



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:32 AM UTC

PDB ID : 1ABB / pdb_00001abb
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 ⓘ 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

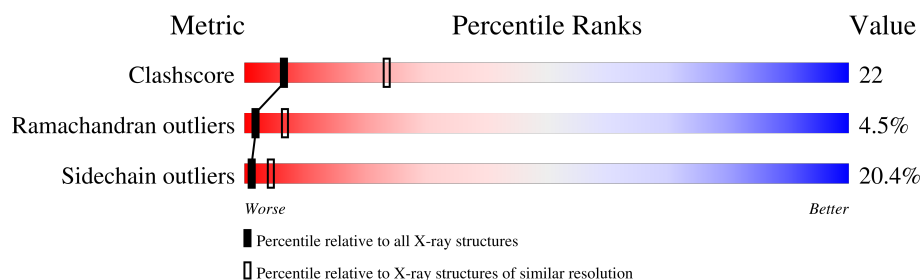
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	828	
1	B	828	
1	C	828	
1	D	828	

2 Entry composition

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.

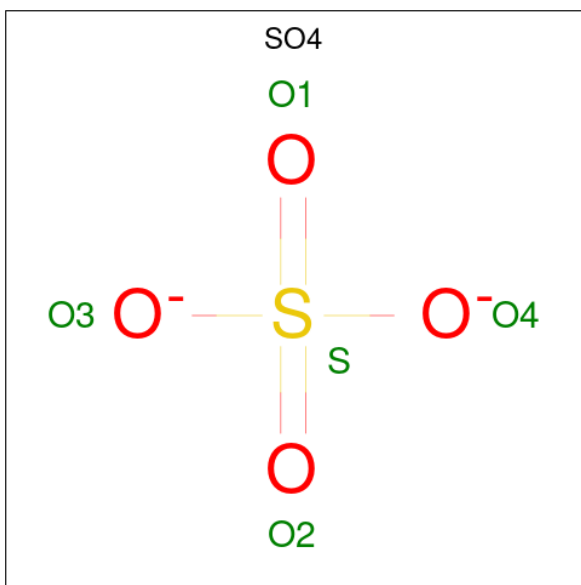
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE B.

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:

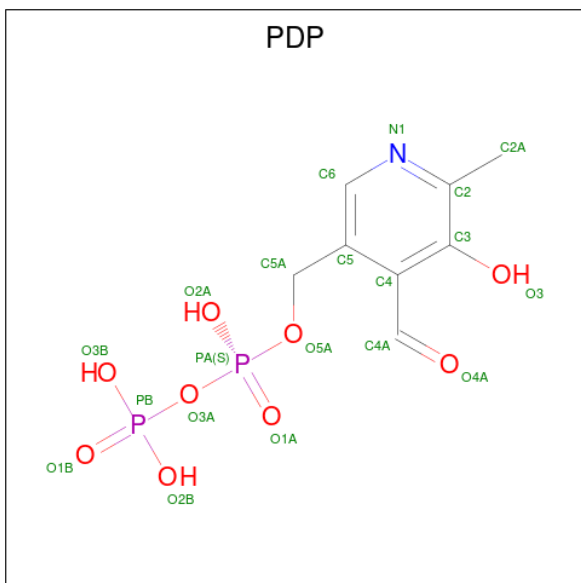
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



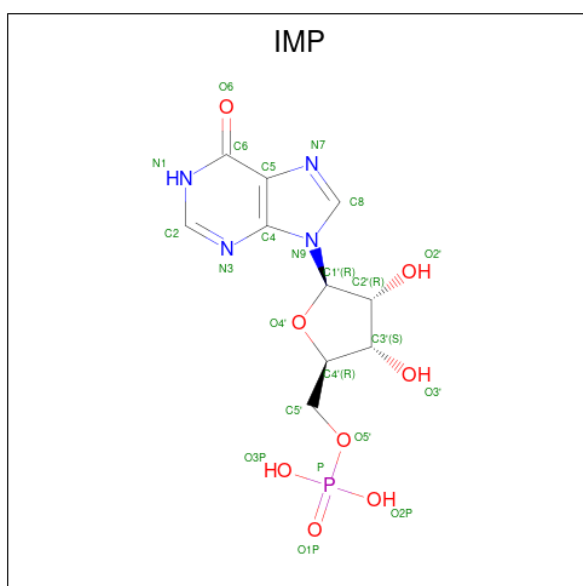
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

- Molecule 3 is PYRIDOXAL-5'-DIPHOSPHATE (CCD ID: PDP) (formula: $\text{C}_8\text{H}_{11}\text{NO}_9\text{P}_2$).



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 (CCD ID: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



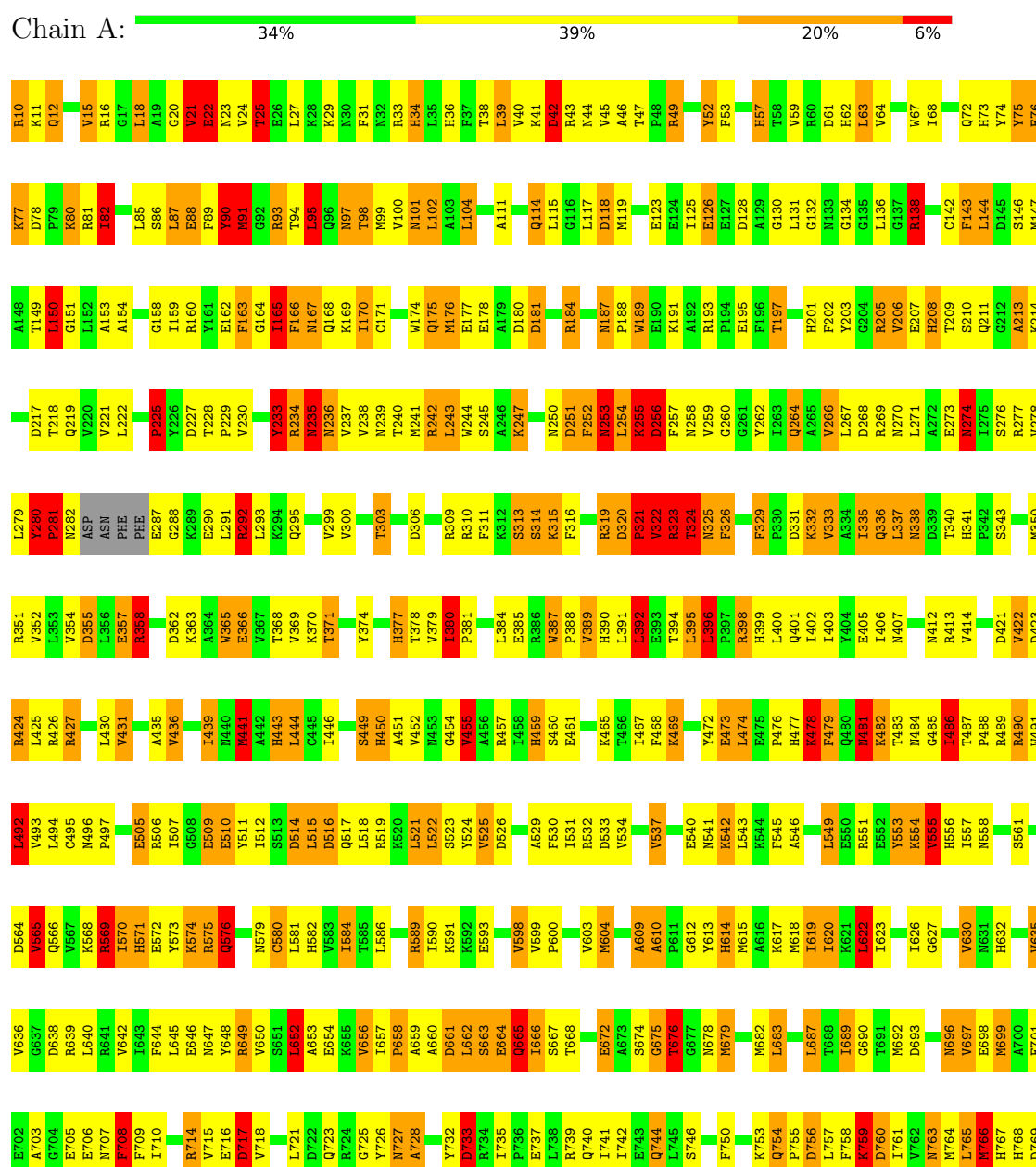
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

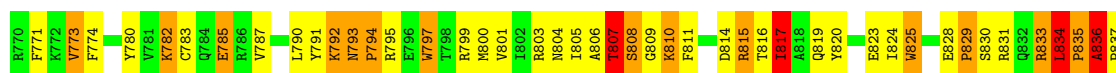
3 Residue-property plots

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.

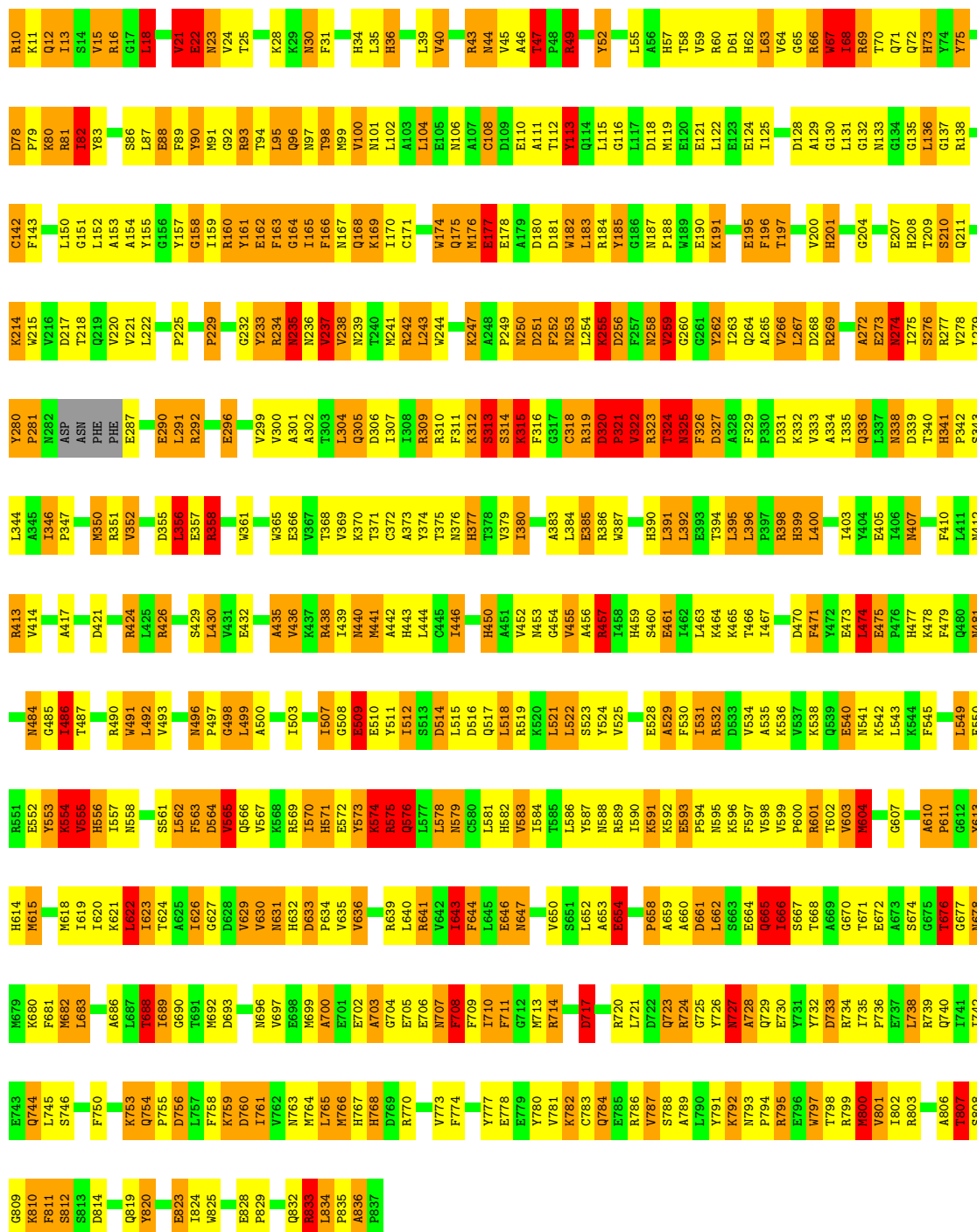
• Molecule 1: GLYCOGEN PHOSPHORYLASE B





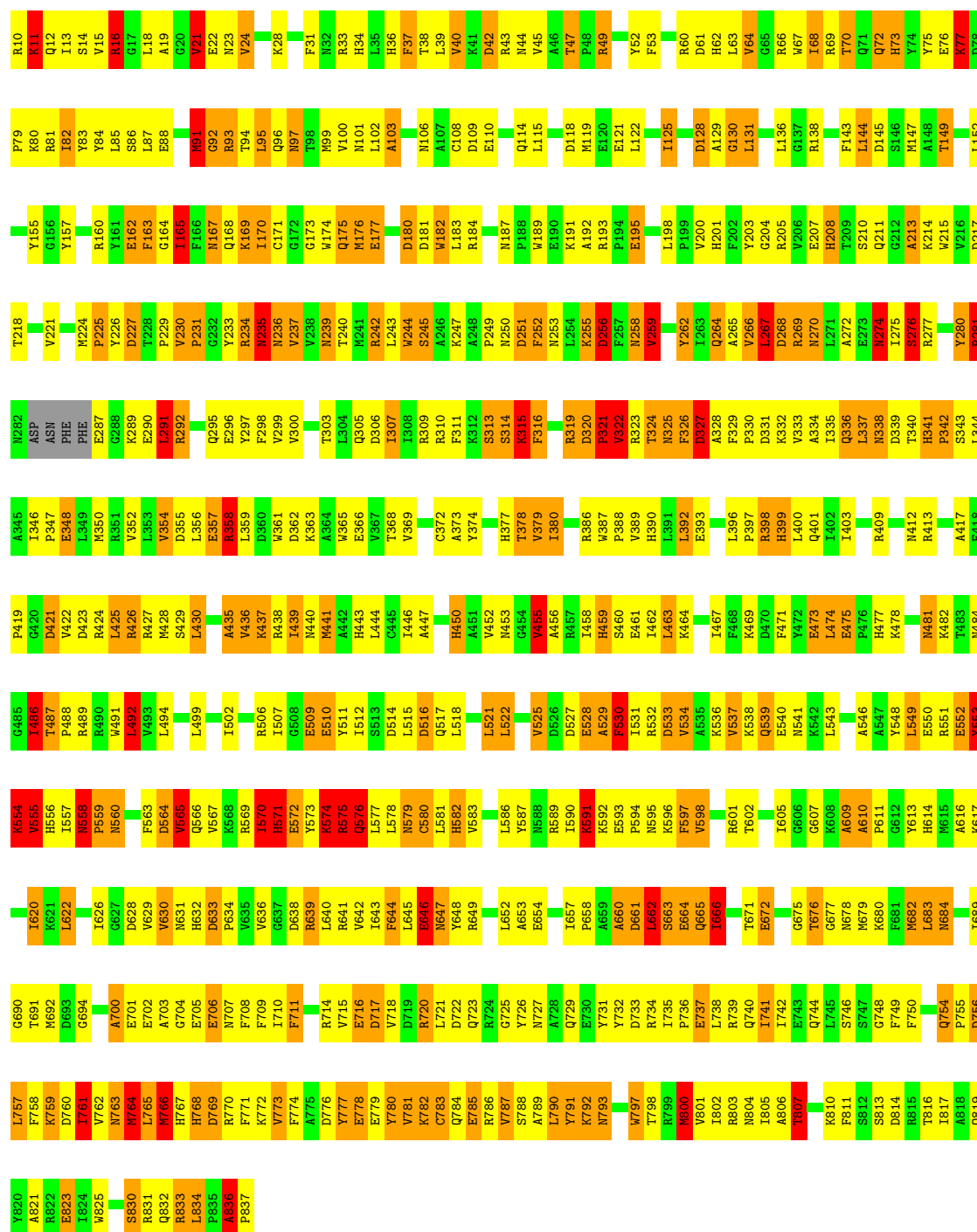
• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain B: 29% 39% 26% 6%



• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain C: 31% 42% 21% 5%



• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain D: 27% 38% 25% 9%





4 Data and refinement statistics

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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.38	52/6843 (0.8%)	2.47	463/9258 (5.0%)
1	B	1.48	59/6843 (0.9%)	2.44	483/9258 (5.2%)
1	C	1.34	49/6843 (0.7%)	2.41	424/9258 (4.6%)
1	D	1.41	55/6843 (0.8%)	2.47	487/9258 (5.3%)
All	All	1.40	215/27372 (0.8%)	2.45	1857/37032 (5.0%)

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 (215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	ILE	N-CA	-37.23	0.99	1.46
1	B	80	LYS	CA-CB	-14.12	1.30	1.53
1	B	68	ILE	CB-CG1	13.90	1.81	1.53
1	A	657	ILE	CA-CB	11.59	1.59	1.54
1	B	69	ARG	CB-CG	10.60	1.84	1.52
1	D	82	ILE	CA-CB	10.03	1.66	1.54
1	D	21	VAL	CA-CB	9.97	1.68	1.54
1	B	82	ILE	CA-CB	9.82	1.66	1.54
1	A	586	LEU	CA-CB	-9.47	1.38	1.53
1	A	225	PRO	CA-CB	-8.82	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	237	VAL	CA-CB	8.80	1.64	1.54
1	D	787	VAL	CA-CB	8.75	1.64	1.54
1	A	82	ILE	CA-CB	8.44	1.64	1.54
1	B	650	VAL	CA-CB	-8.40	1.44	1.54
1	D	263	ILE	CA-CB	8.23	1.65	1.54
1	D	227	ASP	CA-CB	-8.00	1.42	1.53
1	A	565	VAL	CA-CB	7.98	1.66	1.54
1	D	393	GLU	CA-CB	-7.70	1.41	1.53
1	B	81	ARG	CA-C	7.69	1.61	1.52
1	C	582	HIS	CD2-NE2	-7.63	1.29	1.37
1	C	237	VAL	CA-CB	7.61	1.62	1.54
1	D	750	PHE	CA-CB	-7.57	1.40	1.53
1	C	459	HIS	CD2-NE2	-7.49	1.29	1.37
1	D	459	HIS	CD2-NE2	-7.49	1.29	1.37
1	D	377	HIS	CD2-NE2	-7.45	1.29	1.37
1	D	450	HIS	CD2-NE2	-7.41	1.29	1.37
1	C	82	ILE	CA-CB	7.29	1.62	1.54
1	D	582	HIS	CD2-NE2	-7.22	1.29	1.37
1	B	531	ILE	CA-CB	7.15	1.62	1.54
1	A	335	ILE	CA-CB	7.13	1.63	1.54
1	A	443	HIS	CD2-NE2	-7.11	1.30	1.37
1	A	586	LEU	CB-CG	-7.09	1.39	1.53
1	B	21	VAL	CA-CB	7.08	1.64	1.54
1	A	450	HIS	CD2-NE2	-7.06	1.30	1.37
1	A	571	HIS	CD2-NE2	-7.02	1.30	1.37
1	C	335	ILE	CA-CB	6.98	1.63	1.54
1	D	657	ILE	CA-CB	6.94	1.58	1.53
1	A	459	HIS	CD2-NE2	-6.89	1.30	1.37
1	A	201	HIS	CD2-NE2	-6.87	1.30	1.37
1	D	768	HIS	CD2-NE2	-6.87	1.30	1.37
1	C	325	ASN	CA-C	-6.86	1.43	1.52
1	C	443	HIS	CD2-NE2	-6.85	1.30	1.37
1	D	341	HIS	CD2-NE2	-6.83	1.30	1.37
1	D	200	VAL	CA-CB	-6.83	1.45	1.54
1	B	73	HIS	CD2-NE2	-6.80	1.30	1.37
1	A	36	HIS	CG-ND1	-6.76	1.30	1.38
1	A	38	THR	CA-CB	6.72	1.64	1.53
1	C	225	PRO	CA-CB	-6.71	1.45	1.53
1	A	341	HIS	CD2-NE2	-6.70	1.30	1.37
1	D	666	ILE	CA-CB	6.68	1.63	1.54
1	B	36	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	281	PRO	C-N	-6.66	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	PRO	C-N	-6.66	1.24	1.33
1	D	571	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	165	ILE	CA-CB	6.62	1.62	1.55
1	B	582	HIS	CD2-NE2	-6.60	1.30	1.37
1	B	632	HIS	CD2-NE2	-6.59	1.30	1.37
1	B	450	HIS	CG-ND1	-6.57	1.31	1.38
1	D	201	HIS	CG-ND1	-6.54	1.31	1.38
1	B	201	HIS	CD2-NE2	-6.53	1.30	1.37
1	A	443	HIS	CG-ND1	-6.50	1.31	1.38
1	D	791	TYR	CA-CB	6.50	1.63	1.53
1	B	467	ILE	CA-CB	6.50	1.61	1.54
1	A	73	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	571	HIS	CD2-NE2	-6.48	1.30	1.37
1	C	787	VAL	CA-CB	6.47	1.63	1.54
1	A	57	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	450	HIS	CD2-NE2	-6.45	1.30	1.37
1	C	34	HIS	CG-ND1	-6.43	1.31	1.38
1	A	582	HIS	CD2-NE2	-6.43	1.30	1.37
1	C	399	HIS	CG-ND1	-6.41	1.31	1.38
1	C	34	HIS	CD2-NE2	-6.37	1.30	1.37
1	D	230	VAL	CA-CB	6.34	1.59	1.54
1	C	208	HIS	CD2-NE2	-6.34	1.30	1.37
1	D	324	THR	CA-CB	6.32	1.62	1.53
1	D	662	LEU	CA-CB	6.32	1.61	1.53
1	D	201	HIS	CD2-NE2	-6.31	1.30	1.37
1	D	632	HIS	CD2-NE2	-6.31	1.30	1.37
1	B	598	VAL	CA-CB	6.28	1.63	1.54
1	A	377	HIS	CG-ND1	-6.28	1.31	1.38
1	C	437	LYS	CA-CB	-6.26	1.45	1.53
1	B	57	HIS	CG-ND1	-6.26	1.31	1.38
1	B	341	HIS	CD2-NE2	-6.25	1.30	1.37
1	D	487	THR	CA-CB	6.25	1.62	1.53
1	C	632	HIS	CD2-NE2	-6.24	1.30	1.37
1	C	73	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	100	VAL	CA-CB	6.23	1.61	1.54
1	A	62	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	619	ILE	CA-CB	6.21	1.61	1.54
1	A	664	GLU	CA-CB	-6.21	1.43	1.53
1	C	281	PRO	C-N	-6.21	1.24	1.33
1	B	399	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	208	HIS	CD2-NE2	-6.20	1.31	1.37
1	B	73	HIS	CG-ND1	-6.20	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	556	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	553	TYR	CA-CB	6.15	1.63	1.53
1	B	738	LEU	CA-CB	-6.14	1.43	1.53
1	A	632	HIS	CD2-NE2	-6.12	1.31	1.37
1	C	21	VAL	CA-CB	6.11	1.62	1.54
1	C	553	TYR	CA-CB	6.11	1.63	1.53
1	A	614	HIS	CD2-NE2	-6.05	1.31	1.37
1	D	810	LYS	CA-CB	6.03	1.63	1.53
1	B	443	HIS	CG-ND1	-6.00	1.31	1.38
1	D	477	HIS	CD2-NE2	-5.99	1.31	1.37
1	B	258	ASN	CA-CB	5.98	1.62	1.53
1	C	768	HIS	CD2-NE2	-5.98	1.31	1.37
1	D	281	PRO	C-N	-5.97	1.25	1.33
1	A	767	HIS	CD2-NE2	-5.97	1.31	1.37
1	D	377	HIS	CG-ND1	-5.97	1.31	1.38
1	C	377	HIS	CD2-NE2	-5.96	1.31	1.37
1	D	827	VAL	CA-CB	5.92	1.63	1.54
1	D	68	ILE	CA-CB	-5.91	1.47	1.54
1	A	341	HIS	CG-ND1	-5.88	1.31	1.38
1	B	443	HIS	CD2-NE2	-5.86	1.31	1.37
1	D	36	HIS	CD2-NE2	-5.84	1.31	1.37
1	D	565	VAL	CA-CB	5.84	1.63	1.54
1	B	380	ILE	CA-CB	5.82	1.61	1.54
1	C	460	SER	CA-CB	-5.82	1.44	1.53
1	A	34	HIS	CD2-NE2	-5.81	1.31	1.37
1	C	556	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	571	HIS	CA-CB	-5.78	1.43	1.53
1	B	57	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	229	PRO	CA-C	5.73	1.59	1.52
1	D	73	HIS	CD2-NE2	-5.72	1.31	1.37
1	B	459	HIS	CD2-NE2	-5.71	1.31	1.37
1	C	477	HIS	CD2-NE2	-5.71	1.31	1.37
1	B	162	GLU	CA-CB	-5.69	1.44	1.53
1	C	259	VAL	CA-CB	5.68	1.62	1.54
1	D	244	TRP	NE1-CE2	-5.67	1.31	1.37
1	B	714	ARG	CA-CB	5.66	1.61	1.53
1	D	443	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	402	ILE	CA-CB	-5.65	1.47	1.54
1	A	208	HIS	CD2-NE2	-5.65	1.31	1.37
1	B	768	HIS	CD2-NE2	-5.64	1.31	1.37
1	D	767	HIS	CD2-NE2	-5.63	1.31	1.37
1	C	341	HIS	CD2-NE2	-5.63	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	438	ARG	CA-CB	-5.62	1.45	1.53
1	B	556	HIS	CD2-NE2	-5.62	1.31	1.37
1	B	237	VAL	CA-CB	5.61	1.61	1.54
1	A	829	PRO	CA-CB	-5.60	1.45	1.53
1	A	36	HIS	CD2-NE2	-5.60	1.31	1.37
1	B	161	TYR	CA-C	-5.60	1.46	1.52
1	D	170	ILE	CA-CB	5.60	1.60	1.53
1	D	399	HIS	CD2-NE2	-5.59	1.31	1.37
1	C	399	HIS	CD2-NE2	-5.58	1.31	1.37
1	B	322	VAL	CA-CB	5.58	1.62	1.54
1	B	630	VAL	CA-CB	5.58	1.60	1.54
1	B	395	LEU	CA-C	-5.57	1.45	1.52
1	A	477	HIS	CB-CG	5.56	1.57	1.50
1	B	390	HIS	CD2-NE2	-5.55	1.31	1.37
1	D	390	HIS	CD2-NE2	-5.55	1.31	1.37
1	B	98	THR	CA-CB	-5.54	1.44	1.53
1	C	201	HIS	CD2-NE2	-5.54	1.31	1.37
1	C	767	HIS	CD2-NE2	-5.52	1.31	1.37
1	D	208	HIS	CD2-NE2	-5.51	1.31	1.37
1	B	182	TRP	CG-CD2	-5.51	1.33	1.43
1	B	34	HIS	CG-ND1	-5.49	1.32	1.38
1	C	487	THR	CA-CB	5.48	1.62	1.52
1	B	632	HIS	CG-ND1	-5.47	1.32	1.38
1	A	556	HIS	CB-CG	5.46	1.57	1.50
1	A	399	HIS	CD2-NE2	-5.46	1.31	1.37
1	B	477	HIS	CD2-NE2	-5.46	1.31	1.37
1	B	352	VAL	CA-CB	-5.44	1.48	1.54
1	C	552	GLU	CA-CB	5.43	1.61	1.52
1	A	170	ILE	CA-CB	5.43	1.60	1.54
1	C	455	VAL	N-CA	-5.42	1.40	1.46
1	B	377	HIS	CD2-NE2	-5.42	1.31	1.37
1	D	62	HIS	CD2-NE2	-5.42	1.31	1.37
1	D	798	THR	CA-CB	5.41	1.62	1.53
1	C	390	HIS	CD2-NE2	-5.39	1.31	1.37
1	B	34	HIS	CD2-NE2	-5.36	1.31	1.37
1	B	512	ILE	CA-CB	-5.35	1.45	1.54
1	A	34	HIS	CG-ND1	-5.35	1.32	1.38
1	A	436	VAL	CA-CB	5.35	1.61	1.54
1	D	582	HIS	CG-ND1	-5.33	1.32	1.38
1	C	450	HIS	CD2-NE2	-5.32	1.31	1.37
1	C	330	PRO	CA-CB	-5.31	1.46	1.53
1	D	614	HIS	CD2-NE2	-5.30	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	VAL	CA-CB	-5.30	1.47	1.54
1	B	767	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	390	HIS	CD2-NE2	-5.29	1.32	1.37
1	C	62	HIS	CD2-NE2	-5.29	1.32	1.37
1	C	614	HIS	CD2-NE2	-5.27	1.32	1.37
1	C	201	HIS	CG-ND1	-5.26	1.32	1.38
1	C	660	ALA	CA-CB	-5.25	1.45	1.53
1	B	604	MET	CA-CB	5.24	1.61	1.53
1	D	486	ILE	CA-CB	-5.24	1.46	1.54
1	B	191	LYS	CA-C	-5.24	1.46	1.52
1	B	635	VAL	CA-CB	5.24	1.61	1.54
1	B	346	ILE	CA-C	-5.22	1.47	1.52
1	C	36	HIS	CD2-NE2	-5.22	1.32	1.37
1	C	267	LEU	N-CA	-5.21	1.40	1.46
1	D	459	HIS	CG-ND1	-5.21	1.32	1.38
1	A	537	VAL	CA-C	-5.21	1.46	1.52
1	C	387	TRP	NE1-CE2	-5.20	1.31	1.37
1	D	341	HIS	CG-ND1	-5.19	1.32	1.38
1	A	230	VAL	N-CA	5.19	1.50	1.46
1	D	203	TYR	CA-CB	-5.19	1.44	1.53
1	A	450	HIS	CG-ND1	-5.17	1.32	1.38
1	C	310	ARG	CA-CB	-5.17	1.44	1.53
1	C	555	VAL	CA-CB	5.17	1.61	1.54
1	C	450	HIS	CG-ND1	-5.15	1.32	1.38
1	A	477	HIS	CD2-NE2	-5.15	1.32	1.37
1	C	374	TYR	CA-CB	-5.10	1.46	1.53
1	C	93	ARG	CA-C	5.08	1.59	1.52
1	C	571	HIS	CD2-NE2	-5.08	1.32	1.37
1	B	477	HIS	CB-CG	5.08	1.57	1.50
1	A	57	HIS	CG-ND1	-5.06	1.32	1.38
1	D	630	VAL	CA-CB	5.06	1.60	1.54
1	A	424	ARG	CA-CB	-5.05	1.45	1.53
1	D	250	ASN	CA-CB	5.04	1.59	1.53
1	B	170	ILE	CA-CB	5.02	1.61	1.54
1	D	494	LEU	CA-CB	-5.01	1.45	1.53
1	A	571	HIS	CG-ND1	-5.01	1.32	1.38
1	C	230	VAL	CA-CB	5.00	1.59	1.53

All (1857) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	HIS	CA-CB-CG	25.28	139.08	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	N-CA-C	17.30	131.87	111.11
1	C	455	VAL	N-CA-CB	-16.68	90.47	112.16
1	A	61	ASP	CA-CB-CG	16.39	128.99	112.60
1	B	68	ILE	CB-CG1-CD1	16.11	147.63	113.80
1	A	575	ARG	N-CA-C	15.68	135.35	113.56
1	B	275	ILE	N-CA-C	-15.52	95.25	110.30
1	A	477	HIS	CA-CB-CG	15.30	129.10	113.80
1	B	181	ASP	CA-CB-CG	14.87	127.47	112.60
1	B	69	ARG	CA-CB-CG	-13.38	87.35	114.10
1	C	324	THR	N-CA-C	-13.24	94.47	111.02
1	B	455	VAL	N-CA-CB	-13.02	89.75	111.23
1	C	267	LEU	CA-C-O	-12.94	107.37	120.70
1	C	455	VAL	CB-CA-C	12.78	127.24	111.65
1	B	81	ARG	CA-C-O	12.61	134.31	120.32
1	D	676	THR	CA-CB-OG1	-12.41	90.98	109.60
1	D	61	ASP	CA-CB-CG	12.30	124.90	112.60
1	A	253	ASN	CA-CB-CG	12.22	124.82	112.60
1	A	324	THR	N-CA-C	-12.05	95.95	111.02
1	A	76	GLU	CA-CB-CG	11.99	138.08	114.10
1	B	80	LYS	N-CA-CB	11.93	127.62	109.85
1	A	676	THR	CA-CB-OG1	-11.86	91.82	109.60
1	C	453	ASN	CA-CB-CG	11.71	124.31	112.60
1	A	760	ASP	CA-CB-CG	11.67	124.27	112.60
1	A	541	ASN	OD1-CG-ND2	-11.58	111.02	122.60
1	A	351	ARG	CA-C-O	-11.45	108.79	120.82
1	D	258	ASN	N-CA-C	-11.40	96.53	111.24
1	A	716	GLU	CB-CG-CD	11.36	131.91	112.60
1	C	507	ILE	N-CA-C	11.29	124.06	113.10
1	A	668	THR	CA-C-O	-11.24	109.71	120.95
1	C	181	ASP	CA-CB-CG	11.09	123.69	112.60
1	C	268	ASP	CA-CB-CG	11.06	123.66	112.60
1	D	16	ARG	N-CA-C	11.03	124.47	111.02
1	C	274	ASN	CA-CB-CG	10.95	123.55	112.60
1	B	47	THR	CA-CB-OG1	-10.84	93.35	109.60
1	C	631	ASN	CA-CB-CG	10.82	123.42	112.60
1	C	579	ASN	CA-CB-CG	10.82	123.42	112.60
1	B	564	ASP	CA-CB-CG	10.77	123.37	112.60
1	C	807	THR	N-CA-CB	-10.75	94.58	110.49
1	D	514	ASP	CA-CB-CG	10.64	123.24	112.60
1	C	258	ASN	CA-CB-CG	10.57	123.17	112.60
1	A	163	PHE	CA-CB-CG	-10.56	103.24	113.80
1	A	555	VAL	N-CA-C	10.52	131.22	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ALA	O-C-N	10.42	135.08	123.10
1	C	541	ASN	OD1-CG-ND2	-10.38	112.22	122.60
1	C	306	ASP	CA-CB-CG	10.28	122.88	112.60
1	C	325	ASN	O-C-N	10.23	136.61	123.01
1	D	324	THR	N-CA-C	-10.22	98.24	111.02
1	C	325	ASN	OD1-CG-ND2	-10.18	112.42	122.60
1	A	564	ASP	CA-CB-CG	10.15	122.75	112.60
1	A	727	ASN	OD1-CG-ND2	-10.14	112.46	122.60
1	D	235	ASN	OD1-CG-ND2	-10.10	112.50	122.60
1	D	575	ARG	N-CA-C	9.92	127.98	113.40
1	B	325	ASN	N-CA-C	9.91	124.87	110.10
1	C	552	GLU	CB-CG-CD	9.87	129.37	112.60
1	D	727	ASN	OD1-CG-ND2	-9.86	112.74	122.60
1	B	477	HIS	CA-CB-CG	9.84	123.64	113.80
1	B	571	HIS	CB-CG-CD2	-9.84	118.41	131.20
1	D	264	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	D	268	ASP	CA-CB-CG	9.78	122.38	112.60
1	A	380	ILE	N-CA-CB	-9.77	100.99	110.08
1	A	435	ALA	N-CA-C	-9.75	92.84	108.73
1	D	807	THR	N-CA-CB	-9.74	95.17	110.46
1	B	327	ASP	CA-CB-CG	-9.71	102.89	112.60
1	B	463	LEU	N-CA-C	-9.71	100.66	111.14
1	C	473	GLU	N-CA-C	9.70	121.45	111.07
1	A	793	ASN	CA-CB-CG	9.69	122.29	112.60
1	B	81	ARG	CB-CA-C	-9.67	92.20	109.70
1	D	322	VAL	O-C-N	-9.63	113.36	122.71
1	A	676	THR	CA-CB-CG2	9.61	126.84	110.50
1	A	571	HIS	CB-CG-CD2	-9.59	118.73	131.20
1	C	93	ARG	N-CA-C	9.57	131.18	110.80
1	D	322	VAL	N-CA-CB	-9.54	100.99	112.35
1	B	258	ASN	OD1-CG-ND2	-9.54	113.06	122.60
1	B	180	ASP	CA-CB-CG	9.54	122.14	112.60
1	D	435	ALA	N-CA-C	-9.52	93.65	109.46
1	D	325	ASN	O-C-N	9.49	134.47	122.89
1	B	61	ASP	CA-CB-CG	9.48	122.08	112.60
1	A	258	ASN	N-CA-C	-9.42	99.91	111.40
1	D	735	ILE	N-CA-CB	-9.40	98.05	111.21
1	D	564	ASP	CA-CB-CG	9.40	122.00	112.60
1	B	717	ASP	CA-CB-CG	9.38	121.98	112.60
1	B	473	GLU	N-CA-C	9.36	124.50	112.89
1	D	251	ASP	CA-CB-CG	9.34	121.94	112.60
1	D	323	ARG	CA-CB-CG	9.33	132.76	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	788	SER	O-C-N	9.33	132.01	122.12
1	A	268	ASP	CA-CB-CG	9.28	121.88	112.60
1	C	481	ASN	OD1-CG-ND2	-9.28	113.32	122.60
1	C	295	GLN	OE1-CD-NE2	-9.23	113.36	122.60
1	D	479	PHE	CA-CB-CG	-9.23	104.57	113.80
1	A	394	THR	CA-C-O	-9.22	111.31	121.00
1	A	325	ASN	N-CA-C	9.21	123.77	109.96
1	D	810	LYS	N-CA-C	-9.21	101.47	112.89
1	A	490	ARG	NE-CZ-NH2	-9.20	110.92	119.20
1	A	659	ALA	N-CA-C	9.20	124.30	112.89
1	D	667	SER	CA-C-O	-9.19	110.90	121.47
1	A	693	ASP	CA-CB-CG	9.19	121.79	112.60
1	A	509	GLU	CB-CA-C	-9.15	95.30	110.85
1	B	435	ALA	N-CA-C	-9.11	93.88	108.73
1	A	455	VAL	N-CA-CB	-9.11	96.21	111.23
1	A	727	ASN	CA-CB-CG	9.11	121.71	112.60
1	B	338	ASN	OD1-CG-ND2	-9.10	113.50	122.60
1	B	168	GLN	OE1-CD-NE2	-9.09	113.51	122.60
1	A	744	GLN	OE1-CD-NE2	-9.08	113.52	122.60
1	A	825	TRP	N-CA-C	-9.08	101.63	112.89
1	A	338	ASN	OD1-CG-ND2	-9.07	113.53	122.60
1	A	332	LYS	CA-CB-CG	-9.07	95.97	114.10
1	B	258	ASN	CA-CB-CG	9.05	121.66	112.60
1	B	356	LEU	N-CA-C	9.05	121.22	111.36
1	A	459	HIS	CB-CG-CD2	-9.03	119.46	131.20
1	A	42	ASP	N-CA-CB	-9.02	97.57	111.46
1	C	95	LEU	N-CA-C	8.97	120.83	111.14
1	C	652	LEU	N-CA-C	-8.97	100.65	111.69
1	C	213	ALA	N-CA-C	-8.96	96.53	110.42
1	D	391	LEU	N-CA-C	-8.95	100.48	111.40
1	D	676	THR	CA-CB-CG2	8.95	125.71	110.50
1	C	275	ILE	CA-C-O	8.91	129.87	120.25
1	B	744	GLN	OE1-CD-NE2	-8.90	113.70	122.60
1	C	45	VAL	N-CA-CB	-8.90	100.07	112.35
1	D	191	LYS	CA-CB-CG	-8.89	96.33	114.10
1	C	163	PHE	CA-CB-CG	-8.88	104.92	113.80
1	A	380	ILE	CB-CA-C	8.87	120.47	110.89
1	C	160	ARG	NE-CZ-NH2	-8.85	111.23	119.20
1	A	229	PRO	N-CA-CB	-8.82	94.81	103.19
1	C	804	ASN	CA-CB-CG	-8.80	103.80	112.60
1	B	666	ILE	N-CA-C	8.79	127.63	109.34
1	D	571	HIS	CB-CG-ND1	8.77	135.86	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	571	HIS	CB-CG-CD2	-8.76	119.82	131.20
1	C	42	ASP	CA-CB-CG	8.75	121.35	112.60
1	B	563	PHE	CA-CB-CG	8.74	122.54	113.80
1	A	385	GLU	N-CA-C	8.73	122.23	110.35
1	C	676	THR	N-CA-CB	-8.73	96.97	110.06
1	D	274	ASN	CA-CB-CG	8.72	121.32	112.60
1	D	647	ASN	CA-CB-CG	8.72	121.32	112.60
1	C	187	ASN	CA-C-O	-8.72	112.79	119.59
1	C	380	ILE	N-CA-CB	-8.72	101.97	110.08
1	D	455	VAL	N-CA-CB	-8.71	96.85	111.23
1	B	68	ILE	N-CA-C	8.70	127.43	109.34
1	D	676	THR	N-CA-CB	-8.69	97.28	110.13
1	C	579	ASN	OD1-CG-ND2	-8.68	113.92	122.60
1	D	499	LEU	N-CA-CB	8.68	123.85	110.14
1	A	377	HIS	CA-CB-CG	8.66	122.47	113.80
1	A	313	SER	N-CA-C	8.64	120.32	111.07
1	A	509	GLU	N-CA-CB	8.64	122.95	110.16
1	D	493	VAL	CB-CA-C	-8.64	100.48	112.14
1	D	18	LEU	N-CA-C	8.63	122.33	112.57
1	A	807	THR	N-CA-CB	-8.63	96.91	110.46
1	B	602	THR	N-CA-C	-8.63	93.29	108.13
1	B	832	GLN	OE1-CD-NE2	-8.63	113.97	122.60
1	B	746	SER	N-CA-C	8.62	120.67	111.28
1	B	727	ASN	CB-CG-ND2	8.60	129.31	116.40
1	A	250	ASN	OD1-CG-ND2	-8.60	114.00	122.60
1	C	325	ASN	CA-CB-CG	-8.59	104.01	112.60
1	D	52	TYR	N-CA-C	-8.59	101.86	111.14
1	A	16	ARG	O-C-N	-8.58	113.17	122.09
1	B	163	PHE	N-CA-C	8.58	122.54	112.93
1	A	661	ASP	CA-CB-CG	8.57	121.17	112.60
1	C	338	ASN	CA-CB-CG	8.57	121.17	112.60
1	A	150	LEU	CD1-CG-CD2	-8.56	91.96	110.80
1	B	491	TRP	N-CA-C	8.56	122.52	112.93
1	C	37	PHE	N-CA-C	8.55	120.60	111.28
1	A	507	ILE	N-CA-C	8.55	120.32	112.29
1	C	272	ALA	N-CA-C	-8.55	100.42	112.13
1	B	47	THR	CA-CB-CG2	8.52	124.99	110.50
1	C	443	HIS	CA-CB-CG	8.52	122.32	113.80
1	C	649	ARG	CG-CD-NE	-8.49	93.33	112.00
1	D	385	GLU	CA-CB-CG	8.48	131.06	114.10
1	C	322	VAL	CA-C-O	-8.44	110.23	120.78
1	D	118	ASP	CA-CB-CG	8.44	121.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	GLN	OE1-CD-NE2	-8.44	114.17	122.60
1	C	244	TRP	CG-CD2-CE3	8.44	142.34	133.90
1	C	44	ASN	CA-CB-CG	8.43	121.03	112.60
1	C	413	ARG	N-CA-C	-8.43	101.12	111.40
1	D	325	ASN	N-CA-C	8.41	122.73	110.28
1	D	262	TYR	N-CA-C	8.40	122.23	107.61
1	A	727	ASN	CB-CG-ND2	8.39	128.99	116.40
1	C	101	ASN	CA-CB-CG	-8.37	104.23	112.60
1	A	406	ILE	N-CA-C	-8.36	101.58	110.36
1	B	266	VAL	N-CA-C	-8.36	102.28	110.72
1	A	661	ASP	N-CA-C	-8.35	102.91	113.43
1	B	555	VAL	N-CA-C	8.35	126.70	109.34
1	C	365	TRP	CG-CD2-CE3	8.34	142.24	133.90
1	C	435	ALA	N-CA-C	-8.33	96.50	109.25
1	D	534	VAL	CA-C-O	-8.33	112.75	121.41
1	D	80	LYS	N-CA-C	-8.32	98.16	110.48
1	C	231	PRO	N-CA-C	8.32	123.36	110.80
1	A	366	GLU	N-CA-C	-8.32	100.87	111.02
1	D	91	MET	N-CA-C	8.31	121.08	111.11
1	D	541	ASN	OD1-CG-ND2	-8.30	114.30	122.60
1	B	710	ILE	O-C-N	-8.29	115.35	122.65
1	C	592	LYS	N-CA-C	-8.29	102.33	111.36
1	D	37	PHE	N-CA-C	8.29	123.75	112.90
1	A	450	HIS	N-CA-C	8.28	122.16	112.72
1	B	221	VAL	N-CA-C	-8.28	96.08	108.17
1	D	160	ARG	N-CA-C	-8.26	95.77	109.07
1	C	19	ALA	N-CA-C	8.23	128.34	110.80
1	A	768	HIS	CA-CB-CG	8.23	122.03	113.80
1	A	235	ASN	CB-CG-ND2	8.23	128.74	116.40
1	D	42	ASP	CA-CB-CG	8.23	120.83	112.60
1	A	491	TRP	CG-CD2-CE3	8.22	142.12	133.90
1	A	329	PHE	N-CA-C	-8.21	101.00	112.17
1	D	154	ALA	N-CA-C	8.21	122.85	109.72
1	B	250	ASN	OD1-CG-ND2	-8.18	114.42	122.60
1	C	348	GLU	CA-C-O	-8.16	111.81	120.55
1	B	575	ARG	CB-CG-CD	-8.16	92.54	111.30
1	D	365	TRP	CG-CD2-CE3	8.15	142.06	133.90
1	A	825	TRP	CG-CD2-CE3	8.15	142.05	133.90
1	B	473	GLU	CA-CB-CG	-8.14	97.81	114.10
1	D	162	GLU	N-CA-C	8.14	120.16	111.28
1	D	567	VAL	O-C-N	8.13	130.43	122.30
1	B	561	SER	N-CA-C	8.12	121.07	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	486	ILE	N-CA-CB	-8.12	97.49	112.43
1	C	145	ASP	CA-CB-CG	8.12	120.72	112.60
1	C	338	ASN	OD1-CG-ND2	-8.11	114.49	122.60
1	A	352	VAL	CB-CA-C	-8.11	101.20	112.14
1	A	554	LYS	CA-C-O	-8.10	111.66	121.06
1	A	160	ARG	CB-CG-CD	-8.09	92.70	111.30
1	D	322	VAL	N-CA-C	8.09	121.00	106.61
1	C	509	GLU	CB-CG-CD	8.08	126.34	112.60
1	A	699	MET	N-CA-C	-8.07	100.83	111.24
1	D	30	ASN	CA-CB-CG	8.06	120.67	112.60
1	B	341	HIS	O-C-N	-8.05	114.02	120.38
1	B	385	GLU	N-CA-C	8.05	123.48	109.96
1	B	579	ASN	CB-CG-ND2	8.04	128.47	116.40
1	D	688	THR	N-CA-C	8.04	123.05	108.17
1	A	47	THR	CA-C-N	8.03	128.47	119.32
1	A	47	THR	C-N-CA	8.03	128.47	119.32
1	A	718	VAL	N-CA-C	-8.02	102.52	110.30
1	A	94	THR	O-C-N	-8.01	112.49	122.35
1	C	52	TYR	N-CA-C	-8.00	102.56	111.28
1	A	537	VAL	CA-C-O	-7.99	112.64	120.95
1	A	555	VAL	CB-CA-C	-7.99	98.19	111.29
1	C	165	ILE	N-CA-C	-7.99	96.81	108.23
1	C	380	ILE	CB-CA-C	7.99	119.52	110.89
1	D	563	PHE	O-C-N	7.98	132.68	122.87
1	D	496	ASN	CA-CB-CG	-7.97	104.63	112.60
1	A	326	PHE	CA-CB-CG	-7.97	105.83	113.80
1	C	516	ASP	CA-C-O	7.97	129.10	120.10
1	D	16	ARG	O-C-N	-7.96	113.56	122.08
1	B	253	ASN	OD1-CG-ND2	-7.94	114.66	122.60
1	D	746	SER	CA-CB-OG	-7.94	95.22	111.10
1	A	128	ASP	CA-CB-CG	7.94	120.54	112.60
1	C	777	TYR	N-CA-C	7.93	119.92	111.28
1	A	708	PHE	O-C-N	-7.93	112.92	123.23
1	B	555	VAL	CB-CA-C	-7.93	98.29	111.29
1	D	230	VAL	CA-C-O	7.93	124.06	119.94
1	C	239	ASN	CA-CB-CG	7.92	120.52	112.60
1	D	810	LYS	CA-CB-CG	7.91	129.91	114.10
1	A	355	ASP	CA-C-O	-7.90	112.50	120.80
1	D	554	LYS	CA-CB-CG	7.90	129.91	114.10
1	B	267	LEU	CA-C-O	-7.90	112.53	120.82
1	C	72	GLN	N-CA-C	-7.89	102.27	111.03
1	D	565	VAL	N-CA-C	7.89	120.22	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	60	ARG	N-CA-C	7.88	119.87	111.28
1	D	507	ILE	N-CA-C	7.87	125.71	109.34
1	D	603	VAL	CB-CA-C	-7.87	100.20	110.98
1	B	178	GLU	CA-C-O	-7.86	112.70	121.89
1	D	526	ASP	CA-CB-CG	-7.85	104.75	112.60
1	C	486	ILE	CA-C-O	-7.85	112.74	121.92
1	A	759	LYS	N-CA-C	7.84	119.83	111.28
1	D	760	ASP	CA-CB-CG	7.84	120.44	112.60
1	D	253	ASN	CA-CB-CG	7.83	120.42	112.60
1	D	713	MET	CG-SD-CE	-7.83	83.69	100.90
1	D	579	ASN	CA-CB-CG	7.82	120.42	112.60
1	A	387	TRP	CA-C-O	-7.81	112.81	119.76
1	A	325	ASN	O-C-N	7.81	132.53	122.93
1	B	486	ILE	CB-CG1-CD1	-7.81	97.40	113.80
1	B	365	TRP	CG-CD2-CE3	7.80	141.70	133.90
1	D	244	TRP	CG-CD2-CE3	7.78	141.68	133.90
1	B	626	ILE	N-CA-C	-7.78	102.75	110.30
1	A	403	ILE	N-CA-C	-7.77	102.70	110.62
1	A	258	ASN	CA-CB-CG	7.76	120.36	112.60
1	A	716	GLU	CA-CB-CG	7.76	129.62	114.10
1	D	733	ASP	CA-CB-CG	-7.75	104.85	112.60
1	A	690	GLY	CA-C-O	-7.74	114.06	121.49
1	D	94	THR	CA-CB-OG1	-7.74	97.99	109.60
1	A	439	ILE	N-CA-C	-7.74	97.34	108.48
1	D	443	HIS	CA-CB-CG	7.74	121.54	113.80
1	A	541	ASN	CB-CG-ND2	7.73	127.99	116.40
1	B	170	ILE	O-C-N	-7.70	112.94	122.57
1	C	560	ASN	N-CA-C	7.69	122.77	113.23
1	A	325	ASN	OD1-CG-ND2	-7.69	114.91	122.60
1	B	823	GLU	N-CA-C	7.68	121.91	112.23
1	C	641	ARG	CA-CB-CG	-7.68	98.73	114.10
1	C	654	GLU	CA-CB-CG	7.68	129.46	114.10
1	C	325	ASN	CB-CG-ND2	7.68	127.92	116.40
1	B	571	HIS	CB-CG-ND1	7.68	134.22	122.70
1	A	41	LYS	N-CA-C	-7.67	98.15	108.74
1	D	566	GLN	CA-CB-CG	7.67	129.44	114.10
1	C	306	ASP	N-CA-C	-7.66	103.01	111.36
1	A	699	MET	CA-CB-CG	7.66	129.42	114.10
1	D	295	GLN	OE1-CD-NE2	-7.66	114.94	122.60
1	B	455	VAL	CB-CA-C	7.65	123.84	111.29
1	A	649	ARG	O-C-N	-7.64	115.64	123.29
1	D	338	ASN	OD1-CG-ND2	-7.64	114.95	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	507	ILE	CB-CA-C	-7.64	98.75	111.29
1	C	662	LEU	N-CA-C	-7.64	96.94	109.40
1	A	118	ASP	CA-CB-CG	7.64	120.24	112.60
1	A	280	TYR	CA-C-O	7.64	126.89	119.55
1	A	490	ARG	NE-CZ-NH1	7.63	129.13	121.50
1	C	316	PHE	N-CA-C	-7.62	103.98	113.28
1	C	477	HIS	CA-CB-CG	7.62	121.42	113.80
1	C	252	PHE	CA-CB-CG	7.62	121.42	113.80
1	A	306	ASP	CA-CB-CG	7.62	120.22	112.60
1	C	807	THR	CB-CA-C	7.61	122.80	110.09
1	A	230	VAL	CB-CA-C	-7.61	102.43	111.18
1	D	247	LYS	CA-CB-CG	-7.60	98.90	114.10
1	D	522	LEU	N-CA-C	-7.60	102.94	111.07
1	B	309	ARG	N-CA-C	-7.59	102.69	110.97
1	A	653	ALA	CA-C-O	-7.59	112.78	120.90
1	B	374	TYR	N-CA-C	7.59	120.78	108.34
1	D	643	ILE	O-C-N	7.58	131.26	123.07
1	C	276	SER	N-CA-C	-7.57	103.61	112.92
1	B	553	TYR	O-C-N	-7.57	112.53	122.59
1	A	666	ILE	N-CA-C	7.55	125.04	109.34
1	C	797	TRP	N-CA-C	-7.54	102.66	111.03
1	C	327	ASP	CA-CB-CG	-7.53	105.07	112.60
1	D	21	VAL	CA-C-O	-7.53	111.37	120.78
1	A	803	ARG	CA-CB-CG	-7.52	99.05	114.10
1	B	485	GLY	CA-C-N	7.52	135.30	122.67
1	B	485	GLY	C-N-CA	7.52	135.30	122.67
1	C	95	LEU	O-C-N	-7.52	113.97	122.09
1	B	666	ILE	O-C-N	-7.51	113.18	122.57
1	A	251	ASP	CA-CB-CG	7.51	120.11	112.60
1	D	644	PHE	CA-CB-CG	-7.51	106.29	113.80
1	D	62	HIS	CA-CB-CG	-7.49	106.31	113.80
1	D	184	ARG	CB-CG-CD	-7.49	94.08	111.30
1	A	609	ALA	N-CA-C	7.49	120.15	111.02
1	C	766	MET	CG-SD-CE	7.49	117.37	100.90
1	B	814	ASP	CA-CB-CG	7.48	120.08	112.60
1	C	591	LYS	CB-CG-CD	-7.48	94.10	111.30
1	C	240	THR	N-CA-C	7.48	121.11	109.07
1	D	555	VAL	N-CA-C	7.46	124.86	109.34
1	B	258	ASN	CB-CG-ND2	7.46	127.59	116.40
1	D	228	THR	N-CA-C	-7.46	99.06	110.32
1	B	439	ILE	N-CA-C	-7.45	97.67	108.11
1	A	689	ILE	O-C-N	-7.45	115.23	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	ASN	N-CA-C	7.45	121.27	112.93
1	C	638	ASP	CA-CB-CG	7.44	120.04	112.60
1	C	516	ASP	CA-CB-CG	-7.42	105.18	112.60
1	B	689	ILE	O-C-N	-7.42	114.23	122.83
1	D	487	THR	N-CA-C	-7.40	98.89	109.62
1	C	366	GLU	N-CA-C	-7.40	103.15	111.07
1	C	118	ASP	CA-CB-CG	7.39	119.99	112.60
1	C	91	MET	N-CA-C	7.38	119.11	111.14
1	B	166	PHE	CA-CB-CG	7.38	121.18	113.80
1	A	238	VAL	O-C-N	-7.38	113.35	122.57
1	D	784	GLN	N-CA-C	-7.38	103.32	111.36
1	B	57	HIS	CA-C-O	-7.38	112.73	120.55
1	C	555	VAL	CB-CA-C	-7.38	99.19	111.29
1	D	552	GLU	N-CA-C	-7.37	94.90	108.02
1	A	622	LEU	N-CA-C	-7.37	102.85	111.03
1	B	634	PRO	N-CA-C	7.37	123.59	113.65
1	C	280	TYR	CA-CB-CG	-7.37	100.64	113.90
1	C	447	ALA	O-C-N	-7.37	114.14	122.09
1	B	509	GLU	CB-CG-CD	7.35	125.09	112.60
1	A	33	ARG	CA-C-O	-7.34	113.11	120.82
1	B	372	CYS	N-CA-C	7.34	121.64	109.46
1	D	708	PHE	O-C-N	-7.32	114.70	123.27
1	A	181	ASP	CA-C-O	7.32	129.59	121.39
1	A	495	CYS	N-CA-C	7.32	121.96	112.89
1	A	834	LEU	N-CA-C	-7.31	100.21	110.29
1	A	25	THR	CA-CB-OG1	-7.30	98.64	109.60
1	D	57	HIS	CB-CG-CD2	-7.30	121.70	131.20
1	D	93	ARG	N-CA-C	7.30	126.36	110.80
1	D	341	HIS	CB-CG-CD2	-7.30	121.71	131.20
1	C	491	TRP	CG-CD2-CE3	7.30	141.20	133.90
1	B	727	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	D	175	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	A	321	PRO	N-CA-C	7.28	127.47	112.47
1	A	80	LYS	CA-C-O	-7.26	112.46	120.81
1	A	491	TRP	N-CA-C	7.26	121.73	113.02
1	D	250	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	B	229	PRO	N-CA-C	7.25	122.37	110.55
1	A	254	LEU	N-CA-C	-7.24	103.55	113.18
1	A	733	ASP	CA-CB-CG	-7.24	105.36	112.60
1	C	647	ASN	CA-CB-CG	7.24	119.84	112.60
1	D	258	ASN	CA-CB-CG	7.24	119.84	112.60
1	A	351	ARG	N-CA-C	-7.23	103.33	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	ASN	N-CA-C	-7.22	98.37	109.64
1	A	274	ASN	N-CA-C	7.22	121.79	112.26
1	A	387	TRP	CA-C-N	7.21	127.20	119.78
1	A	387	TRP	C-N-CA	7.21	127.20	119.78
1	C	365	TRP	CB-CG-CD1	-7.20	116.10	126.90
1	D	804	ASN	CA-CB-CG	7.20	119.80	112.60
1	B	711	PHE	O-C-N	-7.20	116.50	123.26
1	B	101	ASN	OD1-CG-ND2	-7.19	115.41	122.60
1	A	159	ILE	N-CA-C	-7.18	99.63	109.55
1	A	579	ASN	CA-CB-CG	7.18	119.78	112.60
1	D	708	PHE	CA-CB-CG	7.17	120.97	113.80
1	A	689	ILE	N-CA-C	-7.17	98.00	108.89
1	D	249	PRO	O-C-N	-7.16	114.36	123.03
1	B	532	ARG	CA-CB-CG	7.16	128.42	114.10
1	B	252	PHE	CA-CB-CG	7.16	120.96	113.80
1	A	531	ILE	CA-C-O	-7.16	113.51	120.95
1	B	429	SER	N-CA-C	7.15	120.32	110.24
1	A	449	SER	N-CA-C	7.15	120.60	109.52
1	D	388	PRO	CA-C-O	-7.14	113.59	121.23
1	D	348	GLU	CB-CG-CD	7.13	124.73	112.60
1	A	38	THR	N-CA-C	-7.13	104.20	113.12
1	C	558	ASN	N-CA-C	-7.13	95.78	108.55
1	B	576	GLN	OE1-CD-NE2	-7.13	115.47	122.60
1	C	481	ASN	CB-CG-ND2	7.13	127.09	116.40
1	D	233	TYR	CB-CA-C	-7.12	98.88	110.77
1	D	733	ASP	N-CA-C	7.12	122.05	113.23
1	C	387	TRP	CG-CD2-CE3	7.11	141.01	133.90
1	D	326	PHE	CA-CB-CG	-7.11	106.69	113.80
1	D	233	TYR	N-CA-CB	7.11	121.31	109.94
1	C	754	GLN	CA-C-N	7.11	126.94	119.05
1	C	754	GLN	C-N-CA	7.11	126.94	119.05
1	B	75	TYR	CB-CA-C	7.10	123.70	110.70
1	C	661	ASP	N-CA-C	7.10	122.37	112.93
1	B	400	LEU	N-CA-C	-7.10	103.62	111.36
1	B	454	GLY	N-CA-C	-7.09	103.02	112.81
1	B	44	ASN	N-CA-C	-7.09	104.10	112.89
1	D	678	ASN	CA-CB-CG	7.08	119.69	112.60
1	B	157	TYR	O-C-N	-7.08	113.98	123.19
1	B	268	ASP	CA-CB-CG	7.08	119.68	112.60
1	B	487	THR	CA-C-N	7.08	126.78	119.56
1	B	487	THR	C-N-CA	7.08	126.78	119.56
1	B	253	ASN	CB-CG-ND2	7.08	127.02	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	764	MET	O-C-N	7.07	129.44	122.09
1	D	181	ASP	CA-CB-CG	7.07	119.67	112.60
1	D	338	ASN	CA-CB-CG	7.07	119.67	112.60
1	C	676	THR	CA-CB-OG1	-7.06	99.01	109.60
1	D	270	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	B	274	ASN	CA-CB-CG	7.06	119.66	112.60
1	B	247	LYS	CA-CB-CG	-7.06	99.98	114.10
1	A	229	PRO	CB-CA-C	7.05	120.80	110.85
1	B	124	GLU	CB-CG-CD	7.05	124.59	112.60
1	B	335	ILE	CA-C-O	-7.05	112.41	120.66
1	C	453	ASN	OD1-CG-ND2	-7.05	115.55	122.60
1	B	598	VAL	CB-CA-C	7.05	121.12	110.62
1	D	735	ILE	N-CA-C	7.05	124.10	108.88
1	A	235	ASN	OD1-CG-ND2	-7.04	115.56	122.60
1	C	31	PHE	N-CA-C	-7.04	103.30	110.97
1	D	574	LYS	CG-CD-CE	-7.04	95.11	111.30
1	A	771	PHE	N-CA-C	7.03	122.85	112.94
1	B	481	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	B	710	ILE	CA-C-O	-7.03	115.08	121.97
1	A	219	GLN	N-CA-C	-7.03	100.08	110.48
1	C	764	MET	CA-CB-CG	7.03	128.15	114.10
1	A	481	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	D	650	VAL	CG1-CB-CG2	-7.02	95.36	110.80
1	C	773	VAL	CA-CB-CG2	-7.02	98.47	110.40
1	C	239	ASN	O-C-N	-7.01	113.50	122.20
1	B	650	VAL	CA-C-O	-7.01	113.74	121.17
1	D	769	ASP	CA-CB-CG	7.01	119.61	112.60
1	C	731	TYR	N-CA-C	-7.00	103.65	111.28
1	A	652	LEU	N-CA-C	-7.00	102.73	112.45
1	A	389	VAL	CA-CB-CG2	6.99	122.29	110.40
1	C	92	GLY	O-C-N	-6.99	113.61	122.70
1	D	337	LEU	O-C-N	-6.99	112.97	122.48
1	A	728	ALA	N-CA-C	6.97	125.64	110.80
1	D	274	ASN	CB-CG-ND2	6.97	126.85	116.40
1	D	786	ARG	N-CA-C	-6.97	103.76	111.36
1	B	507	ILE	N-CA-C	6.97	119.59	112.90
1	B	365	TRP	CB-CG-CD1	-6.96	116.47	126.90
1	C	274	ASN	N-CA-C	6.96	121.71	112.25
1	B	324	THR	N-CA-C	-6.95	101.78	111.52
1	B	484	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	B	93	ARG	N-CA-C	6.95	125.60	110.80
1	D	763	ASN	CA-CB-CG	6.95	119.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	ILE	O-C-N	-6.94	115.00	121.94
1	D	555	VAL	CA-C-N	6.94	134.80	121.54
1	D	555	VAL	C-N-CA	6.94	134.80	121.54
1	B	541	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	D	727	ASN	CB-CG-ND2	6.92	126.78	116.40
1	C	235	ASN	OD1-CG-ND2	-6.92	115.69	122.60
1	A	707	ASN	CA-CB-CG	-6.90	105.70	112.60
1	C	646	GLU	CA-CB-CG	6.90	127.90	114.10
1	D	393	GLU	CB-CA-C	-6.90	99.12	110.85
1	B	258	ASN	N-CA-C	-6.89	103.85	111.36
1	A	329	PHE	CA-C-O	-6.89	112.79	119.13
1	B	761	ILE	CB-CA-C	-6.89	103.26	111.94
1	A	21	VAL	CA-C-O	-6.88	112.18	120.78
1	A	491	TRP	CB-CG-CD1	-6.88	116.58	126.90
1	D	225	PRO	N-CA-C	6.88	121.73	111.41
1	C	362	ASP	CA-CB-CG	-6.88	105.72	112.60
1	C	595	ASN	CA-CB-CG	6.88	119.48	112.60
1	A	644	PHE	CA-C-O	-6.88	113.77	120.92
1	B	808	SER	N-CA-C	6.87	120.77	112.38
1	D	177	GLU	CA-CB-CG	6.87	127.85	114.10
1	D	688	THR	CB-CA-C	-6.87	100.07	111.41
1	B	137	GLY	O-C-N	-6.87	115.53	122.19
1	A	16	ARG	CA-C-O	-6.87	113.55	120.90
1	C	597	PHE	CA-C-O	6.87	128.30	120.54
1	C	666	ILE	N-CA-C	6.87	123.62	109.34
1	B	175	GLN	CG-CD-NE2	6.84	126.66	116.40
1	A	679	MET	CG-SD-CE	-6.84	85.85	100.90
1	B	412	ASN	CA-CB-CG	-6.84	105.76	112.60
1	B	714	ARG	O-C-N	-6.84	113.20	122.36
1	C	633	ASP	CA-C-N	6.84	126.47	119.56
1	C	633	ASP	C-N-CA	6.84	126.47	119.56
1	D	602	THR	N-CA-C	-6.83	97.27	108.41
1	C	200	VAL	N-CA-C	-6.83	98.28	108.46
1	D	784	GLN	OE1-CD-NE2	-6.83	115.77	122.60
1	A	229	PRO	O-C-N	-6.83	114.46	123.06
1	D	623	ILE	CA-CB-CG2	-6.83	98.89	110.50
1	B	574	LYS	CG-CD-CE	-6.83	95.60	111.30
1	B	340	THR	N-CA-C	6.82	121.46	113.20
1	C	439	ILE	N-CA-C	-6.82	98.66	108.48
1	D	490	ARG	CG-CD-NE	-6.82	96.99	112.00
1	D	615	MET	N-CA-C	-6.82	103.54	110.97
1	B	766	MET	N-CA-C	6.81	119.54	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	B	650	VAL	CG1-CB-CG2	-6.81	95.82	110.80
1	C	239	ASN	N-CA-C	6.81	120.92	110.36
1	C	556	HIS	CA-CB-CG	-6.81	106.99	113.80
1	D	314	SER	CA-CB-OG	6.81	124.72	111.10
1	A	780	TYR	O-C-N	6.81	129.44	122.09
1	B	394	THR	CA-C-N	-6.80	110.66	122.36
1	B	394	THR	C-N-CA	-6.80	110.66	122.36
1	D	255	LYS	O-C-N	6.80	131.53	122.96
1	A	814	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	352	VAL	N-CA-CB	6.79	119.77	110.54
1	B	178	GLU	O-C-N	-6.79	114.74	122.68
1	B	410	PHE	N-CA-C	-6.79	103.81	111.14
1	B	664	GLU	N-CA-CB	-6.78	100.81	110.58
1	D	362	ASP	N-CA-CB	-6.78	99.86	110.30
1	D	450	HIS	CB-CG-CD2	-6.78	122.39	131.20
1	A	236	ASN	CA-CB-CG	-6.78	105.83	112.60
1	B	583	VAL	N-CA-C	-6.76	103.63	111.00
1	C	149	THR	OG1-CB-CG2	-6.75	95.79	109.30
1	C	529	ALA	N-CA-C	-6.75	102.53	111.24
1	C	610	ALA	N-CA-CB	6.75	122.39	110.37
1	D	365	TRP	CB-CG-CD1	-6.75	116.77	126.90
1	B	667	SER	CA-C-O	-6.75	113.60	121.16
1	A	403	ILE	O-C-N	-6.74	115.33	121.87
1	B	350	MET	CB-CA-C	-6.74	99.59	110.79
1	A	181	ASP	CA-CB-CG	6.74	119.34	112.60
1	B	824	ILE	CB-CA-C	-6.73	104.31	110.91
1	C	389	VAL	O-C-N	-6.73	114.19	121.80
1	C	530	PHE	CA-CB-CG	6.72	120.53	113.80
1	D	459	HIS	CA-C-O	-6.72	113.29	120.42
1	A	638	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	657	ILE	CA-C-O	-6.72	113.60	118.71
1	A	740	GLN	CA-CB-CG	6.72	127.54	114.10
1	B	97	ASN	CA-CB-CG	-6.72	105.88	112.60
1	C	73	HIS	CB-CG-CD2	-6.72	122.47	131.20
1	C	800	MET	CA-CB-CG	-6.72	100.67	114.10
1	A	336	GLN	CG-CD-NE2	-6.71	106.33	116.40
1	B	272	ALA	N-CA-C	-6.71	96.50	110.80
1	C	264	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	B	740	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	A	676	THR	N-CA-CB	-6.70	99.90	110.22
1	B	708	PHE	CA-CB-CG	-6.70	107.10	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	280	TYR	N-CA-C	6.70	120.10	109.64
1	B	610	ALA	N-CA-CB	6.70	122.29	110.37
1	A	509	GLU	CB-CG-CD	6.69	123.97	112.60
1	C	464	LYS	CB-CG-CD	-6.69	95.91	111.30
1	B	175	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	D	443	HIS	N-CA-C	-6.69	104.38	112.54
1	D	166	PHE	N-CA-C	6.68	119.44	110.35
1	A	510	GLU	N-CA-C	6.68	120.30	111.75
1	D	442	ALA	CA-C-O	-6.68	113.82	120.70
1	D	47	THR	CA-CB-OG1	-6.68	99.58	109.60
1	C	244	TRP	CB-CG-CD1	-6.67	116.89	126.90
1	D	641	ARG	N-CA-C	6.67	119.78	108.90
1	C	221	VAL	N-CA-C	-6.67	98.75	108.89
1	D	197	THR	O-C-N	-6.67	115.06	123.06
1	C	430	LEU	N-CA-C	-6.67	105.15	113.28
1	D	211	GLN	OE1-CD-NE2	-6.67	115.94	122.60
1	A	371	THR	O-C-N	-6.66	113.30	122.30
1	B	81	ARG	N-CA-C	-6.66	97.51	108.76
1	B	376	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	B	380	ILE	N-CA-CB	-6.66	101.89	111.21
1	B	161	TYR	N-CA-C	-6.66	98.35	109.07
1	B	81	ARG	CB-CG-CD	-6.66	95.99	111.30
1	D	563	PHE	CA-C-N	6.66	132.62	122.77
1	D	563	PHE	C-N-CA	6.66	132.62	122.77
1	A	757	LEU	O-C-N	-6.65	115.17	122.09
1	A	773	VAL	CA-C-O	-6.65	112.46	120.78
1	D	142	CYS	CB-CA-C	-6.65	99.75	110.79
1	A	804	ASN	CB-CA-C	-6.65	99.75	110.79
1	B	259	VAL	N-CA-C	6.65	123.17	109.34
1	C	114	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	C	235	ASN	CB-CG-ND2	6.65	126.37	116.40
1	A	236	ASN	N-CA-C	6.64	124.95	110.80
1	C	106	ASN	CA-C-O	-6.64	114.03	121.00
1	C	482	LYS	N-CA-C	-6.64	95.92	107.20
1	C	564	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	167	ASN	OD1-CG-ND2	-6.63	115.97	122.60
1	B	384	LEU	CA-C-O	-6.63	113.89	121.19
1	A	744	GLN	CG-CD-NE2	6.63	126.35	116.40
1	D	804	ASN	OD1-CG-ND2	-6.63	115.97	122.60
1	B	682	MET	CB-CG-SD	-6.63	92.81	112.70
1	A	571	HIS	CB-CG-ND1	6.62	132.63	122.70
1	D	746	SER	N-CA-C	6.62	120.82	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	773	VAL	CA-CB-CG1	6.62	121.65	110.40
1	A	274	ASN	CA-CB-CG	6.62	119.22	112.60
1	B	615	MET	N-CA-C	-6.62	103.76	110.97
1	C	193	ARG	CA-C-N	6.61	126.86	119.32
1	C	193	ARG	C-N-CA	6.61	126.86	119.32
1	D	809	GLY	N-CA-C	6.61	121.73	114.40
1	D	836	ALA	O-C-N	-6.61	113.72	121.32
1	C	97	ASN	N-CA-C	6.60	118.56	111.36
1	D	36	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	D	187	ASN	CA-C-N	6.60	126.29	119.56
1	D	187	ASN	C-N-CA	6.60	126.29	119.56
1	B	575	ARG	N-CA-C	6.60	120.28	111.30
1	D	789	ALA	CA-C-O	-6.59	113.84	120.90
1	A	167	ASN	CA-CB-CG	-6.59	106.01	112.60
1	D	445	CYS	CA-C-O	-6.59	113.56	120.55
1	A	180	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	792	LYS	CA-CB-CG	6.58	127.26	114.10
1	B	763	ASN	CA-CB-CG	-6.58	106.02	112.60
1	D	481	ASN	CB-CG-ND2	6.58	126.26	116.40
1	D	400	LEU	N-CA-C	-6.57	104.29	112.90
1	B	67	TRP	NE1-CE2-CZ2	-6.57	120.25	130.10
1	B	745	LEU	N-CA-C	-6.57	103.81	110.97
1	B	807	THR	N-CA-CB	-6.56	100.78	110.49
1	B	811	PHE	CA-CB-CG	-6.56	107.24	113.80
1	D	259	VAL	N-CA-C	6.56	122.98	109.34
1	A	558	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	A	98	THR	N-CA-CB	-6.55	100.47	110.16
1	A	676	THR	O-C-N	-6.55	114.56	122.22
1	B	812	SER	N-CA-C	-6.55	98.59	109.46
1	C	82	ILE	CB-CA-C	6.55	120.58	110.83
1	D	101	ASN	OD1-CG-ND2	6.54	129.14	122.60
1	A	12	GLN	CA-CB-CG	6.54	127.17	114.10
1	D	707	ASN	N-CA-C	6.54	121.11	113.20
1	C	757	LEU	CA-C-O	-6.53	113.91	120.90
1	D	467	ILE	O-C-N	-6.53	114.41	122.57
1	C	160	ARG	CB-CG-CD	-6.53	96.28	111.30
1	B	292	ARG	N-CA-C	-6.53	104.08	111.07
1	D	164	GLY	O-C-N	6.53	131.19	122.70
1	D	180	ASP	O-C-N	-6.53	114.67	122.63
1	A	505	GLU	CA-CB-CG	6.52	127.14	114.10
1	A	165	ILE	N-CA-C	-6.52	98.89	107.88
1	A	491	TRP	CE2-CD2-CG	-6.52	99.38	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	407	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	B	258	ASN	CA-C-O	6.51	127.33	120.42
1	D	589	ARG	CA-CB-CG	-6.51	101.07	114.10
1	B	296	GLU	N-CA-C	-6.51	103.81	111.03
1	A	430	LEU	O-C-N	-6.50	113.48	122.46
1	B	309	ARG	CA-C-O	-6.50	114.17	121.00
1	D	49	ARG	CA-CB-CG	6.50	127.10	114.10
1	D	708	PHE	N-CA-C	6.50	119.00	108.34
1	C	47	THR	CA-CB-OG1	-6.50	99.85	109.60
1	C	390	HIS	CA-CB-CG	6.50	120.30	113.80
1	B	174	TRP	CG-CD2-CE3	6.50	140.40	133.90
1	B	811	PHE	N-CA-C	6.50	120.51	112.59
1	C	258	ASN	N-CA-C	-6.50	101.62	111.56
1	B	554	LYS	CA-C-O	-6.49	113.72	120.99
1	D	89	PHE	O-C-N	-6.49	115.67	123.27
1	D	791	TYR	O-C-N	6.49	128.75	122.07
1	C	421	ASP	N-CA-C	-6.49	98.64	108.96
1	D	561	SER	N-CA-C	6.49	118.70	110.33
1	A	493	VAL	N-CA-C	6.48	116.62	110.53
1	A	782	LYS	CB-CG-CD	6.48	126.20	111.30
1	B	529	ALA	N-CA-C	-6.48	103.84	111.03
1	B	759	LYS	CB-CA-C	-6.48	99.67	110.68
1	B	786	ARG	N-CA-C	-6.47	104.14	111.07
1	A	206	VAL	O-C-N	6.47	129.97	123.18
1	C	776	ASP	CA-CB-CG	-6.46	106.14	112.60
1	B	93	ARG	CA-C-O	6.46	129.75	120.51
1	C	469	LYS	N-CA-C	6.46	120.26	112.38
1	D	569	ARG	CA-C-O	-6.46	114.04	121.15
1	B	598	VAL	O-C-N	-6.46	116.20	123.18
1	D	819	GLN	CB-CG-CD	-6.46	101.62	112.60
1	B	828	GLU	CA-C-O	-6.45	114.54	119.32
1	C	765	LEU	N-CA-CB	-6.45	100.63	110.12
1	D	615	MET	CA-C-O	-6.45	114.22	121.00
1	D	534	VAL	N-CA-C	-6.45	103.52	110.23
1	A	72	GLN	N-CA-C	-6.45	103.94	110.97
1	B	351	ARG	N-CA-C	-6.45	103.94	110.97
1	D	686	ALA	O-C-N	-6.45	114.85	123.23
1	B	615	MET	CA-C-O	-6.45	114.23	121.00
1	D	603	VAL	N-CA-CB	6.45	118.75	111.21
1	B	387	TRP	CA-C-N	6.44	127.89	119.84
1	B	387	TRP	C-N-CA	6.44	127.89	119.84
1	B	644	PHE	O-C-N	-6.43	115.88	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	ILE	O-C-N	-6.43	114.86	122.58
1	C	429	SER	N-CA-C	6.43	118.60	110.24
1	B	700	ALA	N-CA-C	-6.43	104.19	111.07
1	C	552	GLU	CA-C-N	6.43	133.82	121.54
1	C	552	GLU	C-N-CA	6.43	133.82	121.54
1	C	770	ARG	CA-CB-CG	6.43	126.95	114.10
1	A	737	GLU	CB-CA-C	-6.42	101.07	110.96
1	B	523	SER	O-C-N	-6.42	113.82	122.43
1	B	538	LYS	CB-CA-C	-6.42	100.13	110.79
1	C	766	MET	N-CA-C	6.42	118.36	111.36
1	D	793	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	C	459	HIS	CB-CG-CD2	-6.42	122.86	131.20
1	B	424	ARG	CB-CG-CD	-6.41	96.55	111.30
1	D	583	VAL	N-CA-C	-6.41	102.85	111.44
1	D	81	ARG	CA-C-N	-6.41	114.74	123.14
1	D	81	ARG	C-N-CA	-6.41	114.74	123.14
1	D	193	ARG	O-C-N	-6.41	115.60	121.37
1	A	59	VAL	CA-CB-CG1	6.41	121.30	110.40
1	C	754	GLN	N-CA-CB	6.41	119.80	111.40
1	D	808	SER	N-CA-C	6.41	120.20	112.38
1	C	610	ALA	N-CA-C	-6.40	95.66	109.81
1	B	708	PHE	O-C-N	-6.40	115.08	123.21
1	D	19	ALA	N-CA-C	6.40	118.92	108.55
1	C	341	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	C	201	HIS	CA-CB-CG	6.40	120.20	113.80
1	A	238	VAL	CG1-CB-CG2	-6.40	96.73	110.80
1	A	88	GLU	O-C-N	-6.39	116.13	123.42
1	B	611	PRO	N-CA-C	-6.39	101.15	111.19
1	C	170	ILE	N-CA-CB	-6.39	103.75	110.72
1	C	536	LYS	O-C-N	6.39	128.65	122.07
1	D	810	LYS	CG-CD-CE	6.39	125.99	111.30
1	A	95	LEU	N-CA-C	6.38	117.93	110.97
1	C	93	ARG	N-CA-CB	-6.38	99.70	110.49
1	C	230	VAL	CA-C-N	6.38	126.60	119.90
1	C	230	VAL	C-N-CA	6.38	126.60	119.90
1	D	768	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	B	723	GLN	CA-CB-CG	6.37	126.85	114.10
1	D	244	TRP	CB-CG-CD1	-6.37	117.34	126.90
1	D	828	GLU	CA-C-O	6.37	125.54	120.19
1	A	59	VAL	CA-CB-CG2	-6.37	99.57	110.40
1	B	778	GLU	CA-CB-CG	6.37	126.84	114.10
1	D	360	ASP	CA-CB-CG	6.37	118.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	339	ASP	O-C-N	-6.36	114.13	122.59
1	B	52	TYR	N-CA-C	-6.36	104.27	111.14
1	A	492	LEU	CA-C-O	-6.36	111.42	120.51
1	B	80	LYS	CG-CD-CE	-6.36	96.68	111.30
1	A	31	PHE	N-CA-C	-6.35	104.43	111.36
1	C	33	ARG	CB-CA-C	-6.35	100.91	110.88
1	C	77	LYS	CA-CB-CG	6.35	126.80	114.10
1	B	797	TRP	N-CA-C	-6.35	103.98	111.03
1	D	201	HIS	CA-CB-CG	-6.35	107.45	113.80
1	C	683	LEU	N-CA-C	6.35	124.32	110.80
1	B	750	PHE	CA-CB-CG	-6.34	107.46	113.80
1	B	336	GLN	N-CA-C	6.34	118.62	108.41
1	C	473	GLU	CA-CB-CG	-6.34	101.42	114.10
1	B	474	LEU	N-CA-C	-6.34	103.64	112.45
1	A	785	GLU	N-CA-C	-6.33	103.67	111.33
1	B	500	ALA	CA-C-N	6.33	129.09	120.54
1	B	500	ALA	C-N-CA	6.33	129.09	120.54
1	D	717	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	146	SER	CA-C-O	-6.33	114.38	120.90
1	D	68	ILE	CA-C-O	-6.33	114.46	121.17
1	B	563	PHE	O-C-N	6.33	130.65	122.87
1	C	511	TYR	CA-C-O	-6.32	113.80	120.63
1	C	565	VAL	N-CA-C	6.32	117.81	108.45
1	B	761	ILE	N-CA-C	-6.32	104.88	111.58
1	B	40	VAL	O-C-N	6.32	130.47	122.57
1	B	18	LEU	N-CA-C	6.31	119.70	112.57
1	A	63	LEU	CA-C-O	-6.31	114.20	120.70
1	A	144	LEU	CA-C-O	-6.31	113.86	120.55
1	C	102	LEU	N-CA-C	-6.31	104.90	112.59
1	D	36	HIS	N-CA-C	-6.31	104.29	112.68
1	A	138	ARG	CA-C-N	6.30	128.73	120.28
1	A	138	ARG	C-N-CA	6.30	128.73	120.28
1	B	100	VAL	N-CA-CB	6.30	117.92	110.55
1	B	210	SER	CA-CB-OG	6.30	123.70	111.10
1	D	619	ILE	O-C-N	-6.30	115.74	121.91
1	D	716	GLU	CB-CG-CD	6.30	123.31	112.60
1	B	69	ARG	CB-CG-CD	6.29	125.78	111.30
1	B	331	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	457	ARG	N-CA-C	6.29	117.81	111.07
1	B	633	ASP	CA-C-N	6.29	126.20	119.28
1	B	633	ASP	C-N-CA	6.29	126.20	119.28
1	C	109	ASP	N-CA-C	-6.29	104.35	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	ALA	N-CA-C	6.29	119.11	111.82
1	B	133	ASN	CA-CB-CG	6.29	118.89	112.60
1	B	154	ALA	N-CA-C	6.28	119.71	109.59
1	B	185	TYR	N-CA-C	-6.28	103.97	112.26
1	D	740	GLN	OE1-CD-NE2	-6.28	116.32	122.60
1	D	82	ILE	CB-CG1-CD1	6.28	126.98	113.80
1	A	571	HIS	CA-C-O	-6.27	114.08	121.16
1	C	598	VAL	N-CA-C	-6.26	99.10	108.12
1	A	45	VAL	N-CA-CB	-6.26	104.22	112.36
1	A	626	ILE	N-CA-C	-6.26	104.41	110.42
1	B	11	LYS	N-CA-C	6.26	124.13	110.80
1	B	803	ARG	CA-CB-CG	-6.26	101.58	114.10
1	B	174	TRP	CB-CG-CD1	-6.26	117.52	126.90
1	B	556	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	C	525	VAL	CB-CA-C	-6.25	103.70	112.14
1	C	541	ASN	CB-CG-ND2	6.25	125.78	116.40
1	B	708	PHE	CA-C-O	-6.25	114.08	120.71
1	B	470	ASP	CA-CB-CG	6.25	118.85	112.60
1	D	455	VAL	CB-CA-C	6.25	121.54	111.29
1	A	40	VAL	CA-C-O	6.25	128.59	120.78
1	B	166	PHE	N-CA-C	6.25	119.31	110.50
1	D	456	ALA	CA-C-O	-6.24	113.06	120.43
1	C	144	LEU	CA-C-O	-6.24	113.93	120.55
1	B	325	ASN	O-C-N	6.24	130.69	122.95
1	D	666	ILE	O-C-N	-6.24	114.77	122.57
1	C	33	ARG	N-CA-CB	6.23	119.05	110.01
1	A	167	ASN	CB-CG-ND2	6.23	125.75	116.40
1	B	68	ILE	CG1-CB-CG2	-6.23	92.01	110.70
1	C	552	GLU	N-CA-C	-6.23	94.48	107.37
1	A	604	MET	O-C-N	-6.22	116.05	123.27
1	B	235	ASN	CA-CB-CG	6.22	118.83	112.60
1	B	650	VAL	CB-CA-C	-6.22	104.00	111.97
1	C	701	GLU	O-C-N	-6.22	115.52	122.12
1	D	499	LEU	CB-CA-C	-6.22	98.40	110.46
1	B	740	GLN	CA-CB-CG	6.21	126.53	114.10
1	A	271	LEU	N-CA-C	-6.21	105.46	113.16
1	D	459	HIS	O-C-N	-6.21	115.07	122.15
1	C	160	ARG	NE-CZ-NH1	6.21	127.71	121.50
1	C	571	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	D	339	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	746	SER	O-C-N	-6.20	115.68	122.07
1	C	676	THR	CA-CB-CG2	6.20	121.04	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	579	ASN	N-CA-CB	-6.20	101.01	110.12
1	D	773	VAL	CA-CB-CG2	-6.20	99.86	110.40
1	C	325	ASN	N-CA-CB	6.19	119.30	109.51
1	D	38	THR	N-CA-C	-6.19	103.84	112.45
1	A	430	LEU	CD1-CG-CD2	-6.19	97.18	110.80
1	D	309	ARG	CA-C-O	-6.19	114.53	120.90
1	D	619	ILE	N-CA-C	6.19	116.36	110.42
1	A	576	GLN	OE1-CD-NE2	-6.18	116.42	122.60
1	D	512	ILE	CB-CG1-CD1	6.18	126.78	113.80
1	B	686	ALA	N-CA-C	-6.17	97.76	108.69
1	B	210	SER	N-CA-C	6.17	123.94	110.80
1	B	291	LEU	CA-C-O	-6.17	113.88	120.42
1	B	395	LEU	CA-C-N	-6.17	115.87	123.21
1	B	395	LEU	C-N-CA	-6.17	115.87	123.21
1	B	385	GLU	CA-CB-CG	6.17	126.44	114.10
1	C	224	MET	CA-C-N	6.17	126.68	120.14
1	C	224	MET	C-N-CA	6.17	126.68	120.14
1	C	428	MET	CA-CB-CG	-6.17	101.77	114.10
1	A	250	ASN	CA-C-N	6.17	129.68	120.31
1	A	250	ASN	C-N-CA	6.17	129.68	120.31
1	B	699	MET	N-CA-C	-6.16	104.47	112.23
1	D	530	PHE	CB-CA-C	-6.16	100.61	110.84
1	B	187	ASN	O-C-N	-6.16	114.32	121.47
1	D	487	THR	CA-C-N	6.16	126.34	119.32
1	D	487	THR	C-N-CA	6.16	126.34	119.32
1	D	611	PRO	N-CA-C	-6.16	101.52	111.19
1	B	100	VAL	CA-C-O	-6.16	114.64	121.17
1	A	389	VAL	CA-CB-CG1	-6.16	99.94	110.40
1	A	763	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	A	497	PRO	N-CA-C	-6.15	105.15	113.40
1	A	619	ILE	N-CA-CB	-6.15	103.35	110.55
1	D	454	GLY	N-CA-C	-6.15	103.81	112.60
1	B	96	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	C	291	LEU	CD1-CG-CD2	-6.15	97.28	110.80
1	C	453	ASN	CB-CG-ND2	6.15	125.62	116.40
1	A	260	GLY	CA-C-N	6.14	126.76	119.94
1	A	260	GLY	C-N-CA	6.14	126.76	119.94
1	D	85	LEU	CD1-CG-CD2	-6.14	97.29	110.80
1	D	680	LYS	CA-C-O	-6.14	114.37	120.82
1	B	558	ASN	CA-CB-CG	6.14	118.74	112.60
1	C	471	PHE	N-CA-C	-6.14	104.50	112.23
1	B	532	ARG	CA-C-O	-6.13	114.58	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	534	VAL	CG1-CB-CG2	-6.13	97.31	110.80
1	A	146	SER	CA-CB-OG	-6.13	98.85	111.10
1	D	530	PHE	N-CA-CB	6.13	120.14	109.72
1	D	494	LEU	N-CA-CB	-6.12	101.07	110.07
1	B	782	LYS	N-CA-C	-6.12	104.61	111.28
1	C	250	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	D	16	ARG	CA-C-O	-6.12	114.34	121.07
1	B	426	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	D	836	ALA	CA-C-O	-6.12	111.78	120.16
1	C	94	THR	CA-CB-OG1	-6.12	100.43	109.60
1	B	643	ILE	CB-CG1-CD1	-6.11	100.96	113.80
1	C	184	ARG	NE-CZ-NH2	-6.11	113.70	119.20
1	C	554	LYS	CA-C-O	-6.10	113.28	120.60
1	A	401	GLN	O-C-N	6.10	128.35	122.07
1	A	663	SER	CA-CB-OG	6.10	123.30	111.10
1	B	703	ALA	CA-C-O	6.10	126.89	119.38
1	D	224	MET	CA-C-N	6.10	126.07	120.03
1	D	224	MET	C-N-CA	6.10	126.07	120.03
1	A	240	THR	CA-C-N	-6.10	114.51	123.05
1	A	240	THR	C-N-CA	-6.10	114.51	123.05
1	D	533	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	556	HIS	CB-CG-ND1	6.10	131.84	122.70
1	A	62	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	B	101	ASN	CB-CG-ND2	6.09	125.54	116.40
1	B	614	HIS	N-CA-C	6.09	118.71	111.71
1	C	16	ARG	N-CA-C	6.09	123.76	110.80
1	C	676	THR	CB-CA-C	6.08	121.03	110.68
1	A	422	VAL	N-CA-C	-6.08	105.79	111.45
1	A	697	VAL	O-C-N	-6.08	114.97	122.57
1	C	180	ASP	CA-C-N	-6.08	113.03	122.16
1	C	180	ASP	C-N-CA	-6.08	113.03	122.16
1	C	70	THR	N-CA-C	-6.08	104.57	111.14
1	A	620	ILE	O-C-N	-6.08	115.97	121.87
1	A	756	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	262	TYR	N-CA-C	6.08	118.35	108.26
1	D	136	LEU	N-CA-CB	-6.08	100.54	110.14
1	D	537	VAL	N-CA-C	-6.08	103.91	110.23
1	C	387	TRP	CB-CG-CD1	-6.08	117.78	126.90
1	A	332	LYS	N-CA-C	6.07	119.43	112.57
1	B	44	ASN	CA-CB-CG	6.07	118.67	112.60
1	B	600	PRO	CB-CA-C	6.07	119.29	111.46
1	B	514	ASP	O-C-N	-6.07	116.24	123.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	797	TRP	N-CA-C	-6.07	104.36	110.97
1	C	684	ASN	CA-C-O	6.07	126.75	119.59
1	B	754	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	D	136	LEU	CA-C-N	6.06	126.55	119.94
1	D	136	LEU	C-N-CA	6.06	126.55	119.94
1	B	290	GLU	CB-CA-C	-6.06	98.71	110.46
1	D	716	GLU	CA-CB-CG	6.06	126.21	114.10
1	A	22	GLU	O-C-N	6.05	130.64	122.59
1	A	718	VAL	N-CA-CB	6.05	117.22	110.62
1	B	150	LEU	N-CA-C	-6.05	103.26	111.55
1	D	125	ILE	N-CA-C	-6.05	104.78	113.07
1	C	326	PHE	N-CA-C	-6.05	105.00	112.38
1	B	672	GLU	CA-C-O	6.04	128.61	121.36
1	C	486	ILE	N-CA-CB	-6.04	101.31	112.43
1	B	442	ALA	N-CA-C	-6.04	104.82	111.82
1	A	654	GLU	N-CA-C	6.04	120.37	113.19
1	C	558	ASN	CA-CB-CG	6.04	118.64	112.60
1	B	88	GLU	CA-CB-CG	6.03	126.16	114.10
1	C	750	PHE	CA-CB-CG	-6.03	107.77	113.80
1	D	567	VAL	CA-CB-CG1	-6.03	100.15	110.40
1	C	184	ARG	N-CA-C	6.03	123.63	110.80
1	C	611	PRO	N-CA-C	-6.03	101.73	111.19
1	A	571	HIS	CA-CB-CG	-6.02	107.78	113.80
1	D	399	HIS	CB-CG-CD2	-6.02	123.37	131.20
1	D	579	ASN	O-C-N	-6.02	115.33	122.20
1	B	678	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	C	475	GLU	CA-C-N	6.02	125.70	119.56
1	C	475	GLU	C-N-CA	6.02	125.70	119.56
1	D	47	THR	CA-CB-CG2	6.02	120.73	110.50
1	B	545	PHE	CA-CB-CG	-6.01	107.79	113.80
1	C	491	TRP	CE2-CD2-CG	-6.01	99.98	107.20
1	C	611	PRO	CB-CA-C	6.01	119.20	111.21
1	A	469	LYS	N-CA-C	6.01	118.32	111.11
1	B	36	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	D	380	ILE	CB-CA-C	6.01	116.53	110.94
1	A	542	LYS	CA-CB-CG	-6.01	102.09	114.10
1	D	217	ASP	N-CA-C	6.00	119.82	111.90
1	B	578	LEU	CA-C-O	6.00	127.30	121.00
1	D	646	GLU	CA-C-O	6.00	127.60	120.70
1	B	554	LYS	CA-CB-CG	6.00	126.09	114.10
1	A	452	VAL	N-CA-C	-5.99	99.85	108.48
1	A	831	ARG	N-CA-C	-5.99	105.80	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	PHE	N-CA-C	-5.99	103.65	111.74
1	B	623	ILE	CA-C-O	-5.99	114.11	120.64
1	D	13	ILE	N-CA-C	-5.99	97.99	107.15
1	A	63	LEU	N-CA-C	-5.99	104.67	111.14
1	A	690	GLY	O-C-N	-5.99	117.82	123.87
1	B	395	LEU	CA-CB-CG	5.99	137.25	116.30
1	C	620	ILE	O-C-N	-5.98	115.83	121.87
1	B	239	ASN	CA-CB-CG	-5.98	106.62	112.60
1	C	325	ASN	CA-C-O	5.98	127.58	120.70
1	D	731	TYR	N-CA-C	-5.98	104.67	111.07
1	B	610	ALA	CB-CA-C	-5.98	98.39	110.17
1	D	595	ASN	O-C-N	-5.98	115.00	122.24
1	C	325	ASN	CB-CA-C	-5.98	101.55	110.16
1	D	71	GLN	CA-C-O	-5.98	114.08	120.42
1	D	323	ARG	CB-CA-C	-5.98	101.49	111.23
1	D	761	ILE	CA-CB-CG2	-5.98	100.34	110.50
1	A	57	HIS	CB-CG-CD2	-5.97	123.43	131.20
1	C	555	VAL	N-CA-C	5.97	121.76	109.34
1	A	766	MET	N-CA-C	5.97	119.39	111.75
1	A	455	VAL	CB-CA-C	5.97	121.08	111.29
1	C	101	ASN	CB-CG-ND2	5.97	125.35	116.40
1	A	178	GLU	N-CA-C	-5.97	102.83	110.53
1	B	159	ILE	N-CA-CB	-5.97	101.38	111.23
1	B	300	VAL	N-CA-CB	-5.96	104.12	110.62
1	A	529	ALA	N-CA-C	-5.96	104.42	111.03
1	C	182	TRP	CD1-CG-CD2	5.96	115.83	106.30
1	C	461	GLU	CA-C-O	-5.96	114.11	120.42
1	D	555	VAL	CB-CA-C	-5.96	101.52	111.29
1	A	97	ASN	CB-CG-ND2	5.95	125.33	116.40
1	A	723	GLN	CA-C-O	-5.95	114.53	120.90
1	A	276	SER	CA-CB-OG	5.95	123.00	111.10
1	C	652	LEU	N-CA-CB	5.95	119.06	110.20
1	D	807	THR	CB-CA-C	5.95	121.14	109.72
1	B	67	TRP	CE2-CD2-CG	-5.95	100.07	107.20
1	A	323	ARG	CB-CA-C	-5.94	101.55	111.23
1	B	280	TYR	CA-CB-CG	-5.94	103.20	113.90
1	D	205	ARG	N-CA-CB	-5.94	101.00	111.39
1	A	303	THR	N-CA-CB	-5.94	101.46	110.07
1	B	579	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	C	215	TRP	CG-CD1-NE1	-5.93	102.49	110.20
1	D	45	VAL	CG1-CB-CG2	-5.93	97.75	110.80
1	D	491	TRP	N-CA-CB	-5.93	101.86	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	598	VAL	N-CA-CB	-5.93	101.07	111.39
1	A	678	ASN	CA-C-O	5.93	126.71	120.42
1	A	274	ASN	CA-C-O	5.93	127.72	120.55
1	A	514	ASP	O-C-N	-5.93	114.71	122.59
1	C	491	TRP	CB-CG-CD1	-5.92	118.02	126.90
1	B	280	TYR	N-CA-C	5.92	118.87	109.40
1	B	466	THR	CA-CB-OG1	-5.92	100.72	109.60
1	C	437	LYS	CB-CG-CD	-5.92	97.69	111.30
1	C	556	HIS	N-CA-CB	5.92	120.49	110.49
1	D	124	GLU	CB-CG-CD	5.92	122.66	112.60
1	D	811	PHE	CA-CB-CG	-5.92	107.89	113.80
1	A	187	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	D	206	VAL	N-CA-C	-5.91	99.22	107.80
1	B	184	ARG	N-CA-C	5.91	118.20	111.11
1	D	101	ASN	CB-CG-ND2	-5.91	107.53	116.40
1	B	563	PHE	CA-C-N	5.91	131.09	122.41
1	B	563	PHE	C-N-CA	5.91	131.09	122.41
1	A	33	ARG	N-CA-CB	5.91	118.58	110.01
1	B	211	GLN	N-CA-C	-5.91	105.73	113.17
1	B	760	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	575	ARG	O-C-N	-5.90	114.62	122.00
1	D	32	ASN	CA-CB-CG	-5.90	106.70	112.60
1	B	177	GLU	CA-CB-CG	5.90	125.91	114.10
1	A	75	TYR	N-CA-C	-5.90	104.20	111.40
1	A	374	TYR	N-CA-C	5.90	118.02	108.34
1	A	530	PHE	CA-C-O	-5.90	114.58	121.07
1	B	22	GLU	CA-C-O	5.90	128.95	120.51
1	D	762	VAL	CA-C-N	5.90	128.78	120.28
1	D	762	VAL	C-N-CA	5.90	128.78	120.28
1	A	473	GLU	O-C-N	-5.90	115.90	122.03
1	A	551	ARG	N-CA-C	5.90	120.09	113.01
1	C	321	PRO	N-CA-C	5.90	124.62	112.47
1	D	329	PHE	CA-CB-CG	5.89	119.69	113.80
1	D	755	PRO	CA-C-O	5.89	128.58	120.03
1	A	441	MET	N-CA-C	5.89	120.08	113.01
1	D	176	MET	N-CA-C	-5.89	99.40	109.24
1	C	478	LYS	CA-CB-CG	-5.89	102.33	114.10
1	C	554	LYS	CA-CB-CG	5.88	125.87	114.10
1	A	93	ARG	N-CA-C	5.88	123.33	110.80
1	B	272	ALA	CA-C-O	-5.88	112.10	120.51
1	C	322	VAL	O-C-N	-5.88	115.22	122.57
1	C	507	ILE	CB-CA-C	-5.88	104.46	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	TYR	CA-CB-CG	-5.88	103.32	113.90
1	B	80	LYS	N-CA-C	-5.88	101.15	109.96
1	D	386	ARG	CB-CG-CD	-5.88	97.79	111.30
1	A	233	TYR	CA-CB-CG	-5.87	103.33	113.90
1	D	250	ASN	CA-C-N	5.87	129.23	120.31
1	D	250	ASN	C-N-CA	5.87	129.23	120.31
1	C	572	GLU	N-CA-C	5.87	118.46	111.71
1	B	321	PRO	N-CA-C	5.86	124.55	112.47
1	A	258	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	C	702	GLU	N-CA-CB	5.86	119.95	110.40
1	C	771	PHE	N-CA-C	5.86	120.02	112.41
1	A	708	PHE	N-CA-C	5.86	118.95	109.40
1	A	564	ASP	O-C-N	-5.85	115.91	122.93
1	B	759	LYS	N-CA-CB	5.85	118.84	110.06
1	D	640	LEU	N-CA-C	5.85	118.73	107.44
1	A	101	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	77	LYS	CA-CB-CG	5.85	125.79	114.10
1	B	10	ARG	CB-CG-CD	5.84	124.74	111.30
1	B	417	ALA	N-CA-C	5.84	117.73	111.36
1	B	601	ARG	CA-CB-CG	-5.84	102.41	114.10
1	C	663	SER	CA-CB-OG	5.84	122.78	111.10
1	D	441	MET	N-CA-CB	-5.84	101.23	110.28
1	B	440	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	C	128	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	452	VAL	N-CA-C	-5.83	100.08	108.48
1	C	270	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	A	805	ILE	CA-C-O	-5.83	114.58	121.05
1	D	210	SER	N-CA-C	5.83	123.22	110.80
1	A	614	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	B	250	ASN	CB-CG-ND2	5.83	125.14	116.40
1	C	412	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	D	676	THR	N-CA-C	-5.83	104.29	111.40
1	A	95	LEU	CD1-CG-CD2	-5.83	97.98	110.80
1	A	45	VAL	N-CA-C	5.83	118.75	113.10
1	A	64	VAL	CB-CA-C	-5.82	104.19	112.22
1	C	672	GLU	N-CA-C	5.82	119.13	109.46
1	C	749	PHE	O-C-N	5.82	128.07	122.07
1	C	790	LEU	CA-C-O	-5.82	114.38	120.55
1	A	12	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	B	828	GLU	N-CA-C	5.82	117.32	109.24
1	C	553	TYR	O-C-N	-5.82	114.86	122.59
1	B	658	PRO	CA-N-CD	-5.81	103.86	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	PHE	CA-C-O	-5.81	114.35	120.63
1	D	236	ASN	CA-CB-CG	5.81	118.41	112.60
1	D	828	GLU	N-CA-C	-5.81	102.75	110.07
1	A	193	ARG	CG-CD-NE	-5.81	99.23	112.00
1	D	711	PHE	CA-C-N	5.81	132.79	121.41
1	D	711	PHE	C-N-CA	5.81	132.79	121.41
1	A	717	ASP	CA-CB-CG	5.80	118.41	112.60
1	B	496	ASN	CA-C-O	5.80	128.05	120.74
1	C	300	VAL	CA-C-N	5.80	127.98	120.44
1	C	300	VAL	C-N-CA	5.80	127.98	120.44
1	D	456	ALA	O-C-N	-5.80	116.87	123.48
1	D	493	VAL	CA-CB-CG1	-5.80	100.54	110.40
1	C	665	GLN	N-CA-C	5.80	119.49	111.55
1	C	463	LEU	N-CA-C	-5.80	104.87	111.07
1	A	160	ARG	N-CA-C	-5.79	99.74	109.07
1	B	278	VAL	N-CA-CB	-5.79	103.06	111.52
1	B	471	PHE	N-CA-C	-5.79	104.40	112.45
1	A	33	ARG	CB-CA-C	-5.79	101.79	110.88
1	A	817	ILE	CA-C-O	-5.79	115.09	121.29
1	A	454	GLY	O-C-N	-5.79	118.19	122.71
1	B	222	LEU	CD1-CG-CD2	-5.79	98.07	110.80
1	B	399	HIS	N-CA-C	-5.79	105.71	112.89
1	A	558	ASN	CA-C-N	5.79	125.41	119.56
1	A	558	ASN	C-N-CA	5.79	125.41	119.56
1	B	162	GLU	CA-CB-CG	-5.79	102.53	114.10
1	B	453	ASN	CA-CB-CG	5.79	118.39	112.60
1	A	808	SER	CB-CA-C	-5.78	101.14	110.74
1	B	365	TRP	CE2-CD2-CG	-5.78	100.26	107.20
1	C	546	ALA	N-CA-C	-5.78	104.33	111.33
1	D	832	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	A	767	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	B	493	VAL	N-CA-CB	-5.78	104.10	110.51
1	C	249	PRO	N-CA-C	-5.78	102.08	110.80
1	B	184	ARG	CB-CG-CD	-5.77	98.03	111.30
1	C	440	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	A	405	GLU	CA-C-N	5.77	128.04	120.60
1	A	405	GLU	C-N-CA	5.77	128.04	120.60
1	D	163	PHE	N-CA-C	5.77	119.29	112.72
1	A	34	HIS	CA-C-O	-5.76	114.31	120.42
1	D	759	LYS	CB-CA-C	-5.76	100.88	110.68
1	A	213	ALA	N-CA-C	-5.76	101.49	110.42
1	D	332	LYS	N-CA-C	5.76	120.59	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	554	LYS	CA-C-O	-5.76	114.54	120.99
1	A	780	TYR	CA-C-O	-5.76	114.77	120.70
1	B	767	HIS	O-C-N	-5.76	116.00	122.34
1	C	276	SER	N-CA-CB	-5.76	102.15	110.56
1	D	566	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	B	94	THR	N-CA-CB	-5.76	102.93	110.59
1	D	392	LEU	CA-C-N	5.76	128.46	120.29
1	D	392	LEU	C-N-CA	5.76	128.46	120.29
1	D	735	ILE	CA-C-N	5.75	125.43	119.05
1	D	735	ILE	C-N-CA	5.75	125.43	119.05
1	D	450	HIS	CB-CG-ND1	5.75	131.32	122.70
1	A	769	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	290	GLU	CA-CB-CG	5.75	125.59	114.10
1	D	493	VAL	O-C-N	-5.75	116.30	121.87
1	D	757	LEU	CA-C-O	-5.74	114.75	121.07
1	C	336	GLN	N-CA-C	5.74	118.09	107.99
1	A	610	ALA	N-CA-CB	5.74	120.58	110.37
1	C	533	ASP	CA-C-O	-5.74	114.47	120.55
1	B	658	PRO	CA-C-N	5.73	129.02	120.31
1	B	658	PRO	C-N-CA	5.73	129.02	120.31
1	C	660	ALA	N-CA-C	5.73	118.58	109.81
1	D	216	VAL	N-CA-CB	-5.73	105.81	112.34
1	D	268	ASP	N-CA-C	-5.73	104.94	111.07
1	A	459	HIS	CB-CG-ND1	5.73	131.29	122.70
1	A	47	THR	CA-CB-CG2	5.73	120.24	110.50
1	A	266	VAL	N-CA-C	-5.73	104.63	113.16
1	B	493	VAL	N-CA-C	5.73	116.37	110.36
1	B	31	PHE	CA-C-O	5.73	126.83	120.82
1	C	291	LEU	N-CA-C	-5.73	104.94	111.07
1	D	174	TRP	CB-CG-CD1	-5.72	118.31	126.90
1	C	13	ILE	CA-CB-CG2	-5.72	100.77	110.50
1	A	187	ASN	N-CA-C	-5.72	96.17	108.64
1	C	82	ILE	N-CA-CB	-5.72	103.47	111.25
1	B	313	SER	N-CA-C	5.72	117.38	111.03
1	B	603	VAL	N-CA-CB	-5.72	104.52	111.21
1	D	699	MET	N-CA-C	-5.72	104.97	111.14
1	A	541	ASN	CA-CB-CG	5.71	118.31	112.60
1	C	297	TYR	CA-C-N	5.71	128.73	120.79
1	C	297	TYR	C-N-CA	5.71	128.73	120.79
1	A	598	VAL	N-CA-C	-5.71	99.32	107.77
1	B	630	VAL	O-C-N	-5.71	116.23	121.94
1	D	178	GLU	O-C-N	-5.71	116.58	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	ASN	CB-CA-C	-5.71	99.38	110.46
1	C	464	LYS	CA-CB-CG	5.70	125.51	114.10
1	A	746	SER	N-CA-C	5.70	117.17	111.07
1	C	551	ARG	N-CA-C	5.70	120.51	113.50
1	B	25	THR	N-CA-CB	-5.70	101.71	110.20
1	B	643	ILE	CA-CB-CG1	-5.70	100.71	110.40
1	A	830	SER	N-CA-C	-5.70	98.66	110.80
1	C	182	TRP	CG-CD1-NE1	-5.70	102.79	110.20
1	D	743	GLU	N-CA-C	5.70	118.43	111.82
1	B	343	SER	N-CA-C	5.70	118.43	111.82
1	C	763	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	C	475	GLU	O-C-N	-5.69	116.62	121.23
1	C	11	LYS	CA-CB-CG	5.69	125.49	114.10
1	C	36	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	A	825	TRP	CB-CG-CD1	-5.69	118.36	126.90
1	D	322	VAL	CA-C-O	-5.69	114.54	120.51
1	C	221	VAL	O-C-N	-5.69	117.06	122.98
1	A	496	ASN	CA-CB-CG	-5.69	106.91	112.60
1	B	18	LEU	N-CA-CB	-5.69	101.92	110.91
1	D	811	PHE	CA-C-N	-5.69	113.98	122.74
1	D	811	PHE	C-N-CA	-5.69	113.98	122.74
1	C	13	ILE	N-CA-C	-5.68	97.17	106.32
1	C	823	GLU	CB-CG-CD	5.68	122.26	112.60
1	B	325	ASN	CB-CA-C	-5.68	101.04	109.90
1	D	180	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	815	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	A	797	TRP	CE2-CD2-CE3	5.68	124.48	118.80
1	A	687	LEU	CA-C-N	5.67	130.19	122.19
1	A	687	LEU	C-N-CA	5.67	130.19	122.19
1	B	493	VAL	CA-C-O	5.67	127.17	121.27
1	B	615	MET	N-CA-CB	5.67	118.19	109.91
1	B	164	GLY	O-C-N	5.67	130.07	122.70
1	A	389	VAL	CA-C-O	-5.67	114.64	120.71
1	D	294	LYS	CA-C-O	-5.67	114.87	120.82
1	A	653	ALA	N-CA-C	-5.66	104.31	111.11
1	B	260	GLY	CA-C-N	5.66	126.23	119.94
1	B	260	GLY	C-N-CA	5.66	126.23	119.94
1	D	273	GLU	CA-C-N	-5.66	114.11	122.83
1	D	273	GLU	C-N-CA	-5.66	114.11	122.83
1	C	346	ILE	O-C-N	-5.66	114.65	121.10
1	B	484	ASN	CA-CB-CG	5.66	118.26	112.60
1	C	270	ASN	CA-CB-CG	-5.66	106.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	237	VAL	N-CA-CB	5.66	117.78	110.99
1	D	174	TRP	CE2-CD2-CG	-5.66	100.41	107.20
1	D	320	ASP	CA-C-N	5.66	126.91	119.84
1	D	320	ASP	C-N-CA	5.66	126.91	119.84
1	D	449	SER	O-C-N	-5.65	116.03	123.21
1	A	267	LEU	CA-C-O	-5.65	114.88	120.70
1	C	368	THR	CA-C-O	-5.65	114.86	120.90
1	C	715	VAL	CB-CA-C	-5.64	104.75	111.97
1	D	747	SER	CA-C-O	5.64	126.20	119.60
1	A	126	GLU	CA-CB-CG	-5.64	102.81	114.10
1	B	241	MET	CA-CB-CG	-5.64	102.81	114.10
1	C	250	ASN	CA-CB-CG	5.64	118.24	112.60
1	D	71	GLN	N-CA-C	-5.64	105.21	111.36
1	A	564	ASP	N-CA-CB	-5.63	101.25	110.21
1	C	203	TYR	CB-CG-CD2	-5.63	112.35	120.80
1	D	367	VAL	N-CA-CB	-5.63	104.25	110.51
1	D	224	MET	CB-CA-C	-5.63	104.59	110.17
1	B	160	ARG	N-CA-C	-5.63	100.01	109.07
1	B	490	ARG	CG-CD-NE	-5.63	99.62	112.00
1	D	336	GLN	CB-CA-C	-5.63	101.78	110.78
1	A	143	PHE	CA-C-O	-5.62	113.75	120.10
1	B	668	THR	CA-C-O	-5.62	114.97	121.15
1	B	832	GLN	CG-CD-NE2	5.62	124.83	116.40
1	C	574	LYS	CA-C-O	5.62	126.48	119.12
1	D	190	GLU	CB-CG-CD	5.62	122.16	112.60
1	D	336	GLN	CA-C-O	-5.62	114.69	120.54
1	A	805	ILE	O-C-N	-5.62	116.06	121.90
1	B	664	GLU	N-CA-C	5.62	118.30	108.52
1	C	298	PHE	CA-CB-CG	5.62	119.42	113.80
1	C	781	VAL	O-C-N	5.62	128.47	122.06
1	D	402	ILE	CA-C-O	-5.62	115.11	120.95
1	A	146	SER	N-CA-C	-5.62	104.80	111.03
1	A	323	ARG	CA-CB-CG	5.62	125.33	114.10
1	A	510	GLU	CA-CB-CG	-5.62	102.87	114.10
1	B	200	VAL	N-CA-C	-5.62	99.97	108.17
1	C	175	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	D	244	TRP	CE2-CD2-CG	-5.62	100.46	107.20
1	A	613	TYR	N-CA-C	-5.61	99.98	108.67
1	A	622	LEU	N-CA-CB	5.61	118.11	109.98
1	A	412	ASN	CA-C-O	-5.60	114.55	120.55
1	B	660	ALA	CA-C-O	-5.60	114.37	120.81
1	A	362	ASP	CA-CB-CG	-5.60	107.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	VAL	CG1-CB-CG2	-5.60	98.48	110.80
1	A	189	TRP	CD2-CE2-CZ2	-5.60	116.80	122.40
1	B	602	THR	O-C-N	5.60	131.01	123.34
1	C	244	TRP	CE2-CD2-CG	-5.60	100.48	107.20
1	A	114	GLN	OE1-CD-NE2	-5.59	117.00	122.60
1	B	325	ASN	CA-C-O	5.59	127.30	120.92
1	C	103	ALA	CA-C-O	-5.59	112.51	120.51
1	D	240	THR	O-C-N	-5.59	116.22	122.93
1	D	590	ILE	O-C-N	-5.59	115.58	122.57
1	C	269	ARG	O-C-N	-5.59	116.10	122.08
1	C	773	VAL	N-CA-CB	-5.59	102.01	111.23
1	B	491	TRP	CB-CG-CD1	-5.58	118.53	126.90
1	C	700	ALA	N-CA-C	-5.58	104.83	111.03
1	A	737	GLU	N-CA-CB	5.58	118.06	109.91
1	B	208	HIS	CB-CG-CD2	-5.58	123.94	131.20
1	A	264	GLN	O-C-N	-5.58	115.01	122.43
1	D	556	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	B	113	TYR	N-CA-C	-5.58	105.12	111.14
1	D	118	ASP	CA-C-O	-5.58	114.74	120.54
1	C	702	GLU	CB-CA-C	-5.58	98.34	109.99
1	D	67	TRP	CG-CD2-CE3	5.58	139.47	133.90
1	D	702	GLU	N-CA-C	5.58	117.16	111.14
1	A	250	ASN	N-CA-C	5.57	119.73	111.87
1	A	516	ASP	CA-CB-CG	-5.57	107.03	112.60
1	B	302	ALA	N-CA-CB	-5.57	101.93	110.01
1	D	223	ALA	CA-C-O	-5.57	114.75	120.54
1	B	475	GLU	CA-C-N	5.57	125.24	119.56
1	B	475	GLU	C-N-CA	5.57	125.24	119.56
1	B	249	PRO	O-C-N	-5.57	116.30	123.03
1	C	422	VAL	N-CA-C	-5.57	107.02	111.81
1	A	486	ILE	O-C-N	-5.56	116.87	123.04
1	B	706	GLU	CB-CA-C	-5.56	100.34	110.63
1	C	331	ASP	N-CA-C	-5.56	106.46	113.18
1	C	792	LYS	CA-CB-CG	5.56	125.22	114.10
1	A	603	VAL	O-C-N	-5.56	116.16	122.94
1	B	556	HIS	CA-C-O	5.55	128.45	120.51
1	B	412	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	D	759	LYS	N-CA-CB	5.55	118.38	110.06
1	D	764	MET	N-CA-C	-5.54	105.14	111.07
1	A	365	TRP	CE2-CD2-CG	-5.54	100.55	107.20
1	B	724	ARG	CA-CB-CG	5.54	125.19	114.10
1	C	167	ASN	N-CA-C	-5.54	101.25	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	589	ARG	CB-CG-CD	5.54	124.05	111.30
1	D	792	LYS	CA-CB-CG	5.54	125.18	114.10
1	D	459	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	B	491	TRP	N-CA-CB	-5.54	102.92	110.56
1	C	68	ILE	N-CA-C	-5.54	104.93	110.30
1	D	12	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	A	555	VAL	CA-C-N	5.54	132.11	121.54
1	A	555	VAL	C-N-CA	5.54	132.11	121.54
1	A	586	LEU	CB-CA-C	-5.54	101.95	110.81
1	B	30	ASN	N-CA-CB	5.54	118.89	110.14
1	C	729	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	D	828	GLU	N-CA-CB	5.53	117.76	110.29
1	B	344	LEU	N-CA-C	-5.53	106.61	113.19
1	A	98	THR	O-C-N	-5.53	115.84	122.15
1	C	354	VAL	N-CA-C	-5.53	106.31	111.45
1	C	589	ARG	O-C-N	-5.53	116.12	122.09
1	D	492	LEU	CD1-CG-CD2	5.53	122.97	110.80
1	A	687	LEU	CA-C-O	-5.53	114.85	120.71
1	C	265	ALA	CA-C-N	5.53	129.82	120.64
1	C	265	ALA	C-N-CA	5.53	129.82	120.64
1	D	104	LEU	N-CA-C	5.53	122.57	110.80
1	D	596	LYS	CG-CD-CE	5.53	124.01	111.30
1	A	735	ILE	CA-C-N	5.53	125.05	119.19
1	A	735	ILE	C-N-CA	5.53	125.05	119.19
1	D	751	SER	CA-C-N	5.53	125.88	119.47
1	D	751	SER	C-N-CA	5.53	125.88	119.47
1	A	73	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	A	581	LEU	N-CA-C	-5.52	105.34	111.36
1	D	458	ILE	CB-CA-C	-5.52	104.69	112.14
1	C	280	TYR	O-C-N	5.52	126.30	121.39
1	D	198	LEU	CD1-CG-CD2	-5.52	98.65	110.80
1	B	498	GLY	CA-C-O	-5.52	115.36	121.05
1	C	644	PHE	N-CA-C	-5.52	98.76	108.20
1	D	570	ILE	O-C-N	-5.52	115.67	122.57
1	A	833	ARG	N-CA-C	-5.52	102.12	110.28
1	B	801	VAL	N-CA-CB	-5.52	102.13	111.23
1	B	800	MET	N-CA-C	-5.51	104.91	111.69
1	D	110	GLU	N-CA-C	-5.51	105.18	111.14
1	D	565	VAL	CA-C-O	5.51	126.84	120.67
1	B	631	ASN	CA-CB-CG	5.51	118.11	112.60
1	D	583	VAL	CA-C-O	-5.51	114.30	120.25
1	D	169	LYS	CG-CD-CE	5.50	123.96	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	LYS	CA-C-N	5.50	128.04	120.39
1	A	247	LYS	C-N-CA	5.50	128.04	120.39
1	A	365	TRP	NE1-CE2-CZ2	-5.50	121.84	130.10
1	D	160	ARG	CB-CG-CD	-5.50	98.64	111.30
1	C	572	GLU	O-C-N	-5.50	115.78	122.22
1	A	773	VAL	N-CA-C	-5.50	97.90	109.34
1	B	485	GLY	O-C-N	5.50	128.68	123.56
1	D	531	ILE	CA-C-O	-5.50	115.33	121.05
1	D	682	MET	CA-CB-CG	5.50	125.10	114.10
1	B	45	VAL	CA-C-O	5.49	127.65	120.78
1	C	182	TRP	CD2-CE2-CZ2	-5.49	116.91	122.40
1	C	525	VAL	O-C-N	5.49	127.20	121.87
1	C	773	VAL	CA-CB-CG1	5.49	119.73	110.40
1	D	186	GLY	O-C-N	-5.49	117.16	122.87
1	D	658	PRO	O-C-N	-5.49	115.64	122.23
1	B	665	GLN	N-CA-C	5.49	118.77	112.57
1	A	481	ASN	CB-CG-ND2	5.49	124.63	116.40
1	B	322	VAL	O-C-N	-5.49	115.71	122.57
1	B	467	ILE	N-CA-CB	-5.49	104.42	110.51
1	D	478	LYS	N-CA-C	-5.49	106.43	113.23
1	D	804	ASN	N-CA-C	-5.49	105.20	111.07
1	B	73	HIS	CA-C-O	-5.48	115.06	120.82
1	B	23	ASN	N-CA-C	-5.48	99.33	108.32
1	C	352	VAL	N-CA-CB	-5.48	102.18	111.23
1	D	613	TYR	CA-C-O	5.48	126.80	120.60
1	B	142	CYS	N-CA-C	-5.48	104.71	111.40
1	B	744	GLN	CG-CD-NE2	5.48	124.62	116.40
1	B	12	GLN	CB-CG-CD	-5.48	103.29	112.60
1	C	537	VAL	N-CA-C	-5.48	104.53	110.23
1	C	165	ILE	CB-CA-C	5.47	119.85	110.38
1	D	322	VAL	CB-CA-C	5.47	117.16	111.09
1	D	506	ARG	CA-C-O	-5.47	113.68	119.97
1	D	267	LEU	CA-C-O	-5.47	114.62	120.42
1	D	486	ILE	CB-CA-C	5.47	119.01	111.19
1	A	407	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	D	149	THR	N-CA-CB	-5.46	101.51	110.14
1	B	479	PHE	N-CA-C	5.46	117.63	108.23
1	C	33	ARG	N-CA-C	-5.46	105.22	111.07
1	A	184	ARG	CA-C-O	-5.46	112.70	120.51
1	B	89	PHE	N-CA-C	-5.46	98.30	108.02
1	B	322	VAL	CA-C-O	-5.46	113.95	120.78
1	D	163	PHE	CA-CB-CG	-5.46	108.34	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	574	LYS	N-CA-C	-5.46	105.75	112.90
1	B	665	GLN	N-CA-CB	-5.46	102.28	110.91
1	D	493	VAL	N-CA-CB	5.46	117.96	110.54
1	D	160	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	D	707	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	B	310	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	B	413	ARG	CB-CA-C	-5.45	102.28	110.90
1	C	176	MET	N-CA-C	-5.45	99.55	108.76
1	D	170	ILE	O-C-N	-5.45	114.74	122.76
1	B	446	ILE	CB-CG1-CD1	-5.45	102.36	113.80
1	B	220	VAL	CA-C-N	5.45	130.65	122.75
1	B	220	VAL	C-N-CA	5.45	130.65	122.75
1	B	323	ARG	CB-CA-C	-5.45	100.02	110.65
1	D	765	LEU	CB-CA-C	-5.45	101.64	110.79
1	B	430	LEU	O-C-N	-5.45	116.35	122.12
1	B	500	ALA	O-C-N	5.45	127.91	122.08
1	A	111	ALA	CA-C-O	-5.45	115.09	120.70
1	A	656	VAL	N-CA-CB	-5.45	102.68	110.52
1	B	174	TRP	CE2-CD2-CG	-5.45	100.67	107.20
1	C	720	ARG	CB-CA-C	-5.45	102.30	110.90
1	C	778	GLU	CA-CB-CG	5.45	124.99	114.10
1	C	602	THR	N-CA-CB	5.44	119.74	110.87
1	B	296	GLU	CA-C-O	-5.44	115.30	120.90
1	C	533	ASP	N-CA-C	-5.44	105.35	111.28
1	D	726	TYR	O-C-N	-5.44	115.75	122.82
1	D	73	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	B	704	GLY	O-C-N	5.44	129.77	122.70
1	D	556	HIS	CB-CG-ND1	5.44	130.86	122.70
1	A	47	THR	N-CA-CB	-5.43	103.53	109.72
1	D	240	THR	CA-C-O	-5.43	114.77	120.58
1	D	505	GLU	CA-CB-CG	5.43	124.97	114.10
1	D	676	THR	CB-CA-C	5.43	119.92	110.79
1	B	688	THR	N-CA-C	5.43	117.59	108.73
1	D	213	ALA	N-CA-C	-5.43	101.27	109.85
1	D	791	TYR	CA-C-N	5.43	131.91	121.54
1	D	791	TYR	C-N-CA	5.43	131.91	121.54
1	B	122	LEU	CA-C-O	-5.43	115.31	120.90
1	D	33	ARG	N-CA-CB	5.43	117.89	110.01
1	B	394	THR	CA-C-O	-5.43	115.12	120.82
1	B	405	GLU	CB-CG-CD	5.43	121.83	112.60
1	B	632	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	C	67	TRP	CE2-CD2-CG	-5.43	100.68	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	ASN	CB-CG-ND2	5.43	124.54	116.40
1	A	474	LEU	CA-CB-CG	5.43	135.30	116.30
1	A	18	LEU	N-CA-CB	-5.42	102.35	110.91
1	A	610	ALA	CB-CA-C	-5.42	99.49	110.17
1	D	647	ASN	N-CA-C	-5.42	103.81	111.56
1	D	172	GLY	CA-C-O	5.42	125.29	119.06
1	A	278	VAL	N-CA-C	5.42	116.17	108.42
1	B	313	SER	CA-CB-OG	5.42	121.93	111.10
1	C	340	THR	CA-CB-OG1	-5.42	101.47	109.60
1	D	346	ILE	CA-C-O	-5.42	112.69	119.95
1	B	591	LYS	CA-CB-CG	-5.42	103.27	114.10
1	B	16	ARG	N-CA-C	5.41	122.32	110.80
1	B	62	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	C	97	ASN	CA-CB-CG	-5.41	107.19	112.60
1	D	422	VAL	N-CA-C	-5.41	106.53	111.67
1	D	496	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	B	461	GLU	CA-C-O	-5.41	115.13	120.70
1	D	365	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	D	553	TYR	O-C-N	-5.41	115.40	122.59
1	C	182	TRP	CE2-CD2-CG	-5.40	100.72	107.20
1	D	372	CYS	N-CA-C	5.40	118.46	110.46
1	A	230	VAL	CA-C-O	-5.40	114.00	119.89
1	B	67	TRP	CB-CG-CD1	-5.40	118.80	126.90
1	C	365	TRP	CE2-CD2-CG	-5.40	100.72	107.20
1	D	477	HIS	CA-CB-CG	5.40	119.20	113.80
1	C	61	ASP	CA-C-N	5.40	127.78	120.44
1	C	61	ASP	C-N-CA	5.40	127.78	120.44
1	B	163	PHE	CA-CB-CG	-5.40	108.40	113.80
1	D	94	THR	CA-CB-CG2	5.40	119.68	110.50
1	B	467	ILE	N-CA-C	5.39	116.02	110.36
1	D	739	ARG	N-CA-C	-5.39	105.30	111.07
1	C	570	ILE	O-C-N	-5.39	115.83	122.57
1	D	526	ASP	N-CA-C	5.39	120.13	113.50
1	D	25	THR	N-CA-CB	-5.39	102.59	110.40
1	B	320	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	728	ALA	N-CA-C	5.39	122.28	110.80
1	B	209	THR	N-CA-C	5.39	117.53	107.99
1	B	326	PHE	N-CA-CB	-5.39	101.16	110.32
1	A	27	LEU	CA-C-O	-5.38	114.02	120.10
1	D	92	GLY	O-C-N	-5.38	115.70	122.70
1	A	42	ASP	CB-CA-C	5.38	121.72	111.17
1	A	490	ARG	CG-CD-NE	-5.38	100.16	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	667	SER	N-CA-CB	5.38	118.47	110.29
1	B	182	TRP	CE2-CD2-CG	-5.38	100.74	107.20
1	B	647	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	180	ASP	O-C-N	-5.38	115.52	122.56
1	C	602	THR	N-CA-C	-5.38	96.46	107.70
1	C	711	PHE	N-CA-C	5.38	115.34	108.24
1	C	295	GLN	CG-CD-NE2	5.38	124.46	116.40
1	C	661	ASP	CA-C-O	5.38	127.33	120.07
1	B	565	VAL	CA-C-O	5.37	126.69	120.67
1	D	72	GLN	CA-C-N	5.37	127.43	120.44
1	D	72	GLN	C-N-CA	5.37	127.43	120.44
1	D	159	ILE	N-CA-C	-5.37	100.89	109.17
1	D	264	GLN	CG-CD-NE2	5.37	124.46	116.40
1	D	558	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	438	ARG	CA-CB-CG	-5.37	103.36	114.10
1	C	201	HIS	O-C-N	-5.37	116.95	123.29
1	D	787	VAL	CG1-CB-CG2	-5.37	98.98	110.80
1	C	170	ILE	CB-CA-C	5.37	117.57	110.91
1	C	467	ILE	CA-C-O	-5.37	115.54	121.29
1	C	792	LYS	N-CA-CB	-5.37	101.42	110.49
1	B	383	ALA	CA-C-N	5.36	128.32	120.71
1	B	383	ALA	C-N-CA	5.36	128.32	120.71
1	C	718	VAL	O-C-N	5.36	127.36	121.83
1	A	584	ILE	N-CA-C	-5.36	106.03	113.00
1	A	211	GLN	CG-CD-NE2	5.36	124.44	116.40
1	A	255	LYS	O-C-N	5.36	130.01	122.77
1	A	486	ILE	N-CA-CB	-5.36	103.43	112.44
1	C	240	THR	CA-C-O	5.36	126.22	120.38
1	D	391	LEU	O-C-N	-5.36	115.68	122.17
1	C	387	TRP	CE2-CD2-CG	-5.36	100.77	107.20
1	D	371	THR	CA-C-O	-5.36	113.33	119.60
1	A	492	LEU	N-CA-C	-5.36	99.39	110.80
1	A	829	PRO	O-C-N	-5.36	115.41	122.64
1	B	323	ARG	CA-CB-CG	5.36	124.81	114.10
1	C	639	ARG	CA-C-O	5.36	125.55	119.18
1	C	677	GLY	CA-C-N	5.36	127.40	120.44
1	C	677	GLY	C-N-CA	5.36	127.40	120.44
1	B	759	LYS	CA-C-O	-5.35	114.85	120.63
1	A	47	THR	CA-CB-OG1	-5.35	101.57	109.60
1	A	431	VAL	N-CA-C	5.35	115.28	107.37
1	B	459	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	B	538	LYS	N-CA-CB	5.35	117.98	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	THR	CA-C-O	-5.35	115.19	120.70
1	A	336	GLN	CA-C-O	-5.34	114.64	120.36
1	C	646	GLU	N-CA-C	5.34	116.84	109.15
1	A	36	HIS	N-CA-C	5.34	117.91	111.40
1	A	325	ASN	CB-CG-ND2	5.34	124.41	116.40
1	A	654	GLU	CA-CB-CG	5.34	124.78	114.10
1	D	780	TYR	CB-CG-CD2	-5.34	112.79	120.80
1	A	598	VAL	N-CA-CB	-5.34	104.56	111.82
1	A	517	GLN	N-CA-CB	-5.33	101.25	110.32
1	D	525	VAL	N-CA-C	5.33	118.53	111.17
1	B	519	ARG	CB-CG-CD	5.33	123.56	111.30
1	C	769	ASP	O-C-N	-5.33	116.53	122.93
1	C	830	SER	O-C-N	-5.33	116.85	123.36
1	C	554	LYS	CB-CA-C	-5.33	98.56	109.38
1	D	78	ASP	N-CA-C	5.33	121.59	109.81
1	D	502	ILE	CA-CB-CG1	5.33	119.46	110.40
1	B	108	CYS	CA-C-O	-5.33	114.77	120.42
1	C	109	ASP	CA-CB-CG	-5.33	107.27	112.60
1	C	517	GLN	OE1-CD-NE2	5.33	127.93	122.60
1	C	575	ARG	N-CA-C	5.33	122.15	110.80
1	D	744	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	C	356	LEU	N-CA-C	5.33	116.89	111.14
1	A	354	VAL	O-C-N	5.33	129.23	122.57
1	B	318	CYS	N-CA-C	-5.32	104.91	111.40
1	A	546	ALA	N-CA-C	-5.32	105.56	111.36
1	A	402	ILE	N-CA-C	5.32	115.53	110.42
1	B	836	ALA	O-C-N	-5.32	115.20	121.32
1	C	533	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	85	LEU	O-C-N	-5.32	117.16	123.22
1	A	754	GLN	CA-C-N	5.32	126.48	119.84
1	A	754	GLN	C-N-CA	5.32	126.48	119.84
1	B	238	VAL	N-CA-C	-5.32	100.47	108.12
1	C	163	PHE	N-CA-C	5.32	119.74	112.88
1	D	441	MET	N-CA-C	5.31	117.98	111.82
1	B	305	GLN	N-CA-C	-5.31	105.53	112.23
1	D	462	ILE	CB-CG1-CD1	-5.31	102.65	113.80
1	D	361	TRP	CE2-CD2-CG	-5.31	100.83	107.20
1	D	695	ALA	O-C-N	5.31	127.54	122.07
1	C	821	ALA	CA-C-O	-5.31	115.42	121.00
1	D	321	PRO	CA-N-CD	-5.31	104.57	112.00
1	D	714	ARG	CB-CG-CD	5.31	123.51	111.30
1	C	717	ASP	CB-CA-C	-5.31	101.83	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	667	SER	CB-CA-C	-5.31	99.70	109.46
1	A	665	GLN	O-C-N	-5.31	115.53	122.59
1	C	514	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	241	MET	N-CA-C	-5.31	101.82	110.20
1	A	455	VAL	CA-C-O	5.30	127.41	120.78
1	A	455	VAL	CG1-CB-CG2	5.30	122.47	110.80
1	A	484	ASN	CA-CB-CG	-5.30	107.30	112.60
1	B	211	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	C	227	ASP	CB-CA-C	-5.30	100.54	109.72
1	D	618	MET	CA-CB-CG	-5.30	103.49	114.10
1	A	450	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	468	PHE	CA-CB-CG	-5.30	108.50	113.80
1	A	493	VAL	CA-C-O	5.30	126.94	121.05
1	C	617	LYS	CA-C-O	-5.30	114.93	120.55
1	D	374	TYR	N-CA-CB	-5.30	102.13	110.77
1	D	331	ASP	CA-CB-CG	5.30	117.90	112.60
1	D	467	ILE	CB-CG1-CD1	5.30	124.93	113.80
1	C	610	ALA	CB-CA-C	-5.30	99.73	110.17
1	D	226	TYR	CB-CA-C	-5.30	102.50	110.24
1	A	250	ASN	CA-C-O	5.30	127.16	120.65
1	A	280	TYR	N-CA-C	5.30	118.81	108.85
1	D	125	ILE	CA-CB-CG1	5.30	119.41	110.40
1	D	771	PHE	N-CA-C	5.30	120.40	113.30
1	B	671	THR	N-CA-C	5.29	119.84	112.90
1	A	175	GLN	O-C-N	5.29	129.23	123.04
1	B	670	GLY	N-CA-C	-5.29	108.04	114.92
1	A	174	TRP	CE2-CD2-CG	-5.29	100.85	107.20
1	C	389	VAL	CA-C-O	-5.29	114.76	120.47
1	C	816	THR	CA-CB-CG2	-5.29	101.51	110.50
1	D	654	GLU	O-C-N	-5.29	115.56	122.59
1	B	46	ALA	CA-C-N	5.29	130.38	121.92
1	B	46	ALA	C-N-CA	5.29	130.38	121.92
1	C	47	THR	CA-CB-CG2	5.29	119.49	110.50
1	C	804	ASN	CA-C-O	-5.29	115.25	120.80
1	A	338	ASN	CA-C-N	5.29	131.63	121.54
1	A	338	ASN	C-N-CA	5.29	131.63	121.54
1	B	158	GLY	O-C-N	-5.29	118.65	123.78
1	B	197	THR	N-CA-CB	-5.29	100.61	109.28
1	C	539	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	262	TYR	CA-C-O	5.28	127.39	120.15
1	B	292	ARG	N-CA-CB	5.28	117.67	110.01
1	C	387	TRP	CG-CD1-NE1	-5.28	103.34	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	778	GLU	CA-C-O	-5.28	115.47	120.90
1	C	834	LEU	N-CA-C	-5.28	103.00	109.65
1	A	509	GLU	CA-C-O	-5.28	114.83	120.42
1	A	646	GLU	CA-C-O	5.28	127.06	121.05
1	B	459	HIS	CB-CG-ND1	5.28	130.61	122.70
1	A	20	GLY	CA-C-N	5.27	131.46	121.97
1	A	20	GLY	C-N-CA	5.27	131.46	121.97
1	B	394	THR	CA-CB-OG1	-5.27	101.69	109.60
1	A	785	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	565	VAL	N-CA-CB	5.27	120.08	111.44
1	A	579	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	723	GLN	CA-CB-CG	5.27	124.63	114.10
1	C	706	GLU	CA-CB-CG	5.27	124.64	114.10
1	D	222	LEU	N-CA-C	5.26	118.39	109.76
1	C	215	TRP	N-CA-C	-5.26	100.59	108.96
1	A	576	GLN	O-C-N	-5.26	115.59	122.59
1	A	635	VAL	O-C-N	5.26	126.97	121.87
1	A	485	GLY	CA-C-N	5.26	130.99	122.68
1	A	485	GLY	C-N-CA	5.26	130.99	122.68
1	D	475	GLU	O-C-N	-5.25	116.70	121.17
1	A	556	HIS	CA-CB-CG	-5.25	108.55	113.80
1	C	426	ARG	O-C-N	-5.25	115.81	122.27
1	B	267	LEU	CA-CB-CG	-5.25	97.92	116.30
1	B	833	ARG	CB-CA-C	-5.25	102.00	110.77
1	C	761	ILE	N-CA-CB	5.25	116.58	110.65
1	A	478	LYS	N-CA-C	5.25	118.15	111.69
1	B	602	THR	N-CA-CB	5.25	119.25	110.59
1	B	269	ARG	CA-CB-CG	5.25	124.59	114.10
1	D	266	VAL	N-CA-C	-5.25	104.34	111.89
1	A	15	VAL	CA-C-N	5.25	127.62	120.54
1	A	15	VAL	C-N-CA	5.25	127.62	120.54
1	B	13	ILE	N-CA-C	-5.25	99.55	107.73
1	B	196	PHE	CA-CB-CG	5.25	119.05	113.80
1	C	575	ARG	O-C-N	-5.24	115.62	122.59
1	D	33	ARG	CB-CA-C	-5.24	102.65	110.88
1	C	664	GLU	N-CA-CB	-5.24	101.63	110.49
1	D	180	ASP	CA-C-O	-5.24	115.52	121.39
1	D	405	GLU	O-C-N	-5.24	116.09	122.22
1	A	495	CYS	CA-C-O	5.24	125.81	119.31
1	A	525	VAL	N-CA-C	5.24	116.59	110.62
1	D	181	ASP	N-CA-CB	5.24	116.92	110.53
1	A	534	VAL	O-C-N	-5.24	116.70	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	10	ARG	CA-C-O	-5.24	111.90	120.80
1	A	205	ARG	CB-CG-CD	-5.23	99.27	111.30
1	A	598	VAL	CB-CA-C	5.23	117.48	110.42
1	C	36	HIS	CB-CG-ND1	5.23	130.55	122.70
1	C	177	GLU	O-C-N	-5.23	117.12	123.13
1	C	230	VAL	N-CA-C	5.23	113.19	107.60
1	A	811	PHE	N-CA-C	5.23	119.62	112.88
1	B	622	LEU	O-C-N	5.23	127.67	122.08
1	C	108	CYS	CA-CB-SG	-5.23	102.38	114.40
1	C	119	MET	CA-CB-CG	-5.22	103.65	114.10
1	D	33	ARG	CA-C-O	-5.22	115.33	120.82
1	A	91	MET	CB-CG-SD	-5.22	97.03	112.70
1	C	565	VAL	CA-CB-CG2	5.22	119.28	110.40
1	A	273	GLU	CA-C-N	-5.22	114.87	122.86
1	A	273	GLU	C-N-CA	-5.22	114.87	122.86
1	B	10	ARG	O-C-N	-5.22	114.65	123.00
1	C	386	ARG	N-CA-C	5.22	116.55	107.93
1	A	515	LEU	N-CA-C	5.22	121.92	110.80
1	B	118	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	372	CYS	N-CA-C	5.22	118.62	110.32
1	C	556	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	C	791	TYR	O-C-N	5.22	127.65	122.12
1	C	95	LEU	CA-C-O	-5.22	115.33	120.70
1	C	215	TRP	CA-CB-CG	5.21	123.51	113.60
1	A	491	TRP	N-CA-CB	-5.21	102.91	110.47
1	D	234	ARG	O-C-N	-5.21	115.66	122.59
1	A	574	LYS	CA-C-N	5.21	133.01	124.31
1	A	574	LYS	C-N-CA	5.21	133.01	124.31
1	C	359	LEU	N-CA-C	-5.21	102.77	110.48
1	C	830	SER	N-CA-CB	-5.21	102.06	110.81
1	A	553	TYR	CA-CB-CG	5.21	123.28	113.90
1	B	309	ARG	N-CA-CB	5.21	117.52	109.91
1	A	243	LEU	CA-C-N	5.21	130.34	123.05
1	A	243	LEU	C-N-CA	5.21	130.34	123.05
1	A	427	ARG	O-C-N	-5.21	114.32	122.13
1	C	13	ILE	CB-CA-C	-5.21	105.99	112.45
1	A	388	PRO	CA-C-O	-5.20	115.52	121.56
1	C	13	ILE	CA-CB-CG1	5.20	119.25	110.40
1	D	602	THR	CA-C-N	5.20	129.56	122.90
1	D	602	THR	C-N-CA	5.20	129.56	122.90
1	B	707	ASN	N-CA-C	5.20	119.72	113.17
1	B	607	GLY	CA-C-O	5.20	126.48	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	583	VAL	N-CA-C	-5.20	105.33	111.00
1	A	300	VAL	CA-CB-CG2	-5.20	101.56	110.40
1	B	765	LEU	N-CA-C	-5.20	104.87	111.11
1	C	88	GLU	O-C-N	-5.20	116.22	123.34
1	D	679	MET	CA-C-N	5.20	127.20	120.44
1	D	679	MET	C-N-CA	5.20	127.20	120.44
1	A	558	ASN	CB-CA-C	5.19	115.60	109.47
1	C	94	THR	CA-CB-CG2	5.19	119.33	110.50
1	D	266	VAL	N-CA-CB	-5.19	100.50	110.78
1	D	556	HIS	N-CA-CB	5.19	119.26	110.49
1	A	197	THR	N-CA-CB	-5.19	102.42	110.04
1	A	701	GLU	O-C-N	-5.19	115.69	122.59
1	B	766	MET	CB-CA-C	-5.19	101.03	110.63
1	D	26	GLU	O-C-N	-5.19	116.24	122.15
1	D	502	ILE	CA-C-O	-5.19	115.74	121.29
1	B	768	HIS	CB-CG-CD2	-5.18	124.46	131.20
1	C	388	PRO	CA-C-O	-5.18	115.35	121.67
1	D	834	LEU	CA-C-N	5.18	126.32	119.84
1	D	834	LEU	C-N-CA	5.18	126.32	119.84
1	C	61	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	810	LYS	CG-CD-CE	5.18	123.21	111.30
1	C	832	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	B	241	MET	N-CA-C	-5.18	99.97	108.41
1	A	36	HIS	CA-CB-CG	-5.18	108.62	113.80
1	C	628	ASP	CB-CA-C	-5.18	102.20	110.79
1	A	533	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	627	GLY	CA-C-O	-5.17	114.81	120.40
1	A	750	PHE	N-CA-C	5.17	119.59	113.28
1	B	75	TYR	N-CA-CB	-5.17	102.50	110.20
1	C	666	ILE	O-C-N	-5.17	116.11	122.57
1	C	339	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	46	ALA	CA-C-N	5.16	133.20	123.55
1	A	46	ALA	C-N-CA	5.16	133.20	123.55
1	C	450	HIS	CB-CG-ND1	5.16	130.44	122.70
1	A	243	LEU	CA-CB-CG	5.16	134.36	116.30
1	B	373	ALA	CA-C-O	-5.16	115.08	121.11
1	C	706	GLU	CB-CA-C	-5.16	98.63	110.18
1	A	571	HIS	N-CA-CB	-5.15	102.61	110.85
1	B	552	GLU	N-CA-C	-5.15	97.50	107.44
1	B	611	PRO	N-CD-CG	-5.15	95.47	103.20
1	A	614	HIS	CA-CB-CG	5.15	118.95	113.80
1	B	396	LEU	O-C-N	-5.15	116.21	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	108	CYS	N-CA-C	5.15	117.63	111.71
1	D	815	ARG	N-CA-C	-5.15	105.31	111.03
1	B	486	ILE	O-C-N	-5.15	117.62	123.03
1	C	80	LYS	N-CA-C	-5.15	102.24	109.96
1	D	270	ASN	N-CA-C	5.15	116.97	111.36
1	D	814	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	403	ILE	CB-CG1-CD1	-5.14	103.00	113.80
1	B	676	THR	O-C-N	-5.14	115.44	122.33
1	C	84	TYR	CA-C-N	-5.14	116.15	122.84
1	C	84	TYR	C-N-CA	-5.14	116.15	122.84
1	D	690	GLY	N-CA-C	5.14	118.61	111.00
1	D	362	ASP	CB-CA-C	5.14	120.87	110.38
1	C	64	VAL	CA-C-N	5.14	125.64	119.94
1	C	64	VAL	C-N-CA	5.14	125.64	119.94
1	D	764	MET	O-C-N	5.14	127.36	122.07
1	B	188	PRO	CA-C-O	-5.14	111.13	118.89
1	D	795	ARG	CB-CG-CD	5.14	123.11	111.30
1	B	215	TRP	CG-CD1-NE1	-5.13	103.52	110.20
1	C	69	ARG	O-C-N	-5.13	116.68	122.12
1	A	163	PHE	N-CA-C	5.13	119.03	112.26
1	B	380	ILE	CB-CA-C	5.13	120.69	111.36
1	D	342	PRO	N-CA-C	5.13	120.60	113.98
1	A	396	LEU	CA-C-N	5.13	126.25	119.84
1	A	396	LEU	C-N-CA	5.13	126.25	119.84
1	B	540	GLU	CA-CB-CG	5.13	124.35	114.10
1	C	569	ARG	CB-CG-CD	-5.13	99.51	111.30
1	C	525	VAL	N-CA-CB	5.12	117.51	110.54
1	D	25	THR	CB-CA-C	5.12	117.28	109.34
1	A	580	CYS	N-CA-CB	5.12	117.83	110.20
1	C	425	LEU	CA-C-O	-5.12	115.42	120.90
1	B	820	TYR	O-C-N	5.12	127.41	122.09
1	D	604	MET	CG-SD-CE	5.12	112.16	100.90
1	A	25	THR	CA-CB-CG2	5.12	119.20	110.50
1	A	696	ASN	CB-CG-ND2	5.12	124.08	116.40
1	B	455	VAL	N-CA-C	5.12	119.98	109.34
1	C	571	HIS	CB-CG-ND1	5.12	130.38	122.70
1	B	641	ARG	CB-CG-CD	5.12	123.06	111.30
1	D	428	MET	CA-C-O	-5.12	113.29	119.27
1	A	537	VAL	N-CA-C	-5.11	105.40	110.62
1	A	413	ARG	CA-CB-CG	5.11	124.32	114.10
1	B	116	GLY	O-C-N	5.11	129.35	122.70
1	B	309	ARG	CB-CA-C	-5.11	103.09	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	600	PRO	CA-C-N	5.11	130.49	122.21
1	B	600	PRO	C-N-CA	5.11	130.49	122.21
1	A	18	LEU	N-CA-C	5.11	118.34	112.57
1	D	408	GLN	CB-CG-CD	-5.11	103.91	112.60
1	B	619	ILE	CA-C-O	-5.11	115.82	121.29
1	A	205	ARG	N-CA-C	-5.11	100.69	108.76
1	C	460	SER	CA-CB-OG	-5.11	100.88	111.10
1	D	730	GLU	N-CA-C	5.11	117.24	111.11
1	D	764	MET	CA-CB-CG	5.11	124.31	114.10
1	B	190	GLU	N-CA-C	5.10	118.39	110.17
1	B	197	THR	CA-C-O	-5.10	115.29	120.80
1	D	191	LYS	N-CA-C	-5.10	99.97	108.34
1	B	106	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	B	143	PHE	CA-CB-CG	5.10	118.90	113.80
1	B	508	GLY	CA-C-O	-5.10	117.31	122.56
1	D	390	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	D	730	GLU	CA-CB-CG	5.10	124.30	114.10
1	D	325	ASN	CA-C-O	5.10	126.87	121.16
1	D	820	TYR	CA-C-N	5.10	127.38	120.65
1	D	820	TYR	C-N-CA	5.10	127.38	120.65
1	A	407	ASN	N-CA-C	5.09	116.52	111.07
1	B	255	LYS	N-CA-C	5.09	116.49	109.15
1	B	646	GLU	N-CA-C	5.09	117.42	110.24
1	D	538	LYS	N-CA-CB	-5.09	102.37	110.22
1	D	756	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	86	SER	O-C-N	-5.09	117.68	123.48
1	B	491	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	718	VAL	O-C-N	5.09	127.18	121.94
1	D	799	ARG	CA-CB-CG	-5.09	103.92	114.10
1	C	307	ILE	CB-CA-C	-5.09	105.46	111.97
1	D	481	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	B	371	THR	OG1-CB-CG2	-5.09	99.13	109.30
1	B	676	THR	CA-CB-OG1	-5.09	101.97	109.60
1	D	585	THR	CA-CB-OG1	-5.09	101.97	109.60
1	D	813	SER	CA-CB-OG	5.09	121.28	111.10
1	D	693	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	658	PRO	CA-C-N	5.08	130.03	121.14
1	A	658	PRO	C-N-CA	5.08	130.03	121.14
1	A	660	ALA	CA-C-O	-5.08	115.26	121.36
1	D	647	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	A	481	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	265	ALA	N-CA-C	-5.08	107.59	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	567	VAL	CA-CB-CG2	5.08	119.03	110.40
1	C	723	GLN	CB-CG-CD	-5.08	103.97	112.60
1	B	661	ASP	N-CA-CB	5.08	117.82	110.26
1	C	70	THR	O-C-N	-5.08	116.61	122.09
1	C	814	ASP	N-CA-C	-5.08	105.93	111.82
1	D	168	GLN	CA-C-O	-5.08	114.90	120.69
1	C	564	ASP	O-C-N	-5.07	117.30	123.13
1	D	684	ASN	CA-C-O	5.07	126.52	120.53
1	A	758	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	767	HIS	N-CA-CB	-5.07	104.16	110.90
1	C	331	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	645	LEU	O-C-N	-5.07	116.57	122.96
1	A	824	ILE	N-CA-C	5.07	119.88	109.34
1	C	45	VAL	CB-CA-C	5.07	116.40	110.88
1	B	702	GLU	N-CA-C	5.07	116.61	111.14
1	C	189	TRP	CB-CG-CD1	-5.07	119.30	126.90
1	C	276	SER	CA-C-O	-5.07	113.63	119.56
1	D	735	ILE	CB-CG1-CD1	5.07	124.44	113.80
1	A	638	ASP	CA-C-O	5.06	125.65	119.78
1	A	371	THR	CA-CB-CG2	5.06	119.11	110.50
1	D	88	GLU	N-CA-C	-5.06	100.02	108.32
1	A	569	ARG	CB-CG-CD	-5.06	99.66	111.30
1	A	782	LYS	CA-C-O	-5.06	115.19	120.55
1	C	602	THR	CB-CA-C	-5.06	103.38	111.17
1	D	173	GLY	N-CA-C	-5.06	107.11	114.90
1	D	363	LYS	N-CA-C	-5.06	105.95	111.82
1	A	73	HIS	CB-CG-ND1	5.06	130.28	122.70
1	A	650	VAL	N-CA-C	5.06	116.39	110.62
1	C	806	ALA	CA-C-O	5.06	125.61	119.49
1	A	392	LEU	N-CA-C	-5.05	105.96	111.82
1	A	486	ILE	N-CA-C	-5.05	100.61	108.95
1	B	350	MET	N-CA-CB	5.05	117.55	110.12
1	C	557	ILE	O-C-N	-5.05	116.25	122.57
1	A	217	ASP	N-CA-C	5.05	118.41	111.54
1	A	574	LYS	CA-CB-CG	-5.05	104.00	114.10
1	B	49	ARG	CA-C-N	5.05	127.36	120.54
1	B	49	ARG	C-N-CA	5.05	127.36	120.54
1	D	581	LEU	N-CA-C	-5.05	105.69	111.14
1	A	292	ARG	CA-C-O	-5.05	115.70	121.00
1	D	83	TYR	O-C-N	-5.05	116.66	122.87
1	A	407	ASN	CA-C-O	-5.04	115.52	120.82
1	B	312	LYS	O-C-N	-5.04	116.77	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	571	HIS	CA-CB-CG	5.04	118.84	113.80
1	D	67	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	D	707	ASN	CA-C-N	5.04	129.88	122.77
1	D	707	ASN	C-N-CA	5.04	129.88	122.77
1	D	114	GLN	CA-CB-CG	-5.04	104.02	114.10
1	D	830	SER	CA-CB-OG	-5.04	101.02	111.10
1	B	66	ARG	N-CA-C	-5.04	107.13	113.28
1	C	708	PHE	CA-CB-CG	5.04	118.84	113.80
1	C	70	THR	OG1-CB-CG2	-5.04	99.22	109.30
1	B	183	LEU	CA-C-N	5.04	127.34	120.54
1	B	183	LEU	C-N-CA	5.04	127.34	120.54
1	D	87	LEU	N-CA-C	5.04	119.06	113.02
1	C	73	HIS	CB-CG-ND1	5.04	130.25	122.70
1	C	530	PHE	CA-C-O	-5.03	115.13	121.02
1	B	241	MET	CG-SD-CE	5.03	111.97	100.90
1	B	338	ASN	CB-CG-ND2	5.03	123.94	116.40
1	B	770	ARG	CA-CB-CG	5.03	124.16	114.10
1	A	229	PRO	N-CA-C	5.03	119.92	111.32
1	B	78	ASP	N-CA-C	5.03	120.92	109.81
1	B	93	ARG	CG-CD-NE	-5.03	100.94	112.00
1	C	559	PRO	CA-C-N	5.03	130.51	121.66
1	C	559	PRO	C-N-CA	5.03	130.51	121.66
1	B	90	TYR	CA-CB-CG	5.03	122.95	113.90
1	B	46	ALA	O-C-N	5.02	128.92	123.04
1	D	365	TRP	CG-CD1-NE1	-5.02	103.67	110.20
1	D	280	TYR	CA-CB-CG	-5.02	104.86	113.90
1	B	374	TYR	N-CA-CB	-5.02	102.89	110.77
1	B	535	ALA	CA-C-O	5.02	125.53	119.31
1	B	290	GLU	N-CA-CB	5.01	118.06	110.14
1	B	374	TYR	O-C-N	-5.01	117.40	123.27
1	A	202	PHE	CA-CB-CG	-5.01	108.79	113.80
1	B	201	HIS	CA-CB-CG	5.01	118.81	113.80
1	B	499	LEU	N-CA-CB	5.01	118.05	110.28
1	A	667	SER	CA-C-O	-5.01	115.55	121.16
1	B	654	GLU	CA-C-O	-5.01	113.34	120.51
1	C	266	VAL	CA-C-O	5.01	126.06	119.85
1	D	654	GLU	CA-CB-CG	5.01	124.12	114.10
1	D	812	SER	O-C-N	5.01	129.17	123.31
1	D	311	PHE	O-C-N	-5.01	116.88	122.09
1	A	491	TRP	CD1-CG-CD2	5.01	114.31	106.30
1	C	236	ASN	CA-C-O	-5.01	113.35	120.51
1	A	98	THR	CB-CA-C	5.00	119.36	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	784	GLN	N-CA-CB	-5.00	102.77	110.12
1	C	76	GLU	CB-CG-CD	5.00	121.10	112.60
1	A	482	LYS	CG-CD-CE	-5.00	99.80	111.30
1	B	174	TRP	CG-CD1-NE1	-5.00	103.70	110.20
1	D	169	LYS	O-C-N	-5.00	116.73	123.23
1	D	255	LYS	CB-CG-CD	5.00	122.80	111.30
1	D	650	VAL	CA-C-O	-5.00	115.75	120.95
1	D	665	GLN	O-C-N	-5.00	115.78	122.68

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 ⓘ

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	247	3
1	B	6693	0	6653	300	3
1	C	6693	0	6653	284	0
1	D	6693	0	6653	356	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	1	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	1	0
All	All	26960	0	26682	1167	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 22.

All (1167) 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:A:441:MET:HE3	1:A:444:LEU:HD12	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:692:MET:HE2	1:A:710:ILE:HG21	1.60	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:A:574:LYS:HZ2	1:A:672:GLU:CD	1.96	0.73
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:B:503:ILE:HG23	1:B:521:LEU:HD11	1.71	0.73
1:D:766:MET:HE3	1:D:774:PHE:CE2	2.23	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:766:MET:HE3	1:B:774:PHE:HE2	1.53	0.72
1:B:99:MET:HE1	1:B:119: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
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: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: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:C:96:GLN:HA	1:C:99:MET:HE3	1.75	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:91:MET:HE1	1:A:144:LEU:HD12	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:C:682:MET:HE3	1:C:807:THR:HG22	1.80	0.64
1:D:712:GLY:H	1:D:779:GLU:HG2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:798:THR:O	1:D:802:ILE:HG13	1.97	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
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:C:766:MET:HE3	1:C:774:PHE:HE2	1.65	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:D:91:MET:HE1	1:D:144:LEU:HD12	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ARG:HG2	1:B:153:ALA:CB	2.31	0.61
1:D:682:MET:HE2	1:D:808:SER:HA	1.83	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:A:565:VAL:HG12	1:A:604:MET:HE3	1.82	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:C:91:MET:HE1	1:C:144:LEU:HD12	1.84	0.60
1:C:421:ASP:CG	1:C:424:ARG:HB2	2.26	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: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:C:766:MET:HA	1:C:766:MET:CE	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:VAL:H	1:C:459:HIS:HD2	1.51	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:B:78:ASP:OD2	1:B:332:LYS:NZ	2.34	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
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:A:766:MET:HE3	1:A:774:PHE:CE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:363:LYS:HZ2	1:A:366:GLU:CD	2.12	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:699:MET:HE2	1:A:708:PHE:HZ	1.70	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
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:D:592:LYS:C	1:D:594:PRO:HD3	2.31	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:564:ASP:CG	1:C:601:ARG:HH21	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:456:ALA:C	1:B:481:ASN:HD21	2.14	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:A:766:MET:HE3	1:A:774:PHE:HE2	1.68	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
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:D:241:MET:HE3	1:D:243:LEU:HD21	1.89	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: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:766:MET:HA	1:B:766:MET:HE2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:LYS:HZ1	1:C:672:GLU:CD	2.16	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
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:B:255:LYS:O	1:B:256:ASP:HB2	2.07	0.53
1:D:732:TYR:CE1	1:D:739:ARG:HA	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PHE:HB3	1:A:147:MET:HE2	1.90	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
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: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:99:MET:HE1	1:A:119:MET:SD	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:49:ARG:NH2	1:D:125:ILE:O	2.43	0.52
1:D:99:MET:HE1	1:D:119:MET:SD	2.50	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:A:350:MET:SD	1:A:368:THR:OG1	2.62	0.51
1:A:609:ALA:HB2	1:A:620:ILE:HD12	1.91	0.51
1:B:592:LYS:NZ	1:B:593:GLU:CD	2.68	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:MET:HE3	1:C:774:PHE:CE2	2.45	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:D:575:ARG:HB3	1:D:666:ILE:HG13	1.92	0.51
1:C:198:LEU:HD13	1:C:305:GLN:CD	2.36	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:C:766:MET:HA	1:C:766:MET:HE2	1.93	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:357:GLU:O	1:C:358:ARG:HB2	2.10	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:314:SER:C	1:A:316:PHE:H	2.20	0.49
1:B:457:ARG:HA	1:B:481:ASN:ND2	2.27	0.49
1:B:682:MET:HE1	1:B:811:PHE:CE2	2.47	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:C:205:ARG:HH21	1:C:217:ASP:CG	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:165:ILE:HD11	1:C:281:PRO:C	2.37	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:A:253:ASN:C	1:A:254:LEU:HD12	2.38	0.49
1:A:714:ARG:H	1:A:717:ASP:CG	2.21	0.49
1:C:66:ARG:NH1	1:C:236:ASN:OD1	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:596:LYS:HD3	1:B:596:LYS:C	2.38	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:C:591:LYS:HZ2	1:C:633:ASP:CG	2.21	0.48
1:A:138:ARG:NH1	1:A:142:CYS:SG	2.87	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:O	1:D:493:VAL:HG12	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
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:A:764:MET:C	1:A:764:MET:SD	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:75:TYR:CE2	1:A:314:SER:OG	2.60	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:505:GLU:CD	1:A:506:ARG:HH21	2.22	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
1:B:21:VAL:O	1:B:23:ASN:N	2.48	0.47
1:B:730:GLU:O	1:B:734:ARG:HG3	2.15	0.47
1:B:732:TYR:HB2	1:B:766:MET:HE1	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:591:LYS:NZ	1:C:633:ASP:CG	2.73	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: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:253:ASN:C	1:D:254:LEU:HD12	2.39	0.47
1:D:515:LEU:O	1:D:518:LEU:HD23	2.15	0.47
1:D:682:MET:HE3	1:D:807:THR:HG22	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:ILE:HD11	1:B:783:CYS:HB3	1.97	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:604:MET:HE2	1:B:604:MET:HB2	1.71	0.46
1:B:615:MET:HE1	1:B:761:ILE:HA	1.98	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: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: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:A:22:GLU:CD	1:A:104:LEU:HA	2.41	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:96:GLN:HA	1:C:99:MET:CE	2.45	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
1:D:721:LEU:HD21	1:D:726:TYR:CD1	2.48	0.45
1:A:235:ASN:C	1:A:235:ASN:HD22	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:GLY:O	1:A:679:MET:HE3	2.16	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:529:ALA:O	1:D:530:PHE:C	2.60	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: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: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:D:789:ALA:O	1:D:792:LYS:NZ	2.49	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:456:ALA:C	1:C:481:ASN:HD21	2.25	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:314:SER:C	1:B:316:PHE:H	2.26	0.44
1:B:680:LYS:NZ	3:B:932:PDP:O3	2.50	0.44
1:D:192:ALA:HB1	1:D:224:MET:HE3	1.99	0.44
1:D:259:VAL:CG1	1:D:263:ILE:HA	2.48	0.44
1:B:350:MET:HE3	1:B:350:MET:HB3	1.80	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
1:C:417:ALA:C	1:C:419:PRO:HD3	2.42	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLN:NE2	1:C:267:LEU:HD22	2.33	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:D:227:ASP:CG	1:D:242:ARG:HH11	2.25	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: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:C:682:MET:CE	1:C:807:THR:HG22	2.47	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:572:GLU:H	1:B:613:TYR:HH	1.65	0.43
1:C:11:LYS:HB3	1:C:11:LYS:HE3	1.84	0.43
1:C:790:LEU:CD2	1:C:800:MET:HE2	2.48	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:B:726:TYR:HH	1:B:774:PHE:HB2	1.81	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:A:482:LYS:HZ2	1:A:823:GLU:CD	2.27	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:502:ILE:O	1:D:503:ILE:C	2.62	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:B:177:GLU:OE1	1:B:611:PRO:HB3	2.18	0.43
1:C:267:LEU:O	1:C:268:ASP:C	2.61	0.43
1:D:381:PRO:C	1:D:383:ALA:H	2.26	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:A:395:LEU:C	1:A:396:LEU:HD22	2.44	0.43
1:B:413:ARG:HH12	1:B:475:GLU:CD	2.26	0.43
1:B:565:VAL:HB	1:B:604:MET:HE2	2.00	0.43
1:D:567:VAL:HG12	1:D:606:GLY:HA3	2.01	0.43
1:A:95:LEU:HD22	1:A:99:MET:HE2	2.00	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: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:C:195:GLU:H	1:C:195:GLU:HG3	1.38	0.43
1:C:230:VAL:CG2	1:C:239:ASN:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:766:MET:CE	1:B:774:PHE:HE2	2.29	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:A:387:TRP:HA	1:A:387:TRP:CE3	2.54	0.42
1:A:682:MET:HE2	1:A:808:SER:HA	2.01	0.42
1:B:315:LYS:HZ1	4:B:920:IMP:HN1	1.66	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:C:759:LYS:NZ	1:C:763:ASN:OD1	2.48	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:C:722:ASP:OD2	1:C:772:LYS:NZ	2.50	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:182:TRP:H	1:B:182:TRP:CD1	2.36	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: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:519:ARG:HA	1:A:806:ALA:O	2.19	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
1:C:758:PHE:HB3	1:C:761:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:258:ASN:CG	1:B:259:VAL:HG13	2.44	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:591:LYS:NZ	1:D:633:ASP:CG	2.77	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:A:622:LEU:O	1:A:623:ILE:C	2.63	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: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:22:GLU:CD	1:B:104:LEU:HA	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:ASP:O	1:B:696:ASN:HB2	2.20	0.42
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:314:SER:C	1:D:316:PHE:H	2.27	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:642:VAL:C	1:C:643:ILE:HG13	2.44	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:455:VAL:HG22	1:D:484:ASN:CG	2.45	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:B:550:GLU:CD	1:B:556:HIS:H	2.28	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:679:MET:HE2	1:C:811:PHE:CD1	2.55	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:224:MET:HE2	1:D:226:TYR:CE1	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:HB	1:A:241:MET:HE3	2.01	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:D:322:VAL:HG22	1:D:325:ASN:ND2	2.36	0.41
1:D:650:VAL:CG2	3:D:934:PDP:H2A2	2.50	0.41
1:D:651:SER:HA	1:D:654:GLU:HG2	2.02	0.41
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:D:766:MET:HA	1:D:766:MET:HE2	2.02	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:91:MET:HE1	1:D:144:LEU:CD1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:692:MET:HE2	1:B:710:ILE:HG21	2.03	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
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: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:592:LYS:NZ	1:D:593:GLU:CD	2.79	0.41
1:D:597:PHE:HE2	1:D:792:LYS:CD	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:363:LYS:HZ1	1:D:366:GLU:CD	2.29	0.40
1:D:509:GLU:O	1:D:511:TYR:N	2.54	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:B:272:ALA:O	1:B:273:GLU:C	2.64	0.40
1:C:581:LEU:HD22	1:C:741:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:509:GLU:O	1:B:510:GLU:C	2.63	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:143:PHE:HB3	1:D:147:MET:HE2	2.04	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%)	1	6
1	B	820/828 (99%)	699 (85%)	83 (10%)	38 (5%)	2	6
1	C	820/828 (99%)	680 (83%)	107 (13%)	33 (4%)	2	8
1	D	820/828 (99%)	665 (81%)	117 (14%)	38 (5%)	2	6
All	All	3280/3312 (99%)	2720 (83%)	411 (12%)	149 (4%)	2	7

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	569 (80%)	143 (20%)	1	4
1	B	712/717 (99%)	574 (81%)	138 (19%)	1	5
1	C	712/717 (99%)	575 (81%)	137 (19%)	1	5
1	D	712/717 (99%)	549 (77%)	163 (23%)	1	3
All	All	2848/2868 (99%)	2267 (80%)	581 (20%)	1	4

All (581) 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
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	102	LEU
1	A	104	LEU
1	A	117	LEU
1	A	118	ASP
1	A	131	LEU
1	A	136	LEU
1	A	150	LEU
1	A	162	GLU
1	A	165	ILE
1	A	167	ASN
1	A	169	LYS
1	A	176	MET
1	A	177	GLU
1	A	187	ASN
1	A	191	LYS
1	A	195	GLU
1	A	205	ARG
1	A	221	VAL
1	A	225	PRO
1	A	234	ARG
1	A	235	ASN
1	A	237	VAL
1	A	242	ARG
1	A	245	SER
1	A	247	LYS

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Mol	Chain	Res	Type
1	A	251	ASP
1	A	255	LYS
1	A	256	ASP
1	A	266	VAL
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	322	VAL
1	A	323	ARG
1	A	324	THR
1	A	332	LYS
1	A	333	VAL
1	A	337	LEU
1	A	340	THR
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	467	ILE
1	A	478	LYS
1	A	481	ASN
1	A	486	ILE
1	A	487	THR
1	A	492	LEU

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Mol	Chain	Res	Type
1	A	516	ASP
1	A	521	LEU
1	A	522	LEU
1	A	523	SER
1	A	537	VAL
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	575	ARG
1	A	589	ARG
1	A	591	LYS
1	A	593	GLU
1	A	598	VAL
1	A	614	HIS
1	A	622	LEU
1	A	630	VAL
1	A	640	LEU
1	A	649	ARG
1	A	652	LEU
1	A	658	PRO
1	A	662	LEU
1	A	663	SER
1	A	665	GLN
1	A	672	GLU
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	715	VAL
1	A	717	ASP
1	A	727	ASN
1	A	733	ASP
1	A	753	LYS
1	A	754	GLN
1	A	755	PRO

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Mol	Chain	Res	Type
1	A	756	ASP
1	A	759	LYS
1	A	760	ASP
1	A	765	LEU
1	A	766	MET
1	A	782	LYS
1	A	792	LYS
1	A	794	PRO
1	A	800	MET
1	A	807	THR
1	A	810	LYS
1	A	815	ARG
1	A	817	ILE
1	A	828	GLU
1	A	833	ARG
1	A	834	LEU
1	B	10	ARG
1	B	12	GLN
1	B	15	VAL
1	B	16	ARG
1	B	18	LEU
1	B	43	ARG
1	B	47	THR
1	B	49	ARG
1	B	63	LEU
1	B	80	LYS
1	B	82	ILE
1	B	87	LEU
1	B	91	MET
1	B	95	LEU
1	B	104	LEU
1	B	112	THR
1	B	121	GLU
1	B	128	ASP
1	B	131	LEU
1	B	136	LEU
1	B	152	LEU
1	B	165	ILE
1	B	167	ASN
1	B	169	LYS
1	B	176	MET
1	B	177	GLU

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Mol	Chain	Res	Type
1	B	191	LYS
1	B	195	GLU
1	B	197	THR
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	247	LYS
1	B	250	ASN
1	B	251	ASP
1	B	254	LEU
1	B	255	LYS
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	304	LEU
1	B	313	SER
1	B	315	LYS
1	B	318	CYS
1	B	319	ARG
1	B	321	PRO
1	B	322	VAL
1	B	324	THR
1	B	327	ASP
1	B	356	LEU
1	B	358	ARG
1	B	361	TRP
1	B	368	THR
1	B	379	VAL
1	B	380	ILE
1	B	391	LEU
1	B	392	LEU
1	B	395	LEU
1	B	396	LEU
1	B	398	ARG

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Mol	Chain	Res	Type
1	B	400	LEU
1	B	441	MET
1	B	444	LEU
1	B	455	VAL
1	B	457	ARG
1	B	474	LEU
1	B	478	LYS
1	B	486	ILE
1	B	492	LEU
1	B	509	GLU
1	B	517	GLN
1	B	518	LEU
1	B	521	LEU
1	B	522	LEU
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
1	B	586	LEU
1	B	589	ARG
1	B	591	LYS
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	643	ILE
1	B	652	LEU
1	B	654	GLU
1	B	658	PRO
1	B	662	LEU
1	B	665	GLN

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Mol	Chain	Res	Type
1	B	666	ILE
1	B	676	THR
1	B	683	LEU
1	B	688	THR
1	B	697	VAL
1	B	705	GLU
1	B	708	PHE
1	B	714	ARG
1	B	717	ASP
1	B	721	LEU
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	787	VAL
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	B	834	LEU
1	C	10	ARG
1	C	12	GLN
1	C	15	VAL
1	C	16	ARG
1	C	18	LEU
1	C	24	VAL
1	C	40	VAL
1	C	42	ASP
1	C	43	ARG
1	C	47	THR
1	C	49	ARG
1	C	77	LYS
1	C	82	ILE
1	C	91	MET

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Mol	Chain	Res	Type
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	162	GLU
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	237	VAL
1	C	242	ARG
1	C	243	LEU
1	C	245	SER
1	C	247	LYS
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	290	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
1	C	322	VAL
1	C	324	THR

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Mol	Chain	Res	Type
1	C	327	ASP
1	C	332	LYS
1	C	337	LEU
1	C	358	ARG
1	C	378	THR
1	C	379	VAL
1	C	380	ILE
1	C	392	LEU
1	C	396	LEU
1	C	398	ARG
1	C	400	LEU
1	C	430	LEU
1	C	441	MET
1	C	444	LEU
1	C	455	VAL
1	C	473	GLU
1	C	474	LEU
1	C	486	ILE
1	C	487	THR
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	528	GLU
1	C	530	PHE
1	C	540	GLU
1	C	549	LEU
1	C	553	TYR
1	C	554	LYS
1	C	555	VAL
1	C	558	ASN
1	C	565	VAL
1	C	571	HIS
1	C	574	LYS
1	C	575	ARG
1	C	576	GLN
1	C	579	ASN
1	C	580	CYS
1	C	591	LYS

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Mol	Chain	Res	Type
1	C	593	GLU
1	C	598	VAL
1	C	622	LEU
1	C	629	VAL
1	C	630	VAL
1	C	640	LEU
1	C	646	GLU
1	C	658	PRO
1	C	662	LEU
1	C	663	SER
1	C	665	GLN
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	737	GLU
1	C	741	ILE
1	C	756	ASP
1	C	759	LYS
1	C	760	ASP
1	C	761	ILE
1	C	764	MET
1	C	765	LEU
1	C	766	MET
1	C	773	VAL
1	C	782	LYS
1	C	783	CYS
1	C	785	GLU
1	C	792	LYS
1	C	800	MET
1	C	801	VAL
1	C	807	THR
1	C	810	LYS
1	C	830	SER
1	C	833	ARG
1	D	12	GLN
1	D	16	ARG
1	D	18	LEU

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Mol	Chain	Res	Type
1	D	21	VAL
1	D	25	THR
1	D	45	VAL
1	D	47	THR
1	D	49	ARG
1	D	80	LYS
1	D	81	ARG
1	D	82	ILE
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	177	GLU
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	247	LYS
1	D	251	ASP
1	D	254	LEU
1	D	255	LYS
1	D	257	PHE
1	D	258	ASN
1	D	259	VAL
1	D	262	TYR

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Mol	Chain	Res	Type
1	D	266	VAL
1	D	267	LEU
1	D	269	ARG
1	D	274	ASN
1	D	275	ILE
1	D	276	SER
1	D	287	GLU
1	D	290	GLU
1	D	291	LEU
1	D	292	ARG
1	D	304	LEU
1	D	308	ILE
1	D	313	SER
1	D	315	LYS
1	D	319	ARG
1	D	321	PRO
1	D	322	VAL
1	D	323	ARG
1	D	324	THR
1	D	332	LYS
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	379	VAL
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	398	ARG
1	D	400	LEU
1	D	441	MET
1	D	444	LEU
1	D	455	VAL
1	D	460	SER

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Mol	Chain	Res	Type
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	510	GLU
1	D	518	LEU
1	D	521	LEU
1	D	522	LEU
1	D	527	ASP
1	D	530	PHE
1	D	532	ARG
1	D	537	VAL
1	D	538	LYS
1	D	540	GLU
1	D	543	LEU
1	D	549	LEU
1	D	554	LYS
1	D	555	VAL
1	D	561	SER
1	D	565	VAL
1	D	567	VAL
1	D	574	LYS
1	D	575	ARG
1	D	576	GLN
1	D	579	ASN
1	D	591	LYS
1	D	594	PRO
1	D	598	VAL
1	D	602	THR
1	D	603	VAL
1	D	604	MET
1	D	621	LYS
1	D	622	LEU
1	D	629	VAL
1	D	636	VAL
1	D	640	LEU
1	D	642	VAL
1	D	652	LEU
1	D	658	PRO
1	D	662	LEU

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Mol	Chain	Res	Type
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	714	ARG
1	D	717	ASP
1	D	727	ASN
1	D	740	GLN
1	D	741	ILE
1	D	742	ILE
1	D	756	ASP
1	D	759	LYS
1	D	760	ASP
1	D	761	ILE
1	D	764	MET
1	D	765	LEU
1	D	766	MET
1	D	773	VAL
1	D	782	LYS
1	D	785	GLU
1	D	787	VAL
1	D	792	LYS
1	D	800	MET
1	D	802	ILE
1	D	807	THR
1	D	810	LYS
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 (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	167	ASN
1	A	168	GLN
1	A	211	GLN

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Mol	Chain	Res	Type
1	A	235	ASN
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	517	GLN
1	A	541	ASN
1	A	566	GLN
1	A	740	GLN
1	A	744	GLN
1	A	793	ASN
1	B	12	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	412	ASN
1	B	453	ASN
1	B	459	HIS
1	B	481	ASN
1	B	517	GLN
1	B	541	ASN
1	B	576	GLN
1	B	665	GLN
1	B	707	ASN
1	B	744	GLN
1	C	34	HIS
1	C	168	GLN
1	C	211	GLN
1	C	219	GLN
1	C	235	ASN
1	C	270	ASN
1	C	336	GLN
1	C	338	ASN
1	C	377	HIS
1	C	399	HIS

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Mol	Chain	Res	Type
1	C	450	HIS
1	C	453	ASN
1	C	459	HIS
1	C	481	ASN
1	C	566	GLN
1	C	576	GLN
1	C	579	ASN
1	C	665	GLN
1	C	744	GLN
1	D	30	ASN
1	D	71	GLN
1	D	167	ASN
1	D	168	GLN
1	D	235	ASN
1	D	274	ASN
1	D	336	GLN
1	D	377	HIS
1	D	390	HIS
1	D	412	ASN
1	D	453	ASN
1	D	459	HIS
1	D	481	ASN
1	D	576	GLN
1	D	614	HIS
1	D	647	ASN
1	D	665	GLN
1	D	744	GLN
1	D	754	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 oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PDP	B	932	1	18,19,20	2.02	4 (22%)	26,29,30	1.41	5 (19%)
2	SO4	C	900	-	4,4,4	0.22	0	6,6,6	0.52	0
4	IMP	D	920	-	25,25,25	1.35	3 (12%)	37,38,38	1.51	5 (13%)
3	PDP	A	931	1	18,19,20	2.15	2 (11%)	26,29,30	1.32	4 (15%)
2	SO4	D	900	-	4,4,4	0.11	0	6,6,6	0.40	0
4	IMP	B	920	-	25,25,25	1.60	4 (16%)	37,38,38	1.83	7 (18%)
2	SO4	B	900	-	4,4,4	0.35	0	6,6,6	0.53	0
3	PDP	D	934	1	18,19,20	2.77	4 (22%)	26,29,30	1.17	3 (11%)
4	IMP	A	920	-	25,25,25	1.68	5 (20%)	37,38,38	1.75	7 (18%)
3	PDP	C	933	1	18,19,20	1.35	3 (16%)	26,29,30	1.16	3 (11%)
4	IMP	C	920	-	25,25,25	1.55	6 (24%)	37,38,38	1.81	9 (24%)
2	SO4	A	900	-	4,4,4	0.34	0	6,6,6	0.42	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
3	PDP	B	932	1	-	4/12/12/14	0/1/1/1
4	IMP	D	920	-	-	1/10/26/26	0/3/3/3
3	PDP	A	931	1	-	5/12/12/14	0/1/1/1
4	IMP	B	920	-	-	1/10/26/26	0/3/3/3
4	IMP	A	920	-	-	0/10/26/26	0/3/3/3
3	PDP	D	934	1	-	5/12/12/14	0/1/1/1
3	PDP	C	933	1	-	5/12/12/14	0/1/1/1
4	IMP	C	920	-	-	0/10/26/26	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	934	PDP	PA-O3A	9.31	1.69	1.59
3	A	931	PDP	PA-O3A	7.41	1.67	1.59
3	D	934	PDP	C3-C2	-5.04	1.35	1.41
3	B	932	PDP	C3-C2	-4.66	1.36	1.41
4	A	920	IMP	O6-C6	4.49	1.32	1.23
4	C	920	IMP	O6-C6	4.39	1.31	1.23
4	D	920	IMP	O6-C6	3.87	1.30	1.23
3	B	932	PDP	PA-O3A	3.78	1.63	1.59
4	A	920	IMP	O4'-C4'	-3.78	1.36	1.45
4	B	920	IMP	O4'-C4'	-3.57	1.37	1.45
3	B	932	PDP	C2-N1	3.55	1.40	1.33
4	B	920	IMP	O6-C6	3.43	1.30	1.23
4	B	920	IMP	C5'-C4'	3.40	1.61	1.51
4	B	920	IMP	C6-N1	-3.35	1.32	1.39
3	C	933	PDP	C3-C2	-2.95	1.37	1.41
4	A	920	IMP	P-O3P	-2.70	1.44	1.54
4	D	920	IMP	C6-N1	-2.66	1.33	1.39
3	C	933	PDP	C2-N1	2.59	1.38	1.33
4	C	920	IMP	C5'-C4'	2.54	1.59	1.51
4	D	920	IMP	O4'-C4'	-2.52	1.39	1.45
3	C	933	PDP	PA-O3A	2.46	1.62	1.59
3	B	932	PDP	C2A-C2	2.34	1.54	1.50
3	D	934	PDP	C2A-C2	-2.29	1.46	1.50
4	C	920	IMP	C2-N3	2.27	1.34	1.30
3	D	934	PDP	C4A-C4	-2.22	1.47	1.51
4	C	920	IMP	P-O3P	-2.17	1.46	1.54
4	C	920	IMP	C1'-N9	-2.14	1.41	1.47
3	A	931	PDP	C3-C2	-2.09	1.38	1.41
4	A	920	IMP	C6-N1	-2.03	1.35	1.39
4	C	920	IMP	C4-N9	-2.03	1.32	1.38
4	A	920	IMP	P-O5'	2.03	1.66	1.60

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	920	IMP	C2-N1-C6	-5.24	117.91	125.09
4	B	920	IMP	C5-C6-N1	5.02	118.00	110.78
4	D	920	IMP	C5-C6-N1	4.78	117.66	110.78
4	A	920	IMP	C5-C6-N1	4.70	117.54	110.78
4	B	920	IMP	C2-N1-C6	-4.61	118.77	125.09
4	C	920	IMP	N1-C2-N3	4.61	130.81	125.50
4	A	920	IMP	N1-C2-N3	4.27	130.41	125.50
4	C	920	IMP	C2-N1-C6	-4.07	119.51	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	920	IMP	O5'-C5'-C4'	3.84	122.06	108.99
4	D	920	IMP	C2-N1-C6	-3.54	120.24	125.09
4	B	920	IMP	N1-C2-N3	3.44	129.45	125.50
4	B	920	IMP	O4'-C1'-N9	-3.37	100.73	108.36
3	B	932	PDP	O5A-C5A-C5	3.28	115.51	109.36
3	A	931	PDP	O3A-PA-O1A	-3.17	101.16	110.70
4	C	920	IMP	O3P-P-O5'	-3.10	98.57	106.67
4	C	920	IMP	C2-N3-C4	-3.02	106.21	111.53
4	C	920	IMP	C5-C6-N1	2.95	115.03	110.78
4	C	920	IMP	O2P-P-O5'	2.93	114.31	106.67
4	A	920	IMP	O5'-C5'-C4'	2.73	118.30	108.99
3	B	932	PDP	C5-C6-N1	-2.72	119.41	123.83
4	D	920	IMP	N1-C2-N3	2.71	128.62	125.50
3	D	934	PDP	O3B-PB-O2B	2.66	117.79	107.80
4	D	920	IMP	O4'-C4'-C5'	-2.64	100.89	109.33
3	B	932	PDP	O3A-PA-O1A	-2.63	102.79	110.70
4	C	920	IMP	O4'-C1'-N9	-2.63	102.41	108.36
3	A	931	PDP	C4A-C4-C5	-2.47	118.40	120.94
3	B	932	PDP	C6-C5-C4	2.46	120.12	118.10
3	D	934	PDP	C5-C6-N1	-2.46	119.83	123.83
3	C	933	PDP	O2A-PA-O3A	-2.28	101.12	107.27
4	C	920	IMP	O5'-C5'-C4'	2.25	116.64	108.99
3	A	931	PDP	C5-C6-N1	-2.20	120.25	123.83
4	A	920	IMP	O2P-P-O5'	2.17	112.33	106.67
4	B	920	IMP	O2P-P-O5'	2.14	112.24	106.67
3	C	933	PDP	O3A-PB-O1B	-2.14	99.79	111.04
3	C	933	PDP	O3B-PB-O2B	2.14	115.81	107.80
4	A	920	IMP	O4'-C1'-N9	-2.12	103.56	108.36
4	D	920	IMP	O4'-C1'-N9	-2.11	103.58	108.36
3	D	934	PDP	O3A-PA-O1A	-2.10	104.40	110.70
4	C	920	IMP	C8-N7-C5	-2.06	100.59	104.26
3	A	931	PDP	O3B-PB-O2B	2.03	115.41	107.80
3	B	932	PDP	O3B-PB-O2B	2.03	115.40	107.80
4	B	920	IMP	O2'-C2'-C1'	-2.02	103.14	110.10
4	A	920	IMP	O3P-P-O5'	-2.02	101.41	106.67

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
3	A	931	PDP	C5A-O5A-PA-O3A

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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-O3A
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	B	932	PDP	PB-O3A-PA-O1A
3	B	932	PDP	C5A-O5A-PA-O1A
3	C	933	PDP	C5A-O5A-PA-O1A
3	C	933	PDP	C5A-O5A-PA-O3A
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	C	933	PDP	PB-O3A-PA-O1A

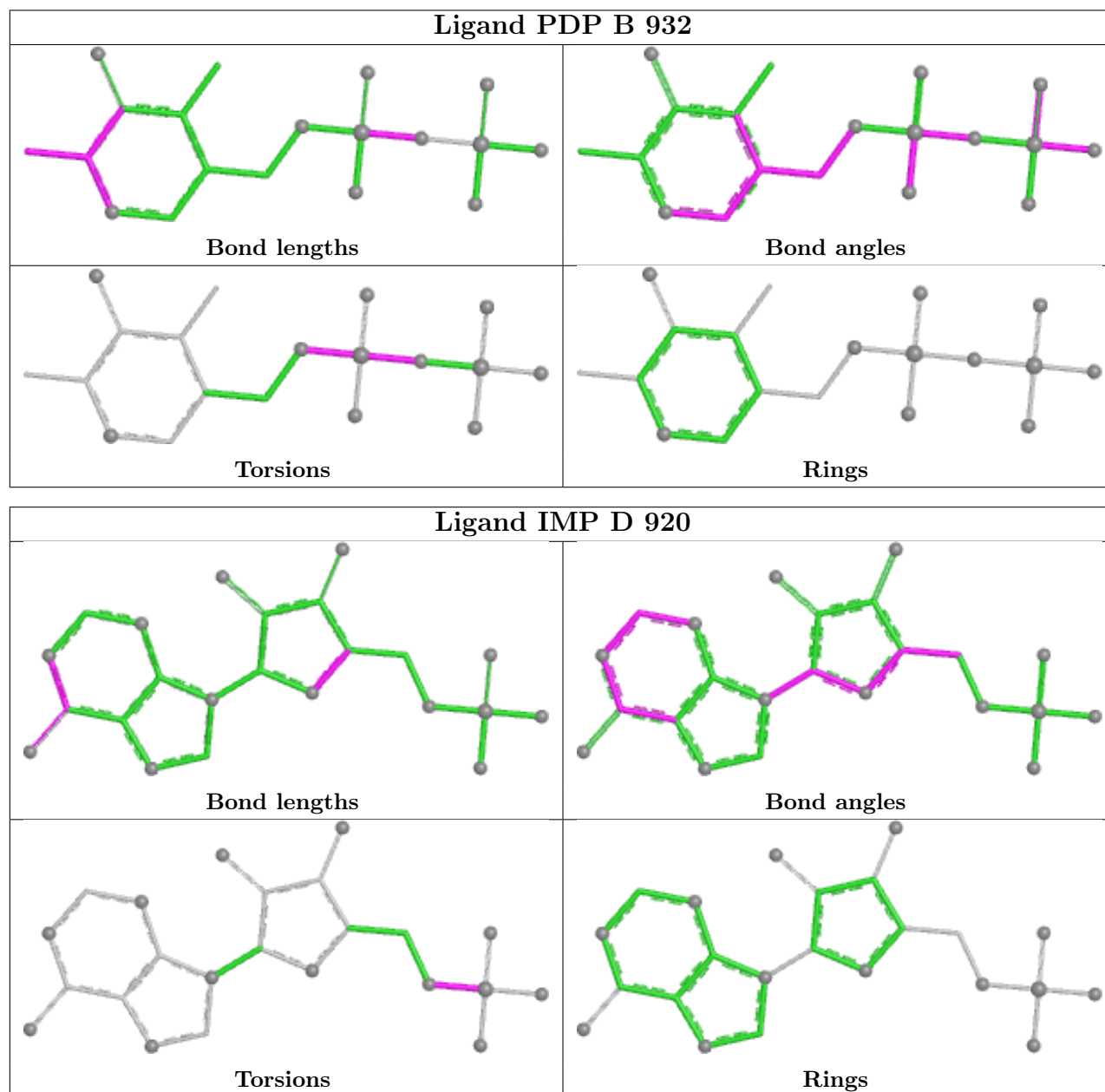
There are no ring outliers.

9 monomers are involved in 15 short contacts:

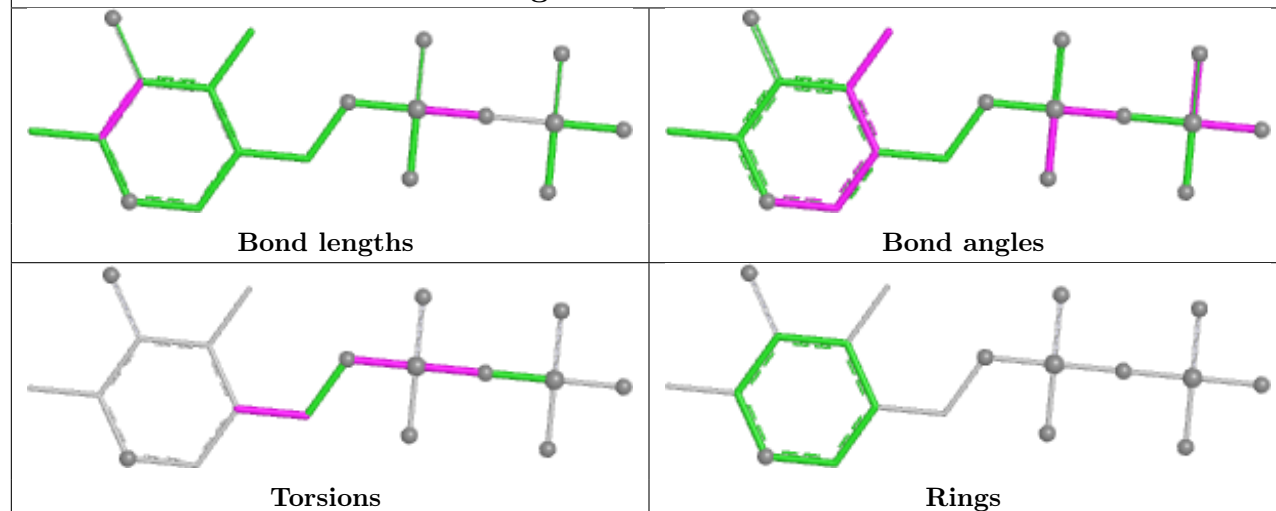
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	932	PDP	2	0
4	D	920	IMP	1	0
3	A	931	PDP	2	0
2	D	900	SO4	1	0
4	B	920	IMP	4	0
3	D	934	PDP	1	0
4	A	920	IMP	2	0
3	C	933	PDP	1	0
4	C	920	IMP	1	0

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 than 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

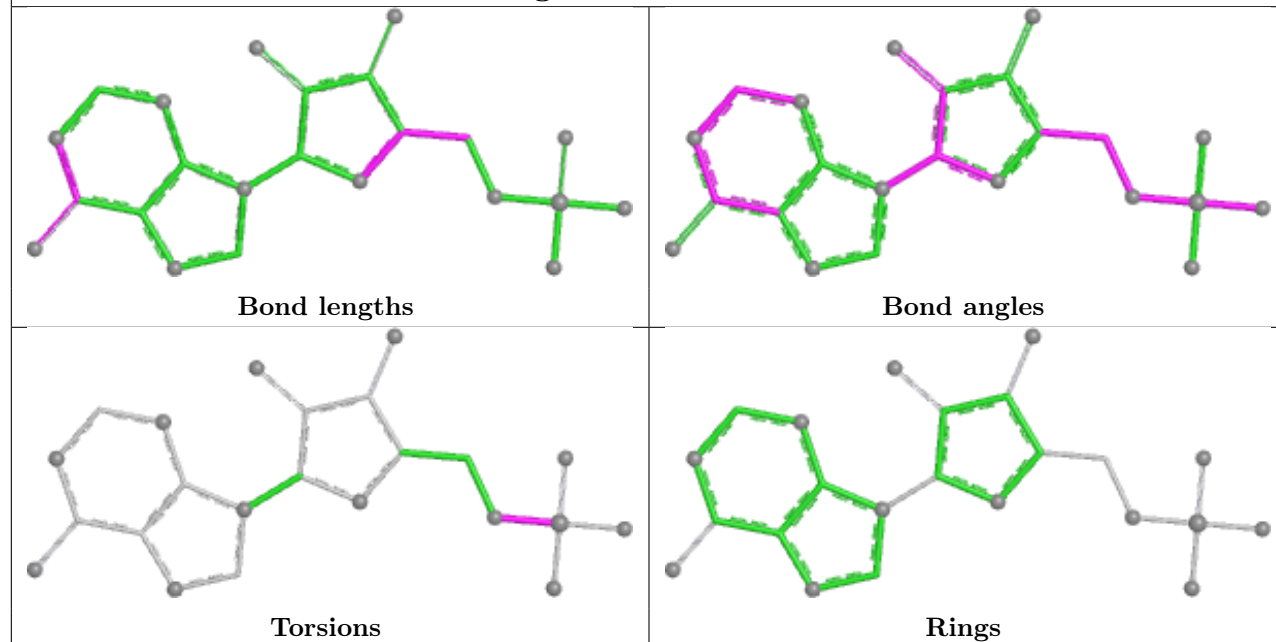
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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



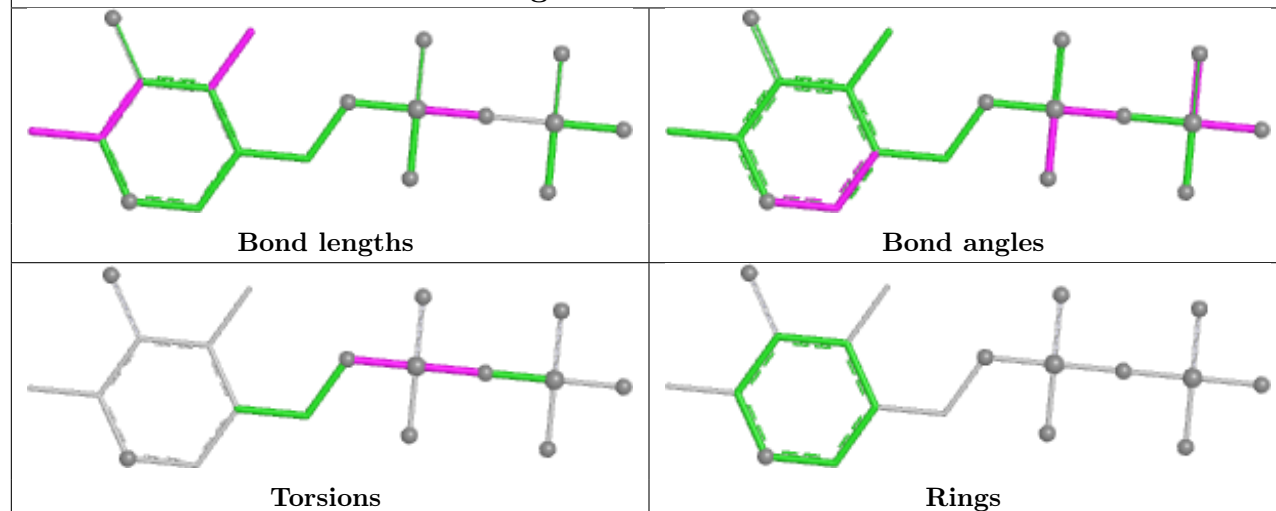
Ligand PDP A 931



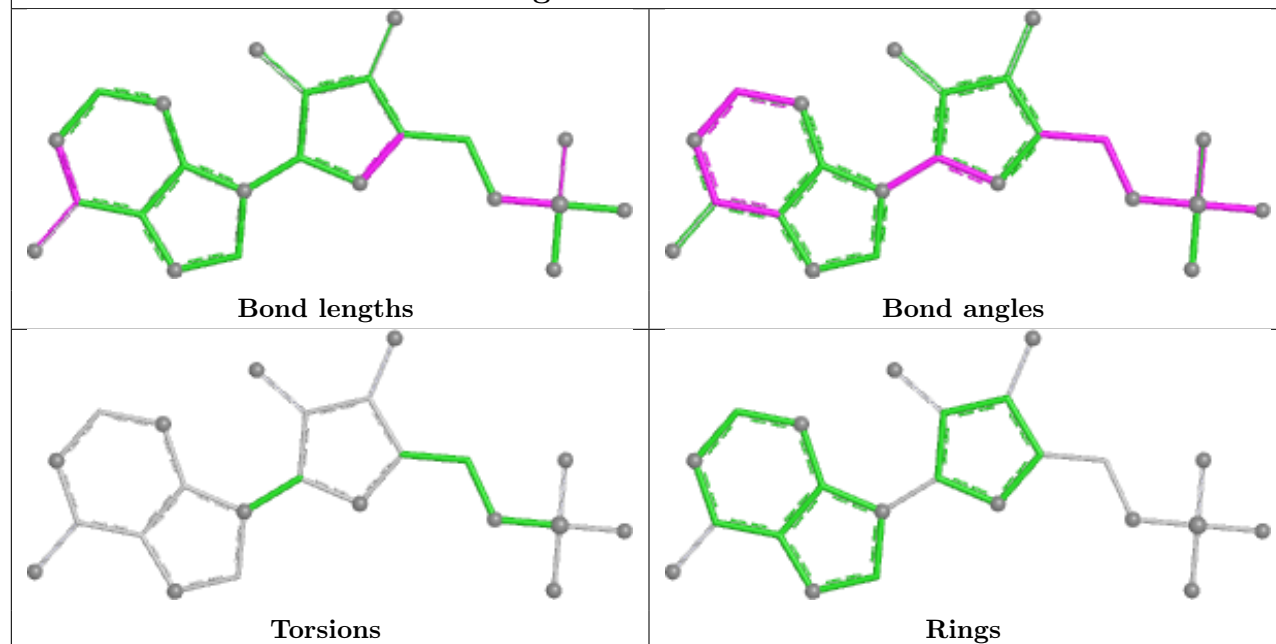
Ligand IMP B 920

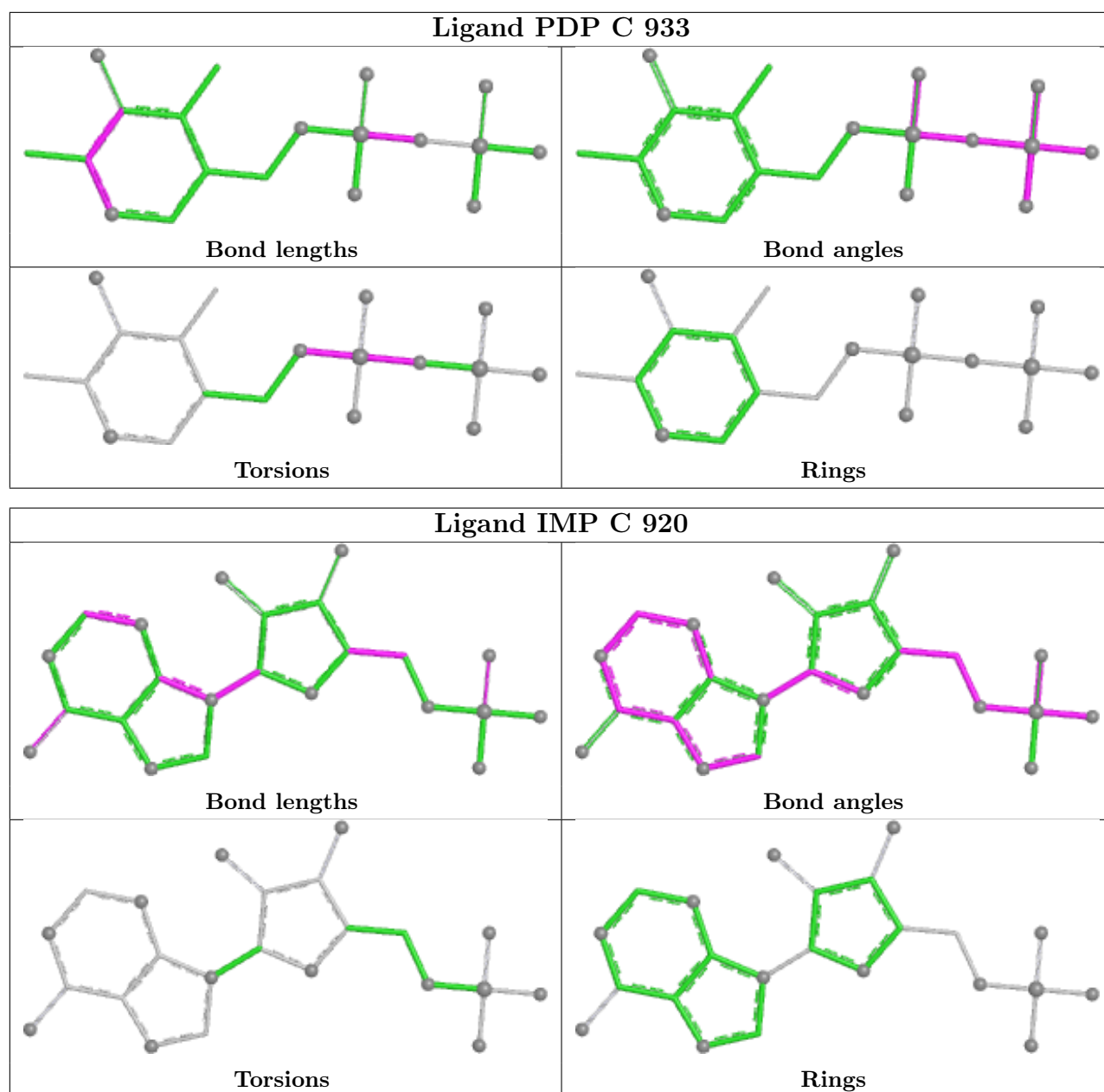


Ligand PDP D 934



Ligand IMP A 920





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.