



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:33 AM UTC

PDB ID : 1GPB / pdb_00001gpb
Title : GLYCOGEN PHOSPHORYLASE B: DESCRIPTION OF THE PROTEIN
STRUCTURE
Authors : Johnson, L.N.; Acharya, K.R.; Stuart, D.I.
Deposited on : 1990-06-04
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

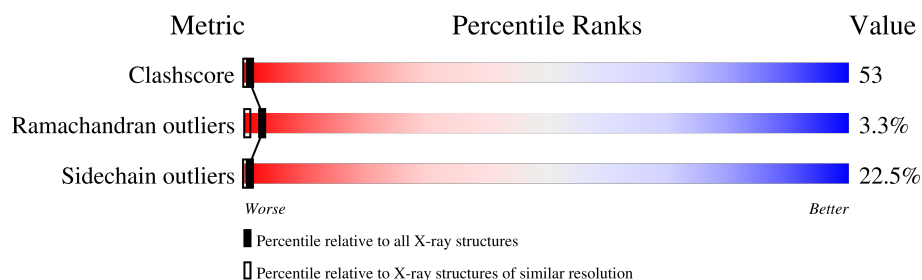
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

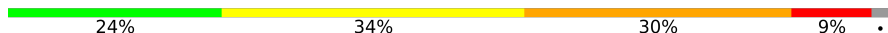
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7397 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.

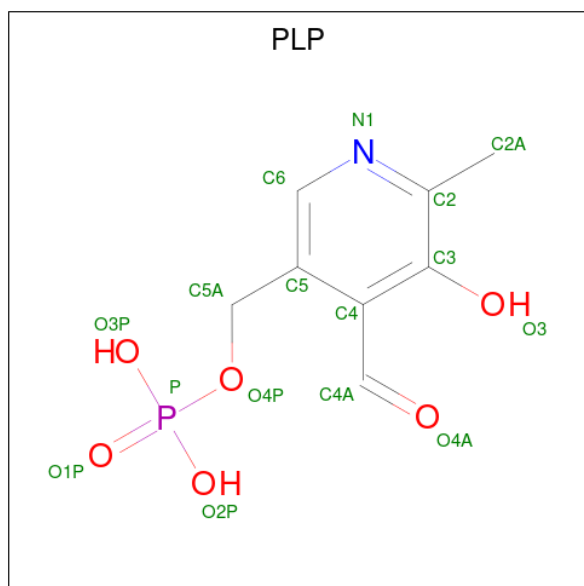
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	823	6691	4264	1178	1219	30	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 3 is water.

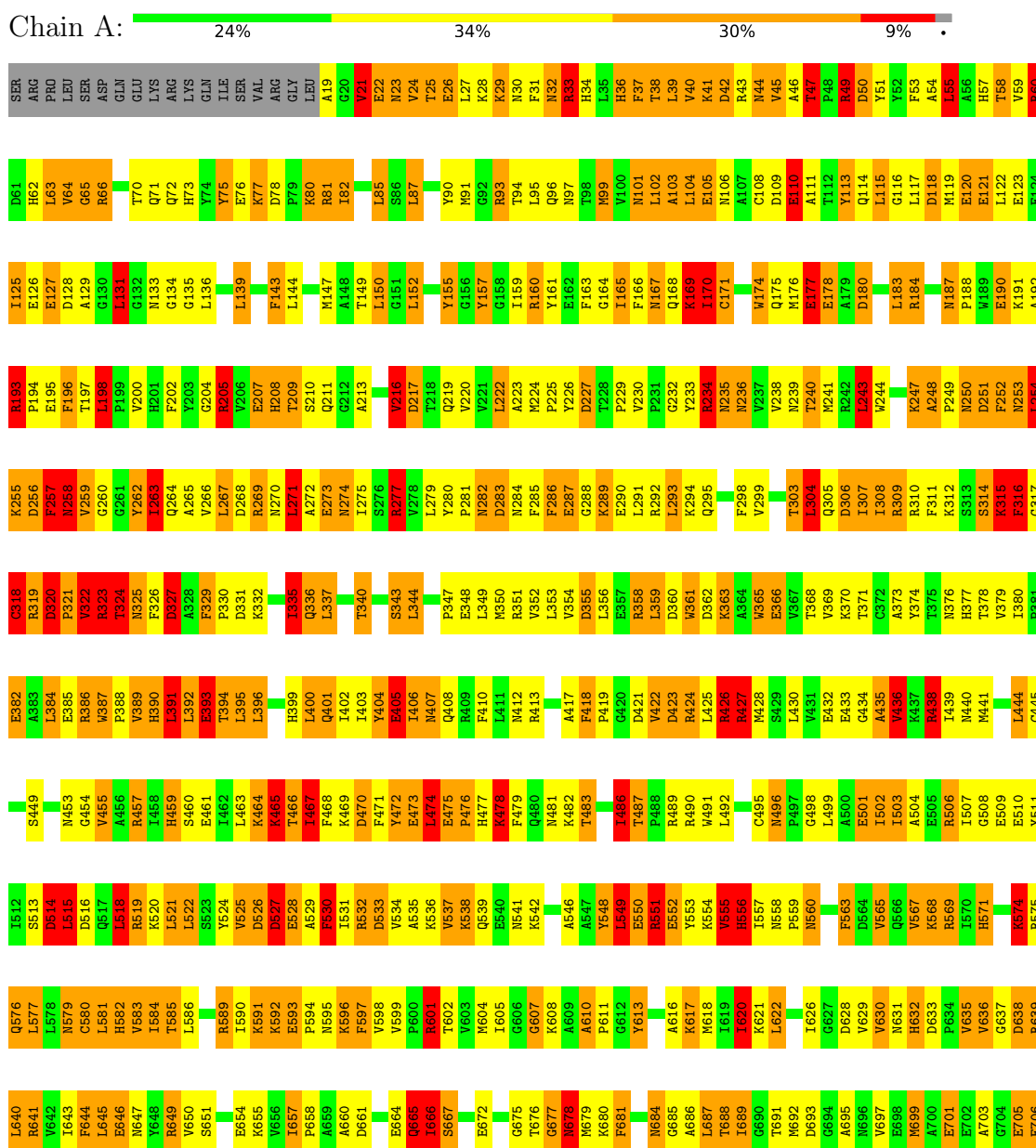
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	691	Total 691	O 691	0	0

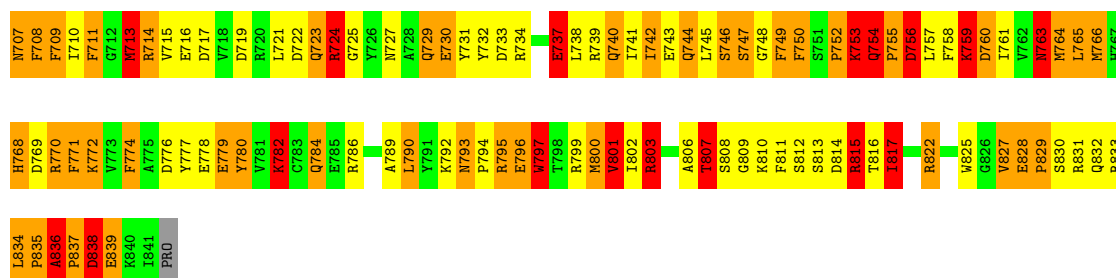
3 Residue-property plots

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





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.50Å 128.50Å 116.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7397	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.53	56/6844 (0.8%)	2.74	615/9265 (6.6%)

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	17

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	678	ASN	CA-CB	9.80	1.70	1.53
1	A	496	ASN	N-CA	9.36	1.56	1.46
1	A	675	GLY	N-CA	8.78	1.54	1.45
1	A	230	VAL	N-CA	8.78	1.57	1.46
1	A	620	ILE	CA-CB	8.62	1.64	1.54
1	A	490	ARG	NE-CZ	7.89	1.41	1.33
1	A	836	ALA	N-CA	-7.28	1.35	1.46
1	A	688	THR	CA-CB	7.19	1.64	1.53
1	A	55	LEU	N-CA	7.08	1.55	1.46
1	A	163	PHE	CA-C	7.06	1.60	1.52
1	A	94	THR	CA-CB	7.01	1.64	1.54
1	A	487	THR	CA-CB	6.88	1.64	1.52
1	A	279	LEU	N-CA	6.76	1.54	1.46
1	A	321	PRO	C-O	6.46	1.32	1.24
1	A	316	PHE	CA-C	6.37	1.60	1.52
1	A	165	ILE	CA-CB	6.33	1.61	1.54
1	A	40	VAL	N-CA	6.22	1.54	1.46
1	A	169	LYS	N-CA	6.17	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	THR	CA-CB	6.15	1.63	1.53
1	A	519	ARG	N-CA	6.14	1.53	1.46
1	A	725	GLY	CA-C	6.09	1.56	1.52
1	A	164	GLY	N-CA	6.04	1.51	1.45
1	A	241	MET	CA-C	6.02	1.60	1.52
1	A	178	GLU	N-CA	5.99	1.53	1.45
1	A	815	ARG	N-CA	5.91	1.53	1.46
1	A	834	LEU	N-CA	5.89	1.53	1.45
1	A	533	ASP	N-CA	5.86	1.53	1.46
1	A	453	ASN	N-CA	5.75	1.53	1.45
1	A	58	THR	N-CA	5.72	1.53	1.46
1	A	348	GLU	N-CA	5.68	1.53	1.46
1	A	171	CYS	N-CA	5.59	1.53	1.46
1	A	227	ASP	N-CA	5.58	1.52	1.46
1	A	230	VAL	CA-C	5.58	1.58	1.52
1	A	613	TYR	N-CA	5.55	1.54	1.46
1	A	368	THR	CB-OG1	5.53	1.52	1.43
1	A	665	GLN	N-CA	5.49	1.54	1.46
1	A	789	ALA	N-CA	5.49	1.52	1.46
1	A	117	LEU	CA-CB	5.46	1.61	1.54
1	A	287	GLU	N-CA	5.40	1.52	1.46
1	A	223	ALA	N-CA	5.32	1.52	1.46
1	A	723	GLN	N-CA	5.28	1.52	1.46
1	A	459	HIS	N-CA	5.24	1.52	1.46
1	A	303	THR	C-O	5.24	1.30	1.24
1	A	248	ALA	N-CA	5.23	1.53	1.46
1	A	507	ILE	CA-CB	5.22	1.60	1.54
1	A	457	ARG	N-CA	5.19	1.52	1.46
1	A	157	TYR	N-CA	5.18	1.52	1.46
1	A	772	LYS	N-CA	5.15	1.53	1.46
1	A	834	LEU	CA-CB	-5.15	1.45	1.53
1	A	377	HIS	CA-CB	5.12	1.61	1.54
1	A	38	THR	CA-CB	5.04	1.61	1.53
1	A	729	GLN	N-CA	5.03	1.52	1.46
1	A	239	ASN	N-CA	5.02	1.51	1.45
1	A	66	ARG	CD-NE	-5.02	1.39	1.46
1	A	797	TRP	CA-CB	-5.01	1.45	1.53
1	A	247	LYS	N-CA	5.00	1.52	1.46

All (615) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ARG	CD-NE-CZ	33.46	171.24	124.40
1	A	277	ARG	CD-NE-CZ	20.79	153.51	124.40
1	A	839	GLU	CB-CG-CD	17.52	142.38	112.60
1	A	207	GLU	CA-CB-CG	17.43	148.96	114.10
1	A	193	ARG	CD-NE-CZ	16.72	147.81	124.40
1	A	384	LEU	CB-CA-C	15.83	136.72	109.65
1	A	117	LEU	N-CA-C	15.83	134.73	114.31
1	A	632	HIS	CA-CB-CG	-15.81	97.99	113.80
1	A	316	PHE	N-CA-C	-15.07	94.13	113.72
1	A	665	GLN	CB-CA-C	14.42	132.96	111.76
1	A	257	PHE	N-CA-C	-14.40	95.71	113.28
1	A	678	ASN	CA-CB-CG	-14.29	98.31	112.60
1	A	64	VAL	N-CA-C	13.88	123.58	110.53
1	A	208	HIS	CA-CB-CG	-13.55	100.25	113.80
1	A	321	PRO	N-CA-C	13.54	140.35	112.47
1	A	834	LEU	CB-CA-C	13.14	130.29	109.52
1	A	309	ARG	CA-CB-CG	13.03	140.17	114.10
1	A	253	ASN	N-CA-C	-12.87	98.41	113.21
1	A	478	LYS	CA-CB-CG	12.56	139.22	114.10
1	A	62	HIS	CA-CB-CG	-12.24	101.56	113.80
1	A	509	GLU	N-CA-C	12.04	129.37	113.72
1	A	322	VAL	N-CA-C	-12.01	98.89	110.42
1	A	325	ASN	CA-CB-CG	-11.98	100.61	112.60
1	A	807	THR	N-CA-CB	-11.79	94.28	110.56
1	A	836	ALA	N-CA-C	11.76	135.81	109.81
1	A	135	GLY	N-CA-C	11.56	126.63	112.64
1	A	257	PHE	CA-C-O	11.56	132.94	119.18
1	A	727	ASN	CA-CB-CG	11.50	124.10	112.60
1	A	749	PHE	CA-CB-CG	-11.27	102.53	113.80
1	A	227	ASP	CA-CB-CG	11.10	123.70	112.60
1	A	556	HIS	N-CA-CB	10.91	128.93	110.49
1	A	322	VAL	N-CA-CB	10.79	123.17	110.55
1	A	478	LYS	CG-CD-CE	10.67	135.84	111.30
1	A	571	HIS	CA-CB-CG	10.65	124.45	113.80
1	A	252	PHE	CA-C-O	10.58	132.13	119.97
1	A	740	GLN	CB-CG-CD	10.57	130.57	112.60
1	A	309	ARG	CD-NE-CZ	10.48	139.08	124.40
1	A	438	ARG	CD-NE-CZ	10.41	138.97	124.40
1	A	340	THR	OG1-CB-CG2	10.40	130.09	109.30
1	A	576	GLN	N-CA-C	-10.34	99.82	111.71
1	A	501	GLU	O-C-N	10.22	133.13	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ARG	CD-NE-CZ	-10.19	110.14	124.40
1	A	97	ASN	CA-C-O	-10.17	109.77	120.55
1	A	678	ASN	N-CA-CB	-10.04	93.53	110.49
1	A	835	PRO	CA-C-N	10.01	146.22	121.80
1	A	835	PRO	C-N-CA	10.01	146.22	121.80
1	A	196	PHE	CA-CB-CG	10.00	123.80	113.80
1	A	272	ALA	N-CA-C	10.00	122.18	111.28
1	A	226	TYR	CA-C-O	-9.83	109.78	120.30
1	A	37	PHE	N-CA-C	9.82	122.89	111.11
1	A	595	ASN	CA-CB-CG	-9.77	102.83	112.60
1	A	340	THR	N-CA-CB	-9.74	94.64	110.42
1	A	677	GLY	N-CA-C	-9.72	100.50	113.24
1	A	675	GLY	N-CA-C	-9.71	100.45	112.68
1	A	526	ASP	N-CA-C	-9.69	88.52	107.62
1	A	490	ARG	NE-CZ-NH2	-9.61	110.55	119.20
1	A	554	LYS	N-CA-CB	9.51	126.01	110.32
1	A	586	LEU	CB-CA-C	9.47	125.75	110.88
1	A	37	PHE	CA-CB-CG	-9.43	104.37	113.80
1	A	323	ARG	CA-C-N	9.40	139.49	121.54
1	A	323	ARG	C-N-CA	9.40	139.49	121.54
1	A	407	ASN	CA-CB-CG	9.36	121.96	112.60
1	A	178	GLU	CA-CB-CG	9.32	132.75	114.10
1	A	822	ARG	CD-NE-CZ	-9.31	111.37	124.40
1	A	519	ARG	CA-CB-CG	9.31	132.71	114.10
1	A	839	GLU	N-CA-C	9.23	123.77	107.80
1	A	251	ASP	N-CA-C	9.21	125.16	113.55
1	A	532	ARG	CD-NE-CZ	9.21	137.29	124.40
1	A	613	TYR	N-CA-C	-9.13	92.68	108.56
1	A	666	ILE	N-CA-C	9.09	128.24	109.34
1	A	491	TRP	N-CA-C	9.04	123.61	113.21
1	A	253	ASN	N-CA-CB	-9.01	97.51	110.57
1	A	495	CYS	CA-C-N	-9.01	112.94	122.85
1	A	495	CYS	C-N-CA	-9.01	112.94	122.85
1	A	567	VAL	CA-C-O	8.98	129.34	120.27
1	A	577	LEU	O-C-N	8.96	131.62	122.12
1	A	838	ASP	N-CA-C	8.92	129.80	110.80
1	A	678	ASN	CA-C-O	8.91	133.26	120.51
1	A	263	ILE	O-C-N	8.89	131.15	121.90
1	A	454	GLY	N-CA-C	-8.84	98.92	112.89
1	A	490	ARG	NH1-CZ-NH2	8.74	130.67	119.30
1	A	772	LYS	N-CA-CB	-8.73	98.44	111.71
1	A	649	ARG	CA-C-O	-8.72	111.90	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ASP	CA-CB-CG	-8.66	103.94	112.60
1	A	822	ARG	N-CA-C	8.62	120.76	111.36
1	A	766	MET	N-CA-C	8.62	121.82	111.82
1	A	387	TRP	N-CA-C	8.58	120.46	109.65
1	A	360	ASP	N-CA-CB	-8.54	97.48	110.04
1	A	807	THR	OG1-CB-CG2	8.54	126.37	109.30
1	A	314	SER	N-CA-C	8.52	122.78	108.20
1	A	774	PHE	CA-CB-CG	8.49	122.29	113.80
1	A	803	ARG	CD-NE-CZ	-8.48	112.53	124.40
1	A	722	ASP	O-C-N	8.47	131.81	122.15
1	A	646	GLU	CA-CB-CG	8.46	131.02	114.10
1	A	768	HIS	N-CA-C	8.45	122.14	110.06
1	A	553	TYR	CA-C-N	8.38	135.15	121.58
1	A	553	TYR	C-N-CA	8.38	135.15	121.58
1	A	666	ILE	CA-C-N	8.33	133.33	120.75
1	A	666	ILE	C-N-CA	8.33	133.33	120.75
1	A	834	LEU	N-CA-C	-8.31	99.09	109.64
1	A	316	PHE	N-CA-CB	8.27	122.80	110.65
1	A	78	ASP	CA-CB-CG	8.24	120.84	112.60
1	A	167	ASN	CA-CB-CG	-8.24	104.36	112.60
1	A	530	PHE	CA-CB-CG	-8.24	105.56	113.80
1	A	487	THR	CA-C-O	8.20	125.39	119.32
1	A	436	VAL	N-CA-CB	8.19	124.75	111.23
1	A	822	ARG	O-C-N	8.13	131.42	122.15
1	A	360	ASP	CA-C-O	-8.11	112.96	121.55
1	A	750	PHE	CA-CB-CG	-8.06	105.74	113.80
1	A	737	GLU	CA-CB-CG	8.03	130.16	114.10
1	A	532	ARG	O-C-N	8.01	132.12	122.27
1	A	287	GLU	CA-CB-CG	8.01	130.12	114.10
1	A	677	GLY	CA-C-N	8.01	136.83	121.54
1	A	677	GLY	C-N-CA	8.01	136.83	121.54
1	A	396	LEU	N-CA-CB	-7.98	101.69	110.71
1	A	666	ILE	CB-CG1-CD1	7.96	130.51	113.80
1	A	310	ARG	CD-NE-CZ	-7.92	113.31	124.40
1	A	835	PRO	CA-C-O	7.92	132.21	119.86
1	A	117	LEU	N-CA-CB	-7.88	100.43	110.90
1	A	63	LEU	N-CA-CB	-7.83	98.23	110.44
1	A	42	ASP	CA-CB-CG	7.83	120.43	112.60
1	A	257	PHE	CA-C-N	7.78	136.40	121.54
1	A	257	PHE	C-N-CA	7.78	136.40	121.54
1	A	800	MET	O-C-N	7.78	130.08	122.07
1	A	490	ARG	CD-NE-CZ	-7.76	113.53	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	ARG	NE-CZ-NH2	7.74	126.16	119.20
1	A	127	GLU	CB-CG-CD	7.73	125.74	112.60
1	A	321	PRO	CA-C-O	-7.73	106.54	120.60
1	A	621	LYS	O-C-N	7.72	130.31	122.12
1	A	377	HIS	CA-CB-CG	-7.72	106.08	113.80
1	A	286	PHE	CA-CB-CG	7.70	121.50	113.80
1	A	482	LYS	CA-C-O	-7.70	111.11	120.89
1	A	610	ALA	CB-CA-C	7.69	121.49	109.42
1	A	538	LYS	CG-CD-CE	7.69	128.98	111.30
1	A	335	ILE	N-CA-CB	7.68	122.01	111.41
1	A	324	THR	N-CA-CB	7.66	123.44	110.49
1	A	325	ASN	CA-C-O	7.66	129.30	120.80
1	A	360	ASP	CA-CB-CG	-7.62	104.98	112.60
1	A	250	ASN	N-CA-C	7.61	122.39	113.18
1	A	143	PHE	CA-C-O	7.61	129.04	120.90
1	A	114	GLN	CB-CG-CD	7.60	125.52	112.60
1	A	481	ASN	CA-CB-CG	-7.57	105.03	112.60
1	A	105	GLU	N-CA-C	7.54	120.15	111.11
1	A	422	VAL	CA-C-O	-7.53	112.34	120.47
1	A	118	ASP	N-CA-CB	7.52	123.20	110.49
1	A	217	ASP	CA-CB-CG	-7.52	105.08	112.60
1	A	644	PHE	CA-CB-CG	-7.51	106.29	113.80
1	A	160	ARG	CD-NE-CZ	-7.47	113.94	124.40
1	A	217	ASP	CB-CA-C	7.46	123.14	111.95
1	A	475	GLU	CG-CD-OE1	7.45	135.53	118.40
1	A	269	ARG	CD-NE-CZ	7.43	134.80	124.40
1	A	152	LEU	CA-C-O	-7.41	112.47	121.36
1	A	282	ASN	OD1-CG-ND2	7.41	130.01	122.60
1	A	433	GLU	N-CA-CB	7.40	120.84	109.97
1	A	701	GLU	CB-CA-C	7.40	122.35	110.96
1	A	406	ILE	O-C-N	7.38	129.15	121.91
1	A	817	ILE	N-CA-CB	7.38	120.58	110.54
1	A	24	VAL	CA-CB-CG2	7.38	122.95	110.40
1	A	678	ASN	CA-C-N	7.36	130.74	120.29
1	A	678	ASN	C-N-CA	7.36	130.74	120.29
1	A	268	ASP	CA-CB-CG	-7.36	105.25	112.60
1	A	527	ASP	N-CA-CB	7.35	122.91	110.49
1	A	21	VAL	N-CA-C	7.34	124.61	109.34
1	A	793	ASN	CA-CB-CG	7.30	119.91	112.60
1	A	782	LYS	CB-CA-C	7.30	122.20	110.96
1	A	298	PHE	CA-CB-CG	7.29	121.09	113.80
1	A	26	GLU	CA-C-N	7.29	130.05	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	GLU	C-N-CA	7.29	130.05	120.28
1	A	811	PHE	CA-CB-CG	-7.29	106.52	113.80
1	A	507	ILE	O-C-N	7.28	128.79	122.16
1	A	753	LYS	N-CA-CB	-7.27	99.11	109.94
1	A	597	PHE	CA-CB-CG	-7.27	106.53	113.80
1	A	831	ARG	N-CA-C	-7.26	104.29	113.72
1	A	121	GLU	CA-CB-CG	7.25	128.60	114.10
1	A	325	ASN	CB-CA-C	7.24	121.64	109.48
1	A	133	ASN	O-C-N	7.23	132.05	122.36
1	A	82	ILE	O-C-N	7.22	130.76	123.18
1	A	40	VAL	CA-C-O	7.21	129.79	120.78
1	A	135	GLY	CA-C-O	7.21	128.47	121.05
1	A	198	LEU	CA-CB-CG	7.21	141.52	116.30
1	A	575	ARG	CA-C-O	7.18	129.83	121.28
1	A	115	LEU	N-CA-C	-7.15	104.52	113.18
1	A	315	LYS	CA-C-N	7.14	133.61	122.26
1	A	315	LYS	C-N-CA	7.14	133.61	122.26
1	A	601	ARG	CA-CB-CG	7.13	128.35	114.10
1	A	519	ARG	N-CA-CB	7.11	120.58	110.12
1	A	208	HIS	CA-C-O	-7.09	112.58	120.60
1	A	678	ASN	CB-CG-ND2	-7.09	105.76	116.40
1	A	24	VAL	O-C-N	7.09	129.03	121.87
1	A	424	ARG	CD-NE-CZ	-7.08	114.49	124.40
1	A	709	PHE	CA-CB-CG	-7.07	106.73	113.80
1	A	390	HIS	CA-CB-CG	7.07	120.87	113.80
1	A	677	GLY	CA-C-O	7.06	128.03	120.40
1	A	412	ASN	CA-CB-CG	7.04	119.64	112.60
1	A	174	TRP	CA-C-O	7.03	129.11	121.16
1	A	404	TYR	CA-C-O	7.02	128.00	120.55
1	A	828	GLU	CB-CA-C	-7.02	100.72	110.13
1	A	822	ARG	CA-C-O	-7.01	112.98	120.42
1	A	209	THR	N-CA-C	6.98	119.44	107.93
1	A	646	GLU	CB-CA-C	-6.97	97.73	109.65
1	A	526	ASP	CB-CA-C	6.96	123.20	111.22
1	A	529	ALA	N-CA-C	-6.96	103.74	111.82
1	A	473	GLU	CB-CG-CD	6.96	124.43	112.60
1	A	65	GLY	O-C-N	6.94	128.85	122.19
1	A	40	VAL	N-CA-CB	-6.91	99.82	111.23
1	A	379	VAL	N-CA-CB	-6.91	104.11	112.33
1	A	277	ARG	NE-CZ-NH1	6.89	128.39	121.50
1	A	608	LYS	O-C-N	6.88	131.02	123.10
1	A	745	LEU	CA-C-N	6.85	129.46	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	745	LEU	C-N-CA	6.85	129.46	120.28
1	A	366	GLU	CB-CG-CD	6.84	124.22	112.60
1	A	406	ILE	CB-CA-C	-6.83	103.22	111.97
1	A	335	ILE	CB-CA-C	6.83	120.74	110.63
1	A	217	ASP	CA-C-O	6.83	130.02	122.03
1	A	771	PHE	CA-CB-CG	-6.82	106.98	113.80
1	A	21	VAL	CA-C-O	-6.82	112.26	120.78
1	A	248	ALA	N-CA-CB	-6.81	101.10	110.29
1	A	574	LYS	CB-CG-CD	-6.80	95.66	111.30
1	A	91	MET	N-CA-C	6.80	119.70	111.82
1	A	472	TYR	CA-CB-CG	-6.79	101.67	113.90
1	A	495	CYS	O-C-N	6.79	131.84	122.46
1	A	532	ARG	CA-C-N	-6.77	111.43	120.63
1	A	532	ARG	C-N-CA	-6.77	111.43	120.63
1	A	274	ASN	OD1-CG-ND2	6.77	129.37	122.60
1	A	216	VAL	N-CA-C	6.76	118.56	108.96
1	A	386	ARG	CD-NE-CZ	6.76	133.87	124.40
1	A	259	VAL	N-CA-C	-6.75	99.70	109.29
1	A	723	GLN	CB-CA-C	6.75	121.48	110.88
1	A	193	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	A	324	THR	N-CA-C	-6.71	96.50	110.80
1	A	324	THR	CA-C-N	-6.71	112.66	122.65
1	A	324	THR	C-N-CA	-6.71	112.66	122.65
1	A	396	LEU	O-C-N	6.69	126.08	121.19
1	A	307	ILE	CA-C-N	6.68	128.97	120.56
1	A	307	ILE	C-N-CA	6.68	128.97	120.56
1	A	582	HIS	CA-CB-CG	-6.66	107.14	113.80
1	A	737	GLU	N-CA-CB	6.65	119.85	109.94
1	A	198	LEU	N-CA-CB	-6.64	99.03	110.72
1	A	121	GLU	N-CA-CB	6.62	120.54	110.28
1	A	178	GLU	CB-CA-C	6.62	123.21	109.38
1	A	63	LEU	CA-C-O	-6.61	111.54	119.27
1	A	81	ARG	O-C-N	6.59	131.46	123.16
1	A	410	PHE	CA-CB-CG	-6.58	107.22	113.80
1	A	768	HIS	CA-CB-CG	6.58	120.38	113.80
1	A	177	GLU	CA-C-N	-6.56	112.39	122.62
1	A	177	GLU	C-N-CA	-6.56	112.39	122.62
1	A	771	PHE	CB-CA-C	6.55	121.63	110.56
1	A	348	GLU	CA-CB-CG	6.55	127.20	114.10
1	A	325	ASN	N-CA-C	6.55	120.50	109.76
1	A	474	LEU	CA-C-N	-6.55	116.52	122.28
1	A	474	LEU	C-N-CA	-6.55	116.52	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	ARG	CB-CA-C	6.54	121.64	110.79
1	A	639	ARG	CB-CA-C	6.53	123.42	110.42
1	A	822	ARG	NE-CZ-NH1	-6.51	114.99	121.50
1	A	433	GLU	CA-CB-CG	6.50	127.11	114.10
1	A	630	VAL	N-CA-C	6.48	116.64	110.42
1	A	312	LYS	CB-CA-C	-6.48	100.04	110.79
1	A	433	GLU	N-CA-C	-6.46	100.72	110.28
1	A	638	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	230	VAL	CA-CB-CG2	6.44	121.35	110.40
1	A	49	ARG	N-CA-CB	6.43	119.57	110.12
1	A	247	LYS	CB-CA-C	6.43	122.07	109.35
1	A	583	VAL	N-CA-C	6.43	117.18	110.62
1	A	647	ASN	N-CA-CB	-6.42	102.20	111.70
1	A	800	MET	CA-CB-CG	-6.42	101.26	114.10
1	A	25	THR	N-CA-CB	6.42	119.66	110.16
1	A	558	ASN	OD1-CG-ND2	6.41	129.01	122.60
1	A	150	LEU	O-C-N	6.39	130.01	122.34
1	A	746	SER	N-CA-C	6.39	118.25	111.28
1	A	96	GLN	OE1-CD-NE2	6.38	128.98	122.60
1	A	495	CYS	CA-C-O	-6.38	111.40	119.31
1	A	376	ASN	CB-CA-C	6.38	120.19	109.48
1	A	99	MET	O-C-N	6.37	128.87	122.12
1	A	176	MET	O-C-N	6.37	130.76	123.31
1	A	304	LEU	O-C-N	6.36	128.87	122.12
1	A	686	ALA	CB-CA-C	6.36	121.87	109.33
1	A	731	TYR	CA-C-O	6.36	127.25	120.70
1	A	589	ARG	CD-NE-CZ	6.36	133.30	124.40
1	A	829	PRO	CB-CA-C	-6.35	102.92	111.12
1	A	392	LEU	N-CA-C	6.34	117.99	111.14
1	A	620	ILE	CB-CA-C	-6.34	103.76	111.88
1	A	39	LEU	O-C-N	6.34	131.21	122.46
1	A	689	ILE	N-CA-C	-6.33	99.31	108.36
1	A	482	LYS	O-C-N	6.32	130.61	123.28
1	A	45	VAL	CB-CA-C	6.32	116.57	110.63
1	A	772	LYS	CB-CA-C	-6.31	102.15	112.06
1	A	253	ASN	CA-CB-CG	6.30	118.90	112.60
1	A	839	GLU	CB-CA-C	-6.30	101.42	110.62
1	A	269	ARG	NE-CZ-NH1	6.30	127.80	121.50
1	A	565	VAL	N-CA-C	6.29	117.55	108.48
1	A	834	LEU	CA-C-N	6.29	126.04	119.05
1	A	834	LEU	C-N-CA	6.29	126.04	119.05
1	A	714	ARG	N-CA-C	-6.28	100.69	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	LEU	CA-C-O	-6.27	112.22	119.56
1	A	54	ALA	O-C-N	6.26	129.29	122.15
1	A	368	THR	CA-C-O	6.26	127.40	120.82
1	A	331	ASP	CB-CA-C	6.26	123.07	109.99
1	A	230	VAL	N-CA-CB	-6.25	102.45	111.21
1	A	393	GLU	CA-C-O	6.24	127.37	120.63
1	A	93	ARG	NH1-CZ-NH2	-6.23	111.20	119.30
1	A	33	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	A	103	ALA	N-CA-CB	-6.21	102.87	112.30
1	A	32	ASN	CA-CB-CG	-6.20	106.40	112.60
1	A	586	LEU	CA-CB-CG	6.20	138.00	116.30
1	A	202	PHE	CA-CB-CG	6.19	119.99	113.80
1	A	649	ARG	N-CA-CB	-6.19	101.31	110.97
1	A	312	LYS	N-CA-C	6.19	118.03	111.28
1	A	732	TYR	O-C-N	6.17	128.50	122.09
1	A	617	LYS	O-C-N	6.16	129.18	122.15
1	A	650	VAL	CB-CA-C	6.16	119.59	111.70
1	A	282	ASN	CA-CB-CG	-6.15	106.45	112.60
1	A	51	TYR	CB-CA-C	6.14	120.52	110.88
1	A	129	ALA	N-CA-C	-6.14	95.66	107.57
1	A	165	ILE	N-CA-CB	-6.13	100.56	110.13
1	A	213	ALA	N-CA-C	6.12	119.34	110.28
1	A	401	GLN	N-CA-CB	6.11	118.87	110.01
1	A	467	ILE	O-C-N	6.11	127.87	121.89
1	A	602	THR	N-CA-C	-6.10	97.34	108.02
1	A	756	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	530	PHE	N-CA-CB	6.08	118.79	109.91
1	A	630	VAL	CA-C-O	-6.07	114.73	121.17
1	A	571	HIS	O-C-N	6.07	129.92	123.42
1	A	216	VAL	CA-C-O	6.07	128.10	121.67
1	A	779	GLU	CA-CB-CG	6.07	126.23	114.10
1	A	365	TRP	CA-C-O	6.06	127.19	120.82
1	A	579	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	45	VAL	CA-C-O	-6.06	112.68	119.35
1	A	66	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	A	577	LEU	CA-C-O	-6.06	114.13	120.55
1	A	487	THR	CA-CB-OG1	-6.06	100.51	109.60
1	A	502	ILE	CA-CB-CG1	6.05	120.69	110.40
1	A	731	TYR	CA-CB-CG	-6.05	103.01	113.90
1	A	816	THR	O-C-N	6.05	128.30	122.07
1	A	514	ASP	CB-CA-C	6.05	122.46	110.42
1	A	220	VAL	N-CA-C	6.05	117.30	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASP	CA-C-O	-6.04	115.10	122.41
1	A	526	ASP	N-CA-CB	6.04	120.67	110.46
1	A	251	ASP	N-CA-CB	-6.03	101.66	110.40
1	A	483	THR	CA-CB-OG1	-6.02	100.57	109.60
1	A	580	CYS	O-C-N	6.01	128.49	122.12
1	A	646	GLU	CB-CG-CD	6.01	122.82	112.60
1	A	123	GLU	OE1-CD-OE2	-6.01	108.48	122.90
1	A	797	TRP	CA-CB-CG	6.00	125.00	113.60
1	A	444	LEU	N-CA-CB	-6.00	101.30	110.12
1	A	459	HIS	CA-C-O	6.00	127.32	120.90
1	A	742	ILE	O-C-N	5.99	128.11	121.94
1	A	310	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	A	555	VAL	N-CA-CB	-5.98	101.37	111.23
1	A	501	GLU	CB-CA-C	-5.97	101.46	110.90
1	A	24	VAL	N-CA-CB	5.97	120.86	110.65
1	A	80	LYS	N-CA-C	-5.97	101.45	110.28
1	A	243	LEU	N-CA-CB	-5.97	101.34	110.65
1	A	459	HIS	O-C-N	-5.95	115.90	122.09
1	A	713	MET	O-C-N	5.95	129.88	122.86
1	A	684	ASN	CA-CB-CG	-5.94	106.66	112.60
1	A	101	ASN	CB-CA-C	5.94	120.65	110.79
1	A	234	ARG	N-CA-CB	-5.93	100.47	110.49
1	A	686	ALA	N-CA-C	-5.93	100.23	109.72
1	A	277	ARG	CA-C-N	-5.92	114.75	122.51
1	A	277	ARG	C-N-CA	-5.92	114.75	122.51
1	A	814	ASP	O-C-N	5.92	128.90	122.15
1	A	654	GLU	CB-CG-CD	-5.91	102.55	112.60
1	A	687	LEU	CB-CA-C	5.91	119.61	109.51
1	A	240	THR	CA-C-N	5.90	131.49	123.11
1	A	240	THR	C-N-CA	5.90	131.49	123.11
1	A	133	ASN	OD1-CG-ND2	5.90	128.50	122.60
1	A	224	MET	N-CA-CB	-5.89	99.50	110.05
1	A	455	VAL	N-CA-CB	-5.89	104.66	112.26
1	A	167	ASN	N-CA-C	-5.89	100.40	109.76
1	A	479	PHE	N-CA-C	5.89	119.23	109.46
1	A	354	VAL	CA-C-N	5.88	128.16	120.28
1	A	354	VAL	C-N-CA	5.88	128.16	120.28
1	A	814	ASP	N-CA-CB	5.87	118.85	110.16
1	A	534	VAL	CA-C-O	-5.87	115.31	121.41
1	A	577	LEU	N-CA-CB	5.86	118.74	110.12
1	A	316	PHE	CB-CA-C	-5.86	99.70	109.55
1	A	555	VAL	CA-CB-CG1	5.86	120.36	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	763	ASN	CA-C-N	5.86	128.06	120.44
1	A	763	ASN	C-N-CA	5.86	128.06	120.44
1	A	466	THR	N-CA-C	5.85	123.26	110.80
1	A	392	LEU	CA-C-N	5.85	128.39	120.38
1	A	392	LEU	C-N-CA	5.85	128.39	120.38
1	A	552	GLU	N-CA-C	5.85	119.94	112.34
1	A	391	LEU	N-CA-C	-5.84	104.84	111.14
1	A	193	ARG	CB-CA-C	5.83	118.84	111.21
1	A	816	THR	N-CA-CB	5.83	118.46	110.01
1	A	784	GLN	CB-CG-CD	-5.81	102.72	112.60
1	A	309	ARG	CB-CA-C	5.81	120.15	110.92
1	A	283	ASP	N-CA-CB	-5.80	101.44	110.55
1	A	81	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	A	40	VAL	CB-CA-C	5.79	120.79	111.29
1	A	267	LEU	O-C-N	5.79	128.75	122.15
1	A	160	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	A	518	LEU	O-C-N	5.79	129.91	122.39
1	A	507	ILE	N-CA-CB	-5.79	104.80	112.26
1	A	511	TYR	CA-C-O	-5.78	111.54	119.05
1	A	754	GLN	CB-CA-C	-5.78	98.79	110.17
1	A	533	ASP	O-C-N	5.77	128.26	122.03
1	A	471	PHE	CA-C-O	5.77	126.88	120.82
1	A	742	ILE	CB-CA-C	5.76	119.02	111.81
1	A	293	LEU	N-CA-CB	-5.76	101.65	110.12
1	A	95	LEU	N-CA-C	5.75	117.22	111.07
1	A	209	THR	CA-C-O	5.75	127.00	119.98
1	A	62	HIS	CA-C-O	5.74	126.44	119.49
1	A	51	TYR	N-CA-C	-5.74	104.93	111.07
1	A	550	GLU	CA-C-O	-5.74	114.97	121.00
1	A	355	ASP	O-C-N	5.73	128.20	122.12
1	A	401	GLN	CB-CA-C	-5.73	101.88	110.88
1	A	596	LYS	CA-C-N	5.71	128.99	120.87
1	A	596	LYS	C-N-CA	5.71	128.99	120.87
1	A	90	TYR	CA-C-N	5.71	128.99	120.31
1	A	90	TYR	C-N-CA	5.71	128.99	120.31
1	A	269	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	A	749	PHE	CB-CA-C	5.71	120.31	110.84
1	A	167	ASN	OD1-CG-ND2	5.70	128.30	122.60
1	A	689	ILE	CA-C-O	-5.70	114.47	120.57
1	A	318	CYS	CB-CA-C	5.70	121.76	110.42
1	A	705	GLU	CB-CG-CD	5.70	122.29	112.60
1	A	113	TYR	N-CA-CB	5.70	120.12	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLU	N-CA-CB	5.69	119.77	110.90
1	A	418	PHE	O-C-N	5.69	126.59	121.42
1	A	711	PHE	O-C-N	5.68	128.97	123.29
1	A	509	GLU	CB-CA-C	-5.68	100.00	109.55
1	A	335	ILE	CA-CB-CG2	5.68	120.15	110.50
1	A	537	VAL	O-C-N	5.67	127.37	121.87
1	A	324	THR	CA-C-O	-5.67	112.40	120.51
1	A	200	VAL	CA-C-O	-5.67	114.04	120.67
1	A	777	TYR	O-C-N	5.67	128.21	122.09
1	A	506	ARG	NE-CZ-NH1	5.66	127.16	121.50
1	A	304	LEU	CA-C-O	-5.66	114.55	120.55
1	A	556	HIS	N-CA-C	-5.66	98.75	110.80
1	A	222	LEU	CA-C-N	-5.66	115.24	122.77
1	A	222	LEU	C-N-CA	-5.66	115.24	122.77
1	A	187	ASN	CA-C-N	5.66	125.33	119.56
1	A	187	ASN	C-N-CA	5.66	125.33	119.56
1	A	689	ILE	N-CA-CB	5.66	117.78	110.99
1	A	607	GLY	N-CA-C	-5.65	102.63	111.00
1	A	766	MET	CB-CA-C	-5.64	99.84	110.67
1	A	435	ALA	CA-C-N	5.64	132.12	121.97
1	A	435	ALA	C-N-CA	5.64	132.12	121.97
1	A	745	LEU	CA-C-O	5.62	126.49	120.70
1	A	279	LEU	CA-C-O	-5.62	114.64	121.05
1	A	176	MET	N-CA-C	-5.62	99.27	108.76
1	A	630	VAL	CB-CA-C	5.62	119.16	111.97
1	A	808	SER	N-CA-C	5.61	120.13	113.28
1	A	243	LEU	O-C-N	5.61	129.78	123.27
1	A	190	GLU	CG-CD-OE2	5.61	131.30	118.40
1	A	292	ARG	N-CA-CB	-5.59	101.89	110.16
1	A	227	ASP	CA-C-O	5.58	127.00	120.80
1	A	252	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	706	GLU	CA-CB-CG	-5.58	102.94	114.10
1	A	802	ILE	O-C-N	5.57	127.27	121.87
1	A	565	VAL	CB-CA-C	-5.56	102.33	110.62
1	A	802	ILE	N-CA-CB	5.56	118.10	110.54
1	A	81	ARG	CA-C-O	-5.56	114.88	121.16
1	A	178	GLU	CB-CG-CD	-5.56	103.15	112.60
1	A	320	ASP	CA-C-N	5.55	126.78	119.84
1	A	320	ASP	C-N-CA	5.55	126.78	119.84
1	A	87	LEU	CB-CA-C	5.55	120.00	110.01
1	A	139	LEU	CA-C-O	5.55	126.64	120.82
1	A	724	ARG	CA-CB-CG	5.54	125.17	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	807	THR	CA-CB-CG2	5.54	119.91	110.50
1	A	532	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	A	60	ARG	CB-CA-C	5.53	120.08	110.68
1	A	23	ASN	CA-C-O	-5.52	114.67	120.63
1	A	744	GLN	CA-CB-CG	5.52	125.14	114.10
1	A	275	ILE	CA-C-O	-5.52	115.31	121.05
1	A	628	ASP	O-C-N	5.51	127.96	122.12
1	A	657	ILE	N-CA-CB	5.51	118.93	111.21
1	A	750	PHE	N-CA-C	5.51	119.63	113.02
1	A	362	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	219	GLN	N-CA-C	-5.51	100.73	109.76
1	A	647	ASN	N-CA-C	5.51	118.99	111.39
1	A	701	GLU	CB-CG-CD	5.51	121.96	112.60
1	A	828	GLU	CB-CG-CD	5.50	121.95	112.60
1	A	701	GLU	CA-CB-CG	5.50	125.10	114.10
1	A	317	GLY	CA-C-O	5.49	126.05	120.45
1	A	317	GLY	O-C-N	5.49	127.85	122.19
1	A	152	LEU	O-C-N	5.47	129.19	123.06
1	A	688	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	391	LEU	CB-CA-C	5.47	119.54	110.90
1	A	465	LYS	O-C-N	5.47	129.81	122.49
1	A	475	GLU	O-C-N	5.46	125.38	121.12
1	A	321	PRO	CB-CA-C	-5.46	102.55	111.56
1	A	684	ASN	CA-C-O	5.46	126.28	119.78
1	A	630	VAL	O-C-N	5.46	127.26	121.91
1	A	428	MET	CA-C-O	5.45	125.67	119.18
1	A	550	GLU	N-CA-CB	5.45	117.87	109.91
1	A	110	GLU	O-C-N	5.44	129.83	122.59
1	A	538	LYS	N-CA-CB	5.44	118.12	110.12
1	A	687	LEU	N-CA-C	-5.42	101.69	110.32
1	A	740	GLN	CA-C-O	5.42	126.21	119.97
1	A	258	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	178	GLU	CG-CD-OE1	-5.42	105.94	118.40
1	A	393	GLU	CA-CB-CG	5.42	124.93	114.10
1	A	688	THR	CA-C-O	-5.42	114.48	120.38
1	A	686	ALA	CA-C-O	-5.41	114.99	121.11
1	A	515	LEU	O-C-N	5.41	128.55	122.22
1	A	632	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	47	THR	N-CA-C	-5.41	102.15	110.58
1	A	343	SER	N-CA-C	5.40	118.97	112.38
1	A	806	ALA	N-CA-C	5.39	117.85	111.33
1	A	350	MET	CA-C-O	5.38	126.26	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	MET	CA-C-O	-5.37	113.79	119.97
1	A	496	ASN	N-CA-CB	-5.37	103.81	110.79
1	A	219	GLN	CA-C-O	-5.36	114.85	120.80
1	A	97	ASN	O-C-N	5.36	127.80	122.12
1	A	538	LYS	CB-CG-CD	-5.36	98.98	111.30
1	A	253	ASN	CB-CA-C	5.35	120.19	110.72
1	A	503	ILE	CB-CA-C	-5.35	104.83	112.22
1	A	134	GLY	O-C-N	5.34	129.64	122.70
1	A	752	PRO	CA-C-N	5.33	127.74	120.54
1	A	752	PRO	C-N-CA	5.33	127.74	120.54
1	A	222	LEU	CA-C-O	-5.33	114.79	120.92
1	A	49	ARG	CD-NE-CZ	-5.33	116.94	124.40
1	A	336	GLN	CB-CG-CD	-5.33	103.55	112.60
1	A	136	LEU	CB-CA-C	5.32	119.24	110.88
1	A	714	ARG	N-CA-CB	5.32	119.08	110.51
1	A	535	ALA	N-CA-C	5.32	117.82	111.71
1	A	814	ASP	CA-C-O	-5.32	114.79	120.42
1	A	329	PHE	CB-CA-C	5.31	120.64	110.17
1	A	486	ILE	CA-CB-CG2	5.31	119.53	110.50
1	A	575	ARG	N-CA-C	5.31	118.91	111.74
1	A	50	ASP	CB-CG-OD2	5.31	130.60	118.40
1	A	707	ASN	CA-CB-CG	5.30	117.90	112.60
1	A	560	ASN	CB-CA-C	5.29	119.82	111.72
1	A	149	THR	CA-CB-CG2	5.29	119.49	110.50
1	A	379	VAL	N-CA-C	-5.29	108.13	113.47
1	A	506	ARG	CD-NE-CZ	5.28	131.80	124.40
1	A	549	LEU	N-CA-C	-5.28	104.57	111.02
1	A	478	LYS	CB-CG-CD	5.28	123.44	111.30
1	A	75	TYR	CA-CB-CG	-5.28	104.41	113.90
1	A	120	GLU	CB-CA-C	5.27	119.64	110.68
1	A	26	GLU	N-CA-C	5.27	117.45	111.02
1	A	205	ARG	N-CA-C	-5.27	101.11	108.96
1	A	115	LEU	CA-CB-CG	5.26	134.70	116.30
1	A	271	LEU	CA-C-N	5.25	127.32	120.28
1	A	271	LEU	C-N-CA	5.25	127.32	120.28
1	A	71	GLN	CA-C-O	-5.25	115.30	120.82
1	A	585	THR	CA-C-O	5.25	126.33	120.82
1	A	801	VAL	CB-CA-C	-5.25	105.16	112.04
1	A	763	ASN	CB-CA-C	5.25	119.21	110.81
1	A	168	GLN	CA-C-O	5.24	125.97	120.36
1	A	131	LEU	CA-C-O	-5.23	113.03	120.51
1	A	440	ASN	CB-CA-C	5.23	119.44	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	THR	O-C-N	5.23	129.55	122.59
1	A	273	GLU	N-CA-C	-5.23	106.85	113.18
1	A	599	VAL	N-CA-C	-5.23	103.83	108.95
1	A	650	VAL	N-CA-C	5.23	115.67	110.23
1	A	292	ARG	CA-CB-CG	-5.22	103.65	114.10
1	A	489	ARG	CB-CA-C	5.22	120.81	110.42
1	A	502	ILE	N-CA-CB	5.21	117.63	110.54
1	A	554	LYS	N-CA-C	-5.21	99.33	107.93
1	A	541	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	A	800	MET	CG-SD-CE	5.20	112.33	100.90
1	A	808	SER	CA-CB-OG	5.19	121.48	111.10
1	A	47	THR	O-C-N	5.19	124.87	121.14
1	A	309	ARG	CA-C-N	5.18	127.48	120.38
1	A	309	ARG	C-N-CA	5.18	127.48	120.38
1	A	470	ASP	CA-C-N	5.18	127.18	120.44
1	A	470	ASP	C-N-CA	5.18	127.18	120.44
1	A	327	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	322	VAL	O-C-N	5.18	126.98	121.91
1	A	405	GLU	CB-CA-C	-5.18	102.20	110.79
1	A	359	LEU	N-CA-CB	-5.17	102.20	110.63
1	A	244	TRP	N-CA-C	5.17	118.37	110.20
1	A	253	ASN	CA-C-N	5.17	131.41	121.54
1	A	253	ASN	C-N-CA	5.17	131.41	121.54
1	A	170	ILE	N-CA-CB	5.17	118.36	111.64
1	A	238	VAL	O-C-N	5.16	127.61	122.97
1	A	386	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	A	530	PHE	O-C-N	5.16	127.39	122.03
1	A	378	THR	O-C-N	5.15	128.56	123.46
1	A	183	LEU	CB-CA-C	5.15	119.26	110.56
1	A	593	GLU	CA-CB-CG	5.14	124.39	114.10
1	A	796	GLU	CB-CA-C	5.14	120.87	110.38
1	A	23	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	251	ASP	CA-C-O	-5.13	113.78	119.67
1	A	184	ARG	CD-NE-CZ	5.12	131.57	124.40
1	A	308	ILE	N-CA-CB	-5.12	104.56	110.55
1	A	780	TYR	CA-C-N	5.12	127.01	120.56
1	A	780	TYR	C-N-CA	5.12	127.01	120.56
1	A	136	LEU	N-CA-CB	-5.12	102.59	110.01
1	A	639	ARG	CG-CD-NE	5.11	123.24	112.00
1	A	744	GLN	CB-CA-C	-5.10	100.88	110.67
1	A	681	PHE	O-C-N	5.08	128.52	122.27
1	A	236	ASN	CA-CB-CG	5.08	117.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	155	TYR	O-C-N	5.07	129.24	123.31
1	A	310	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	A	556	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	295	GLN	N-CA-CB	5.06	117.35	110.01
1	A	165	ILE	CB-CA-C	5.06	118.95	111.26
1	A	620	ILE	N-CA-CB	-5.05	104.90	110.51
1	A	265	ALA	CB-CA-C	-5.05	101.28	110.63
1	A	149	THR	CA-CB-OG1	-5.05	102.02	109.60
1	A	38	THR	O-C-N	5.05	127.97	122.11
1	A	171	CYS	CB-CA-C	5.05	118.83	109.70
1	A	225	PRO	N-CA-C	5.05	119.95	111.32
1	A	699	MET	N-CA-C	-5.04	105.48	110.97
1	A	192	ALA	CA-C-N	-5.04	117.25	122.89
1	A	192	ALA	C-N-CA	-5.04	117.25	122.89
1	A	744	GLN	N-CA-CB	5.03	118.08	110.28
1	A	39	LEU	CA-C-O	-5.03	113.07	119.31
1	A	253	ASN	CA-C-O	5.03	128.46	119.36
1	A	120	GLU	CG-CD-OE2	5.03	129.96	118.40
1	A	427	ARG	N-CA-C	5.03	116.76	111.28
1	A	285	PHE	O-C-N	5.02	129.14	123.42
1	A	262	TYR	CB-CA-C	-5.01	102.33	110.85
1	A	688	THR	N-CA-C	5.01	117.14	109.07
1	A	489	ARG	CD-NE-CZ	5.01	131.41	124.40
1	A	219	GLN	OE1-CD-NE2	5.01	127.61	122.60
1	A	599	VAL	CB-CA-C	5.01	116.30	110.89
1	A	723	GLN	CA-CB-CG	-5.00	104.09	114.10
1	A	169	LYS	CA-C-O	-5.00	115.46	121.11

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ARG	Sidechain
1	A	234	ARG	Sidechain
1	A	323	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	358	ARG	Sidechain
1	A	413	ARG	Sidechain
1	A	426	ARG	Sidechain
1	A	427	ARG	Sidechain
1	A	49	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	569	ARG	Sidechain
1	A	60	ARG	Sidechain
1	A	601	ARG	Sidechain
1	A	649	ARG	Sidechain
1	A	770	ARG	Sidechain
1	A	803	ARG	Sidechain
1	A	822	ARG	Sidechain
1	A	833	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6691	0	6616	712	1
2	A	15	0	7	1	0
3	A	691	0	0	56	0
All	All	7397	0	6623	712	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

All (712) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:MET:HE1	1:A:119:MET:CE	1.19	1.54
1:A:666:ILE:HG21	1:A:711:PHE:CZ	1.53	1.44
1:A:99:MET:CE	1:A:119:MET:HE1	1.49	1.42
1:A:320:ASP:HB3	1:A:321:PRO:CD	1.48	1.36
1:A:320:ASP:CB	1:A:321:PRO:HD3	1.55	1.36
1:A:584:ILE:HD11	1:A:741:ILE:CD1	1.61	1.31
1:A:322:VAL:HG11	1:A:325:ASN:CB	1.63	1.29
1:A:322:VAL:CG1	1:A:325:ASN:HB2	1.65	1.26
1:A:160:ARG:NH1	1:A:190:GLU:OE1	1.70	1.24
1:A:549:LEU:C	1:A:555:VAL:HG21	1.64	1.21
1:A:251:ASP:O	1:A:255:LYS:N	1.71	1.20
1:A:756:ASP:HB2	1:A:759:LYS:CE	1.71	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:CG2	1:A:711:PHE:HZ	1.56	1.19
1:A:99:MET:CE	1:A:119:MET:CE	2.14	1.17
1:A:666:ILE:CG2	1:A:711:PHE:CZ	2.29	1.16
1:A:474:LEU:HD13	1:A:474:LEU:O	1.48	1.14
1:A:160:ARG:HH12	1:A:190:GLU:CD	1.55	1.14
1:A:256:ASP:HB2	1:A:258:ASN:HB2	1.30	1.13
1:A:474:LEU:HD12	1:A:475:GLU:HG3	1.24	1.13
1:A:687:LEU:HD21	1:A:801:VAL:HG23	1.31	1.11
1:A:832:GLN:HG3	3:A:1038:HOH:O	1.49	1.10
1:A:404:TYR:HB3	3:A:1267:HOH:O	1.50	1.10
1:A:555:VAL:HG13	1:A:557:ILE:HG23	1.21	1.08
1:A:474:LEU:O	1:A:474:LEU:CD1	2.01	1.07
1:A:85:LEU:HG	1:A:335:ILE:HD13	1.38	1.06
1:A:687:LEU:HD21	1:A:801:VAL:CG2	1.85	1.06
1:A:99:MET:HE1	1:A:119:MET:HE2	1.32	1.05
1:A:723:GLN:HA	3:A:1375:HOH:O	1.54	1.05
1:A:536:LYS:HD2	1:A:539:GLN:HE21	1.18	1.04
1:A:584:ILE:CD1	1:A:741:ILE:HD13	1.88	1.04
1:A:198:LEU:HD21	1:A:305:GLN:CB	1.87	1.03
1:A:527:ASP:O	1:A:531:ILE:HD13	1.60	1.02
1:A:311:PHE:CE1	1:A:316:PHE:HE2	1.76	1.02
1:A:316:PHE:HD1	1:A:319:ARG:CB	1.72	1.02
1:A:316:PHE:CD1	1:A:319:ARG:HG3	1.94	1.02
1:A:518:LEU:O	1:A:521:LEU:HB2	1.60	1.02
1:A:555:VAL:CG1	1:A:557:ILE:HG23	1.91	1.01
1:A:198:LEU:HD21	1:A:305:GLN:HB2	1.44	1.00
1:A:778:GLU:HB3	3:A:1540:HOH:O	1.60	1.00
1:A:256:ASP:CB	1:A:258:ASN:HB2	1.92	0.99
1:A:251:ASP:O	1:A:254:LEU:C	2.05	0.99
1:A:325:ASN:HD22	1:A:326:PHE:H	1.12	0.98
1:A:106:ASN:OD1	3:A:1406:HOH:O	1.81	0.97
1:A:316:PHE:HD1	1:A:319:ARG:CG	1.76	0.97
1:A:99:MET:CE	1:A:108:CYS:CB	2.43	0.96
1:A:43:ARG:NH1	3:A:1002:HOH:O	1.94	0.96
1:A:316:PHE:HE1	1:A:319:ARG:NE	1.63	0.96
1:A:756:ASP:HB2	1:A:759:LYS:HE3	1.45	0.96
1:A:549:LEU:C	1:A:555:VAL:CG2	2.39	0.96
1:A:426:ARG:NH1	1:A:427:ARG:HG3	1.81	0.95
1:A:314:SER:HB3	3:A:1581:HOH:O	1.65	0.95
1:A:82:ILE:HD11	1:A:827:VAL:HG21	1.49	0.95
1:A:427:ARG:NH1	1:A:470:ASP:OD1	1.99	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:ASP:O	1:A:723:GLN:HG3	1.67	0.95
1:A:549:LEU:HB3	1:A:555:VAL:HG21	1.47	0.95
1:A:24:VAL:HG12	1:A:28:LYS:HE2	1.49	0.94
1:A:252:PHE:C	1:A:254:LEU:H	1.66	0.94
1:A:316:PHE:CE1	1:A:319:ARG:NE	2.36	0.94
1:A:426:ARG:HH12	1:A:427:ARG:CG	1.81	0.94
1:A:474:LEU:CD1	1:A:474:LEU:C	2.41	0.93
1:A:108:CYS:CB	1:A:119:MET:HE1	1.98	0.93
1:A:834:LEU:HD23	1:A:836:ALA:HB2	1.48	0.93
1:A:108:CYS:HB3	1:A:119:MET:CE	1.98	0.93
1:A:709:PHE:CZ	1:A:800:MET:HE1	2.04	0.93
1:A:150:LEU:HD12	1:A:817:ILE:HG22	1.52	0.92
1:A:536:LYS:HD2	1:A:539:GLN:NE2	1.83	0.92
1:A:593:GLU:OE2	1:A:596:LYS:HD2	1.69	0.92
1:A:678:ASN:HB3	1:A:679:MET:HG3	1.52	0.92
1:A:646:GLU:HG3	3:A:1127:HOH:O	1.68	0.92
1:A:666:ILE:HG23	1:A:691:THR:HG23	1.51	0.91
1:A:108:CYS:HB3	1:A:119:MET:HE1	1.50	0.91
1:A:584:ILE:HD11	1:A:741:ILE:HD13	0.93	0.90
1:A:421:ASP:O	1:A:425:LEU:HD13	1.70	0.90
1:A:361:TRP:CH2	1:A:406:ILE:HD13	2.05	0.90
1:A:316:PHE:CD1	1:A:319:ARG:CG	2.53	0.90
1:A:550:GLU:N	1:A:555:VAL:HG21	1.87	0.90
1:A:99:MET:HE2	1:A:108:CYS:HB2	1.54	0.90
1:A:198:LEU:HD23	1:A:305:GLN:CD	1.96	0.90
1:A:256:ASP:HB2	1:A:258:ASN:CB	2.01	0.90
1:A:779:GLU:HG2	3:A:1684:HOH:O	1.72	0.89
1:A:335:ILE:HD11	1:A:337:LEU:HD13	1.55	0.89
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.02	0.88
1:A:252:PHE:HA	1:A:255:LYS:HB2	1.54	0.87
1:A:271:LEU:O	1:A:274:ASN:HB2	1.74	0.87
1:A:435:ALA:O	1:A:436:VAL:HG23	1.75	0.87
1:A:304:LEU:O	1:A:308:ILE:HG12	1.73	0.86
1:A:311:PHE:CE1	1:A:316:PHE:CE2	2.63	0.86
1:A:211:GLN:O	3:A:1068:HOH:O	1.94	0.86
1:A:548:TYR:CD2	1:A:655:LYS:HE2	2.09	0.86
1:A:474:LEU:HD12	1:A:475:GLU:CG	2.05	0.86
1:A:551:ARG:HG3	1:A:552:GLU:H	1.41	0.85
1:A:790:LEU:O	1:A:790:LEU:CD1	2.24	0.85
1:A:316:PHE:HA	1:A:319:ARG:HB2	1.58	0.85
1:A:252:PHE:HA	1:A:255:LYS:CB	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:CG2	1:A:691:THR:HG23	2.05	0.85
1:A:790:LEU:O	1:A:790:LEU:HD13	1.75	0.85
1:A:455:VAL:H	1:A:459:HIS:HD2	1.24	0.85
1:A:546:ALA:HB2	1:A:557:ILE:HD11	1.58	0.85
1:A:752:PRO:HB2	1:A:753:LYS:HZ3	1.42	0.85
1:A:252:PHE:CA	1:A:255:LYS:HB2	2.08	0.84
1:A:80:LYS:HE2	1:A:825:TRP:O	1.78	0.84
1:A:752:PRO:HB2	1:A:753:LYS:NZ	1.92	0.84
1:A:759:LYS:O	1:A:763:ASN:ND2	2.10	0.83
1:A:549:LEU:HB3	1:A:555:VAL:CG2	2.06	0.83
1:A:474:LEU:HD12	1:A:474:LEU:C	2.04	0.83
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.61	0.82
1:A:584:ILE:HD13	1:A:585:THR:N	1.94	0.82
1:A:549:LEU:CB	1:A:555:VAL:HG21	2.09	0.82
1:A:311:PHE:CZ	1:A:316:PHE:CE2	2.68	0.82
1:A:102:LEU:HB3	1:A:104:LEU:HD22	1.62	0.82
1:A:426:ARG:HH12	1:A:427:ARG:HG3	1.38	0.81
1:A:756:ASP:HB2	1:A:759:LYS:CD	2.11	0.81
1:A:63:LEU:HD21	1:A:229:PRO:HG3	1.62	0.81
1:A:85:LEU:HG	1:A:335:ILE:CD1	2.10	0.81
1:A:555:VAL:HG12	1:A:556:HIS:H	1.45	0.81
1:A:160:ARG:NH1	1:A:190:GLU:CD	2.28	0.81
1:A:322:VAL:O	1:A:323:ARG:HG2	1.81	0.81
1:A:316:PHE:CD1	1:A:319:ARG:CB	2.64	0.80
1:A:423:ASP:HB3	3:A:1289:HOH:O	1.81	0.80
1:A:266:VAL:O	1:A:269:ARG:HG3	1.82	0.80
1:A:311:PHE:CZ	1:A:316:PHE:HE2	1.98	0.80
1:A:549:LEU:CA	1:A:555:VAL:HG21	2.11	0.80
1:A:743:GLU:O	1:A:747:SER:OG	1.99	0.80
1:A:584:ILE:CD1	1:A:741:ILE:CD1	2.55	0.80
1:A:111:ALA:O	1:A:115:LEU:HD13	1.82	0.80
1:A:361:TRP:CZ2	1:A:406:ILE:HD13	2.16	0.80
1:A:463:LEU:HD22	1:A:467:ILE:HD11	1.63	0.79
1:A:579:ASN:O	1:A:583:VAL:HG23	1.83	0.79
1:A:322:VAL:CG2	1:A:325:ASN:OD1	2.30	0.79
1:A:699:MET:HE2	1:A:708:PHE:HZ	1.48	0.79
1:A:159:ILE:CG1	1:A:299:VAL:HG23	2.13	0.79
1:A:474:LEU:O	1:A:474:LEU:HD12	1.83	0.78
1:A:742:ILE:HG21	1:A:766:MET:HE3	1.63	0.78
1:A:19:ALA:N	1:A:106:ASN:HB3	1.98	0.78
1:A:314:SER:C	1:A:316:PHE:H	1.89	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HG13	1:A:299:VAL:CG2	2.14	0.77
1:A:536:LYS:HE3	3:A:1321:HOH:O	1.82	0.77
1:A:661:ASP:O	1:A:797:TRP:HH2	1.66	0.77
1:A:316:PHE:CA	1:A:319:ARG:HB2	2.15	0.77
1:A:147:MET:HE2	1:A:825:TRP:CH2	2.19	0.77
1:A:236:ASN:ND2	1:A:834:LEU:O	2.12	0.77
1:A:322:VAL:HG21	1:A:325:ASN:OD1	1.84	0.77
1:A:402:ILE:O	1:A:406:ILE:HG12	1.85	0.77
1:A:75:TYR:HE1	3:A:1557:HOH:O	1.67	0.76
1:A:99:MET:CE	1:A:108:CYS:HB2	2.11	0.76
1:A:716:GLU:HA	3:A:1527:HOH:O	1.85	0.76
1:A:177:GLU:OE1	1:A:611:PRO:HG3	1.85	0.76
1:A:248:ALA:HB1	1:A:253:ASN:OD1	1.86	0.76
1:A:630:VAL:HG11	1:A:640:LEU:HD13	1.68	0.75
1:A:251:ASP:HB2	1:A:255:LYS:HG3	1.68	0.75
1:A:555:VAL:HG13	1:A:557:ILE:CG2	2.12	0.75
1:A:666:ILE:HG21	1:A:711:PHE:HZ	0.66	0.75
1:A:208:HIS:O	1:A:209:THR:OG1	2.05	0.74
1:A:340:THR:HG23	1:A:374:TYR:HE1	1.50	0.74
1:A:528:GLU:O	1:A:532:ARG:HG3	1.87	0.74
1:A:304:LEU:HD12	1:A:307:ILE:HD12	1.69	0.74
1:A:426:ARG:NH1	1:A:427:ARG:CG	2.46	0.74
1:A:380:ILE:O	1:A:384:LEU:HD12	1.87	0.74
1:A:198:LEU:CD2	1:A:305:GLN:CD	2.61	0.74
1:A:756:ASP:HB2	1:A:759:LYS:HE2	1.67	0.74
1:A:288:GLY:C	1:A:289:LYS:HD2	2.13	0.74
1:A:322:VAL:O	1:A:323:ARG:CG	2.35	0.73
1:A:549:LEU:HD23	1:A:557:ILE:HG21	1.70	0.73
1:A:322:VAL:HG11	1:A:325:ASN:HB2	0.78	0.73
1:A:43:ARG:HD3	3:A:1412:HOH:O	1.89	0.73
1:A:340:THR:HG23	1:A:374:TYR:CE1	2.23	0.73
1:A:729:GLN:O	1:A:733:ASP:HB2	1.88	0.73
1:A:756:ASP:HA	1:A:759:LYS:HG3	1.70	0.73
1:A:55:LEU:HD11	1:A:119:MET:HE3	1.71	0.73
1:A:160:ARG:NH1	1:A:190:GLU:OE2	2.16	0.73
1:A:522:LEU:O	1:A:525:VAL:HG22	1.87	0.73
1:A:737:GLU:O	1:A:740:GLN:HG2	1.89	0.73
1:A:486:ILE:HD11	1:A:680:LYS:HE3	1.71	0.72
1:A:546:ALA:CB	1:A:557:ILE:HD11	2.18	0.72
1:A:589:ARG:NH2	1:A:737:GLU:OE1	2.22	0.72
1:A:834:LEU:HD23	1:A:836:ALA:CB	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:MET:HE2	1:A:710:ILE:HD13	1.70	0.72
1:A:486:ILE:CD1	1:A:676:THR:HB	2.18	0.72
1:A:763:ASN:N	1:A:763:ASN:HD22	1.87	0.72
1:A:380:ILE:CG2	1:A:382:GLU:CD	2.61	0.72
1:A:99:MET:HE2	1:A:108:CYS:CB	2.12	0.72
1:A:499:LEU:HD12	1:A:502:ILE:HD11	1.71	0.72
1:A:633:ASP:OD1	1:A:635:VAL:HG23	1.89	0.72
1:A:198:LEU:HD21	1:A:305:GLN:HB3	1.70	0.71
1:A:498:GLY:O	1:A:501:GLU:HB3	1.90	0.71
1:A:19:ALA:HB1	3:A:1206:HOH:O	1.89	0.71
1:A:76:GLU:HA	1:A:315:LYS:NZ	2.05	0.71
1:A:208:HIS:C	1:A:209:THR:OG1	2.34	0.71
1:A:380:ILE:HG23	1:A:382:GLU:CD	2.16	0.71
1:A:21:VAL:HG23	3:A:1592:HOH:O	1.91	0.71
1:A:665:GLN:NE2	3:A:1400:HOH:O	2.22	0.71
1:A:108:CYS:HB2	1:A:119:MET:HE1	1.72	0.71
1:A:270:ASN:O	1:A:271:LEU:C	2.33	0.71
1:A:31:PHE:CD2	1:A:115:LEU:HD21	2.26	0.71
1:A:30:ASN:HB3	1:A:58:THR:HG23	1.73	0.70
1:A:82:ILE:HD13	1:A:825:TRP:CE3	2.25	0.70
1:A:325:ASN:HD22	1:A:326:PHE:N	1.86	0.70
1:A:630:VAL:HG11	1:A:640:LEU:CD1	2.22	0.70
1:A:549:LEU:HB3	1:A:555:VAL:CG1	2.22	0.70
1:A:198:LEU:HD23	1:A:305:GLN:NE2	2.06	0.70
1:A:335:ILE:HD11	1:A:337:LEU:CD1	2.22	0.70
1:A:687:LEU:CD2	1:A:801:VAL:CG2	2.69	0.70
1:A:75:TYR:O	1:A:315:LYS:HE3	1.92	0.69
1:A:193:ARG:HD3	1:A:196:PHE:HE2	1.57	0.69
1:A:604:MET:HB3	1:A:645:LEU:HD22	1.73	0.69
1:A:661:ASP:O	1:A:797:TRP:CH2	2.45	0.69
1:A:828:GLU:CD	3:A:1405:HOH:O	2.35	0.69
1:A:709:PHE:HZ	1:A:800:MET:HE1	1.55	0.69
1:A:752:PRO:CB	1:A:753:LYS:HZ3	2.04	0.69
1:A:460:SER:O	1:A:464:LYS:HG3	1.91	0.69
1:A:551:ARG:CG	1:A:552:GLU:H	2.05	0.69
1:A:709:PHE:CE2	1:A:800:MET:HE1	2.26	0.69
1:A:250:ASN:HA	1:A:269:ARG:NH2	2.08	0.69
1:A:198:LEU:CD2	1:A:305:GLN:HB2	2.19	0.69
1:A:43:ARG:HB2	3:A:1412:HOH:O	1.91	0.69
1:A:63:LEU:HD21	1:A:229:PRO:CG	2.23	0.68
1:A:426:ARG:HH12	1:A:427:ARG:HG2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLU:O	1:A:734:ARG:HG3	1.92	0.68
1:A:687:LEU:HD21	1:A:801:VAL:HG22	1.73	0.68
1:A:744:GLN:HB3	1:A:749:PHE:HB3	1.73	0.68
1:A:252:PHE:N	1:A:255:LYS:HB2	2.09	0.68
1:A:252:PHE:C	1:A:254:LEU:N	2.45	0.68
1:A:99:MET:HE1	1:A:119:MET:HE1	0.68	0.68
1:A:466:THR:HA	1:A:469:LYS:HD3	1.75	0.68
1:A:519:ARG:C	1:A:521:LEU:H	2.01	0.67
1:A:118:ASP:HB3	1:A:121:GLU:HG3	1.75	0.67
1:A:584:ILE:HD13	1:A:585:THR:H	1.56	0.67
1:A:251:ASP:O	1:A:255:LYS:CA	2.42	0.67
1:A:538:LYS:NZ	1:A:684:ASN:O	2.28	0.67
1:A:108:CYS:HB3	1:A:119:MET:HE3	1.74	0.67
1:A:289:LYS:HD2	1:A:289:LYS:N	2.08	0.67
1:A:85:LEU:CG	1:A:335:ILE:HD13	2.22	0.67
1:A:513:SER:O	1:A:514:ASP:HB2	1.94	0.67
1:A:790:LEU:HD12	1:A:797:TRP:CD1	2.30	0.67
1:A:665:GLN:NE2	1:A:678:ASN:HA	2.09	0.66
1:A:763:ASN:HB3	3:A:1083:HOH:O	1.95	0.66
1:A:633:ASP:HB3	1:A:636:VAL:HG23	1.77	0.66
1:A:152:LEU:HD11	1:A:829:PRO:HA	1.77	0.66
1:A:504:ALA:O	1:A:508:GLY:N	2.27	0.66
1:A:256:ASP:HB2	1:A:258:ASN:CG	2.20	0.66
1:A:426:ARG:HG3	1:A:427:ARG:N	2.11	0.65
1:A:31:PHE:CD2	1:A:115:LEU:CD2	2.79	0.65
1:A:475:GLU:HB3	1:A:477:HIS:CE1	2.31	0.65
1:A:519:ARG:C	1:A:521:LEU:N	2.53	0.65
1:A:250:ASN:HA	1:A:269:ARG:HH22	1.60	0.65
1:A:361:TRP:HH2	1:A:406:ILE:HD13	1.59	0.65
1:A:466:THR:O	1:A:469:LYS:HD3	1.96	0.65
1:A:591:LYS:NZ	3:A:1100:HOH:O	2.29	0.65
1:A:581:LEU:O	1:A:584:ILE:CD1	2.43	0.65
1:A:404:TYR:CB	3:A:1267:HOH:O	2.23	0.65
1:A:761:ILE:HG22	1:A:765:LEU:CD2	2.26	0.65
1:A:742:ILE:CG2	1:A:766:MET:HE3	2.27	0.65
1:A:351:ARG:O	1:A:355:ASP:HB2	1.97	0.65
1:A:549:LEU:HB3	1:A:555:VAL:HG11	1.77	0.65
1:A:790:LEU:HD11	1:A:797:TRP:N	2.12	0.65
1:A:834:LEU:CD2	1:A:836:ALA:HB2	2.26	0.65
1:A:438:ARG:HG2	1:A:438:ARG:HH11	1.62	0.64
1:A:43:ARG:O	1:A:43:ARG:HG3	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HD11	1:A:119:MET:CE	2.27	0.64
1:A:113:TYR:O	1:A:116:GLY:HA2	1.96	0.64
1:A:753:LYS:HB2	1:A:754:GLN:HE21	1.63	0.64
1:A:538:LYS:O	1:A:538:LYS:HG3	1.98	0.64
1:A:582:HIS:HB2	1:A:780:TYR:HE2	1.61	0.64
1:A:167:ASN:ND2	1:A:180:ASP:HA	2.12	0.64
1:A:316:PHE:HD1	1:A:319:ARG:HB2	1.62	0.64
1:A:657:ILE:HG23	1:A:681:PHE:CD1	2.32	0.64
1:A:569:ARG:O	1:A:574:LYS:HE2	1.98	0.64
1:A:99:MET:HE3	1:A:108:CYS:SG	2.38	0.64
1:A:525:VAL:O	1:A:531:ILE:HD11	1.97	0.64
1:A:552:GLU:O	3:A:1326:HOH:O	2.15	0.64
1:A:251:ASP:C	1:A:255:LYS:HB2	2.22	0.64
1:A:548:TYR:CD1	1:A:548:TYR:C	2.75	0.64
1:A:687:LEU:HD23	1:A:797:TRP:CZ3	2.33	0.63
1:A:159:ILE:HG13	1:A:299:VAL:HG23	1.75	0.63
1:A:102:LEU:HB3	1:A:104:LEU:CD2	2.27	0.63
1:A:101:ASN:ND2	1:A:233:TYR:HA	2.14	0.63
1:A:758:PHE:C	1:A:760:ASP:H	2.06	0.63
1:A:810:LYS:O	1:A:810:LYS:HG3	1.97	0.63
1:A:99:MET:CE	1:A:108:CYS:HB3	2.27	0.62
1:A:113:TYR:O	1:A:116:GLY:N	2.30	0.62
1:A:335:ILE:HD12	1:A:336:GLN:N	2.14	0.62
1:A:551:ARG:HG3	1:A:552:GLU:N	2.15	0.62
1:A:253:ASN:O	1:A:254:LEU:HB3	1.98	0.62
1:A:316:PHE:C	1:A:318:CYS:N	2.57	0.62
1:A:631:ASN:O	1:A:632:HIS:CD2	2.52	0.62
1:A:527:ASP:O	1:A:531:ILE:CD1	2.44	0.61
1:A:582:HIS:HB2	1:A:780:TYR:CE2	2.34	0.61
1:A:76:GLU:HA	1:A:315:LYS:HZ2	1.65	0.61
1:A:803:ARG:O	1:A:807:THR:HB	2.00	0.61
1:A:436:VAL:O	1:A:438:ARG:HD2	1.99	0.61
1:A:170:ILE:HD11	1:A:644:PHE:CE1	2.35	0.61
1:A:790:LEU:O	1:A:790:LEU:HD12	2.00	0.61
1:A:455:VAL:H	1:A:459:HIS:CD2	2.12	0.61
1:A:756:ASP:CB	1:A:759:LYS:CE	2.64	0.61
1:A:101:ASN:HD22	1:A:232:GLY:C	2.09	0.61
1:A:753:LYS:CG	1:A:754:GLN:H	2.14	0.61
1:A:395:LEU:C	1:A:396:LEU:HG	2.26	0.61
1:A:423:ASP:O	1:A:426:ARG:HG2	2.00	0.61
1:A:555:VAL:HG12	1:A:556:HIS:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:GLU:N	1:A:555:VAL:CG2	2.61	0.61
1:A:756:ASP:CB	1:A:759:LYS:HE3	2.26	0.60
1:A:99:MET:CE	1:A:108:CYS:SG	2.89	0.60
1:A:687:LEU:CD2	1:A:801:VAL:HG22	2.30	0.60
1:A:766:MET:HE2	1:A:774:PHE:HZ	1.66	0.60
1:A:746:SER:HB3	3:A:1534:HOH:O	2.01	0.60
1:A:24:VAL:O	1:A:28:LYS:HG3	2.01	0.60
1:A:208:HIS:C	1:A:209:THR:HG1	2.04	0.60
1:A:81:ARG:NH2	3:A:1581:HOH:O	2.34	0.60
1:A:110:GLU:O	1:A:113:TYR:N	2.35	0.60
1:A:252:PHE:C	1:A:255:LYS:H	2.09	0.60
1:A:325:ASN:ND2	1:A:326:PHE:H	1.92	0.60
1:A:542:LYS:HE3	1:A:661:ASP:OD2	2.01	0.60
1:A:703:ALA:CB	1:A:807:THR:HG21	2.32	0.60
1:A:426:ARG:NH1	3:A:1289:HOH:O	2.34	0.60
1:A:797:TRP:HZ3	3:A:1662:HOH:O	1.83	0.60
1:A:72:GLN:NE2	1:A:76:GLU:OE1	2.35	0.60
1:A:322:VAL:CG1	1:A:325:ASN:CB	2.47	0.60
1:A:790:LEU:HD12	1:A:797:TRP:HD1	1.67	0.59
1:A:327:ASP:HA	1:A:363:LYS:HZ1	1.67	0.59
1:A:251:ASP:CG	1:A:255:LYS:HZ1	2.10	0.59
1:A:356:LEU:N	1:A:356:LEU:HD12	2.17	0.59
1:A:102:LEU:O	1:A:103:ALA:HB3	2.03	0.59
1:A:803:ARG:NH1	1:A:803:ARG:HG3	2.15	0.59
1:A:667:SER:HB3	1:A:693:ASP:OD2	2.02	0.59
1:A:764:MET:HE1	1:A:769:ASP:HA	1.85	0.59
1:A:147:MET:HE2	1:A:825:TRP:HH2	1.67	0.59
1:A:463:LEU:HD22	1:A:467:ILE:CD1	2.31	0.59
1:A:705:GLU:HG2	1:A:710:ILE:HD12	1.84	0.59
1:A:75:TYR:CE1	3:A:1557:HOH:O	2.48	0.58
1:A:327:ASP:HA	1:A:363:LYS:NZ	2.18	0.58
1:A:99:MET:CE	1:A:119:MET:HE2	2.08	0.58
1:A:169:LYS:HG3	1:A:170:ILE:N	2.17	0.58
1:A:716:GLU:HB2	3:A:1114:HOH:O	2.03	0.58
1:A:72:GLN:O	1:A:75:TYR:HB3	2.03	0.58
1:A:629:VAL:HG23	3:A:1536:HOH:O	2.03	0.58
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.85	0.58
1:A:327:ASP:CA	1:A:363:LYS:HZ1	2.14	0.58
1:A:758:PHE:C	1:A:760:ASP:N	2.61	0.58
1:A:105:GLU:HB3	3:A:1428:HOH:O	2.04	0.58
1:A:536:LYS:HE2	3:A:1320:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:TYR:CE2	1:A:655:LYS:HE2	2.39	0.58
1:A:314:SER:C	1:A:316:PHE:N	2.61	0.58
1:A:47:THR:N	1:A:50:ASP:OD2	2.29	0.58
1:A:60:ARG:O	1:A:63:LEU:HB3	2.04	0.58
1:A:235:ASN:HD22	1:A:235:ASN:H	1.52	0.57
1:A:753:LYS:HG2	1:A:754:GLN:H	1.68	0.57
1:A:175:GLN:HG2	1:A:177:GLU:OE2	2.04	0.57
1:A:198:LEU:CD2	1:A:305:GLN:CB	2.74	0.57
1:A:555:VAL:CG1	1:A:556:HIS:H	2.06	0.57
1:A:664:GLU:OE1	1:A:666:ILE:CD1	2.51	0.57
1:A:752:PRO:CG	1:A:753:LYS:HZ3	2.17	0.57
1:A:322:VAL:HG22	1:A:323:ARG:HG3	1.86	0.57
1:A:41:LYS:HE3	3:A:1576:HOH:O	2.04	0.57
1:A:466:THR:O	1:A:469:LYS:CD	2.52	0.57
1:A:752:PRO:O	1:A:755:PRO:HD3	2.04	0.57
1:A:536:LYS:CE	3:A:1321:HOH:O	2.46	0.57
1:A:42:ASP:H	1:A:45:VAL:HG13	1.70	0.57
1:A:80:LYS:CE	1:A:825:TRP:O	2.49	0.57
1:A:205:ARG:HH21	1:A:216:VAL:HG21	1.69	0.57
1:A:763:ASN:CB	3:A:1083:HOH:O	2.52	0.57
1:A:150:LEU:CD1	1:A:817:ILE:HG22	2.32	0.57
1:A:380:ILE:HG23	1:A:382:GLU:OE2	2.05	0.57
1:A:476:PRO:HB3	3:A:1203:HOH:O	2.04	0.57
1:A:474:LEU:CD1	1:A:475:GLU:HG3	2.16	0.56
1:A:274:ASN:HA	1:A:277:ARG:HH11	1.70	0.56
1:A:327:ASP:CB	1:A:363:LYS:HZ1	2.16	0.56
1:A:761:ILE:HG22	1:A:765:LEU:HD22	1.85	0.56
1:A:280:TYR:OH	1:A:291:LEU:HB3	2.06	0.56
1:A:171:CYS:N	1:A:174:TRP:O	2.33	0.56
1:A:111:ALA:O	1:A:115:LEU:CD1	2.52	0.56
1:A:337:LEU:HD22	1:A:373:ALA:O	2.05	0.56
1:A:581:LEU:O	1:A:584:ILE:HD13	2.05	0.56
1:A:590:ILE:HD13	1:A:636:VAL:HG13	1.87	0.56
1:A:678:ASN:OD1	1:A:695:ALA:HB3	2.05	0.56
1:A:159:ILE:HG12	1:A:299:VAL:HG23	1.87	0.56
1:A:687:LEU:N	1:A:687:LEU:HD22	2.20	0.56
1:A:538:LYS:HE2	1:A:660:ALA:O	2.06	0.56
1:A:703:ALA:HB2	1:A:807:THR:HG21	1.88	0.56
1:A:705:GLU:HG2	1:A:710:ILE:CD1	2.36	0.56
1:A:113:TYR:O	1:A:116:GLY:CA	2.53	0.56
1:A:538:LYS:CE	1:A:660:ALA:O	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HG22	1:A:691:THR:HG23	1.88	0.56
1:A:837:PRO:HG2	1:A:838:ASP:H	1.70	0.56
1:A:666:ILE:CG2	1:A:711:PHE:CE1	2.87	0.55
1:A:756:ASP:CA	1:A:759:LYS:HG3	2.36	0.55
1:A:349:LEU:HD12	1:A:353:LEU:HG	1.86	0.55
1:A:256:ASP:CA	1:A:258:ASN:HB2	2.37	0.55
1:A:251:ASP:OD1	1:A:252:PHE:N	2.40	0.55
1:A:65:GLY:HA3	1:A:838:ASP:OD1	2.05	0.55
1:A:343:SER:OG	1:A:441:MET:HG3	2.07	0.55
1:A:713:MET:HB2	1:A:717:ASP:HB2	1.88	0.55
1:A:252:PHE:CE2	1:A:255:LYS:HE2	2.41	0.55
1:A:340:THR:CG2	1:A:374:TYR:CE1	2.89	0.55
1:A:343:SER:HB3	1:A:445:CYS:SG	2.47	0.55
1:A:790:LEU:HD11	1:A:796:GLU:C	2.32	0.54
1:A:532:ARG:O	1:A:536:LYS:HB2	2.08	0.54
1:A:183:LEU:HD23	1:A:187:ASN:HB2	1.89	0.54
1:A:252:PHE:CA	1:A:255:LYS:H	2.20	0.54
1:A:754:GLN:HB3	1:A:757:LEU:HB2	1.90	0.54
1:A:150:LEU:O	1:A:152:LEU:CD1	2.55	0.54
1:A:571:HIS:HB2	1:A:574:LYS:HD2	1.89	0.54
1:A:41:LYS:CE	3:A:1576:HOH:O	2.55	0.54
1:A:557:ILE:HG13	1:A:557:ILE:O	2.07	0.54
1:A:322:VAL:C	1:A:323:ARG:CG	2.80	0.54
1:A:22:GLU:O	1:A:25:THR:N	2.41	0.54
1:A:565:VAL:HG21	1:A:660:ALA:HB2	1.90	0.54
1:A:571:HIS:HB2	1:A:574:LYS:CD	2.37	0.54
1:A:790:LEU:CD1	1:A:790:LEU:C	2.80	0.54
1:A:36:HIS:HB2	3:A:1000:HOH:O	2.08	0.53
1:A:42:ASP:H	1:A:45:VAL:CG1	2.21	0.53
1:A:487:THR:HG23	1:A:487:THR:O	2.08	0.53
1:A:703:ALA:HA	1:A:807:THR:HG21	1.91	0.53
1:A:205:ARG:HE	1:A:216:VAL:HG23	1.72	0.53
1:A:314:SER:O	1:A:316:PHE:N	2.41	0.53
1:A:519:ARG:O	1:A:521:LEU:N	2.41	0.53
1:A:76:GLU:HA	1:A:315:LYS:CE	2.37	0.53
1:A:147:MET:CE	1:A:825:TRP:HH2	2.21	0.53
1:A:666:ILE:HG23	1:A:711:PHE:CZ	2.37	0.53
1:A:676:THR:CA	1:A:678:ASN:HB2	2.39	0.53
1:A:113:TYR:C	1:A:113:TYR:CD1	2.86	0.53
1:A:528:GLU:OE1	1:A:532:ARG:NH2	2.37	0.53
1:A:584:ILE:HG13	1:A:741:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ALA:CA	1:A:807:THR:HG21	2.39	0.53
1:A:55:LEU:CD2	1:A:59:VAL:HG23	2.39	0.53
1:A:322:VAL:HG22	1:A:325:ASN:OD1	2.07	0.53
1:A:235:ASN:H	1:A:235:ASN:ND2	2.07	0.53
1:A:400:LEU:HD13	1:A:404:TYR:CE2	2.44	0.53
1:A:810:LYS:O	1:A:810:LYS:CG	2.56	0.53
1:A:263:ILE:O	1:A:267:LEU:HG	2.09	0.52
1:A:753:LYS:HG3	1:A:754:GLN:NE2	2.24	0.52
1:A:197:THR:CG2	1:A:222:LEU:HB3	2.40	0.52
1:A:763:ASN:HD22	1:A:763:ASN:H	1.58	0.52
1:A:347:PRO:HB3	1:A:402:ILE:HG22	1.91	0.52
1:A:486:ILE:HD12	1:A:676:THR:HB	1.90	0.52
1:A:306:ASP:HA	1:A:309:ARG:HD3	1.90	0.52
1:A:685:GLY:HA2	3:A:1667:HOH:O	2.09	0.52
1:A:387:TRP:HD1	1:A:441:MET:SD	2.33	0.52
1:A:549:LEU:HD23	1:A:557:ILE:HD13	1.92	0.52
1:A:689:ILE:CD1	1:A:784:GLN:HG2	2.40	0.52
1:A:259:VAL:HG22	1:A:260:GLY:H	1.75	0.52
1:A:427:ARG:NH1	1:A:470:ASP:CG	2.67	0.51
1:A:316:PHE:CE1	1:A:319:ARG:CD	2.93	0.51
1:A:380:ILE:CG2	1:A:382:GLU:OE1	2.59	0.51
1:A:252:PHE:HA	1:A:255:LYS:H	1.75	0.51
1:A:577:LEU:O	1:A:580:CYS:HB2	2.09	0.51
1:A:483:THR:O	1:A:815:ARG:NH2	2.43	0.51
1:A:658:PRO:HA	1:A:684:ASN:HB3	1.91	0.51
1:A:664:GLU:HB3	1:A:666:ILE:HD12	1.92	0.51
1:A:455:VAL:N	1:A:459:HIS:HD2	2.02	0.51
1:A:76:GLU:HA	1:A:315:LYS:HE3	1.93	0.51
1:A:198:LEU:CD2	1:A:305:GLN:NE2	2.72	0.51
1:A:311:PHE:CZ	1:A:325:ASN:O	2.63	0.51
1:A:31:PHE:CE2	1:A:115:LEU:HD23	2.45	0.50
1:A:472:TYR:O	1:A:476:PRO:HG3	2.11	0.50
1:A:590:ILE:HG22	1:A:591:LYS:N	2.25	0.50
1:A:557:ILE:HD12	1:A:563:PHE:CZ	2.45	0.50
1:A:753:LYS:HB2	1:A:754:GLN:NE2	2.27	0.50
1:A:721:LEU:HA	1:A:724:ARG:HG3	1.92	0.50
1:A:738:LEU:O	1:A:742:ILE:HG12	2.12	0.50
1:A:616:ALA:O	1:A:620:ILE:HG12	2.11	0.50
1:A:73:HIS:O	1:A:77:LYS:HB2	2.11	0.50
1:A:382:GLU:OE2	1:A:770:ARG:NH1	2.39	0.50
1:A:321:PRO:O	1:A:322:VAL:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:MET:HE1	1:A:108:CYS:HB3	1.92	0.50
1:A:386:ARG:HA	1:A:439:ILE:O	2.12	0.50
1:A:810:LYS:O	1:A:815:ARG:HD2	2.12	0.50
1:A:384:LEU:HD23	3:A:1260:HOH:O	2.11	0.49
1:A:322:VAL:HG11	1:A:325:ASN:CG	2.32	0.49
1:A:322:VAL:C	1:A:323:ARG:HG3	2.37	0.49
1:A:503:ILE:HG12	1:A:521:LEU:HD21	1.94	0.49
1:A:584:ILE:HG12	1:A:741:ILE:HG12	1.94	0.49
1:A:191:LYS:HE3	1:A:193:ARG:NH2	2.28	0.49
1:A:363:LYS:HD2	1:A:363:LYS:C	2.37	0.49
1:A:402:ILE:O	1:A:405:GLU:HB2	2.13	0.49
1:A:70:THR:O	1:A:73:HIS:HB3	2.13	0.49
1:A:227:ASP:HB3	1:A:240:THR:HG23	1.94	0.49
1:A:666:ILE:HD13	1:A:780:TYR:CE1	2.47	0.49
1:A:198:LEU:HD23	1:A:305:GLN:OE1	2.13	0.49
1:A:589:ARG:HH21	1:A:737:GLU:CD	2.20	0.49
1:A:337:LEU:CD2	1:A:373:ALA:O	2.61	0.49
1:A:699:MET:HE2	1:A:708:PHE:CZ	2.38	0.49
1:A:742:ILE:HG21	1:A:766:MET:CE	2.38	0.49
1:A:748:GLY:O	1:A:749:PHE:C	2.56	0.49
1:A:304:LEU:CD1	1:A:307:ILE:HD12	2.39	0.48
1:A:667:SER:OG	1:A:672:GLU:HB2	2.13	0.48
1:A:744:GLN:NE2	1:A:750:PHE:CZ	2.81	0.48
1:A:492:LEU:O	1:A:496:ASN:N	2.40	0.48
1:A:316:PHE:CD1	1:A:319:ARG:HB3	2.47	0.48
1:A:417:ALA:C	1:A:419:PRO:HD3	2.38	0.48
1:A:287:GLU:OE1	1:A:289:LYS:HG2	2.13	0.48
1:A:322:VAL:O	1:A:323:ARG:HG3	2.13	0.48
1:A:93:ARG:NE	1:A:126:GLU:O	2.46	0.48
1:A:550:GLU:O	1:A:551:ARG:C	2.54	0.48
1:A:408:GLN:OE1	3:A:1191:HOH:O	2.20	0.48
1:A:703:ALA:HB2	1:A:807:THR:CG2	2.43	0.48
1:A:793:ASN:HD21	1:A:796:GLU:HG3	1.78	0.48
1:A:320:ASP:CB	1:A:321:PRO:CD	2.37	0.48
1:A:764:MET:C	1:A:764:MET:SD	2.97	0.48
1:A:790:LEU:HD12	1:A:797:TRP:CB	2.44	0.48
1:A:311:PHE:HZ	1:A:325:ASN:O	1.96	0.48
1:A:661:ASP:C	1:A:797:TRP:HH2	2.20	0.48
1:A:692:MET:CE	1:A:710:ILE:HD13	2.41	0.48
1:A:99:MET:HE3	1:A:108:CYS:CB	2.41	0.47
1:A:709:PHE:CE2	1:A:800:MET:CE	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ARG:HD3	3:A:1469:HOH:O	2.13	0.47
1:A:131:LEU:HG	1:A:161:TYR:HD2	1.79	0.47
1:A:311:PHE:CE1	1:A:332:LYS:HD2	2.49	0.47
1:A:463:LEU:HD23	1:A:467:ILE:HD11	1.92	0.47
1:A:466:THR:O	1:A:469:LYS:CG	2.62	0.47
1:A:568:LYS:O	1:A:607:GLY:HA3	2.14	0.47
1:A:441:MET:HG2	3:A:1471:HOH:O	2.13	0.47
1:A:715:VAL:HG23	1:A:716:GLU:N	2.30	0.47
1:A:315:LYS:N	1:A:315:LYS:CD	2.76	0.47
1:A:316:PHE:C	1:A:318:CYS:H	2.21	0.47
1:A:387:TRP:HA	1:A:388:PRO:HD3	1.85	0.47
1:A:795:ARG:HE	1:A:795:ARG:HB3	1.21	0.47
1:A:46:ALA:HA	1:A:50:ASP:OD2	2.14	0.47
1:A:75:TYR:CE2	1:A:315:LYS:HE2	2.50	0.47
1:A:422:VAL:HG13	3:A:1643:HOH:O	2.13	0.47
1:A:631:ASN:C	1:A:632:HIS:CD2	2.93	0.47
1:A:678:ASN:HB3	1:A:679:MET:H	1.26	0.47
1:A:316:PHE:HA	1:A:319:ARG:CB	2.39	0.47
1:A:347:PRO:HB3	1:A:402:ILE:CG2	2.45	0.47
1:A:551:ARG:CG	1:A:552:GLU:N	2.73	0.47
1:A:688:THR:HB	1:A:708:PHE:CE2	2.50	0.47
1:A:44:ASN:ND2	3:A:1001:HOH:O	2.47	0.47
1:A:147:MET:CE	1:A:825:TRP:CH2	2.93	0.47
1:A:315:LYS:H	1:A:315:LYS:HD3	1.79	0.47
1:A:557:ILE:O	1:A:559:PRO:HD3	2.15	0.47
1:A:177:GLU:OE1	1:A:611:PRO:CG	2.60	0.47
1:A:113:TYR:O	1:A:113:TYR:HD1	1.98	0.46
1:A:193:ARG:HD3	1:A:196:PHE:CE2	2.43	0.46
1:A:424:ARG:NH2	1:A:473:GLU:OE1	2.48	0.46
1:A:113:TYR:C	1:A:113:TYR:HD1	2.23	0.46
1:A:119:MET:O	1:A:120:GLU:C	2.59	0.46
1:A:251:ASP:OD2	1:A:255:LYS:NZ	2.36	0.46
1:A:315:LYS:N	1:A:315:LYS:HD3	2.31	0.46
1:A:399:HIS:O	1:A:403:ILE:HG13	2.16	0.46
1:A:803:ARG:NH1	1:A:803:ARG:CG	2.74	0.46
1:A:101:ASN:ND2	1:A:233:TYR:CA	2.79	0.46
1:A:177:GLU:H	1:A:177:GLU:HG2	1.52	0.46
1:A:355:ASP:C	1:A:356:LEU:HD12	2.39	0.46
1:A:356:LEU:N	1:A:356:LEU:CD1	2.78	0.46
1:A:640:LEU:O	1:A:641:ARG:HD2	2.16	0.46
1:A:697:VAL:O	1:A:701:GLU:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:GLN:O	1:A:729:GLN:HG3	2.15	0.46
1:A:160:ARG:HH11	1:A:160:ARG:HD2	1.42	0.46
1:A:93:ARG:NH1	3:A:1014:HOH:O	2.41	0.46
1:A:159:ILE:HG13	1:A:299:VAL:HG21	1.96	0.46
1:A:257:PHE:HD1	1:A:257:PHE:HA	1.65	0.46
1:A:290:GLU:O	1:A:294:LYS:HG3	2.16	0.46
1:A:584:ILE:CG1	1:A:741:ILE:HG12	2.46	0.46
1:A:771:PHE:O	1:A:772:LYS:HB2	2.15	0.46
1:A:167:ASN:HD22	1:A:180:ASP:HA	1.79	0.46
1:A:252:PHE:CE2	1:A:255:LYS:CE	2.98	0.46
1:A:251:ASP:CG	1:A:255:LYS:NZ	2.73	0.46
1:A:316:PHE:CD1	1:A:319:ARG:HB2	2.44	0.46
1:A:335:ILE:HD12	1:A:335:ILE:C	2.41	0.46
1:A:455:VAL:O	1:A:483:THR:HA	2.16	0.46
1:A:764:MET:HE1	3:A:1654:HOH:O	2.15	0.46
1:A:483:THR:HB	1:A:815:ARG:NH2	2.31	0.45
1:A:502:ILE:HG21	1:A:533:ASP:HB3	1.98	0.45
1:A:756:ASP:CB	1:A:759:LYS:HE2	2.41	0.45
1:A:28:LYS:O	1:A:32:ASN:ND2	2.49	0.45
1:A:309:ARG:HG2	3:A:1253:HOH:O	2.15	0.45
1:A:47:THR:OG1	1:A:50:ASP:OD2	2.34	0.45
1:A:118:ASP:CB	1:A:121:GLU:HG3	2.43	0.45
1:A:273:GLU:C	1:A:277:ARG:NH1	2.74	0.45
1:A:407:ASN:O	1:A:408:GLN:C	2.60	0.45
1:A:676:THR:C	1:A:678:ASN:HB2	2.42	0.45
1:A:103:ALA:HB2	1:A:234:ARG:NE	2.32	0.45
1:A:157:TYR:CG	1:A:303:THR:HG23	2.52	0.45
1:A:593:GLU:N	1:A:594:PRO:HD3	2.32	0.45
1:A:676:THR:C	1:A:678:ASN:N	2.72	0.45
1:A:39:LEU:N	1:A:39:LEU:HD12	2.31	0.45
1:A:109:ASP:OD2	3:A:1205:HOH:O	2.21	0.45
1:A:467:ILE:HD12	1:A:468:PHE:CE2	2.52	0.45
1:A:753:LYS:O	1:A:755:PRO:HD2	2.17	0.45
1:A:150:LEU:HD12	1:A:817:ILE:CG2	2.35	0.45
1:A:322:VAL:CG1	1:A:325:ASN:CG	2.89	0.45
1:A:461:GLU:HA	1:A:464:LYS:HD2	1.99	0.45
1:A:597:PHE:HD1	3:A:1327:HOH:O	1.98	0.45
1:A:592:LYS:C	1:A:594:PRO:HD3	2.40	0.45
1:A:666:ILE:HD13	1:A:780:TYR:HE1	1.82	0.45
1:A:837:PRO:CG	1:A:838:ASP:H	2.29	0.45
1:A:175:GLN:HE21	1:A:177:GLU:CD	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:THR:O	1:A:487:THR:CG2	2.65	0.45
1:A:57:HIS:HE1	3:A:1007:HOH:O	2.00	0.45
1:A:187:ASN:HA	1:A:188:PRO:HD2	1.85	0.45
1:A:252:PHE:CE1	1:A:255:LYS:HD2	2.52	0.45
1:A:204:GLY:HA2	1:A:217:ASP:O	2.16	0.45
1:A:382:GLU:OE2	1:A:770:ARG:NH2	2.47	0.45
1:A:382:GLU:H	1:A:382:GLU:HG3	1.23	0.45
1:A:417:ALA:HB3	1:A:418:PHE:CD1	2.51	0.45
1:A:39:LEU:HD21	1:A:53:PHE:HB3	1.99	0.44
1:A:249:PRO:O	1:A:269:ARG:NH2	2.50	0.44
1:A:466:THR:O	1:A:469:LYS:HG2	2.17	0.44
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.99	0.44
1:A:796:GLU:OE1	1:A:799:ARG:HD3	2.16	0.44
1:A:43:ARG:O	1:A:43:ARG:CG	2.62	0.44
1:A:262:TYR:O	1:A:266:VAL:HG23	2.17	0.44
1:A:335:ILE:CD1	1:A:337:LEU:HD13	2.35	0.44
1:A:390:HIS:CE1	1:A:391:LEU:HD12	2.53	0.44
1:A:752:PRO:HB2	1:A:753:LYS:HZ2	1.76	0.44
1:A:365:TRP:O	1:A:369:VAL:HG23	2.17	0.44
1:A:208:HIS:HB2	3:A:1268:HOH:O	2.18	0.44
1:A:390:HIS:O	1:A:394:THR:OG1	2.32	0.44
1:A:549:LEU:CB	1:A:555:VAL:CG2	2.81	0.44
1:A:567:VAL:O	1:A:568:LYS:HB3	2.18	0.44
1:A:834:LEU:CD2	1:A:836:ALA:CB	2.91	0.43
1:A:306:ASP:OD1	1:A:309:ARG:HD3	2.18	0.43
1:A:713:MET:HG2	1:A:776:ASP:OD1	2.18	0.43
1:A:24:VAL:HG12	1:A:24:VAL:O	2.17	0.43
1:A:29:LYS:HB3	1:A:29:LYS:HE2	1.78	0.43
1:A:31:PHE:CE2	1:A:115:LEU:CD2	3.02	0.43
1:A:184:ARG:HE	1:A:184:ARG:HB2	1.25	0.43
1:A:36:HIS:O	1:A:40:VAL:N	2.52	0.43
1:A:744:GLN:HB3	1:A:749:PHE:CB	2.44	0.43
1:A:344:LEU:O	1:A:347:PRO:HD2	2.17	0.43
1:A:766:MET:HE2	1:A:774:PHE:CZ	2.50	0.43
1:A:835:PRO:HG2	1:A:836:ALA:H	1.84	0.43
1:A:36:HIS:CB	3:A:1000:HOH:O	2.65	0.43
1:A:589:ARG:NH2	1:A:737:GLU:CD	2.75	0.43
1:A:170:ILE:HA	1:A:174:TRP:O	2.19	0.43
1:A:329:PHE:N	1:A:330:PRO:HD2	2.34	0.43
1:A:366:GLU:O	1:A:370:LYS:HG3	2.19	0.43
1:A:252:PHE:CZ	1:A:255:LYS:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:TRP:CZ2	1:A:406:ILE:CD1	2.94	0.43
1:A:389:VAL:O	1:A:393:GLU:HB2	2.19	0.43
1:A:344:LEU:C	1:A:347:PRO:HD2	2.44	0.43
1:A:678:ASN:HA	1:A:678:ASN:HD22	0.99	0.43
1:A:680:LYS:NZ	2:A:999:PLP:O3	2.52	0.43
1:A:327:ASP:HB3	1:A:363:LYS:HZ1	1.84	0.43
1:A:515:LEU:HD22	1:A:518:LEU:CD2	2.49	0.43
1:A:193:ARG:N	1:A:194:PRO:CD	2.82	0.42
1:A:758:PHE:O	1:A:760:ASP:N	2.52	0.42
1:A:159:ILE:CG1	1:A:299:VAL:CG2	2.80	0.42
1:A:753:LYS:CG	1:A:754:GLN:N	2.80	0.42
1:A:75:TYR:CZ	1:A:315:LYS:HE2	2.55	0.42
1:A:465:LYS:HD2	1:A:465:LYS:HA	1.67	0.42
1:A:530:PHE:HD1	1:A:530:PHE:HA	1.47	0.42
1:A:665:GLN:HE21	1:A:678:ASN:HA	1.83	0.42
1:A:752:PRO:HG2	1:A:753:LYS:HZ3	1.82	0.42
1:A:49:ARG:HH11	1:A:49:ARG:HD2	1.67	0.42
1:A:251:ASP:CG	1:A:255:LYS:HE2	2.44	0.42
1:A:688:THR:HG21	1:A:708:PHE:CE2	2.55	0.42
1:A:316:PHE:HE1	1:A:319:ARG:CD	2.27	0.42
1:A:103:ALA:HB2	1:A:234:ARG:HE	1.84	0.42
1:A:548:TYR:HA	1:A:551:ARG:HG2	2.02	0.42
1:A:584:ILE:HD11	1:A:741:ILE:CG1	2.40	0.42
1:A:139:LEU:HD21	1:A:143:PHE:CZ	2.53	0.42
1:A:160:ARG:HB2	1:A:243:LEU:HB3	2.02	0.42
1:A:688:THR:HG21	1:A:708:PHE:HE2	1.84	0.42
1:A:152:LEU:CD1	1:A:829:PRO:HA	2.46	0.42
1:A:605:ILE:O	1:A:644:PHE:HA	2.20	0.42
1:A:449:SER:O	1:A:478:LYS:HD3	2.20	0.42
1:A:778:GLU:HG2	1:A:782:LYS:HE3	2.02	0.42
1:A:36:HIS:HD2	1:A:37:PHE:CE2	2.38	0.42
1:A:33:ARG:HG2	1:A:37:PHE:HD2	1.85	0.41
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.55	0.41
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.73	0.41
1:A:441:MET:HA	1:A:441:MET:HE3	2.01	0.41
1:A:464:LYS:HG3	1:A:464:LYS:H	1.65	0.41
1:A:516:ASP:C	1:A:518:LEU:N	2.77	0.41
1:A:322:VAL:CG1	1:A:325:ASN:OD1	2.68	0.41
1:A:786:ARG:HH11	1:A:786:ARG:HD3	1.75	0.41
1:A:363:LYS:HD2	1:A:363:LYS:O	2.19	0.41
1:A:365:TRP:CE3	1:A:365:TRP:HA	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:HA	1:A:255:LYS:N	2.35	0.41
1:A:516:ASP:C	1:A:518:LEU:H	2.29	0.41
1:A:618:MET:HB3	1:A:761:ILE:HD11	2.03	0.41
1:A:283:ASP:O	1:A:284:ASN:HB2	2.19	0.41
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.68	0.41
1:A:677:GLY:O	1:A:681:PHE:HD2	2.04	0.41
1:A:39:LEU:O	1:A:40:VAL:HB	2.20	0.41
1:A:316:PHE:CE1	1:A:319:ARG:HG3	2.50	0.41
1:A:524:TYR:CD1	1:A:524:TYR:N	2.89	0.41
1:A:549:LEU:HD12	1:A:549:LEU:HA	1.82	0.41
1:A:666:ILE:HG23	1:A:711:PHE:CE1	2.55	0.41
1:A:282:ASN:ND2	1:A:610:ALA:HB1	2.35	0.41
1:A:349:LEU:O	1:A:353:LEU:HG	2.20	0.41
1:A:352:VAL:O	1:A:353:LEU:C	2.63	0.41
1:A:522:LEU:HG	3:A:1312:HOH:O	2.20	0.41
1:A:676:THR:N	1:A:678:ASN:HB2	2.36	0.41
1:A:707:ASN:ND2	1:A:803:ARG:HD2	2.36	0.41
1:A:316:PHE:CD1	1:A:319:ARG:NE	2.87	0.41
1:A:325:ASN:HD22	1:A:325:ASN:HA	1.44	0.41
1:A:637:GLY:C	1:A:639:ARG:N	2.79	0.41
1:A:128:ASP:OD1	1:A:651:SER:OG	2.36	0.41
1:A:622:LEU:HD22	1:A:626:ILE:HD12	2.03	0.41
1:A:793:ASN:ND2	1:A:796:GLU:HB2	2.35	0.41
1:A:76:GLU:H	1:A:76:GLU:HG2	1.62	0.41
1:A:85:LEU:N	1:A:85:LEU:HD23	2.36	0.41
1:A:99:MET:O	1:A:103:ALA:N	2.54	0.41
1:A:254:LEU:O	1:A:254:LEU:HD13	2.21	0.41
1:A:457:ARG:HH12	1:A:701:GLU:CD	2.29	0.41
1:A:593:GLU:OE2	1:A:596:LYS:CD	2.54	0.41
1:A:125:ILE:O	1:A:125:ILE:HG22	2.21	0.40
1:A:166:PHE:CD1	1:A:166:PHE:C	2.99	0.40
1:A:758:PHE:HD2	1:A:761:ILE:HD12	1.87	0.40
1:A:293:LEU:HB2	1:A:387:TRP:CH2	2.57	0.40
1:A:380:ILE:HG21	1:A:382:GLU:OE1	2.22	0.40
1:A:41:LYS:NZ	3:A:1576:HOH:O	2.54	0.40
1:A:170:ILE:HD11	1:A:644:PHE:HE1	1.84	0.40
1:A:254:LEU:O	1:A:254:LEU:CD1	2.69	0.40
1:A:269:ARG:O	1:A:273:GLU:HG3	2.22	0.40
1:A:790:LEU:HD11	1:A:797:TRP:CA	2.51	0.40
1:A:81:ARG:HB3	1:A:155:TYR:HE1	1.87	0.40
1:A:400:LEU:CD2	1:A:439:ILE:HD11	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ALA:HA	1:A:611:PRO:HD3	1.80	0.40
1:A:715:VAL:HG23	1:A:716:GLU:H	1.86	0.40
1:A:790:LEU:CD1	1:A:797:TRP:N	2.83	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:O	1:A:254:LEU:CD1[7_556]	1.88	0.32

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	821/842 (98%)	735 (90%)	59 (7%)	27 (3%)	3 0

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	LEU
1	A	256	ASP
1	A	258	ASN
1	A	315	LYS
1	A	319	ARG
1	A	320	ASP
1	A	436	VAL
1	A	837	PRO
1	A	838	ASP
1	A	21	VAL
1	A	323	ARG
1	A	527	ASP
1	A	551	ARG

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Mol	Chain	Res	Type
1	A	271	LEU
1	A	324	THR
1	A	434	GLY
1	A	514	ASP
1	A	556	HIS
1	A	836	ALA
1	A	210	SER
1	A	555	VAL
1	A	36	HIS
1	A	131	LEU
1	A	520	LYS
1	A	678	ASN
1	A	759	LYS
1	A	755	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	711/731 (97%)	551 (78%)	160 (22%)	1 0

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	22	GLU
1	A	23	ASN
1	A	26	GLU
1	A	27	LEU
1	A	29	LYS
1	A	41	LYS
1	A	44	ASN
1	A	47	THR
1	A	55	LEU
1	A	60	ARG
1	A	64	VAL

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Mol	Chain	Res	Type
1	A	66	ARG
1	A	77	LYS
1	A	85	LEU
1	A	87	LEU
1	A	102	LEU
1	A	104	LEU
1	A	110	GLU
1	A	122	LEU
1	A	125	ILE
1	A	127	GLU
1	A	144	LEU
1	A	165	ILE
1	A	169	LYS
1	A	170	ILE
1	A	177	GLU
1	A	178	GLU
1	A	193	ARG
1	A	195	GLU
1	A	198	LEU
1	A	207	GLU
1	A	216	VAL
1	A	234	ARG
1	A	235	ASN
1	A	243	LEU
1	A	247	LYS
1	A	254	LEU
1	A	255	LYS
1	A	257	PHE
1	A	258	ASN
1	A	263	ILE
1	A	264	GLN
1	A	271	LEU
1	A	277	ARG
1	A	281	PRO
1	A	289	LYS
1	A	304	LEU
1	A	306	ASP
1	A	315	LYS
1	A	316	PHE
1	A	318	CYS
1	A	320	ASP
1	A	322	VAL

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Mol	Chain	Res	Type
1	A	323	ARG
1	A	324	THR
1	A	327	ASP
1	A	335	ILE
1	A	337	LEU
1	A	344	LEU
1	A	358	ARG
1	A	359	LEU
1	A	361	TRP
1	A	363	LYS
1	A	382	GLU
1	A	389	VAL
1	A	391	LEU
1	A	392	LEU
1	A	393	GLU
1	A	394	THR
1	A	395	LEU
1	A	400	LEU
1	A	401	GLN
1	A	405	GLU
1	A	426	ARG
1	A	430	LEU
1	A	432	GLU
1	A	438	ARG
1	A	444	LEU
1	A	464	LYS
1	A	465	LYS
1	A	467	ILE
1	A	474	LEU
1	A	476	PRO
1	A	478	LYS
1	A	486	ILE
1	A	506	ARG
1	A	510	GLU
1	A	515	LEU
1	A	518	LEU
1	A	521	LEU
1	A	522	LEU
1	A	525	VAL
1	A	526	ASP
1	A	528	GLU
1	A	530	PHE

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Mol	Chain	Res	Type
1	A	537	VAL
1	A	548	TYR
1	A	549	LEU
1	A	551	ARG
1	A	560	ASN
1	A	568	LYS
1	A	574	LYS
1	A	576	GLN
1	A	581	LEU
1	A	584	ILE
1	A	591	LYS
1	A	592	LYS
1	A	598	VAL
1	A	601	ARG
1	A	613	TYR
1	A	617	LYS
1	A	620	ILE
1	A	622	LEU
1	A	635	VAL
1	A	636	VAL
1	A	638	ASP
1	A	640	LEU
1	A	641	ARG
1	A	643	ILE
1	A	645	LEU
1	A	665	GLN
1	A	666	ILE
1	A	667	SER
1	A	678	ASN
1	A	706	GLU
1	A	708	PHE
1	A	713	MET
1	A	714	ARG
1	A	724	ARG
1	A	730	GLU
1	A	737	GLU
1	A	739	ARG
1	A	747	SER
1	A	753	LYS
1	A	754	GLN
1	A	756	ASP
1	A	759	LYS

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Mol	Chain	Res	Type
1	A	760	ASP
1	A	763	ASN
1	A	764	MET
1	A	765	LEU
1	A	768	HIS
1	A	782	LYS
1	A	790	LEU
1	A	792	LYS
1	A	794	PRO
1	A	795	ARG
1	A	797	TRP
1	A	801	VAL
1	A	803	ARG
1	A	807	THR
1	A	812	SER
1	A	813	SER
1	A	815	ARG
1	A	817	ILE
1	A	827	VAL
1	A	830	SER
1	A	838	ASP
1	A	839	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	36	HIS
1	A	71	GLN
1	A	101	ASN
1	A	106	ASN
1	A	235	ASN
1	A	282	ASN
1	A	412	ASN
1	A	459	HIS
1	A	477	HIS
1	A	481	ASN
1	A	484	ASN
1	A	539	GLN
1	A	560	ASN
1	A	566	GLN
1	A	576	GLN

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Mol	Chain	Res	Type
1	A	579	ASN
1	A	632	HIS
1	A	678	ASN
1	A	754	GLN
1	A	763	ASN
1	A	793	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLP	A	999	1	15,15,16	2.05	6 (40%)	21,22,23	2.91	8 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	999	1	-	2/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	PLP	C4A-C4	-4.05	1.43	1.51
2	A	999	PLP	C5A-C5	3.42	1.59	1.50
2	A	999	PLP	P-O4P	3.31	1.70	1.60
2	A	999	PLP	P-O2P	-2.35	1.46	1.54
2	A	999	PLP	C2A-C2	2.03	1.53	1.50
2	A	999	PLP	P-O3P	-2.00	1.47	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	PLP	C6-N1-C2	5.64	129.42	119.20
2	A	999	PLP	O4P-C5A-C5	-5.49	99.06	109.36
2	A	999	PLP	C5-C6-N1	-5.28	115.23	123.83
2	A	999	PLP	C3-C2-N1	-4.60	115.16	120.96
2	A	999	PLP	C2A-C2-N1	4.35	125.83	117.64
2	A	999	PLP	C6-C5-C4	4.00	121.37	118.10
2	A	999	PLP	O2P-P-O4P	-3.71	97.00	106.67
2	A	999	PLP	O2P-P-O1P	2.83	121.87	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	PLP	C4-C5-C5A-O4P
2	A	999	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	PLP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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.