



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:16 PM BST

PDB ID : 4AAU
EMDB ID: : EMD-2001
Title : ATP-triggered molecular mechanics of the chaperonin GroEL
Authors : Clare, D.K.; Vasishtan, D.; Stagg, S.; Quispe, J.; Farr, G.W.; Topf, M.; Horwich, A.L.; Saibil, H.R.
Deposited on : 2011-12-05
Resolution : 8.50 Å(reported)
Based on PDB ID : 1OEL

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

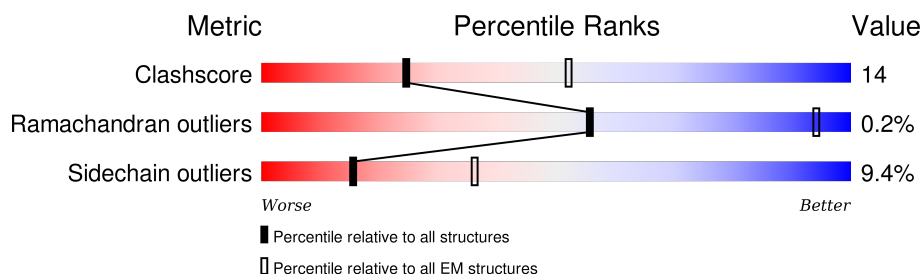
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	548	60% 25% 9% . .
1	B	548	60% 25% 9% . .
1	C	548	61% 25% 9% . .
1	D	548	60% 25% 9% . .
1	E	548	61% 25% 9% . .
1	F	548	61% 25% 9% . .
1	G	548	61% 25% 9% . .
1	H	548	65% 25% 5% .
1	I	548	65% 25% 5% .

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Mol	Chain	Length	Quality of chain
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	

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
3	PO4	A	1527	-	-	X	-
3	PO4	B	1527	-	-	X	-
3	PO4	C	1527	-	-	X	-
3	PO4	D	1527	-	-	X	-
3	PO4	E	1527	-	-	X	-
3	PO4	F	1527	-	-	X	-
3	PO4	G	1527	-	-	X	-
3	PO4	H	1526	-	-	X	-
3	PO4	I	1526	-	-	X	-
3	PO4	J	1526	-	-	X	-
3	PO4	K	1526	-	-	X	-
3	PO4	L	1526	-	-	X	-
3	PO4	M	1526	-	-	X	-
3	PO4	N	1526	-	-	X	-
4	ATP	M	1527	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 54474 atoms, of which 168 are hydrogens and 0 are deuteriums.

In the tables below, 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 60 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	B	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	C	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	D	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	E	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	F	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	G	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	H	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	I	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	J	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	K	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	L	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	M	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	N	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
B	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
D	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
E	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
F	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
G	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
H	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
I	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
J	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
K	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
L	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
M	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
N	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

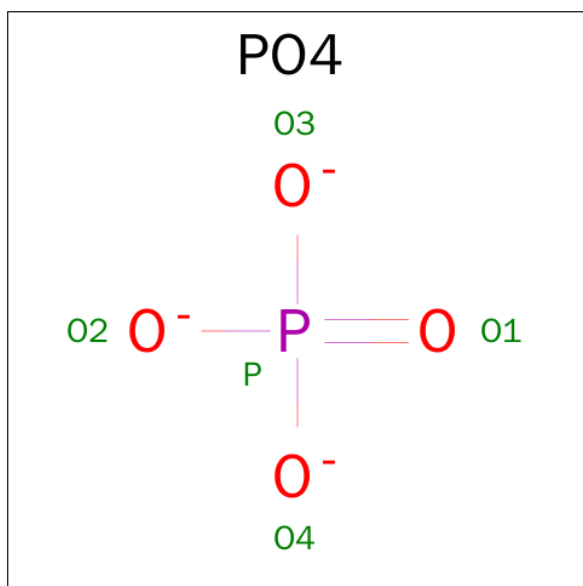
Mol	Chain	Residues	Atoms	AltConf
2	G	1	Total Mg 1 1	0
2	J	1	Total Mg 1 1	0
2	D	1	Total Mg 1 1	0
2	K	1	Total Mg 1 1	0
2	E	1	Total Mg 1 1	0
2	H	1	Total Mg 1 1	0
2	B	1	Total Mg 1 1	0
2	I	1	Total Mg 1 1	0
2	C	1	Total Mg 1 1	0
2	A	1	Total Mg 1 1	0
2	N	1	Total Mg 1 1	0
2	L	1	Total Mg 1 1	0
2	F	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
2	M	1	Total	Mg	0
			1	1	

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



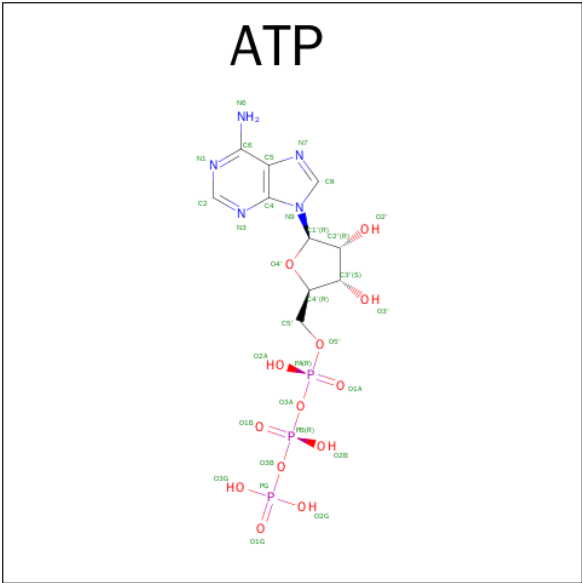
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	P	0
			1	1	
3	B	1	Total	P	0
			1	1	
3	C	1	Total	P	0
			1	1	
3	D	1	Total	P	0
			1	1	
3	E	1	Total	P	0
			1	1	
3	F	1	Total	P	0
			1	1	
3	G	1	Total	P	0
			1	1	
3	H	1	Total	P	0
			1	1	
3	I	1	Total	P	0
			1	1	
3	J	1	Total	P	0
			1	1	

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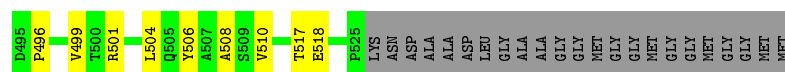
Mol	Chain	Residues	Atoms		AltConf
3	K	1	Total	P	0
			1	1	
3	L	1	Total	P	0
			1	1	
3	M	1	Total	P	0
			1	1	
3	N	1	Total	P	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



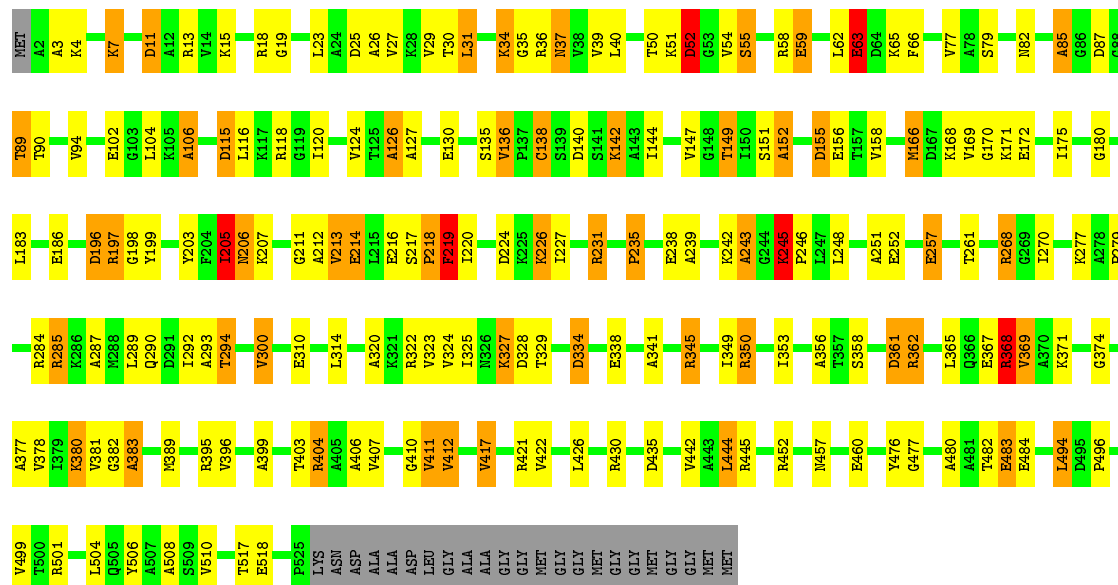
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Mol	Chain	Residues	Atoms						AltConf
4	H	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	I	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	J	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	K	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	L	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	M	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	N	1	Total 43	C 10	H 12	N 5	O 13	P 3	0



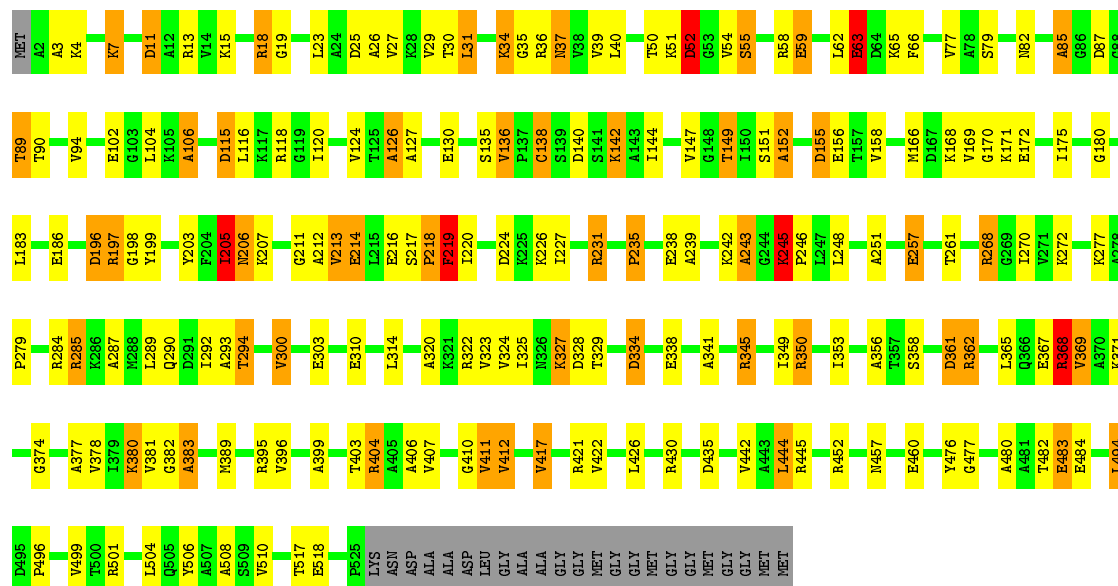
• Molecule 1: 60 KDA CHAPERONIN

Chain C: 61% 25% 9% . .



• Molecule 1: 60 KDA CHAPERONIN

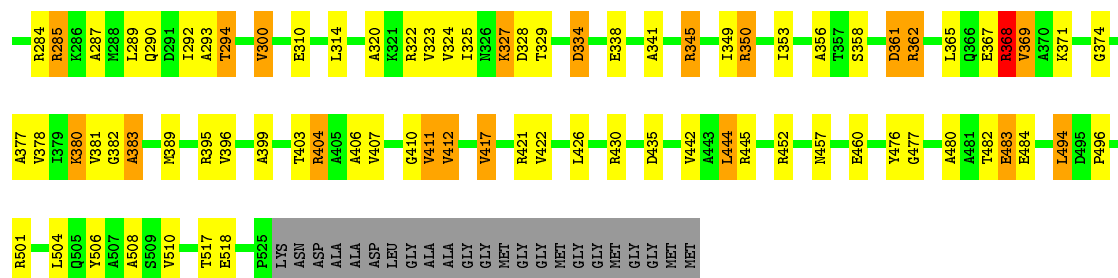
Chain D: 60% 25% 9% . .



• Molecule 1: 60 KDA CHAPERONIN

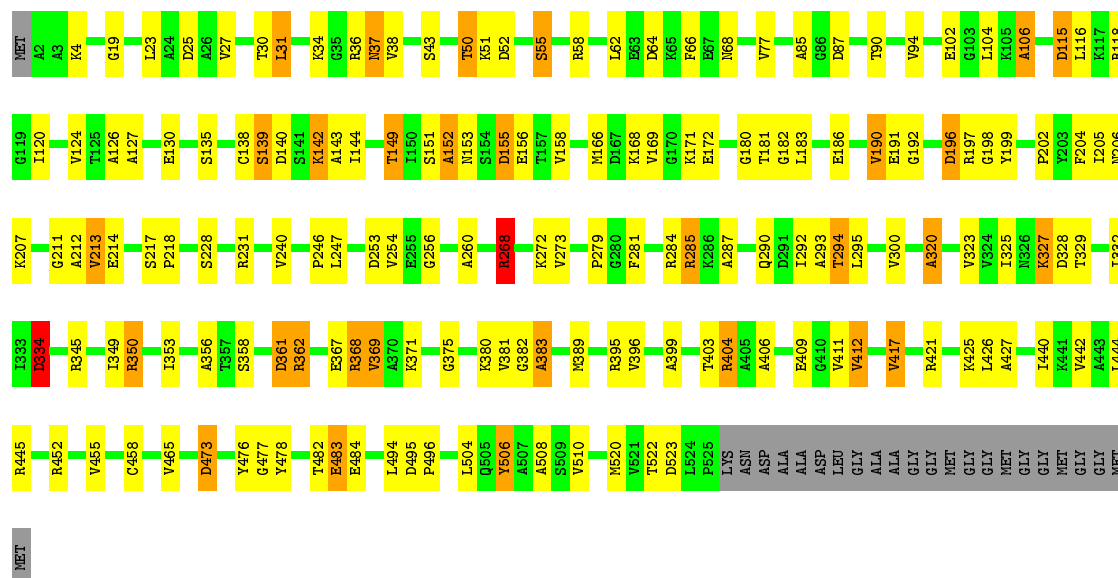
Chain E: 61% 25% 9% . .





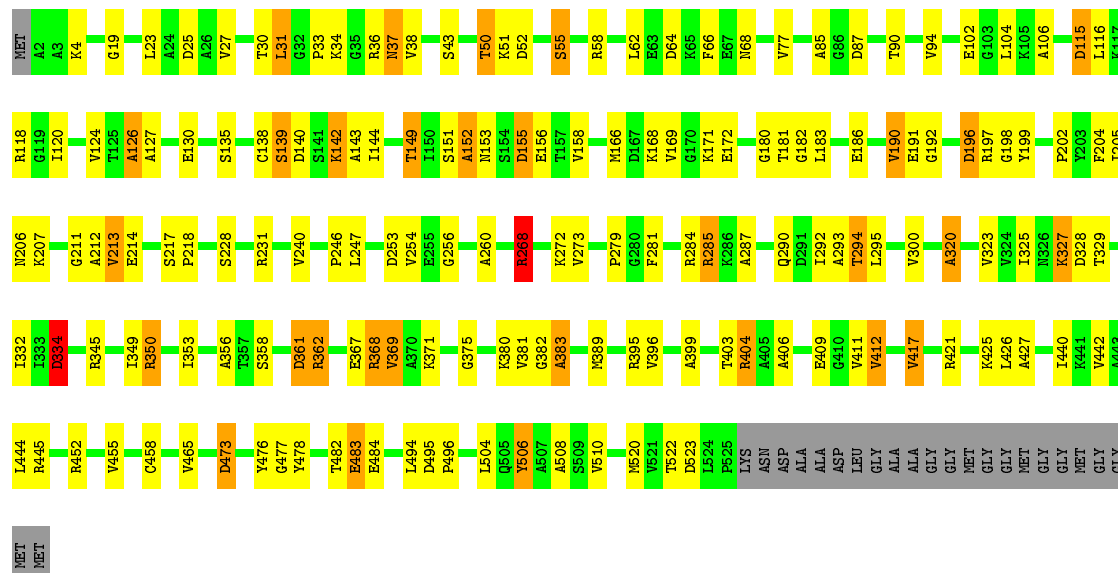
• Molecule 1: 60 KDA CHAPERONIN

Chain H: 65% 25% 5% •



• Molecule 1: 60 KDA CHAPERONIN

Chain I: 65% 25% 5% •



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE WAS PHASE FLIPPED, Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 4K CCD CAM- ERA	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ATP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.01	0/3873	1.46	68/5229 (1.3%)
1	B	1.01	0/3873	1.46	67/5229 (1.3%)
1	C	1.01	0/3873	1.46	66/5229 (1.3%)
1	D	1.01	0/3873	1.46	67/5229 (1.3%)
1	E	1.01	0/3873	1.45	67/5229 (1.3%)
1	F	1.01	0/3873	1.46	67/5229 (1.3%)
1	G	1.01	0/3873	1.46	68/5229 (1.3%)
1	H	1.00	0/3871	1.40	57/5223 (1.1%)
1	I	1.00	0/3871	1.39	55/5223 (1.1%)
1	J	1.00	0/3871	1.39	53/5223 (1.0%)
1	K	1.00	0/3871	1.40	55/5223 (1.1%)
1	L	1.00	0/3871	1.39	56/5223 (1.1%)
1	M	1.08	1/3871 (0.0%)	1.40	58/5223 (1.1%)
1	N	1.00	0/3871	1.40	57/5223 (1.1%)
All	All	1.01	1/54208 (0.0%)	1.43	861/73164 (1.2%)

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	10
1	B	0	10
1	C	0	10
1	D	0	10
1	E	0	10
1	F	0	10
1	G	0	10
1	H	0	10
1	I	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	10
1	K	0	10
1	L	0	10
1	M	0	10
1	N	1	10
All	All	1	140

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	493	ILE	CG1-CD1	26.52	3.33	1.50

All (861) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	245	LYS	N-CA-CB	-14.08	85.26	110.60
1	D	245	LYS	N-CA-CB	-14.05	85.30	110.60
1	B	245	LYS	N-CA-CB	-14.05	85.31	110.60
1	A	245	LYS	N-CA-CB	-14.05	85.31	110.60
1	G	245	LYS	N-CA-CB	-14.04	85.33	110.60
1	C	245	LYS	N-CA-CB	-14.04	85.33	110.60
1	E	245	LYS	N-CA-CB	-14.02	85.37	110.60
1	B	63	GLU	N-CA-CB	-13.54	86.22	110.60
1	C	63	GLU	N-CA-CB	-13.53	86.24	110.60
1	G	63	GLU	N-CA-CB	-13.53	86.25	110.60
1	F	63	GLU	N-CA-CB	-13.52	86.27	110.60
1	A	63	GLU	N-CA-CB	-13.50	86.30	110.60
1	D	63	GLU	N-CA-CB	-13.49	86.31	110.60
1	E	63	GLU	N-CA-CB	-13.48	86.34	110.60
1	N	383	ALA	N-CA-CB	11.86	126.70	110.10
1	H	383	ALA	N-CA-CB	11.85	126.69	110.10
1	M	383	ALA	N-CA-CB	11.85	126.69	110.10
1	L	383	ALA	N-CA-CB	11.84	126.67	110.10
1	I	383	ALA	N-CA-CB	11.83	126.67	110.10
1	K	383	ALA	N-CA-CB	11.82	126.64	110.10
1	J	383	ALA	N-CA-CB	11.79	126.60	110.10
1	B	383	ALA	N-CA-CB	11.24	125.83	110.10
1	C	383	ALA	N-CA-CB	11.23	125.83	110.10
1	A	383	ALA	N-CA-CB	11.23	125.82	110.10
1	F	383	ALA	N-CA-CB	11.23	125.82	110.10
1	G	383	ALA	N-CA-CB	11.20	125.78	110.10
1	D	383	ALA	N-CA-CB	11.17	125.74	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	383	ALA	N-CA-CB	11.15	125.71	110.10
1	K	231	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	I	231	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	L	231	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	J	231	ARG	NE-CZ-NH1	9.55	125.07	120.30
1	M	231	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	N	231	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	H	231	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	K	153	ASN	CB-CA-C	9.16	128.73	110.40
1	K	87	ASP	CB-CG-OD2	9.08	126.47	118.30
1	J	153	ASN	CB-CA-C	8.73	127.87	110.40
1	N	153	ASN	CB-CA-C	8.73	127.86	110.40
1	I	153	ASN	CB-CA-C	8.72	127.83	110.40
1	L	153	ASN	CB-CA-C	8.71	127.83	110.40
1	H	153	ASN	CB-CA-C	8.69	127.78	110.40
1	E	115	ASP	CB-CA-C	8.61	127.63	110.40
1	G	115	ASP	CB-CA-C	8.61	127.62	110.40
1	D	115	ASP	CB-CA-C	8.61	127.61	110.40
1	A	115	ASP	CB-CA-C	8.60	127.60	110.40
1	B	115	ASP	CB-CA-C	8.60	127.61	110.40
1	C	115	ASP	CB-CA-C	8.60	127.61	110.40
1	F	115	ASP	CB-CA-C	8.60	127.59	110.40
1	M	493	ILE	N-CA-CB	8.59	130.54	110.80
1	I	362	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	N	362	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	M	362	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	L	231	ARG	CB-CA-C	-8.31	93.79	110.40
1	M	231	ARG	CB-CA-C	-8.30	93.79	110.40
1	N	231	ARG	CB-CA-C	-8.30	93.79	110.40
1	K	231	ARG	CB-CA-C	-8.30	93.80	110.40
1	I	231	ARG	CB-CA-C	-8.29	93.82	110.40
1	J	231	ARG	CB-CA-C	-8.29	93.81	110.40
1	H	231	ARG	CB-CA-C	-8.29	93.82	110.40
1	K	362	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	H	362	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	J	362	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	L	362	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	L	473	ASP	N-CA-CB	8.19	125.34	110.60
1	N	473	ASP	N-CA-CB	8.19	125.34	110.60
1	I	473	ASP	N-CA-CB	8.18	125.33	110.60
1	J	473	ASP	N-CA-CB	8.16	125.29	110.60
1	K	473	ASP	N-CA-CB	8.16	125.30	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	473	ASP	N-CA-CB	8.16	125.28	110.60
1	M	473	ASP	N-CA-CB	8.15	125.27	110.60
1	M	153	ASN	CB-CA-C	8.14	126.69	110.40
1	H	152	ALA	CB-CA-C	8.14	122.30	110.10
1	E	285	ARG	CB-CA-C	-8.12	94.17	110.40
1	L	152	ALA	CB-CA-C	8.12	122.28	110.10
1	N	152	ALA	CB-CA-C	8.11	122.27	110.10
1	C	285	ARG	CB-CA-C	-8.11	94.19	110.40
1	D	285	ARG	CB-CA-C	-8.10	94.19	110.40
1	G	285	ARG	CB-CA-C	-8.10	94.20	110.40
1	I	152	ALA	CB-CA-C	8.10	122.25	110.10
1	B	285	ARG	CB-CA-C	-8.10	94.20	110.40
1	B	362	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	285	ARG	CB-CA-C	-8.09	94.21	110.40
1	J	152	ALA	CB-CA-C	8.09	122.23	110.10
1	M	152	ALA	CB-CA-C	8.08	122.22	110.10
1	E	362	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	F	285	ARG	CB-CA-C	-8.07	94.27	110.40
1	F	362	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	K	152	ALA	CB-CA-C	8.02	122.14	110.10
1	C	362	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	D	362	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	362	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	G	362	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	F	404	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	C	404	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	B	404	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	404	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	C	37	ASN	N-CA-CB	-7.71	96.73	110.60
1	D	404	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	E	37	ASN	N-CA-CB	-7.70	96.74	110.60
1	C	138	CYS	N-CA-CB	7.69	124.44	110.60
1	G	37	ASN	N-CA-CB	-7.69	96.75	110.60
1	G	404	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	A	37	ASN	N-CA-CB	-7.69	96.76	110.60
1	D	37	ASN	N-CA-CB	-7.69	96.77	110.60
1	B	138	CYS	N-CA-CB	7.68	124.43	110.60
1	B	37	ASN	N-CA-CB	-7.68	96.78	110.60
1	G	138	CYS	N-CA-CB	7.68	124.42	110.60
1	A	138	CYS	N-CA-CB	7.67	124.41	110.60
1	D	138	CYS	N-CA-CB	7.67	124.41	110.60
1	E	138	CYS	N-CA-CB	7.67	124.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	37	ASN	N-CA-CB	-7.66	96.81	110.60
1	F	452	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	F	138	CYS	N-CA-CB	7.64	124.36	110.60
1	A	452	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	G	452	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	D	452	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	E	152	ALA	CB-CA-C	7.58	121.46	110.10
1	G	152	ALA	CB-CA-C	7.56	121.44	110.10
1	A	152	ALA	CB-CA-C	7.55	121.42	110.10
1	E	452	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	D	152	ALA	CB-CA-C	7.55	121.42	110.10
1	B	152	ALA	CB-CA-C	7.54	121.41	110.10
1	F	152	ALA	CB-CA-C	7.53	121.39	110.10
1	H	404	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	C	152	ALA	CB-CA-C	7.52	121.38	110.10
1	C	452	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	E	404	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	M	404	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	B	452	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	J	404	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	L	404	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	K	404	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	J	115	ASP	CB-CA-C	7.43	125.27	110.40
1	C	87	ASP	CB-CG-OD2	7.42	124.97	118.30
1	H	115	ASP	CB-CA-C	7.41	125.22	110.40
1	B	87	ASP	CB-CG-OD2	7.41	124.97	118.30
1	K	115	ASP	CB-CA-C	7.41	125.21	110.40
1	M	115	ASP	CB-CA-C	7.41	125.21	110.40
1	L	115	ASP	CB-CA-C	7.40	125.20	110.40
1	I	115	ASP	CB-CA-C	7.39	125.19	110.40
1	N	115	ASP	CB-CA-C	7.39	125.19	110.40
1	I	404	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	E	87	ASP	CB-CG-OD2	7.36	124.93	118.30
1	D	87	ASP	CB-CG-OD2	7.35	124.91	118.30
1	G	87	ASP	CB-CG-OD2	7.34	124.91	118.30
1	A	87	ASP	CB-CG-OD2	7.33	124.89	118.30
1	F	87	ASP	CB-CG-OD2	7.33	124.89	118.30
1	A	59	GLU	CB-CA-C	7.32	125.05	110.40
1	C	59	GLU	CB-CA-C	7.32	125.05	110.40
1	F	59	GLU	CB-CA-C	7.32	125.04	110.40
1	D	59	GLU	CB-CA-C	7.32	125.03	110.40
1	B	59	GLU	CB-CA-C	7.31	125.03	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	59	GLU	CB-CA-C	7.30	125.00	110.40
1	M	87	ASP	CB-CG-OD1	7.30	124.87	118.30
1	E	59	GLU	CB-CA-C	7.29	124.98	110.40
1	N	404	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	G	268	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	E	268	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	E	216	GLU	N-CA-CB	-7.21	97.63	110.60
1	H	55	SER	CB-CA-C	-7.20	96.41	110.10
1	N	55	SER	CB-CA-C	-7.20	96.42	110.10
1	K	55	SER	CB-CA-C	-7.20	96.43	110.10
1	F	216	GLU	N-CA-CB	-7.19	97.65	110.60
1	C	216	GLU	N-CA-CB	-7.18	97.67	110.60
1	A	268	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	216	GLU	N-CA-CB	-7.18	97.68	110.60
1	L	55	SER	CB-CA-C	-7.17	96.47	110.10
1	B	268	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	G	216	GLU	N-CA-CB	-7.17	97.69	110.60
1	I	55	SER	CB-CA-C	-7.17	96.48	110.10
1	D	55	SER	N-CA-CB	7.17	121.25	110.50
1	A	216	GLU	N-CA-CB	-7.17	97.70	110.60
1	B	55	SER	N-CA-CB	7.16	121.23	110.50
1	D	216	GLU	N-CA-CB	-7.16	97.72	110.60
1	D	268	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	55	SER	N-CA-CB	7.13	121.20	110.50
1	G	55	SER	N-CA-CB	7.12	121.19	110.50
1	F	268	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	J	55	SER	CB-CA-C	-7.12	96.57	110.10
1	E	55	SER	N-CA-CB	7.12	121.17	110.50
1	H	231	ARG	CA-CB-CG	7.11	129.05	113.40
1	J	87	ASP	CB-CG-OD2	7.11	124.70	118.30
1	C	55	SER	N-CA-CB	7.11	121.16	110.50
1	I	231	ARG	CA-CB-CG	7.10	129.01	113.40
1	M	231	ARG	CA-CB-CG	7.10	129.01	113.40
1	N	231	ARG	CA-CB-CG	7.10	129.01	113.40
1	L	231	ARG	CA-CB-CG	7.09	129.01	113.40
1	K	231	ARG	CA-CB-CG	7.09	129.00	113.40
1	J	231	ARG	CA-CB-CG	7.09	128.99	113.40
1	F	55	SER	N-CA-CB	7.08	121.13	110.50
1	I	87	ASP	CB-CG-OD2	7.08	124.67	118.30
1	L	87	ASP	CB-CG-OD2	7.06	124.65	118.30
1	C	268	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	K	482	THR	N-CA-CB	6.98	123.56	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	322	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	D	483	GLU	CB-CG-CD	6.93	132.91	114.20
1	E	483	GLU	CB-CG-CD	6.93	132.91	114.20
1	F	483	GLU	CB-CG-CD	6.92	132.89	114.20
1	A	483	GLU	CB-CG-CD	6.92	132.89	114.20
1	B	483	GLU	CB-CG-CD	6.92	132.88	114.20
1	C	483	GLU	CB-CG-CD	6.91	132.87	114.20
1	G	483	GLU	CB-CG-CD	6.91	132.85	114.20
1	H	87	ASP	CB-CG-OD2	6.90	124.51	118.30
1	M	52	ASP	CB-CA-C	6.89	124.18	110.40
1	G	322	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	F	322	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	J	482	THR	N-CA-CB	6.86	123.34	110.30
1	M	294	THR	CA-CB-CG2	-6.85	102.81	112.40
1	B	322	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	322	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	H	294	THR	CA-CB-CG2	-6.83	102.84	112.40
1	G	235	PRO	N-CA-CB	6.83	111.49	103.30
1	I	294	THR	CA-CB-CG2	-6.82	102.85	112.40
1	B	235	PRO	N-CA-CB	6.82	111.48	103.30
1	C	235	PRO	N-CA-CB	6.82	111.48	103.30
1	E	235	PRO	N-CA-CB	6.82	111.48	103.30
1	C	322	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	D	235	PRO	N-CA-CB	6.81	111.47	103.30
1	E	322	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	J	294	THR	CA-CB-CG2	-6.80	102.87	112.40
1	N	294	THR	CA-CB-CG2	-6.80	102.87	112.40
1	L	294	THR	CA-CB-CG2	-6.80	102.88	112.40
1	K	294	THR	CA-CB-CG2	-6.80	102.89	112.40
1	A	235	PRO	N-CA-CB	6.79	111.45	103.30
1	F	235	PRO	N-CA-CB	6.77	111.43	103.30
1	N	87	ASP	CB-CG-OD2	6.76	124.39	118.30
1	N	479	ASN	CB-CA-C	6.71	123.83	110.40
1	N	139	SER	CB-CA-C	6.70	122.84	110.10
1	E	367	GLU	CB-CA-C	-6.69	97.02	110.40
1	I	139	SER	CB-CA-C	6.69	122.81	110.10
1	C	367	GLU	CB-CA-C	-6.69	97.03	110.40
1	A	367	GLU	CB-CA-C	-6.69	97.03	110.40
1	B	367	GLU	CB-CA-C	-6.68	97.03	110.40
1	J	139	SER	CB-CA-C	6.68	122.79	110.10
1	F	367	GLU	CB-CA-C	-6.67	97.05	110.40
1	L	139	SER	CB-CA-C	6.67	122.78	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	367	GLU	CB-CA-C	-6.66	97.08	110.40
1	G	367	GLU	CB-CA-C	-6.66	97.08	110.40
1	H	139	SER	CB-CA-C	6.65	122.74	110.10
1	M	139	SER	CB-CA-C	6.65	122.73	110.10
1	K	139	SER	CB-CA-C	6.63	122.69	110.10
1	B	417	VAL	CA-CB-CG2	-6.62	100.97	110.90
1	D	417	VAL	CA-CB-CG2	-6.61	100.98	110.90
1	M	55	SER	CB-CA-C	-6.61	97.54	110.10
1	C	412	VAL	CB-CA-C	-6.60	98.85	111.40
1	B	85	ALA	N-CA-CB	-6.60	100.86	110.10
1	F	417	VAL	CA-CB-CG2	-6.60	101.00	110.90
1	L	285	ARG	CB-CA-C	-6.60	97.20	110.40
1	I	285	ARG	CB-CA-C	-6.60	97.20	110.40
1	G	482	THR	N-CA-CB	6.59	122.82	110.30
1	E	85	ALA	N-CA-CB	-6.59	100.88	110.10
1	G	412	VAL	CB-CA-C	-6.59	98.88	111.40
1	M	285	ARG	CB-CA-C	-6.59	97.22	110.40
1	C	417	VAL	CA-CB-CG2	-6.59	101.02	110.90
1	G	417	VAL	CA-CB-CG2	-6.59	101.02	110.90
1	B	412	VAL	CB-CA-C	-6.58	98.89	111.40
1	E	417	VAL	CA-CB-CG2	-6.58	101.02	110.90
1	E	482	THR	N-CA-CB	6.58	122.81	110.30
1	H	285	ARG	CB-CA-C	-6.58	97.23	110.40
1	D	482	THR	N-CA-CB	6.58	122.80	110.30
1	E	412	VAL	CB-CA-C	-6.58	98.90	111.40
1	F	482	THR	N-CA-CB	6.58	122.80	110.30
1	A	412	VAL	CB-CA-C	-6.58	98.91	111.40
1	N	285	ARG	CB-CA-C	-6.58	97.25	110.40
1	C	482	THR	N-CA-CB	6.57	122.79	110.30
1	F	412	VAL	CB-CA-C	-6.57	98.91	111.40
1	K	285	ARG	CB-CA-C	-6.57	97.25	110.40
1	K	334	ASP	CB-CG-OD1	6.57	124.22	118.30
1	B	482	THR	N-CA-CB	6.57	122.79	110.30
1	A	482	THR	N-CA-CB	6.57	122.78	110.30
1	D	412	VAL	CB-CA-C	-6.57	98.92	111.40
1	G	85	ALA	N-CA-CB	-6.57	100.91	110.10
1	J	285	ARG	CB-CA-C	-6.57	97.27	110.40
1	F	85	ALA	N-CA-CB	-6.54	100.94	110.10
1	N	334	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	417	VAL	CA-CB-CG2	-6.53	101.10	110.90
1	I	334	ASP	CB-CG-OD1	6.53	124.18	118.30
1	H	334	ASP	CB-CG-OD1	6.52	124.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	140	ASP	N-CA-CB	-6.51	98.88	110.60
1	M	140	ASP	N-CA-CB	-6.51	98.88	110.60
1	H	140	ASP	N-CA-CB	-6.50	98.90	110.60
1	K	425	LYS	CB-CA-C	6.50	123.40	110.40
1	K	140	ASP	N-CA-CB	-6.50	98.91	110.60
1	H	367	GLU	CB-CA-C	-6.49	97.42	110.40
1	M	334	ASP	CB-CG-OD1	6.49	124.14	118.30
1	N	140	ASP	N-CA-CB	-6.49	98.92	110.60
1	I	140	ASP	N-CA-CB	-6.48	98.93	110.60
1	J	140	ASP	N-CA-CB	-6.48	98.93	110.60
1	L	334	ASP	CB-CG-OD1	6.48	124.14	118.30
1	L	367	GLU	CB-CA-C	-6.48	97.44	110.40
1	I	367	GLU	CB-CA-C	-6.48	97.44	110.40
1	M	425	LYS	CB-CA-C	6.47	123.35	110.40
1	J	367	GLU	CB-CA-C	-6.47	97.46	110.40
1	N	367	GLU	CB-CA-C	-6.47	97.46	110.40
1	K	367	GLU	CB-CA-C	-6.47	97.47	110.40
1	L	425	LYS	CB-CA-C	6.47	123.33	110.40
1	J	425	LYS	CB-CA-C	6.46	123.31	110.40
1	M	367	GLU	CB-CA-C	-6.46	97.49	110.40
1	I	425	LYS	CB-CA-C	6.45	123.31	110.40
1	H	425	LYS	CB-CA-C	6.45	123.31	110.40
1	N	425	LYS	CB-CA-C	6.45	123.30	110.40
1	J	334	ASP	CB-CG-OD1	6.45	124.10	118.30
1	M	371	LYS	CB-CA-C	6.40	123.20	110.40
1	K	371	LYS	CB-CA-C	6.39	123.19	110.40
1	A	126	ALA	CB-CA-C	6.39	119.68	110.10
1	N	371	LYS	CB-CA-C	6.39	123.18	110.40
1	H	350	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	H	371	LYS	CB-CA-C	6.38	123.16	110.40
1	I	371	LYS	CB-CA-C	6.38	123.16	110.40
1	L	371	LYS	CB-CA-C	6.37	123.15	110.40
1	J	371	LYS	CB-CA-C	6.37	123.14	110.40
1	F	444	LEU	CB-CA-C	-6.37	98.10	110.20
1	C	126	ALA	CB-CA-C	6.37	119.65	110.10
1	B	126	ALA	CB-CA-C	6.37	119.65	110.10
1	E	126	ALA	CB-CA-C	6.37	119.65	110.10
1	L	482	THR	N-CA-CB	6.37	122.39	110.30
1	C	444	LEU	CB-CA-C	-6.36	98.12	110.20
1	G	444	LEU	CB-CA-C	-6.36	98.12	110.20
1	D	444	LEU	CB-CA-C	-6.35	98.13	110.20
1	G	155	ASP	CB-CA-C	6.35	123.10	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	444	LEU	CB-CA-C	-6.35	98.13	110.20
1	B	444	LEU	CB-CA-C	-6.35	98.14	110.20
1	A	444	LEU	CB-CA-C	-6.34	98.15	110.20
1	F	126	ALA	CB-CA-C	6.34	119.61	110.10
1	G	126	ALA	CB-CA-C	6.34	119.61	110.10
1	D	126	ALA	CB-CA-C	6.33	119.60	110.10
1	C	155	ASP	CB-CA-C	6.33	123.06	110.40
1	D	155	ASP	CB-CA-C	6.33	123.06	110.40
1	F	353	ILE	CB-CA-C	-6.32	98.96	111.60
1	F	155	ASP	CB-CA-C	6.32	123.04	110.40
1	I	482	THR	N-CA-CB	6.32	122.31	110.30
1	A	155	ASP	CB-CA-C	6.32	123.03	110.40
1	C	353	ILE	CB-CA-C	-6.32	98.97	111.60
1	B	155	ASP	CB-CA-C	6.31	123.03	110.40
1	E	353	ILE	CB-CA-C	-6.30	98.99	111.60
1	B	353	ILE	CB-CA-C	-6.30	98.99	111.60
1	E	155	ASP	CB-CA-C	6.30	123.01	110.40
1	G	353	ILE	CB-CA-C	-6.30	99.00	111.60
1	D	353	ILE	CB-CA-C	-6.30	99.01	111.60
1	A	85	ALA	N-CA-CB	-6.29	101.29	110.10
1	C	85	ALA	N-CA-CB	-6.29	101.29	110.10
1	N	350	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	353	ILE	CB-CA-C	-6.29	99.02	111.60
1	D	85	ALA	N-CA-CB	-6.29	101.30	110.10
1	K	510	VAL	CB-CA-C	-6.29	99.46	111.40
1	L	510	VAL	CB-CA-C	-6.28	99.47	111.40
1	H	482	THR	N-CA-CB	6.27	122.22	110.30
1	L	350	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	M	510	VAL	CB-CA-C	-6.26	99.50	111.40
1	M	493	ILE	CB-CG1-CD1	6.26	131.43	113.90
1	M	482	THR	N-CA-CB	6.25	122.17	110.30
1	H	452	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	M	350	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	I	350	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	M	89	THR	CB-CA-C	-6.22	94.80	111.60
1	H	510	VAL	CB-CA-C	-6.22	99.58	111.40
1	I	510	VAL	CB-CA-C	-6.22	99.58	111.40
1	J	510	VAL	CB-CA-C	-6.22	99.58	111.40
1	N	510	VAL	CB-CA-C	-6.21	99.60	111.40
1	I	452	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	K	350	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	219	PHE	CB-CG-CD1	6.16	125.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	140	ASP	N-CA-CB	-6.14	99.54	110.60
1	E	140	ASP	N-CA-CB	-6.14	99.55	110.60
1	G	219	PHE	CB-CG-CD1	6.14	125.10	120.80
1	C	63	GLU	CA-CB-CG	6.13	126.89	113.40
1	F	140	ASP	N-CA-CB	-6.13	99.56	110.60
1	D	140	ASP	N-CA-CB	-6.13	99.57	110.60
1	J	350	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	140	ASP	N-CA-CB	-6.12	99.58	110.60
1	C	140	ASP	N-CA-CB	-6.12	99.58	110.60
1	A	140	ASP	N-CA-CB	-6.12	99.58	110.60
1	G	206	ASN	CA-CB-CG	6.12	126.86	113.40
1	B	206	ASN	CA-CB-CG	6.12	126.85	113.40
1	D	206	ASN	CA-CB-CG	6.11	126.85	113.40
1	D	219	PHE	CB-CG-CD1	6.11	125.08	120.80
1	F	510	VAL	CB-CA-C	-6.11	99.80	111.40
1	G	63	GLU	CA-CB-CG	6.11	126.84	113.40
1	E	219	PHE	CB-CG-CD1	6.10	125.07	120.80
1	A	219	PHE	CB-CG-CD1	6.10	125.07	120.80
1	D	11	ASP	CB-CA-C	6.10	122.60	110.40
1	F	206	ASN	CA-CB-CG	6.10	126.82	113.40
1	G	510	VAL	CB-CA-C	-6.10	99.81	111.40
1	K	231	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	63	GLU	CA-CB-CG	6.09	126.81	113.40
1	E	206	ASN	CA-CB-CG	6.09	126.81	113.40
1	B	510	VAL	CB-CA-C	-6.09	99.82	111.40
1	M	452	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	F	63	GLU	CA-CB-CG	6.09	126.80	113.40
1	C	206	ASN	CA-CB-CG	6.09	126.79	113.40
1	C	510	VAL	CB-CA-C	-6.09	99.84	111.40
1	E	11	ASP	CB-CA-C	6.09	122.57	110.40
1	E	510	VAL	CB-CA-C	-6.09	99.84	111.40
1	A	510	VAL	CB-CA-C	-6.08	99.84	111.40
1	J	231	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	11	ASP	CB-CA-C	6.08	122.56	110.40
1	D	63	GLU	CA-CB-CG	6.08	126.78	113.40
1	B	11	ASP	CB-CA-C	6.08	122.55	110.40
1	C	219	PHE	CB-CG-CD1	6.08	125.05	120.80
1	N	231	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	206	ASN	CA-CB-CG	6.07	126.76	113.40
1	K	452	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	G	11	ASP	CB-CA-C	6.07	122.54	110.40
1	A	63	GLU	CA-CB-CG	6.07	126.75	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	510	VAL	CB-CA-C	-6.07	99.88	111.40
1	A	11	ASP	CB-CA-C	6.06	122.52	110.40
1	J	452	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	F	219	PHE	CB-CG-CD1	6.05	125.04	120.80
1	J	43	SER	N-CA-CB	6.05	119.58	110.50
1	K	43	SER	N-CA-CB	6.05	119.58	110.50
1	F	11	ASP	CB-CA-C	6.05	122.50	110.40
1	F	34	LYS	CB-CA-C	6.05	122.50	110.40
1	I	43	SER	N-CA-CB	6.04	119.57	110.50
1	L	231	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	34	LYS	CB-CA-C	6.04	122.49	110.40
1	G	34	LYS	CB-CA-C	6.04	122.48	110.40
1	H	43	SER	N-CA-CB	6.04	119.56	110.50
1	N	452	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	34	LYS	CB-CA-C	6.03	122.47	110.40
1	J	181	THR	N-CA-CB	6.03	121.76	110.30
1	K	181	THR	N-CA-CB	6.03	121.76	110.30
1	N	181	THR	N-CA-CB	6.03	121.76	110.30
1	D	34	LYS	CB-CA-C	6.03	122.46	110.40
1	K	89	THR	CB-CA-C	-6.03	95.32	111.60
1	E	63	GLU	CA-CB-CG	6.02	126.65	113.40
1	K	52	ASP	CB-CA-C	6.02	122.45	110.40
1	H	181	THR	N-CA-CB	6.02	121.73	110.30
1	B	34	LYS	CB-CA-C	6.02	122.44	110.40
1	M	43	SER	N-CA-CB	6.02	119.52	110.50
1	N	43	SER	N-CA-CB	6.01	119.52	110.50
1	L	181	THR	N-CA-CB	6.01	121.72	110.30
1	J	52	ASP	CB-CA-C	6.01	122.42	110.40
1	L	43	SER	N-CA-CB	6.01	119.51	110.50
1	E	34	LYS	CB-CA-C	6.01	122.42	110.40
1	I	52	ASP	CB-CA-C	6.01	122.42	110.40
1	M	231	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	E	203	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	L	52	ASP	CB-CA-C	5.99	122.38	110.40
1	N	479	ASN	N-CA-CB	5.99	121.38	110.60
1	K	85	ALA	N-CA-CB	-5.99	101.72	110.10
1	M	181	THR	N-CA-CB	5.99	121.68	110.30
1	I	181	THR	N-CA-CB	5.99	121.67	110.30
1	H	231	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	411	VAL	CB-CA-C	-5.98	100.04	111.40
1	J	85	ALA	N-CA-CB	-5.98	101.73	110.10
1	N	85	ALA	N-CA-CB	-5.98	101.73	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	231	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	F	411	VAL	CB-CA-C	-5.97	100.05	111.40
1	H	52	ASP	CB-CA-C	5.97	122.34	110.40
1	E	411	VAL	CB-CA-C	-5.96	100.07	111.40
1	L	85	ALA	N-CA-CB	-5.96	101.75	110.10
1	L	452	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	D	411	VAL	CB-CA-C	-5.96	100.07	111.40
1	H	85	ALA	N-CA-CB	-5.96	101.76	110.10
1	C	411	VAL	CB-CA-C	-5.96	100.08	111.40
1	A	203	TYR	CB-CG-CD2	-5.96	117.43	121.00
1	G	203	TYR	CB-CG-CD2	-5.96	117.43	121.00
1	B	411	VAL	CB-CA-C	-5.95	100.09	111.40
1	N	52	ASP	CB-CA-C	5.95	122.31	110.40
1	I	85	ALA	N-CA-CB	-5.95	101.78	110.10
1	F	261	THR	N-CA-CB	5.94	121.59	110.30
1	G	411	VAL	CB-CA-C	-5.94	100.11	111.40
1	F	203	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	C	261	THR	N-CA-CB	5.92	121.56	110.30
1	B	203	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	G	261	THR	N-CA-CB	5.92	121.54	110.30
1	M	155	ASP	CB-CA-C	5.92	122.23	110.40
1	D	261	THR	N-CA-CB	5.91	121.54	110.30
1	J	353	ILE	CB-CA-C	-5.91	99.77	111.60
1	K	353	ILE	CB-CA-C	-5.90	99.81	111.60
1	M	353	ILE	CB-CA-C	-5.89	99.82	111.60
1	B	261	THR	N-CA-CB	5.89	121.49	110.30
1	C	87	ASP	OD1-CG-OD2	-5.89	112.11	123.30
1	A	261	THR	N-CA-CB	5.89	121.49	110.30
1	N	353	ILE	CB-CA-C	-5.88	99.83	111.60
1	E	261	THR	N-CA-CB	5.88	121.48	110.30
1	I	353	ILE	CB-CA-C	-5.88	99.84	111.60
1	L	353	ILE	CB-CA-C	-5.88	99.84	111.60
1	D	203	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	H	353	ILE	CB-CA-C	-5.87	99.86	111.60
1	N	30	THR	N-CA-CB	5.87	121.46	110.30
1	B	87	ASP	OD1-CG-OD2	-5.87	112.15	123.30
1	J	204	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	I	204	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	K	204	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	E	87	ASP	OD1-CG-OD2	-5.86	112.17	123.30
1	G	87	ASP	OD1-CG-OD2	-5.86	112.17	123.30
1	C	203	TYR	CB-CG-CD2	-5.85	117.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	30	THR	N-CA-CB	5.85	121.42	110.30
1	A	87	ASP	OD1-CG-OD2	-5.85	112.19	123.30
1	E	196	ASP	N-CA-CB	-5.85	100.07	110.60
1	G	196	ASP	N-CA-CB	-5.85	100.07	110.60
1	H	30	THR	N-CA-CB	5.85	121.41	110.30
1	C	196	ASP	N-CA-CB	-5.85	100.08	110.60
1	A	196	ASP	N-CA-CB	-5.84	100.09	110.60
1	F	87	ASP	OD1-CG-OD2	-5.84	112.20	123.30
1	F	196	ASP	N-CA-CB	-5.84	100.09	110.60
1	I	30	THR	N-CA-CB	5.84	121.39	110.30
1	M	204	PHE	CB-CG-CD2	-5.84	116.72	120.80
1	N	204	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	B	196	ASP	N-CA-CB	-5.83	100.11	110.60
1	D	501	ARG	N-CA-CB	-5.83	100.11	110.60
1	G	501	ARG	N-CA-CB	-5.83	100.11	110.60
1	D	58	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	F	501	ARG	N-CA-CB	-5.82	100.12	110.60
1	M	417	VAL	CA-CB-CG2	-5.81	102.18	110.90
1	D	196	ASP	N-CA-CB	-5.81	100.14	110.60
1	I	87	ASP	OD1-CG-OD2	-5.81	112.26	123.30
1	M	87	ASP	OD1-CG-OD2	-5.81	112.26	123.30
1	L	87	ASP	OD1-CG-OD2	-5.81	112.27	123.30
1	B	501	ARG	N-CA-CB	-5.81	100.15	110.60
1	D	87	ASP	OD1-CG-OD2	-5.80	112.27	123.30
1	K	417	VAL	CA-CB-CG2	-5.80	102.19	110.90
1	I	155	ASP	CB-CA-C	5.80	122.00	110.40
1	N	417	VAL	CA-CB-CG2	-5.80	102.19	110.90
1	E	501	ARG	N-CA-CB	-5.80	100.16	110.60
1	I	149	THR	N-CA-CB	5.80	121.32	110.30
1	D	149	THR	N-CA-CB	5.80	121.32	110.30
1	A	501	ARG	N-CA-CB	-5.80	100.17	110.60
1	L	155	ASP	CB-CA-C	5.80	121.99	110.40
1	J	87	ASP	OD1-CG-OD2	-5.79	112.29	123.30
1	L	204	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	C	501	ARG	N-CA-CB	-5.79	100.18	110.60
1	F	58	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	F	149	THR	N-CA-CB	5.79	121.30	110.30
1	H	417	VAL	CA-CB-CG2	-5.79	102.22	110.90
1	H	87	ASP	OD1-CG-OD2	-5.78	112.32	123.30
1	J	417	VAL	CA-CB-CG2	-5.78	102.23	110.90
1	L	149	THR	N-CA-CB	5.78	121.28	110.30
1	A	58	ARG	NE-CZ-NH1	5.78	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	155	ASP	CB-CA-C	5.78	121.95	110.40
1	L	417	VAL	CA-CB-CG2	-5.77	102.24	110.90
1	G	149	THR	N-CA-CB	5.77	121.26	110.30
1	A	149	THR	N-CA-CB	5.76	121.25	110.30
1	N	149	THR	N-CA-CB	5.76	121.24	110.30
1	M	58	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	149	THR	N-CA-CB	5.76	121.24	110.30
1	I	417	VAL	CA-CB-CG2	-5.76	102.26	110.90
1	A	380	LYS	N-CA-CB	-5.75	100.25	110.60
1	C	149	THR	N-CA-CB	5.75	121.22	110.30
1	C	380	LYS	N-CA-CB	-5.75	100.25	110.60
1	B	380	LYS	N-CA-CB	-5.75	100.26	110.60
1	H	149	THR	N-CA-CB	5.75	121.22	110.30
1	H	204	PHE	CB-CG-CD2	-5.75	116.78	120.80
1	G	166	MET	CG-SD-CE	-5.75	91.01	100.20
1	E	149	THR	N-CA-CB	5.74	121.21	110.30
1	B	166	MET	CG-SD-CE	-5.74	91.02	100.20
1	D	166	MET	CG-SD-CE	-5.73	91.03	100.20
1	D	411	VAL	CA-CB-CG2	5.73	119.49	110.90
1	E	380	LYS	N-CA-CB	-5.73	100.29	110.60
1	N	87	ASP	OD1-CG-OD2	-5.73	112.42	123.30
1	A	166	MET	CG-SD-CE	-5.72	91.04	100.20
1	D	380	LYS	N-CA-CB	-5.72	100.30	110.60
1	H	155	ASP	CB-CA-C	5.72	121.84	110.40
1	G	58	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	G	380	LYS	N-CA-CB	-5.71	100.32	110.60
1	N	155	ASP	CB-CA-C	5.71	121.82	110.40
1	C	166	MET	CG-SD-CE	-5.71	91.07	100.20
1	C	411	VAL	CA-CB-CG2	5.71	119.46	110.90
1	F	166	MET	CG-SD-CE	-5.70	91.08	100.20
1	E	166	MET	CG-SD-CE	-5.70	91.08	100.20
1	F	380	LYS	N-CA-CB	-5.70	100.34	110.60
1	L	285	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	411	VAL	CA-CB-CG2	5.69	119.44	110.90
1	F	411	VAL	CA-CB-CG2	5.69	119.43	110.90
1	M	285	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	F	257	GLU	N-CA-CB	-5.68	100.37	110.60
1	C	257	GLU	N-CA-CB	-5.68	100.38	110.60
1	E	257	GLU	N-CA-CB	-5.68	100.38	110.60
1	A	257	GLU	N-CA-CB	-5.67	100.40	110.60
1	B	257	GLU	N-CA-CB	-5.67	100.39	110.60
1	G	411	VAL	CA-CB-CG2	5.67	119.40	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	257	GLU	N-CA-CB	-5.66	100.41	110.60
1	E	58	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	411	VAL	CA-CB-CG2	5.66	119.39	110.90
1	E	411	VAL	CA-CB-CG2	5.66	119.39	110.90
1	G	257	GLU	N-CA-CB	-5.66	100.41	110.60
1	L	412	VAL	CB-CA-C	-5.65	100.67	111.40
1	I	412	VAL	CB-CA-C	-5.65	100.67	111.40
1	K	412	VAL	CB-CA-C	-5.64	100.68	111.40
1	J	412	VAL	CB-CA-C	-5.64	100.68	111.40
1	F	334	ASP	CB-CG-OD1	5.64	123.38	118.30
1	N	412	VAL	CB-CA-C	-5.64	100.68	111.40
1	H	412	VAL	CB-CA-C	-5.63	100.69	111.40
1	M	85	ALA	N-CA-CB	-5.63	102.21	110.10
1	E	334	ASP	CB-CG-OD1	5.63	123.37	118.30
1	K	58	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	M	412	VAL	CB-CA-C	-5.61	100.74	111.40
1	B	58	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	334	ASP	CB-CG-OD1	5.60	123.34	118.30
1	G	334	ASP	CB-CG-OD1	5.59	123.33	118.30
1	K	285	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	K	126	ALA	CB-CA-C	5.59	118.49	110.10
1	I	285	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	J	126	ALA	CB-CA-C	5.59	118.48	110.10
1	M	30	THR	N-CA-CB	5.59	120.92	110.30
1	N	126	ALA	CB-CA-C	5.59	118.48	110.10
1	I	126	ALA	CB-CA-C	5.59	118.48	110.10
1	L	126	ALA	CB-CA-C	5.59	118.48	110.10
1	H	285	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	N	285	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	H	126	ALA	CB-CA-C	5.57	118.45	110.10
1	C	58	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	334	ASP	CB-CG-OD1	5.55	123.30	118.30
1	E	368	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	M	126	ALA	CB-CA-C	5.55	118.43	110.10
1	C	334	ASP	CB-CG-OD1	5.54	123.29	118.30
1	J	166	MET	CG-SD-CE	-5.53	91.36	100.20
1	I	166	MET	CG-SD-CE	-5.50	91.39	100.20
1	I	58	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	N	369	VAL	N-CA-CB	5.49	123.58	111.50
1	H	58	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	N	166	MET	CG-SD-CE	-5.49	91.42	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	294	THR	CA-CB-CG2	-5.49	104.72	112.40
1	J	285	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	C	368	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	H	369	VAL	N-CA-CB	5.48	123.55	111.50
1	F	338	GLU	N-CA-CB	5.47	120.45	110.60
1	K	155	ASP	CB-CA-C	5.47	121.35	110.40
1	C	294	THR	CA-CB-CG2	-5.47	104.74	112.40
1	M	369	VAL	N-CA-CB	5.47	123.53	111.50
1	A	368	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	231	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	J	58	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	E	294	THR	CA-CB-CG2	-5.46	104.75	112.40
1	F	368	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	H	166	MET	CG-SD-CE	-5.46	91.46	100.20
1	M	166	MET	CG-SD-CE	-5.46	91.46	100.20
1	L	369	VAL	N-CA-CB	5.46	123.51	111.50
1	G	368	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	294	THR	CA-CB-CG2	-5.46	104.76	112.40
1	A	338	GLU	N-CA-CB	5.45	120.42	110.60
1	G	294	THR	CA-CB-CG2	-5.45	104.76	112.40
1	J	369	VAL	N-CA-CB	5.45	123.50	111.50
1	B	294	THR	CA-CB-CG2	-5.45	104.77	112.40
1	C	338	GLU	N-CA-CB	5.45	120.41	110.60
1	G	338	GLU	N-CA-CB	5.45	120.41	110.60
1	I	369	VAL	N-CA-CB	5.45	123.49	111.50
1	F	294	THR	CA-CB-CG2	-5.45	104.77	112.40
1	K	369	VAL	N-CA-CB	5.45	123.48	111.50
1	L	166	MET	CG-SD-CE	-5.45	91.49	100.20
1	D	338	GLU	N-CA-CB	5.44	120.40	110.60
1	B	338	GLU	N-CA-CB	5.44	120.39	110.60
1	F	285	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	E	338	GLU	N-CA-CB	5.44	120.39	110.60
1	B	300	VAL	CB-CA-C	-5.43	101.08	111.40
1	K	87	ASP	OD1-CG-OD2	-5.43	112.98	123.30
1	G	285	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	E	231	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	F	300	VAL	CB-CA-C	-5.42	101.10	111.40
1	E	300	VAL	CB-CA-C	-5.42	101.10	111.40
1	B	231	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	H	409	GLU	N-CA-CB	5.42	120.35	110.60
1	C	226	LYS	N-CA-CB	-5.41	100.86	110.60
1	A	231	ARG	NE-CZ-NH1	5.41	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	300	VAL	CB-CA-C	-5.41	101.12	111.40
1	E	226	LYS	N-CA-CB	-5.41	100.86	110.60
1	J	409	GLU	N-CA-CB	5.41	120.34	110.60
1	L	409	GLU	N-CA-CB	5.41	120.33	110.60
1	N	473	ASP	CB-CA-C	5.41	121.21	110.40
1	A	300	VAL	CB-CA-C	-5.41	101.13	111.40
1	D	231	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	G	300	VAL	CB-CA-C	-5.41	101.13	111.40
1	C	300	VAL	CB-CA-C	-5.40	101.14	111.40
1	B	285	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	368	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	K	473	ASP	CB-CA-C	5.39	121.19	110.40
1	L	473	ASP	CB-CA-C	5.39	121.19	110.40
1	G	226	LYS	N-CA-CB	-5.39	100.89	110.60
1	H	506	TYR	CB-CG-CD1	5.39	124.24	121.00
1	N	58	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	N	409	GLU	N-CA-CB	5.39	120.31	110.60
1	I	473	ASP	CB-CA-C	5.39	121.18	110.40
1	H	473	ASP	CB-CA-C	5.38	121.17	110.40
1	I	409	GLU	N-CA-CB	5.38	120.29	110.60
1	K	409	GLU	N-CA-CB	5.38	120.28	110.60
1	M	473	ASP	CB-CA-C	5.38	121.16	110.40
1	J	473	ASP	CB-CA-C	5.38	121.15	110.40
1	F	226	LYS	N-CA-CB	-5.37	100.93	110.60
1	D	368	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	E	285	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	F	231	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	M	409	GLU	N-CA-CB	5.37	120.26	110.60
1	A	226	LYS	N-CA-CB	-5.36	100.95	110.60
1	E	369	VAL	CA-CB-CG2	5.36	118.93	110.90
1	B	369	VAL	CA-CB-CG2	5.34	118.92	110.90
1	M	140	ASP	CB-CG-OD1	5.34	123.11	118.30
1	F	369	VAL	CA-CB-CG2	5.34	118.91	110.90
1	G	369	VAL	CA-CB-CG2	5.34	118.91	110.90
1	D	285	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	I	506	TYR	CB-CG-CD1	5.33	124.20	121.00
1	L	58	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	G	231	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	N	506	TYR	CB-CG-CD1	5.31	124.19	121.00
1	K	166	MET	CG-SD-CE	-5.31	91.71	100.20
1	A	369	VAL	N-CA-CB	5.30	123.16	111.50
1	B	226	LYS	N-CA-CB	-5.30	101.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	190	VAL	CB-CA-C	5.30	121.47	111.40
1	K	140	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	285	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	G	369	VAL	N-CA-CB	5.30	123.15	111.50
1	A	369	VAL	CA-CB-CG2	5.29	118.84	110.90
1	D	369	VAL	CA-CB-CG2	5.29	118.84	110.90
1	L	140	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	369	VAL	N-CA-CB	5.29	123.13	111.50
1	L	196	ASP	N-CA-CB	-5.28	101.09	110.60
1	C	369	VAL	CA-CB-CG2	5.28	118.82	110.90
1	J	506	TYR	CB-CG-CD1	5.28	124.17	121.00
1	M	368	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	E	369	VAL	N-CA-CB	5.28	123.11	111.50
1	B	218	PRO	N-CA-CB	5.28	109.63	103.30
1	A	218	PRO	N-CA-CB	5.28	109.63	103.30
1	N	196	ASP	N-CA-CB	-5.28	101.10	110.60
1	K	196	ASP	N-CA-CB	-5.27	101.11	110.60
1	B	369	VAL	N-CA-CB	5.27	123.10	111.50
1	I	190	VAL	CB-CA-C	5.27	121.42	111.40
1	M	190	VAL	CB-CA-C	5.27	121.42	111.40
1	C	369	VAL	N-CA-CB	5.27	123.09	111.50
1	L	190	VAL	CB-CA-C	5.27	121.41	111.40
1	N	190	VAL	CB-CA-C	5.27	121.41	111.40
1	C	218	PRO	N-CA-CB	5.27	109.62	103.30
1	H	196	ASP	N-CA-CB	-5.26	101.12	110.60
1	J	190	VAL	CB-CA-C	5.26	121.40	111.40
1	F	369	VAL	N-CA-CB	5.26	123.08	111.50
1	J	196	ASP	N-CA-CB	-5.26	101.13	110.60
1	L	268	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	H	140	ASP	CB-CG-OD1	5.26	123.03	118.30
1	K	190	VAL	CB-CA-C	5.26	121.39	111.40
1	D	226	LYS	N-CA-CB	-5.26	101.14	110.60
1	M	196	ASP	N-CA-CB	-5.26	101.14	110.60
1	A	341	ALA	N-CA-CB	5.25	117.45	110.10
1	I	196	ASP	N-CA-CB	-5.25	101.15	110.60
1	D	218	PRO	N-CA-CB	5.25	109.60	103.30
1	E	218	PRO	N-CA-CB	5.24	109.59	103.30
1	A	411	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	F	218	PRO	N-CA-CB	5.24	109.59	103.30
1	D	203	TYR	CB-CG-CD1	5.24	124.14	121.00
1	G	203	TYR	CB-CG-CD1	5.24	124.14	121.00
1	G	218	PRO	N-CA-CB	5.24	109.58	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	203	TYR	CB-CG-CD1	5.23	124.14	121.00
1	F	341	ALA	N-CA-CB	5.23	117.43	110.10
1	C	411	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	D	411	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	E	411	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	F	411	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	J	368	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	F	203	TYR	CB-CG-CD1	5.23	124.14	121.00
1	L	284	ARG	CB-CA-C	-5.23	99.94	110.40
1	C	203	TYR	CB-CG-CD1	5.23	124.14	121.00
1	G	341	ALA	N-CA-CB	5.23	117.42	110.10
1	I	284	ARG	CB-CA-C	-5.23	99.94	110.40
1	H	284	ARG	CB-CA-C	-5.23	99.95	110.40
1	K	284	ARG	CB-CA-C	-5.22	99.95	110.40
1	C	285	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	203	TYR	CB-CG-CD1	5.22	124.13	121.00
1	G	243	ALA	N-CA-CB	5.22	117.41	110.10
1	M	284	ARG	CB-CA-C	-5.22	99.97	110.40
1	N	284	ARG	CB-CA-C	-5.21	99.97	110.40
1	I	320	ALA	N-CA-CB	5.21	117.40	110.10
1	J	284	ARG	CB-CA-C	-5.21	99.98	110.40
1	J	320	ALA	N-CA-CB	5.21	117.39	110.10
1	K	320	ALA	N-CA-CB	5.21	117.39	110.10
1	H	140	ASP	CA-CB-CG	5.21	124.85	113.40
1	L	320	ALA	N-CA-CB	5.21	117.39	110.10
1	B	411	VAL	CG1-CB-CG2	-5.20	102.57	110.90
1	E	341	ALA	N-CA-CB	5.20	117.39	110.10
1	J	268	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	341	ALA	N-CA-CB	5.20	117.38	110.10
1	D	341	ALA	N-CA-CB	5.20	117.38	110.10
1	C	341	ALA	N-CA-CB	5.20	117.37	110.10
1	H	320	ALA	N-CA-CB	5.20	117.37	110.10
1	N	320	ALA	N-CA-CB	5.19	117.37	110.10
1	N	495	ASP	CB-CA-C	-5.19	100.01	110.40
1	G	411	VAL	CG1-CB-CG2	-5.19	102.60	110.90
1	A	284	ARG	CB-CA-C	-5.19	100.02	110.40
1	M	320	ALA	N-CA-CB	5.18	117.36	110.10
1	H	368	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	284	ARG	CB-CA-C	-5.18	100.04	110.40
1	F	284	ARG	CB-CA-C	-5.18	100.04	110.40
1	B	243	ALA	N-CA-CB	5.17	117.34	110.10
1	D	284	ARG	CB-CA-C	-5.17	100.06	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	284	ARG	CB-CA-C	-5.17	100.06	110.40
1	G	284	ARG	CB-CA-C	-5.17	100.06	110.40
1	H	268	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	L	140	ASP	CA-CB-CG	5.17	124.78	113.40
1	F	243	ALA	N-CA-CB	5.17	117.34	110.10
1	B	203	TYR	CB-CG-CD1	5.17	124.10	121.00
1	D	18	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	K	140	ASP	CA-CB-CG	5.16	124.74	113.40
1	A	243	ALA	N-CA-CB	5.15	117.32	110.10
1	M	140	ASP	CA-CB-CG	5.15	124.74	113.40
1	L	368	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	205	ILE	CB-CA-C	5.15	121.90	111.60
1	K	368	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	284	ARG	CB-CA-C	-5.15	100.10	110.40
1	E	243	ALA	N-CA-CB	5.15	117.31	110.10
1	L	361	ASP	CB-CA-C	5.15	120.69	110.40
1	M	361	ASP	CB-CA-C	5.15	120.69	110.40
1	J	361	ASP	CB-CA-C	5.14	120.69	110.40
1	B	205	ILE	CB-CA-C	5.14	121.89	111.60
1	K	361	ASP	CB-CA-C	5.14	120.69	110.40
1	D	243	ALA	N-CA-CB	5.14	117.29	110.10
1	I	268	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	E	205	ILE	CB-CA-C	5.14	121.87	111.60
1	C	205	ILE	CB-CA-C	5.13	121.86	111.60
1	C	243	ALA	N-CA-CB	5.13	117.28	110.10
1	F	284	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	G	205	ILE	CB-CA-C	5.13	121.86	111.60
1	N	361	ASP	CB-CA-C	5.13	120.66	110.40
1	F	205	ILE	CB-CA-C	5.13	121.86	111.60
1	N	268	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	H	361	ASP	CB-CA-C	5.12	120.65	110.40
1	I	361	ASP	CB-CA-C	5.12	120.64	110.40
1	B	106	ALA	CB-CA-C	5.12	117.78	110.10
1	C	106	ALA	CB-CA-C	5.12	117.78	110.10
1	D	205	ILE	CB-CA-C	5.12	121.84	111.60
1	G	106	ALA	CB-CA-C	5.12	117.78	110.10
1	A	106	ALA	CB-CA-C	5.11	117.77	110.10
1	M	104	LEU	CB-CA-C	5.11	119.91	110.20
1	N	368	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	284	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	E	106	ALA	CB-CA-C	5.11	117.76	110.10
1	L	104	LEU	CB-CA-C	5.11	119.90	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	F	106	ALA	CB-CA-C	5.09	117.74	110.10
1	M	268	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	K	104	LEU	CB-CA-C	5.08	119.86	110.20
1	J	104	LEU	CB-CA-C	5.08	119.85	110.20
1	N	104	LEU	CB-CA-C	5.08	119.86	110.20
1	D	106	ALA	CB-CA-C	5.08	117.72	110.10
1	E	18	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	I	104	LEU	CB-CA-C	5.08	119.85	110.20
1	K	268	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	J	204	PHE	CB-CG-CD1	5.07	124.35	120.80
1	H	104	LEU	CB-CA-C	5.07	119.83	110.20
1	N	369	VAL	CB-CA-C	-5.07	101.77	111.40
1	G	18	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	I	369	VAL	CB-CA-C	-5.06	101.78	111.40
1	I	204	PHE	CB-CG-CD1	5.05	124.34	120.80
1	K	369	VAL	CB-CA-C	-5.04	101.82	111.40
1	L	369	VAL	CB-CA-C	-5.04	101.83	111.40
1	M	369	VAL	CB-CA-C	-5.04	101.83	111.40
1	H	369	VAL	CB-CA-C	-5.03	101.83	111.40
1	A	322	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	J	369	VAL	CB-CA-C	-5.03	101.85	111.40
1	M	501	ARG	N-CA-CB	-5.03	101.55	110.60
1	L	501	ARG	N-CA-CB	-5.03	101.56	110.60
1	I	368	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	G	322	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	361	ASP	CB-CA-C	5.01	120.43	110.40
1	N	501	ARG	N-CA-CB	-5.01	101.58	110.60
1	H	106	ALA	CB-CA-C	5.01	117.61	110.10
1	A	361	ASP	CB-CA-C	5.01	120.42	110.40
1	B	153	ASN	CB-CA-C	5.01	120.41	110.40
1	G	361	ASP	CB-CA-C	5.01	120.41	110.40
1	D	361	ASP	CB-CA-C	5.00	120.41	110.40
1	F	361	ASP	CB-CA-C	5.00	120.41	110.40
1	C	361	ASP	CB-CA-C	5.00	120.40	110.40
1	K	501	ARG	N-CA-CB	-5.00	101.60	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	N	479	ASN	CA

All (140) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Sidechain
1	A	18	ARG	Sidechain
1	A	197	ARG	Sidechain
1	A	345	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	368	ARG	Sidechain
1	A	395	ARG	Sidechain
1	A	404	ARG	Sidechain
1	A	445	ARG	Sidechain
1	B	118	ARG	Sidechain
1	B	18	ARG	Sidechain
1	B	197	ARG	Sidechain
1	B	345	ARG	Sidechain
1	B	350	ARG	Sidechain
1	B	362	ARG	Sidechain
1	B	368	ARG	Sidechain
1	B	395	ARG	Sidechain
1	B	404	ARG	Sidechain
1	B	445	ARG	Sidechain
1	C	118	ARG	Sidechain
1	C	18	ARG	Sidechain
1	C	197	ARG	Sidechain
1	C	345	ARG	Sidechain
1	C	350	ARG	Sidechain
1	C	362	ARG	Sidechain
1	C	368	ARG	Sidechain
1	C	395	ARG	Sidechain
1	C	404	ARG	Sidechain
1	C	445	ARG	Sidechain
1	D	118	ARG	Sidechain
1	D	18	ARG	Sidechain
1	D	197	ARG	Sidechain
1	D	345	ARG	Sidechain
1	D	350	ARG	Sidechain
1	D	362	ARG	Sidechain
1	D	368	ARG	Sidechain
1	D	395	ARG	Sidechain
1	D	404	ARG	Sidechain
1	D	445	ARG	Sidechain
1	E	118	ARG	Sidechain
1	E	18	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	197	ARG	Sidechain
1	E	345	ARG	Sidechain
1	E	350	ARG	Sidechain
1	E	362	ARG	Sidechain
1	E	368	ARG	Sidechain
1	E	395	ARG	Sidechain
1	E	404	ARG	Sidechain
1	E	445	ARG	Sidechain
1	F	118	ARG	Sidechain
1	F	18	ARG	Sidechain
1	F	197	ARG	Sidechain
1	F	345	ARG	Sidechain
1	F	350	ARG	Sidechain
1	F	362	ARG	Sidechain
1	F	368	ARG	Sidechain
1	F	395	ARG	Sidechain
1	F	404	ARG	Sidechain
1	F	445	ARG	Sidechain
1	G	118	ARG	Sidechain
1	G	18	ARG	Sidechain
1	G	197	ARG	Sidechain
1	G	345	ARG	Sidechain
1	G	350	ARG	Sidechain
1	G	362	ARG	Sidechain
1	G	368	ARG	Sidechain
1	G	395	ARG	Sidechain
1	G	404	ARG	Sidechain
1	G	445	ARG	Sidechain
1	H	118	ARG	Sidechain
1	H	197	ARG	Sidechain
1	H	268	ARG	Sidechain
1	H	36	ARG	Sidechain
1	H	362	ARG	Sidechain
1	H	395	ARG	Sidechain
1	H	404	ARG	Sidechain
1	H	445	ARG	Sidechain
1	H	478	TYR	Sidechain
1	H	483	GLU	Sidechain
1	I	118	ARG	Sidechain
1	I	197	ARG	Sidechain
1	I	268	ARG	Sidechain
1	I	36	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	362	ARG	Sidechain
1	I	395	ARG	Sidechain
1	I	404	ARG	Sidechain
1	I	445	ARG	Sidechain
1	I	478	TYR	Sidechain
1	I	483	GLU	Sidechain
1	J	118	ARG	Sidechain
1	J	197	ARG	Sidechain
1	J	268	ARG	Sidechain
1	J	36	ARG	Sidechain
1	J	362	ARG	Sidechain
1	J	395	ARG	Sidechain
1	J	404	ARG	Sidechain
1	J	445	ARG	Sidechain
1	J	478	TYR	Sidechain
1	J	483	GLU	Sidechain
1	K	118	ARG	Sidechain
1	K	197	ARG	Sidechain
1	K	268	ARG	Sidechain
1	K	36	ARG	Sidechain
1	K	362	ARG	Sidechain
1	K	395	ARG	Sidechain
1	K	404	ARG	Sidechain
1	K	445	ARG	Sidechain
1	K	478	TYR	Sidechain
1	K	483	GLU	Sidechain
1	L	118	ARG	Sidechain
1	L	197	ARG	Sidechain
1	L	268	ARG	Sidechain
1	L	36	ARG	Sidechain
1	L	362	ARG	Sidechain
1	L	395	ARG	Sidechain
1	L	404	ARG	Sidechain
1	L	445	ARG	Sidechain
1	L	478	TYR	Sidechain
1	L	483	GLU	Sidechain
1	M	118	ARG	Sidechain
1	M	197	ARG	Sidechain
1	M	268	ARG	Sidechain
1	M	36	ARG	Sidechain
1	M	362	ARG	Sidechain
1	M	395	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	M	404	ARG	Sidechain
1	M	445	ARG	Sidechain
1	M	478	TYR	Sidechain
1	M	58	ARG	Sidechain
1	N	118	ARG	Sidechain
1	N	197	ARG	Sidechain
1	N	268	ARG	Sidechain
1	N	36	ARG	Sidechain
1	N	362	ARG	Sidechain
1	N	395	ARG	Sidechain
1	N	404	ARG	Sidechain
1	N	445	ARG	Sidechain
1	N	478	TYR	Sidechain
1	N	483	GLU	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	3846	0	3970	127	0
1	B	3846	0	3970	126	0
1	C	3846	0	3970	125	0
1	D	3846	0	3970	122	0
1	E	3846	0	3970	122	0
1	F	3846	0	3970	123	0
1	G	3846	0	3970	123	0
1	H	3846	0	3968	86	0
1	I	3846	0	3968	89	0
1	J	3846	0	3968	88	0
1	K	3846	0	3968	89	0
1	L	3846	0	3968	87	0
1	M	3846	0	3968	108	0
1	N	3846	0	3968	87	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	1	0	0	5	0
3	B	1	0	0	5	0
3	C	1	0	0	5	0
3	D	1	0	0	5	0
3	E	1	0	0	4	0
3	F	1	0	0	5	0
3	G	1	0	0	4	0
3	H	1	0	0	5	0
3	I	1	0	0	5	0
3	J	1	0	0	5	0
3	K	1	0	0	5	0
3	L	1	0	0	5	0
3	M	1	0	0	5	0
3	N	1	0	0	4	0
4	A	31	12	12	4	0
4	B	31	12	12	4	0
4	C	31	12	12	4	0
4	D	31	12	12	4	0
4	E	31	12	12	3	0
4	F	31	12	12	4	0
4	G	31	12	12	3	0
4	H	31	12	12	4	0
4	I	31	12	12	5	0
4	J	31	12	12	5	0
4	K	31	12	12	5	0
4	L	31	12	12	5	0
4	M	31	12	12	34	0
4	N	31	12	12	5	0
All	All	54306	168	55734	1536	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1536) 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)
4:M:1527:ATP:C4	4:M:1527:ATP:C5	1.93	1.55
4:M:1527:ATP:C8	4:M:1527:ATP:N7	1.72	1.54
4:M:1527:ATP:N7	4:M:1527:ATP:C5	1.93	1.37
4:M:1527:ATP:C8	4:M:1527:ATP:N9	1.94	1.36
4:M:1527:ATP:C4	4:M:1527:ATP:N9	2.02	1.26
1:M:493:ILE:CD1	4:M:1527:ATP:C4	2.28	1.17
1:M:493:ILE:CD1	4:M:1527:ATP:C5	2.27	1.16
1:M:493:ILE:CG1	4:M:1527:ATP:C4	2.29	1.15
1:M:493:ILE:CD1	4:M:1527:ATP:C8	2.31	1.13
1:M:493:ILE:CG1	4:M:1527:ATP:C5	2.30	1.13
1:M:493:ILE:CG1	4:M:1527:ATP:C8	2.33	1.11
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.35	1.08
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.42	1.02
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.42	1.02
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.42	1.02
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.42	1.01
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.42	1.01
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.42	1.01
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.42	1.01
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.49	0.94
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.49	0.93
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.49	0.93
1:M:493:ILE:CD1	4:M:1527:ATP:N9	2.32	0.93
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.49	0.92
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.50	0.91
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.51	0.91
1:B:4:LYS:H	1:C:63:GLU:HB2	1.38	0.89
1:M:493:ILE:CG1	4:M:1527:ATP:N9	2.37	0.88
1:D:4:LYS:H	1:E:63:GLU:HB2	1.38	0.88
1:A:63:GLU:HB2	1:G:4:LYS:H	1.38	0.88
1:C:4:LYS:H	1:D:63:GLU:HB2	1.37	0.88
1:M:493:ILE:CD1	4:M:1527:ATP:N7	2.36	0.88
1:E:4:LYS:H	1:F:63:GLU:HB2	1.37	0.87
1:N:37:ASN:C	1:N:50:THR:O	2.13	0.87
1:I:37:ASN:C	1:I:50:THR:O	2.13	0.87
1:H:37:ASN:C	1:H:50:THR:O	2.13	0.87
1:A:4:LYS:H	1:B:63:GLU:HB2	1.37	0.86
1:M:37:ASN:C	1:M:50:THR:O	2.13	0.86
1:K:37:ASN:C	1:K:50:THR:O	2.13	0.86
1:F:4:LYS:H	1:G:63:GLU:HB2	1.38	0.86
1:L:37:ASN:C	1:L:50:THR:O	2.13	0.86
1:J:37:ASN:C	1:J:50:THR:O	2.13	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:493:ILE:HD12	4:M:1527:ATP:C4	2.10	0.85
1:M:493:ILE:HG13	4:M:1527:ATP:C5	2.10	0.84
1:M:493:ILE:HD13	4:M:1527:ATP:C8	2.12	0.83
1:M:493:ILE:CG1	4:M:1527:ATP:N7	2.41	0.83
1:C:183:LEU:O	1:C:382:GLY:HA3	1.82	0.80
1:B:183:LEU:O	1:B:382:GLY:HA3	1.82	0.80
1:D:183:LEU:O	1:D:382:GLY:HA3	1.82	0.80
1:A:183:LEU:O	1:A:382:GLY:HA3	1.82	0.80
1:K:183:LEU:O	1:K:382:GLY:HA3	1.82	0.80
1:L:183:LEU:O	1:L:382:GLY:HA3	1.82	0.80
1:F:183:LEU:O	1:F:382:GLY:HA3	1.82	0.79
1:E:183:LEU:O	1:E:382:GLY:HA3	1.82	0.79
1:G:183:LEU:O	1:G:382:GLY:HA3	1.82	0.79
1:J:183:LEU:O	1:J:382:GLY:HA3	1.82	0.79
1:M:183:LEU:O	1:M:382:GLY:HA3	1.82	0.79
1:M:493:ILE:HD11	4:M:1527:ATP:C5	2.16	0.78
1:N:183:LEU:O	1:N:382:GLY:HA3	1.82	0.78
1:H:183:LEU:O	1:H:382:GLY:HA3	1.82	0.78
1:L:135:SER:HA	1:L:412:VAL:HG12	1.66	0.78
1:M:135:SER:HA	1:M:412:VAL:HG12	1.66	0.78
1:K:135:SER:HA	1:K:412:VAL:HG12	1.66	0.78
1:I:183:LEU:O	1:I:382:GLY:HA3	1.82	0.78
1:N:135:SER:HA	1:N:412:VAL:HG12	1.66	0.77
3:F:1527:PO4:P	4:F:1528:ATP:O1G	2.43	0.77
3:D:1527:PO4:P	4:D:1528:ATP:O1G	2.43	0.77
3:A:1527:PO4:P	4:A:1528:ATP:O1G	2.43	0.77
3:E:1527:PO4:P	4:E:1528:ATP:O1G	2.43	0.77
1:J:135:SER:HA	1:J:412:VAL:HG12	1.66	0.77
3:G:1527:PO4:P	4:G:1528:ATP:O1G	2.43	0.77
1:H:135:SER:HA	1:H:412:VAL:HG12	1.66	0.77
1:K:199:TYR:CD2	1:K:205:ILE:HD11	2.21	0.76
1:I:135:SER:HA	1:I:412:VAL:HG12	1.66	0.76
1:K:198:GLY:HA2	1:K:327:LYS:O	1.86	0.76
1:M:198:GLY:HA2	1:M:327:LYS:O	1.86	0.76
1:J:199:TYR:CD2	1:J:205:ILE:HD11	2.21	0.76
1:L:199:TYR:CD2	1:L:205:ILE:HD11	2.21	0.76
3:C:1527:PO4:P	4:C:1528:ATP:O1G	2.43	0.76
3:B:1527:PO4:P	4:B:1528:ATP:O1G	2.43	0.76
1:N:199:TYR:CD2	1:N:205:ILE:HD11	2.21	0.76
1:M:199:TYR:CD2	1:M:205:ILE:HD11	2.21	0.76
1:I:199:TYR:CD2	1:I:205:ILE:HD11	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:TYR:CD2	1:H:205:ILE:HD11	2.21	0.76
1:D:138:CYS:N	1:D:410:GLY:HA2	2.01	0.75
1:E:138:CYS:N	1:E:410:GLY:HA2	2.01	0.75
1:C:138:CYS:N	1:C:410:GLY:HA2	2.01	0.75
1:J:198:GLY:HA2	1:J:327:LYS:O	1.86	0.75
1:A:138:CYS:N	1:A:410:GLY:HA2	2.01	0.75
1:B:138:CYS:N	1:B:410:GLY:HA2	2.01	0.75
1:G:138:CYS:N	1:G:410:GLY:HA2	2.01	0.75
1:L:198:GLY:HA2	1:L:327:LYS:O	1.86	0.75
1:H:198:GLY:HA2	1:H:327:LYS:O	1.86	0.74
1:I:198:GLY:HA2	1:I:327:LYS:O	1.86	0.74
1:N:198:GLY:HA2	1:N:327:LYS:O	1.86	0.74
1:F:138:CYS:N	1:F:410:GLY:HA2	2.01	0.74
1:F:127:ALA:HB2	1:F:426:LEU:HD11	1.69	0.74
1:A:127:ALA:HB2	1:A:426:LEU:HD11	1.69	0.74
1:B:127:ALA:HB2	1:B:426:LEU:HD11	1.69	0.74
1:C:127:ALA:HB2	1:C:426:LEU:HD11	1.69	0.73
1:G:127:ALA:HB2	1:G:426:LEU:HD11	1.69	0.73
1:E:147:VAL:HG22	1:E:494:LEU:HD11	1.71	0.73
1:B:147:VAL:HG22	1:B:494:LEU:HD11	1.71	0.73
1:D:127:ALA:HB2	1:D:426:LEU:HD11	1.69	0.73
1:F:147:VAL:HG22	1:F:494:LEU:HD11	1.71	0.73
1:E:127:ALA:HB2	1:E:426:LEU:HD11	1.69	0.73
3:J:1526:PO4:P	4:J:1527:ATP:O1G	2.47	0.73
1:C:147:VAL:HG22	1:C:494:LEU:HD11	1.71	0.73
1:D:147:VAL:HG22	1:D:494:LEU:HD11	1.71	0.73
1:A:147:VAL:HG22	1:A:494:LEU:HD11	1.71	0.73
1:G:147:VAL:HG22	1:G:494:LEU:HD11	1.71	0.72
3:L:1526:PO4:P	4:L:1527:ATP:O1G	2.47	0.72
1:B:214:GLU:HA	1:B:323:VAL:O	1.90	0.72
1:E:214:GLU:HA	1:E:323:VAL:O	1.90	0.72
1:F:214:GLU:HA	1:F:323:VAL:O	1.90	0.72
1:B:29:VAL:O	1:B:35:GLY:HA3	1.90	0.72
3:I:1526:PO4:P	4:I:1527:ATP:O1G	2.48	0.72
1:D:214:GLU:HA	1:D:323:VAL:O	1.90	0.72
1:A:214:GLU:HA	1:A:323:VAL:O	1.90	0.72
1:G:214:GLU:HA	1:G:323:VAL:O	1.90	0.72
1:F:138:CYS:HA	1:F:411:VAL:HG13	1.72	0.71
1:D:29:VAL:O	1:D:35:GLY:HA3	1.90	0.71
1:G:138:CYS:HA	1:G:411:VAL:HG13	1.73	0.71
1:E:138:CYS:HA	1:E:411:VAL:HG13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:CYS:HA	1:A:411:VAL:HG13	1.73	0.71
1:E:29:VAL:O	1:E:35:GLY:HA3	1.90	0.71
1:F:29:VAL:O	1:F:35:GLY:HA3	1.90	0.71
1:C:214:GLU:HA	1:C:323:VAL:O	1.90	0.70
1:G:29:VAL:O	1:G:35:GLY:HA3	1.90	0.70
1:L:191:GLU:O	1:L:334:ASP:HA	1.92	0.70
1:C:29:VAL:O	1:C:35:GLY:HA3	1.90	0.70
3:N:1526:PO4:P	4:N:1527:ATP:O1A	2.50	0.70
1:K:191:GLU:O	1:K:334:ASP:HA	1.92	0.70
1:M:31:LEU:HB3	1:M:90:THR:HG21	1.73	0.70
1:B:138:CYS:HA	1:B:411:VAL:HG13	1.73	0.70
1:D:198:GLY:HA2	1:D:327:LYS:O	1.92	0.70
1:M:191:GLU:O	1:M:334:ASP:HA	1.92	0.70
1:J:191:GLU:O	1:J:334:ASP:HA	1.92	0.70
1:M:493:ILE:HG13	4:M:1527:ATP:C4	2.26	0.69
3:H:1526:PO4:P	4:H:1527:ATP:O1A	2.50	0.69
3:H:1526:PO4:P	4:H:1527:ATP:O1G	2.49	0.69
1:E:198:GLY:HA2	1:E:327:LYS:O	1.92	0.69
1:A:29:VAL:O	1:A:35:GLY:HA3	1.90	0.69
1:G:199:TYR:CD2	1:G:205:ILE:HD11	2.28	0.69
1:M:31:LEU:CB	1:M:90:THR:HG21	2.22	0.69
1:C:198:GLY:HA2	1:C:327:LYS:O	1.92	0.69
1:A:199:TYR:CD2	1:A:205:ILE:HD11	2.28	0.69
1:E:31:LEU:HA	3:E:1527:PO4:P	2.32	0.69
1:D:138:CYS:HA	1:D:411:VAL:HG13	1.73	0.69
1:A:31:LEU:HA	3:A:1527:PO4:P	2.32	0.69
1:F:199:TYR:CD2	1:F:205:ILE:HD11	2.28	0.69
1:G:31:LEU:HA	3:G:1527:PO4:P	2.32	0.69
3:N:1526:PO4:P	4:N:1527:ATP:O1G	2.50	0.69
1:N:191:GLU:O	1:N:334:ASP:HA	1.92	0.69
1:G:198:GLY:HA2	1:G:327:LYS:O	1.92	0.69
1:F:198:GLY:HA2	1:F:327:LYS:O	1.92	0.69
1:B:31:LEU:HA	3:B:1527:PO4:P	2.32	0.69
1:D:31:LEU:HA	3:D:1527:PO4:P	2.33	0.69
1:B:199:TYR:CD2	1:B:205:ILE:HD11	2.28	0.69
1:F:31:LEU:HA	3:F:1527:PO4:P	2.32	0.69
1:C:138:CYS:HA	1:C:411:VAL:HG13	1.73	0.69
1:B:198:GLY:HA2	1:B:327:LYS:O	1.92	0.69
3:M:1526:PO4:P	4:M:1527:ATP:O3G	2.51	0.68
1:A:198:GLY:HA2	1:A:327:LYS:O	1.92	0.68
1:C:31:LEU:HA	3:C:1527:PO4:P	2.32	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:TYR:CD2	1:E:205:ILE:HD11	2.28	0.68
1:I:191:GLU:O	1:I:334:ASP:HA	1.92	0.68
1:H:191:GLU:O	1:H:334:ASP:HA	1.92	0.68
3:L:1526:PO4:P	4:L:1527:ATP:O1A	2.52	0.68
3:J:1526:PO4:P	4:J:1527:ATP:O1A	2.52	0.68
1:C:199:TYR:CD2	1:C:205:ILE:HD11	2.28	0.68
1:M:493:ILE:HG12	4:M:1527:ATP:C8	2.27	0.67
3:I:1526:PO4:P	4:I:1527:ATP:O1A	2.52	0.67
1:D:199:TYR:CD2	1:D:205:ILE:HD11	2.28	0.67
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.77	0.67
1:F:180:GLY:HA2	1:F:380:LYS:HB3	1.77	0.67
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.77	0.67
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.77	0.66
1:C:180:GLY:HA2	1:C:380:LYS:HB3	1.77	0.66
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.78	0.66
3:K:1526:PO4:P	4:K:1527:ATP:O1G	2.53	0.66
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.77	0.66
1:C:27:VAL:HG12	1:C:90:THR:CG2	2.24	0.66
1:D:135:SER:HA	1:D:412:VAL:HG12	1.77	0.66
1:C:138:CYS:CB	1:C:407:VAL:HA	2.27	0.65
1:B:138:CYS:CB	1:B:407:VAL:HA	2.26	0.65
1:B:135:SER:HA	1:B:412:VAL:HG12	1.77	0.65
1:L:180:GLY:HA2	1:L:380:LYS:HB3	1.78	0.65
1:E:135:SER:HA	1:E:412:VAL:HG12	1.77	0.65
3:M:1526:PO4:P	4:M:1527:ATP:O1A	2.54	0.65
1:N:37:ASN:C	1:N:50:THR:C	2.55	0.65
1:G:138:CYS:CB	1:G:407:VAL:HA	2.27	0.65
1:A:135:SER:HA	1:A:412:VAL:HG12	1.77	0.65
1:H:37:ASN:C	1:H:50:THR:C	2.55	0.65
1:J:37:ASN:C	1:J:50:THR:C	2.55	0.65
1:A:138:CYS:CB	1:A:407:VAL:HA	2.27	0.65
1:K:180:GLY:HA2	1:K:380:LYS:HB3	1.78	0.65
1:M:180:GLY:HA2	1:M:380:LYS:HB3	1.78	0.65
1:F:138:CYS:CB	1:F:407:VAL:HA	2.26	0.65
1:E:138:CYS:CB	1:E:407:VAL:HA	2.26	0.65
1:C:135:SER:HA	1:C:412:VAL:HG12	1.77	0.65
1:N:180:GLY:HA2	1:N:380:LYS:HB3	1.78	0.65
1:I:37:ASN:C	1:I:50:THR:C	2.55	0.65
1:L:37:ASN:C	1:L:50:THR:C	2.55	0.65
1:F:135:SER:HA	1:F:412:VAL:HG12	1.77	0.65
1:M:37:ASN:C	1:M:50:THR:C	2.55	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:ASN:C	1:K:50:THR:C	2.55	0.65
1:B:206:ASN:HB2	1:B:213:VAL:HA	1.79	0.65
1:G:135:SER:HA	1:G:412:VAL:HG12	1.77	0.65
1:A:206:ASN:HB2	1:A:213:VAL:HA	1.79	0.65
1:D:138:CYS:CB	1:D:407:VAL:HA	2.26	0.64
1:C:206:ASN:HB2	1:C:213:VAL:HA	1.79	0.64
1:N:27:VAL:HG12	1:N:90:THR:CG2	2.26	0.64
1:J:180:GLY:HA2	1:J:380:LYS:HB3	1.78	0.64
1:G:206:ASN:HB2	1:G:213:VAL:HA	1.79	0.64
1:D:27:VAL:HG12	1:D:90:THR:CG2	2.24	0.64
1:H:180:GLY:HA2	1:H:380:LYS:HB3	1.78	0.64
1:H:27:VAL:HG12	1:H:90:THR:CG2	2.26	0.64
1:F:206:ASN:HB2	1:F:213:VAL:HA	1.79	0.64
1:I:180:GLY:HA2	1:I:380:LYS:HB3	1.78	0.64
3:E:1527:PO4:P	4:E:1528:ATP:O1A	2.57	0.63
1:I:27:VAL:HG12	1:I:90:THR:CG2	2.26	0.63
1:D:206:ASN:HB2	1:D:213:VAL:HA	1.79	0.63
1:M:493:ILE:HG12	4:M:1527:ATP:N7	2.11	0.63
3:C:1527:PO4:P	4:C:1528:ATP:O1A	2.57	0.63
1:L:27:VAL:HG12	1:L:90:THR:CG2	2.26	0.63
1:J:27:VAL:HG12	1:J:90:THR:CG2	2.27	0.63
3:B:1527:PO4:P	4:B:1528:ATP:O1A	2.57	0.63
3:D:1527:PO4:P	4:D:1528:ATP:O1A	2.57	0.63
1:E:206:ASN:HB2	1:E:213:VAL:HA	1.79	0.63
3:F:1527:PO4:P	4:F:1528:ATP:O1A	2.57	0.62
3:A:1527:PO4:P	4:A:1528:ATP:O1A	2.57	0.62
3:G:1527:PO4:P	4:G:1528:ATP:O1A	2.57	0.62
1:E:411:VAL:HG12	1:E:494:LEU:HD13	1.81	0.62
1:E:27:VAL:HG12	1:E:90:THR:CG2	2.24	0.62
1:A:149:THR:HA	1:A:152:ALA:HB3	1.82	0.62
1:B:149:THR:HA	1:B:152:ALA:HB3	1.82	0.62
1:J:31:LEU:HB3	1:J:90:THR:HG21	1.82	0.62
1:D:411:VAL:HG12	1:D:494:LEU:HD13	1.81	0.62
1:C:149:THR:HA	1:C:152:ALA:HB3	1.82	0.62
1:G:149:THR:HA	1:G:152:ALA:HB3	1.82	0.62
1:E:149:THR:HA	1:E:152:ALA:HB3	1.82	0.62
1:L:37:ASN:O	1:L:38:VAL:N	2.33	0.62
1:F:411:VAL:HG12	1:F:494:LEU:HD13	1.81	0.62
1:D:149:THR:HA	1:D:152:ALA:HB3	1.82	0.62
1:F:149:THR:HA	1:F:152:ALA:HB3	1.82	0.62
1:N:37:ASN:O	1:N:38:VAL:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:ASN:O	1:I:38:VAL:N	2.33	0.61
1:F:3:ALA:HA	1:G:63:GLU:CA	2.31	0.61
1:L:31:LEU:HB3	1:L:90:THR:HG21	1.82	0.61
1:B:411:VAL:HG12	1:B:494:LEU:HD13	1.81	0.61
1:A:63:GLU:CA	1:G:3:ALA:HA	2.31	0.61
1:B:26:ALA:O	1:B:30:THR:HG23	2.00	0.61
1:D:26:ALA:O	1:D:30:THR:HG23	2.01	0.61
1:K:37:ASN:O	1:K:38:VAL:N	2.33	0.61
1:F:27:VAL:HG12	1:F:90:THR:CG2	2.24	0.61
1:I:31:LEU:HB3	1:I:90:THR:HG21	1.82	0.61
1:E:3:ALA:HA	1:F:63:GLU:CA	2.30	0.61
1:A:3:ALA:HA	1:B:63:GLU:CA	2.31	0.61
1:C:411:VAL:HG12	1:C:494:LEU:HD13	1.81	0.61
1:A:411:VAL:HG12	1:A:494:LEU:HD13	1.81	0.61
1:F:26:ALA:O	1:F:30:THR:HG23	2.01	0.61
1:G:26:ALA:O	1:G:30:THR:HG23	2.01	0.61
1:G:411:VAL:HG12	1:G:494:LEU:HD13	1.81	0.61
1:A:26:ALA:O	1:A:30:THR:HG23	2.01	0.61
1:A:27:VAL:HG12	1:A:90:THR:CG2	2.24	0.61
1:M:37:ASN:O	1:M:38:VAL:N	2.33	0.61
1:K:27:VAL:HG12	1:K:90:THR:CG2	2.28	0.60
1:E:26:ALA:O	1:E:30:THR:HG23	2.00	0.60
1:G:130:GLU:HB3	1:G:422:VAL:HG12	1.83	0.60
1:D:3:ALA:HA	1:E:63:GLU:CA	2.31	0.60
1:H:37:ASN:O	1:H:38:VAL:N	2.33	0.60
1:J:37:ASN:O	1:J:38:VAL:N	2.33	0.60
1:H:31:LEU:HB3	1:H:90:THR:HG21	1.82	0.60
1:B:3:ALA:HA	1:C:63:GLU:CA	2.31	0.60
1:C:26:ALA:O	1:C:30:THR:HG23	2.01	0.60
1:A:63:GLU:HA	1:G:3:ALA:HA	1.84	0.60
1:C:3:ALA:HA	1:D:63:GLU:CA	2.31	0.60
1:I:417:VAL:HG21	1:I:477:GLY:HA3	1.84	0.60
1:G:27:VAL:HG12	1:G:90:THR:CG2	2.24	0.60
1:L:246:PRO:HB3	1:L:272:LYS:HB2	1.84	0.60
1:B:27:VAL:HG12	1:B:90:THR:CG2	2.24	0.60
1:F:3:ALA:HA	1:G:63:GLU:HA	1.84	0.60
1:K:417:VAL:HG21	1:K:477:GLY:HA3	1.84	0.60
1:F:130:GLU:HB3	1:F:422:VAL:HG12	1.83	0.60
1:N:31:LEU:HB3	1:N:90:THR:HG21	1.82	0.60
1:M:417:VAL:HG21	1:M:477:GLY:HA3	1.84	0.60
1:A:130:GLU:HB3	1:A:422:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:417:VAL:HG21	1:H:477:GLY:HA3	1.84	0.60
1:K:246:PRO:HB3	1:K:272:LYS:HB2	1.84	0.60
1:J:417:VAL:HG21	1:J:477:GLY:HA3	1.84	0.59
1:N:417:VAL:HG21	1:N:477:GLY:HA3	1.84	0.59
1:G:30:THR:HG22	1:G:36:ARG:O	2.03	0.59
1:A:30:THR:HG22	1:A:36:ARG:O	2.03	0.59
1:A:3:ALA:HA	1:B:63:GLU:HA	1.84	0.59
1:L:417:VAL:HG21	1:L:477:GLY:HA3	1.84	0.59
1:A:279:PRO:HG3	1:A:292:ILE:HD11	1.85	0.59
1:D:30:THR:HG22	1:D:36:ARG:O	2.03	0.59
1:I:151:SER:HB3	1:I:399:ALA:HA	1.85	0.59
1:G:279:PRO:HG3	1:G:292:ILE:HD11	1.85	0.59
1:F:31:LEU:HB3	1:F:90:THR:HG21	1.85	0.59
1:F:30:THR:HG22	1:F:36:ARG:O	2.03	0.59
1:M:151:SER:HB3	1:M:399:ALA:HA	1.84	0.59
1:B:279:PRO:HG3	1:B:292:ILE:HD11	1.85	0.59
1:C:130:GLU:HB3	1:C:422:VAL:HG12	1.83	0.59
1:G:31:LEU:HB3	1:G:90:THR:HG21	1.85	0.59
1:E:31:LEU:HB3	1:E:90:THR:HG21	1.85	0.59
1:F:279:PRO:HG3	1:F:292:ILE:HD11	1.85	0.59
1:K:31:LEU:HB2	1:K:90:THR:HG21	1.84	0.59
1:M:246:PRO:HB3	1:M:272:LYS:HB2	1.84	0.59
1:D:130:GLU:HB3	1:D:422:VAL:HG12	1.84	0.59
1:A:31:LEU:HB3	1:A:90:THR:HG21	1.85	0.59
1:E:3:ALA:HA	1:F:63:GLU:HA	1.84	0.59
1:E:279:PRO:HG3	1:E:292:ILE:HD11	1.85	0.59
1:H:246:PRO:HB3	1:H:272:LYS:HB2	1.84	0.59
1:J:246:PRO:HB3	1:J:272:LYS:HB2	1.84	0.59
1:K:31:LEU:CB	1:K:90:THR:HG21	2.33	0.59
1:B:3:ALA:HA	1:C:63:GLU:HA	1.84	0.59
1:C:30:THR:HG22	1:C:36:ARG:O	2.03	0.58
1:C:31:LEU:HB3	1:C:90:THR:HG21	1.85	0.58
1:E:130:GLU:HB3	1:E:422:VAL:HG12	1.83	0.58
1:D:31:LEU:HB3	1:D:90:THR:HG21	1.85	0.58
1:E:30:THR:HG22	1:E:36:ARG:O	2.03	0.58
1:B:130:GLU:HB3	1:B:422:VAL:HG12	1.84	0.58
1:H:151:SER:HB3	1:H:399:ALA:HA	1.85	0.58
1:L:151:SER:HB3	1:L:399:ALA:HA	1.85	0.58
1:J:151:SER:CB	1:J:399:ALA:HA	2.34	0.58
1:B:31:LEU:HB3	1:B:90:THR:HG21	1.85	0.58
1:B:30:THR:HG22	1:B:36:ARG:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:151:SER:CB	1:L:399:ALA:HA	2.34	0.58
1:N:246:PRO:HB3	1:N:272:LYS:HB2	1.84	0.58
1:D:279:PRO:HG3	1:D:292:ILE:HD11	1.85	0.58
1:C:279:PRO:HG3	1:C:292:ILE:HD11	1.85	0.58
3:K:1526:PO4:P	4:K:1527:ATP:O1A	2.61	0.58
1:I:246:PRO:HB3	1:I:272:LYS:HB2	1.84	0.58
1:I:151:SER:CB	1:I:399:ALA:HA	2.34	0.58
1:J:151:SER:HB3	1:J:399:ALA:HA	1.85	0.58
1:H:192:GLY:O	1:H:375:GLY:HA2	2.04	0.58
1:C:3:ALA:HA	1:D:63:GLU:HA	1.84	0.57
1:M:214:GLU:HA	1:M:323:VAL:O	2.04	0.57
1:K:214:GLU:HA	1:K:323:VAL:O	2.04	0.57
1:D:3:ALA:HA	1:E:63:GLU:HA	1.84	0.57
1:M:151:SER:CB	1:M:399:ALA:HA	2.34	0.57
1:H:151:SER:CB	1:H:399:ALA:HA	2.34	0.57
1:N:151:SER:HB3	1:N:399:ALA:HA	1.85	0.57
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.86	0.57
1:J:214:GLU:HA	1:J:323:VAL:O	2.04	0.57
1:L:127:ALA:HB2	1:L:426:LEU:HD11	1.87	0.57
1:K:127:ALA:HB2	1:K:426:LEU:HD11	1.86	0.57
3:K:1526:PO4:P	4:K:1527:ATP:O3B	2.63	0.57
1:E:212:ALA:HA	1:E:325:ILE:O	2.05	0.57
1:K:192:GLY:O	1:K:375:GLY:HA2	2.04	0.57
1:L:192:GLY:O	1:L:375:GLY:HA2	2.04	0.57
1:G:417:VAL:HG21	1:G:477:GLY:HA3	1.86	0.57
1:B:417:VAL:HG21	1:B:477:GLY:HA3	1.86	0.57
1:C:417:VAL:HG21	1:C:477:GLY:HA3	1.86	0.57
1:G:212:ALA:HA	1:G:325:ILE:O	2.05	0.57
1:M:127:ALA:HB2	1:M:426:LEU:HD11	1.87	0.57
1:C:217:SER:HA	1:C:320:ALA:O	2.05	0.57
1:N:151:SER:CB	1:N:399:ALA:HA	2.34	0.57
1:I:192:GLY:O	1:I:375:GLY:HA2	2.04	0.57
1:E:217:SER:HA	1:E:320:ALA:O	2.05	0.57
1:F:217:SER:HA	1:F:320:ALA:O	2.05	0.57
1:D:217:SER:HA	1:D:320:ALA:O	2.05	0.57
1:I:214:GLU:HA	1:I:323:VAL:O	2.04	0.57
1:A:138:CYS:HB2	1:A:407:VAL:HA	1.87	0.57
1:D:212:ALA:HA	1:D:325:ILE:O	2.05	0.57
1:G:217:SER:HA	1:G:320:ALA:O	2.05	0.57
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.86	0.57
1:N:192:GLY:O	1:N:375:GLY:HA2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:VAL:HB	1:E:377:ALA:HB2	1.87	0.57
1:B:217:SER:HA	1:B:320:ALA:O	2.05	0.57
1:L:214:GLU:HA	1:L:323:VAL:O	2.04	0.57
1:C:138:CYS:HB2	1:C:407:VAL:HA	1.87	0.56
1:C:212:ALA:HA	1:C:325:ILE:O	2.05	0.56
1:J:192:GLY:O	1:J:375:GLY:HA2	2.04	0.56
1:F:169:VAL:HB	1:F:377:ALA:HB2	1.87	0.56
1:I:217:SER:HA	1:I:320:ALA:O	2.05	0.56
1:H:214:GLU:HA	1:H:323:VAL:O	2.04	0.56
1:F:138:CYS:HB2	1:F:407:VAL:HA	1.87	0.56
1:N:214:GLU:HA	1:N:323:VAL:O	2.04	0.56
1:I:212:ALA:HA	1:I:325:ILE:O	2.05	0.56
1:J:127:ALA:HB2	1:J:426:LEU:HD11	1.87	0.56
1:C:169:VAL:HB	1:C:377:ALA:HB2	1.87	0.56
1:A:212:ALA:HA	1:A:325:ILE:O	2.05	0.56
1:A:217:SER:HA	1:A:320:ALA:O	2.05	0.56
1:D:417:VAL:HG21	1:D:477:GLY:HA3	1.86	0.56
1:D:169:VAL:HB	1:D:377:ALA:HB2	1.87	0.56
1:J:217:SER:HA	1:J:320:ALA:O	2.05	0.56
1:E:138:CYS:HB2	1:E:407:VAL:HA	1.87	0.56
1:B:138:CYS:HB2	1:B:407:VAL:HA	1.87	0.56
1:F:186:GLU:H	1:F:380:LYS:HB2	1.71	0.56
1:N:212:ALA:HA	1:N:325:ILE:O	2.06	0.56
1:A:186:GLU:H	1:A:380:LYS:HB2	1.71	0.56
1:H:127:ALA:HB2	1:H:426:LEU:HD11	1.86	0.56
1:E:417:VAL:HG21	1:E:477:GLY:HA3	1.86	0.56
1:M:192:GLY:O	1:M:375:GLY:HA2	2.04	0.56
1:C:186:GLU:H	1:C:380:LYS:HB2	1.71	0.56
1:N:217:SER:HA	1:N:320:ALA:O	2.05	0.56
1:N:127:ALA:HB2	1:N:426:LEU:HD11	1.87	0.56
1:H:217:SER:HA	1:H:320:ALA:O	2.05	0.56
1:J:212:ALA:HA	1:J:325:ILE:O	2.06	0.56
1:G:138:CYS:HB2	1:G:407:VAL:HA	1.87	0.56
1:F:212:ALA:HA	1:F:325:ILE:O	2.05	0.56
1:M:217:SER:HA	1:M:320:ALA:O	2.05	0.56
1:I:127:ALA:HB2	1:I:426:LEU:HD11	1.87	0.56
4:M:1527:ATP:C8	4:M:1527:ATP:C5	2.94	0.56
1:B:212:ALA:HA	1:B:325:ILE:O	2.05	0.56
1:M:212:ALA:HA	1:M:325:ILE:O	2.05	0.56
1:G:169:VAL:HB	1:G:377:ALA:HB2	1.87	0.56
1:B:169:VAL:HB	1:B:377:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:212:ALA:HA	1:K:325:ILE:O	2.05	0.56
1:E:186:GLU:H	1:E:380:LYS:HB2	1.71	0.56
1:I:206:ASN:HB2	1:I:213:VAL:HA	1.88	0.56
1:K:217:SER:HA	1:K:320:ALA:O	2.05	0.56
1:L:217:SER:HA	1:L:320:ALA:O	2.05	0.56
1:H:206:ASN:HB2	1:H:213:VAL:HA	1.88	0.55
1:D:186:GLU:H	1:D:380:LYS:HB2	1.71	0.55
1:L:212:ALA:HA	1:L:325:ILE:O	2.06	0.55
1:H:212:ALA:HA	1:H:325:ILE:O	2.06	0.55
1:A:169:VAL:HB	1:A:377:ALA:HB2	1.88	0.55
1:G:186:GLU:H	1:G:380:LYS:HB2	1.71	0.55
1:E:144:ILE:HG23	1:E:403:THR:CG2	2.37	0.55
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.37	0.55
1:F:151:SER:CB	1:F:399:ALA:HA	2.37	0.55
3:I:1526:PO4:P	4:I:1527:ATP:O3B	2.65	0.55
1:J:206:ASN:HB2	1:J:213:VAL:HA	1.88	0.55
1:G:151:SER:CB	1:G:399:ALA:HA	2.37	0.55
1:E:151:SER:CB	1:E:399:ALA:HA	2.37	0.55
1:K:186:GLU:H	1:K:380:LYS:HB2	1.72	0.55
1:N:206:ASN:HB2	1:N:213:VAL:HA	1.88	0.55
1:L:206:ASN:HB2	1:L:213:VAL:HA	1.88	0.55
1:A:151:SER:CB	1:A:399:ALA:HA	2.37	0.55
1:D:151:SER:CB	1:D:399:ALA:HA	2.37	0.55
1:M:186:GLU:H	1:M:380:LYS:HB2	1.72	0.55
1:D:235:PRO:HB2	1:D:310:GLU:HA	1.89	0.55
1:B:151:SER:CB	1:B:399:ALA:HA	2.37	0.55
1:D:138:CYS:HB2	1:D:407:VAL:HA	1.87	0.55
1:E:235:PRO:HB2	1:E:310:GLU:HA	1.89	0.55
1:K:151:SER:CB	1:K:399:ALA:HA	2.36	0.55
3:L:1526:PO4:P	4:L:1527:ATP:O3B	2.65	0.54
1:N:218:PRO:HG2	1:N:320:ALA:HB3	1.90	0.54
1:C:151:SER:CB	1:C:399:ALA:HA	2.37	0.54
1:E:31:LEU:CB	1:E:90:THR:HG21	2.37	0.54
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.37	0.54
1:F:235:PRO:HB2	1:F:310:GLU:HA	1.89	0.54
1:D:31:LEU:CB	1:D:90:THR:HG21	2.37	0.54
1:J:186:GLU:H	1:J:380:LYS:HB2	1.72	0.54
1:J:218:PRO:HG2	1:J:320:ALA:HB3	1.90	0.54
1:K:206:ASN:HB2	1:K:213:VAL:HA	1.88	0.54
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.37	0.54
1:C:235:PRO:HB2	1:C:310:GLU:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:LEU:CB	1:F:90:THR:HG21	2.37	0.54
1:G:31:LEU:CB	1:G:90:THR:HG21	2.37	0.54
1:B:186:GLU:H	1:B:380:LYS:HB2	1.71	0.54
1:K:218:PRO:HG2	1:K:320:ALA:HB3	1.90	0.54
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.37	0.54
1:L:186:GLU:H	1:L:380:LYS:HB2	1.72	0.54
1:H:218:PRO:HG2	1:H:320:ALA:HB3	1.90	0.54
1:M:218:PRO:HG2	1:M:320:ALA:HB3	1.90	0.54
1:B:31:LEU:CB	1:B:90:THR:HG21	2.37	0.54
1:A:31:LEU:CB	1:A:90:THR:HG21	2.37	0.54
1:M:206:ASN:HB2	1:M:213:VAL:HA	1.88	0.54
1:C:31:LEU:CB	1:C:90:THR:HG21	2.37	0.54
1:H:186:GLU:H	1:H:380:LYS:HB2	1.72	0.54
1:I:218:PRO:HG2	1:I:320:ALA:HB3	1.90	0.54
1:L:218:PRO:HG2	1:L:320:ALA:HB3	1.90	0.54
1:C:239:ALA:HB1	1:C:314:LEU:HG	1.90	0.54
1:D:144:ILE:HG23	1:D:403:THR:CG2	2.37	0.54
3:N:1526:PO4:P	4:N:1527:ATP:O3B	2.65	0.54
1:B:239:ALA:HB1	1:B:314:LEU:HG	1.90	0.54
1:D:239:ALA:HB1	1:D:314:LEU:HG	1.90	0.54
1:I:186:GLU:H	1:I:380:LYS:HB2	1.72	0.54
1:A:239:ALA:HB1	1:A:314:LEU:HG	1.90	0.54
3:H:1526:PO4:P	4:H:1527:ATP:O3B	2.66	0.53
1:D:147:VAL:CG2	1:D:494:LEU:HD11	2.38	0.53
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.37	0.53
1:G:235:PRO:HB2	1:G:310:GLU:HA	1.89	0.53
1:N:31:LEU:CB	1:N:90:THR:HG21	2.38	0.53
3:J:1526:PO4:P	4:J:1527:ATP:O3B	2.67	0.53
1:F:151:SER:HB3	1:F:399:ALA:HA	1.91	0.53
1:C:106:ALA:CB	1:C:116:LEU:HD21	2.39	0.53
1:D:106:ALA:CB	1:D:116:LEU:HD21	2.39	0.53
1:N:186:GLU:H	1:N:380:LYS:HB2	1.72	0.53
1:A:235:PRO:HB2	1:A:310:GLU:HA	1.89	0.53
1:B:235:PRO:HB2	1:B:310:GLU:HA	1.89	0.53
1:G:239:ALA:HB1	1:G:314:LEU:HG	1.90	0.53
1:A:206:ASN:CB	1:A:213:VAL:HA	2.38	0.53
1:D:151:SER:HB3	1:D:399:ALA:HA	1.91	0.53
1:E:106:ALA:CB	1:E:116:LEU:HD21	2.39	0.53
1:E:239:ALA:HB1	1:E:314:LEU:HG	1.90	0.53
1:J:411:VAL:HB	1:J:494:LEU:HB3	1.91	0.53
1:E:147:VAL:CG2	1:E:494:LEU:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ASN:CB	1:B:213:VAL:HA	2.38	0.53
1:G:151:SER:HB3	1:G:399:ALA:HA	1.91	0.53
1:H:411:VAL:HB	1:H:494:LEU:HB3	1.91	0.53
1:F:239:ALA:HB1	1:F:314:LEU:HG	1.90	0.53
1:C:172:GLU:H	1:C:172:GLU:CD	2.12	0.53
1:B:106:ALA:CB	1:B:116:LEU:HD21	2.39	0.53
1:K:411:VAL:HB	1:K:494:LEU:HB3	1.91	0.53
1:F:172:GLU:H	1:F:172:GLU:CD	2.12	0.53
1:B:147:VAL:CG2	1:B:494:LEU:HD11	2.38	0.53
1:C:151:SER:HB3	1:C:399:ALA:HA	1.91	0.53
1:G:172:GLU:H	1:G:172:GLU:CD	2.13	0.53
1:H:31:LEU:CB	1:H:90:THR:HG21	2.38	0.52
1:L:31:LEU:CB	1:L:90:THR:HG21	2.38	0.52
1:I:31:LEU:CB	1:I:90:THR:HG21	2.38	0.52
1:J:205:ILE:HD12	1:J:211:GLY:O	2.10	0.52
1:D:206:ASN:CB	1:D:213:VAL:HA	2.38	0.52
1:G:106:ALA:CB	1:G:116:LEU:HD21	2.39	0.52
1:B:172:GLU:CD	1:B:172:GLU:H	2.13	0.52
1:M:205:ILE:HD12	1:M:211:GLY:O	2.10	0.52
1:H:144:ILE:HG23	1:H:403:THR:CG2	2.40	0.52
1:A:251:ALA:O	1:A:277:LYS:HA	2.09	0.52
1:D:172:GLU:H	1:D:172:GLU:CD	2.12	0.52
3:D:1527:PO4:P	4:D:1528:ATP:O3B	2.68	0.52
3:E:1527:PO4:P	4:E:1528:ATP:O3B	2.68	0.52
1:J:31:LEU:CB	1:J:90:THR:HG21	2.39	0.52
1:L:205:ILE:HD12	1:L:211:GLY:O	2.09	0.52
1:N:205:ILE:HD12	1:N:211:GLY:O	2.09	0.52
1:F:206:ASN:CB	1:F:213:VAL:HA	2.38	0.52
1:G:206:ASN:CB	1:G:213:VAL:HA	2.38	0.52
1:M:152:ALA:HB1	1:M:155:ASP:HB3	1.92	0.52
1:I:411:VAL:HB	1:I:494:LEU:HB3	1.91	0.52
1:L:144:ILE:HG23	1:L:403:THR:CG2	2.39	0.52
1:A:172:GLU:H	1:A:172:GLU:CD	2.12	0.52
3:C:1527:PO4:P	4:C:1528:ATP:O3B	2.68	0.52
3:B:1527:PO4:P	4:B:1528:ATP:O3B	2.68	0.52
1:E:206:ASN:CB	1:E:213:VAL:HA	2.38	0.52
1:E:151:SER:HB3	1:E:399:ALA:HA	1.91	0.52
1:M:144:ILE:HG23	1:M:403:THR:CG2	2.40	0.52
1:N:411:VAL:HB	1:N:494:LEU:HB3	1.91	0.52
1:G:251:ALA:O	1:G:277:LYS:HA	2.09	0.52
3:A:1527:PO4:P	4:A:1528:ATP:O3B	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASN:CB	1:C:213:VAL:HA	2.38	0.52
1:I:144:ILE:HG23	1:I:403:THR:CG2	2.40	0.52
1:E:172:GLU:H	1:E:172:GLU:CD	2.13	0.52
1:B:206:ASN:HB2	1:B:213:VAL:CB	2.40	0.52
1:A:206:ASN:HB2	1:A:213:VAL:CB	2.40	0.52
1:A:151:SER:HB3	1:A:399:ALA:HA	1.91	0.52
1:N:144:ILE:HG23	1:N:403:THR:CG2	2.40	0.52
1:B:251:ALA:O	1:B:277:LYS:HA	2.09	0.52
1:H:205:ILE:HD12	1:H:211:GLY:O	2.09	0.52
1:F:218:PRO:HG2	1:F:320:ALA:HB3	1.92	0.52
1:B:151:SER:HB3	1:B:399:ALA:HA	1.91	0.52
1:C:147:VAL:CG2	1:C:494:LEU:HD11	2.38	0.52
1:E:218:PRO:HG2	1:E:320:ALA:HB3	1.92	0.52
1:F:206:ASN:HB2	1:F:213:VAL:CB	2.40	0.52
1:E:152:ALA:HB1	1:E:155:ASP:HB3	1.92	0.52
1:F:106:ALA:CB	1:F:116:LEU:HD21	2.39	0.52
1:E:251:ALA:O	1:E:277:LYS:HA	2.09	0.52
1:A:106:ALA:CB	1:A:116:LEU:HD21	2.39	0.52
3:M:1526:PO4:P	4:M:1527:ATP:PA	3.07	0.52
1:D:251:ALA:O	1:D:277:LYS:HA	2.09	0.52
1:N:152:ALA:HB1	1:N:155:ASP:HB3	1.92	0.52
1:L:152:ALA:HB1	1:L:155:ASP:HB3	1.92	0.52
1:M:31:LEU:HB2	1:M:90:THR:HG21	1.91	0.52
1:F:147:VAL:CG2	1:F:494:LEU:HD11	2.38	0.52
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.40	0.52
1:I:247:LEU:O	1:I:273:VAL:HA	2.10	0.52
1:L:411:VAL:HB	1:L:494:LEU:HB3	1.91	0.52
1:I:31:LEU:HA	3:I:1526:PO4:P	2.50	0.51
1:K:205:ILE:HD12	1:K:211:GLY:O	2.10	0.51
1:G:147:VAL:CG2	1:G:494:LEU:HD11	2.38	0.51
1:D:218:PRO:HG2	1:D:320:ALA:HB3	1.92	0.51
1:G:206:ASN:HB2	1:G:213:VAL:CB	2.40	0.51
1:C:206:ASN:HB2	1:C:213:VAL:CB	2.40	0.51
1:A:152:ALA:HB1	1:A:155:ASP:HB3	1.92	0.51
1:D:152:ALA:HB1	1:D:155:ASP:HB3	1.92	0.51
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.40	0.51
1:M:247:LEU:O	1:M:273:VAL:HA	2.10	0.51
1:H:142:LYS:HD2	1:H:142:LYS:H	1.75	0.51
3:G:1527:PO4:P	4:G:1528:ATP:O3B	2.68	0.51
1:D:206:ASN:HB2	1:D:213:VAL:CB	2.40	0.51
1:G:218:PRO:HG2	1:G:320:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ALA:O	1:C:277:LYS:HA	2.09	0.51
1:J:144:ILE:HG23	1:J:403:THR:CG2	2.40	0.51
3:F:1527:PO4:P	4:F:1528:ATP:O3B	2.68	0.51
1:B:152:ALA:HB1	1:B:155:ASP:HB3	1.92	0.51
1:C:152:ALA:HB1	1:C:155:ASP:HB3	1.91	0.51
1:F:251:ALA:O	1:F:277:LYS:HA	2.09	0.51
1:N:247:LEU:O	1:N:273:VAL:HA	2.10	0.51
1:H:247:LEU:O	1:H:273:VAL:HA	2.10	0.51
1:D:124:VAL:HG21	1:D:508:ALA:CB	2.40	0.51
1:K:144:ILE:HG23	1:K:403:THR:CG2	2.40	0.51
1:L:142:LYS:HD2	1:L:142:LYS:H	1.75	0.51
1:B:127:ALA:N	1:B:426:LEU:HD21	2.25	0.51
1:C:169:VAL:HG13	1:C:170:GLY:O	2.11	0.51
1:M:411:VAL:HB	1:M:494:LEU:HB3	1.91	0.51
1:L:247:LEU:O	1:L:273:VAL:HA	2.10	0.51
1:F:127:ALA:N	1:F:426:LEU:HD21	2.26	0.51
1:E:206:ASN:HB2	1:E:213:VAL:CB	2.40	0.51
1:F:152:ALA:HB1	1:F:155:ASP:HB3	1.91	0.51
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.40	0.51
1:K:247:LEU:O	1:K:273:VAL:HA	2.10	0.51
1:L:31:LEU:HA	3:L:1526:PO4:P	2.50	0.51
1:I:205:ILE:HD12	1:I:211:GLY:O	2.10	0.51
1:A:147:VAL:CG2	1:A:494:LEU:HD11	2.38	0.51
1:G:152:ALA:HB1	1:G:155:ASP:HB3	1.92	0.51
1:M:142:LYS:H	1:M:142:LYS:HD2	1.76	0.51
1:M:493:ILE:HG21	4:M:1527:ATP:H2'	1.92	0.51
1:E:411:VAL:HB	1:E:494:LEU:HB2	1.93	0.51
1:A:127:ALA:N	1:A:426:LEU:HD21	2.26	0.51
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.40	0.51
1:D:411:VAL:HB	1:D:494:LEU:HB2	1.93	0.51
1:C:127:ALA:N	1:C:426:LEU:HD21	2.25	0.51
1:E:127:ALA:N	1:E:426:LEU:HD21	2.26	0.51
1:E:124:VAL:HG21	1:E:508:ALA:CB	2.40	0.51
1:J:247:LEU:O	1:J:273:VAL:HA	2.10	0.51
1:M:493:ILE:CG2	4:M:1527:ATP:H2'	2.40	0.51
1:F:411:VAL:HB	1:F:494:LEU:HB2	1.93	0.51
1:H:149:THR:HA	1:H:152:ALA:HB3	1.93	0.51
1:C:411:VAL:HB	1:C:494:LEU:HB2	1.93	0.51
1:D:127:ALA:N	1:D:426:LEU:HD21	2.26	0.51
1:G:180:GLY:HA3	1:G:381:VAL:O	2.11	0.51
1:D:169:VAL:HG13	1:D:170:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:149:THR:HA	1:M:152:ALA:HB3	1.93	0.51
1:H:152:ALA:HB1	1:H:155:ASP:HB3	1.92	0.51
1:I:149:THR:HA	1:I:152:ALA:HB3	1.93	0.51
3:K:1526:PO4:P	4:K:1527:ATP:PG	3.09	0.50
1:G:127:ALA:N	1:G:426:LEU:HD21	2.26	0.50
3:M:1526:PO4:P	4:M:1527:ATP:O2A	2.69	0.50
1:C:218:PRO:HG2	1:C:320:ALA:HB3	1.92	0.50
1:F:169:VAL:HG13	1:F:170:GLY:O	2.11	0.50
1:A:169:VAL:HG13	1:A:170:GLY:O	2.11	0.50
1:N:149:THR:HA	1:N:152:ALA:HB3	1.93	0.50
1:L:149:THR:HA	1:L:152:ALA:HB3	1.93	0.50
1:B:411:VAL:HB	1:B:494:LEU:HB2	1.93	0.50
1:G:411:VAL:HB	1:G:494:LEU:HB2	1.93	0.50
1:A:218:PRO:HG2	1:A:320:ALA:HB3	1.92	0.50
1:D:180:GLY:HA3	1:D:381:VAL:O	2.11	0.50
1:B:169:VAL:HG13	1:B:170:GLY:O	2.11	0.50
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.40	0.50
1:C:180:GLY:HA3	1:C:381:VAL:O	2.11	0.50
1:A:135:SER:HA	1:A:412:VAL:CG1	2.42	0.50
1:J:152:ALA:HB1	1:J:155:ASP:HB3	1.92	0.50
1:K:142:LYS:HD2	1:K:142:LYS:H	1.75	0.50
1:F:206:ASN:HB2	1:F:213:VAL:HB	1.94	0.50
1:G:206:ASN:HB2	1:G:213:VAL:HB	1.94	0.50
1:E:180:GLY:HA3	1:E:381:VAL:O	2.11	0.50
1:E:169:VAL:HG13	1:E:170:GLY:O	2.11	0.50
1:B:218:PRO:HG2	1:B:320:ALA:HB3	1.92	0.50
1:B:135:SER:HA	1:B:412:VAL:CG1	2.42	0.50
1:J:149:THR:HA	1:J:152:ALA:HB3	1.94	0.50
1:A:411:VAL:HB	1:A:494:LEU:HB2	1.93	0.50
1:E:206:ASN:HB2	1:E:213:VAL:HB	1.94	0.50
1:A:206:ASN:HB2	1:A:213:VAL:HB	1.94	0.50
1:C:206:ASN:HB2	1:C:213:VAL:HB	1.94	0.50
1:B:206:ASN:HB2	1:B:213:VAL:HB	1.94	0.50
1:F:180:GLY:HA3	1:F:381:VAL:O	2.11	0.50
1:D:517:THR:HG23	1:E:39:VAL:HB	1.94	0.50
1:E:517:THR:HG23	1:F:39:VAL:HB	1.94	0.50
1:B:142:LYS:H	1:B:142:LYS:HD2	1.76	0.50
1:J:172:GLU:H	1:J:172:GLU:CD	2.14	0.50
1:D:206:ASN:HB2	1:D:213:VAL:HB	1.94	0.50
1:G:169:VAL:HG13	1:G:170:GLY:O	2.11	0.50
1:K:138:CYS:HA	1:K:411:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:152:ALA:HB1	1:I:155:ASP:HB3	1.92	0.50
1:F:293:ALA:HB2	1:F:300:VAL:CG2	2.42	0.50
1:N:33:PRO:HG3	4:N:1527:ATP:C5	2.47	0.49
1:F:169:VAL:HG11	1:F:175:ILE:CG1	2.42	0.49
1:J:138:CYS:HA	1:J:411:VAL:HG22	1.94	0.49
1:K:152:ALA:HB1	1:K:155:ASP:HB3	1.93	0.49
1:A:90:THR:HG22	1:A:94:VAL:HG23	1.95	0.49
1:K:149:THR:HA	1:K:152:ALA:HB3	1.94	0.49
1:A:349:ILE:HG22	1:A:369:VAL:HG13	1.95	0.49
1:D:349:ILE:HG22	1:D:369:VAL:HG13	1.95	0.49
1:A:142:LYS:HD2	1:A:142:LYS:H	1.76	0.49
1:L:172:GLU:H	1:L:172:GLU:CD	2.16	0.49
1:N:172:GLU:H	1:N:172:GLU:CD	2.14	0.49
1:G:293:ALA:HB2	1:G:300:VAL:CG2	2.42	0.49
1:F:90:THR:HG22	1:F:94:VAL:HG23	1.95	0.49
1:E:90:THR:HG22	1:E:94:VAL:HG23	1.95	0.49
1:B:180:GLY:HA3	1:B:381:VAL:O	2.11	0.49
1:C:169:VAL:HG11	1:C:175:ILE:CG1	2.43	0.49
1:D:169:VAL:HG11	1:D:175:ILE:CG1	2.42	0.49
1:B:169:VAL:HG11	1:B:175:ILE:CG1	2.43	0.49
1:N:138:CYS:HA	1:N:411:VAL:HG22	1.94	0.49
1:F:517:THR:HG23	1:G:39:VAL:HB	1.94	0.49
1:D:224:ASP:HA	1:D:289:LEU:CD1	2.43	0.49
1:C:349:ILE:HG22	1:C:369:VAL:HG13	1.95	0.49
1:F:142:LYS:H	1:F:142:LYS:HD2	1.77	0.49
1:C:517:THR:HG23	1:D:39:VAL:HB	1.94	0.49
1:G:90:THR:HG22	1:G:94:VAL:HG23	1.95	0.49
1:E:349:ILE:HG22	1:E:369:VAL:HG13	1.94	0.49
1:G:349:ILE:HG22	1:G:369:VAL:HG13	1.95	0.49
1:H:106:ALA:HB3	1:H:116:LEU:HD21	1.95	0.49
1:F:224:ASP:HA	1:F:289:LEU:CD1	2.43	0.49
1:E:142:LYS:HD2	1:E:142:LYS:H	1.76	0.49
1:A:224:ASP:HA	1:A:289:LEU:CD1	2.43	0.49
1:L:106:ALA:HB3	1:L:116:LEU:HD21	1.95	0.49
1:N:106:ALA:HB3	1:N:116:LEU:HD21	1.95	0.49
1:M:172:GLU:H	1:M:172:GLU:CD	2.16	0.49
1:G:169:VAL:HG11	1:G:175:ILE:CG1	2.42	0.49
1:I:138:CYS:HA	1:I:411:VAL:HG22	1.94	0.49
1:I:106:ALA:HB3	1:I:116:LEU:HD21	1.95	0.49
1:A:39:VAL:HB	1:G:517:THR:HG23	1.94	0.49
1:B:349:ILE:HG22	1:B:369:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:106:ALA:HB3	1:M:116:LEU:HD21	1.95	0.49
1:D:90:THR:HG22	1:D:94:VAL:HG23	1.95	0.49
1:A:180:GLY:HA3	1:A:381:VAL:O	2.11	0.49
1:F:349:ILE:HG22	1:F:369:VAL:HG13	1.94	0.49
1:F:406:ALA:HB2	1:F:496:PRO:HG3	1.95	0.49
1:D:142:LYS:HD2	1:D:142:LYS:H	1.77	0.49
1:E:169:VAL:HG11	1:E:175:ILE:CG1	2.43	0.49
1:C:293:ALA:HB2	1:C:300:VAL:CG2	2.42	0.49
1:K:106:ALA:HB3	1:K:116:LEU:HD21	1.95	0.49
1:K:172:GLU:CD	1:K:172:GLU:H	2.16	0.49
1:K:151:SER:HB3	1:K:399:ALA:HA	1.94	0.49
1:L:138:CYS:HA	1:L:411:VAL:HG22	1.94	0.49
1:E:293:ALA:HB2	1:E:300:VAL:CG2	2.42	0.49
1:I:172:GLU:CD	1:I:172:GLU:H	2.14	0.49
1:B:90:THR:HG22	1:B:94:VAL:HG23	1.95	0.48
1:G:135:SER:HA	1:G:412:VAL:CG1	2.42	0.48
1:A:169:VAL:HG11	1:A:175:ILE:CG1	2.42	0.48
1:J:106:ALA:HB3	1:J:116:LEU:HD21	1.95	0.48
1:D:293:ALA:HB2	1:D:300:VAL:CG2	2.42	0.48
1:G:142:LYS:H	1:G:142:LYS:HD2	1.76	0.48
1:J:142:LYS:H	1:J:142:LYS:HD2	1.78	0.48
1:B:224:ASP:HA	1:B:289:LEU:CD1	2.43	0.48
1:N:142:LYS:H	1:N:142:LYS:HD2	1.78	0.48
1:E:135:SER:HA	1:E:412:VAL:CG1	2.42	0.48
1:B:293:ALA:HB2	1:B:300:VAL:CG2	2.42	0.48
1:B:517:THR:HG23	1:C:39:VAL:HB	1.94	0.48
1:D:406:ALA:HB2	1:D:496:PRO:HG3	1.95	0.48
1:H:138:CYS:HA	1:H:411:VAL:HG22	1.94	0.48
1:M:138:CYS:HA	1:M:411:VAL:HG22	1.94	0.48
1:C:224:ASP:HA	1:C:289:LEU:CD1	2.43	0.48
1:E:224:ASP:HA	1:E:289:LEU:CD1	2.43	0.48
1:I:142:LYS:HD2	1:I:142:LYS:H	1.78	0.48
1:C:142:LYS:H	1:C:142:LYS:HD2	1.76	0.48
1:M:206:ASN:HB2	1:M:213:VAL:CB	2.44	0.48
1:H:172:GLU:H	1:H:172:GLU:CD	2.16	0.48
1:G:224:ASP:HA	1:G:289:LEU:CD1	2.43	0.48
1:D:135:SER:HA	1:D:412:VAL:CG1	2.42	0.48
1:L:206:ASN:HB2	1:L:213:VAL:CB	2.44	0.48
1:A:293:ALA:HB2	1:A:300:VAL:CG2	2.42	0.48
1:A:158:VAL:HG22	1:A:396:VAL:HG22	1.96	0.48
1:J:206:ASN:HB2	1:J:213:VAL:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:THR:HG23	1:B:39:VAL:HB	1.94	0.48
1:E:205:ILE:HD12	1:E:211:GLY:O	2.14	0.48
1:N:206:ASN:HB2	1:N:213:VAL:CB	2.44	0.48
1:D:158:VAL:HG22	1:D:396:VAL:HG22	1.96	0.48
1:A:205:ILE:HD12	1:A:211:GLY:O	2.14	0.48
1:F:135:SER:HA	1:F:412:VAL:CG1	2.42	0.48
1:D:205:ILE:HD12	1:D:211:GLY:O	2.14	0.48
1:G:205:ILE:HD12	1:G:211:GLY:O	2.14	0.48
1:I:206:ASN:HB2	1:I:213:VAL:CB	2.43	0.48
1:A:144:ILE:HG23	1:A:403:THR:HG21	1.96	0.48
1:C:144:ILE:HG23	1:C:403:THR:HG21	1.96	0.48
1:M:496:PRO:HB2	1:M:499:VAL:HG13	1.94	0.48
1:K:27:VAL:CG1	1:K:90:THR:HG23	2.34	0.47
1:H:206:ASN:HB2	1:H:213:VAL:CB	2.44	0.47
1:B:144:ILE:HG23	1:B:403:THR:HG21	1.96	0.47
1:C:158:VAL:HG22	1:C:396:VAL:HG22	1.96	0.47
1:F:205:ILE:HD12	1:F:211:GLY:O	2.14	0.47
1:K:206:ASN:HB2	1:K:213:VAL:CB	2.43	0.47
1:E:144:ILE:HG23	1:E:403:THR:HG21	1.96	0.47
1:F:144:ILE:HG23	1:F:403:THR:HG21	1.96	0.47
1:G:158:VAL:HG22	1:G:396:VAL:HG22	1.96	0.47
1:B:158:VAL:HG22	1:B:396:VAL:HG22	1.96	0.47
1:C:90:THR:HG22	1:C:94:VAL:HG23	1.95	0.47
1:B:205:ILE:HD12	1:B:211:GLY:O	2.14	0.47
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.96	0.47
1:D:496:PRO:HB2	1:D:499:VAL:HG13	1.96	0.47
1:E:406:ALA:HB2	1:E:496:PRO:HG3	1.95	0.47
1:G:406:ALA:HB2	1:G:496:PRO:HG3	1.95	0.47
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.97	0.47
1:C:406:ALA:HB2	1:C:496:PRO:HG3	1.95	0.47
1:K:158:VAL:HG22	1:K:396:VAL:HG22	1.96	0.47
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.97	0.47
1:A:126:ALA:HB3	1:A:426:LEU:HD22	1.97	0.47
1:H:106:ALA:CB	1:H:116:LEU:HD21	2.45	0.47
1:M:106:ALA:CB	1:M:116:LEU:HD21	2.45	0.47
1:M:158:VAL:HG22	1:M:396:VAL:HG22	1.96	0.47
1:A:496:PRO:HB2	1:A:499:VAL:HG13	1.96	0.47
1:B:126:ALA:HB3	1:B:426:LEU:HD22	1.97	0.47
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.96	0.47
1:B:406:ALA:HB2	1:B:496:PRO:HG3	1.95	0.47
1:H:158:VAL:HG22	1:H:396:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:VAL:HG22	1:F:396:VAL:HG22	1.96	0.47
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.97	0.47
1:M:493:ILE:CB	4:M:1527:ATP:N9	2.77	0.47
1:E:136:VAL:O	1:E:410:GLY:HA3	2.15	0.47
1:B:136:VAL:O	1:B:410:GLY:HA3	2.15	0.47
1:C:199:TYR:CE2	1:C:327:LYS:HB3	2.50	0.47
1:C:496:PRO:HB2	1:C:499:VAL:HG13	1.96	0.47
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.34	0.47
1:F:426:LEU:HB2	1:F:444:LEU:HD22	1.97	0.47
1:C:426:LEU:HB2	1:C:444:LEU:HD22	1.97	0.47
1:G:126:ALA:HB3	1:G:426:LEU:HD22	1.97	0.47
1:D:126:ALA:HB3	1:D:426:LEU:HD22	1.97	0.47
1:C:135:SER:HA	1:C:412:VAL:CG1	2.42	0.47
1:L:427:ALA:HA	1:L:444:LEU:CD1	2.45	0.47
1:D:426:LEU:HB2	1:D:444:LEU:HD22	1.97	0.47
1:E:426:LEU:HB2	1:E:444:LEU:HD22	1.97	0.47
1:D:199:TYR:CE2	1:D:327:LYS:HB3	2.50	0.47
1:A:199:TYR:CE2	1:A:327:LYS:HB3	2.50	0.47
1:F:199:TYR:CE2	1:F:327:LYS:HB3	2.50	0.47
1:B:199:TYR:CE2	1:B:327:LYS:HB3	2.50	0.47
1:L:144:ILE:HG23	1:L:403:THR:HG21	1.97	0.47
1:M:196:ASP:HA	1:M:329:THR:HA	1.97	0.47
1:I:158:VAL:HG22	1:I:396:VAL:HG22	1.97	0.47
1:N:158:VAL:HG22	1:N:396:VAL:HG22	1.97	0.47
1:E:158:VAL:HG22	1:E:396:VAL:HG22	1.96	0.47
1:A:371:LYS:O	1:A:374:GLY:HA3	2.15	0.47
1:J:158:VAL:HG22	1:J:396:VAL:HG22	1.97	0.47
1:D:136:VAL:O	1:D:410:GLY:HA3	2.15	0.46
1:F:136:VAL:O	1:F:410:GLY:HA3	2.15	0.46
1:C:126:ALA:HB3	1:C:426:LEU:HD22	1.97	0.46
1:E:126:ALA:HB3	1:E:426:LEU:HD22	1.97	0.46
1:E:199:TYR:CE2	1:E:327:LYS:HB3	2.50	0.46
1:I:106:ALA:CB	1:I:116:LEU:HD21	2.45	0.46
1:A:406:ALA:HB2	1:A:496:PRO:HG3	1.95	0.46
1:C:371:LYS:O	1:C:374:GLY:HA3	2.15	0.46
1:B:34:LYS:HB2	1:B:457:ASN:HB3	1.97	0.46
1:K:196:ASP:HA	1:K:329:THR:HA	1.97	0.46
1:B:371:LYS:O	1:B:374:GLY:HA3	2.15	0.46
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.34	0.46
1:C:136:VAL:O	1:C:410:GLY:HA3	2.15	0.46
1:G:136:VAL:O	1:G:410:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:TYR:CE2	1:G:327:LYS:HB3	2.50	0.46
1:L:106:ALA:CB	1:L:116:LEU:HD21	2.45	0.46
1:K:106:ALA:CB	1:K:116:LEU:HD21	2.45	0.46
1:D:371:LYS:O	1:D:374:GLY:HA3	2.15	0.46
1:L:196:ASP:HA	1:L:329:THR:HA	1.97	0.46
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.97	0.46
1:F:371:LYS:O	1:F:374:GLY:HA3	2.15	0.46
1:N:427:ALA:HA	1:N:444:LEU:CD1	2.45	0.46
1:L:158:VAL:HG22	1:L:396:VAL:HG22	1.97	0.46
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.35	0.46
1:B:426:LEU:HB2	1:B:444:LEU:HD22	1.97	0.46
1:H:124:VAL:HG21	1:H:508:ALA:CB	2.46	0.46
1:K:287:ALA:HB1	1:K:368:ARG:CZ	2.45	0.46
1:M:427:ALA:HA	1:M:444:LEU:CD1	2.45	0.46
1:G:426:LEU:HB2	1:G:444:LEU:HD22	1.97	0.46
1:C:205:ILE:HD12	1:C:211:GLY:O	2.14	0.46
1:N:240:VAL:HG11	1:N:247:LEU:HB2	1.97	0.46
1:H:240:VAL:HG11	1:H:247:LEU:HB2	1.96	0.46
1:A:120:ILE:O	1:A:124:VAL:HG23	2.16	0.46
1:G:120:ILE:O	1:G:124:VAL:HG23	2.16	0.46
1:N:124:VAL:HG21	1:N:508:ALA:CB	2.46	0.46
1:N:196:ASP:HA	1:N:329:THR:HA	1.97	0.46
1:N:139:SER:HB3	1:N:143:ALA:HB2	1.98	0.46
1:H:427:ALA:HA	1:H:444:LEU:CD1	2.45	0.46
1:G:371:LYS:O	1:G:374:GLY:HA3	2.15	0.46
1:N:287:ALA:HB1	1:N:368:ARG:CZ	2.45	0.46
1:L:120:ILE:O	1:L:124:VAL:HG23	2.16	0.46
1:H:287:ALA:HB1	1:H:368:ARG:CZ	2.45	0.46
1:M:493:ILE:HD11	4:M:1527:ATP:N7	2.29	0.46
1:D:219:PHE:CE2	1:D:314:LEU:HD22	2.51	0.46
1:M:240:VAL:HG11	1:M:247:LEU:HB2	1.97	0.46
1:F:120:ILE:O	1:F:124:VAL:HG23	2.15	0.46
1:J:106:ALA:CB	1:J:116:LEU:HD21	2.45	0.46
1:H:120:ILE:O	1:H:124:VAL:HG23	2.16	0.46
1:E:371:LYS:O	1:E:374:GLY:HA3	2.15	0.46
1:K:124:VAL:HG21	1:K:508:ALA:CB	2.46	0.46
1:C:34:LYS:HB2	1:C:457:ASN:HB3	1.97	0.46
1:C:383:ALA:HB3	1:C:389:MET:HB2	1.97	0.46
1:C:219:PHE:CE2	1:C:314:LEU:HD22	2.51	0.46
1:A:219:PHE:CE2	1:A:314:LEU:HD22	2.51	0.46
1:C:120:ILE:O	1:C:124:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.97	0.46
1:N:106:ALA:CB	1:N:116:LEU:HD21	2.45	0.46
1:M:406:ALA:HB2	1:M:496:PRO:HG3	1.98	0.46
1:K:120:ILE:O	1:K:124:VAL:HG23	2.16	0.46
1:L:287:ALA:HB1	1:L:368:ARG:CZ	2.45	0.46
1:J:120:ILE:O	1:J:124:VAL:HG23	2.16	0.46
1:I:427:ALA:HA	1:I:444:LEU:CD1	2.45	0.46
1:K:51:LYS:O	3:K:1526:PO4:P	2.74	0.46
1:A:136:VAL:O	1:A:410:GLY:HA3	2.15	0.46
1:B:219:PHE:CE2	1:B:314:LEU:HD22	2.51	0.46
1:L:139:SER:HB3	1:L:143:ALA:HB2	1.98	0.46
1:J:287:ALA:HB1	1:J:368:ARG:CZ	2.45	0.46
1:J:427:ALA:HA	1:J:444:LEU:CD1	2.45	0.46
1:K:427:ALA:HA	1:K:444:LEU:CD1	2.45	0.46
1:A:426:LEU:HB2	1:A:444:LEU:HD22	1.97	0.46
1:G:219:PHE:CE2	1:G:314:LEU:HD22	2.51	0.46
1:I:144:ILE:HG23	1:I:403:THR:HG21	1.97	0.46
1:I:240:VAL:HG11	1:I:247:LEU:HB2	1.97	0.46
1:K:240:VAL:HG11	1:K:247:LEU:HB2	1.97	0.46
1:A:34:LYS:HB2	1:A:457:ASN:HB3	1.98	0.46
1:J:196:ASP:HA	1:J:329:THR:HA	1.97	0.46
1:K:139:SER:HB3	1:K:143:ALA:HB2	1.98	0.46
1:M:139:SER:HB3	1:M:143:ALA:HB2	1.98	0.46
1:N:27:VAL:CG1	1:N:90:THR:HG23	2.34	0.46
1:H:27:VAL:CG1	1:H:90:THR:HG23	2.34	0.46
1:C:411:VAL:CG1	1:C:494:LEU:HD22	2.46	0.46
1:E:219:PHE:CE2	1:E:314:LEU:HD22	2.51	0.46
1:M:144:ILE:HG23	1:M:403:THR:HG21	1.98	0.46
1:B:120:ILE:O	1:B:124:VAL:HG23	2.15	0.46
1:L:240:VAL:HG21	1:L:247:LEU:HD13	1.98	0.46
1:H:139:SER:HB3	1:H:143:ALA:HB2	1.98	0.46
1:H:196:ASP:HA	1:H:329:THR:HA	1.97	0.46
1:L:356:ALA:HB1	1:L:361:ASP:HB2	1.98	0.46
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.98	0.46
1:N:356:ALA:HB1	1:N:361:ASP:HB2	1.97	0.46
1:M:124:VAL:HG21	1:M:508:ALA:CB	2.46	0.46
1:H:356:ALA:HB1	1:H:361:ASP:HB2	1.97	0.46
1:A:345:ARG:HA	1:A:345:ARG:HD3	1.96	0.46
1:K:356:ALA:HB1	1:K:361:ASP:HB2	1.98	0.46
1:E:411:VAL:CG1	1:E:494:LEU:HD22	2.46	0.46
1:F:126:ALA:HB3	1:F:426:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:240:VAL:HG21	1:M:247:LEU:HD13	1.98	0.46
1:F:34:LYS:HB2	1:F:457:ASN:HB3	1.97	0.46
1:E:345:ARG:HD3	1:E:345:ARG:HA	1.96	0.46
1:L:383:ALA:HB3	1:L:389:MET:HB2	1.98	0.46
1:M:287:ALA:HB1	1:M:368:ARG:CZ	2.45	0.46
1:N:127:ALA:CB	1:N:426:LEU:HD11	2.47	0.45
1:E:120:ILE:O	1:E:124:VAL:HG23	2.16	0.45
1:L:124:VAL:HG21	1:L:508:ALA:CB	2.46	0.45
1:J:124:VAL:HG21	1:J:508:ALA:CB	2.46	0.45
1:I:287:ALA:HB1	1:I:368:ARG:CZ	2.45	0.45
1:K:349:ILE:HG22	1:K:369:VAL:HG13	1.99	0.45
1:E:34:LYS:HB2	1:E:457:ASN:HB3	1.97	0.45
1:A:411:VAL:CG1	1:A:494:LEU:HD22	2.46	0.45
1:D:417:VAL:HG13	1:D:476:TYR:O	2.17	0.45
1:H:127:ALA:CB	1:H:426:LEU:HD11	2.46	0.45
1:L:240:VAL:HG11	1:L:247:LEU:HB2	1.96	0.45
1:I:427:ALA:HA	1:I:444:LEU:HD11	1.98	0.45
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.98	0.45
1:I:124:VAL:HG21	1:I:508:ALA:CB	2.46	0.45
1:J:139:SER:HB3	1:J:143:ALA:HB2	1.97	0.45
1:F:383:ALA:HB3	1:F:389:MET:HB2	1.97	0.45
1:J:349:ILE:HG22	1:J:369:VAL:HG13	1.99	0.45
1:K:150:ILE:HA	4:K:1527:ATP:C8	2.52	0.45
1:E:169:VAL:HG11	1:E:175:ILE:HG13	1.99	0.45
1:F:169:VAL:HG11	1:F:175:ILE:HG13	1.99	0.45
1:H:144:ILE:HG23	1:H:403:THR:HG21	1.97	0.45
1:F:287:ALA:HB1	1:F:368:ARG:CZ	2.47	0.45
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.97	0.45
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.98	0.45
1:L:127:ALA:CB	1:L:426:LEU:HD11	2.47	0.45
1:D:169:VAL:HG11	1:D:175:ILE:HG13	1.98	0.45
1:I:127:ALA:CB	1:I:426:LEU:HD11	2.47	0.45
1:K:240:VAL:HG21	1:K:247:LEU:HD13	1.98	0.45
1:I:196:ASP:HA	1:I:329:THR:HA	1.97	0.45
1:B:287:ALA:HB1	1:B:368:ARG:CZ	2.47	0.45
1:I:356:ALA:HB1	1:I:361:ASP:HB2	1.97	0.45
1:D:34:LYS:HB2	1:D:457:ASN:HB3	1.97	0.45
1:D:411:VAL:CG1	1:D:494:LEU:HD22	2.46	0.45
1:G:411:VAL:HG11	1:G:494:LEU:HD22	1.99	0.45
1:G:169:VAL:HG11	1:G:175:ILE:HG13	1.99	0.45
1:N:144:ILE:HG23	1:N:403:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:240:VAL:HG21	1:I:247:LEU:HD13	1.98	0.45
1:H:240:VAL:HG21	1:H:247:LEU:HD13	1.98	0.45
1:J:427:ALA:HA	1:J:444:LEU:HD11	1.99	0.45
1:I:120:ILE:O	1:I:124:VAL:HG23	2.16	0.45
1:F:345:ARG:HD3	1:F:345:ARG:HA	1.96	0.45
1:L:349:ILE:HG22	1:L:369:VAL:HG13	1.99	0.45
1:I:139:SER:HB3	1:I:143:ALA:HB2	1.98	0.45
1:I:349:ILE:HG22	1:I:369:VAL:HG13	1.99	0.45
1:K:406:ALA:HB2	1:K:496:PRO:HG3	1.99	0.45
1:K:127:ALA:CB	1:K:426:LEU:HD11	2.46	0.45
1:C:417:VAL:HG13	1:C:476:TYR:O	2.17	0.45
1:N:120:ILE:O	1:N:124:VAL:HG23	2.16	0.45
1:M:120:ILE:O	1:M:124:VAL:HG23	2.16	0.45
1:G:34:LYS:HB2	1:G:457:ASN:HB3	1.97	0.45
1:A:287:ALA:HB1	1:A:368:ARG:CZ	2.47	0.45
1:B:417:VAL:HG13	1:B:476:TYR:O	2.17	0.45
1:J:127:ALA:CB	1:J:426:LEU:HD11	2.46	0.45
1:D:120:ILE:O	1:D:124:VAL:HG23	2.16	0.45
1:C:287:ALA:HB1	1:C:368:ARG:CZ	2.47	0.45
1:A:411:VAL:HG11	1:A:494:LEU:HD22	1.99	0.45
1:F:411:VAL:CG1	1:F:494:LEU:HD22	2.46	0.45
1:F:411:VAL:HG11	1:F:494:LEU:HD22	1.99	0.45
1:D:127:ALA:CB	1:D:426:LEU:HD11	2.44	0.45
1:G:417:VAL:HG13	1:G:476:TYR:O	2.17	0.45
1:F:417:VAL:HG13	1:F:476:TYR:O	2.17	0.45
1:F:219:PHE:CE2	1:F:314:LEU:HD22	2.51	0.45
1:M:349:ILE:HG22	1:M:369:VAL:HG13	1.99	0.45
1:J:406:ALA:HB2	1:J:496:PRO:HG3	1.99	0.45
1:L:406:ALA:HB2	1:L:496:PRO:HG3	1.99	0.45
1:C:51:LYS:O	1:C:55:SER:HB2	2.17	0.45
1:C:23:LEU:O	1:C:27:VAL:HG23	2.17	0.45
1:E:23:LEU:O	1:E:27:VAL:HG23	2.17	0.45
1:G:411:VAL:CG1	1:G:494:LEU:HD22	2.46	0.45
1:B:127:ALA:CB	1:B:426:LEU:HD11	2.44	0.45
1:E:287:ALA:HB1	1:E:368:ARG:CZ	2.47	0.45
1:H:406:ALA:HB2	1:H:496:PRO:HG3	1.99	0.45
1:M:383:ALA:HB3	1:M:389:MET:HB2	1.98	0.45
1:H:34:LYS:HE2	1:H:458:CYS:HA	1.99	0.45
1:A:23:LEU:O	1:A:27:VAL:HG23	2.17	0.45
1:B:411:VAL:CG1	1:B:494:LEU:HD22	2.46	0.45
1:C:127:ALA:CB	1:C:426:LEU:HD11	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:SER:O	1:E:245:LYS:HG2	2.17	0.45
1:N:240:VAL:HG21	1:N:247:LEU:HD13	1.98	0.45
1:D:51:LYS:O	1:D:55:SER:HB2	2.17	0.45
1:M:356:ALA:HB1	1:M:361:ASP:HB2	1.98	0.45
1:F:51:LYS:O	1:F:55:SER:HB2	2.17	0.45
1:G:51:LYS:O	1:G:55:SER:HB2	2.17	0.45
1:B:411:VAL:HG11	1:B:494:LEU:HD22	1.99	0.44
1:G:287:ALA:HB1	1:G:368:ARG:CZ	2.47	0.44
1:F:37:ASN:HB2	1:F:50:THR:O	2.18	0.44
1:H:349:ILE:HG22	1:H:369:VAL:HG13	1.99	0.44
1:D:23:LEU:O	1:D:27:VAL:HG23	2.17	0.44
1:J:31:LEU:HA	3:J:1526:PO4:P	2.57	0.44
1:A:417:VAL:HG13	1:A:476:TYR:O	2.17	0.44
1:H:383:ALA:HB3	1:H:389:MET:HB2	1.98	0.44
1:J:356:ALA:HB1	1:J:361:ASP:HB2	1.97	0.44
1:D:287:ALA:HB1	1:D:368:ARG:CZ	2.47	0.44
1:M:27:VAL:CG1	1:M:90:THR:HG23	2.25	0.44
1:D:217:SER:O	1:D:245:LYS:HG2	2.17	0.44
1:G:217:SER:O	1:G:245:LYS:HG2	2.17	0.44
1:C:217:SER:O	1:C:245:LYS:HG2	2.17	0.44
1:K:206:ASN:CB	1:K:213:VAL:HA	2.48	0.44
1:G:106:ALA:HB3	1:G:116:LEU:HD21	1.99	0.44
1:J:144:ILE:HG23	1:J:403:THR:HG21	1.98	0.44
1:E:54:VAL:HG13	1:E:89:THR:HG21	1.99	0.44
1:E:102:GLU:HB2	1:E:442:VAL:HG13	1.99	0.44
1:N:349:ILE:HG22	1:N:369:VAL:HG13	1.99	0.44
1:D:54:VAL:HG13	1:D:89:THR:HG21	1.99	0.44
1:G:37:ASN:HB2	1:G:50:THR:O	2.18	0.44
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.98	0.44
1:F:23:LEU:O	1:F:27:VAL:HG23	2.17	0.44
1:E:127:ALA:CB	1:E:426:LEU:HD11	2.44	0.44
1:A:217:SER:O	1:A:245:LYS:HG2	2.17	0.44
1:N:417:VAL:HG13	1:N:476:TYR:O	2.18	0.44
1:M:127:ALA:CB	1:M:426:LEU:HD11	2.47	0.44
1:E:417:VAL:HG13	1:E:476:TYR:O	2.17	0.44
1:J:240:VAL:HG21	1:J:247:LEU:HD13	1.98	0.44
1:L:427:ALA:HA	1:L:444:LEU:HD11	1.99	0.44
1:H:427:ALA:HA	1:H:444:LEU:HD11	1.98	0.44
1:K:34:LYS:HE2	1:K:458:CYS:HA	1.99	0.44
1:L:279:PRO:HG3	1:L:292:ILE:HD11	2.00	0.44
1:M:279:PRO:HG3	1:M:292:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LYS:O	1:B:55:SER:HB2	2.17	0.44
1:E:411:VAL:HG11	1:E:494:LEU:HD22	1.99	0.44
1:L:206:ASN:CB	1:L:213:VAL:HA	2.48	0.44
1:C:106:ALA:HB3	1:C:116:LEU:HD21	1.99	0.44
1:M:427:ALA:HA	1:M:444:LEU:HD11	1.98	0.44
1:K:427:ALA:HA	1:K:444:LEU:HD11	1.98	0.44
1:D:102:GLU:HB2	1:D:442:VAL:HG13	1.99	0.44
1:F:54:VAL:HG13	1:F:89:THR:HG21	1.99	0.44
1:N:279:PRO:HG3	1:N:292:ILE:HD11	2.00	0.44
1:C:37:ASN:HB2	1:C:50:THR:O	2.18	0.44
1:C:411:VAL:HG11	1:C:494:LEU:HD22	1.99	0.44
1:F:217:SER:O	1:F:245:LYS:HG2	2.17	0.44
1:C:169:VAL:HG11	1:C:175:ILE:HG13	1.99	0.44
1:B:37:ASN:HB2	1:B:50:THR:O	2.18	0.44
1:L:412:VAL:HG22	1:L:495:ASP:O	2.18	0.44
1:B:217:SER:O	1:B:245:LYS:HG2	2.17	0.44
1:K:440:ILE:O	1:K:444:LEU:HG	2.18	0.44
1:D:37:ASN:HB2	1:D:50:THR:O	2.18	0.44
1:F:102:GLU:HB2	1:F:442:VAL:HG13	1.99	0.44
1:H:279:PRO:HG3	1:H:292:ILE:HD11	2.00	0.44
1:C:213:VAL:O	1:C:324:VAL:HA	2.18	0.44
1:G:152:ALA:HB1	1:G:155:ASP:O	2.18	0.44
1:M:417:VAL:HG13	1:M:476:TYR:O	2.18	0.44
1:H:417:VAL:HG13	1:H:476:TYR:O	2.18	0.44
1:J:206:ASN:CB	1:J:213:VAL:HA	2.48	0.44
1:E:106:ALA:HB3	1:E:116:LEU:HD21	1.99	0.44
1:F:106:ALA:HB3	1:F:116:LEU:HD21	1.99	0.44
1:I:440:ILE:O	1:I:444:LEU:HG	2.18	0.44
1:N:406:ALA:HB2	1:N:496:PRO:HG3	1.99	0.44
1:C:54:VAL:HG13	1:C:89:THR:HG21	1.99	0.44
1:H:455:VAL:HG11	1:H:465:VAL:HG21	2.00	0.44
1:A:51:LYS:O	1:A:55:SER:HB2	2.17	0.44
1:J:90:THR:HG22	1:J:94:VAL:HG23	2.00	0.44
1:M:412:VAL:HG22	1:M:495:ASP:O	2.18	0.44
1:B:213:VAL:O	1:B:324:VAL:HA	2.18	0.44
1:J:417:VAL:HG13	1:J:476:TYR:O	2.18	0.44
1:A:169:VAL:HG11	1:A:175:ILE:HG13	1.99	0.44
1:H:440:ILE:O	1:H:444:LEU:HG	2.18	0.44
1:K:279:PRO:HG3	1:K:292:ILE:HD11	2.00	0.44
1:I:406:ALA:HB2	1:I:496:PRO:HG3	1.99	0.44
1:E:37:ASN:HB2	1:E:50:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:455:VAL:HG11	1:I:465:VAL:HG21	2.00	0.44
1:H:256:GLY:O	1:H:260:ALA:HB3	2.18	0.44
1:B:356:ALA:HB1	1:B:361:ASP:HB2	2.00	0.44
1:N:455:VAL:HG11	1:N:465:VAL:HG21	2.00	0.44
1:G:23:LEU:O	1:G:27:VAL:HG23	2.17	0.43
1:H:31:LEU:HA	3:H:1526:PO4:P	2.58	0.43
1:F:152:ALA:HB1	1:F:155:ASP:O	2.18	0.43
1:M:206:ASN:CB	1:M:213:VAL:HA	2.48	0.43
1:M:206:ASN:HB2	1:M:213:VAL:HB	2.00	0.43
1:L:440:ILE:O	1:L:444:LEU:HG	2.18	0.43
1:J:440:ILE:O	1:J:444:LEU:HG	2.18	0.43
1:M:256:GLY:O	1:M:260:ALA:HB3	2.18	0.43
1:A:54:VAL:HG13	1:A:89:THR:HG21	1.99	0.43
1:C:102:GLU:HB2	1:C:442:VAL:HG13	1.99	0.43
1:M:64:ASP:O	1:M:68:ASN:HB2	2.18	0.43
3:M:1526:PO4:P	4:M:1527:ATP:O1B	2.76	0.43
1:B:23:LEU:O	1:B:27:VAL:HG23	2.17	0.43
1:N:412:VAL:HG22	1:N:495:ASP:O	2.18	0.43
1:J:412:VAL:HG22	1:J:495:ASP:O	2.18	0.43
1:H:412:VAL:HG22	1:H:495:ASP:O	2.18	0.43
1:I:412:VAL:HG22	1:I:495:ASP:O	2.18	0.43
1:D:411:VAL:HG11	1:D:494:LEU:HD22	1.99	0.43
1:B:169:VAL:HG11	1:B:175:ILE:HG13	1.99	0.43
1:F:196:ASP:HA	1:F:329:THR:HA	2.00	0.43
1:I:256:GLY:O	1:I:260:ALA:HB3	2.18	0.43
1:G:183:LEU:C	1:G:382:GLY:HA3	2.38	0.43
1:G:127:ALA:CB	1:G:426:LEU:HD11	2.44	0.43
1:K:417:VAL:HG13	1:K:476:TYR:O	2.18	0.43
1:I:206:ASN:CB	1:I:213:VAL:HA	2.48	0.43
1:J:455:VAL:HG11	1:J:465:VAL:HG21	2.00	0.43
1:E:51:LYS:O	1:E:55:SER:HB2	2.17	0.43
1:A:102:GLU:HB2	1:A:442:VAL:HG13	1.99	0.43
1:E:196:ASP:HA	1:E:329:THR:HA	2.01	0.43
3:L:1526:PO4:P	4:L:1527:ATP:PG	3.17	0.43
1:A:213:VAL:O	1:A:324:VAL:HA	2.18	0.43
1:E:152:ALA:HB1	1:E:155:ASP:O	2.18	0.43
1:H:383:ALA:HB3	1:H:389:MET:N	2.34	0.43
1:L:256:GLY:O	1:L:260:ALA:HB3	2.18	0.43
1:D:196:ASP:HA	1:D:329:THR:HA	2.01	0.43
1:N:34:LYS:HE2	1:N:458:CYS:HA	2.01	0.43
3:J:1526:PO4:P	4:J:1527:ATP:PG	3.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ALA:HB1	1:A:155:ASP:O	2.18	0.43
1:N:427:ALA:HA	1:N:444:LEU:HD11	1.99	0.43
1:N:440:ILE:O	1:N:444:LEU:HG	2.18	0.43
1:I:383:ALA:HB3	1:I:389:MET:N	2.34	0.43
1:M:383:ALA:HB3	1:M:389:MET:N	2.34	0.43
1:N:383:ALA:HB3	1:N:389:MET:N	2.34	0.43
1:J:279:PRO:HG3	1:J:292:ILE:HD11	2.00	0.43
1:L:455:VAL:HG11	1:L:465:VAL:HG21	2.00	0.43
1:C:356:ALA:HB1	1:C:361:ASP:HB2	2.00	0.43
1:J:102:GLU:HB2	1:J:442:VAL:HG13	2.01	0.43
1:N:180:GLY:HA3	1:N:381:VAL:O	2.19	0.43
1:L:417:VAL:HG13	1:L:476:TYR:O	2.18	0.43
1:L:206:ASN:HB2	1:L:213:VAL:HB	2.00	0.43
1:H:206:ASN:CB	1:H:213:VAL:HA	2.48	0.43
1:N:34:LYS:HZ1	1:N:483:GLU:CD	2.21	0.43
1:H:102:GLU:HB2	1:H:442:VAL:HG13	2.01	0.43
1:K:64:ASP:O	1:K:68:ASN:HB2	2.18	0.43
1:G:54:VAL:HG13	1:G:89:THR:HG21	1.99	0.43
1:A:37:ASN:HB2	1:A:50:THR:O	2.18	0.43
1:J:34:LYS:HE2	1:J:458:CYS:HA	2.01	0.43
1:I:279:PRO:HG3	1:I:292:ILE:HD11	2.00	0.43
1:M:493:ILE:HG21	4:M:1527:ATP:C8	2.52	0.43
1:I:182:GLY:O	1:I:382:GLY:HA2	2.19	0.43
1:G:213:VAL:O	1:G:324:VAL:HA	2.18	0.43
1:N:206:ASN:HB2	1:N:213:VAL:HB	2.00	0.43
1:D:106:ALA:HB3	1:D:116:LEU:HD21	1.99	0.43
1:G:227:ILE:H	1:G:251:ALA:HB1	1.84	0.43
1:E:227:ILE:H	1:E:251:ALA:HB1	1.84	0.43
1:A:106:ALA:HB3	1:A:116:LEU:HD21	1.99	0.43
1:J:383:ALA:HB3	1:J:389:MET:N	2.34	0.43
1:A:356:ALA:HB1	1:A:361:ASP:HB2	2.00	0.43
1:G:345:ARG:HA	1:G:345:ARG:HD3	1.96	0.43
1:I:34:LYS:HE2	1:I:458:CYS:HA	2.01	0.43
1:D:356:ALA:HB1	1:D:361:ASP:HB2	2.00	0.43
1:L:90:THR:HG22	1:L:94:VAL:HG23	2.01	0.43
1:I:90:THR:HG22	1:I:94:VAL:HG23	2.01	0.43
1:K:182:GLY:O	1:K:382:GLY:HA2	2.19	0.43
1:H:182:GLY:O	1:H:382:GLY:HA2	2.19	0.43
1:M:180:GLY:HA3	1:M:381:VAL:O	2.19	0.43
1:G:152:ALA:HB1	1:G:155:ASP:CA	2.49	0.43
1:F:152:ALA:HB1	1:F:155:ASP:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:417:VAL:HG13	1:I:476:TYR:O	2.18	0.43
1:K:213:VAL:HG13	1:K:325:ILE:HB	2.01	0.43
1:M:440:ILE:O	1:M:444:LEU:HG	2.18	0.43
1:I:34:LYS:HZ1	1:I:483:GLU:CD	2.22	0.43
1:K:455:VAL:HG11	1:K:465:VAL:HG21	2.01	0.43
1:F:356:ALA:HB1	1:F:361:ASP:HB2	2.00	0.43
1:C:220:ILE:HD12	1:C:248:LEU:HD23	2.01	0.43
1:G:102:GLU:HB2	1:G:442:VAL:HG13	1.99	0.43
1:K:102:GLU:HB2	1:K:442:VAL:HG13	2.01	0.43
1:L:102:GLU:HB2	1:L:442:VAL:HG13	2.01	0.43
1:I:102:GLU:HB2	1:I:442:VAL:HG13	2.01	0.43
1:N:102:GLU:HB2	1:N:442:VAL:HG13	2.01	0.43
1:K:31:LEU:HB3	1:K:90:THR:HG21	2.00	0.43
1:D:183:LEU:C	1:D:382:GLY:HA3	2.38	0.43
1:N:182:GLY:O	1:N:382:GLY:HA2	2.19	0.43
1:D:213:VAL:O	1:D:324:VAL:HA	2.18	0.43
1:K:180:GLY:HA3	1:K:381:VAL:O	2.19	0.43
1:J:180:GLY:HA3	1:J:381:VAL:O	2.19	0.43
1:H:180:GLY:HA3	1:H:381:VAL:O	2.19	0.43
1:M:213:VAL:HG13	1:M:325:ILE:HB	2.01	0.43
1:N:206:ASN:CB	1:N:213:VAL:HA	2.48	0.43
1:I:206:ASN:HB2	1:I:213:VAL:HB	2.00	0.43
1:J:206:ASN:HB2	1:J:213:VAL:HB	2.00	0.43
1:D:227:ILE:H	1:D:251:ALA:HB1	1.84	0.43
1:L:383:ALA:HB3	1:L:389:MET:N	2.34	0.43
1:G:196:ASP:HA	1:G:329:THR:HA	2.00	0.43
1:B:54:VAL:HG13	1:B:89:THR:HG21	1.99	0.43
1:K:293:ALA:HB2	1:K:300:VAL:CG2	2.49	0.43
1:L:293:ALA:HB2	1:L:300:VAL:CG2	2.49	0.43
1:M:182:GLY:O	1:M:382:GLY:HA2	2.19	0.43
1:I:180:GLY:HA3	1:I:381:VAL:O	2.19	0.43
1:E:152:ALA:HB1	1:E:155:ASP:CA	2.49	0.43
1:L:213:VAL:HG13	1:L:325:ILE:HB	2.01	0.43
1:K:206:ASN:HB2	1:K:213:VAL:HB	2.00	0.43
1:I:64:ASP:O	1:I:68:ASN:HB2	2.19	0.43
1:E:356:ALA:HB1	1:E:361:ASP:HB2	2.00	0.43
1:F:147:VAL:HG22	1:F:494:LEU:CD1	2.46	0.42
1:F:213:VAL:O	1:F:324:VAL:HA	2.18	0.42
1:H:206:ASN:HB2	1:H:213:VAL:HB	2.00	0.42
1:H:213:VAL:HG13	1:H:325:ILE:HB	2.01	0.42
1:K:383:ALA:HB3	1:K:389:MET:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:ALA:O	1:C:483:GLU:CG	2.67	0.42
1:B:102:GLU:HB2	1:B:442:VAL:HG13	2.00	0.42
1:M:102:GLU:HB2	1:M:442:VAL:HG13	2.01	0.42
1:J:293:ALA:HB2	1:J:300:VAL:CG2	2.49	0.42
1:B:220:ILE:HD12	1:B:248:LEU:HD23	2.01	0.42
1:C:196:ASP:HA	1:C:329:THR:HA	2.01	0.42
1:K:256:GLY:O	1:K:260:ALA:HB3	2.18	0.42
1:A:480:ALA:O	1:A:483:GLU:CG	2.67	0.42
1:N:293:ALA:HB2	1:N:300:VAL:CG2	2.49	0.42
1:H:90:THR:HG22	1:H:94:VAL:HG23	2.01	0.42
1:K:50:THR:HG1	1:K:51:LYS:N	2.16	0.42
1:C:183:LEU:C	1:C:382:GLY:HA3	2.38	0.42
1:A:183:LEU:C	1:A:382:GLY:HA3	2.38	0.42
1:L:182:GLY:O	1:L:382:GLY:HA2	2.19	0.42
1:A:152:ALA:HB1	1:A:155:ASP:CA	2.49	0.42
1:B:152:ALA:HB1	1:B:155:ASP:CA	2.49	0.42
1:D:106:ALA:HB1	1:D:116:LEU:HD21	2.01	0.42
1:F:227:ILE:H	1:F:251:ALA:HB1	1.84	0.42
1:K:144:ILE:HG23	1:K:403:THR:HG21	2.01	0.42
1:D:349:ILE:HB	1:D:369:VAL:HG12	2.02	0.42
1:L:294:THR:HG21	1:L:345:ARG:HG3	2.01	0.42
1:L:34:LYS:HE2	1:L:458:CYS:HA	2.01	0.42
1:H:64:ASP:O	1:H:68:ASN:HB2	2.19	0.42
1:J:256:GLY:O	1:J:260:ALA:HB3	2.18	0.42
1:I:293:ALA:HB2	1:I:300:VAL:CG2	2.49	0.42
1:K:23:LEU:O	1:K:27:VAL:HG23	2.20	0.42
1:K:412:VAL:HG22	1:K:495:ASP:O	2.18	0.42
1:C:152:ALA:HB1	1:C:155:ASP:CA	2.49	0.42
1:C:152:ALA:HB1	1:C:155:ASP:O	2.18	0.42
1:D:152:ALA:HB1	1:D:155:ASP:O	2.18	0.42
1:N:213:VAL:HG13	1:N:325:ILE:HB	2.01	0.42
1:C:106:ALA:HB1	1:C:116:LEU:HD21	2.01	0.42
1:D:480:ALA:O	1:D:483:GLU:CG	2.67	0.42
1:J:64:ASP:O	1:J:68:ASN:HB2	2.18	0.42
1:N:256:GLY:O	1:N:260:ALA:HB3	2.18	0.42
1:K:294:THR:HG21	1:K:345:ARG:HG3	2.01	0.42
1:D:220:ILE:HD12	1:D:248:LEU:HD23	2.01	0.42
1:M:455:VAL:HG11	1:M:465:VAL:HG21	2.01	0.42
3:I:1526:PO4:P	4:I:1527:ATP:PG	3.17	0.42
1:E:213:VAL:O	1:E:324:VAL:HA	2.18	0.42
1:B:106:ALA:HB3	1:B:116:LEU:HD21	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ILE:H	1:B:251:ALA:HB1	1.84	0.42
1:C:349:ILE:HG23	1:C:365:LEU:CD1	2.50	0.42
1:C:349:ILE:HB	1:C:369:VAL:HG12	2.01	0.42
1:E:349:ILE:HG23	1:E:365:LEU:CD1	2.50	0.42
1:G:356:ALA:HB1	1:G:361:ASP:HB2	2.00	0.42
1:L:19:GLY:HA2	1:L:62:LEU:CD1	2.50	0.42
1:L:64:ASP:O	1:L:68:ASN:HB2	2.20	0.42
1:B:15:LYS:HB3	1:B:66:PHE:HB3	2.02	0.42
1:N:90:THR:HG22	1:N:94:VAL:HG23	2.01	0.42
1:I:23:LEU:O	1:I:27:VAL:HG23	2.20	0.42
1:J:182:GLY:O	1:J:382:GLY:HA2	2.19	0.42
1:K:202:PRO:O	1:K:205:ILE:HB	2.20	0.42
1:B:152:ALA:HB1	1:B:155:ASP:O	2.18	0.42
1:C:15:LYS:HB3	1:C:66:PHE:HB3	2.02	0.42
1:M:293:ALA:HB2	1:M:300:VAL:CG2	2.49	0.42
1:C:285:ARG:HH11	1:C:285:ARG:HG3	1.85	0.42
1:A:147:VAL:HG22	1:A:494:LEU:CD1	2.46	0.42
1:F:138:CYS:SG	1:F:407:VAL:HA	2.60	0.42
1:F:206:ASN:ND2	1:F:214:GLU:H	2.18	0.42
1:D:152:ALA:HB1	1:D:155:ASP:CA	2.49	0.42
1:C:227:ILE:H	1:C:251:ALA:HB1	1.84	0.42
1:A:349:ILE:HB	1:A:369:VAL:HG12	2.02	0.42
1:D:349:ILE:HG23	1:D:365:LEU:CD1	2.49	0.42
1:E:349:ILE:HB	1:E:369:VAL:HG12	2.02	0.42
1:I:383:ALA:HB3	1:I:389:MET:CA	2.50	0.42
1:H:34:LYS:HZ1	1:H:483:GLU:CD	2.22	0.42
1:M:19:GLY:HA2	1:M:62:LEU:CD1	2.50	0.42
1:M:294:THR:HG21	1:M:345:ARG:HG3	2.02	0.42
1:N:23:LEU:O	1:N:27:VAL:HG23	2.20	0.42
1:J:50:THR:HG1	1:J:51:LYS:N	2.18	0.42
1:M:135:SER:CA	1:M:412:VAL:HG12	2.45	0.42
1:D:138:CYS:SG	1:D:407:VAL:HA	2.60	0.42
1:F:127:ALA:CB	1:F:426:LEU:HD11	2.44	0.42
1:F:213:VAL:CG1	1:F:325:ILE:HB	2.50	0.42
1:C:206:ASN:ND2	1:C:214:GLU:H	2.18	0.42
1:C:378:VAL:HG11	1:C:380:LYS:HZ2	1.85	0.42
1:L:180:GLY:HA3	1:L:381:VAL:O	2.19	0.42
1:I:213:VAL:HG13	1:I:325:ILE:HB	2.01	0.42
1:J:213:VAL:HG13	1:J:325:ILE:HB	2.01	0.42
1:C:19:GLY:HA2	1:C:62:LEU:CD1	2.50	0.42
1:G:220:ILE:HD12	1:G:248:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:64:ASP:O	1:N:68:ASN:HB2	2.19	0.42
1:E:7:LYS:HB2	1:E:11:ASP:HB3	2.01	0.42
1:B:480:ALA:O	1:B:483:GLU:CG	2.67	0.42
1:K:19:GLY:HA2	1:K:62:LEU:CD1	2.50	0.42
1:B:19:GLY:HA2	1:B:62:LEU:CD1	2.50	0.42
1:J:268:ARG:NE	1:J:268:ARG:HA	2.35	0.42
1:L:23:LEU:O	1:L:27:VAL:HG23	2.20	0.42
1:E:183:LEU:C	1:E:382:GLY:HA3	2.38	0.42
1:J:202:PRO:O	1:J:205:ILE:HB	2.20	0.42
1:C:138:CYS:SG	1:C:407:VAL:HA	2.60	0.42
1:A:138:CYS:SG	1:A:407:VAL:HA	2.60	0.42
1:B:138:CYS:SG	1:B:407:VAL:HA	2.60	0.42
1:D:213:VAL:CG1	1:D:325:ILE:HB	2.50	0.42
1:G:213:VAL:CG1	1:G:325:ILE:HB	2.50	0.42
1:H:383:ALA:HB3	1:H:389:MET:CA	2.50	0.42
1:A:50:THR:HG21	1:A:59:GLU:HB2	2.01	0.42
1:F:7:LYS:HB2	1:F:11:ASP:HB3	2.02	0.42
1:I:66:PHE:CZ	1:I:522:THR:HG22	2.55	0.42
1:G:19:GLY:HA2	1:G:62:LEU:CD1	2.50	0.42
1:H:293:ALA:HB2	1:H:300:VAL:CG2	2.49	0.42
1:K:268:ARG:NE	1:K:268:ARG:HA	2.35	0.42
4:M:1527:ATP:C4	4:M:1527:ATP:C8	3.07	0.42
1:M:23:LEU:O	1:M:27:VAL:HG23	2.20	0.42
1:B:183:LEU:C	1:B:382:GLY:HA3	2.38	0.42
1:L:202:PRO:O	1:L:205:ILE:HB	2.20	0.42
1:E:213:VAL:CG1	1:E:325:ILE:HB	2.50	0.42
1:E:106:ALA:HB1	1:E:116:LEU:HD21	2.01	0.42
1:A:227:ILE:H	1:A:251:ALA:HB1	1.84	0.42
1:G:349:ILE:HG23	1:G:365:LEU:CD1	2.50	0.42
1:J:383:ALA:HB3	1:J:389:MET:CA	2.50	0.42
1:G:50:THR:HG21	1:G:59:GLU:HB2	2.01	0.42
1:J:294:THR:HG21	1:J:345:ARG:HG3	2.01	0.42
1:B:196:ASP:HA	1:B:329:THR:HA	2.00	0.42
1:G:480:ALA:O	1:G:483:GLU:CG	2.67	0.42
1:D:15:LYS:HB3	1:D:66:PHE:HB3	2.02	0.42
1:F:220:ILE:HD12	1:F:248:LEU:HD23	2.01	0.42
1:A:285:ARG:HG3	1:A:285:ARG:HH11	1.85	0.42
1:I:33:PRO:HG3	4:I:1527:ATP:C4	2.55	0.42
1:J:23:LEU:O	1:J:27:VAL:HG23	2.20	0.42
1:M:152:ALA:HB1	1:M:155:ASP:CA	2.50	0.42
1:H:152:ALA:HB1	1:H:155:ASP:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ILE:HG23	1:B:365:LEU:CD1	2.49	0.42
1:F:349:ILE:HB	1:F:369:VAL:HG12	2.02	0.42
1:G:294:THR:HG21	1:G:345:ARG:HG3	2.02	0.42
1:A:196:ASP:HA	1:A:329:THR:HA	2.01	0.42
1:A:220:ILE:HD12	1:A:248:LEU:HD23	2.01	0.42
1:J:19:GLY:HA2	1:J:62:LEU:CD1	2.50	0.42
1:E:480:ALA:O	1:E:483:GLU:CG	2.67	0.42
1:H:66:PHE:CZ	1:H:522:THR:HG22	2.55	0.42
1:J:66:PHE:CZ	1:J:522:THR:HG22	2.55	0.42
1:A:19:GLY:HA2	1:A:62:LEU:CD1	2.50	0.42
1:A:15:LYS:HB3	1:A:66:PHE:HB3	2.02	0.42
1:I:268:ARG:NE	1:I:268:ARG:HA	2.35	0.42
1:F:218:PRO:HG2	1:F:323:VAL:HG23	2.02	0.41
1:H:323:VAL:HG22	1:H:332:ILE:HA	2.02	0.41
1:N:323:VAL:HG22	1:N:332:ILE:HA	2.02	0.41
1:B:106:ALA:HB1	1:B:116:LEU:HD21	2.01	0.41
1:N:152:ALA:HB1	1:N:155:ASP:CA	2.50	0.41
1:F:349:ILE:HG23	1:F:365:LEU:CD1	2.49	0.41
1:F:383:ALA:HB3	1:F:389:MET:N	2.35	0.41
1:G:240:VAL:HA	1:G:243:ALA:HB3	2.03	0.41
1:N:19:GLY:HA2	1:N:62:LEU:CD1	2.50	0.41
1:F:77:VAL:HG12	1:F:506:TYR:HB3	2.02	0.41
1:N:294:THR:HG21	1:N:345:ARG:HG3	2.02	0.41
1:B:294:THR:HG21	1:B:345:ARG:HG3	2.02	0.41
1:L:268:ARG:NE	1:L:268:ARG:HA	2.35	0.41
1:G:285:ARG:HH11	1:G:285:ARG:HG3	1.85	0.41
1:L:50:THR:HG1	1:L:51:LYS:N	2.18	0.41
1:D:218:PRO:HG2	1:D:323:VAL:HG23	2.02	0.41
1:C:218:PRO:HG2	1:C:323:VAL:HG23	2.02	0.41
1:E:199:TYR:CD2	1:E:327:LYS:HA	2.56	0.41
1:B:378:VAL:HG11	1:B:380:LYS:HZ2	1.85	0.41
1:I:323:VAL:HG22	1:I:332:ILE:HA	2.02	0.41
1:L:152:ALA:HB1	1:L:155:ASP:CA	2.50	0.41
1:G:349:ILE:HB	1:G:369:VAL:HG12	2.02	0.41
1:K:383:ALA:HB3	1:K:389:MET:CA	2.50	0.41
1:G:383:ALA:HB3	1:G:389:MET:N	2.35	0.41
1:F:50:THR:HG21	1:F:59:GLU:HB2	2.01	0.41
1:B:50:THR:HG21	1:B:59:GLU:HB2	2.01	0.41
1:F:19:GLY:HA2	1:F:62:LEU:CD1	2.50	0.41
1:F:480:ALA:O	1:F:483:GLU:CG	2.67	0.41
1:D:19:GLY:HA2	1:D:62:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ARG:HG3	1:B:285:ARG:HH11	1.85	0.41
1:N:50:THR:HG1	1:N:51:LYS:N	2.18	0.41
1:M:50:THR:HG1	1:M:51:LYS:N	2.18	0.41
1:E:138:CYS:SG	1:E:407:VAL:HA	2.60	0.41
1:B:147:VAL:HG22	1:B:494:LEU:CD1	2.46	0.41
1:D:199:TYR:CD2	1:D:327:LYS:HA	2.56	0.41
1:F:199:TYR:CD2	1:F:327:LYS:HA	2.55	0.41
1:G:106:ALA:HB1	1:G:116:LEU:HD21	2.01	0.41
1:A:106:ALA:HB1	1:A:116:LEU:HD21	2.01	0.41
1:K:152:ALA:HB1	1:K:155:ASP:CA	2.50	0.41
1:A:349:ILE:HG23	1:A:365:LEU:CD1	2.49	0.41
1:A:294:THR:HG21	1:A:345:ARG:HG3	2.03	0.41
1:M:383:ALA:HB3	1:M:389:MET:CA	2.50	0.41
1:N:383:ALA:HB3	1:N:389:MET:CA	2.50	0.41
1:B:51:LYS:HG2	1:B:52:ASP:H	1.85	0.41
1:D:13:ARG:CG	1:D:104:LEU:HD22	2.51	0.41
1:G:7:LYS:HB2	1:G:11:ASP:HB3	2.01	0.41
1:D:77:VAL:HG12	1:D:506:TYR:HB3	2.02	0.41
1:M:268:ARG:NE	1:M:268:ARG:HA	2.35	0.41
1:F:240:VAL:HA	1:F:243:ALA:HB3	2.02	0.41
1:L:33:PRO:HG3	4:L:1527:ATP:C4	2.55	0.41
1:E:218:PRO:HG2	1:E:323:VAL:HG23	2.03	0.41
1:A:206:ASN:ND2	1:A:214:GLU:H	2.18	0.41
1:A:213:VAL:CG1	1:A:325:ILE:HB	2.50	0.41
1:C:199:TYR:CD2	1:C:327:LYS:HA	2.56	0.41
1:D:378:VAL:HG11	1:D:380:LYS:HZ2	1.84	0.41
1:I:152:ALA:HB1	1:I:155:ASP:CA	2.51	0.41
1:C:383:ALA:HB3	1:C:389:MET:N	2.35	0.41
1:F:294:THR:HG21	1:F:345:ARG:HG3	2.03	0.41
1:C:13:ARG:CG	1:C:104:LEU:HD22	2.51	0.41
1:F:13:ARG:CG	1:F:104:LEU:HD22	2.51	0.41
1:A:240:VAL:HA	1:A:243:ALA:HB3	2.02	0.41
1:H:19:GLY:HA2	1:H:62:LEU:CD1	2.50	0.41
1:G:13:ARG:CG	1:G:104:LEU:HD22	2.51	0.41
1:D:285:ARG:HH11	1:D:285:ARG:HG3	1.85	0.41
1:C:294:THR:HG21	1:C:345:ARG:HG3	2.02	0.41
1:F:183:LEU:C	1:F:382:GLY:HA3	2.38	0.41
1:I:205:ILE:HA	1:I:205:ILE:HD13	1.91	0.41
1:B:218:PRO:HG2	1:B:323:VAL:HG23	2.03	0.41
1:D:206:ASN:ND2	1:D:214:GLU:H	2.18	0.41
1:G:206:ASN:ND2	1:G:214:GLU:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:PRO:HG2	1:G:323:VAL:HG23	2.03	0.41
1:A:85:ALA:HB1	1:A:499:VAL:HA	2.03	0.41
1:A:383:ALA:HB3	1:A:389:MET:N	2.35	0.41
1:L:383:ALA:HB3	1:L:389:MET:CA	2.50	0.41
1:C:51:LYS:HG2	1:C:52:ASP:H	1.85	0.41
1:C:50:THR:HG21	1:C:59:GLU:HB2	2.01	0.41
1:D:50:THR:HG21	1:D:59:GLU:HB2	2.01	0.41
1:E:50:THR:HG21	1:E:59:GLU:HB2	2.01	0.41
1:D:7:LYS:HB2	1:D:11:ASP:HB3	2.02	0.41
1:C:77:VAL:HG12	1:C:506:TYR:HB3	2.02	0.41
1:K:117:LYS:HZ2	1:K:121:ASP:CG	2.24	0.41
1:E:220:ILE:HD12	1:E:248:LEU:HD23	2.01	0.41
1:E:77:VAL:HG12	1:E:506:TYR:HB3	2.03	0.41
1:M:117:LYS:HZ2	1:M:121:ASP:CG	2.24	0.41
1:G:77:VAL:HG12	1:G:506:TYR:HB3	2.02	0.41
1:E:285:ARG:HH11	1:E:285:ARG:HG3	1.85	0.41
1:H:268:ARG:NE	1:H:268:ARG:HA	2.35	0.41
1:M:202:PRO:O	1:M:205:ILE:HB	2.20	0.41
1:H:202:PRO:O	1:H:205:ILE:HB	2.20	0.41
1:G:147:VAL:HG22	1:G:494:LEU:CD1	2.46	0.41
1:B:213:VAL:CG1	1:B:325:ILE:HB	2.50	0.41
1:C:213:VAL:CG1	1:C:325:ILE:HB	2.50	0.41
1:J:126:ALA:HB3	1:J:426:LEU:HD22	2.03	0.41
1:B:383:ALA:HB3	1:B:389:MET:N	2.35	0.41
1:D:51:LYS:HG2	1:D:52:ASP:H	1.85	0.41
1:K:34:LYS:HZ1	1:K:483:GLU:CD	2.23	0.41
1:M:66:PHE:CZ	1:M:522:THR:HG22	2.55	0.41
1:G:15:LYS:HB3	1:G:66:PHE:HB3	2.01	0.41
1:E:13:ARG:CG	1:E:104:LEU:HD22	2.51	0.41
1:I:50:THR:HG1	1:I:51:LYS:N	2.18	0.41
1:A:218:PRO:HG2	1:A:323:VAL:HG23	2.03	0.41
3:N:1526:PO4:P	4:N:1527:ATP:PG	3.19	0.41
1:M:323:VAL:HG22	1:M:332:ILE:HA	2.02	0.41
1:J:323:VAL:HG22	1:J:332:ILE:HA	2.02	0.41
1:K:126:ALA:HB3	1:K:426:LEU:HD22	2.03	0.41
1:F:106:ALA:HB1	1:F:116:LEU:HD21	2.01	0.41
1:J:152:ALA:HB1	1:J:155:ASP:CA	2.50	0.41
1:B:349:ILE:HB	1:B:369:VAL:HG12	2.01	0.41
1:C:85:ALA:HB1	1:C:499:VAL:HA	2.03	0.41
1:G:383:ALA:HB3	1:G:389:MET:CA	2.51	0.41
1:A:51:LYS:HG2	1:A:52:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:66:PHE:CZ	1:N:522:THR:HG22	2.55	0.41
1:I:294:THR:HG21	1:I:345:ARG:HG3	2.02	0.41
1:I:19:GLY:HA2	1:I:62:LEU:CD1	2.50	0.41
1:H:23:LEU:O	1:H:27:VAL:HG23	2.20	0.41
1:E:147:VAL:HG22	1:E:494:LEU:CD1	2.46	0.41
1:G:138:CYS:SG	1:G:407:VAL:HA	2.60	0.41
1:E:206:ASN:ND2	1:E:214:GLU:H	2.18	0.41
1:B:199:TYR:CD2	1:B:327:LYS:HA	2.55	0.41
1:A:166:MET:HA	1:A:175:ILE:HD11	2.03	0.41
1:D:85:ALA:HB1	1:D:499:VAL:HA	2.03	0.41
1:B:383:ALA:HB3	1:B:389:MET:CA	2.51	0.41
1:A:383:ALA:HB3	1:A:389:MET:CA	2.51	0.41
1:E:294:THR:HG21	1:E:345:ARG:HG3	2.03	0.41
1:F:383:ALA:HB3	1:F:389:MET:CA	2.51	0.41
1:D:294:THR:HG21	1:D:345:ARG:HG3	2.02	0.41
1:I:77:VAL:HG12	1:I:506:TYR:HB3	2.03	0.41
1:F:15:LYS:HB3	1:F:66:PHE:HB3	2.01	0.41
1:F:85:ALA:O	1:F:499:VAL:HG12	2.21	0.41
1:H:281:PHE:HA	1:H:285:ARG:HB2	2.03	0.41
3:F:1527:PO4:P	4:F:1528:ATP:PG	3.19	0.41
3:H:1526:PO4:P	4:H:1527:ATP:PG	3.19	0.41
1:I:202:PRO:O	1:I:205:ILE:HB	2.20	0.41
1:B:206:ASN:ND2	1:B:214:GLU:H	2.18	0.41
1:A:206:ASN:HB2	1:A:213:VAL:CA	2.49	0.41
1:G:199:TYR:CD2	1:G:327:LYS:HA	2.56	0.41
1:I:126:ALA:HB3	1:I:426:LEU:HD22	2.03	0.41
1:B:166:MET:HA	1:B:175:ILE:HD11	2.03	0.41
1:E:383:ALA:HB3	1:E:389:MET:N	2.36	0.41
1:E:51:LYS:HG2	1:E:52:ASP:H	1.85	0.41
1:B:13:ARG:CG	1:B:104:LEU:HD22	2.51	0.41
1:E:19:GLY:HA2	1:E:62:LEU:CD1	2.50	0.41
1:M:281:PHE:HA	1:M:285:ARG:HB2	2.03	0.41
1:H:294:THR:HG21	1:H:345:ARG:HG3	2.02	0.41
1:N:268:ARG:HA	1:N:268:ARG:NE	2.35	0.41
1:L:281:PHE:HA	1:L:285:ARG:HB2	2.03	0.41
1:J:77:VAL:HG12	1:J:506:TYR:HB3	2.03	0.41
1:E:85:ALA:O	1:E:499:VAL:HG12	2.21	0.41
1:N:281:PHE:HA	1:N:285:ARG:HB2	2.03	0.41
3:B:1527:PO4:P	4:B:1528:ATP:PG	3.19	0.41
1:M:205:ILE:HG23	1:M:211:GLY:HA2	2.03	0.41
1:B:426:LEU:HB2	1:B:444:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ASN:HB2	1:B:213:VAL:CA	2.49	0.41
1:G:378:VAL:HG11	1:G:380:LYS:HZ2	1.85	0.41
1:L:126:ALA:HB3	1:L:426:LEU:HD22	2.03	0.41
1:C:166:MET:HA	1:C:175:ILE:HD11	2.03	0.41
1:A:197:ARG:HD2	1:A:277:LYS:HB2	2.03	0.41
1:G:197:ARG:HD2	1:G:277:LYS:HB2	2.03	0.41
1:E:197:ARG:HD2	1:E:277:LYS:HB2	2.03	0.41
1:D:197:ARG:HD2	1:D:277:LYS:HB2	2.03	0.41
1:L:66:PHE:CZ	1:L:522:THR:HG22	2.55	0.41
1:H:77:VAL:HG12	1:H:506:TYR:HB3	2.03	0.41
1:A:13:ARG:CG	1:A:104:LEU:HD22	2.51	0.41
1:B:240:VAL:HA	1:B:243:ALA:HB3	2.02	0.41
1:B:7:LYS:HB2	1:B:11:ASP:HB3	2.01	0.41
1:F:285:ARG:HG3	1:F:285:ARG:HH11	1.85	0.41
1:N:77:VAL:HG12	1:N:506:TYR:HB3	2.03	0.41
3:C:1527:PO4:P	4:C:1528:ATP:PG	3.19	0.40
1:A:378:VAL:HG11	1:A:380:LYS:HZ2	1.85	0.40
1:L:323:VAL:HG22	1:L:332:ILE:HA	2.02	0.40
1:B:197:ARG:HD2	1:B:277:LYS:HB2	2.03	0.40
1:C:197:ARG:HD2	1:C:277:LYS:HB2	2.03	0.40
1:I:281:PHE:HA	1:I:285:ARG:HB2	2.03	0.40
1:B:77:VAL:HG12	1:B:506:TYR:HB3	2.03	0.40
1:C:226:LYS:HA	1:C:252:GLU:H	1.86	0.40
1:B:85:ALA:O	1:B:499:VAL:HG12	2.21	0.40
3:A:1527:PO4:P	4:A:1528:ATP:PG	3.19	0.40
1:A:199:TYR:CD2	1:A:327:LYS:HA	2.56	0.40
1:K:323:VAL:HG22	1:K:332:ILE:HA	2.02	0.40
1:F:197:ARG:HD2	1:F:277:LYS:HB2	2.03	0.40
1:J:117:LYS:HZ2	1:J:121:ASP:CG	2.25	0.40
1:K:66:PHE:CZ	1:K:522:THR:HG22	2.55	0.40
1:E:15:LYS:HB3	1:E:66:PHE:HB3	2.02	0.40
1:N:197:ARG:HA	1:N:197:ARG:HD3	1.95	0.40
3:D:1527:PO4:P	4:D:1528:ATP:PG	3.19	0.40
1:J:205:ILE:HG23	1:J:211:GLY:HA2	2.04	0.40
1:N:205:ILE:HG23	1:N:211:GLY:HA2	2.04	0.40
1:F:426:LEU:HB2	1:F:444:LEU:CD2	2.52	0.40
1:C:426:LEU:HB2	1:C:444:LEU:CD2	2.52	0.40
1:D:383:ALA:HB3	1:D:389:MET:CA	2.51	0.40
1:D:383:ALA:HB3	1:D:389:MET:N	2.35	0.40
1:E:383:ALA:HB3	1:E:389:MET:CA	2.51	0.40
1:C:383:ALA:HB3	1:C:389:MET:CA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:LYS:HG2	1:G:52:ASP:H	1.85	0.40
1:C:7:LYS:HB2	1:C:11:ASP:HB3	2.02	0.40
1:A:7:LYS:HB2	1:A:11:ASP:HB3	2.01	0.40
1:J:33:PRO:HG3	4:J:1527:ATP:C4	2.57	0.40
1:H:50:THR:HG1	1:H:51:LYS:N	2.18	0.40
1:K:205:ILE:HG23	1:K:211:GLY:HA2	2.03	0.40
1:I:205:ILE:HG23	1:I:211:GLY:HA2	2.03	0.40
1:H:205:ILE:HG23	1:H:211:GLY:HA2	2.03	0.40
1:M:206:ASN:HD22	1:M:214:GLU:H	1.70	0.40
1:L:206:ASN:HD22	1:L:214:GLU:H	1.70	0.40
1:A:77:VAL:HG12	1:A:506:TYR:HB3	2.03	0.40
1:K:281:PHE:HA	1:K:285:ARG:HB2	2.03	0.40
1:N:206:ASN:HD22	1:N:214:GLU:H	1.70	0.40
1:M:85:ALA:HB1	1:M:499:VAL:HA	2.02	0.40
1:A:19:GLY:HA2	1:A:62:LEU:HD13	2.04	0.40
1:L:231:ARG:O	1:L:235:PRO:HD2	2.22	0.40
1:K:166:MET:HA	1:K:175:ILE:HD11	2.04	0.40
1:J:166:MET:HA	1:J:175:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	B	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	C	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	D	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	E	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	F	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	39	80
1	H	518/548 (94%)	513 (99%)	5 (1%)	0	100	100
1	I	518/548 (94%)	513 (99%)	5 (1%)	0	100	100
1	J	518/548 (94%)	513 (99%)	5 (1%)	0	100	100
1	K	518/548 (94%)	513 (99%)	5 (1%)	0	100	100
1	L	518/548 (94%)	513 (99%)	5 (1%)	0	100	100
1	M	518/548 (94%)	513 (99%)	5 (1%)	0	100	100
1	N	518/548 (94%)	513 (99%)	5 (1%)	0	100	100
All	All	7280/7672 (95%)	7217 (99%)	49 (1%)	14 (0%)	56	86

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ALA
1	B	243	ALA
1	C	243	ALA
1	D	243	ALA
1	E	243	ALA
1	F	243	ALA
1	G	243	ALA
1	A	52	ASP
1	B	52	ASP
1	C	52	ASP
1	D	52	ASP
1	E	52	ASP
1	F	52	ASP
1	G	52	ASP

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 PDB entries followed by that with respect to all EM entries.

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	402/414 (97%)	358 (89%)	44 (11%)	8	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	402/414 (97%)	358 (89%)	44 (11%)	8	35
1	C	402/414 (97%)	359 (89%)	43 (11%)	8	36
1	D	402/414 (97%)	357 (89%)	45 (11%)	7	33
1	E	402/414 (97%)	359 (89%)	43 (11%)	8	36
1	F	402/414 (97%)	359 (89%)	43 (11%)	8	36
1	G	402/414 (97%)	359 (89%)	43 (11%)	8	36
1	H	402/414 (97%)	370 (92%)	32 (8%)	15	50
1	I	402/414 (97%)	370 (92%)	32 (8%)	15	50
1	J	402/414 (97%)	370 (92%)	32 (8%)	15	50
1	K	402/414 (97%)	370 (92%)	32 (8%)	15	50
1	L	402/414 (97%)	370 (92%)	32 (8%)	15	50
1	M	402/414 (97%)	370 (92%)	32 (8%)	15	50
1	N	402/414 (97%)	369 (92%)	33 (8%)	14	49
All	All	5628/5796 (97%)	5098 (91%)	530 (9%)	15	42

All (530) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	25	ASP
1	A	31	LEU
1	A	40	LEU
1	A	52	ASP
1	A	63	GLU
1	A	65	LYS
1	A	79	SER
1	A	82	ASN
1	A	89	THR
1	A	115	ASP
1	A	136	VAL
1	A	142	LYS
1	A	156	GLU
1	A	168	LYS
1	A	171	LYS
1	A	205	ILE
1	A	207	LYS
1	A	213	VAL

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Mol	Chain	Res	Type
1	A	214	GLU
1	A	219	PHE
1	A	231	ARG
1	A	238	GLU
1	A	242	LYS
1	A	245	LYS
1	A	246	PRO
1	A	257	GLU
1	A	268	ARG
1	A	270	ILE
1	A	272	LYS
1	A	290	GLN
1	A	327	LYS
1	A	328	ASP
1	A	334	ASP
1	A	350	ARG
1	A	358	SER
1	A	421	ARG
1	A	430	ARG
1	A	435	ASP
1	A	460	GLU
1	A	484	GLU
1	A	494	LEU
1	A	504	LEU
1	A	518	GLU
1	B	7	LYS
1	B	25	ASP
1	B	31	LEU
1	B	40	LEU
1	B	52	ASP
1	B	63	GLU
1	B	65	LYS
1	B	79	SER
1	B	82	ASN
1	B	89	THR
1	B	115	ASP
1	B	136	VAL
1	B	142	LYS
1	B	156	GLU
1	B	168	LYS
1	B	171	LYS
1	B	205	ILE

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Mol	Chain	Res	Type
1	B	207	LYS
1	B	213	VAL
1	B	214	GLU
1	B	219	PHE
1	B	231	ARG
1	B	238	GLU
1	B	242	LYS
1	B	245	LYS
1	B	246	PRO
1	B	257	GLU
1	B	268	ARG
1	B	270	ILE
1	B	290	GLN
1	B	303	GLU
1	B	327	LYS
1	B	328	ASP
1	B	334	ASP
1	B	350	ARG
1	B	358	SER
1	B	421	ARG
1	B	430	ARG
1	B	435	ASP
1	B	460	GLU
1	B	484	GLU
1	B	494	LEU
1	B	504	LEU
1	B	518	GLU
1	C	7	LYS
1	C	25	ASP
1	C	31	LEU
1	C	40	LEU
1	C	52	ASP
1	C	63	GLU
1	C	65	LYS
1	C	79	SER
1	C	82	ASN
1	C	89	THR
1	C	115	ASP
1	C	136	VAL
1	C	142	LYS
1	C	156	GLU
1	C	168	LYS

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Mol	Chain	Res	Type
1	C	171	LYS
1	C	205	ILE
1	C	207	LYS
1	C	213	VAL
1	C	214	GLU
1	C	219	PHE
1	C	231	ARG
1	C	238	GLU
1	C	242	LYS
1	C	245	LYS
1	C	246	PRO
1	C	257	GLU
1	C	268	ARG
1	C	270	ILE
1	C	290	GLN
1	C	327	LYS
1	C	328	ASP
1	C	334	ASP
1	C	350	ARG
1	C	358	SER
1	C	421	ARG
1	C	430	ARG
1	C	435	ASP
1	C	460	GLU
1	C	484	GLU
1	C	494	LEU
1	C	504	LEU
1	C	518	GLU
1	D	7	LYS
1	D	25	ASP
1	D	31	LEU
1	D	40	LEU
1	D	52	ASP
1	D	63	GLU
1	D	65	LYS
1	D	79	SER
1	D	82	ASN
1	D	89	THR
1	D	115	ASP
1	D	136	VAL
1	D	142	LYS
1	D	156	GLU

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Mol	Chain	Res	Type
1	D	168	LYS
1	D	171	LYS
1	D	205	ILE
1	D	207	LYS
1	D	213	VAL
1	D	214	GLU
1	D	219	PHE
1	D	231	ARG
1	D	238	GLU
1	D	242	LYS
1	D	245	LYS
1	D	246	PRO
1	D	257	GLU
1	D	268	ARG
1	D	270	ILE
1	D	272	LYS
1	D	290	GLN
1	D	303	GLU
1	D	327	LYS
1	D	328	ASP
1	D	334	ASP
1	D	350	ARG
1	D	358	SER
1	D	421	ARG
1	D	430	ARG
1	D	435	ASP
1	D	460	GLU
1	D	484	GLU
1	D	494	LEU
1	D	504	LEU
1	D	518	GLU
1	E	7	LYS
1	E	25	ASP
1	E	31	LEU
1	E	40	LEU
1	E	52	ASP
1	E	63	GLU
1	E	65	LYS
1	E	79	SER
1	E	82	ASN
1	E	89	THR
1	E	115	ASP

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Mol	Chain	Res	Type
1	E	136	VAL
1	E	142	LYS
1	E	156	GLU
1	E	168	LYS
1	E	171	LYS
1	E	205	ILE
1	E	207	LYS
1	E	213	VAL
1	E	214	GLU
1	E	219	PHE
1	E	231	ARG
1	E	238	GLU
1	E	242	LYS
1	E	245	LYS
1	E	246	PRO
1	E	257	GLU
1	E	268	ARG
1	E	270	ILE
1	E	290	GLN
1	E	327	LYS
1	E	328	ASP
1	E	334	ASP
1	E	350	ARG
1	E	358	SER
1	E	421	ARG
1	E	430	ARG
1	E	435	ASP
1	E	460	GLU
1	E	484	GLU
1	E	494	LEU
1	E	504	LEU
1	E	518	GLU
1	F	7	LYS
1	F	25	ASP
1	F	31	LEU
1	F	40	LEU
1	F	52	ASP
1	F	63	GLU
1	F	65	LYS
1	F	79	SER
1	F	82	ASN
1	F	89	THR

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Mol	Chain	Res	Type
1	F	115	ASP
1	F	136	VAL
1	F	142	LYS
1	F	156	GLU
1	F	168	LYS
1	F	171	LYS
1	F	205	ILE
1	F	207	LYS
1	F	213	VAL
1	F	214	GLU
1	F	219	PHE
1	F	231	ARG
1	F	238	GLU
1	F	242	LYS
1	F	245	LYS
1	F	246	PRO
1	F	257	GLU
1	F	268	ARG
1	F	270	ILE
1	F	290	GLN
1	F	327	LYS
1	F	328	ASP
1	F	334	ASP
1	F	350	ARG
1	F	358	SER
1	F	421	ARG
1	F	430	ARG
1	F	435	ASP
1	F	460	GLU
1	F	484	GLU
1	F	494	LEU
1	F	504	LEU
1	F	518	GLU
1	G	7	LYS
1	G	25	ASP
1	G	31	LEU
1	G	40	LEU
1	G	52	ASP
1	G	63	GLU
1	G	65	LYS
1	G	79	SER
1	G	82	ASN

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Mol	Chain	Res	Type
1	G	89	THR
1	G	115	ASP
1	G	136	VAL
1	G	142	LYS
1	G	156	GLU
1	G	168	LYS
1	G	171	LYS
1	G	205	ILE
1	G	207	LYS
1	G	213	VAL
1	G	214	GLU
1	G	219	PHE
1	G	231	ARG
1	G	238	GLU
1	G	242	LYS
1	G	245	LYS
1	G	246	PRO
1	G	257	GLU
1	G	268	ARG
1	G	270	ILE
1	G	290	GLN
1	G	327	LYS
1	G	328	ASP
1	G	334	ASP
1	G	350	ARG
1	G	358	SER
1	G	421	ARG
1	G	430	ARG
1	G	435	ASP
1	G	460	GLU
1	G	484	GLU
1	G	494	LEU
1	G	504	LEU
1	G	518	GLU
1	H	4	LYS
1	H	25	ASP
1	H	31	LEU
1	H	37	ASN
1	H	50	THR
1	H	55	SER
1	H	115	ASP
1	H	130	GLU

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Mol	Chain	Res	Type
1	H	142	LYS
1	H	156	GLU
1	H	168	LYS
1	H	169	VAL
1	H	171	LYS
1	H	190	VAL
1	H	207	LYS
1	H	213	VAL
1	H	228	SER
1	H	253	ASP
1	H	254	VAL
1	H	290	GLN
1	H	295	LEU
1	H	327	LYS
1	H	328	ASP
1	H	334	ASP
1	H	350	ARG
1	H	358	SER
1	H	421	ARG
1	H	473	ASP
1	H	484	GLU
1	H	504	LEU
1	H	520	MET
1	H	523	ASP
1	I	4	LYS
1	I	25	ASP
1	I	31	LEU
1	I	37	ASN
1	I	50	THR
1	I	55	SER
1	I	115	ASP
1	I	130	GLU
1	I	142	LYS
1	I	156	GLU
1	I	168	LYS
1	I	169	VAL
1	I	171	LYS
1	I	190	VAL
1	I	207	LYS
1	I	213	VAL
1	I	228	SER
1	I	253	ASP

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Mol	Chain	Res	Type
1	I	254	VAL
1	I	290	GLN
1	I	295	LEU
1	I	327	LYS
1	I	328	ASP
1	I	334	ASP
1	I	350	ARG
1	I	358	SER
1	I	421	ARG
1	I	473	ASP
1	I	484	GLU
1	I	504	LEU
1	I	520	MET
1	I	523	ASP
1	J	4	LYS
1	J	25	ASP
1	J	31	LEU
1	J	37	ASN
1	J	50	THR
1	J	55	SER
1	J	115	ASP
1	J	130	GLU
1	J	142	LYS
1	J	156	GLU
1	J	168	LYS
1	J	169	VAL
1	J	171	LYS
1	J	190	VAL
1	J	207	LYS
1	J	213	VAL
1	J	228	SER
1	J	253	ASP
1	J	254	VAL
1	J	290	GLN
1	J	295	LEU
1	J	327	LYS
1	J	328	ASP
1	J	334	ASP
1	J	350	ARG
1	J	358	SER
1	J	421	ARG
1	J	473	ASP

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Mol	Chain	Res	Type
1	J	484	GLU
1	J	504	LEU
1	J	520	MET
1	J	523	ASP
1	K	4	LYS
1	K	25	ASP
1	K	31	LEU
1	K	37	ASN
1	K	50	THR
1	K	55	SER
1	K	115	ASP
1	K	130	GLU
1	K	142	LYS
1	K	156	GLU
1	K	168	LYS
1	K	169	VAL
1	K	171	LYS
1	K	190	VAL
1	K	207	LYS
1	K	213	VAL
1	K	228	SER
1	K	253	ASP
1	K	254	VAL
1	K	290	GLN
1	K	295	LEU
1	K	327	LYS
1	K	328	ASP
1	K	334	ASP
1	K	350	ARG
1	K	358	SER
1	K	421	ARG
1	K	473	ASP
1	K	484	GLU
1	K	504	LEU
1	K	520	MET
1	K	523	ASP
1	L	4	LYS
1	L	25	ASP
1	L	31	LEU
1	L	37	ASN
1	L	50	THR
1	L	55	SER

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Mol	Chain	Res	Type
1	L	115	ASP
1	L	130	GLU
1	L	142	LYS
1	L	156	GLU
1	L	168	LYS
1	L	169	VAL
1	L	171	LYS
1	L	190	VAL
1	L	207	LYS
1	L	213	VAL
1	L	228	SER
1	L	253	ASP
1	L	254	VAL
1	L	290	GLN
1	L	295	LEU
1	L	327	LYS
1	L	328	ASP
1	L	334	ASP
1	L	350	ARG
1	L	358	SER
1	L	421	ARG
1	L	473	ASP
1	L	484	GLU
1	L	504	LEU
1	L	520	MET
1	L	523	ASP
1	M	4	LYS
1	M	25	ASP
1	M	31	LEU
1	M	37	ASN
1	M	50	THR
1	M	55	SER
1	M	115	ASP
1	M	130	GLU
1	M	142	LYS
1	M	156	GLU
1	M	168	LYS
1	M	169	VAL
1	M	171	LYS
1	M	190	VAL
1	M	207	LYS
1	M	213	VAL

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Mol	Chain	Res	Type
1	M	228	SER
1	M	253	ASP
1	M	254	VAL
1	M	290	GLN
1	M	295	LEU
1	M	327	LYS
1	M	328	ASP
1	M	334	ASP
1	M	350	ARG
1	M	358	SER
1	M	421	ARG
1	M	473	ASP
1	M	484	GLU
1	M	504	LEU
1	M	520	MET
1	M	523	ASP
1	N	4	LYS
1	N	25	ASP
1	N	31	LEU
1	N	37	ASN
1	N	50	THR
1	N	55	SER
1	N	115	ASP
1	N	130	GLU
1	N	142	LYS
1	N	156	GLU
1	N	168	LYS
1	N	169	VAL
1	N	171	LYS
1	N	190	VAL
1	N	207	LYS
1	N	213	VAL
1	N	228	SER
1	N	253	ASP
1	N	254	VAL
1	N	290	GLN
1	N	295	LEU
1	N	327	LYS
1	N	328	ASP
1	N	334	ASP
1	N	350	ARG
1	N	358	SER

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Mol	Chain	Res	Type
1	N	421	ARG
1	N	473	ASP
1	N	479	ASN
1	N	484	GLU
1	N	504	LEU
1	N	520	MET
1	N	523	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	453	GLN
1	B	453	GLN
1	C	453	GLN
1	D	453	GLN
1	E	453	GLN
1	F	453	GLN
1	G	453	GLN
1	H	453	GLN
1	I	453	GLN
1	J	453	GLN
1	K	453	GLN
1	L	453	GLN
1	M	453	GLN
1	N	453	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 14 are modelled with single atom and 14 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ATP	A	1528	2	26,33,33	0.89	1 (3%)	26,52,52	1.27	4 (15%)
4	ATP	B	1528	2	26,33,33	0.90	1 (3%)	26,52,52	1.27	4 (15%)
4	ATP	C	1528	2	26,33,33	0.90	1 (3%)	26,52,52	1.27	4 (15%)
4	ATP	D	1528	2	26,33,33	0.88	1 (3%)	26,52,52	1.27	4 (15%)
4	ATP	E	1528	2	26,33,33	0.90	1 (3%)	26,52,52	1.27	4 (15%)
4	ATP	F	1528	2	26,33,33	0.90	1 (3%)	26,52,52	1.27	4 (15%)
4	ATP	G	1528	2	26,33,33	0.89	1 (3%)	26,52,52	1.27	4 (15%)
4	ATP	H	1527	2	26,33,33	0.98	1 (3%)	26,52,52	1.34	5 (19%)
4	ATP	I	1527	2	26,33,33	0.82	0	26,52,52	1.08	2 (7%)
4	ATP	J	1527	2	26,33,33	0.83	1 (3%)	26,52,52	1.11	2 (7%)
4	ATP	K	1527	2	26,33,33	0.89	0	26,52,52	1.42	6 (23%)
4	ATP	L	1527	2	26,33,33	0.82	1 (3%)	26,52,52	1.08	2 (7%)
4	ATP	M	1527	2	26,33,33	6.77	5 (19%)	26,52,52	2.99	6 (23%)
4	ATP	N	1527	2	26,33,33	1.00	1 (3%)	26,52,52	1.39	6 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	1528	2	-	0/18/38/38	0/3/3/3
4	ATP	B	1528	2	-	0/18/38/38	0/3/3/3
4	ATP	C	1528	2	-	0/18/38/38	0/3/3/3
4	ATP	D	1528	2	-	0/18/38/38	0/3/3/3
4	ATP	E	1528	2	-	0/18/38/38	0/3/3/3
4	ATP	F	1528	2	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	G	1528	2	-	0/18/38/38	0/3/3/3
4	ATP	H	1527	2	-	0/18/38/38	0/3/3/3
4	ATP	I	1527	2	-	0/18/38/38	0/3/3/3
4	ATP	J	1527	2	-	0/18/38/38	0/3/3/3
4	ATP	K	1527	2	-	0/18/38/38	0/3/3/3
4	ATP	L	1527	2	-	0/18/38/38	0/3/3/3
4	ATP	M	1527	2	-	0/18/38/38	0/3/3/3
4	ATP	N	1527	2	-	0/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	1527	ATP	C2'-C1'	-3.47	1.48	1.53
4	H	1527	ATP	C2'-C1'	-3.27	1.48	1.53
4	C	1528	ATP	C2'-C1'	-2.78	1.49	1.53
4	F	1528	ATP	C2'-C1'	-2.77	1.49	1.53
4	E	1528	ATP	C2'-C1'	-2.77	1.49	1.53
4	G	1528	ATP	C2'-C1'	-2.75	1.49	1.53
4	B	1528	ATP	C2'-C1'	-2.75	1.49	1.53
4	A	1528	ATP	C2'-C1'	-2.74	1.49	1.53
4	D	1528	ATP	C2'-C1'	-2.72	1.49	1.53
4	M	1527	ATP	C4-N3	-2.14	1.32	1.35
4	L	1527	ATP	C2'-C1'	-2.04	1.50	1.53
4	J	1527	ATP	C2'-C1'	-2.02	1.50	1.53
4	M	1527	ATP	C5'-C4'	2.07	1.58	1.51
4	M	1527	ATP	C5-N7	15.22	1.93	1.39
4	M	1527	ATP	C8-N7	19.77	1.72	1.34
4	M	1527	ATP	C5-C4	23.27	1.93	1.40

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1527	ATP	O3G-PG-O2G	-3.79	93.53	107.44
4	K	1527	ATP	C4'-O4'-C1'	-3.54	105.89	109.64
4	N	1527	ATP	C1'-N9-C4	-2.94	123.53	126.81
4	H	1527	ATP	C4'-O4'-C1'	-2.53	106.96	109.64
4	N	1527	ATP	C4'-O4'-C1'	-2.41	107.08	109.64
4	H	1527	ATP	C1'-N9-C4	-2.19	124.36	126.81
4	C	1528	ATP	C1'-N9-C4	-2.07	124.50	126.81
4	D	1528	ATP	C1'-N9-C4	-2.05	124.52	126.81
4	F	1528	ATP	C1'-N9-C4	-2.05	124.52	126.81
4	E	1528	ATP	C1'-N9-C4	-2.04	124.53	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1528	ATP	C1'-N9-C4	-2.03	124.55	126.81
4	A	1528	ATP	C1'-N9-C4	-2.02	124.55	126.81
4	G	1528	ATP	C1'-N9-C4	-2.01	124.56	126.81
4	E	1528	ATP	O4'-C1'-N9	2.04	111.97	108.11
4	N	1527	ATP	O3'-C3'-C4'	2.04	117.11	111.01
4	C	1528	ATP	O4'-C1'-N9	2.05	111.98	108.11
4	F	1528	ATP	O4'-C1'-N9	2.07	112.02	108.11
4	B	1528	ATP	O4'-C1'-N9	2.08	112.03	108.11
4	G	1528	ATP	O4'-C1'-N9	2.08	112.03	108.11
4	A	1528	ATP	O4'-C1'-N9	2.09	112.05	108.11
4	D	1528	ATP	O4'-C1'-N9	2.09	112.06	108.11
4	M	1527	ATP	O2A-PA-O3A	2.12	114.34	105.27
4	K	1527	ATP	C1'-N9-C4	2.17	129.23	126.81
4	L	1527	ATP	O2A-PA-O3A	2.17	114.59	105.27
4	I	1527	ATP	O2A-PA-O3A	2.19	114.63	105.27
4	B	1528	ATP	O2A-PA-O3A	2.19	114.65	105.27
4	C	1528	ATP	O2A-PA-O3A	2.19	114.67	105.27
4	D	1528	ATP	O2A-PA-O3A	2.20	114.69	105.27
4	A	1528	ATP	O2A-PA-O3A	2.20	114.70	105.27
4	G	1528	ATP	O2A-PA-O3A	2.20	114.71	105.27
4	E	1528	ATP	O2A-PA-O3A	2.21	114.72	105.27
4	F	1528	ATP	O2A-PA-O3A	2.21	114.72	105.27
4	J	1527	ATP	O2A-PA-O3A	2.22	114.80	105.27
4	K	1527	ATP	C2'-C1'-N9	2.29	119.58	113.47
4	K	1527	ATP	O4'-C1'-N9	2.30	112.46	108.11
4	N	1527	ATP	O4'-C1'-N9	2.31	112.47	108.11
4	H	1527	ATP	O2A-PA-O3A	2.32	115.20	105.27
4	H	1527	ATP	O4'-C1'-N9	2.32	112.49	108.11
4	G	1528	ATP	O3G-PG-O2G	2.34	116.03	107.44
4	A	1528	ATP	O3G-PG-O2G	2.34	116.04	107.44
4	D	1528	ATP	O3G-PG-O2G	2.35	116.05	107.44
4	F	1528	ATP	O3G-PG-O2G	2.35	116.07	107.44
4	N	1527	ATP	O3G-PG-O2G	2.36	116.09	107.44
4	E	1528	ATP	O3G-PG-O2G	2.36	116.11	107.44
4	B	1528	ATP	O3G-PG-O2G	2.36	116.11	107.44
4	C	1528	ATP	O3G-PG-O2G	2.37	116.12	107.44
4	N	1527	ATP	O2A-PA-O3A	2.40	115.55	105.27
4	H	1527	ATP	O3G-PG-O2G	2.42	116.34	107.44
4	K	1527	ATP	O2A-PA-O3A	2.45	115.75	105.27
4	K	1527	ATP	O3G-PG-O2G	2.45	116.43	107.44
4	J	1527	ATP	O3G-PG-O2G	2.54	116.76	107.44
4	L	1527	ATP	O3G-PG-O2G	2.55	116.79	107.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1527	ATP	O3G-PG-O2G	2.55	116.81	107.44
4	M	1527	ATP	O3G-PG-O1G	2.82	119.83	110.63
4	M	1527	ATP	C2-N1-C6	3.57	125.13	118.77
4	M	1527	ATP	C1'-N9-C4	8.03	135.77	126.81
4	M	1527	ATP	N3-C2-N1	10.28	136.95	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1528	ATP	4	0
4	B	1528	ATP	4	0
4	C	1528	ATP	4	0
4	D	1528	ATP	4	0
4	E	1528	ATP	3	0
4	F	1528	ATP	4	0
4	G	1528	ATP	3	0
4	H	1527	ATP	4	0
4	I	1527	ATP	5	0
4	J	1527	ATP	5	0
4	K	1527	ATP	5	0
4	L	1527	ATP	5	0
4	M	1527	ATP	34	0
4	N	1527	ATP	5	0

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.