



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 04:32 PM EDT

PDB ID : 7GPB
Title : STRUCTURAL MECHANISM FOR GLYCOGEN PHOSPHORYLASE
CONTROL BY PHOSPHORYLATION AND AMP
Authors : Barford, D.; Hu, S.-H.; Johnson, L.N.
Deposited on : 1990-11-13
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

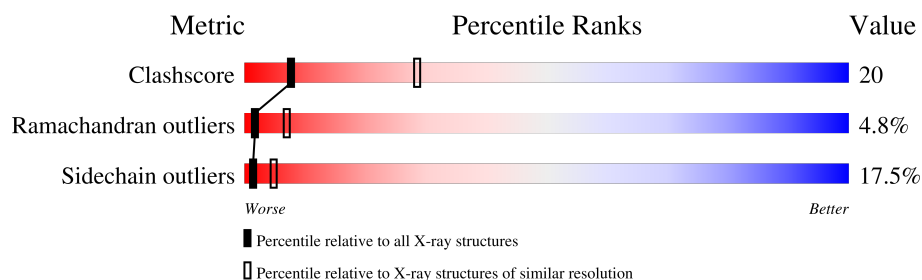
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	
1	B	842	
1	C	842	
1	D	842	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	901	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26955 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
			6692	4264	1185	1213	30			
1	B	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	C	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	D	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			

There are 4 discrepancies between the modelled and reference sequences:

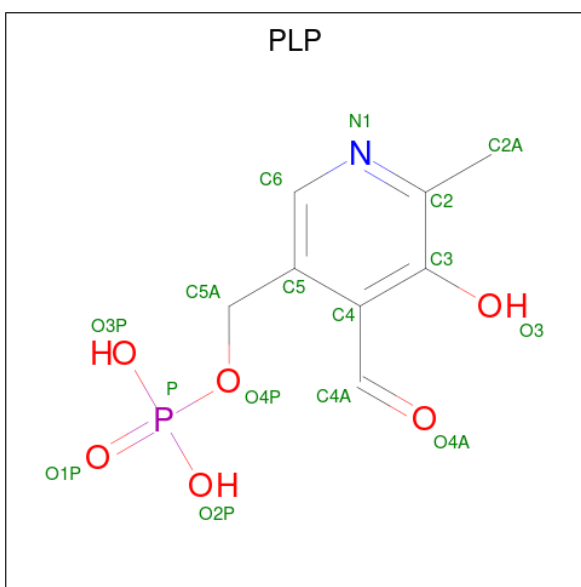
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



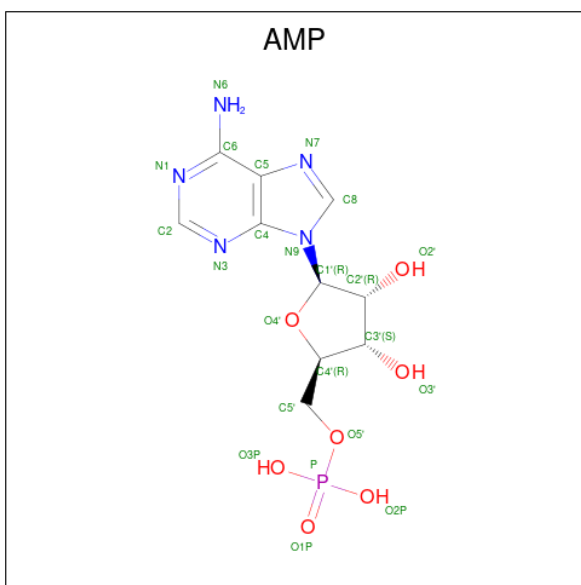
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



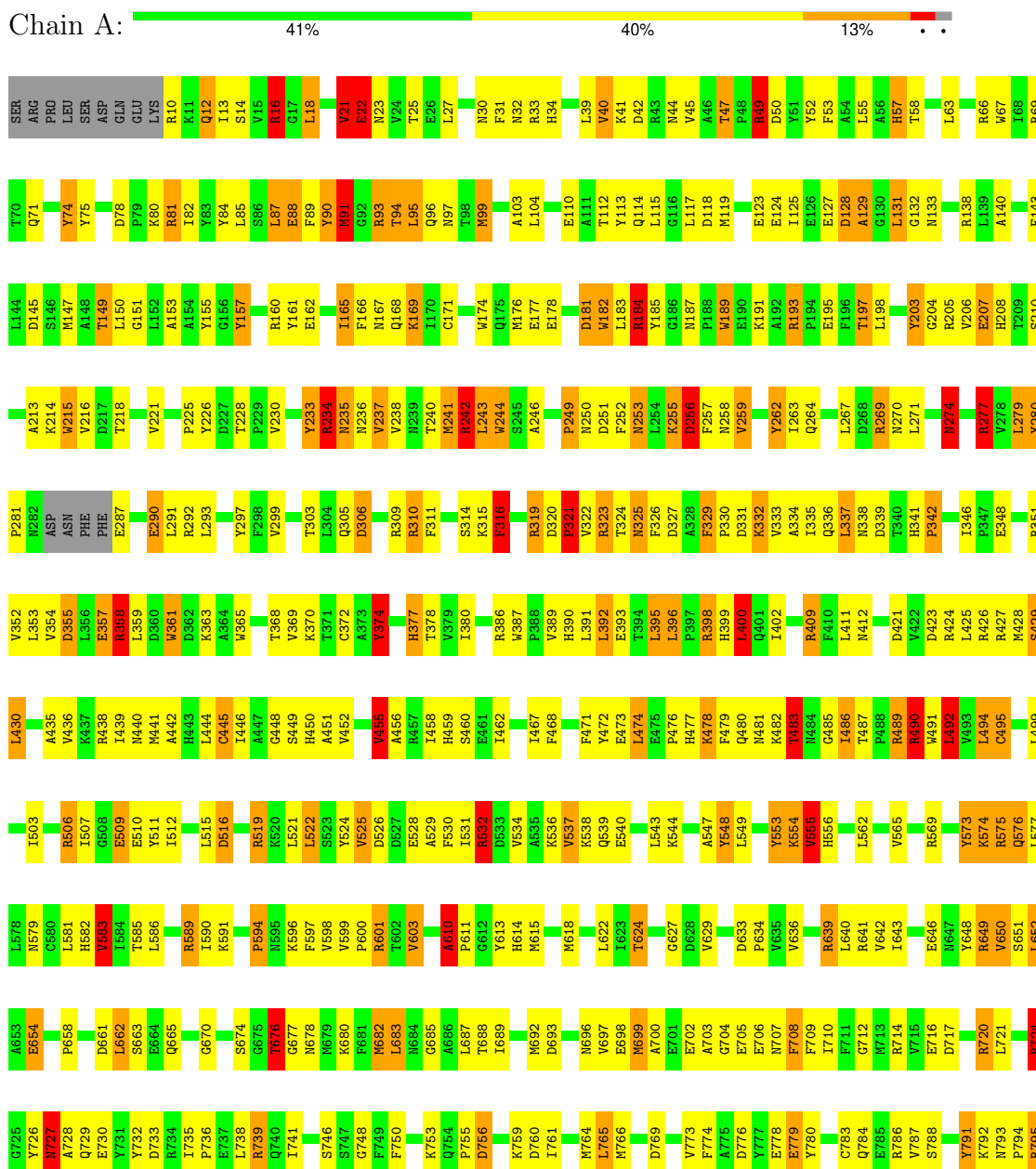
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	D	1	Total 23	C 10	N 5	O 7	P 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

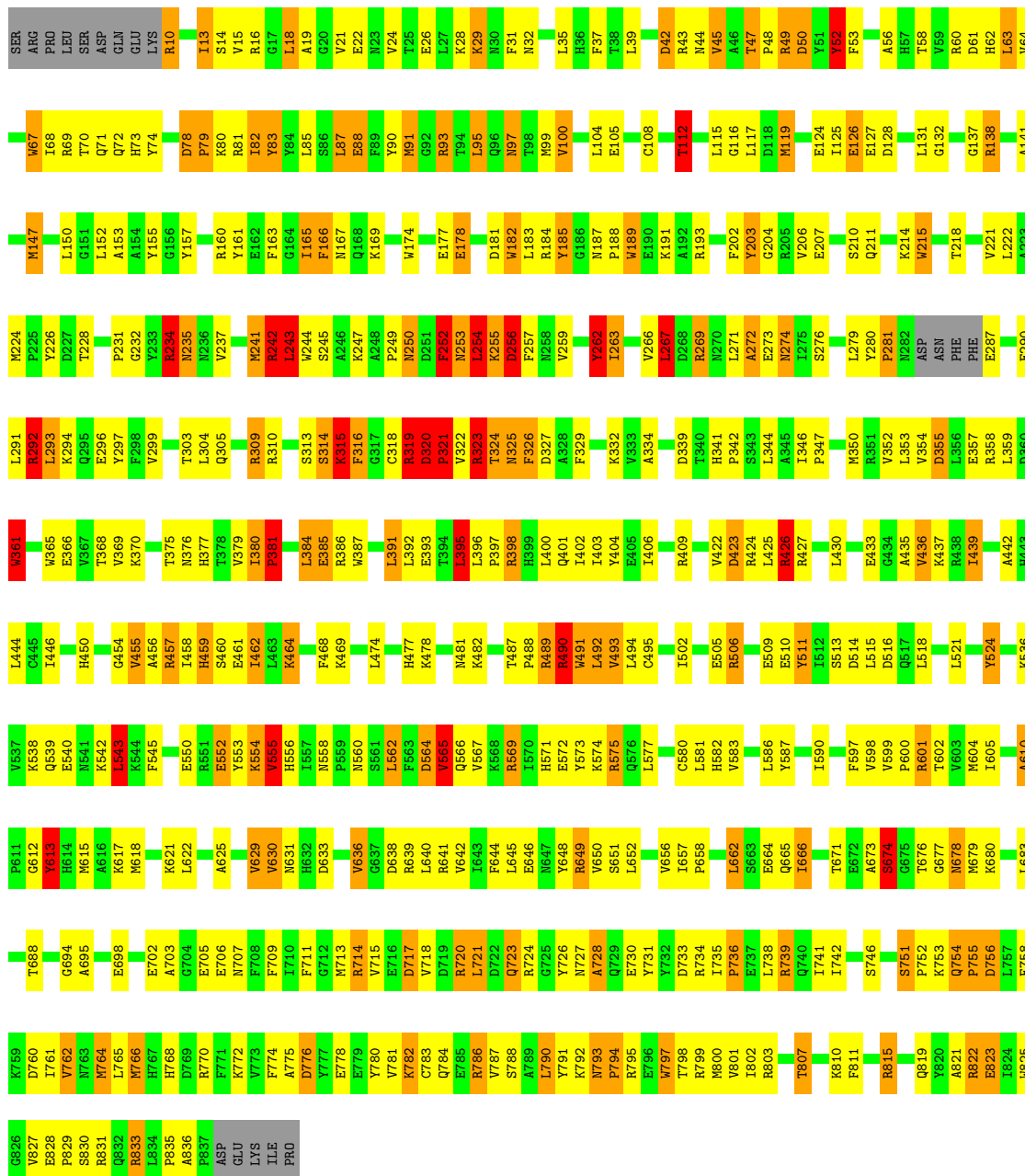
Note EDS was not executed.

• Molecule 1: GLYCOGEN PHOSPHORYLASE B



- Molecule 1: GLYCOGEN PHOSPHORYLASE B

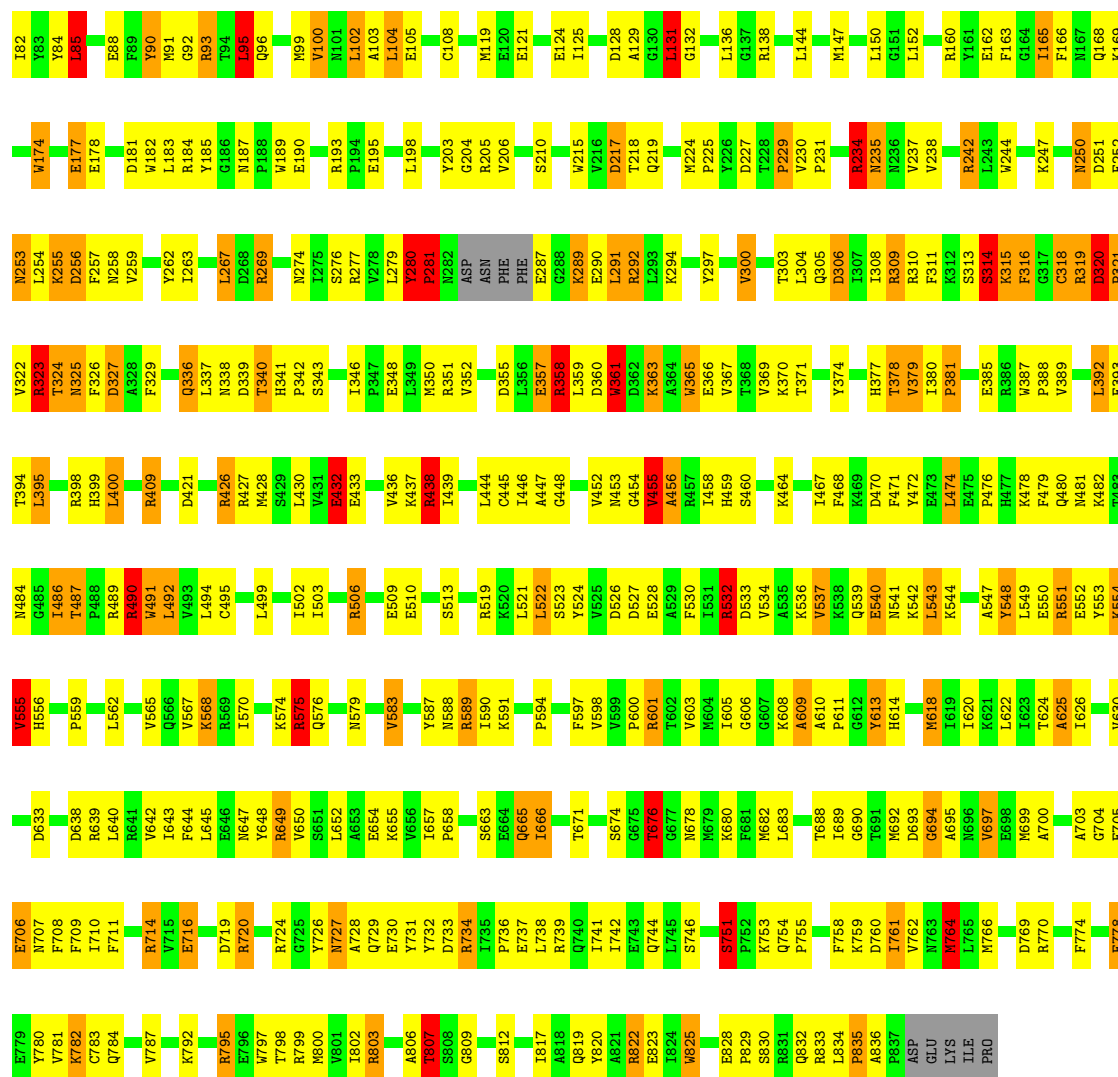
Chain B: 43% 38% 14% 5%



- Molecule 1: GLYCOGEN PHOSPHORYLASE B

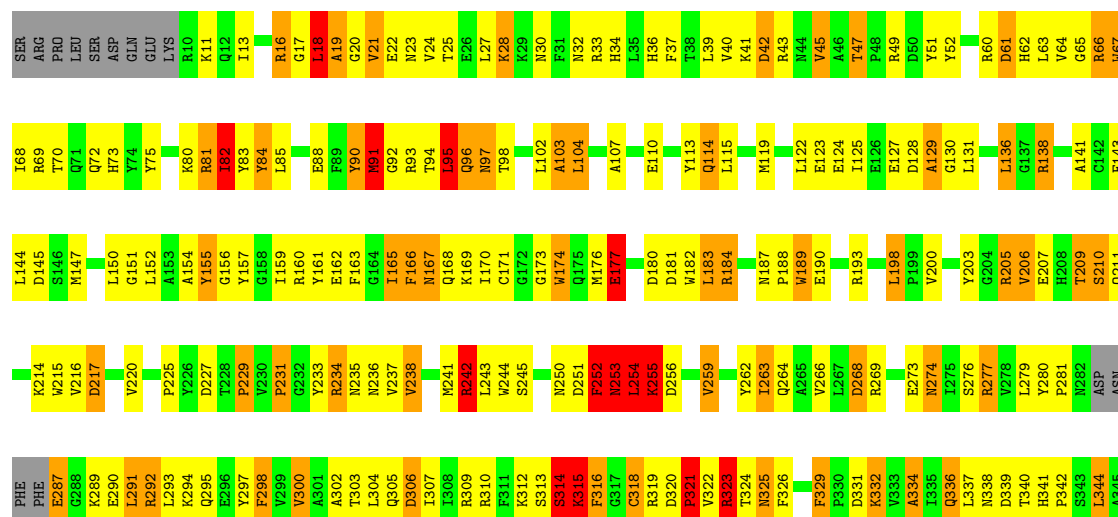
Chain C:  46% 38% 11% 5%





• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain D: 36% 42% 16%





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 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26955	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: AMP, PLP, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	6/6842 (0.1%)	2.02	223/9258 (2.4%)
1	B	1.00	5/6842 (0.1%)	1.90	186/9258 (2.0%)
1	C	1.00	2/6842 (0.0%)	1.96	190/9258 (2.1%)
1	D	0.99	2/6842 (0.0%)	2.00	203/9258 (2.2%)
All	All	1.00	15/27368 (0.1%)	1.97	802/37032 (2.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	5
1	D	0	8
All	All	0	25

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	ARG	CZ-NH1	8.57	1.44	1.33
1	B	100	VAL	CA-CB	7.53	1.70	1.54
1	B	319	ARG	CZ-NH1	7.05	1.42	1.33
1	B	323	ARG	CZ-NH2	6.47	1.41	1.33
1	A	323	ARG	NE-CZ	6.26	1.41	1.33
1	A	22	GLU	CG-CD	6.00	1.60	1.51
1	A	829	PRO	CA-CB	-5.84	1.41	1.53
1	D	361	TRP	CG-CD2	-5.83	1.33	1.43
1	C	215	TRP	CD2-CE2	-5.78	1.34	1.41
1	B	385	GLU	CD-OE2	-5.59	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	ARG	CZ-NH1	5.51	1.40	1.33
1	D	244	TRP	CG-CD2	-5.25	1.34	1.43
1	A	323	ARG	CZ-NH2	5.16	1.39	1.33
1	A	189	TRP	CG-CD2	-5.10	1.34	1.43
1	C	388	PRO	CA-CB	-5.06	1.43	1.53

All (802) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	TRP	CG-CD2-CE3	-40.61	97.35	133.90
1	D	67	TRP	NE1-CE2-CZ2	-33.92	93.09	130.40
1	A	49	ARG	NE-CZ-NH2	-19.84	110.38	120.30
1	A	16	ARG	NE-CZ-NH2	14.98	127.79	120.30
1	D	490	ARG	NE-CZ-NH2	-14.37	113.11	120.30
1	A	277	ARG	NE-CZ-NH1	14.32	127.46	120.30
1	B	398	ARG	NE-CZ-NH2	-14.29	113.16	120.30
1	A	49	ARG	NE-CZ-NH1	13.60	127.10	120.30
1	C	409	ARG	NE-CZ-NH2	-13.39	113.60	120.30
1	C	90	TYR	CB-CG-CD2	-12.48	113.51	121.00
1	C	490	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	C	203	TYR	CB-CG-CD2	-12.38	113.57	121.00
1	A	277	ARG	NH1-CZ-NH2	-12.19	106.00	119.40
1	D	157	TYR	CB-CG-CD2	-12.15	113.71	121.00
1	A	161	TYR	CB-CG-CD2	-12.12	113.73	121.00
1	C	93	ARG	NE-CZ-NH2	-12.05	114.27	120.30
1	D	409	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	A	490	ARG	NE-CZ-NH2	-11.67	114.46	120.30
1	C	160	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	A	613	TYR	CB-CG-CD2	-11.48	114.11	121.00
1	C	310	ARG	NE-CZ-NH2	-11.37	114.61	120.30
1	A	386	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	C	292	ARG	NE-CZ-NH1	11.29	125.94	120.30
1	D	569	ARG	NE-CZ-NH2	-11.19	114.71	120.30
1	B	234	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	C	69	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	B	780	TYR	CB-CG-CD2	-10.96	114.43	121.00
1	D	242	ARG	NE-CZ-NH2	-10.85	114.87	120.30
1	A	193	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	A	242	ARG	NE-CZ-NH2	-10.72	114.94	120.30
1	A	138	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	C	551	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	310	ARG	NE-CZ-NH2	-10.54	115.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	TYR	CB-CG-CD2	-10.53	114.68	121.00
1	D	816	THR	CA-CB-CG2	-10.47	97.74	112.40
1	A	795	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	374	TYR	CB-CG-CD2	-10.37	114.78	121.00
1	A	654	GLU	CA-CB-CG	10.34	136.15	113.40
1	A	67	TRP	NE1-CE2-CZ2	-10.23	119.15	130.40
1	C	428	MET	CA-CB-CG	-10.23	95.92	113.30
1	C	81	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	A	720	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	C	292	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	C	309	ARG	NE-CZ-NH2	-10.09	115.26	120.30
1	C	215	TRP	CD1-CG-CD2	10.02	114.31	106.30
1	D	351	ARG	NE-CZ-NH2	-9.99	115.31	120.30
1	D	325	ASN	CA-C-N	-9.97	95.26	117.20
1	C	490	ARG	NE-CZ-NH1	9.97	125.29	120.30
1	A	182	TRP	CD1-CG-CD2	9.92	114.24	106.30
1	B	174	TRP	CD1-CG-CD2	9.92	114.24	106.30
1	B	831	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	B	193	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	A	398	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	A	90	TYR	CB-CG-CD2	-9.58	115.25	121.00
1	C	532	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	C	374	TYR	CB-CG-CD2	-9.48	115.31	121.00
1	A	244	TRP	CD1-CG-CD2	9.39	113.81	106.30
1	D	506	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	C	825	TRP	CD1-CG-CD2	9.37	113.80	106.30
1	C	40	VAL	CG1-CB-CG2	-9.36	95.93	110.90
1	D	822	ARG	NE-CZ-NH2	9.29	124.95	120.30
1	A	243	LEU	CA-CB-CG	9.25	136.58	115.30
1	C	174	TRP	CD1-CG-CD2	9.18	113.64	106.30
1	C	807	THR	N-CA-CB	-9.16	92.90	110.30
1	B	244	TRP	CD1-CG-CD2	9.10	113.58	106.30
1	C	601	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	D	244	TRP	CD1-CG-CD2	9.01	113.51	106.30
1	D	67	TRP	CD1-CG-CD2	9.00	113.50	106.30
1	D	81	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	D	242	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	174	TRP	CD1-CG-CD2	8.91	113.43	106.30
1	C	351	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	A	649	ARG	CG-CD-NE	-8.75	93.42	111.80
1	A	387	TRP	CD1-CG-CD2	8.71	113.27	106.30
1	C	242	ARG	NE-CZ-NH2	-8.70	115.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	427	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	457	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	B	601	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	B	490	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	C	309	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	C	706	GLU	CA-CB-CG	8.60	132.31	113.40
1	C	93	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	C	319	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	126	GLU	CA-CB-CG	-8.41	94.89	113.40
1	A	650	VAL	CG1-CB-CG2	-8.38	97.50	110.90
1	A	155	TYR	CB-CG-CD1	-8.37	115.98	121.00
1	A	138	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	325	ASN	CA-C-N	-8.34	98.85	117.20
1	C	205	ARG	CA-CB-CG	8.34	131.75	113.40
1	B	387	TRP	CD1-CG-CD2	8.32	112.96	106.30
1	B	477	HIS	CA-CB-CG	8.30	127.72	113.60
1	B	489	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	C	67	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	A	491	TRP	CE2-CD2-CG	-8.27	100.69	107.30
1	A	553	TYR	CB-CG-CD2	-8.25	116.05	121.00
1	A	739	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	C	136	LEU	CA-CB-CG	8.24	134.25	115.30
1	C	205	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	A	424	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	C	825	TRP	CE2-CD2-CG	-8.21	100.73	107.30
1	C	783	CYS	CA-CB-SG	-8.21	99.23	114.00
1	C	552	GLU	N-CA-C	-8.20	88.85	111.00
1	D	780	TYR	CB-CG-CD2	-8.19	116.08	121.00
1	D	365	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	B	244	TRP	CE2-CD2-CG	-8.17	100.76	107.30
1	C	182	TRP	CD1-CG-CD2	8.12	112.79	106.30
1	A	244	TRP	CE2-CD2-CG	-8.11	100.81	107.30
1	D	491	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	D	269	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	C	215	TRP	CG-CD1-NE1	-8.08	102.02	110.10
1	A	610	ALA	N-CA-CB	8.08	121.41	110.10
1	A	676	THR	CA-CB-CG2	8.04	123.66	112.40
1	C	387	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	C	491	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	A	74	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	D	409	ARG	NE-CZ-NH1	7.96	124.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	TYR	CB-CG-CD2	-7.96	116.23	121.00
1	A	682	MET	CG-SD-CE	-7.96	87.47	100.20
1	C	174	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	A	575	ARG	CB-CG-CD	-7.94	90.97	111.60
1	D	292	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	351	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	739	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	D	323	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	B	455	VAL	N-CA-CB	-7.89	94.15	111.50
1	D	734	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	281	PRO	N-CA-C	7.88	132.58	112.10
1	C	350	MET	CG-SD-CE	-7.85	87.63	100.20
1	D	489	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	D	511	TYR	CB-CG-CD2	-7.84	116.30	121.00
1	A	67	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	B	174	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	D	398	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	C	491	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	B	825	TRP	CG-CD2-CE3	7.78	140.90	133.90
1	A	67	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	A	182	TRP	CE2-CD2-CG	-7.77	101.09	107.30
1	D	215	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	C	323	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	639	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	D	649	ARG	NE-CZ-NH1	-7.75	116.43	120.30
1	B	825	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	B	491	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	B	365	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	D	365	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	D	489	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	387	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	B	185	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	D	292	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	B	262	TYR	CB-CG-CD1	-7.64	116.42	121.00
1	C	255	LYS	CA-C-N	-7.63	100.42	117.20
1	D	506	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	C	365	TRP	CD1-CG-CD2	7.62	112.39	106.30
1	C	825	TRP	CG-CD2-CE3	7.62	140.75	133.90
1	C	43	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	90	TYR	CB-CG-CD1	7.57	125.54	121.00
1	C	51	TYR	CB-CG-CD1	-7.55	116.47	121.00
1	C	269	ARG	NE-CZ-NH2	-7.54	116.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	825	TRP	CD1-CG-CD2	7.53	112.32	106.30
1	C	724	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	C	300	VAL	CA-CB-CG2	-7.50	99.65	110.90
1	B	182	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	B	613	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	D	254	LEU	CA-CB-CG	7.45	132.44	115.30
1	B	215	TRP	CD1-CG-CD2	7.42	112.23	106.30
1	D	155	TYR	CB-CG-CD2	-7.40	116.56	121.00
1	D	310	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	C	189	TRP	CD1-CG-CD2	7.38	112.21	106.30
1	B	365	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	B	257	PHE	CA-C-N	-7.36	101.00	117.20
1	B	650	VAL	CG1-CB-CG2	-7.36	99.12	110.90
1	D	395	LEU	CA-CB-CG	7.35	132.21	115.30
1	A	610	ALA	CB-CA-C	-7.35	99.08	110.10
1	A	203	TYR	CB-CG-CD2	-7.34	116.60	121.00
1	B	587	TYR	CB-CG-CD1	-7.34	116.60	121.00
1	A	537	VAL	CA-CB-CG2	-7.33	99.90	110.90
1	D	157	TYR	CG-CD1-CE1	-7.33	115.44	121.30
1	D	67	TRP	CG-CD1-NE1	-7.32	102.78	110.10
1	A	351	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	B	62	HIS	CA-C-N	-7.30	101.13	117.20
1	B	387	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	B	361	TRP	NE1-CE2-CZ2	-7.29	122.39	130.40
1	A	12	GLN	CA-CB-CG	7.28	129.42	113.40
1	C	365	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	B	602	THR	N-CA-C	-7.26	91.39	111.00
1	A	325	ASN	CA-C-N	-7.25	101.25	117.20
1	C	649	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	189	TRP	CD1-CG-CD2	7.21	112.07	106.30
1	D	323	ARG	CA-CB-CG	7.21	129.26	113.40
1	A	84	TYR	CB-CG-CD1	-7.19	116.68	121.00
1	D	49	ARG	CA-CB-CG	7.19	129.21	113.40
1	A	365	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	B	491	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	B	269	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	310	ARG	CG-CD-NE	-7.16	96.77	111.80
1	B	679	MET	CG-SD-CE	-7.15	88.76	100.20
1	C	234	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	D	396	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	A	215	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	B	83	TYR	CB-CG-CD1	-7.12	116.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	332	LYS	CA-CB-CG	-7.12	97.75	113.40
1	A	430	LEU	CA-CB-CG	7.11	131.66	115.30
1	D	314	SER	N-CA-CB	7.10	121.15	110.50
1	B	67	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	C	764	MET	CA-CB-CG	7.10	125.36	113.30
1	D	136	LEU	CA-CB-CG	7.10	131.62	115.30
1	C	255	LYS	O-C-N	7.09	134.05	122.70
1	A	189	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	A	555	VAL	CB-CA-C	-7.09	97.93	111.40
1	A	358	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	365	TRP	CB-CG-CD1	-7.08	117.79	127.00
1	B	825	TRP	CE2-CD2-CG	-7.08	101.63	107.30
1	A	277	ARG	CG-CD-NE	7.07	126.65	111.80
1	C	244	TRP	CE2-CD2-CG	-7.07	101.64	107.30
1	A	306	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	182	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	D	127	GLU	CA-CB-CG	7.05	128.92	113.40
1	B	361	TRP	CD1-CG-CD2	7.04	111.93	106.30
1	B	67	TRP	CD1-CG-CD2	7.04	111.93	106.30
1	B	552	GLU	N-CA-C	-7.04	92.00	111.00
1	C	575	ARG	N-CA-C	7.04	130.00	111.00
1	A	174	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	B	489	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	575	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	C	182	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	D	568	LYS	CA-CB-CG	7.00	128.79	113.40
1	A	613	TYR	CB-CG-CD1	7.00	125.20	121.00
1	B	292	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	C	45	VAL	N-CA-CB	-6.99	96.13	111.50
1	C	244	TRP	CD1-CG-CD2	6.98	111.89	106.30
1	B	138	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	D	90	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	B	18	LEU	N-CA-C	6.97	129.83	111.00
1	C	792	LYS	N-CA-CB	-6.97	98.05	110.60
1	D	491	TRP	CE2-CD2-CG	-6.97	101.73	107.30
1	D	669	ALA	CA-C-N	-6.96	102.27	116.20
1	C	160	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	19	ALA	CA-C-N	6.95	130.09	116.20
1	D	206	VAL	CG1-CB-CG2	-6.94	99.80	110.90
1	B	174	TRP	CG-CD2-CE3	6.92	140.13	133.90
1	D	387	TRP	CD1-CG-CD2	6.90	111.82	106.30
1	A	365	TRP	CD1-CG-CD2	6.89	111.81	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	387	TRP	CE2-CD2-CG	-6.89	101.79	107.30
1	A	491	TRP	CD1-CG-CD2	6.89	111.81	106.30
1	D	244	TRP	CE2-CD2-CG	-6.88	101.79	107.30
1	A	724	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	633	ASP	CB-CG-OD1	6.88	124.49	118.30
1	D	387	TRP	CE2-CD2-CG	-6.87	101.80	107.30
1	A	409	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	67	TRP	CE2-CD2-CG	-6.85	101.82	107.30
1	A	797	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	C	66	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	455	VAL	N-CA-CB	-6.83	96.48	111.50
1	D	174	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	A	400	LEU	CA-CB-CG	6.81	130.97	115.30
1	B	250	ASN	CA-C-N	-6.79	102.25	117.20
1	A	509	GLU	CB-CA-C	-6.78	96.83	110.40
1	D	797	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	D	601	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	509	GLU	N-CA-C	6.76	129.25	111.00
1	C	575	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	D	215	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	B	215	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	361	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	B	797	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	B	323	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	C	138	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	825	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	D	182	TRP	CD1-CG-CD2	6.74	111.69	106.30
1	B	174	TRP	CG-CD1-NE1	-6.73	103.37	110.10
1	B	513	SER	CA-CB-OG	6.72	129.34	111.20
1	A	277	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	233	TYR	CB-CG-CD1	-6.71	116.97	121.00
1	D	501	GLU	CA-CB-CG	6.70	128.14	113.40
1	D	679	MET	CG-SD-CE	-6.70	89.48	100.20
1	D	713	MET	CG-SD-CE	-6.70	89.49	100.20
1	C	215	TRP	CE2-CD2-CG	-6.69	101.95	107.30
1	C	551	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	96	GLN	CA-C-N	6.68	131.91	117.20
1	A	185	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	C	37	PHE	CB-CG-CD2	-6.68	116.12	120.80
1	D	174	TRP	CD1-CG-CD2	6.68	111.65	106.30
1	D	532	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	573	TYR	CB-CG-CD2	-6.67	117.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	649	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	321	PRO	CA-N-CD	-6.66	102.18	111.50
1	D	792	LYS	CA-CB-CG	6.63	127.98	113.40
1	A	795	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	393	GLU	CA-CB-CG	6.60	127.91	113.40
1	C	613	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	D	799	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	D	769	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	815	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	769	ASP	CB-CG-OD1	6.54	124.19	118.30
1	B	720	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	C	85	LEU	CA-CB-CG	6.54	130.35	115.30
1	A	807	THR	N-CA-CB	-6.54	97.88	110.30
1	B	569	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	474	LEU	CA-CB-CG	6.52	130.29	115.30
1	A	532	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	797	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	B	309	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	20	GLY	CA-C-N	-6.49	102.91	117.20
1	C	189	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	A	455	VAL	CG1-CB-CG2	6.49	121.28	110.90
1	C	676	THR	N-CA-CB	-6.49	97.98	110.30
1	C	491	TRP	CG-CD2-CE3	6.48	139.73	133.90
1	B	174	TRP	CB-CG-CD1	-6.47	118.59	127.00
1	C	421	ASP	CA-C-N	-6.47	102.96	117.20
1	D	582	HIS	CA-CB-CG	6.46	124.59	113.60
1	D	51	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	D	351	ARG	CA-CB-CG	6.46	127.61	113.40
1	D	441	MET	CG-SD-CE	6.46	110.53	100.20
1	A	445	CYS	CA-CB-SG	-6.45	102.38	114.00
1	B	310	ARG	CG-CD-NE	-6.45	98.25	111.80
1	D	314	SER	CB-CA-C	-6.45	97.85	110.10
1	B	365	TRP	CG-CD2-CE3	6.44	139.70	133.90
1	A	99	MET	CG-SD-CE	-6.44	89.89	100.20
1	A	778	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	A	803	ARG	CA-CB-CG	-6.42	99.28	113.40
1	D	114	GLN	CA-CB-CG	-6.41	99.29	113.40
1	A	808	SER	CB-CA-C	-6.41	97.92	110.10
1	D	825	TRP	CE2-CD2-CG	-6.40	102.18	107.30
1	A	182	TRP	CG-CD1-NE1	-6.38	103.72	110.10
1	D	569	ARG	CA-CB-CG	6.38	127.43	113.40
1	B	361	TRP	CE2-CD2-CG	-6.37	102.20	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	D	361	TRP	CE2-CD2-CE3	6.37	126.34	118.70
1	C	365	TRP	CG-CD2-CE3	6.35	139.62	133.90
1	A	184	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	B	409	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	C	797	TRP	CE2-CD2-CG	-6.33	102.23	107.30
1	A	244	TRP	CB-CG-CD1	-6.33	118.77	127.00
1	D	650	VAL	CG1-CB-CG2	-6.33	100.77	110.90
1	C	537	VAL	CA-CB-CG1	-6.33	101.41	110.90
1	B	575	ARG	CB-CG-CD	-6.32	95.16	111.60
1	C	244	TRP	CB-CG-CD1	-6.32	118.78	127.00
1	D	474	LEU	CA-CB-CG	6.32	129.84	115.30
1	D	676	THR	CA-CB-OG1	-6.32	95.72	109.00
1	A	519	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	43	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	149	THR	N-CA-CB	-6.31	98.31	110.30
1	A	215	TRP	CE2-CD2-CG	-6.30	102.26	107.30
1	B	464	LYS	CB-CG-CD	-6.30	95.21	111.60
1	A	33	ARG	CA-CB-CG	6.30	127.26	113.40
1	C	575	ARG	CB-CG-CD	-6.30	95.22	111.60
1	B	597	PHE	CA-C-N	-6.29	103.36	117.20
1	C	325	ASN	CA-C-N	-6.28	103.38	117.20
1	C	797	TRP	CD1-CG-CD2	6.28	111.32	106.30
1	B	250	ASN	N-CA-C	6.28	127.94	111.00
1	A	67	TRP	CB-CG-CD1	-6.27	118.85	127.00
1	A	724	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	182	TRP	CE2-CD2-CG	-6.25	102.30	107.30
1	A	332	LYS	CA-CB-CG	-6.24	99.66	113.40
1	D	306	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	226	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	C	365	TRP	CB-CG-CD1	-6.24	118.89	127.00
1	B	203	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	A	50	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	825	TRP	CD1-CG-CD2	6.22	111.28	106.30
1	A	305	GLN	CA-C-N	6.22	130.88	117.20
1	B	780	TYR	CB-CG-CD1	6.21	124.73	121.00
1	D	334	ALA	N-CA-CB	-6.21	101.40	110.10
1	B	426	ARG	CA-CB-CG	6.21	127.06	113.40
1	C	513	SER	N-CA-CB	-6.21	101.19	110.50
1	D	365	TRP	CB-CG-CD1	-6.21	118.93	127.00
1	A	91	MET	CG-SD-CE	6.20	110.12	100.20
1	A	575	ARG	N-CA-C	6.19	127.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	PRO	CA-N-CD	-6.19	102.83	111.50
1	C	185	TYR	CB-CG-CD1	-6.19	117.29	121.00
1	D	323	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	C	314	SER	CA-C-N	-6.16	103.64	117.20
1	A	495	CYS	CA-CB-SG	6.15	125.08	114.00
1	D	400	LEU	CA-CB-CG	6.15	129.45	115.30
1	B	386	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	455	VAL	N-CA-CB	-6.14	98.00	111.50
1	A	332	LYS	N-CA-C	6.13	127.55	111.00
1	A	332	LYS	CB-CG-CD	6.12	127.52	111.60
1	B	69	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	13	ILE	N-CA-C	-6.12	94.47	111.00
1	B	319	ARG	CA-CB-CG	6.12	126.87	113.40
1	C	548	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	555	VAL	N-CA-C	6.12	127.51	111.00
1	C	242	ARG	CB-CG-CD	-6.11	95.70	111.60
1	B	565	VAL	CB-CA-C	-6.10	99.80	111.40
1	A	342	PRO	CA-N-CD	-6.10	102.96	111.50
1	B	42	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	D	435	ALA	N-CA-C	-6.08	94.58	111.00
1	A	509	GLU	CA-C-N	6.08	130.57	117.20
1	D	455	VAL	N-CA-CB	-6.08	98.12	111.50
1	A	66	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	D	687	LEU	CA-CB-CG	6.07	129.26	115.30
1	C	822	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	B	490	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	124	GLU	OE1-CD-OE2	-6.06	116.03	123.30
1	A	316	PHE	N-CA-CB	-6.05	99.71	110.60
1	B	319	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	424	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	624	THR	CA-CB-CG2	-6.04	103.95	112.40
1	B	116	GLY	O-C-N	6.04	132.36	122.70
1	B	464	LYS	CA-CB-CG	6.04	126.68	113.40
1	D	575	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	D	203	TYR	CB-CG-CD2	-6.03	117.39	121.00
1	C	486	ILE	CA-CB-CG1	-6.02	99.55	111.00
1	B	755	PRO	CA-C-N	-6.02	103.95	117.20
1	D	325	ASN	O-C-N	6.02	132.34	122.70
1	A	40	VAL	CA-CB-CG1	-6.02	101.87	110.90
1	A	780	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	A	716	GLU	CB-CG-CD	6.01	130.44	114.20
1	C	714	ARG	NE-CZ-NH2	-6.01	117.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	803	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	D	783	CYS	CA-CB-SG	-6.00	103.20	114.00
1	B	310	ARG	CB-CA-C	-6.00	98.41	110.40
1	A	716	GLU	CA-CB-CG	5.99	126.58	113.40
1	B	293	LEU	CB-CG-CD2	-5.99	100.82	111.00
1	A	93	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	324	THR	N-CA-C	-5.98	94.86	111.00
1	A	246	ALA	CB-CA-C	-5.97	101.14	110.10
1	C	174	TRP	CG-CD1-NE1	-5.97	104.13	110.10
1	B	163	PHE	N-CA-C	5.96	127.10	111.00
1	B	160	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	676	THR	CA-CB-CG2	5.95	120.73	112.40
1	D	329	PHE	CB-CG-CD2	-5.95	116.64	120.80
1	B	555	VAL	N-CA-C	5.95	127.05	111.00
1	D	815	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	A	274	ASN	CB-CG-ND2	5.94	130.94	116.70
1	B	457	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	361	TRP	CE2-CD2-CG	-5.93	102.56	107.30
1	A	181	ASP	CA-CB-CG	5.93	126.44	113.40
1	A	240	THR	CA-C-N	-5.93	104.16	117.20
1	D	613	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	D	189	TRP	CE2-CD2-CG	-5.92	102.56	107.30
1	C	95	LEU	CB-CG-CD1	-5.92	100.93	111.00
1	B	324	THR	N-CA-C	-5.92	95.01	111.00
1	A	361	TRP	CD1-CG-CD2	5.92	111.03	106.30
1	A	662	LEU	CA-CB-CG	5.91	128.89	115.30
1	B	610	ALA	N-CA-CB	5.91	118.37	110.10
1	D	205	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	B	393	GLU	CA-CB-CG	5.90	126.39	113.40
1	B	131	LEU	CA-CB-CG	5.90	128.87	115.30
1	B	91	MET	CG-SD-CE	-5.89	90.77	100.20
1	C	649	ARG	CG-CD-NE	-5.88	99.44	111.80
1	D	676	THR	N-CA-CB	-5.88	99.12	110.30
1	D	770	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	244	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	D	313	SER	CA-C-N	5.87	130.12	117.20
1	C	427	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	640	LEU	CA-CB-CG	5.86	128.78	115.30
1	D	215	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	A	438	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	463	LEU	CA-CB-CG	5.86	128.77	115.30
1	B	18	LEU	CA-CB-CG	5.85	128.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	GLY	CA-C-N	-5.85	104.32	117.20
1	A	52	TYR	O-C-N	-5.85	113.34	122.70
1	D	84	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	D	184	ARG	CA-CB-CG	5.84	126.26	113.40
1	C	119	MET	CA-CB-CG	-5.84	103.37	113.30
1	B	269	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	D	103	ALA	CB-CA-C	-5.84	101.34	110.10
1	D	613	TYR	N-CA-C	-5.84	95.24	111.00
1	B	189	TRP	CD1-CG-CD2	5.83	110.96	106.30
1	A	128	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	B	387	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	A	739	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	D	131	LEU	CA-CB-CG	5.82	128.69	115.30
1	C	182	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	D	90	TYR	CB-CG-CD1	5.81	124.49	121.00
1	A	244	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	D	177	GLU	CA-CB-CG	5.80	126.17	113.40
1	C	587	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	A	355	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	409	ARG	NH1-CZ-NH2	5.79	125.78	119.40
1	B	384	LEU	CA-CB-CG	5.79	128.62	115.30
1	D	361	TRP	CD1-CG-CD2	5.79	110.93	106.30
1	D	797	TRP	CD1-CG-CD2	5.78	110.92	106.30
1	D	273	GLU	CA-CB-CG	5.78	126.11	113.40
1	B	262	TYR	CA-CB-CG	-5.77	102.44	113.40
1	D	558	ASN	N-CA-C	-5.77	95.42	111.00
1	A	589	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	436	VAL	CA-CB-CG1	-5.76	102.26	110.90
1	A	128	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	776	ASP	O-C-N	-5.75	113.50	122.70
1	C	487	THR	CA-CB-CG2	5.75	120.45	112.40
1	D	18	LEU	CA-CB-CG	5.75	128.53	115.30
1	D	325	ASN	CA-C-O	5.75	132.18	120.10
1	D	551	ARG	N-CA-C	-5.75	95.48	111.00
1	A	81	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	575	ARG	N-CA-C	5.74	126.50	111.00
1	C	195	GLU	CB-CA-C	-5.74	98.93	110.40
1	B	49	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	B	189	TRP	CE2-CD2-CG	-5.73	102.72	107.30
1	B	797	TRP	CD1-CG-CD2	5.73	110.88	106.30
1	C	491	TRP	CG-CD1-NE1	-5.73	104.37	110.10
1	B	822	ARG	NE-CZ-NH2	-5.72	117.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	THR	CA-CB-CG2	5.72	120.40	112.40
1	A	193	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	16	ARG	NH1-CZ-NH2	-5.71	113.12	119.40
1	D	67	TRP	CE2-CD2-CG	-5.70	102.74	107.30
1	D	33	ARG	CA-CB-CG	5.70	125.94	113.40
1	D	66	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	203	TYR	CG-CD2-CE2	-5.70	116.74	121.30
1	C	104	LEU	CB-CG-CD2	-5.69	101.32	111.00
1	A	727	ASN	CB-CG-ND2	5.69	130.36	116.70
1	C	438	ARG	O-C-N	5.68	131.79	122.70
1	B	61	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	575	ARG	N-CA-C	5.68	126.34	111.00
1	C	693	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	112	THR	CA-CB-CG2	-5.67	104.46	112.40
1	B	249	PRO	CA-C-N	5.67	129.68	117.20
1	C	281	PRO	N-CA-C	5.67	126.84	112.10
1	D	424	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	C	379	VAL	CA-CB-CG2	-5.66	102.40	110.90
1	D	425	LEU	CA-CB-CG	5.66	128.32	115.30
1	D	138	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	174	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	B	491	TRP	NE1-CE2-CZ2	-5.66	124.18	130.40
1	D	491	TRP	CB-CG-CD1	-5.66	119.65	127.00
1	A	277	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	601	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	124	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	C	215	TRP	CH2-CZ2-CE2	5.65	123.05	117.40
1	D	361	TRP	CE2-CD2-CG	-5.64	102.79	107.30
1	C	648	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	537	VAL	CA-CB-CG1	5.63	119.35	110.90
1	A	776	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D	387	TRP	CG-CD2-CE3	5.63	138.97	133.90
1	D	593	GLU	CA-CB-CG	-5.63	101.02	113.40
1	B	254	LEU	CB-CA-C	-5.63	99.51	110.20
1	D	159	ILE	CG1-CB-CG2	-5.63	99.02	111.40
1	D	16	ARG	N-CA-C	5.62	126.18	111.00
1	C	124	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	A	649	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	676	THR	CA-CB-OG1	-5.61	97.21	109.00
1	D	61	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	697	VAL	O-C-N	-5.61	113.73	122.70
1	D	561	SER	N-CA-C	5.61	126.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	432	GLU	CA-CB-CG	5.60	125.72	113.40
1	C	491	TRP	CB-CG-CD1	-5.60	119.72	127.00
1	C	568	LYS	CA-CB-CG	5.59	125.69	113.40
1	B	243	LEU	CA-CB-CG	5.58	128.15	115.30
1	A	69	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	D	69	ARG	CA-CB-CG	5.58	125.69	113.40
1	A	319	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	791	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	B	178	GLU	O-C-N	-5.58	113.77	122.70
1	B	398	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	D	233	TYR	CA-C-N	-5.56	104.96	117.20
1	A	574	LYS	CB-CG-CD	5.56	126.05	111.60
1	D	613	TYR	CB-CG-CD1	5.56	124.33	121.00
1	D	831	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	837	PRO	N-CA-C	5.55	126.53	112.10
1	B	787	VAL	CG1-CB-CG2	-5.55	102.03	110.90
1	D	287	GLU	N-CA-C	-5.55	96.03	111.00
1	C	309	ARG	CG-CD-NE	-5.54	100.16	111.80
1	D	150	LEU	CA-CB-CG	5.54	128.05	115.30
1	D	96	GLN	CA-CB-CG	-5.54	101.21	113.40
1	B	310	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	601	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	50	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	553	TYR	CB-CG-CD1	5.53	124.31	121.00
1	C	325	ASN	O-C-N	5.53	131.54	122.70
1	A	238	VAL	CG1-CB-CG2	-5.52	102.06	110.90
1	B	556	HIS	N-CA-CB	5.52	120.53	110.60
1	A	244	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	D	103	ALA	N-CA-CB	5.51	117.81	110.10
1	C	184	ARG	CA-CB-CG	5.50	125.51	113.40
1	B	430	LEU	CA-CB-CG	5.50	127.96	115.30
1	C	682	MET	CA-CB-CG	5.50	122.66	113.30
1	A	395	LEU	CA-CB-CG	5.50	127.95	115.30
1	B	67	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	C	51	TYR	CG-CD2-CE2	-5.50	116.90	121.30
1	B	543	LEU	CA-CB-CG	5.49	127.94	115.30
1	D	28	LYS	CA-CB-CG	-5.49	101.31	113.40
1	D	365	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	C	387	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	D	313	SER	CA-C-O	-5.48	108.59	120.10
1	C	371	THR	CA-C-N	5.48	129.25	117.20
1	B	37	PHE	CB-CG-CD2	-5.47	116.97	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	MET	CG-SD-CE	5.47	108.96	100.20
1	C	421	ASP	N-CA-CB	5.47	120.45	110.60
1	D	174	TRP	CB-CG-CD1	-5.47	119.89	127.00
1	A	25	THR	CA-CB-OG1	-5.46	97.54	109.00
1	B	776	ASP	CB-CG-OD1	5.46	123.21	118.30
1	D	797	TRP	CB-CG-CD1	-5.46	119.91	127.00
1	A	583	VAL	CB-CA-C	-5.46	101.03	111.40
1	B	355	ASP	CB-CG-OD1	5.45	123.21	118.30
1	C	269	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	792	LYS	CA-CB-CG	5.45	125.40	113.40
1	C	825	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	B	241	MET	CG-SD-CE	5.45	108.92	100.20
1	C	447	ALA	CA-C-N	5.43	127.07	116.20
1	A	323	ARG	CA-CB-CG	5.43	125.35	113.40
1	C	380	ILE	N-CA-CB	-5.43	98.31	110.80
1	B	404	TYR	CB-CG-CD1	5.42	124.25	121.00
1	D	61	ASP	CA-CB-CG	5.42	125.33	113.40
1	C	281	PRO	N-CA-CB	-5.42	96.64	102.60
1	D	491	TRP	CG-CD1-NE1	-5.42	104.68	110.10
1	B	739	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	47	THR	CA-CB-CG2	5.41	119.97	112.40
1	A	494	LEU	CB-CG-CD1	-5.40	101.82	111.00
1	C	189	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	B	249	PRO	O-C-N	-5.39	114.07	122.70
1	D	255	LYS	O-C-N	5.39	131.33	122.70
1	D	477	HIS	CA-CB-CG	5.39	122.76	113.60
1	A	262	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	C	40	VAL	CA-CB-CG2	5.38	118.98	110.90
1	A	124	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	A	525	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	C	537	VAL	CB-CA-C	-5.38	101.17	111.40
1	C	365	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	C	67	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	C	720	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	756	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	262	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	B	215	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	A	532	ARG	CA-CB-CG	5.36	125.20	113.40
1	C	95	LEU	CB-CA-C	-5.36	100.01	110.20
1	C	297	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	D	138	ARG	CG-CD-NE	5.35	123.04	111.80
1	B	267	LEU	CA-CB-CG	-5.35	102.99	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	ARG	N-CA-CB	5.35	120.23	110.60
1	C	807	THR	OG1-CB-CG2	5.35	122.30	110.00
1	B	723	GLN	CA-CB-CG	5.35	125.16	113.40
1	A	582	HIS	CA-CB-CG	5.34	122.68	113.60
1	A	746	SER	N-CA-CB	-5.34	102.48	110.50
1	B	88	GLU	CA-CB-CG	5.34	125.16	113.40
1	C	486	ILE	N-CA-CB	-5.34	98.51	110.80
1	B	825	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	D	244	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	D	755	PRO	CA-C-N	-5.33	105.48	117.20
1	D	647	ASN	CA-C-N	-5.33	105.48	117.20
1	A	74	TYR	CB-CG-CD1	5.32	124.19	121.00
1	B	491	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	B	320	ASP	OD1-CG-OD2	-5.32	113.19	123.30
1	B	587	TYR	CB-CG-CD2	5.32	124.19	121.00
1	A	393	GLU	CA-CB-CG	5.32	125.10	113.40
1	A	205	ARG	CA-CB-CG	5.32	125.10	113.40
1	C	18	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	438	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	310	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	553	TYR	CA-C-N	5.31	128.88	117.20
1	B	352	VAL	CG1-CB-CG2	-5.31	102.41	110.90
1	C	565	VAL	CB-CA-C	-5.31	101.31	111.40
1	C	300	VAL	CA-CB-CG1	5.31	118.86	110.90
1	D	527	ASP	CA-C-N	-5.31	105.53	117.20
1	D	527	ASP	O-C-N	5.31	131.19	122.70
1	D	753	LYS	CD-CE-NZ	-5.31	99.49	111.70
1	B	439	ILE	CA-CB-CG1	-5.31	100.92	111.00
1	C	131	LEU	CA-CB-CG	5.30	127.50	115.30
1	C	731	TYR	CB-CG-CD1	5.30	124.18	121.00
1	C	280	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	B	422	VAL	N-CA-CB	-5.30	99.84	111.50
1	A	18	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	489	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	145	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	233	TYR	O-C-N	5.28	131.14	122.70
1	A	221	VAL	CA-CB-CG1	-5.27	102.99	110.90
1	C	61	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	16	ARG	CA-C-N	5.27	126.74	116.20
1	C	306	ASP	CB-CG-OD1	5.27	123.04	118.30
1	D	601	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	69	ARG	NE-CZ-NH2	-5.27	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	589	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	A	435	ALA	N-CA-C	-5.26	96.79	111.00
1	B	365	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	A	374	TYR	CB-CG-CD1	5.26	124.16	121.00
1	B	252	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	A	160	ARG	CB-CG-CD	-5.25	97.94	111.60
1	C	234	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	D	220	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	D	238	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	B	203	TYR	CA-CB-CG	-5.25	103.43	113.40
1	C	392	LEU	CA-CB-CG	5.24	127.36	115.30
1	D	184	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	395	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	697	VAL	CA-C-N	5.24	128.73	117.20
1	C	803	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	249	PRO	CA-C-N	5.23	128.71	117.20
1	C	732	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	D	91	MET	CG-SD-CE	-5.23	91.83	100.20
1	D	177	GLU	OE1-CD-OE2	-5.23	117.02	123.30
1	A	16	ARG	O-C-N	-5.22	114.32	123.20
1	B	147	MET	CA-CB-CG	-5.22	104.43	113.30
1	D	205	ARG	N-CA-CB	-5.22	101.21	110.60
1	A	354	VAL	CA-CB-CG2	-5.21	103.08	110.90
1	B	165	ILE	N-CA-C	-5.21	96.92	111.00
1	A	720	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	795	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	B	320	ASP	CA-CB-CG	5.20	124.85	113.40
1	B	116	GLY	CA-C-N	-5.20	105.76	117.20
1	B	244	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	B	365	TRP	NE1-CE2-CZ2	-5.20	124.69	130.40
1	C	455	VAL	CB-CA-C	5.20	121.27	111.40
1	A	765	LEU	CA-CB-CG	5.19	127.24	115.30
1	D	67	TRP	CD1-NE1-CE2	5.19	113.67	109.00
1	D	374	TYR	N-CA-CB	-5.19	101.26	110.60
1	A	769	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	603	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	A	814	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	25	THR	N-CA-CB	-5.18	100.45	110.30
1	C	716	GLU	CA-C-N	-5.18	105.80	117.20
1	A	372	CYS	N-CA-CB	-5.18	101.28	110.60
1	B	193	ARG	CA-C-N	5.17	131.58	117.10
1	C	361	TRP	CD1-CG-CD2	5.17	110.44	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	558	ASN	CA-C-N	5.17	131.57	117.10
1	B	10	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	177	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	D	244	TRP	CG-CD2-CE3	5.16	138.55	133.90
1	A	359	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	823	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	D	160	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	532	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	C	323	ARG	N-CA-C	5.15	124.90	111.00
1	D	640	LEU	CA-CB-CG	5.15	127.14	115.30
1	D	568	LYS	CA-C-N	5.14	128.52	117.20
1	B	52	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	B	646	GLU	CA-C-N	-5.14	105.90	117.20
1	B	721	LEU	CA-CB-CG	5.14	127.11	115.30
1	C	13	ILE	N-CA-C	-5.14	97.13	111.00
1	C	108	CYS	CA-CB-SG	-5.14	104.75	114.00
1	C	203	TYR	CG-CD2-CE2	-5.13	117.19	121.30
1	D	277	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	40	VAL	CA-CB-CG2	5.13	118.59	110.90
1	C	203	TYR	CD1-CG-CD2	5.13	123.54	117.90
1	B	714	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	786	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	D	67	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	A	800	MET	CG-SD-CE	-5.12	92.00	100.20
1	D	765	LEU	CA-CB-CG	5.12	127.09	115.30
1	A	329	PHE	CA-C-N	5.12	131.45	117.10
1	C	66	ARG	CA-CB-CG	-5.12	102.13	113.40
1	A	94	THR	CA-C-N	5.12	128.47	117.20
1	D	314	SER	CA-CB-OG	5.12	125.02	111.20
1	D	348	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	C	575	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	357	GLU	O-C-N	-5.11	114.52	122.70
1	C	177	GLU	CA-CB-CG	5.11	124.64	113.40
1	D	233	TYR	CB-CA-C	-5.11	100.18	110.40
1	D	426	ARG	CA-CB-CG	5.11	124.64	113.40
1	C	45	VAL	CB-CA-C	5.11	121.10	111.40
1	D	479	PHE	CB-CG-CD2	-5.11	117.23	120.80
1	A	515	LEU	N-CA-C	5.10	124.78	111.00
1	A	507	ILE	CB-CA-C	-5.10	101.40	111.60
1	B	762	VAL	CG1-CB-CG2	-5.10	102.75	110.90
1	C	215	TRP	N-CA-C	-5.09	97.24	111.00
1	C	310	ARG	CB-CG-CD	-5.09	98.37	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	TYR	CA-CB-CG	5.09	123.06	113.40
1	B	422	VAL	CA-CB-CG2	-5.09	103.27	110.90
1	C	160	ARG	CB-CG-CD	-5.09	98.38	111.60
1	C	244	TRP	CG-CD2-CE3	5.09	138.48	133.90
1	A	396	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	801	VAL	CG1-CB-CG2	-5.08	102.77	110.90
1	D	573	TYR	CA-CB-CG	5.08	123.06	113.40
1	B	706	GLU	CB-CA-C	-5.08	100.24	110.40
1	C	552	GLU	N-CA-CB	5.08	119.74	110.60
1	C	676	THR	CA-CB-CG2	5.08	119.51	112.40
1	D	82	ILE	CA-C-N	-5.08	106.03	117.20
1	C	650	VAL	CG1-CB-CG2	-5.08	102.78	110.90
1	A	280	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	C	770	ARG	CA-CB-CG	5.07	124.55	113.40
1	D	16	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	506	ARG	CB-CG-CD	5.07	124.77	111.60
1	A	207	GLU	CA-CB-CG	5.06	124.54	113.40
1	B	339	ASP	O-C-N	-5.06	114.60	122.70
1	A	534	VAL	CG1-CB-CG2	-5.06	102.80	110.90
1	A	663	SER	CA-CB-OG	5.06	124.87	111.20
1	C	289	LYS	CA-C-N	-5.05	106.08	117.20
1	A	583	VAL	CA-CB-CG1	-5.05	103.33	110.90
1	B	320	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	825	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	D	610	ALA	N-CA-CB	5.05	117.17	110.10
1	A	21	VAL	CA-C-O	-5.04	109.51	120.10
1	D	455	VAL	CB-CA-C	5.04	120.98	111.40
1	C	583	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	D	268	ASP	CB-CG-OD1	5.04	122.83	118.30
1	C	470	ASP	CB-CG-OD1	5.04	122.83	118.30
1	C	227	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	A	641	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	189	TRP	NE1-CE2-CD2	5.03	112.33	107.30
1	A	554	LYS	CA-C-N	5.03	128.26	117.20
1	B	618	MET	CG-SD-CE	-5.03	92.16	100.20
1	B	754	GLN	N-CA-C	-5.03	97.43	111.00
1	D	649	ARG	NH1-CZ-NH2	5.03	124.93	119.40
1	B	714	ARG	CA-CB-CG	5.02	124.45	113.40
1	A	548	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	B	78	ASP	N-CA-C	5.02	124.56	111.00
1	D	255	LYS	CA-C-N	-5.02	106.15	117.20
1	A	241	MET	N-CA-C	-5.02	97.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	11	LYS	CA-CB-CG	5.02	124.44	113.40
1	D	174	TRP	CG-CD2-CE3	5.02	138.41	133.90
1	A	157	TYR	CG-CD2-CE2	-5.01	117.29	121.30
1	C	487	THR	CA-CB-OG1	-5.01	98.47	109.00
1	B	47	THR	N-CA-CB	-5.01	100.78	110.30
1	D	252	PHE	CB-CG-CD2	-5.01	117.29	120.80
1	A	234	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	240	THR	O-C-N	5.01	130.71	122.70
1	D	387	TRP	CB-CG-CD1	-5.00	120.49	127.00
1	A	67	TRP	CG-CD1-NE1	-5.00	105.10	110.10
1	A	339	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	D	421	ASP	N-CA-C	-5.00	97.49	111.00
1	A	57	HIS	CA-C-N	5.00	128.20	117.20

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	277	ARG	Sidechain
1	A	280	TYR	Peptide
1	A	320	ASP	Peptide
1	A	47	THR	Peptide
1	A	49	ARG	Sidechain
1	B	262	TYR	Sidechain
1	B	320	ASP	Peptide
1	B	52	TYR	Sidechain
1	B	524	TYR	Sidechain
1	B	751	SER	Peptide
1	B	793	ASN	Peptide
1	C	280	TYR	Peptide
1	C	320	ASP	Peptide
1	C	751	SER	Peptide
1	C	820	TYR	Sidechain
1	C	84	TYR	Sidechain
1	D	155	TYR	Sidechain
1	D	280	TYR	Peptide
1	D	320	ASP	Peptide
1	D	52	TYR	Sidechain
1	D	569	ARG	Sidechain
1	D	610	ALA	Peptide
1	D	836	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	D	84	TYR	Sidechain

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	6692	0	6653	248	1
1	B	6692	0	6653	244	0
1	C	6692	0	6653	246	0
1	D	6692	0	6653	337	1
2	A	10	0	0	2	0
2	B	10	0	0	1	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
3	A	15	0	6	2	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
3	D	15	0	7	3	0
4	A	23	0	12	3	0
4	B	23	0	12	1	0
4	C	23	0	12	1	0
4	D	23	0	12	2	0
All	All	26955	0	26687	1056	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1056) 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:D:85:LEU:HD21	1:D:303:THR:HG21	1.43	1.00
1:D:251:ASP:HB3	1:D:255:LYS:HB3	1.46	0.98
1:D:707:ASN:HA	1:D:800:MET:SD	2.04	0.97
1:A:45:VAL:HG21	4:B:920:AMP:H3'	1.44	0.97
1:A:682:MET:SD	1:A:699:MET:HG2	2.09	0.92
1:D:428:MET:SD	1:D:470:ASP:HB3	2.09	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:HD21	1:B:303:THR:HG21	1.50	0.92
1:A:677:GLY:HA2	1:A:680:LYS:HG3	1.52	0.89
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.53	0.88
1:A:103:ALA:HB2	1:A:234:ARG:HH11	1.38	0.88
1:D:326:PHE:HA	1:D:329:PHE:HB2	1.58	0.85
1:B:550:GLU:HA	1:B:554:LYS:HA	1.60	0.84
1:C:486:ILE:HD11	1:C:676:THR:HG23	1.56	0.84
1:D:597:PHE:HE2	1:D:792:LYS:HD2	1.43	0.83
1:C:85:LEU:HD12	1:C:342:PRO:HB3	1.61	0.82
1:A:208:HIS:HA	1:A:213:ALA:HA	1.61	0.81
1:A:799:ARG:HA	1:A:802:ILE:HD12	1.64	0.79
1:A:88:GLU:HG2	1:A:132:GLY:HA2	1.65	0.79
1:A:337:LEU:HD23	1:A:445:CYS:SG	2.23	0.78
1:D:663:SER:HB3	1:D:688:THR:HA	1.66	0.78
1:D:315:LYS:HA	1:D:318:CYS:SG	2.25	0.77
1:A:336:GLN:HE21	1:A:825:TRP:HE1	1.33	0.77
1:A:389:VAL:HG12	1:A:439:ILE:HG13	1.65	0.77
1:C:251:ASP:HB3	1:C:255:LYS:HB3	1.65	0.76
1:A:490:ARG:HA	1:A:494:LEU:HD13	1.67	0.76
1:C:165:ILE:HD11	1:C:281:PRO:HA	1.67	0.76
1:A:337:LEU:HB2	1:A:374:TYR:HB2	1.67	0.76
1:A:492:LEU:HG	1:A:683:LEU:HD22	1.68	0.76
1:A:326:PHE:HA	1:A:329:PHE:HB2	1.69	0.75
1:D:522:LEU:O	1:D:525:VAL:HG23	1.87	0.75
1:D:692:MET:SD	1:D:710:ILE:HG21	2.26	0.74
1:D:326:PHE:HD1	1:D:329:PHE:CD2	2.05	0.74
1:A:423:ASP:HA	1:A:426:ARG:HG2	1.69	0.74
1:C:733:ASP:HA	1:C:739:ARG:HH12	1.53	0.73
1:A:459:HIS:O	1:A:462:ILE:HG12	1.88	0.73
1:D:323:ARG:HG2	1:D:325:ASN:HB2	1.69	0.73
1:A:738:LEU:O	1:A:741:ILE:HG12	1.89	0.73
1:C:486:ILE:HG12	1:C:680:LYS:HG3	1.71	0.73
1:A:738:LEU:HD12	1:A:741:ILE:HD11	1.71	0.72
1:B:316:PHE:HD2	1:B:324:THR:HG23	1.54	0.72
1:C:163:PHE:HE1	1:C:277:ARG:HH11	1.38	0.72
1:C:224:MET:SD	1:C:247:LYS:NZ	2.62	0.72
1:D:143:PHE:O	1:D:147:MET:HG3	1.90	0.72
1:B:755:PRO:HD2	1:C:426:ARG:NH1	2.05	0.71
1:A:783:CYS:O	1:A:787:VAL:HG23	1.91	0.71
1:C:570:ILE:HB	1:C:609:ALA:HA	1.72	0.71
1:B:93:ARG:HG2	1:B:126:GLU:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:692:MET:HG3	1:D:697:VAL:HG22	1.71	0.71
1:A:157:TYR:HE1	1:A:242:ARG:HG2	1.56	0.70
1:B:274:ASN:ND2	1:B:291:LEU:HD21	2.07	0.70
1:D:263:ILE:O	1:D:266:VAL:HG23	1.92	0.70
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.73	0.70
1:B:458:ILE:HD11	1:B:694:GLY:H	1.55	0.70
1:B:766:MET:HE3	1:B:774:PHE:HE2	1.56	0.70
1:C:692:MET:SD	1:C:710:ILE:HG21	2.32	0.70
1:B:346:ILE:HG23	1:B:368:THR:HG21	1.74	0.69
1:D:597:PHE:CE2	1:D:792:LYS:HD2	2.26	0.69
1:A:727:ASN:HD21	1:D:725:GLY:HA3	1.58	0.69
1:C:548:TYR:HE2	1:C:655:LYS:HZ2	1.41	0.69
1:D:80:LYS:HE2	1:D:331:ASP:O	1.92	0.69
1:D:474:LEU:HD13	1:D:475:GLU:HG3	1.73	0.69
1:A:34:HIS:CD2	1:A:57:HIS:HB3	2.28	0.69
1:B:678:ASN:ND2	1:B:695:ALA:HB3	2.08	0.69
1:C:91:MET:HB3	1:C:129:ALA:HB3	1.76	0.69
1:D:557:ILE:HG22	1:D:558:ASN:H	1.58	0.69
1:D:170:ILE:HG12	1:D:646:GLU:HG3	1.75	0.68
1:A:157:TYR:CE1	1:A:242:ARG:HG2	2.28	0.68
1:B:678:ASN:HD22	1:B:695:ALA:HB3	1.59	0.68
1:B:353:LEU:HB3	1:B:359:LEU:HD12	1.74	0.68
1:D:253:ASN:OD1	1:D:254:LEU:HD22	1.94	0.68
1:C:369:VAL:HA	1:C:448:GLY:O	1.94	0.67
1:C:568:LYS:HD2	1:C:574:LYS:HE3	1.76	0.67
1:A:426:ARG:NH2	1:D:754:GLN:HA	2.10	0.67
1:A:629:VAL:HG11	1:A:750:PHE:HE1	1.59	0.67
1:D:64:VAL:HA	1:D:67:TRP:HB3	1.77	0.67
1:C:346:ILE:HD13	1:C:448:GLY:HA3	1.77	0.67
1:A:396:LEU:HB3	1:A:399:HIS:HB2	1.77	0.67
1:A:49:ARG:HH21	1:A:125:ILE:HG22	1.57	0.67
1:D:813:SER:O	1:D:817:ILE:HG12	1.95	0.67
1:B:562:LEU:HG	1:B:791:TYR:CD2	2.29	0.67
1:C:62:HIS:ND1	1:C:104:LEU:HD21	2.11	0.67
1:D:165:ILE:HG12	1:D:279:LEU:HB3	1.75	0.67
1:D:657:ILE:HD13	1:D:680:LYS:HB3	1.76	0.67
1:A:235:ASN:HD21	1:A:237:VAL:HG22	1.60	0.66
1:D:326:PHE:HD1	1:D:329:PHE:HD2	1.42	0.66
1:A:119:MET:O	1:A:123:GLU:HG3	1.96	0.66
1:D:550:GLU:HA	1:D:554:LYS:HA	1.76	0.66
1:C:326:PHE:HA	1:C:329:PHE:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:ASN:ND2	1:C:695:ALA:HB3	2.11	0.66
1:C:168:GLN:OE1	1:C:608:LYS:HA	1.96	0.66
1:D:732:TYR:HA	1:D:738:LEU:HD22	1.78	0.66
1:D:791:TYR:HA	1:D:797:TRP:CD1	2.30	0.66
1:A:783:CYS:SG	1:A:786:ARG:NH2	2.69	0.66
1:A:87:LEU:HD13	1:A:341:HIS:HB3	1.77	0.65
1:D:519:ARG:O	1:D:522:LEU:HB2	1.96	0.65
1:C:85:LEU:HD12	1:C:342:PRO:CB	2.26	0.65
1:D:488:PRO:O	1:D:492:LEU:HB3	1.95	0.65
1:C:365:TRP:O	1:C:369:VAL:HG23	1.96	0.65
1:D:522:LEU:HD11	1:D:803:ARG:HH11	1.60	0.65
1:A:258:ASN:OD1	1:A:259:VAL:HG22	1.97	0.65
1:C:600:PRO:HA	1:C:639:ARG:O	1.97	0.65
1:D:312:LYS:HA	1:D:324:THR:HG21	1.79	0.64
1:D:75:TYR:HE1	1:D:314:SER:HA	1.61	0.64
1:D:235:ASN:HA	1:D:833:ARG:HG3	1.80	0.64
1:B:615:MET:CE	1:B:761:ILE:HG12	2.27	0.64
1:D:424:ARG:HG3	1:D:427:ARG:NH2	2.11	0.64
1:D:804:ASN:O	1:D:807:THR:HB	1.97	0.64
1:B:305:GLN:O	1:B:309:ARG:HB2	1.98	0.64
1:B:738:LEU:HD12	1:B:741:ILE:HD11	1.80	0.64
1:D:225:PRO:HB2	1:D:242:ARG:HD2	1.80	0.64
1:D:63:LEU:HD21	1:D:231:PRO:HB3	1.79	0.64
1:A:732:TYR:CE1	1:A:739:ARG:HA	2.33	0.63
1:A:795:ARG:O	1:A:799:ARG:HG3	1.99	0.63
1:B:581:LEU:HD22	1:B:741:ILE:HD12	1.81	0.63
1:D:60:ARG:HD3	1:D:188:PRO:O	1.99	0.63
1:D:578:LEU:HD23	1:D:666:ILE:HD12	1.79	0.63
1:C:315:LYS:HA	1:C:318:CYS:SG	2.37	0.63
1:D:198:LEU:HD22	1:D:305:GLN:HB3	1.81	0.63
1:A:599:VAL:HG11	1:A:791:TYR:HD2	1.62	0.63
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.81	0.63
1:B:790:LEU:HD23	1:B:797:TRP:CD1	2.34	0.63
1:D:193:ARG:HB2	1:D:225:PRO:HG2	1.80	0.63
1:D:530:PHE:HA	1:D:533:ASP:HB2	1.80	0.63
1:D:316:PHE:HB3	1:D:324:THR:HG23	1.81	0.62
1:D:688:THR:HG22	1:D:689:ILE:O	1.98	0.62
1:B:28:LYS:HB3	1:B:115:LEU:HD21	1.82	0.62
1:A:472:TYR:CD1	1:A:476:PRO:HA	2.34	0.62
1:A:516:ASP:HA	1:A:809:GLY:HA3	1.81	0.62
1:A:91:MET:SD	1:A:241:MET:HE1	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:O	1:A:114:GLN:HG3	1.99	0.62
1:A:215:TRP:CE2	1:A:218:THR:HG21	2.35	0.62
1:B:791:TYR:HA	1:B:797:TRP:CD1	2.35	0.62
1:D:567:VAL:HA	1:D:606:GLY:O	2.00	0.62
1:B:234:ARG:O	1:B:833:ARG:HG3	2.00	0.62
1:D:293:LEU:HD23	1:D:391:LEU:HD22	1.82	0.62
1:D:588:ASN:HD21	1:D:741:ILE:HG22	1.65	0.61
1:A:103:ALA:HB2	1:A:234:ARG:HD2	1.82	0.61
1:C:340:THR:O	1:C:343:SER:HB3	2.00	0.61
1:D:627:GLY:O	1:D:631:ASN:HB2	1.99	0.61
1:D:692:MET:SD	1:D:710:ILE:CG2	2.87	0.61
1:A:733:ASP:HA	1:A:739:ARG:HH12	1.64	0.61
1:B:87:LEU:HD11	1:B:296:GLU:HA	1.82	0.61
1:D:85:LEU:HD13	1:D:300:VAL:HG23	1.82	0.61
1:B:502:ILE:O	1:B:506:ARG:HG2	2.00	0.61
1:D:499:LEU:N	1:D:537:VAL:HG11	2.14	0.61
1:B:666:ILE:HG22	1:B:711:PHE:CE1	2.36	0.61
1:D:91:MET:SD	1:D:241:MET:HE1	2.40	0.61
1:D:498:GLY:O	1:D:501:GLU:HB3	2.01	0.61
1:A:255:LYS:O	1:A:256:ASP:HB2	2.00	0.61
1:D:396:LEU:HB3	1:D:399:HIS:HB2	1.82	0.61
1:D:42:ASP:OD1	1:D:43:ARG:N	2.34	0.61
1:B:166:PHE:HB2	1:B:178:GLU:O	2.00	0.60
1:D:702:GLU:HB2	1:D:807:THR:HG23	1.82	0.60
1:B:316:PHE:HA	1:B:319:ARG:HB3	1.83	0.60
1:C:606:GLY:HA3	1:C:645:LEU:HB2	1.83	0.60
1:B:600:PRO:HA	1:B:639:ARG:O	2.01	0.60
1:C:690:GLY:O	1:C:710:ILE:HA	2.01	0.60
1:D:748:GLY:HA3	1:D:755:PRO:HB3	1.83	0.60
1:A:395:LEU:HG	1:A:396:LEU:HD22	1.84	0.60
1:A:197:THR:O	1:A:198:LEU:HD23	2.02	0.60
1:D:64:VAL:O	1:D:68:ILE:HG12	2.01	0.60
1:D:227:ASP:OD1	1:D:242:ARG:HD3	2.01	0.60
1:A:585:THR:O	1:A:589:ARG:HD3	2.02	0.60
1:D:200:VAL:HG21	1:D:298:PHE:CD1	2.36	0.60
1:C:503:ILE:HG12	1:C:521:LEU:HD21	1.84	0.59
1:A:446:ILE:HG21	1:A:471:PHE:CD2	2.37	0.59
1:C:694:GLY:O	1:C:697:VAL:HB	2.01	0.59
1:D:341:HIS:HB2	1:D:342:PRO:HD3	1.84	0.59
1:D:507:ILE:HB	1:D:520:LYS:NZ	2.16	0.59
1:A:525:VAL:O	1:A:531:ILE:HD11	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:ASP:HA	1:A:739:ARG:NH1	2.17	0.59
1:B:482:LYS:HZ2	1:B:823:GLU:CD	2.05	0.59
1:C:716:GLU:O	1:C:720:ARG:HG2	2.02	0.59
1:D:593:GLU:HB3	1:D:596:LYS:HB2	1.83	0.59
1:A:692:MET:HE2	1:A:710:ILE:HG21	1.85	0.59
1:D:521:LEU:HA	1:D:524:TYR:CD1	2.37	0.59
1:D:357:GLU:O	1:D:358:ARG:HB2	2.01	0.59
1:D:795:ARG:O	1:D:799:ARG:HG3	2.02	0.59
1:A:455:VAL:H	1:A:459:HIS:HD2	1.51	0.59
1:B:290:GLU:HG3	1:B:391:LEU:CD2	2.33	0.59
1:D:18:LEU:HD22	1:D:18:LEU:H	1.68	0.59
1:C:781:VAL:HG23	1:C:782:LYS:HE3	1.85	0.59
1:A:150:LEU:HD13	1:A:829:PRO:HB3	1.85	0.58
1:B:778:GLU:O	1:B:782:LYS:HG2	2.03	0.58
1:D:588:ASN:HD21	1:D:744:GLN:HE22	1.50	0.58
1:A:348:GLU:O	1:A:352:VAL:HG23	2.03	0.58
1:A:392:LEU:HB3	1:A:400:LEU:HB2	1.85	0.58
1:C:316:PHE:O	1:C:324:THR:HG23	2.03	0.58
1:C:336:GLN:HG2	1:C:825:TRP:HE1	1.68	0.58
1:D:703:ALA:HB2	1:D:807:THR:HG21	1.85	0.58
1:A:528:GLU:HB3	1:A:532:ARG:NH2	2.19	0.58
1:A:629:VAL:HG11	1:A:750:PHE:CE1	2.38	0.58
1:C:642:VAL:O	1:C:643:ILE:HG13	2.03	0.58
1:D:91:MET:SD	1:D:241:MET:CE	2.92	0.58
1:D:511:TYR:HA	1:D:514:ASP:O	2.03	0.58
1:B:573:TYR:HD2	1:B:671:THR:HB	1.69	0.58
1:C:692:MET:SD	1:C:710:ILE:HG13	2.44	0.58
1:D:642:VAL:O	1:D:643:ILE:HG13	2.02	0.58
1:D:350:MET:SD	1:D:365:TRP:HE3	2.26	0.58
1:C:68:ILE:O	1:C:72:GLN:HG3	2.04	0.58
1:B:82:ILE:HB	1:B:334:ALA:HB3	1.86	0.58
1:C:711:PHE:CZ	1:C:780:TYR:HD1	2.21	0.58
1:D:98:THR:O	1:D:102:LEU:HB2	2.04	0.58
1:D:336:GLN:HG3	1:D:825:TRP:HE1	1.67	0.58
1:B:458:ILE:HD11	1:B:694:GLY:N	2.19	0.58
1:B:184:ARG:HD2	1:B:185:TYR:CE2	2.39	0.58
1:B:293:LEU:HD23	1:B:395:LEU:HD21	1.86	0.57
1:B:539:GLN:O	1:B:543:LEU:HB2	2.04	0.57
1:C:322:VAL:O	1:C:325:ASN:HB2	2.03	0.57
1:D:675:GLY:HA3	1:D:678:ASN:HD21	1.68	0.57
1:D:721:LEU:HG	1:D:726:TYR:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASP:O	1:A:425:LEU:HD23	2.04	0.57
1:A:600:PRO:HB3	1:A:639:ARG:HA	1.86	0.57
1:B:211:GLN:HG2	1:B:358:ARG:HD2	1.85	0.57
1:C:85:LEU:HD22	1:C:303:THR:HG21	1.84	0.57
1:D:459:HIS:CD2	1:D:673:ALA:HB1	2.39	0.57
1:B:707:ASN:HA	1:B:800:MET:SD	2.44	0.57
1:A:74:TYR:CE2	1:A:153:ALA:HA	2.40	0.57
1:C:150:LEU:HB3	1:C:829:PRO:HB3	1.85	0.57
1:D:97:ASN:HA	1:D:494:LEU:HD11	1.87	0.57
1:D:410:PHE:O	1:D:414:VAL:HG23	2.05	0.57
1:A:30:ASN:HB2	1:A:58:THR:HG23	1.84	0.57
1:A:651:SER:HA	1:A:654:GLU:HG2	1.86	0.57
1:C:96:GLN:O	1:C:100:VAL:HG13	2.05	0.57
1:C:224:MET:HB2	1:C:247:LYS:HE2	1.85	0.57
1:A:336:GLN:NE2	1:A:825:TRP:HE1	2.02	0.57
1:C:129:ALA:HB1	1:C:131:LEU:HD23	1.86	0.57
1:C:751:SER:HB2	1:C:754:GLN:O	2.04	0.57
1:D:661:ASP:HB3	1:D:797:TRP:CH2	2.40	0.57
1:D:456:ALA:HB3	1:D:459:HIS:HB3	1.87	0.56
1:A:181:ASP:O	1:A:184:ARG:HB2	2.05	0.56
1:B:727:ASN:O	1:B:730:GLU:HG2	2.05	0.56
1:C:322:VAL:HG13	1:C:325:ASN:HB2	1.87	0.56
1:A:583:VAL:HG11	1:A:642:VAL:HG22	1.88	0.56
1:B:320:ASP:HA	1:B:324:THR:HA	1.87	0.56
1:B:459:HIS:CD2	1:B:673:ALA:HB1	2.39	0.56
1:D:764:MET:HA	1:D:768:HIS:CE1	2.41	0.56
1:A:411:LEU:HD11	1:A:429:SER:HB2	1.87	0.56
1:B:781:VAL:HG23	1:B:782:LYS:HE3	1.87	0.56
1:D:798:THR:O	1:D:802:ILE:HG13	2.06	0.56
1:B:181:ASP:O	1:B:184:ARG:HB2	2.06	0.56
1:D:316:PHE:HD2	1:D:324:THR:HG23	1.71	0.56
1:A:661:ASP:HB3	1:A:797:TRP:CZ2	2.41	0.56
1:A:590:ILE:HG12	1:A:598:VAL:HG11	1.88	0.56
1:B:253:ASN:O	1:B:254:LEU:HD12	2.05	0.56
1:B:290:GLU:O	1:B:294:LYS:HG3	2.06	0.56
1:C:678:ASN:HD22	1:C:695:ALA:HB3	1.71	0.56
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.41	0.56
1:B:319:ARG:NE	1:B:321:PRO:HD2	2.21	0.56
1:C:609:ALA:HB2	1:C:620:ILE:HD11	1.87	0.56
1:C:726:TYR:OH	1:C:774:PHE:HB2	2.05	0.56
1:D:73:HIS:CD2	1:D:834:LEU:HD11	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:VAL:HG21	1:B:788:SER:O	2.05	0.55
1:C:129:ALA:HB1	1:C:131:LEU:CD2	2.35	0.55
1:B:677:GLY:HA2	1:B:680:LYS:HD2	1.88	0.55
1:C:626:ILE:O	1:C:630:VAL:HG13	2.06	0.55
1:D:235:ASN:HB2	1:D:833:ARG:HA	1.87	0.55
1:B:511:TYR:HA	1:B:514:ASP:O	2.07	0.55
1:C:235:ASN:OD1	1:C:237:VAL:HG22	2.07	0.55
1:C:695:ALA:O	1:C:699:MET:SD	2.65	0.55
1:B:459:HIS:HB2	1:B:673:ALA:O	2.06	0.55
1:A:14:SER:OG	1:A:16:ARG:NH1	2.39	0.55
1:A:468:PHE:HB3	1:A:479:PHE:CZ	2.41	0.55
1:A:322:VAL:HG13	1:A:325:ASN:HD22	1.71	0.55
1:A:492:LEU:HG	1:A:683:LEU:CD2	2.35	0.55
1:A:583:VAL:HG11	1:A:642:VAL:CG2	2.36	0.55
1:C:147:MET:O	1:C:152:LEU:HB2	2.07	0.55
1:C:665:GLN:HE21	1:C:678:ASN:HA	1.72	0.55
1:C:692:MET:SD	1:C:710:ILE:CG2	2.94	0.55
1:D:143:PHE:CD1	1:D:817:ILE:HD11	2.41	0.55
1:D:613:TYR:HE1	1:D:615:MET:HB3	1.71	0.55
1:A:204:GLY:HA3	1:A:218:THR:HG22	1.89	0.55
1:A:689:ILE:HA	1:A:709:PHE:HB2	1.89	0.55
1:D:507:ILE:HB	1:D:520:LYS:HZ2	1.71	0.55
1:D:721:LEU:HD21	1:D:726:TYR:HD1	1.71	0.55
1:A:540:GLU:O	1:A:544:LYS:HD3	2.06	0.55
1:B:161:TYR:HA	1:B:276:SER:O	2.07	0.55
1:B:612:GLY:H	1:B:617:LYS:HE2	1.72	0.55
1:B:728:ALA:O	1:B:731:TYR:HB2	2.07	0.55
1:B:810:LYS:HD3	1:B:811:PHE:HE1	1.72	0.55
1:D:144:LEU:HD21	1:D:156:GLY:HA3	1.89	0.55
1:A:503:ILE:HG23	1:A:521:LEU:HD11	1.90	0.54
1:B:795:ARG:O	1:B:799:ARG:HG3	2.07	0.54
1:C:343:SER:HB2	1:C:445:CYS:SG	2.47	0.54
1:C:834:LEU:HD12	1:C:835:PRO:HD2	1.89	0.54
1:D:650:VAL:HA	3:D:999:PLP:H2A1	1.90	0.54
1:A:458:ILE:HG21	1:A:697:VAL:HG21	1.90	0.54
1:D:486:ILE:HG12	1:D:680:LYS:HG3	1.88	0.54
1:B:355:ASP:OD2	1:B:398:ARG:HD3	2.08	0.54
1:C:96:GLN:HA	1:C:99:MET:CE	2.37	0.54
1:B:204:GLY:HA3	1:B:215:TRP:HE1	1.73	0.54
1:D:28:LYS:HZ2	1:D:114:GLN:HB3	1.72	0.54
1:B:391:LEU:O	1:B:395:LEU:HD23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:576:GLN:O	1:D:580:CYS:SG	2.58	0.54
1:D:818:ALA:O	1:D:821:ALA:HB3	2.08	0.54
1:A:797:TRP:CZ3	1:A:801:VAL:HG21	2.43	0.54
1:C:204:GLY:HA3	1:C:218:THR:HG22	1.90	0.54
1:C:742:ILE:HD11	1:C:774:PHE:CZ	2.43	0.54
1:B:341:HIS:HB2	1:B:342:PRO:HD3	1.89	0.54
1:C:492:LEU:HG	1:C:683:LEU:HD22	1.90	0.54
1:D:138:ARG:HD3	1:D:491:TRP:HZ2	1.72	0.54
1:B:67:TRP:O	1:B:71:GLN:HG2	2.08	0.54
1:C:727:ASN:O	1:C:730:GLU:HG2	2.08	0.54
1:D:707:ASN:CA	1:D:800:MET:SD	2.90	0.54
1:A:482:LYS:HE3	1:A:819:GLN:O	2.06	0.54
1:D:351:ARG:HG2	1:D:398:ARG:HG2	1.89	0.54
1:D:424:ARG:HA	1:D:427:ARG:NH2	2.23	0.54
1:D:527:ASP:OD2	1:D:529:ALA:HB3	2.07	0.54
1:D:665:GLN:HE22	1:D:678:ASN:HA	1.73	0.54
1:B:82:ILE:HD11	1:B:147:MET:SD	2.47	0.53
1:B:456:ALA:HB2	1:B:674:SER:HB2	1.89	0.53
1:B:746:SER:OG	1:B:762:VAL:HG11	2.07	0.53
1:C:340:THR:HB	1:C:385:GLU:OE1	2.08	0.53
1:C:707:ASN:HA	1:C:800:MET:SD	2.48	0.53
1:A:21:VAL:O	1:A:23:ASN:N	2.41	0.53
1:A:129:ALA:HA	1:A:182:TRP:CE3	2.43	0.53
1:A:191:LYS:HD2	1:A:193:ARG:HH11	1.73	0.53
1:D:682:MET:HE3	1:D:808:SER:HA	1.90	0.53
1:A:39:LEU:HD21	1:A:53:PHE:HB2	1.90	0.53
1:A:49:ARG:HG3	1:A:53:PHE:HE2	1.73	0.53
1:C:250:ASN:HD21	1:C:269:ARG:HE	1.56	0.53
1:A:42:ASP:OD2	1:A:44:ASN:HB2	2.08	0.53
1:B:423:ASP:HA	1:B:426:ARG:HG3	1.89	0.53
1:B:574:LYS:NZ	2:B:901:SO4:O2	2.41	0.53
1:B:577:LEU:HD13	1:B:765:LEU:HD13	1.89	0.53
1:B:735:ILE:O	1:B:739:ARG:HB2	2.09	0.53
1:D:436:VAL:HB	1:D:438:ARG:NH2	2.24	0.53
1:B:573:TYR:CD2	1:B:671:THR:HB	2.43	0.53
1:B:590:ILE:HD11	1:B:598:VAL:HG21	1.91	0.53
1:C:363:LYS:O	1:C:367:VAL:HG23	2.07	0.53
1:D:390:HIS:HA	1:D:393:GLU:OE1	2.09	0.53
1:C:224:MET:SD	1:C:247:LYS:CE	2.96	0.53
1:D:322:VAL:O	1:D:325:ASN:N	2.41	0.53
1:D:575:ARG:NH2	1:D:776:ASP:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:VAL:O	1:B:325:ASN:HB2	2.09	0.53
1:B:350:MET:O	1:B:354:VAL:HG23	2.08	0.53
1:A:426:ARG:NH1	1:D:755:PRO:HD2	2.24	0.53
1:C:395:LEU:H	1:C:395:LEU:HD23	1.74	0.53
1:D:231:PRO:HA	1:D:238:VAL:HG22	1.91	0.53
1:C:665:GLN:NE2	1:C:678:ASN:HA	2.24	0.53
1:D:507:ILE:HG21	1:D:520:LYS:HB2	1.89	0.53
1:D:561:SER:HA	1:D:600:PRO:HG2	1.90	0.53
1:D:603:VAL:HG23	1:D:642:VAL:HA	1.91	0.53
1:A:361:TRP:CZ3	1:A:409:ARG:HD2	2.44	0.53
1:B:580:CYS:SG	1:B:622:LEU:HD12	2.49	0.53
1:B:347:PRO:HG3	1:B:403:ILE:HD11	1.91	0.52
1:D:661:ASP:HB3	1:D:797:TRP:HH2	1.72	0.52
1:B:319:ARG:HE	1:B:319:ARG:C	2.13	0.52
1:C:168:GLN:HB2	1:C:608:LYS:HG2	1.91	0.52
1:D:528:GLU:HG2	1:D:532:ARG:HH21	1.73	0.52
1:D:664:GLU:HA	1:D:689:ILE:HG22	1.91	0.52
1:D:675:GLY:HA3	1:D:678:ASN:ND2	2.24	0.52
1:D:677:GLY:HA2	1:D:680:LYS:HD2	1.92	0.52
1:A:264:GLN:NE2	1:C:267:LEU:HD22	2.24	0.52
1:B:157:TYR:CE2	1:B:242:ARG:HG2	2.44	0.52
1:B:183:LEU:HD23	1:B:187:ASN:HB2	1.91	0.52
1:B:783:CYS:SG	1:B:786:ARG:NH2	2.83	0.52
1:C:689:ILE:HA	1:C:709:PHE:HB2	1.90	0.52
1:D:167:ASN:HD22	1:D:180:ASP:HB2	1.72	0.52
1:B:361:TRP:HH2	1:B:406:ILE:HG12	1.74	0.52
1:D:569:ARG:HG2	1:D:574:LYS:HD3	1.92	0.52
1:D:699:MET:HB3	1:D:708:PHE:HE2	1.73	0.52
1:B:90:TYR:HB3	1:B:137:GLY:C	2.30	0.52
1:D:274:ASN:HA	1:D:277:ARG:HG3	1.91	0.52
1:B:82:ILE:HA	1:B:334:ALA:HB3	1.91	0.52
1:D:503:ILE:HG12	1:D:521:LEU:HD21	1.91	0.52
1:C:590:ILE:O	1:C:594:PRO:HA	2.10	0.52
1:C:699:MET:HB3	1:C:708:PHE:HZ	1.74	0.52
1:D:75:TYR:CE1	1:D:314:SER:HA	2.44	0.52
1:D:491:TRP:HA	1:D:495:CYS:SG	2.50	0.52
1:D:735:ILE:HG22	1:D:738:LEU:HB2	1.92	0.52
1:C:63:LEU:HD13	1:C:229:PRO:HG2	1.92	0.52
1:C:253:ASN:H	1:C:259:VAL:HG21	1.74	0.52
1:D:171:CYS:O	1:D:174:TRP:HB2	2.09	0.52
1:A:676:THR:HG22	3:A:999:PLP:C4A	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:MET:HE2	1:B:761:ILE:HG12	1.92	0.51
1:C:355:ASP:OD2	1:C:398:ARG:HD3	2.10	0.51
1:C:579:ASN:O	1:C:583:VAL:HG23	2.09	0.51
1:A:577:LEU:O	1:A:581:LEU:HG	2.11	0.51
1:B:810:LYS:HD3	1:B:811:PHE:CE1	2.45	0.51
1:C:378:THR:O	1:C:459:HIS:CE1	2.63	0.51
1:D:326:PHE:CA	1:D:329:PHE:HB2	2.36	0.51
1:D:567:VAL:HB	1:D:648:TYR:CZ	2.45	0.51
1:B:255:LYS:O	1:B:256:ASP:HB2	2.09	0.51
1:B:571:HIS:CE1	1:B:613:TYR:HH	2.27	0.51
1:B:798:THR:O	1:B:802:ILE:HG13	2.11	0.51
1:C:348:GLU:OE1	1:C:399:HIS:HE1	1.93	0.51
1:C:258:ASN:OD1	1:C:259:VAL:HG22	2.10	0.51
1:B:112:THR:HG22	1:B:117:LEU:HB2	1.92	0.51
1:B:315:LYS:O	1:B:319:ARG:HB2	2.10	0.51
1:C:250:ASN:HD21	1:C:269:ARG:NE	2.08	0.51
1:A:369:VAL:HG22	1:A:448:GLY:HA2	1.92	0.51
1:A:538:LYS:O	1:A:538:LYS:HG3	2.10	0.51
1:B:402:ILE:O	1:B:406:ILE:HG13	2.10	0.51
1:C:96:GLN:HA	1:C:99:MET:HE3	1.91	0.51
1:A:149:THR:HA	1:A:235:ASN:OD1	2.10	0.51
1:B:290:GLU:HG3	1:B:391:LEU:HD21	1.92	0.51
1:C:676:THR:HG22	3:C:999:PLP:C4A	2.40	0.51
1:D:168:GLN:HE22	1:D:644:PHE:HE2	1.59	0.51
1:A:203:TYR:O	1:A:218:THR:HG22	2.11	0.51
1:A:353:LEU:O	1:A:357:GLU:HB2	2.11	0.51
1:C:91:MET:HB3	1:C:129:ALA:CB	2.40	0.51
1:C:472:TYR:CE1	1:C:476:PRO:HA	2.46	0.51
1:A:88:GLU:HG3	1:A:279:LEU:HD11	1.93	0.51
1:C:323:ARG:HB2	1:C:325:ASN:CG	2.32	0.51
1:A:703:ALA:CA	1:A:807:THR:HG21	2.40	0.51
1:B:280:TYR:OH	1:B:291:LEU:HD12	2.11	0.51
1:A:355:ASP:OD2	1:A:398:ARG:HD3	2.10	0.50
1:B:426:ARG:NH2	1:B:427:ARG:HG2	2.27	0.50
1:B:738:LEU:O	1:B:742:ILE:HG12	2.11	0.50
1:C:446:ILE:HG12	1:C:452:VAL:HG21	1.93	0.50
1:D:138:ARG:HD3	1:D:491:TRP:CZ2	2.45	0.50
1:D:637:GLY:O	1:D:641:ARG:NH2	2.44	0.50
1:A:274:ASN:HA	1:A:277:ARG:HB2	1.93	0.50
1:C:315:LYS:CA	1:C:318:CYS:SG	2.99	0.50
1:D:211:GLN:HG3	1:D:358:ARG:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:PHE:HZ	1:D:268:ASP:OD2	1.94	0.50
1:B:99:MET:HB3	1:B:105:GLU:HA	1.93	0.50
1:B:279:LEU:HD23	1:B:280:TYR:H	1.76	0.50
1:C:341:HIS:HB2	1:C:342:PRO:HD3	1.93	0.50
1:D:575:ARG:HH22	1:D:776:ASP:HB2	1.76	0.50
1:D:810:LYS:O	1:D:815:ARG:NH2	2.43	0.50
1:C:357:GLU:O	1:C:358:ARG:HB2	2.11	0.50
1:C:589:ARG:HH11	1:C:737:GLU:HG2	1.77	0.50
1:D:346:ILE:HD13	1:D:445:CYS:HA	1.93	0.50
1:A:529:ALA:O	1:A:532:ARG:HG2	2.12	0.50
1:D:70:THR:O	1:D:73:HIS:HB3	2.11	0.50
1:D:455:VAL:HG12	1:D:459:HIS:HD2	1.76	0.50
1:D:506:ARG:HH22	1:D:533:ASP:CG	2.14	0.50
1:D:677:GLY:O	1:D:681:PHE:HD1	1.95	0.50
1:B:263:ILE:O	1:B:266:VAL:HG23	2.12	0.50
1:A:330:PRO:HG3	1:A:370:LYS:HE3	1.93	0.50
1:B:74:TYR:CZ	1:B:153:ALA:HA	2.47	0.50
1:B:207:GLU:OE2	1:B:214:LYS:NZ	2.45	0.50
1:C:13:ILE:O	1:D:43:ARG:HD3	2.11	0.50
1:A:687:LEU:HD22	1:A:800:MET:HG2	1.94	0.50
1:C:699:MET:HB3	1:C:708:PHE:CZ	2.46	0.50
1:D:373:ALA:HA	1:D:449:SER:HB3	1.93	0.50
1:A:449:SER:O	1:A:478:LYS:HD3	2.12	0.49
1:B:47:THR:H	1:B:50:ASP:HB2	1.77	0.49
1:C:34:HIS:HA	1:C:38:THR:HB	1.93	0.49
1:C:764:MET:SD	1:C:769:ASP:HA	2.52	0.49
1:D:562:LEU:HB2	1:D:600:PRO:O	2.12	0.49
1:A:456:ALA:HA	1:A:483:THR:HG23	1.93	0.49
1:A:601:ARG:NH2	1:A:784:GLN:OE1	2.45	0.49
1:B:48:PRO:HB2	1:B:125:ILE:HD11	1.94	0.49
1:B:742:ILE:HG22	1:B:762:VAL:HG13	1.93	0.49
1:D:60:ARG:HG3	1:D:189:TRP:CE3	2.47	0.49
1:D:82:ILE:HD13	1:D:82:ILE:O	2.12	0.49
1:D:516:ASP:HA	1:D:809:GLY:HA3	1.94	0.49
1:D:713:MET:HG2	1:D:717:ASP:HB2	1.94	0.49
1:A:526:ASP:OD2	1:A:799:ARG:NH1	2.45	0.49
1:B:601:ARG:NH2	1:B:784:GLN:OE1	2.45	0.49
1:B:267:LEU:HD23	1:B:271:LEU:HD21	1.94	0.49
1:C:70:THR:O	1:C:73:HIS:HB3	2.12	0.49
1:C:289:LYS:HG2	1:C:291:LEU:HB2	1.94	0.49
1:D:579:ASN:HB2	1:D:666:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ARG:HB3	1:A:524:TYR:CE2	2.47	0.49
1:B:369:VAL:O	1:B:450:HIS:HB3	2.12	0.49
1:D:531:ILE:HD11	1:D:799:ARG:CD	2.43	0.49
1:B:366:GLU:O	1:B:370:LYS:HB2	2.13	0.49
1:C:605:ILE:O	1:C:644:PHE:HA	2.12	0.49
1:D:507:ILE:CG2	1:D:520:LYS:HD2	2.42	0.49
1:B:93:ARG:HA	1:B:126:GLU:OE2	2.13	0.49
1:B:558:ASN:OD1	1:B:560:ASN:HB2	2.13	0.49
1:C:392:LEU:HB3	1:C:400:LEU:HG	1.94	0.49
1:D:24:VAL:O	1:D:28:LYS:HG3	2.13	0.49
1:D:92:GLY:H	1:D:129:ALA:HB3	1.78	0.49
1:A:614:HIS:O	1:A:618:MET:HG2	2.12	0.49
1:B:91:MET:SD	1:B:141:ALA:CB	3.00	0.49
1:B:538:LYS:HG3	1:B:542:LYS:HD3	1.95	0.49
1:C:487:THR:O	1:C:491:TRP:HB2	2.13	0.49
1:C:711:PHE:CZ	1:C:780:TYR:CD1	3.00	0.49
1:C:784:GLN:HA	1:C:787:VAL:HB	1.93	0.49
1:D:163:PHE:CD1	1:D:181:ASP:HB3	2.48	0.49
1:D:352:VAL:HA	1:D:356:LEU:HD12	1.95	0.49
1:A:169:LYS:HB2	1:A:178:GLU:OE1	2.13	0.49
1:A:310:ARG:O	1:A:314:SER:HB2	2.13	0.49
1:D:170:ILE:O	1:D:170:ILE:HG22	2.13	0.49
1:D:293:LEU:CD2	1:D:391:LEU:HD22	2.43	0.49
1:D:568:LYS:HE2	1:D:665:GLN:OE1	2.11	0.49
1:D:587:TYR:HE2	1:D:749:PHE:CZ	2.31	0.49
1:D:665:GLN:HG2	1:D:696:ASN:OD1	2.13	0.49
1:A:80:LYS:HE3	1:A:825:TRP:O	2.12	0.48
1:A:486:ILE:HD11	1:A:676:THR:HG23	1.95	0.48
1:B:571:HIS:ND1	1:B:613:TYR:OH	2.44	0.48
1:C:455:VAL:O	1:C:674:SER:HB2	2.12	0.48
1:C:726:TYR:CE2	1:C:728:ALA:HB2	2.48	0.48
1:D:486:ILE:HD13	1:D:679:MET:HB2	1.95	0.48
1:D:489:ARG:HD3	1:D:489:ARG:N	2.27	0.48
1:A:665:GLN:HE21	1:A:678:ASN:HA	1.76	0.48
1:C:313:SER:O	1:C:315:LYS:N	2.46	0.48
1:C:522:LEU:HD13	1:C:806:ALA:CB	2.43	0.48
1:D:352:VAL:O	1:D:356:LEU:HB2	2.14	0.48
1:B:64:VAL:O	1:B:68:ILE:HG12	2.13	0.48
1:C:323:ARG:HB2	1:C:325:ASN:HA	1.96	0.48
1:D:558:ASN:OD1	1:D:560:ASN:HB2	2.13	0.48
1:D:699:MET:HB3	1:D:708:PHE:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:816:THR:O	1:D:820:TYR:HD1	1.95	0.48
1:A:55:LEU:HD13	1:A:112:THR:HG21	1.95	0.48
1:A:336:GLN:HG3	1:A:825:TRP:CZ2	2.49	0.48
1:A:712:GLY:H	1:A:779:GLU:HG2	1.78	0.48
1:B:582:HIS:HD2	1:B:781:VAL:HG12	1.79	0.48
1:B:742:ILE:CG2	1:B:762:VAL:HG13	2.43	0.48
1:D:36:HIS:O	1:D:40:VAL:HA	2.14	0.48
1:D:80:LYS:HA	1:D:332:LYS:O	2.13	0.48
1:B:506:ARG:HB3	1:B:524:TYR:CE2	2.49	0.48
1:B:665:GLN:NE2	1:B:678:ASN:HA	2.29	0.48
1:D:713:MET:SD	1:D:718:VAL:HG22	2.53	0.48
1:D:759:LYS:NZ	1:D:763:ASN:OD1	2.38	0.48
1:A:235:ASN:ND2	1:A:237:VAL:HG13	2.29	0.48
1:B:720:ARG:O	1:B:723:GLN:HB3	2.13	0.48
1:A:636:VAL:O	1:A:639:ARG:HD3	2.13	0.48
1:B:506:ARG:HB3	1:B:524:TYR:HE2	1.79	0.48
1:C:43:ARG:HD3	1:D:13:ILE:O	2.12	0.48
1:D:27:LEU:HD11	1:D:107:ALA:HB1	1.96	0.48
1:D:200:VAL:HG11	1:D:298:PHE:HA	1.94	0.48
1:D:374:TYR:OH	1:D:376:ASN:ND2	2.45	0.48
1:A:665:GLN:HG2	1:A:678:ASN:ND2	2.28	0.48
1:C:60:ARG:O	1:C:64:VAL:HG13	2.13	0.48
1:D:27:LEU:CD1	1:D:107:ALA:HB1	2.44	0.48
1:D:91:MET:CE	1:D:144:LEU:HD12	2.43	0.48
1:B:202:PHE:CE1	1:B:297:TYR:HD2	2.32	0.48
1:C:458:ILE:HD11	1:C:694:GLY:H	1.78	0.48
1:C:562:LEU:HB3	1:C:601:ARG:HG2	1.96	0.48
1:C:601:ARG:NH2	1:C:784:GLN:OE1	2.47	0.48
1:D:147:MET:SD	1:D:154:ALA:HB1	2.54	0.48
1:D:395:LEU:HG	1:D:396:LEU:HD13	1.95	0.48
1:D:651:SER:O	1:D:655:LYS:HG3	2.14	0.48
1:B:403:ILE:HG21	1:B:439:ILE:HD13	1.95	0.47
1:B:821:ALA:HB1	1:B:827:VAL:O	2.14	0.47
1:C:55:LEU:HG	1:C:95:LEU:HD11	1.95	0.47
1:D:115:LEU:HD23	1:D:115:LEU:HA	1.67	0.47
1:D:492:LEU:HD11	1:D:511:TYR:OH	2.14	0.47
1:D:765:LEU:HG	1:D:774:PHE:CE1	2.48	0.47
1:A:670:GLY:H	1:A:693:ASP:CG	2.17	0.47
1:C:49:ARG:HA	1:C:125:ILE:HG21	1.96	0.47
1:C:103:ALA:HA	1:C:234:ARG:NH1	2.29	0.47
1:D:615:MET:O	1:D:619:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASP:OD2	1:A:649:ARG:HG3	2.14	0.47
1:C:204:GLY:HA2	1:C:217:ASP:O	2.13	0.47
1:C:589:ARG:NH1	1:C:737:GLU:HG2	2.29	0.47
1:D:163:PHE:CE1	1:D:181:ASP:HB3	2.49	0.47
1:A:40:VAL:HG11	1:B:67:TRP:CZ3	2.49	0.47
1:A:49:ARG:NH2	1:A:125:ILE:HG22	2.27	0.47
1:B:24:VAL:O	1:B:28:LYS:HG3	2.15	0.47
1:B:252:PHE:CE2	1:B:269:ARG:HB2	2.49	0.47
1:C:614:HIS:HE1	1:C:760:ASP:OD2	1.98	0.47
1:A:346:ILE:HG23	1:A:368:THR:CG2	2.44	0.47
1:A:519:ARG:O	1:A:522:LEU:HB2	2.14	0.47
1:A:650:VAL:HA	3:A:999:PLP:H2A1	1.95	0.47
1:C:536:LYS:HG3	1:C:540:GLU:OE1	2.14	0.47
1:C:798:THR:O	1:C:802:ILE:HG13	2.13	0.47
1:D:536:LYS:O	1:D:539:GLN:HB3	2.15	0.47
1:A:499:LEU:HD12	1:A:537:VAL:HG11	1.97	0.47
1:A:536:LYS:HG3	1:A:540:GLU:OE1	2.15	0.47
1:A:574:LYS:NZ	2:A:901:SO4:O4	2.48	0.47
1:B:35:LEU:O	1:B:39:LEU:HB2	2.14	0.47
1:C:235:ASN:ND2	1:C:237:VAL:H	2.13	0.47
1:C:389:VAL:HG22	1:C:437:LYS:O	2.14	0.47
1:C:468:PHE:HB3	1:C:471:PHE:HB2	1.95	0.47
1:A:253:ASN:H	1:A:259:VAL:HG21	1.79	0.47
1:B:491:TRP:HA	1:B:495:CYS:SG	2.54	0.47
1:C:430:LEU:O	1:C:439:ILE:HA	2.13	0.47
1:D:30:ASN:O	1:D:34:HIS:ND1	2.47	0.47
1:D:67:TRP:HB2	1:D:238:VAL:CG1	2.44	0.47
1:D:91:MET:HE1	1:D:144:LEU:HD12	1.97	0.47
1:D:326:PHE:CD1	1:D:329:PHE:HD2	2.28	0.47
1:D:489:ARG:HD3	1:D:489:ARG:H	1.80	0.47
1:A:55:LEU:HD23	1:A:95:LEU:HD11	1.97	0.47
1:A:133:ASN:OD1	1:A:165:ILE:HG21	2.14	0.47
1:A:151:GLY:HA2	1:A:237:VAL:HG11	1.96	0.47
1:C:193:ARG:HB2	1:C:225:PRO:HG2	1.97	0.47
1:C:251:ASP:HB3	1:C:255:LYS:CB	2.41	0.47
1:C:536:LYS:HD2	1:C:536:LYS:HA	1.74	0.47
1:D:207:GLU:OE1	1:D:214:LYS:NZ	2.47	0.47
1:A:80:LYS:HA	1:A:332:LYS:HA	1.97	0.47
1:B:29:LYS:NZ	1:B:29:LYS:HB3	2.29	0.47
1:B:99:MET:CE	1:B:119:MET:SD	3.03	0.47
1:B:564:ASP:OD1	1:B:662:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ALA:CB	1:A:234:ARG:HH11	2.18	0.47
1:A:487:THR:HA	1:A:813:SER:OG	2.15	0.47
1:B:47:THR:HG22	1:B:49:ARG:H	1.80	0.47
1:B:91:MET:SD	1:B:141:ALA:HB2	2.55	0.47
1:B:241:MET:HG2	1:B:243:LEU:CD1	2.45	0.47
1:D:456:ALA:HB3	1:D:459:HIS:CB	2.45	0.47
1:D:754:GLN:HB2	1:D:757:LEU:HB2	1.97	0.47
1:A:369:VAL:O	1:A:450:HIS:HB3	2.16	0.46
1:A:378:THR:O	1:A:459:HIS:HE1	1.97	0.46
1:C:486:ILE:CD1	1:C:676:THR:HG23	2.37	0.46
1:B:70:THR:O	1:B:73:HIS:HB3	2.15	0.46
1:B:206:VAL:HG23	1:B:397:PRO:HB2	1.97	0.46
1:B:426:ARG:NH1	1:C:755:PRO:HD2	2.31	0.46
1:B:698:GLU:O	1:B:702:GLU:HG2	2.14	0.46
1:C:455:VAL:HA	1:C:482:LYS:O	2.16	0.46
1:D:502:ILE:HD12	1:D:533:ASP:HB3	1.97	0.46
1:D:529:ALA:O	1:D:532:ARG:HG2	2.15	0.46
1:D:549:LEU:HD23	1:D:557:ILE:HD11	1.98	0.46
1:D:550:GLU:HA	1:D:553:TYR:O	2.15	0.46
1:D:587:TYR:HE2	1:D:749:PHE:HZ	1.62	0.46
1:A:71:GLN:HB3	4:A:920:AMP:O4'	2.15	0.46
1:A:688:THR:HB	1:A:708:PHE:CE2	2.50	0.46
1:C:575:ARG:HD3	1:C:666:ILE:O	2.16	0.46
1:D:525:VAL:HG12	1:D:799:ARG:NH1	2.30	0.46
1:B:90:TYR:HB3	1:B:138:ARG:N	2.30	0.46
1:B:204:GLY:HA3	1:B:215:TRP:NE1	2.30	0.46
1:B:322:VAL:HG22	1:B:323:ARG:HG2	1.96	0.46
1:B:380:ILE:HA	1:B:381:PRO:HD3	1.90	0.46
1:C:235:ASN:HD21	1:C:237:VAL:HG22	1.81	0.46
1:D:366:GLU:O	1:D:370:LYS:HB2	2.14	0.46
1:A:129:ALA:HA	1:A:182:TRP:CZ3	2.51	0.46
1:A:648:TYR:HA	1:A:652:LEU:HD12	1.97	0.46
1:B:442:ALA:O	1:B:446:ILE:HG13	2.16	0.46
1:C:799:ARG:O	1:C:803:ARG:HG3	2.16	0.46
1:D:37:PHE:CD1	1:D:37:PHE:N	2.80	0.46
1:D:316:PHE:CD2	1:D:324:THR:HG23	2.48	0.46
1:A:89:PHE:CE1	1:A:140:ALA:HB1	2.50	0.46
1:A:440:ASN:OD1	1:A:442:ALA:HB3	2.15	0.46
1:D:302:ALA:O	1:D:305:GLN:HB2	2.15	0.46
1:D:815:ARG:HD2	1:D:819:GLN:OE1	2.15	0.46
1:A:115:LEU:HD22	1:B:13:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:GLU:O	1:A:702:GLU:HG2	2.16	0.46
1:A:707:ASN:HA	1:A:800:MET:SD	2.55	0.46
1:B:703:ALA:HA	1:B:807:THR:HG21	1.97	0.46
1:C:71:GLN:HB3	4:C:920:AMP:O4'	2.16	0.46
1:C:166:PHE:HB2	1:C:178:GLU:O	2.16	0.46
1:C:727:ASN:ND2	1:C:729:GLN:HB3	2.31	0.46
1:D:81:ARG:NH1	1:D:314:SER:OG	2.48	0.46
1:D:783:CYS:SG	1:D:786:ARG:CZ	3.04	0.46
1:D:791:TYR:HD1	1:D:797:TRP:CE2	2.33	0.46
1:A:311:PHE:O	1:A:316:PHE:HB3	2.16	0.46
1:C:314:SER:O	1:C:316:PHE:N	2.49	0.46
1:A:596:LYS:HD3	1:A:597:PHE:N	2.31	0.46
1:B:491:TRP:C	1:B:495:CYS:SG	2.95	0.46
1:B:566:GLN:O	1:B:605:ILE:HA	2.16	0.46
1:C:163:PHE:HE1	1:C:277:ARG:NH1	2.11	0.46
1:C:198:LEU:HD13	1:C:305:GLN:HB2	1.98	0.46
1:C:495:CYS:HB2	1:C:654:GLU:O	2.16	0.46
1:C:603:VAL:HG23	1:C:642:VAL:HG13	1.97	0.46
1:D:80:LYS:HD3	1:D:334:ALA:HB2	1.98	0.46
1:D:170:ILE:HG22	1:D:173:GLY:HA2	1.98	0.46
1:A:95:LEU:O	1:A:99:MET:HG3	2.16	0.46
1:A:189:TRP:O	1:A:228:THR:HG23	2.15	0.46
1:B:60:ARG:O	1:B:64:VAL:HG13	2.15	0.46
1:B:657:ILE:HD13	1:B:680:LYS:HB3	1.98	0.46
1:B:713:MET:SD	1:B:775:ALA:HB1	2.56	0.46
1:C:325:ASN:HB3	1:C:327:ASP:HB2	1.98	0.46
1:C:381:PRO:HG3	1:C:467:ILE:HG13	1.97	0.46
1:C:542:LYS:HE2	1:C:559:PRO:O	2.16	0.46
1:A:78:ASP:O	1:A:332:LYS:NZ	2.49	0.45
1:B:104:LEU:HB3	1:B:108:CYS:SG	2.56	0.45
1:C:70:THR:HG21	1:C:238:VAL:O	2.16	0.45
1:C:253:ASN:N	1:C:259:VAL:HG21	2.31	0.45
1:C:519:ARG:O	1:C:522:LEU:HB2	2.16	0.45
1:D:599:VAL:HG22	1:D:792:LYS:HD3	1.97	0.45
1:D:687:LEU:HD23	1:D:804:ASN:ND2	2.31	0.45
1:C:502:ILE:HG13	1:C:503:ILE:N	2.31	0.45
1:C:738:LEU:HD11	1:C:774:PHE:CE1	2.51	0.45
1:C:778:GLU:O	1:C:782:LYS:HG2	2.16	0.45
1:C:822:ARG:NH1	1:C:828:GLU:OE1	2.50	0.45
1:D:575:ARG:HG3	1:D:773:VAL:HG22	1.98	0.45
1:A:91:MET:SD	1:A:241:MET:CE	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:648:TYR:HA	1:D:652:LEU:HD12	1.98	0.45
1:C:355:ASP:OD1	1:C:398:ARG:NH1	2.49	0.45
1:D:522:LEU:HD13	1:D:522:LEU:HA	1.77	0.45
1:A:165:ILE:HD13	1:A:166:PHE:CD1	2.51	0.45
1:B:95:LEU:HD22	1:B:99:MET:HE2	1.99	0.45
1:B:376:ASN:HD22	1:B:468:PHE:HE2	1.65	0.45
1:B:735:ILE:HG22	1:B:738:LEU:H	1.81	0.45
1:C:308:ILE:HD12	1:C:352:VAL:HG11	1.99	0.45
1:C:657:ILE:HD13	1:C:680:LYS:HB3	1.98	0.45
1:D:136:LEU:HD21	1:D:339:ASP:HB2	1.98	0.45
1:A:555:VAL:HG21	1:A:643:ILE:HD13	1.99	0.45
1:B:433:GLU:CD	1:B:437:LYS:HZ1	2.20	0.45
1:B:631:ASN:O	1:B:641:ARG:NH1	2.50	0.45
1:A:817:ILE:HD13	1:A:817:ILE:HA	1.80	0.45
1:B:567:VAL:HB	1:B:648:TYR:CZ	2.52	0.45
1:B:715:VAL:HA	1:B:718:VAL:HG23	1.97	0.45
1:B:454:GLY:HA3	1:B:460:SER:OG	2.16	0.45
1:B:571:HIS:ND1	1:B:572:GLU:N	2.65	0.45
1:B:793:ASN:N	1:B:794:PRO:HD2	2.30	0.45
1:C:365:TRP:CH2	1:C:448:GLY:HA2	2.52	0.45
1:D:550:GLU:HG2	1:D:555:VAL:H	1.82	0.45
1:D:631:ASN:OD1	1:D:641:ARG:HD3	2.17	0.45
1:A:206:VAL:HG12	1:A:208:HIS:CD2	2.52	0.45
1:B:95:LEU:HD22	1:B:99:MET:CE	2.46	0.45
1:B:630:VAL:O	1:B:636:VAL:HG11	2.17	0.45
1:B:799:ARG:O	1:B:803:ARG:HG3	2.16	0.45
1:C:555:VAL:HG11	1:C:643:ILE:HG12	1.99	0.45
1:C:657:ILE:HD13	1:C:680:LYS:CB	2.46	0.45
1:D:122:LEU:O	1:D:125:ILE:HB	2.17	0.45
1:D:563:PHE:HD2	1:D:659:ALA:O	1.99	0.45
1:B:292:ARG:NH1	1:B:385:GLU:OE2	2.50	0.45
1:B:605:ILE:O	1:B:644:PHE:HA	2.17	0.45
1:B:815:ARG:O	1:B:819:GLN:HG3	2.17	0.45
1:C:44:ASN:ND2	4:D:920:AMP:C2	2.84	0.45
1:C:355:ASP:O	1:C:358:ARG:NH1	2.50	0.45
1:C:400:LEU:HD23	1:C:400:LEU:HA	1.83	0.45
1:C:819:GLN:O	1:C:823:GLU:HB2	2.16	0.45
1:B:515:LEU:HD21	1:B:683:LEU:HD11	1.99	0.44
1:C:703:ALA:HA	1:C:807:THR:HG21	1.98	0.44
1:D:309:ARG:NH2	4:D:920:AMP:P	2.91	0.44
1:A:157:TYR:HA	1:A:242:ARG:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:OE1	1:A:214:LYS:NZ	2.50	0.44
1:A:482:LYS:HD2	1:A:819:GLN:HB3	1.99	0.44
1:A:700:ALA:HB2	1:A:710:ILE:HD11	2.00	0.44
1:C:162:GLU:HB3	1:C:163:PHE:CD1	2.53	0.44
1:D:24:VAL:O	1:D:24:VAL:HG12	2.17	0.44
1:D:314:SER:O	1:D:316:PHE:N	2.51	0.44
1:A:81:ARG:O	1:A:334:ALA:N	2.50	0.44
1:A:452:VAL:HB	1:A:479:PHE:CD1	2.52	0.44
1:A:576:GLN:H	1:A:576:GLN:NE2	2.15	0.44
1:B:26:GLU:OE1	1:B:29:LYS:NZ	2.50	0.44
1:B:206:VAL:HB	1:B:401:GLN:HE22	1.82	0.44
1:D:252:PHE:N	1:D:252:PHE:CD1	2.85	0.44
1:A:398:ARG:O	1:A:402:ILE:HG13	2.18	0.44
1:A:727:ASN:O	1:A:729:GLN:N	2.51	0.44
1:B:53:PHE:HE1	1:B:188:PRO:HD3	1.81	0.44
1:B:326:PHE:HA	1:B:329:PHE:HB2	1.98	0.44
1:C:456:ALA:H	1:C:481:ASN:ND2	2.16	0.44
1:C:528:GLU:O	1:C:532:ARG:HG2	2.16	0.44
1:A:721:LEU:HD21	1:A:726:TYR:CD1	2.53	0.44
4:A:920:AMP:C2	1:B:44:ASN:ND2	2.85	0.44
1:B:83:TYR:CD1	1:B:155:TYR:HB2	2.53	0.44
1:D:187:ASN:ND2	1:D:190:GLU:HB3	2.32	0.44
1:D:466:THR:OG1	1:D:467:ILE:HG13	2.17	0.44
1:A:80:LYS:HG3	1:A:331:ASP:O	2.18	0.44
1:A:85:LEU:HD12	1:A:335:ILE:HG23	1.99	0.44
1:A:235:ASN:ND2	1:A:237:VAL:HG22	2.30	0.44
1:A:499:LEU:O	1:A:503:ILE:HG13	2.18	0.44
1:B:53:PHE:CE1	1:B:188:PRO:HD3	2.52	0.44
1:B:481:ASN:O	1:B:482:LYS:HG2	2.17	0.44
1:B:666:ILE:HG22	1:B:711:PHE:HE1	1.81	0.44
1:D:571:HIS:H	1:D:576:GLN:HE21	1.65	0.44
1:C:289:LYS:HG2	1:C:291:LEU:H	1.81	0.44
1:D:728:ALA:HB3	1:D:766:MET:O	2.18	0.44
1:B:152:LEU:HD22	1:B:827:VAL:HG21	1.99	0.44
1:C:162:GLU:HA	1:C:183:LEU:HD12	2.00	0.44
1:D:205:ARG:HB3	1:D:216:VAL:HG23	1.98	0.44
1:D:235:ASN:OD1	1:D:237:VAL:HG22	2.18	0.44
1:D:531:ILE:HG22	1:D:532:ARG:N	2.33	0.44
1:A:31:PHE:HA	1:A:58:THR:OG1	2.17	0.44
1:A:395:LEU:O	1:A:396:LEU:HD13	2.18	0.44
1:A:455:VAL:O	1:A:483:THR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ASP:HA	1:A:634:PRO:HD3	1.82	0.44
1:B:292:ARG:O	1:B:296:GLU:HG3	2.18	0.44
1:B:316:PHE:HA	1:B:319:ARG:CB	2.47	0.44
1:B:319:ARG:NH2	1:B:320:ASP:O	2.49	0.44
1:C:88:GLU:HG2	1:C:132:GLY:HA2	2.00	0.44
1:C:338:ASN:OD1	1:C:377:HIS:CE1	2.70	0.44
1:C:482:LYS:HE3	1:C:819:GLN:O	2.17	0.44
1:C:609:ALA:HB2	1:C:620:ILE:CD1	2.47	0.44
1:C:803:ARG:HG3	1:C:803:ARG:HH11	1.82	0.44
1:D:277:ARG:NH1	1:D:277:ARG:HG2	2.32	0.44
1:D:446:ILE:O	1:D:478:LYS:HE3	2.18	0.44
1:A:251:ASP:HB3	1:A:255:LYS:NZ	2.33	0.43
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.18	0.43
1:B:52:TYR:OH	1:B:126:GLU:HG3	2.18	0.43
1:C:78:ASP:HB2	1:C:315:LYS:HZ3	1.82	0.43
1:C:144:LEU:HA	1:C:147:MET:HG3	1.99	0.43
1:C:487:THR:HG23	1:C:490:ARG:H	1.82	0.43
1:C:539:GLN:O	1:C:543:LEU:HB2	2.18	0.43
1:C:544:LYS:O	1:C:547:ALA:HB3	2.17	0.43
1:C:574:LYS:NZ	2:C:901:SO4:O2	2.51	0.43
1:C:614:HIS:O	1:C:618:MET:HB2	2.18	0.43
1:D:163:PHE:HE2	1:D:277:ARG:HH11	1.65	0.43
1:D:304:LEU:HD21	1:D:349:LEU:HB2	1.99	0.43
1:A:162:GLU:HA	1:A:183:LEU:HD12	2.01	0.43
1:A:322:VAL:O	1:A:325:ASN:HB2	2.17	0.43
1:A:524:TYR:CD1	1:A:524:TYR:N	2.85	0.43
1:A:703:ALA:HA	1:A:807:THR:HG21	1.99	0.43
1:B:150:LEU:HB3	1:B:829:PRO:HB3	1.99	0.43
1:B:290:GLU:OE1	1:B:294:LYS:NZ	2.51	0.43
1:B:721:LEU:CD1	1:B:726:TYR:HA	2.49	0.43
1:C:523:SER:HB2	1:C:524:TYR:CE1	2.52	0.43
1:C:524:TYR:CD1	1:C:524:TYR:N	2.86	0.43
1:D:297:TYR:CD2	1:D:396:LEU:HD11	2.52	0.43
1:D:713:MET:CE	1:D:775:ALA:HB1	2.48	0.43
1:A:398:ARG:HG3	1:A:402:ILE:HD11	2.00	0.43
1:C:281:PRO:HB2	1:C:611:PRO:CD	2.49	0.43
1:C:456:ALA:H	1:C:481:ASN:HD21	1.66	0.43
1:D:28:LYS:NZ	1:D:114:GLN:HB3	2.33	0.43
1:D:170:ILE:CG2	1:D:173:GLY:HA2	2.49	0.43
1:D:571:HIS:H	1:D:576:GLN:NE2	2.17	0.43
1:D:816:THR:HG22	1:D:820:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:PHE:CD2	1:D:61:ASP:HB3	2.53	0.43
1:C:37:PHE:CE1	1:D:18:LEU:HD23	2.53	0.43
1:D:822:ARG:NH1	1:D:828:GLU:OE1	2.51	0.43
1:A:428:MET:HE1	1:A:474:LEU:HG	1.99	0.43
1:B:379:VAL:HG11	1:B:671:THR:O	2.19	0.43
1:B:657:ILE:CD1	1:B:680:LYS:HD3	2.49	0.43
1:C:165:ILE:HG12	1:C:279:LEU:HB3	2.00	0.43
1:C:454:GLY:HA3	1:C:460:SER:OG	2.18	0.43
1:D:380:ILE:HG13	1:D:382:GLU:OE1	2.19	0.43
1:D:528:GLU:HG2	1:D:532:ARG:NH2	2.31	0.43
1:D:633:ASP:OD2	1:D:636:VAL:HG23	2.18	0.43
1:D:753:LYS:HB2	1:D:754:GLN:OE1	2.18	0.43
1:D:797:TRP:O	1:D:801:VAL:HG23	2.18	0.43
1:A:269:ARG:HH11	1:A:269:ARG:HD3	1.71	0.43
1:B:56:ALA:HB1	1:B:189:TRP:CZ2	2.54	0.43
1:B:730:GLU:HG3	1:B:734:ARG:HH12	1.84	0.43
1:B:822:ARG:HD3	1:B:828:GLU:OE2	2.18	0.43
1:C:280:TYR:HB3	1:C:281:PRO:HD3	1.99	0.43
1:D:19:ALA:C	1:D:21:VAL:H	2.20	0.43
1:D:253:ASN:C	1:D:254:LEU:HD13	2.39	0.43
1:D:603:VAL:HG22	1:D:641:ARG:O	2.18	0.43
1:D:631:ASN:OD1	1:D:641:ARG:HA	2.19	0.43
1:D:677:GLY:CA	3:D:999:PLP:H5A1	2.48	0.43
1:B:455:VAL:HG12	1:B:674:SER:HB3	1.99	0.43
1:C:224:MET:SD	1:C:247:LYS:HE2	2.59	0.43
1:C:311:PHE:CE1	1:C:329:PHE:HA	2.54	0.43
1:D:66:ARG:HH12	1:D:837:PRO:HG3	1.84	0.43
1:D:530:PHE:CA	1:D:533:ASP:HB2	2.47	0.43
1:D:555:VAL:HG23	1:D:556:HIS:H	1.84	0.43
1:D:689:ILE:HG12	1:D:690:GLY:N	2.34	0.43
1:A:727:ASN:ND2	1:D:725:GLY:HA3	2.28	0.43
1:B:78:ASP:O	1:B:332:LYS:NZ	2.51	0.43
1:B:202:PHE:O	1:B:218:THR:HB	2.18	0.43
1:B:433:GLU:OE2	1:B:437:LYS:NZ	2.50	0.43
1:C:570:ILE:HG21	1:C:620:ILE:HG13	2.01	0.43
1:C:603:VAL:CG2	1:C:642:VAL:HG13	2.49	0.43
1:C:746:SER:OG	1:C:762:VAL:HG21	2.18	0.43
1:D:380:ILE:HA	1:D:381:PRO:HD3	1.61	0.43
1:D:592:LYS:NZ	1:D:593:GLU:OE2	2.50	0.43
1:A:94:THR:HB	1:A:189:TRP:NE1	2.33	0.43
1:A:509:GLU:OE2	1:A:512:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:O	1:A:547:ALA:HB3	2.19	0.43
1:B:224:MET:HE3	1:B:226:TYR:HE1	1.83	0.43
1:B:545:PHE:HZ	1:B:645:LEU:HD21	1.84	0.43
1:D:152:LEU:HD22	1:D:827:VAL:HG21	2.01	0.43
1:D:312:LYS:HA	1:D:324:THR:CG2	2.46	0.43
1:D:689:ILE:HA	1:D:709:PHE:HB2	2.01	0.43
1:A:531:ILE:HG12	1:A:802:ILE:HD11	2.01	0.43
1:B:435:ALA:HB2	1:C:174:TRP:CD2	2.54	0.43
1:B:735:ILE:HA	1:B:736:PRO:HD3	1.83	0.43
1:D:338:ASN:OD1	1:D:377:HIS:CE1	2.72	0.43
1:A:55:LEU:HD13	1:A:112:THR:CG2	2.48	0.42
1:B:790:LEU:HD23	1:B:797:TRP:HD1	1.83	0.42
1:C:526:ASP:OD2	1:C:799:ARG:NH1	2.52	0.42
1:C:626:ILE:HG22	1:C:642:VAL:HG21	2.00	0.42
1:D:41:LYS:HD3	1:D:45:VAL:HG12	2.01	0.42
1:D:562:LEU:HD13	1:D:601:ARG:CZ	2.49	0.42
1:A:293:LEU:HD23	1:A:395:LEU:HD21	2.02	0.42
1:A:485:GLY:O	1:A:486:ILE:HD12	2.18	0.42
1:B:182:TRP:CE2	1:B:183:LEU:HG	2.54	0.42
1:C:36:HIS:O	1:C:40:VAL:HA	2.19	0.42
1:C:734:ARG:O	1:C:736:PRO:HD3	2.19	0.42
1:D:91:MET:HE1	1:D:141:ALA:HA	2.00	0.42
1:D:291:LEU:HA	1:D:294:LYS:HB2	2.01	0.42
1:D:316:PHE:HB3	1:D:324:THR:CG2	2.49	0.42
1:D:455:VAL:HG22	1:D:484:ASN:OD1	2.20	0.42
1:A:47:THR:HG22	1:A:49:ARG:N	2.34	0.42
1:A:450:HIS:O	1:A:450:HIS:ND1	2.52	0.42
1:B:31:PHE:HA	1:B:58:THR:OG1	2.19	0.42
1:B:325:ASN:C	1:B:327:ASP:H	2.23	0.42
1:B:423:ASP:O	1:B:427:ARG:N	2.53	0.42
1:C:366:GLU:HG2	1:C:370:LYS:HE3	2.01	0.42
1:C:610:ALA:HA	1:C:611:PRO:HD3	1.83	0.42
1:C:795:ARG:O	1:C:799:ARG:HG3	2.20	0.42
1:D:62:HIS:O	1:D:66:ARG:HG3	2.19	0.42
1:A:21:VAL:HG13	1:A:22:GLU:H	1.84	0.42
1:A:22:GLU:OE1	1:A:104:LEU:HA	2.19	0.42
1:B:253:ASN:H	1:B:259:VAL:HG21	1.84	0.42
1:C:730:GLU:HB2	1:C:734:ARG:NH2	2.34	0.42
1:D:407:ASN:HB2	1:D:430:LEU:HD12	2.01	0.42
1:D:453:ASN:ND2	1:D:482:LYS:HB2	2.33	0.42
1:D:632:HIS:O	1:D:634:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:688:THR:HB	1:D:708:PHE:CE1	2.55	0.42
1:A:75:TYR:CE2	4:A:920:AMP:N7	2.87	0.42
1:A:225:PRO:HB3	1:A:244:TRP:CE3	2.54	0.42
1:A:346:ILE:HG23	1:A:368:THR:HG21	2.02	0.42
1:B:314:SER:O	1:B:316:PHE:N	2.52	0.42
1:C:102:LEU:O	1:C:104:LEU:HD12	2.20	0.42
1:C:144:LEU:HA	1:C:144:LEU:HD23	1.90	0.42
1:C:474:LEU:HD22	1:C:474:LEU:O	2.19	0.42
1:A:233:TYR:OH	1:A:234:ARG:NH2	2.53	0.42
1:A:338:ASN:OD1	1:A:377:HIS:CE1	2.72	0.42
1:A:573:TYR:CZ	1:A:574:LYS:HD2	2.54	0.42
1:A:703:ALA:HB2	1:A:807:THR:HG21	2.02	0.42
1:B:545:PHE:HE2	1:B:604:MET:SD	2.42	0.42
1:C:551:ARG:O	1:C:551:ARG:NH1	2.53	0.42
1:C:590:ILE:HG12	1:C:598:VAL:HG11	2.01	0.42
1:D:82:ILE:CD1	1:D:147:MET:SD	3.07	0.42
1:D:423:ASP:O	1:D:426:ARG:HD3	2.19	0.42
1:D:649:ARG:HH11	1:D:649:ARG:HD2	1.61	0.42
1:A:235:ASN:C	1:A:235:ASN:HD22	2.23	0.42
1:B:379:VAL:HG23	1:B:462:ILE:HD12	2.01	0.42
1:C:64:VAL:O	1:C:68:ILE:HG12	2.20	0.42
1:C:187:ASN:HB3	1:C:190:GLU:OE2	2.19	0.42
1:C:281:PRO:HB2	1:C:611:PRO:HD2	2.01	0.42
1:C:502:ILE:HD13	1:C:534:VAL:HA	2.01	0.42
1:D:60:ARG:HG3	1:D:189:TRP:HE3	1.81	0.42
1:D:110:GLU:O	1:D:113:TYR:HB3	2.19	0.42
1:D:290:GLU:HG3	1:D:391:LEU:HD21	2.00	0.42
1:D:486:ILE:HD11	1:D:680:LYS:HE3	2.01	0.42
1:D:588:ASN:HD21	1:D:744:GLN:NE2	2.18	0.42
1:A:536:LYS:HZ2	1:A:540:GLU:CD	2.23	0.42
1:B:319:ARG:HH21	1:B:320:ASP:C	2.23	0.42
1:B:481:ASN:OD1	1:B:482:LYS:N	2.53	0.42
1:B:629:VAL:HG12	1:B:630:VAL:N	2.33	0.42
1:B:680:LYS:NZ	3:B:999:PLP:O3	2.53	0.42
1:B:783:CYS:HA	1:B:786:ARG:NH1	2.35	0.42
1:D:119:MET:O	1:D:123:GLU:HG3	2.20	0.42
1:D:152:LEU:HD22	1:D:827:VAL:CG2	2.50	0.42
1:D:490:ARG:HG2	1:D:491:TRP:CE2	2.55	0.42
1:D:588:ASN:ND2	1:D:741:ILE:HG22	2.31	0.42
1:A:94:THR:HG21	1:A:189:TRP:CD2	2.55	0.42
1:A:460:SER:OG	1:A:481:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ILE:HA	1:A:736:PRO:HD3	1.79	0.42
1:B:97:ASN:OD1	1:B:490:ARG:NH1	2.53	0.42
1:B:492:LEU:HB3	1:B:493:VAL:H	1.59	0.42
1:C:506:ARG:HH22	1:C:533:ASP:CG	2.23	0.42
1:C:700:ALA:O	1:C:704:GLY:N	2.53	0.42
1:D:206:VAL:HG22	1:D:398:ARG:HD2	2.01	0.42
1:D:461:GLU:OE1	1:D:465:LYS:NZ	2.53	0.42
1:B:14:SER:OG	1:B:15:VAL:N	2.52	0.42
1:B:375:THR:HG22	1:B:377:HIS:CE1	2.55	0.42
1:B:379:VAL:HG23	1:B:462:ILE:CD1	2.50	0.42
1:C:730:GLU:HG3	1:C:734:ARG:NH1	2.35	0.42
1:D:682:MET:CE	1:D:808:SER:HA	2.49	0.42
1:A:32:ASN:OD1	1:B:13:ILE:HA	2.20	0.41
1:A:538:LYS:HD2	1:A:658:PRO:O	2.19	0.41
1:A:540:GLU:HA	1:A:543:LEU:HB2	2.01	0.41
1:A:665:GLN:NE2	1:A:678:ASN:HA	2.35	0.41
1:A:698:GLU:HB3	1:A:810:LYS:HZ3	1.84	0.41
1:B:487:THR:HA	1:B:488:PRO:HD2	1.92	0.41
1:B:515:LEU:O	1:B:518:LEU:HG	2.20	0.41
1:C:37:PHE:N	1:C:37:PHE:CD1	2.88	0.41
1:C:379:VAL:HG11	1:C:671:THR:O	2.20	0.41
1:C:738:LEU:HA	1:C:741:ILE:HG12	2.01	0.41
1:C:817:ILE:HD13	1:C:817:ILE:HA	1.74	0.41
1:D:484:ASN:O	1:D:679:MET:SD	2.78	0.41
1:A:575:ARG:HG2	1:A:773:VAL:CG2	2.50	0.41
1:B:49:ARG:O	1:B:52:TYR:HB3	2.20	0.41
1:B:461:GLU:OE2	1:B:464:LYS:NZ	2.52	0.41
1:B:565:VAL:HG11	1:B:656:VAL:HG21	2.02	0.41
1:B:622:LEU:HA	1:B:758:PHE:CZ	2.55	0.41
1:D:83:TYR:CZ	1:D:307:ILE:HG12	2.55	0.41
1:D:198:LEU:HB3	1:D:305:GLN:OE1	2.20	0.41
1:D:522:LEU:O	1:D:524:TYR:N	2.53	0.41
1:D:613:TYR:CE1	1:D:615:MET:HB3	2.52	0.41
1:D:778:GLU:OE1	1:D:782:LYS:NZ	2.53	0.41
1:A:271:LEU:HA	1:A:274:ASN:ND2	2.34	0.41
1:A:485:GLY:C	1:A:486:ILE:HD12	2.41	0.41
1:A:610:ALA:HA	1:A:611:PRO:HD3	1.84	0.41
1:A:678:ASN:ND2	1:A:696:ASN:OD1	2.52	0.41
1:A:828:GLU:HA	1:A:829:PRO:HD3	1.80	0.41
1:B:469:LYS:HE2	1:B:469:LYS:HB2	1.84	0.41
1:B:583:VAL:HG11	1:B:642:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ASN:HB3	1:C:480:GLN:HB2	2.03	0.41
1:C:567:VAL:HA	1:C:606:GLY:O	2.20	0.41
1:C:622:LEU:O	1:C:625:ALA:HB3	2.20	0.41
1:D:128:ASP:O	1:D:130:GLY:N	2.53	0.41
1:D:209:THR:O	1:D:211:GLN:N	2.53	0.41
1:D:571:HIS:ND1	1:D:572:GLU:N	2.68	0.41
1:C:13:ILE:HG23	1:D:32:ASN:OD1	2.21	0.41
1:C:432:GLU:HB3	1:C:438:ARG:HB2	2.03	0.41
1:C:591:LYS:HZ2	1:C:633:ASP:CG	2.23	0.41
1:D:344:LEU:HD22	1:D:347:PRO:HG3	2.02	0.41
1:D:622:LEU:HG	1:D:761:ILE:HD12	2.01	0.41
1:D:711:PHE:CG	1:D:712:GLY:N	2.87	0.41
1:B:460:SER:OG	1:B:481:ASN:ND2	2.54	0.41
1:C:600:PRO:C	1:C:601:ARG:HG3	2.40	0.41
1:D:206:VAL:HG11	1:D:401:GLN:OE1	2.20	0.41
1:D:463:LEU:O	1:D:468:PHE:HB2	2.20	0.41
1:D:816:THR:HG22	1:D:820:TYR:HE1	1.85	0.41
1:A:482:LYS:CD	1:A:819:GLN:HB3	2.50	0.41
1:A:591:LYS:O	1:A:594:PRO:HD3	2.20	0.41
1:A:738:LEU:O	1:A:741:ILE:N	2.54	0.41
1:B:575:ARG:HH22	1:B:776:ASP:CG	2.24	0.41
1:B:688:THR:O	1:B:709:PHE:HB2	2.21	0.41
1:C:663:SER:HB3	1:C:688:THR:HA	2.02	0.41
1:D:677:GLY:HA3	3:D:999:PLP:H5A1	2.02	0.41
1:A:306:ASP:OD1	1:A:309:ARG:NH1	2.54	0.41
1:A:389:VAL:HG23	1:A:390:HIS:N	2.36	0.41
1:B:78:ASP:HA	1:B:79:PRO:HD3	1.76	0.41
1:B:566:GLN:HG3	1:B:664:GLU:HB2	2.02	0.41
1:B:764:MET:HA	1:B:768:HIS:CE1	2.55	0.41
1:C:588:ASN:HD21	1:C:744:GLN:NE2	2.18	0.41
1:C:830:SER:OG	1:C:832:GLN:HG2	2.20	0.41
1:D:166:PHE:CD1	1:D:177:GLU:HB3	2.56	0.41
1:D:815:ARG:O	1:D:818:ALA:HB3	2.21	0.41
1:A:575:ARG:HG2	1:A:773:VAL:HG22	2.02	0.41
1:A:627:GLY:HA2	1:A:642:VAL:HB	2.02	0.41
1:C:433:GLU:OE2	1:C:437:LYS:NZ	2.54	0.41
1:C:446:ILE:O	1:C:478:LYS:HE3	2.21	0.41
1:D:162:GLU:HA	1:D:183:LEU:HD12	2.02	0.41
1:D:322:VAL:HG13	1:D:325:ASN:HB3	2.03	0.41
1:D:366:GLU:O	1:D:370:LYS:HE3	2.21	0.41
1:A:13:ILE:HA	1:B:32:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD21	1:A:104:LEU:HD22	2.02	0.41
1:A:41:LYS:HD3	1:A:41:LYS:HA	1.74	0.41
1:A:89:PHE:O	1:A:131:LEU:HB2	2.21	0.41
1:A:290:GLU:HG2	1:A:391:LEU:HD21	2.02	0.41
1:A:539:GLN:O	1:A:543:LEU:HD23	2.21	0.41
1:A:569:ARG:HB2	2:A:901:SO4:O2	2.21	0.41
1:B:395:LEU:HG	1:B:396:LEU:HD13	2.02	0.41
1:B:446:ILE:O	1:B:478:LYS:HE3	2.21	0.41
1:B:490:ARG:HA	1:B:494:LEU:HD23	2.03	0.41
1:C:361:TRP:CZ3	1:C:409:ARG:HD2	2.55	0.41
1:D:28:LYS:HZ2	1:D:114:GLN:CB	2.34	0.41
1:D:602:THR:HA	1:D:641:ARG:HB2	2.03	0.41
1:D:655:LYS:O	1:D:658:PRO:HB2	2.21	0.41
1:D:733:ASP:O	1:D:739:ARG:NH1	2.54	0.41
1:D:791:TYR:HA	1:D:797:TRP:NE1	2.35	0.41
1:A:264:GLN:O	1:A:267:LEU:HD12	2.21	0.41
1:B:88:GLU:HG2	1:B:132:GLY:HA2	2.02	0.41
1:B:222:LEU:O	1:B:247:LYS:N	2.49	0.41
1:B:232:GLY:HA3	1:B:235:ASN:ND2	2.36	0.41
1:B:355:ASP:O	1:B:358:ARG:NH1	2.54	0.41
1:C:44:ASN:OD1	1:D:72:GLN:NE2	2.54	0.41
1:C:150:LEU:HA	1:C:830:SER:O	2.21	0.41
1:C:163:PHE:HA	1:C:181:ASP:HA	2.02	0.41
1:C:320:ASP:HA	1:C:324:THR:HA	2.02	0.41
1:D:23:ASN:OD1	1:D:25:THR:HB	2.20	0.41
1:D:95:LEU:HD23	1:D:95:LEU:HA	1.84	0.41
1:D:338:ASN:OD1	1:D:377:HIS:HE1	2.03	0.41
1:A:230:VAL:O	1:A:230:VAL:HG23	2.21	0.40
1:A:426:ARG:NE	1:D:753:LYS:O	2.54	0.40
1:A:724:ARG:HH22	1:A:730:GLU:CD	2.24	0.40
1:B:822:ARG:HD3	1:B:822:ARG:HH11	1.63	0.40
1:C:290:GLU:O	1:C:294:LYS:HG3	2.21	0.40
1:D:386:ARG:HA	1:D:439:ILE:O	2.21	0.40
1:D:466:THR:OG1	1:D:467:ILE:N	2.54	0.40
1:D:622:LEU:O	1:D:625:ALA:HB3	2.22	0.40
1:A:615:MET:HE1	1:A:761:ILE:HG12	2.02	0.40
1:B:63:LEU:HD23	1:B:63:LEU:HA	1.95	0.40
1:B:738:LEU:HA	1:B:741:ILE:HG12	2.02	0.40
1:B:799:ARG:HH11	1:B:799:ARG:HD2	1.67	0.40
1:C:530:PHE:HA	1:C:533:ASP:OD2	2.21	0.40
1:C:733:ASP:HA	1:C:739:ARG:NH1	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:TYR:HA	1:D:276:SER:O	2.21	0.40
1:D:424:ARG:HA	1:D:427:ARG:CZ	2.51	0.40
1:A:47:THR:HG22	1:A:49:ARG:H	1.86	0.40
1:A:143:PHE:O	1:A:147:MET:HG3	2.21	0.40
1:A:168:GLN:HE21	1:A:646:GLU:HA	1.87	0.40
1:A:249:PRO:HD2	1:A:252:PHE:CZ	2.57	0.40
1:A:748:GLY:HA3	1:A:755:PRO:HA	2.02	0.40
1:C:432:GLU:N	1:C:438:ARG:O	2.55	0.40
1:C:758:PHE:HD1	1:C:761:ILE:CD1	2.34	0.40
1:D:369:VAL:O	1:D:450:HIS:HB3	2.21	0.40
1:D:518:LEU:HB3	1:D:806:ALA:HA	2.04	0.40
1:A:682:MET:CE	1:A:808:SER:HA	2.51	0.40
1:C:598:VAL:HG12	1:C:639:ARG:HH21	1.86	0.40
1:D:295:GLN:O	1:D:298:PHE:HB3	2.22	0.40
1:A:409:ARG:O	1:A:412:ASN:N	2.55	0.40
1:B:272:ALA:O	1:B:274:ASN:N	2.55	0.40
1:B:524:TYR:CD1	1:B:524:TYR:N	2.89	0.40
1:B:718:VAL:HG13	1:B:772:LYS:HD2	2.02	0.40
1:C:452:VAL:O	1:C:479:PHE:HA	2.21	0.40
1:C:522:LEU:HD13	1:C:806:ALA:HB3	2.03	0.40
1:C:550:GLU:HA	1:C:554:LYS:HA	2.03	0.40
1:C:647:ASN:O	1:C:649:ARG:HG2	2.21	0.40
1:D:63:LEU:CD2	1:D:231:PRO:HB3	2.48	0.40
1:D:73:HIS:NE2	1:D:834:LEU:HD11	2.36	0.40
1:D:522:LEU:HD11	1:D:803:ARG:HD3	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLU:N	1:D:321:PRO:O[2_646]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	820/842 (97%)	669 (82%)	116 (14%)	35 (4%)	2	8
1	B	820/842 (97%)	687 (84%)	92 (11%)	41 (5%)	1	6
1	C	820/842 (97%)	708 (86%)	82 (10%)	30 (4%)	2	11
1	D	820/842 (97%)	669 (82%)	100 (12%)	51 (6%)	1	3
All	All	3280/3368 (97%)	2733 (83%)	390 (12%)	157 (5%)	2	7

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	A	321	PRO
1	A	358	ARG
1	A	553	TYR
1	A	674	SER
1	A	728	ALA
1	A	793	ASN
1	A	835	PRO
1	B	16	ARG
1	B	93	ARG
1	B	166	PHE
1	B	253	ASN
1	B	281	PRO
1	B	321	PRO
1	B	610	ALA
1	B	752	PRO
1	B	794	PRO
1	B	835	PRO
1	C	210	SER
1	C	253	ASN
1	C	314	SER
1	C	315	LYS
1	C	321	PRO
1	C	323	ARG
1	C	358	ARG
1	C	555	VAL
1	C	556	HIS
1	C	609	ALA
1	C	836	ALA
1	D	129	ALA

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Mol	Chain	Res	Type
1	D	210	SER
1	D	314	SER
1	D	321	PRO
1	D	358	ARG
1	D	609	ALA
1	D	674	SER
1	D	829	PRO
1	A	21	VAL
1	A	91	MET
1	A	253	ASN
1	A	256	ASP
1	A	281	PRO
1	A	451	ALA
1	A	477	HIS
1	A	555	VAL
1	A	610	ALA
1	A	836	ALA
1	B	21	VAL
1	B	22	GLU
1	B	95	LEU
1	B	252	PHE
1	B	256	ASP
1	B	436	VAL
1	C	21	VAL
1	C	256	ASP
1	C	694	GLY
1	C	809	GLY
1	D	16	ARG
1	D	103	ALA
1	D	104	LEU
1	D	151	GLY
1	D	183	LEU
1	D	217	ASP
1	D	234	ARG
1	D	256	ASP
1	D	323	ARG
1	D	429	SER
1	D	489	ARG
1	D	523	SER
1	D	531	ILE
1	D	556	HIS
1	D	561	SER

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Mol	Chain	Res	Type
1	D	610	ALA
1	D	694	GLY
1	A	93	ARG
1	A	210	SER
1	A	316	PHE
1	A	492	LEU
1	A	556	HIS
1	B	19	ALA
1	B	273	GLU
1	B	314	SER
1	B	381	PRO
1	B	555	VAL
1	C	92	GLY
1	C	93	ARG
1	C	436	VAL
1	C	625	ALA
1	D	21	VAL
1	D	95	LEU
1	D	252	PHE
1	D	253	ASN
1	D	555	VAL
1	D	658	PRO
1	A	22	GLU
1	A	88	GLU
1	A	357	GLU
1	B	203	TYR
1	B	272	ALA
1	B	674	SER
1	C	456	ALA
1	C	484	ASN
1	C	778	GLU
1	D	91	MET
1	D	166	PHE
1	D	637	GLY
1	A	129	ALA
1	A	259	VAL
1	A	436	VAL
1	A	483	THR
1	B	254	LEU
1	B	315	LYS
1	B	344	LEU
1	B	728	ALA

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Mol	Chain	Res	Type
1	B	836	ALA
1	C	257	PHE
1	C	394	THR
1	C	835	PRO
1	D	93	ARG
1	D	96	GLN
1	D	254	LEU
1	D	259	VAL
1	D	298	PHE
1	D	315	LYS
1	D	436	VAL
1	D	557	ILE
1	D	751	SER
1	D	830	SER
1	D	835	PRO
1	B	45	VAL
1	B	326	PHE
1	B	625	ALA
1	B	666	ILE
1	B	756	ASP
1	C	357	GLU
1	D	229	PRO
1	D	625	ALA
1	A	263	ILE
1	B	263	ILE
1	B	629	VAL
1	C	697	VAL
1	A	685	GLY
1	B	493	VAL
1	C	263	ILE
1	C	666	ILE
1	A	594	PRO
1	A	704	GLY
1	B	79	PRO
1	B	231	PRO
1	D	263	ILE
1	B	736	PRO
1	C	751	SER
1	D	17	GLY
1	D	710	ILE
1	D	725	GLY
1	A	342	PRO

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Mol	Chain	Res	Type
1	B	751	SER

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	712/731 (97%)	589 (83%)	123 (17%)	1	5
1	B	712/731 (97%)	595 (84%)	117 (16%)	2	6
1	C	712/731 (97%)	592 (83%)	120 (17%)	1	5
1	D	712/731 (97%)	573 (80%)	139 (20%)	1	3
All	All	2848/2924 (97%)	2349 (82%)	499 (18%)	1	5

All (499) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	12	GLN
1	A	16	ARG
1	A	18	LEU
1	A	49	ARG
1	A	63	LEU
1	A	82	ILE
1	A	87	LEU
1	A	90	TYR
1	A	95	LEU
1	A	97	ASN
1	A	117	LEU
1	A	118	ASP
1	A	127	GLU
1	A	131	LEU
1	A	165	ILE
1	A	167	ASN
1	A	169	LYS
1	A	171	CYS
1	A	176	MET

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Mol	Chain	Res	Type
1	A	184	ARG
1	A	187	ASN
1	A	195	GLU
1	A	197	THR
1	A	216	VAL
1	A	234	ARG
1	A	235	ASN
1	A	237	VAL
1	A	242	ARG
1	A	243	LEU
1	A	250	ASN
1	A	255	LYS
1	A	256	ASP
1	A	257	PHE
1	A	262	TYR
1	A	269	ARG
1	A	270	ASN
1	A	274	ASN
1	A	277	ARG
1	A	279	LEU
1	A	287	GLU
1	A	290	GLU
1	A	291	LEU
1	A	292	ARG
1	A	299	VAL
1	A	315	LYS
1	A	319	ARG
1	A	321	PRO
1	A	323	ARG
1	A	324	THR
1	A	327	ASP
1	A	333	VAL
1	A	337	LEU
1	A	358	ARG
1	A	363	LYS
1	A	374	TYR
1	A	377	HIS
1	A	380	ILE
1	A	392	LEU
1	A	400	LEU
1	A	429	SER
1	A	430	LEU

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Mol	Chain	Res	Type
1	A	441	MET
1	A	444	LEU
1	A	455	VAL
1	A	467	ILE
1	A	473	GLU
1	A	478	LYS
1	A	480	GLN
1	A	483	THR
1	A	486	ILE
1	A	489	ARG
1	A	490	ARG
1	A	492	LEU
1	A	495	CYS
1	A	506	ARG
1	A	510	GLU
1	A	516	ASP
1	A	522	LEU
1	A	530	PHE
1	A	532	ARG
1	A	548	TYR
1	A	549	LEU
1	A	554	LYS
1	A	555	VAL
1	A	562	LEU
1	A	565	VAL
1	A	576	GLN
1	A	579	ASN
1	A	583	VAL
1	A	586	LEU
1	A	603	VAL
1	A	622	LEU
1	A	624	THR
1	A	640	LEU
1	A	652	LEU
1	A	662	LEU
1	A	676	THR
1	A	683	LEU
1	A	699	MET
1	A	705	GLU
1	A	706	GLU
1	A	708	PHE
1	A	714	ARG

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Mol	Chain	Res	Type
1	A	717	ASP
1	A	720	ARG
1	A	724	ARG
1	A	727	ASN
1	A	753	LYS
1	A	756	ASP
1	A	759	LYS
1	A	760	ASP
1	A	764	MET
1	A	765	LEU
1	A	766	MET
1	A	779	GLU
1	A	788	SER
1	A	792	LYS
1	A	794	PRO
1	A	807	THR
1	A	810	LYS
1	A	832	GLN
1	A	833	ARG
1	B	10	ARG
1	B	18	LEU
1	B	29	LYS
1	B	42	ASP
1	B	45	VAL
1	B	63	LEU
1	B	72	GLN
1	B	80	LYS
1	B	82	ILE
1	B	87	LEU
1	B	97	ASN
1	B	100	VAL
1	B	112	THR
1	B	127	GLU
1	B	128	ASP
1	B	165	ILE
1	B	167	ASN
1	B	169	LYS
1	B	177	GLU
1	B	191	LYS
1	B	210	SER
1	B	221	VAL
1	B	228	THR

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Mol	Chain	Res	Type
1	B	234	ARG
1	B	235	ASN
1	B	237	VAL
1	B	242	ARG
1	B	243	LEU
1	B	245	SER
1	B	250	ASN
1	B	254	LEU
1	B	255	LYS
1	B	256	ASP
1	B	262	TYR
1	B	267	LEU
1	B	274	ASN
1	B	287	GLU
1	B	292	ARG
1	B	299	VAL
1	B	304	LEU
1	B	313	SER
1	B	315	LYS
1	B	316	PHE
1	B	318	CYS
1	B	319	ARG
1	B	321	PRO
1	B	323	ARG
1	B	361	TRP
1	B	380	ILE
1	B	381	PRO
1	B	384	LEU
1	B	391	LEU
1	B	392	LEU
1	B	395	LEU
1	B	400	LEU
1	B	423	ASP
1	B	425	LEU
1	B	426	ARG
1	B	444	LEU
1	B	457	ARG
1	B	459	HIS
1	B	462	ILE
1	B	474	LEU
1	B	489	ARG
1	B	490	ARG

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Mol	Chain	Res	Type
1	B	492	LEU
1	B	505	GLU
1	B	506	ARG
1	B	509	GLU
1	B	510	GLU
1	B	511	TYR
1	B	516	ASP
1	B	521	LEU
1	B	536	LYS
1	B	540	GLU
1	B	543	LEU
1	B	552	GLU
1	B	553	TYR
1	B	554	LYS
1	B	555	VAL
1	B	562	LEU
1	B	564	ASP
1	B	565	VAL
1	B	569	ARG
1	B	586	LEU
1	B	613	TYR
1	B	621	LYS
1	B	630	VAL
1	B	636	VAL
1	B	638	ASP
1	B	640	LEU
1	B	649	ARG
1	B	651	SER
1	B	652	LEU
1	B	658	PRO
1	B	662	LEU
1	B	674	SER
1	B	676	THR
1	B	678	ASN
1	B	705	GLU
1	B	714	ARG
1	B	717	ASP
1	B	724	ARG
1	B	733	ASP
1	B	753	LYS
1	B	754	GLN
1	B	756	ASP

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Mol	Chain	Res	Type
1	B	760	ASP
1	B	764	MET
1	B	766	MET
1	B	770	ARG
1	B	782	LYS
1	B	790	LEU
1	B	792	LYS
1	B	807	THR
1	B	830	SER
1	B	833	ARG
1	C	12	GLN
1	C	18	LEU
1	C	21	VAL
1	C	27	LEU
1	C	37	PHE
1	C	42	ASP
1	C	45	VAL
1	C	47	THR
1	C	60	ARG
1	C	66	ARG
1	C	77	LYS
1	C	82	ILE
1	C	85	LEU
1	C	90	TYR
1	C	95	LEU
1	C	100	VAL
1	C	102	LEU
1	C	105	GLU
1	C	121	GLU
1	C	128	ASP
1	C	131	LEU
1	C	165	ILE
1	C	169	LYS
1	C	177	GLU
1	C	206	VAL
1	C	217	ASP
1	C	219	GLN
1	C	229	PRO
1	C	230	VAL
1	C	231	PRO
1	C	234	ARG
1	C	235	ASN

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Mol	Chain	Res	Type
1	C	242	ARG
1	C	250	ASN
1	C	252	PHE
1	C	254	LEU
1	C	256	ASP
1	C	267	LEU
1	C	274	ASN
1	C	276	SER
1	C	281	PRO
1	C	287	GLU
1	C	291	LEU
1	C	292	ARG
1	C	300	VAL
1	C	304	LEU
1	C	306	ASP
1	C	309	ARG
1	C	314	SER
1	C	316	PHE
1	C	318	CYS
1	C	319	ARG
1	C	320	ASP
1	C	327	ASP
1	C	336	GLN
1	C	337	LEU
1	C	339	ASP
1	C	340	THR
1	C	358	ARG
1	C	359	LEU
1	C	360	ASP
1	C	361	TRP
1	C	363	LYS
1	C	378	THR
1	C	381	PRO
1	C	395	LEU
1	C	400	LEU
1	C	426	ARG
1	C	432	GLU
1	C	438	ARG
1	C	444	LEU
1	C	455	VAL
1	C	464	LYS
1	C	474	LEU

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Mol	Chain	Res	Type
1	C	489	ARG
1	C	490	ARG
1	C	492	LEU
1	C	494	LEU
1	C	499	LEU
1	C	506	ARG
1	C	509	GLU
1	C	510	GLU
1	C	522	LEU
1	C	527	ASP
1	C	532	ARG
1	C	537	VAL
1	C	540	GLU
1	C	541	ASN
1	C	543	LEU
1	C	549	LEU
1	C	553	TYR
1	C	554	LYS
1	C	555	VAL
1	C	575	ARG
1	C	576	GLN
1	C	597	PHE
1	C	613	TYR
1	C	618	MET
1	C	624	THR
1	C	638	ASP
1	C	652	LEU
1	C	658	PRO
1	C	665	GLN
1	C	676	THR
1	C	705	GLU
1	C	706	GLU
1	C	714	ARG
1	C	719	ASP
1	C	727	ASN
1	C	734	ARG
1	C	751	SER
1	C	753	LYS
1	C	759	LYS
1	C	761	ILE
1	C	764	MET
1	C	766	MET

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Mol	Chain	Res	Type
1	C	782	LYS
1	C	807	THR
1	C	812	SER
1	C	833	ARG
1	D	18	LEU
1	D	22	GLU
1	D	39	LEU
1	D	42	ASP
1	D	45	VAL
1	D	47	THR
1	D	82	ILE
1	D	88	GLU
1	D	90	TYR
1	D	91	MET
1	D	94	THR
1	D	95	LEU
1	D	97	ASN
1	D	104	LEU
1	D	145	ASP
1	D	165	ILE
1	D	167	ASN
1	D	169	LYS
1	D	176	MET
1	D	177	GLU
1	D	184	ARG
1	D	198	LEU
1	D	209	THR
1	D	210	SER
1	D	217	ASP
1	D	229	PRO
1	D	231	PRO
1	D	234	ARG
1	D	236	ASN
1	D	242	ARG
1	D	243	LEU
1	D	245	SER
1	D	250	ASN
1	D	253	ASN
1	D	254	LEU
1	D	255	LYS
1	D	259	VAL
1	D	262	TYR

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Mol	Chain	Res	Type
1	D	264	GLN
1	D	274	ASN
1	D	281	PRO
1	D	287	GLU
1	D	289	LYS
1	D	291	LEU
1	D	292	ARG
1	D	300	VAL
1	D	306	ASP
1	D	315	LYS
1	D	316	PHE
1	D	318	CYS
1	D	319	ARG
1	D	321	PRO
1	D	323	ARG
1	D	336	GLN
1	D	337	LEU
1	D	340	THR
1	D	344	LEU
1	D	358	ARG
1	D	360	ASP
1	D	361	TRP
1	D	363	LYS
1	D	370	LYS
1	D	391	LEU
1	D	392	LEU
1	D	393	GLU
1	D	394	THR
1	D	395	LEU
1	D	396	LEU
1	D	400	LEU
1	D	401	GLN
1	D	424	ARG
1	D	425	LEU
1	D	426	ARG
1	D	429	SER
1	D	450	HIS
1	D	455	VAL
1	D	458	ILE
1	D	459	HIS
1	D	477	HIS
1	D	478	LYS

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Mol	Chain	Res	Type
1	D	480	GLN
1	D	489	ARG
1	D	494	LEU
1	D	499	LEU
1	D	506	ARG
1	D	511	TYR
1	D	516	ASP
1	D	522	LEU
1	D	526	ASP
1	D	530	PHE
1	D	533	ASP
1	D	543	LEU
1	D	549	LEU
1	D	562	LEU
1	D	565	VAL
1	D	569	ARG
1	D	571	HIS
1	D	573	TYR
1	D	575	ARG
1	D	576	GLN
1	D	578	LEU
1	D	591	LYS
1	D	613	TYR
1	D	618	MET
1	D	622	LEU
1	D	640	LEU
1	D	649	ARG
1	D	652	LEU
1	D	658	PRO
1	D	662	LEU
1	D	665	GLN
1	D	676	THR
1	D	678	ASN
1	D	683	LEU
1	D	688	THR
1	D	692	MET
1	D	705	GLU
1	D	706	GLU
1	D	708	PHE
1	D	711	PHE
1	D	719	ASP
1	D	724	ARG

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Mol	Chain	Res	Type
1	D	727	ASN
1	D	733	ASP
1	D	756	ASP
1	D	759	LYS
1	D	760	ASP
1	D	765	LEU
1	D	770	ARG
1	D	787	VAL
1	D	792	LYS
1	D	797	TRP
1	D	798	THR
1	D	803	ARG
1	D	813	SER
1	D	816	THR
1	D	823	GLU
1	D	828	GLU
1	D	833	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	168	GLN
1	A	235	ASN
1	A	264	GLN
1	A	274	ASN
1	A	336	GLN
1	A	399	HIS
1	A	459	HIS
1	A	541	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	665	GLN
1	A	727	ASN
1	A	744	GLN
1	B	235	ASN
1	B	274	ASN
1	B	341	HIS
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN

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Mol	Chain	Res	Type
1	B	566	GLN
1	B	582	HIS
1	B	588	ASN
1	B	614	HIS
1	B	665	GLN
1	B	678	ASN
1	C	36	HIS
1	C	264	GLN
1	C	336	GLN
1	C	377	HIS
1	C	399	HIS
1	C	459	HIS
1	C	477	HIS
1	C	481	ASN
1	C	566	GLN
1	C	576	GLN
1	C	579	ASN
1	C	614	HIS
1	C	727	ASN
1	C	744	GLN
1	D	72	GLN
1	D	168	GLN
1	D	187	ASN
1	D	274	ASN
1	D	336	GLN
1	D	376	ASN
1	D	377	HIS
1	D	453	ASN
1	D	481	ASN
1	D	566	GLN
1	D	576	GLN
1	D	582	HIS
1	D	588	ASN
1	D	665	GLN
1	D	727	ASN
1	D	744	GLN
1	D	804	ASN

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 ⓘ

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PLP	B	999	1	15,15,16	1.60	1 (6%)	21,22,23	1.09	1 (4%)
3	PLP	D	999	1	15,15,16	1.12	1 (6%)	21,22,23	1.87	2 (9%)
4	AMP	D	920	-	21,25,25	0.94	1 (4%)	23,38,38	0.99	0
2	SO4	A	901	-	4,4,4	0.34	0	6,6,6	0.33	0
2	SO4	A	900	-	4,4,4	0.24	0	6,6,6	0.37	0
2	SO4	C	901	-	4,4,4	0.32	0	6,6,6	0.41	0
3	PLP	A	999	1	15,15,16	1.87	5 (33%)	21,22,23	1.07	2 (9%)
2	SO4	B	900	-	4,4,4	0.46	0	6,6,6	0.44	0
2	SO4	C	900	-	4,4,4	0.36	0	6,6,6	0.34	0
2	SO4	B	901	-	4,4,4	0.41	0	6,6,6	0.26	0
2	SO4	D	900	-	4,4,4	0.24	0	6,6,6	0.32	0
4	AMP	A	920	-	21,25,25	0.96	2 (9%)	23,38,38	1.12	1 (4%)
4	AMP	B	920	-	21,25,25	0.93	2 (9%)	23,38,38	0.90	0
4	AMP	C	920	-	21,25,25	0.97	2 (9%)	23,38,38	1.04	0
3	PLP	C	999	1	15,15,16	1.14	1 (6%)	21,22,23	0.98	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	B	999	1	-	0/6/6/8	0/1/1/1
3	PLP	D	999	1	-	0/6/6/8	0/1/1/1
4	AMP	D	920	-	-	3/6/26/26	0/3/3/3
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1
4	AMP	A	920	-	-	3/6/26/26	0/3/3/3
4	AMP	B	920	-	-	2/6/26/26	0/3/3/3
4	AMP	C	920	-	-	3/6/26/26	0/3/3/3
3	PLP	C	999	1	-	0/6/6/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	PLP	C3-C2	-3.98	1.36	1.41
3	A	999	PLP	C3-C2	-3.92	1.36	1.41
3	A	999	PLP	P-O2P	-2.57	1.45	1.54
3	C	999	PLP	C3-C2	-2.55	1.38	1.41
3	A	999	PLP	C5-C4	-2.41	1.37	1.40
4	A	920	AMP	O4'-C1'	2.39	1.44	1.40
3	A	999	PLP	C5A-C5	-2.26	1.45	1.50
4	D	920	AMP	O4'-C1'	2.21	1.43	1.40
4	C	920	AMP	O4'-C1'	2.17	1.43	1.40
4	C	920	AMP	C8-N7	-2.16	1.30	1.34
4	B	920	AMP	O4'-C1'	2.12	1.43	1.40
3	A	999	PLP	C4A-C4	-2.12	1.47	1.51
4	A	920	AMP	C8-N7	-2.07	1.30	1.34
4	B	920	AMP	C8-N7	-2.06	1.30	1.34
3	D	999	PLP	P-O3P	-2.05	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	999	PLP	O4P-C5A-C5	7.49	123.39	109.36
4	A	920	AMP	C4'-O4'-C1'	-2.80	107.36	109.92
3	C	999	PLP	C6-C5-C4	2.34	120.01	118.10
3	A	999	PLP	C5-C6-N1	-2.28	120.12	123.83
3	D	999	PLP	C5-C6-N1	-2.26	120.16	123.83
3	B	999	PLP	O4P-C5A-C5	2.22	113.52	109.36
3	A	999	PLP	O2P-P-O4P	-2.00	101.44	106.67

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	920	AMP	C5'-O5'-P-O2P
4	A	920	AMP	C5'-O5'-P-O3P
4	B	920	AMP	C5'-O5'-P-O2P
4	B	920	AMP	C5'-O5'-P-O3P
4	C	920	AMP	C5'-O5'-P-O2P
4	C	920	AMP	C5'-O5'-P-O3P
4	D	920	AMP	C5'-O5'-P-O2P
4	A	920	AMP	C5'-O5'-P-O1P
4	C	920	AMP	C5'-O5'-P-O1P
4	D	920	AMP	C5'-O5'-P-O3P
4	D	920	AMP	C5'-O5'-P-O1P

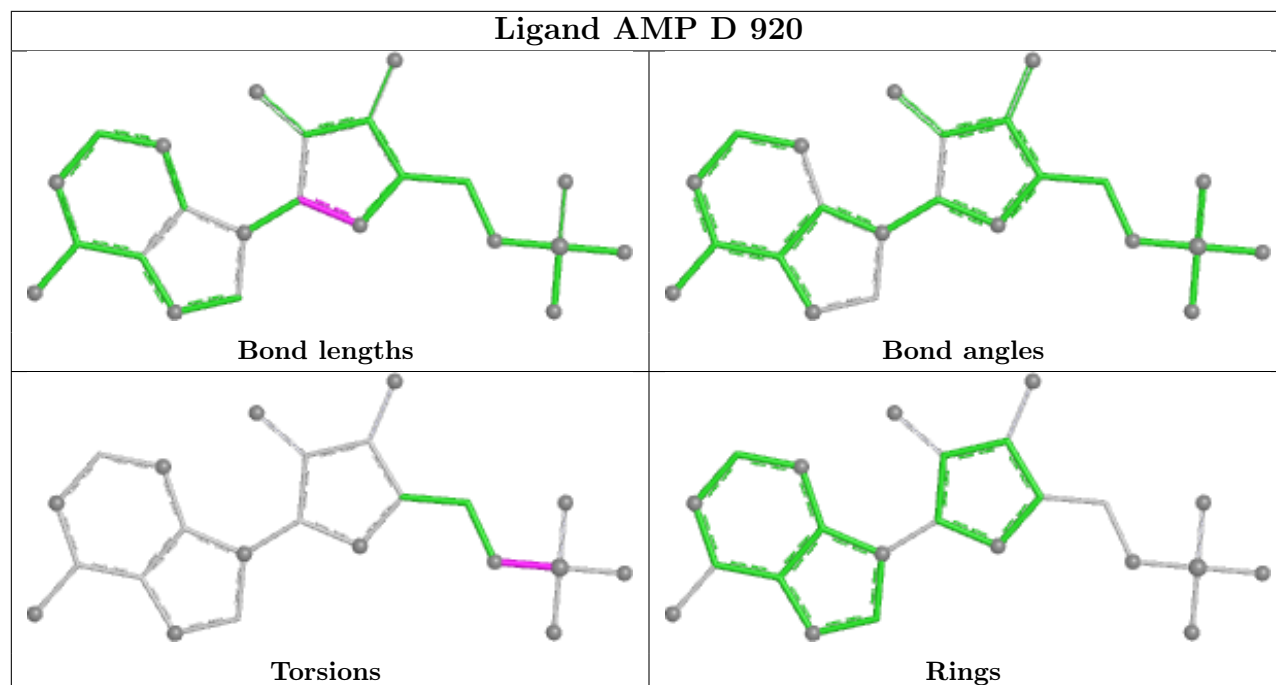
There are no ring outliers.

11 monomers are involved in 18 short contacts:

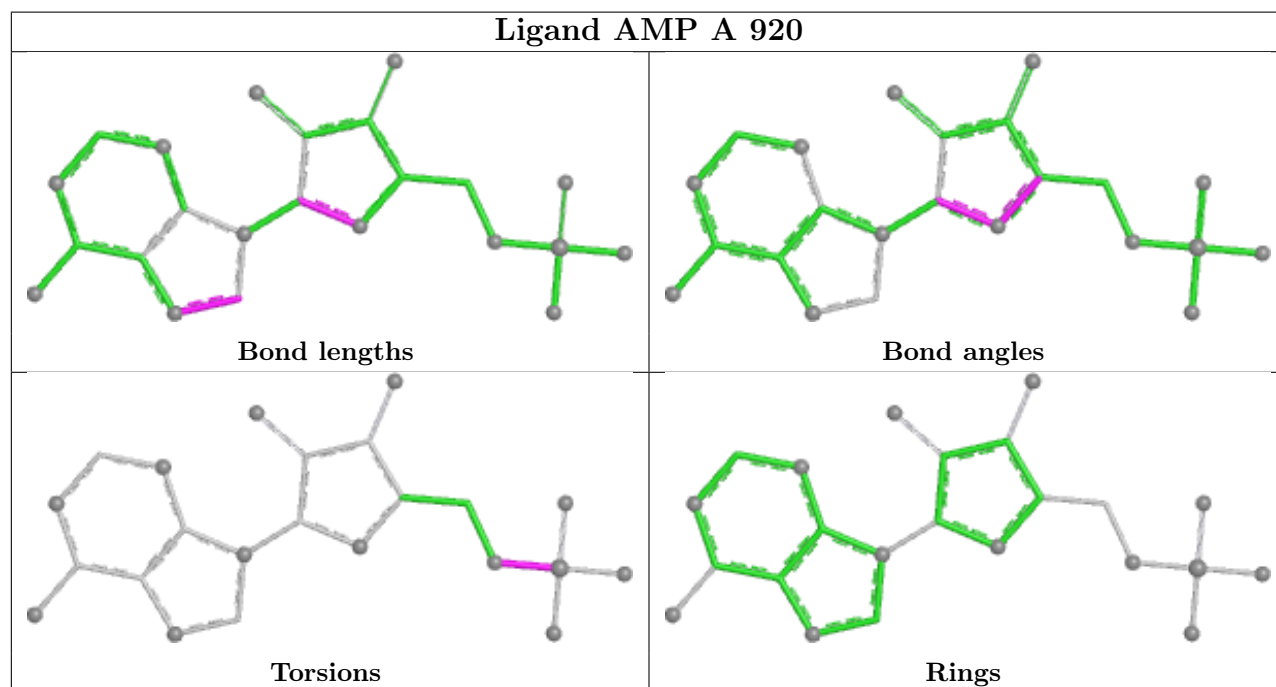
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	999	PLP	1	0
3	D	999	PLP	3	0
4	D	920	AMP	2	0
2	A	901	SO4	2	0
2	C	901	SO4	1	0
3	A	999	PLP	2	0
2	B	901	SO4	1	0
4	A	920	AMP	3	0
4	B	920	AMP	1	0
4	C	920	AMP	1	0
3	C	999	PLP	1	0

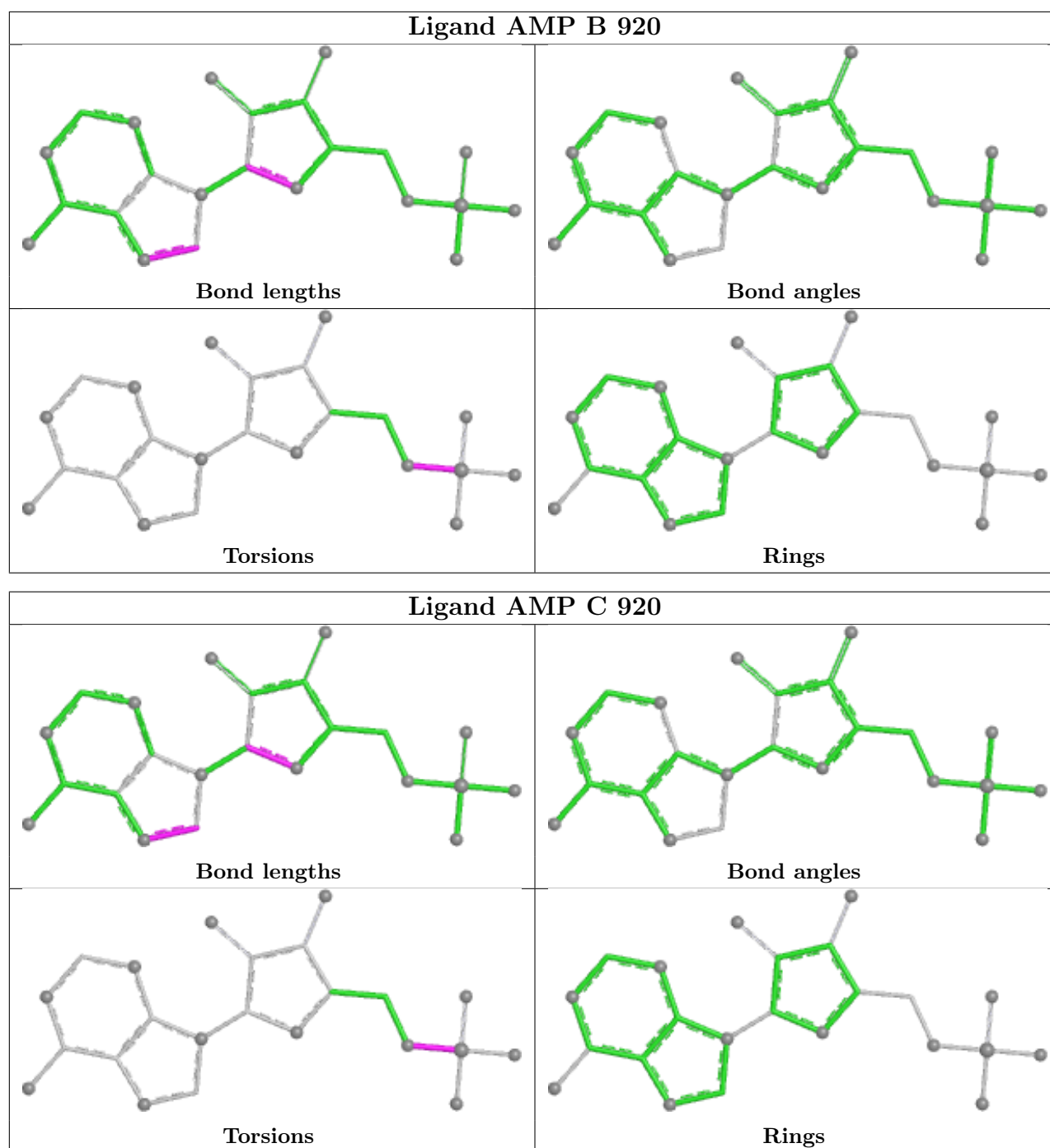
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 AMP D 920



Ligand AMP 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.