5A
3	B	932	PDP	PB-O3A-PA-O5A
3	C	933	PDP	PB-O3A-PA-O5A
3	D	934	PDP	PB-O3A-PA-O5A
3	A	931	PDP	C5A-O5A-PA-O3A
3	C	933	PDP	C5A-O5A-PA-O3A
3	B	932	PDP	PB-O3A-PA-O1A
3	B	932	PDP	C5A-O5A-PA-O1A
3	C	933	PDP	C5A-O5A-PA-O1A
4	D	920	IMP	C5'-O5'-P-O1P
3	A	931	PDP	C6-C5-C5A-O5A
4	B	920	IMP	C5'-O5'-P-O3P
3	D	934	PDP	C5A-O5A-PA-O3A
3	C	933	PDP	PB-O3A-PA-O1A

There are no ring outliers.

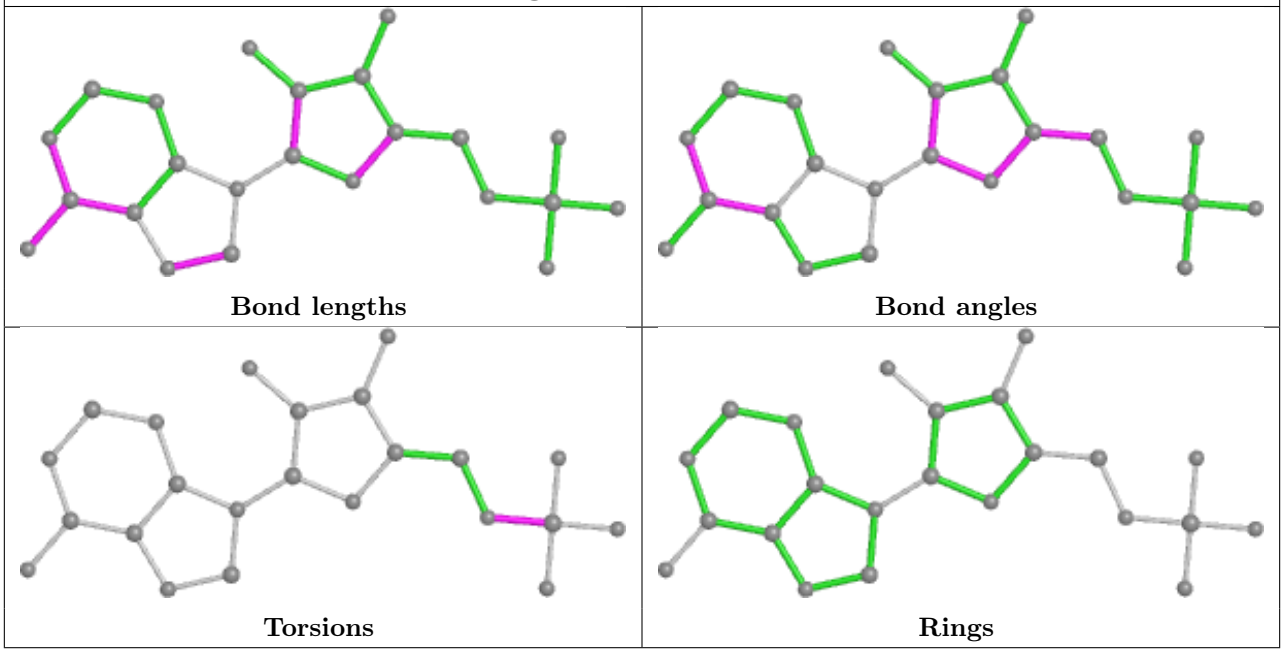
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	920	IMP	2	0
3	B	932	PDP	2	0
3	C	933	PDP	1	0
4	C	920	IMP	1	0
4	B	920	IMP	4	0
2	D	900	SO4	1	0
4	A	920	IMP	2	0
3	A	931	PDP	2	0

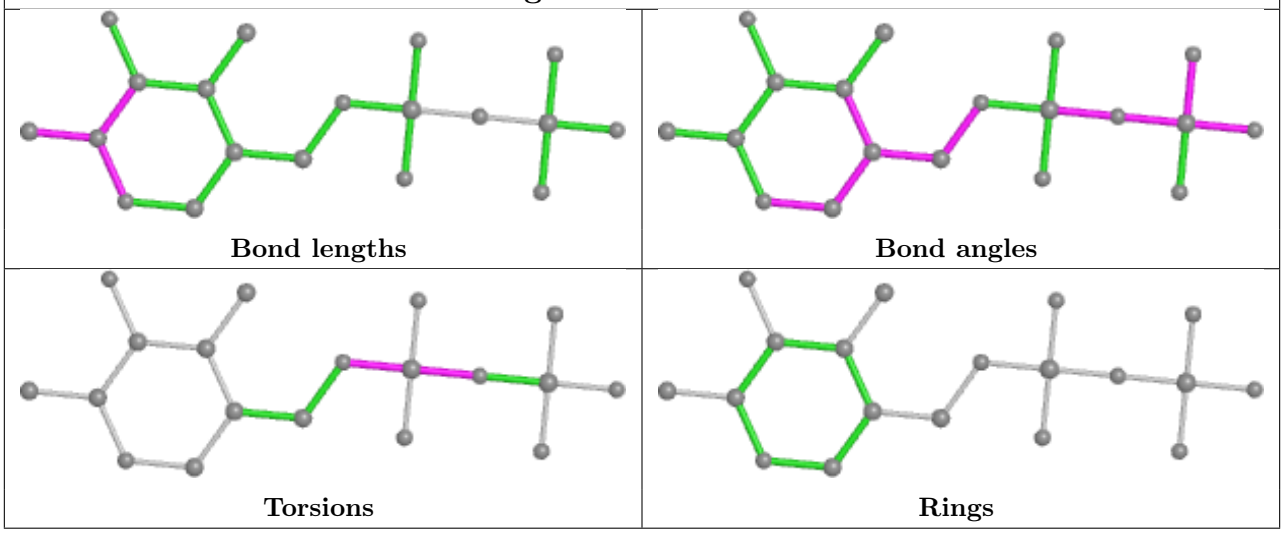
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

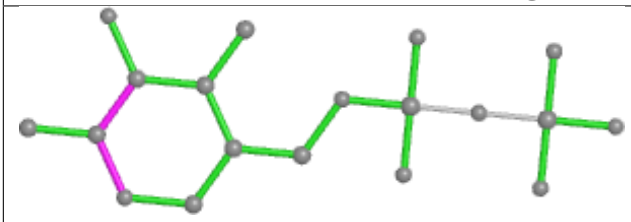
Ligand IMP D 920



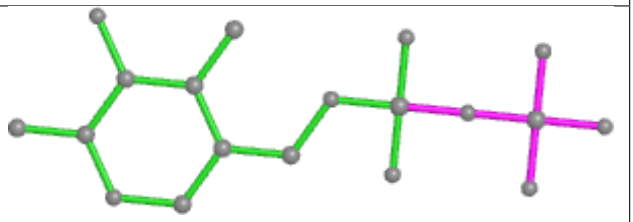
Ligand PDP B 932



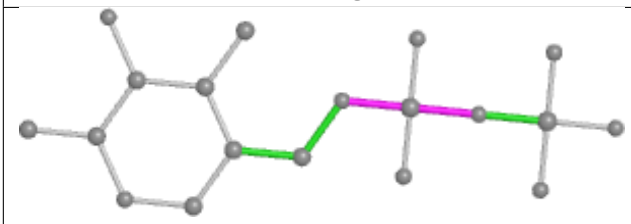
Ligand PDP C 933



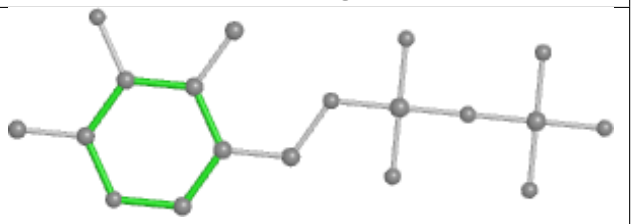
Bond lengths



Bond angles

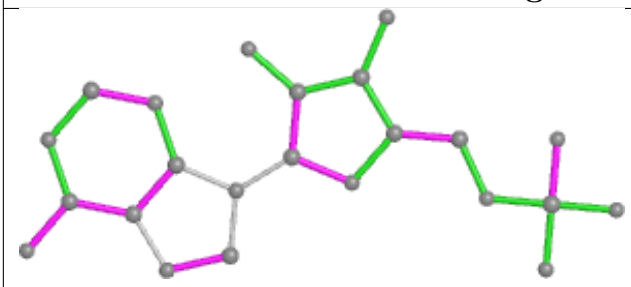


Torsions

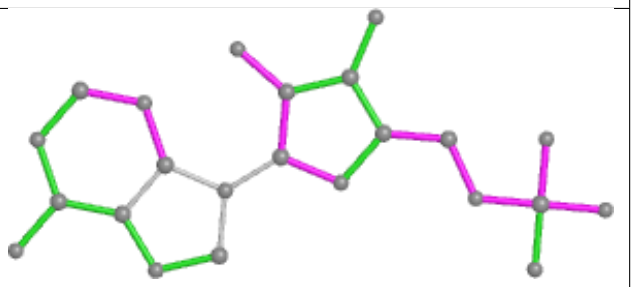


Rings

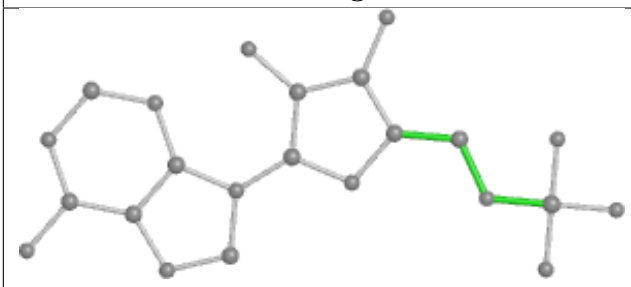
Ligand IMP C 920



Bond lengths



Bond angles



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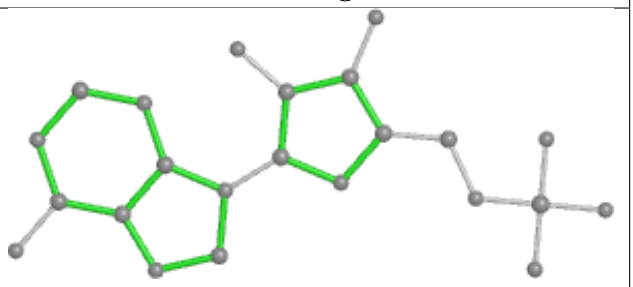
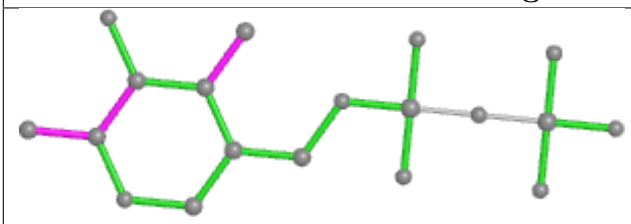
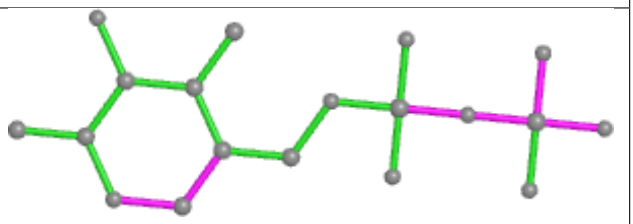


Rings

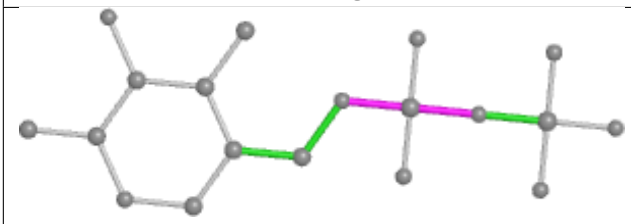
Ligand PDP D 934



Bond lengths



Bond angles



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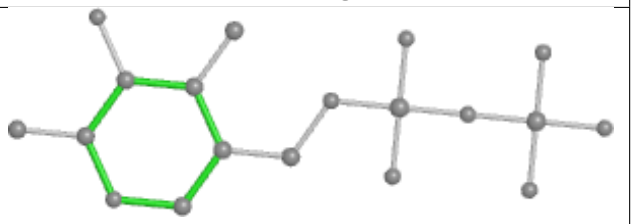
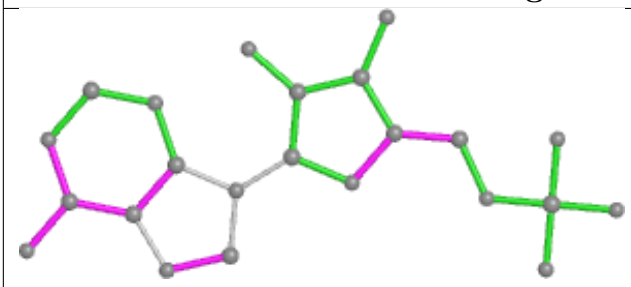
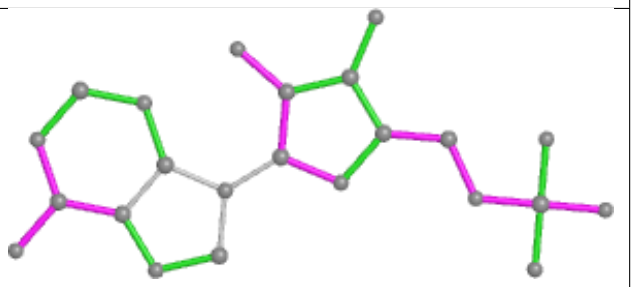


Rings

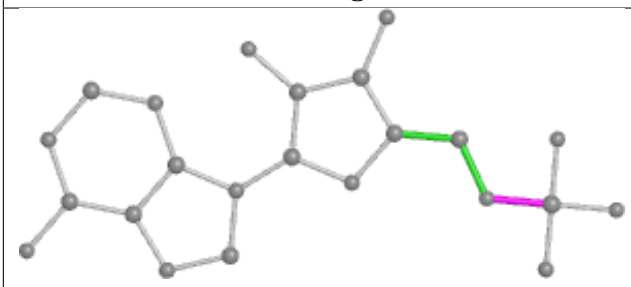
Ligand IMP B 920



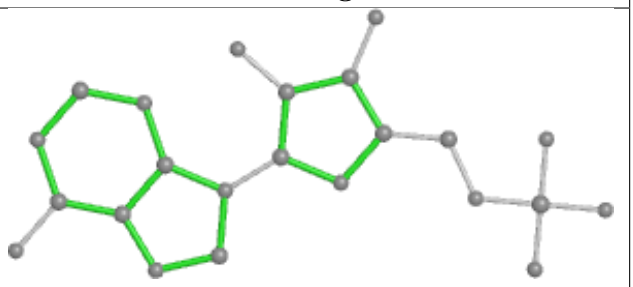
Bond lengths



Bond angles

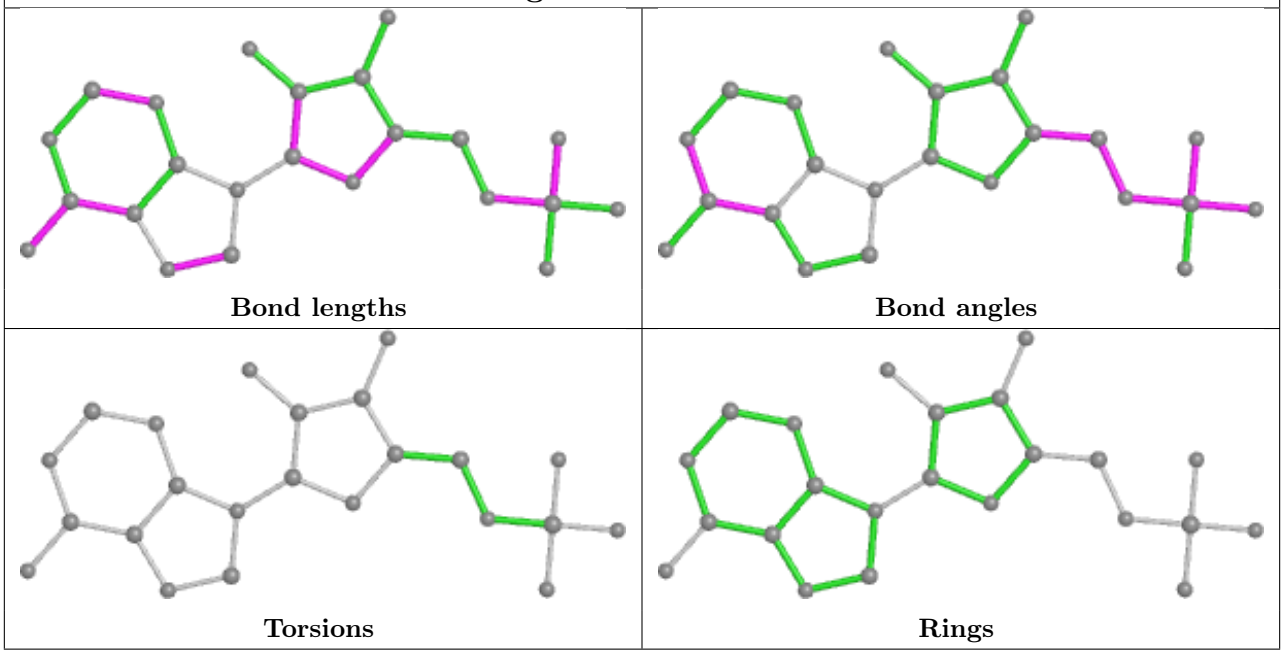


Torsions

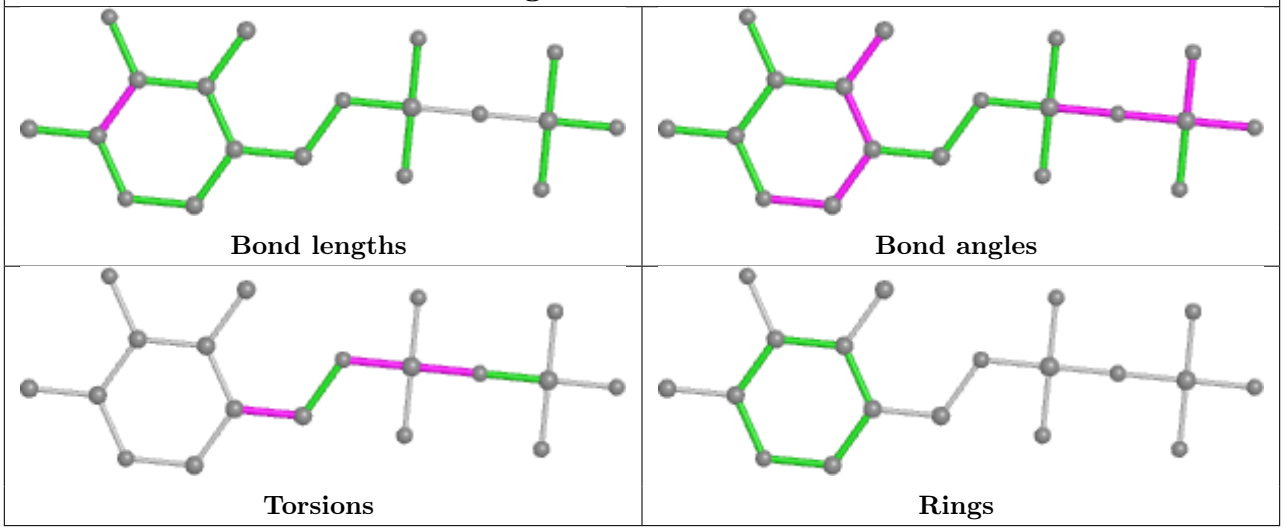


Rings

Ligand IMP A 920



Ligand PDP A 931



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.