



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 05:37 PM UTC

PDB ID : 4AAU / pdb_00004aau
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 initial model : 1OEL

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

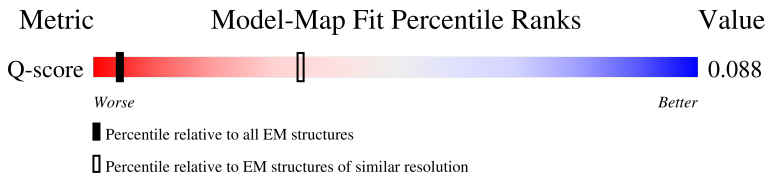
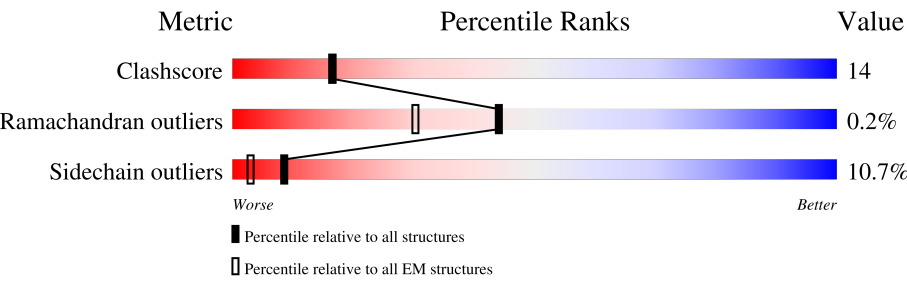
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	328 (8.00 - 9.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	14% 55% 28% 11% • •
1	B	548	15% 55% 28% 11% • •
1	C	548	14% 55% 28% 11% • •
1	D	548	14% 55% 27% 12% • •

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Mol	Chain	Length	Quality of chain
1	E	548	
1	F	548	
1	G	548	
1	H	548	
1	I	548	
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 (CCD ID: MG) (formula: Mg).

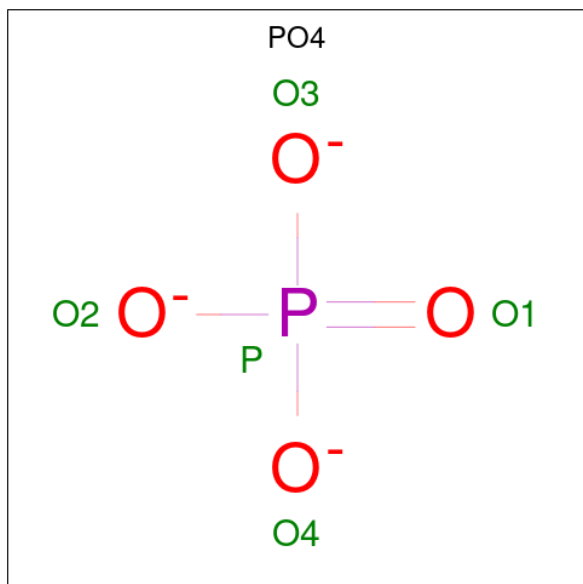
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Mg 1 1	0
2	B	1	Total Mg 1 1	0
2	C	1	Total Mg 1 1	0
2	D	1	Total Mg 1 1	0
2	E	1	Total Mg 1 1	0
2	F	1	Total Mg 1 1	0
2	G	1	Total Mg 1 1	0
2	H	1	Total Mg 1 1	0
2	I	1	Total Mg 1 1	0
2	J	1	Total Mg 1 1	0
2	K	1	Total Mg 1 1	0
2	L	1	Total Mg 1 1	0
2	M	1	Total Mg 1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

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



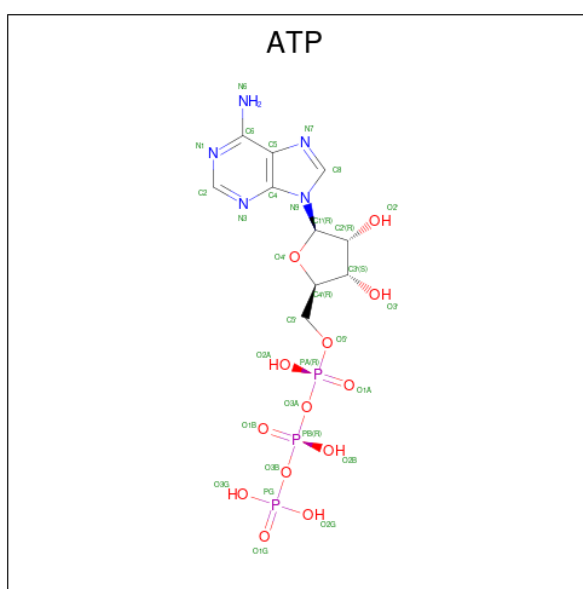
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	P	0
			1	1	
3	B	1	Total	P	0
			1	1	
3	C	1	Total	P	0
			1	1	
3	D	1	Total	P	0
			1	1	
3	E	1	Total	P	0
			1	1	
3	F	1	Total	P	0
			1	1	
3	G	1	Total	P	0
			1	1	
3	H	1	Total	P	0
			1	1	
3	I	1	Total	P	0
			1	1	
3	J	1	Total	P	0
			1	1	

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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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
4	G	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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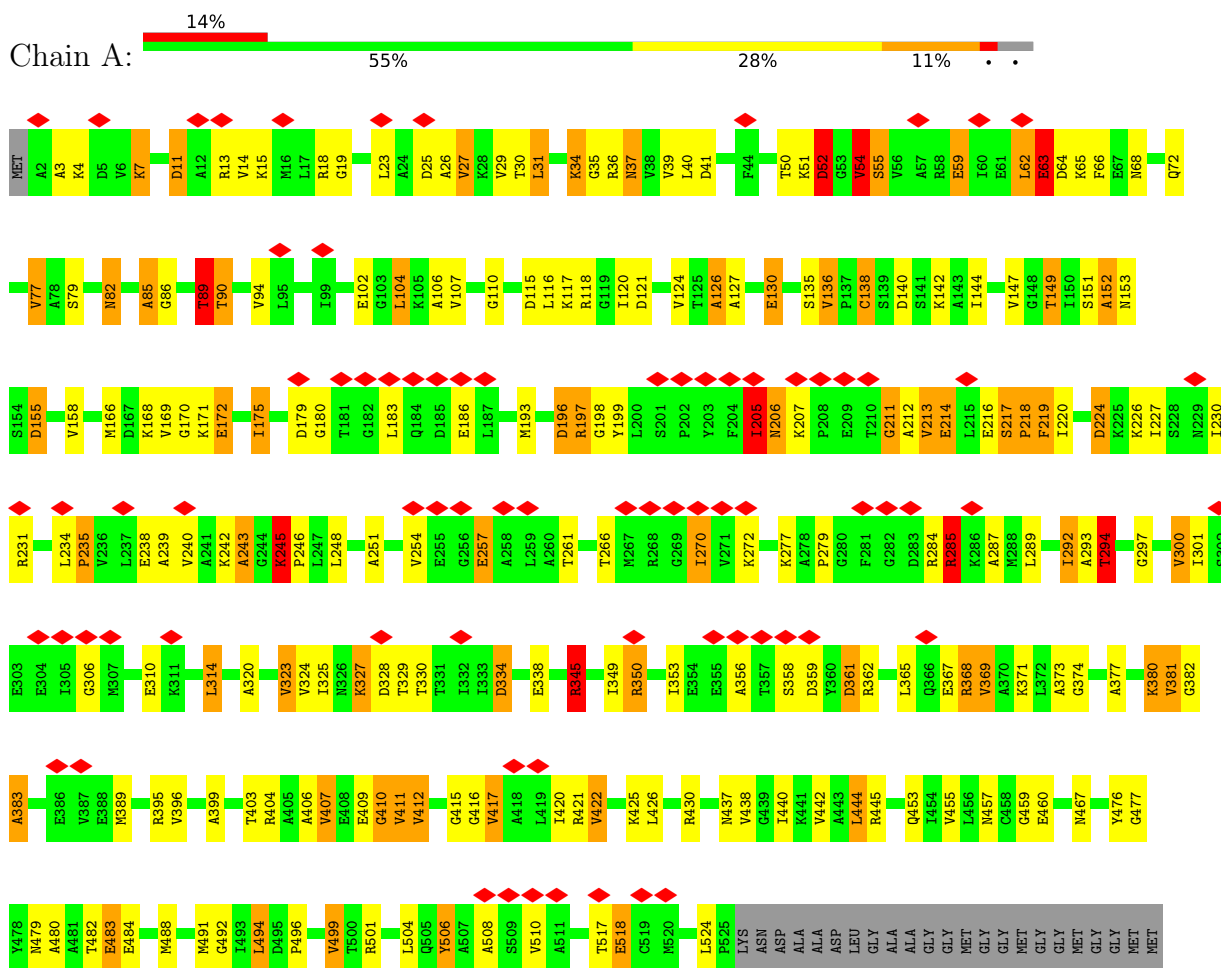
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Mol	Chain	Residues	Atoms						AltConf
4	H	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	I	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	J	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	K	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	L	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
4	M	1	Total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

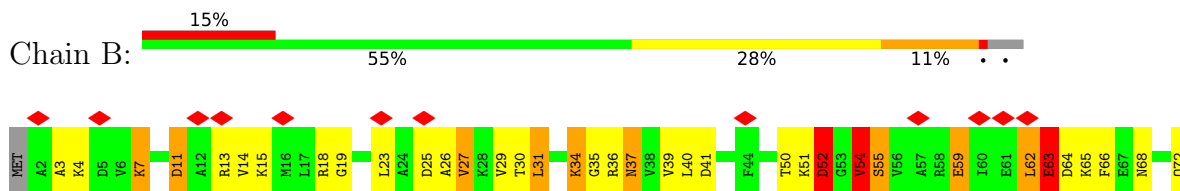
3 Residue-property plots

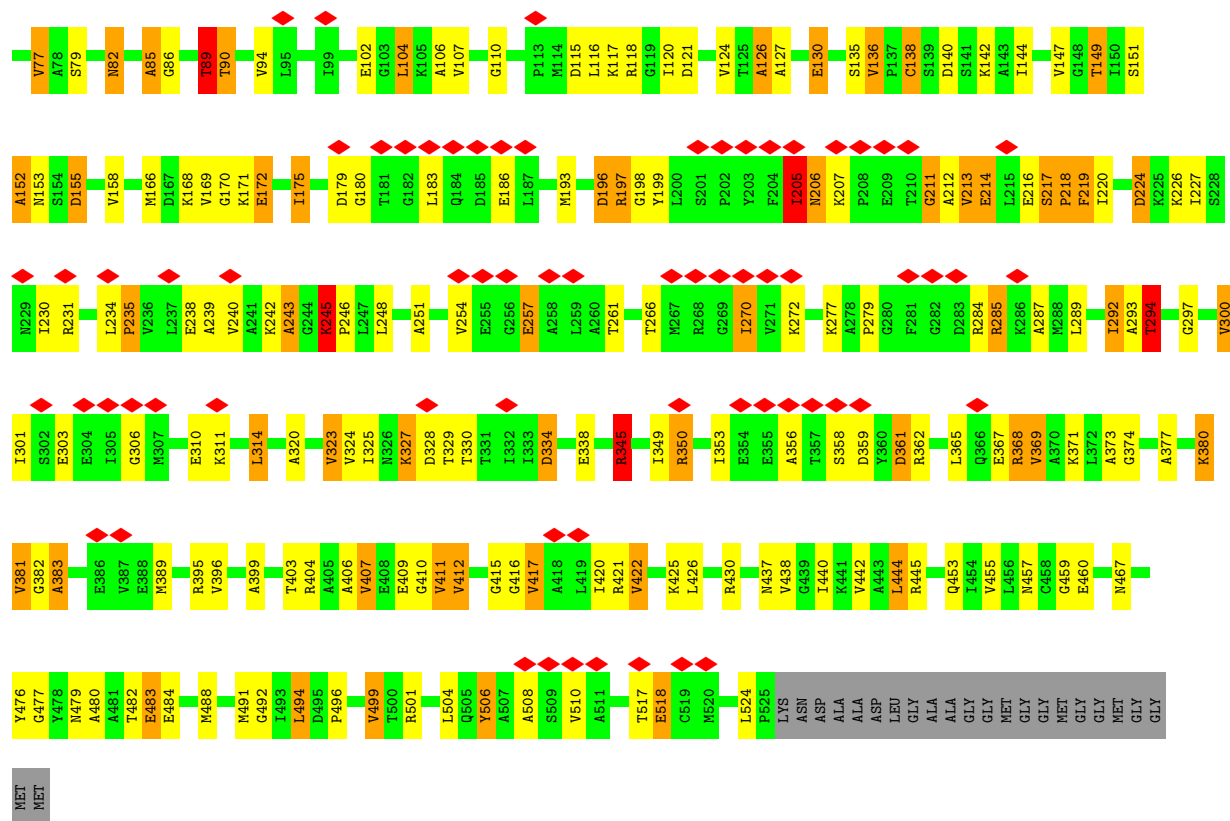
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 60 KDA CHAPERONIN

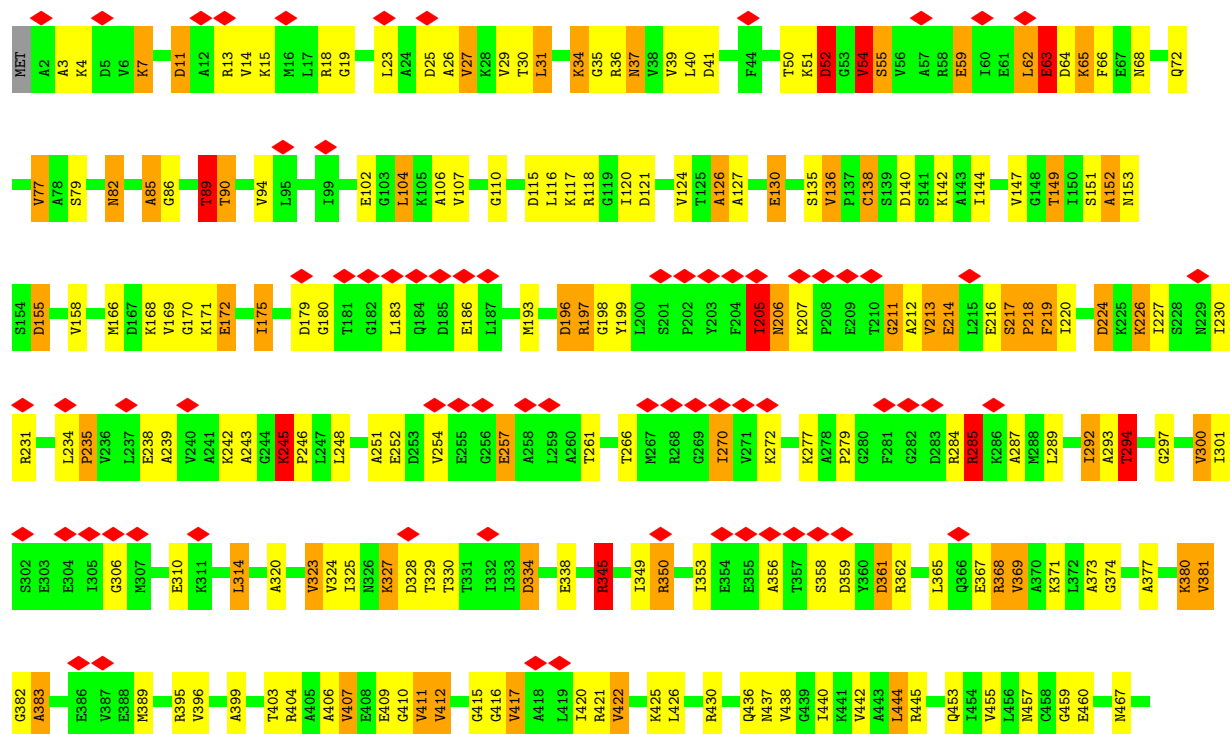


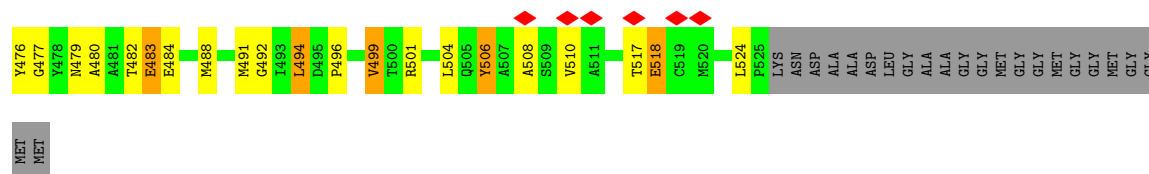
• Molecule 1: 60 KDA CHAPERONIN



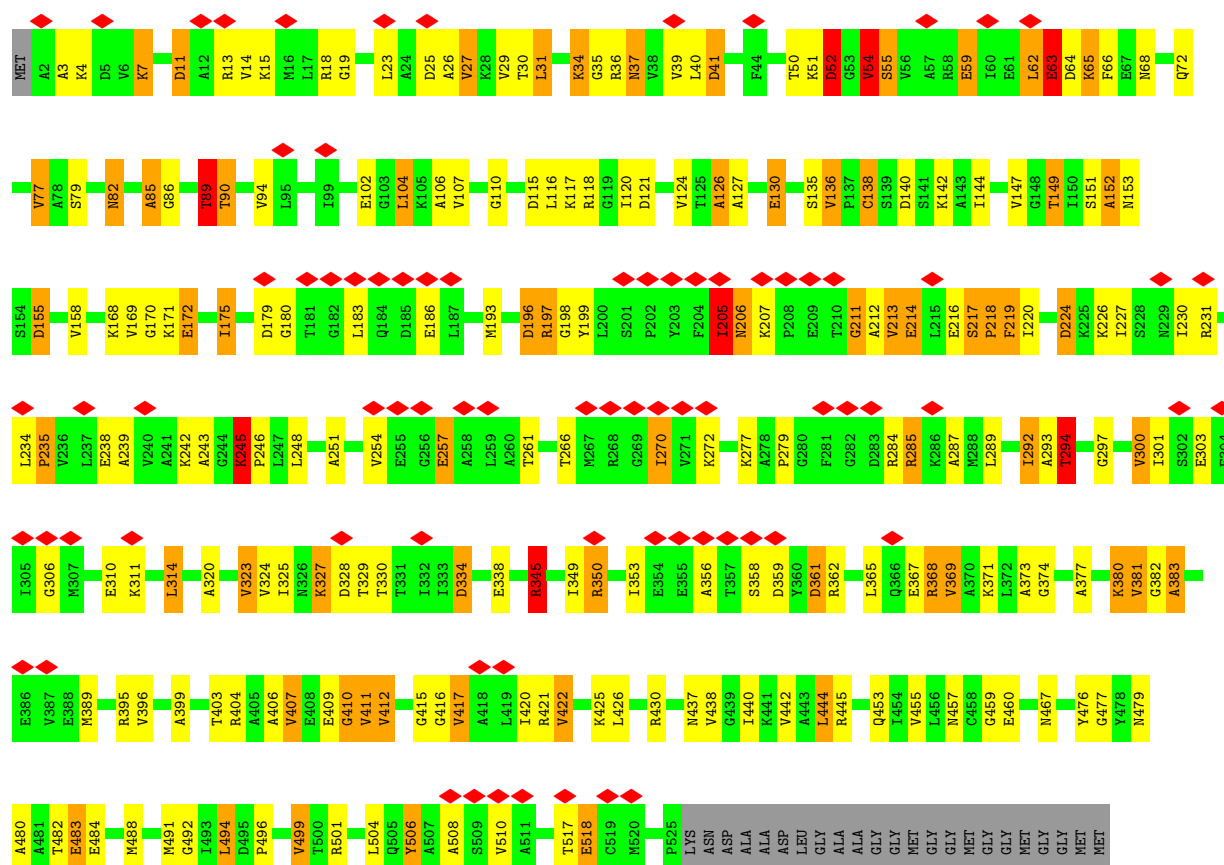


• Molecule 1: 60 KDA CHAPERONIN

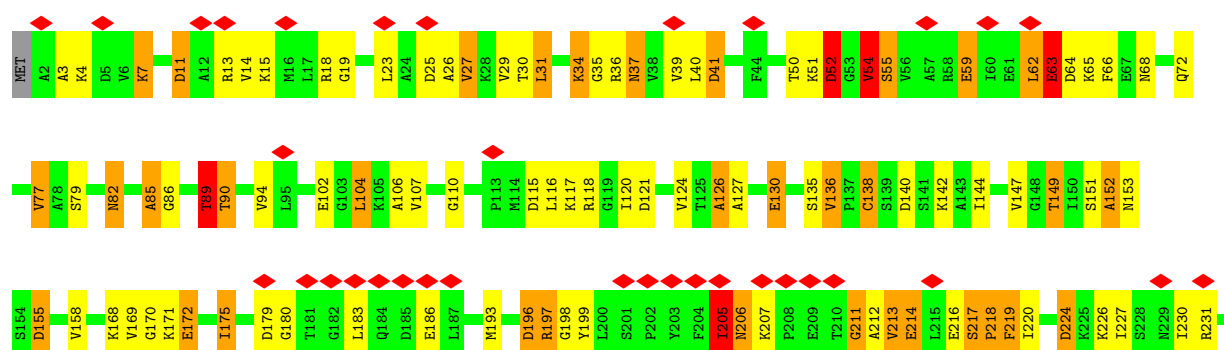


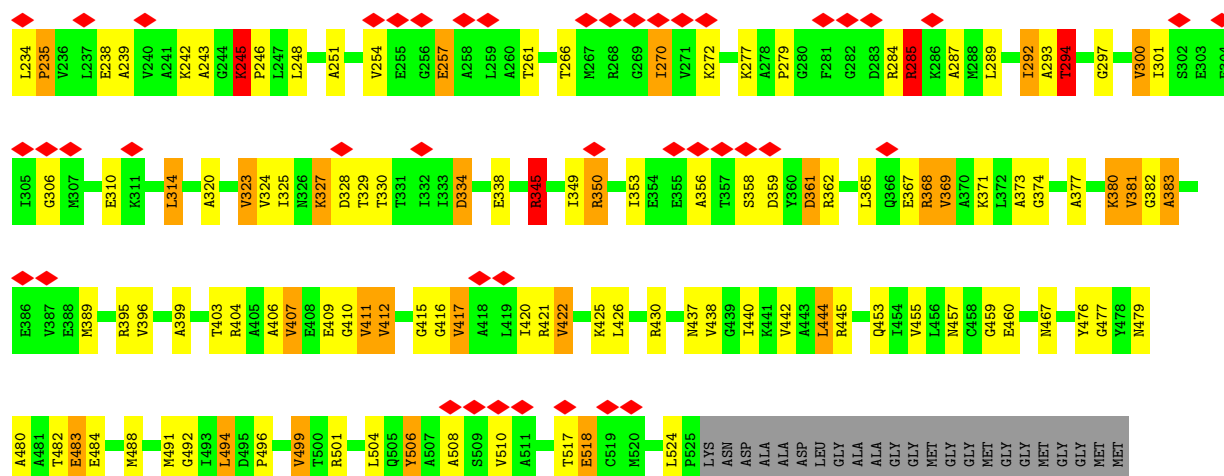


• Molecule 1: 60 KDA CHAPERONIN

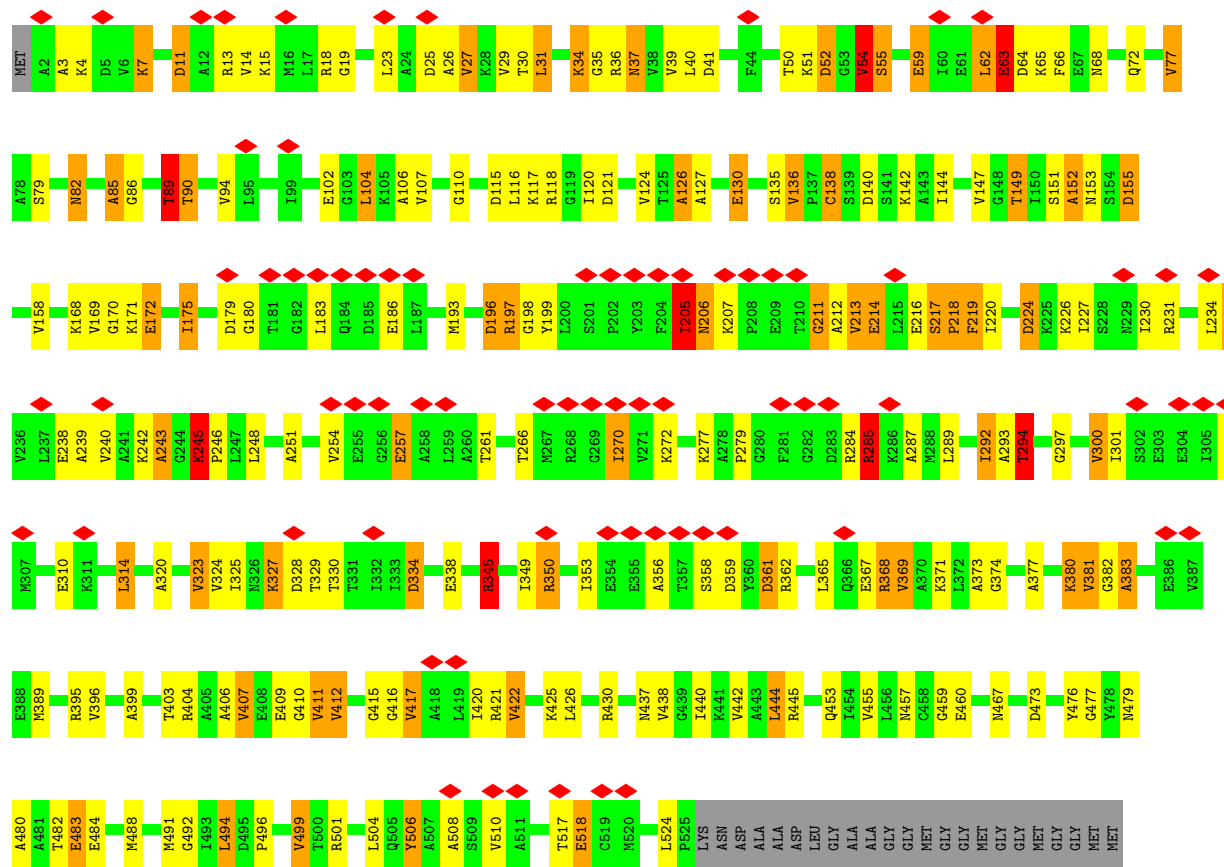


• Molecule 1: 60 KDA CHAPERONIN

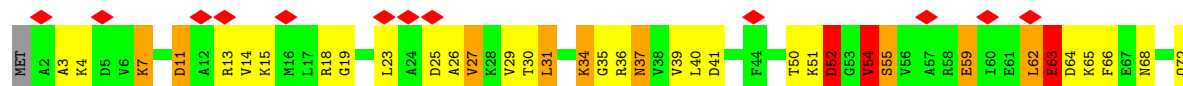


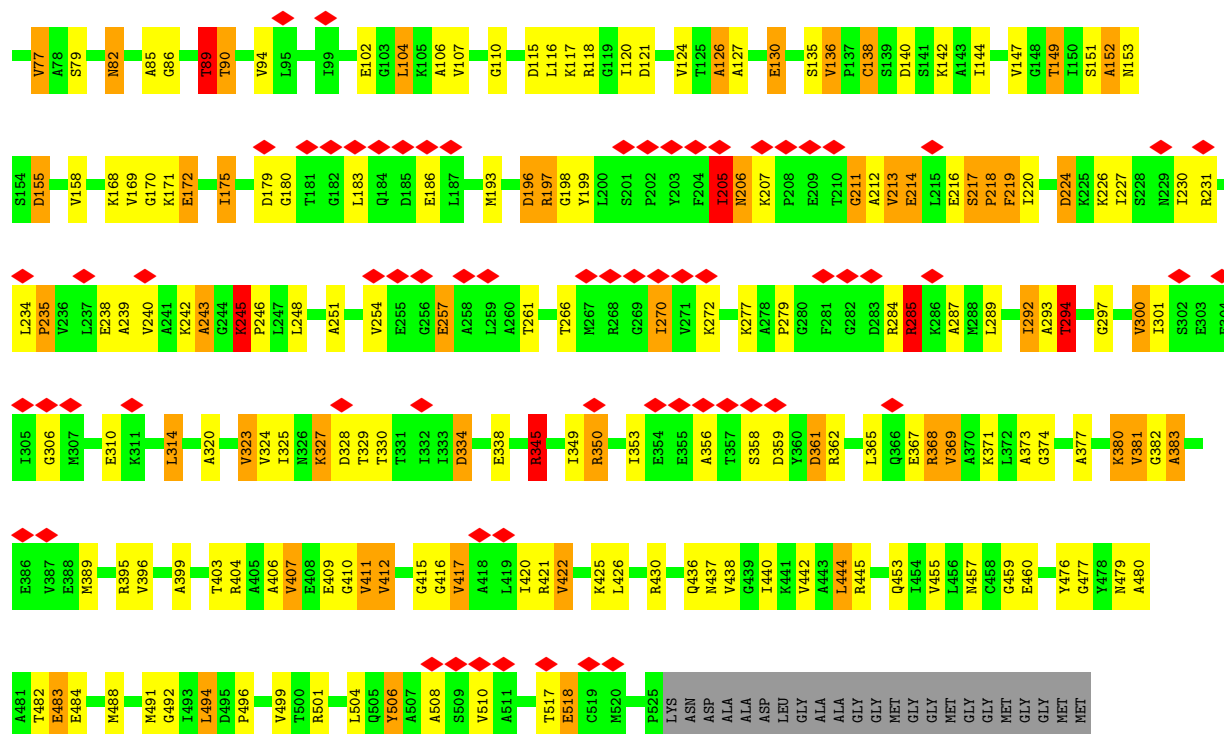


• Molecule 1: 60 KDA CHAPERONIN

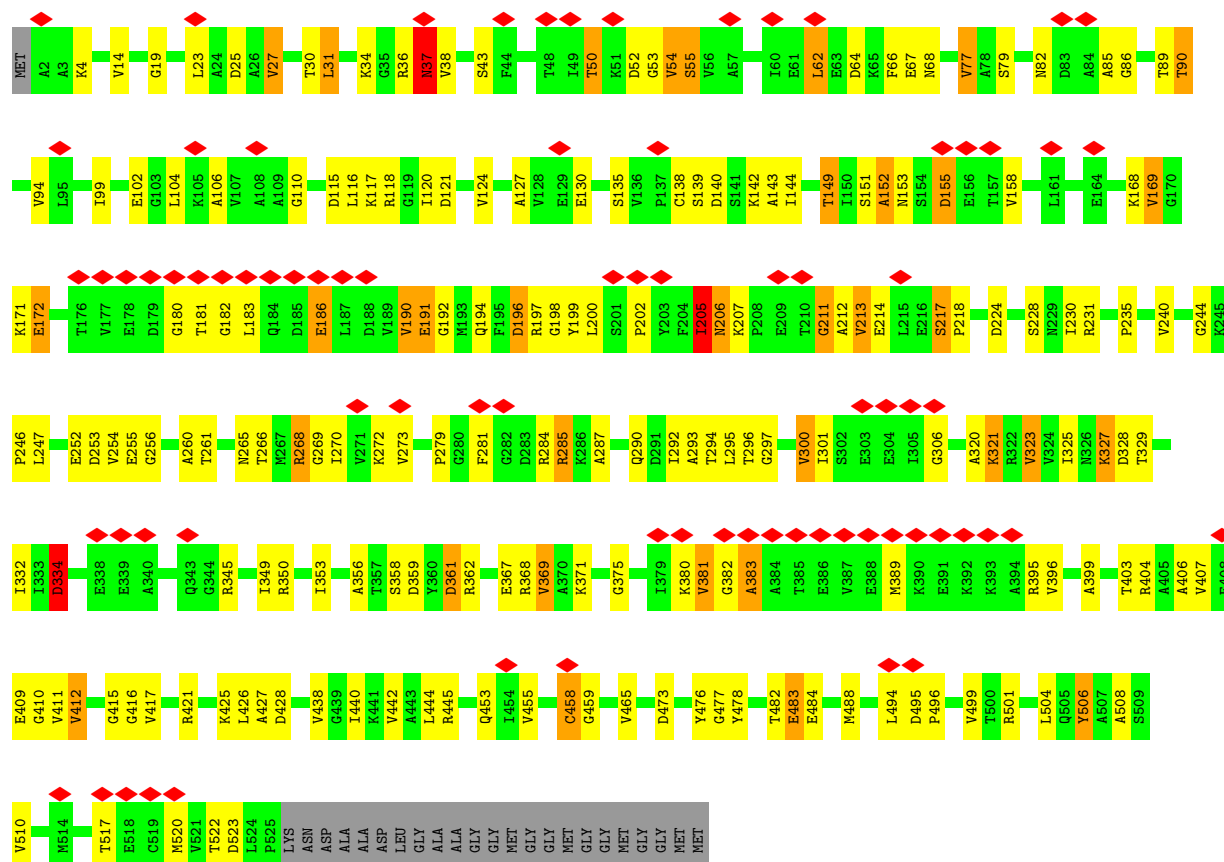


• Molecule 1: 60 KDA CHAPERONIN

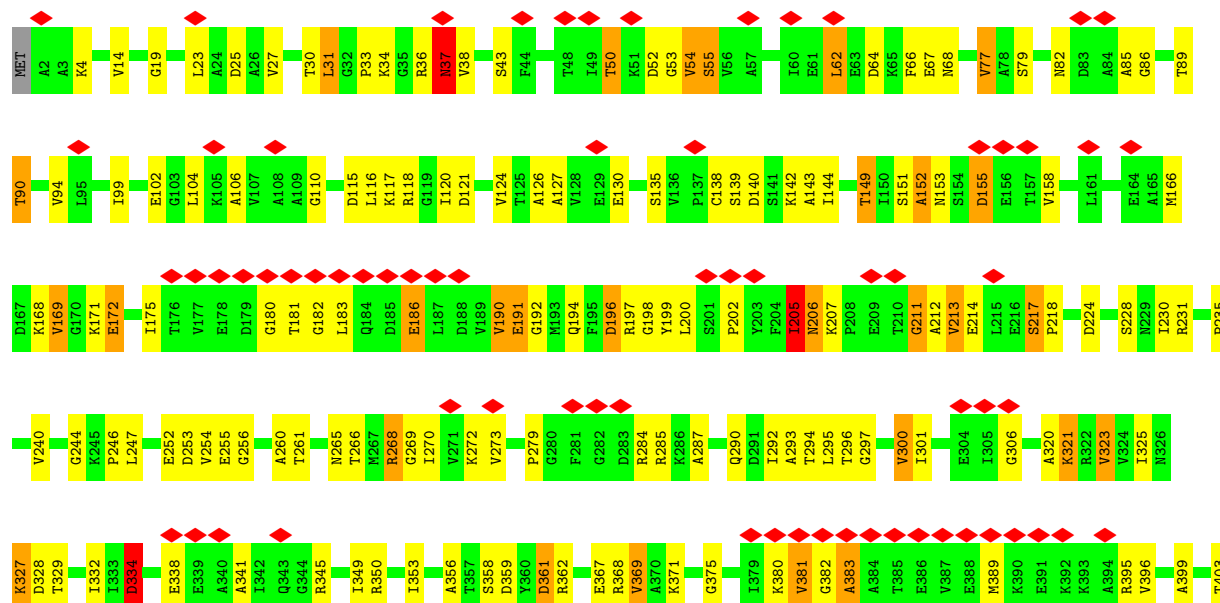


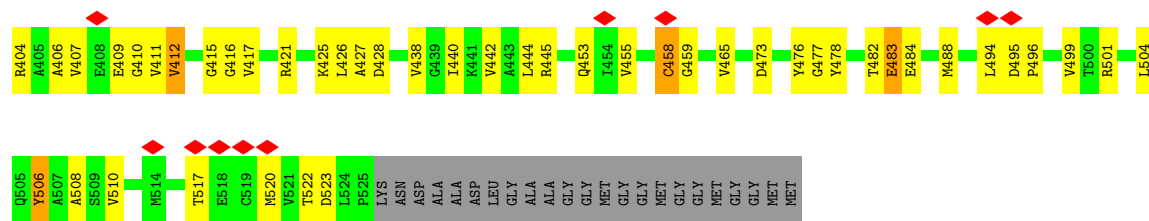


Molecule 1: 60 KDA CHAPERONIN

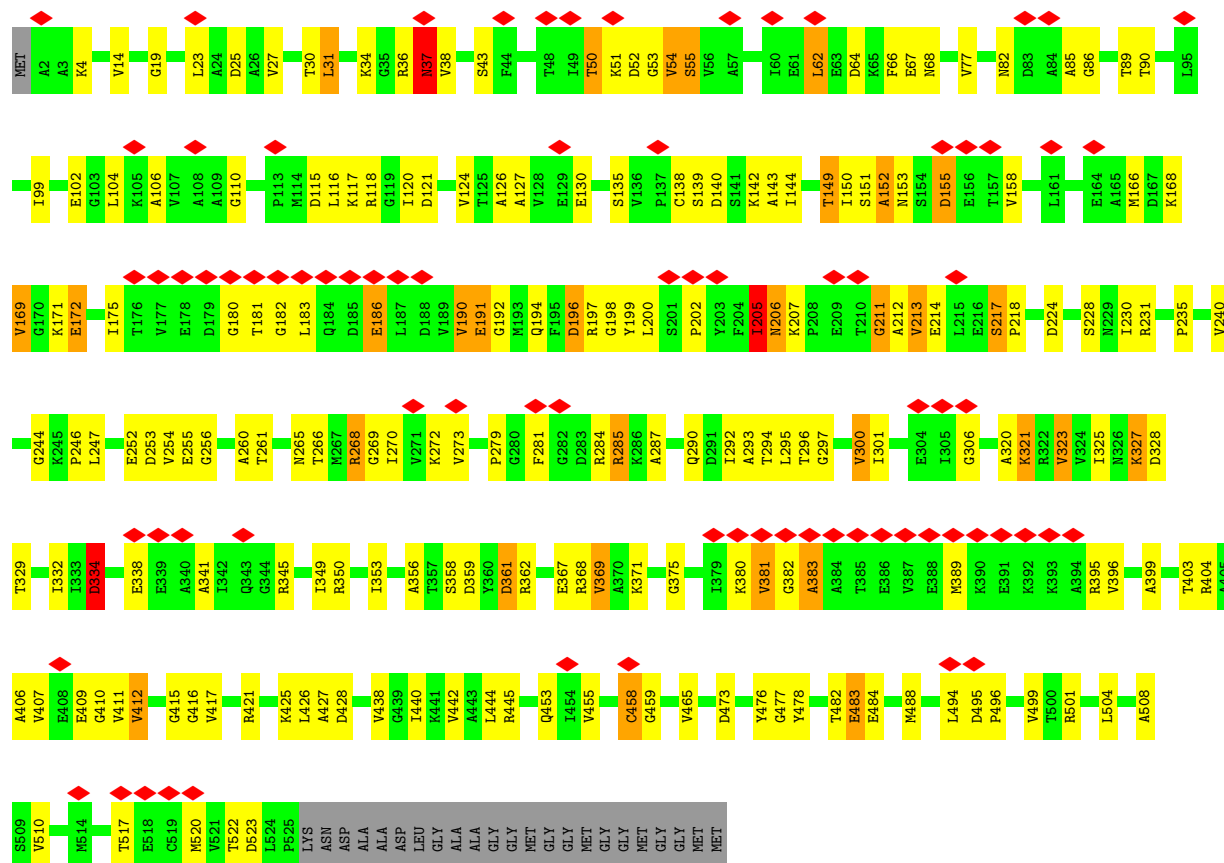


Chain I: 14% 58% 30% 6% . .

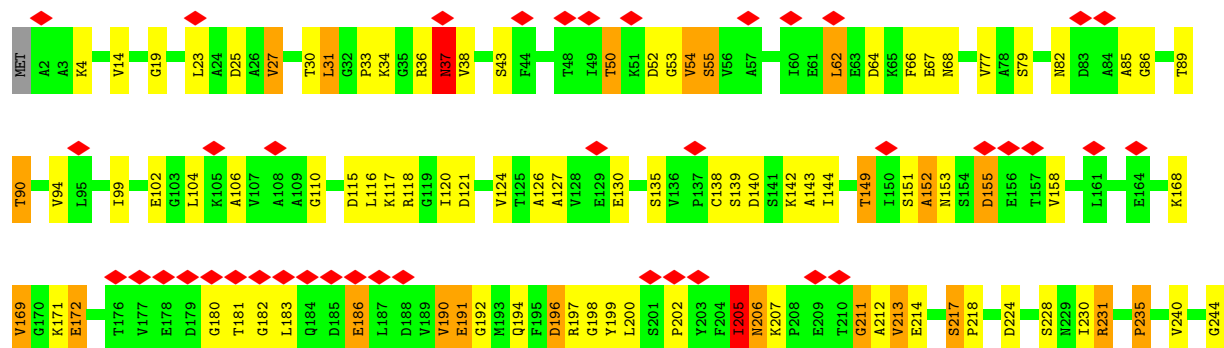


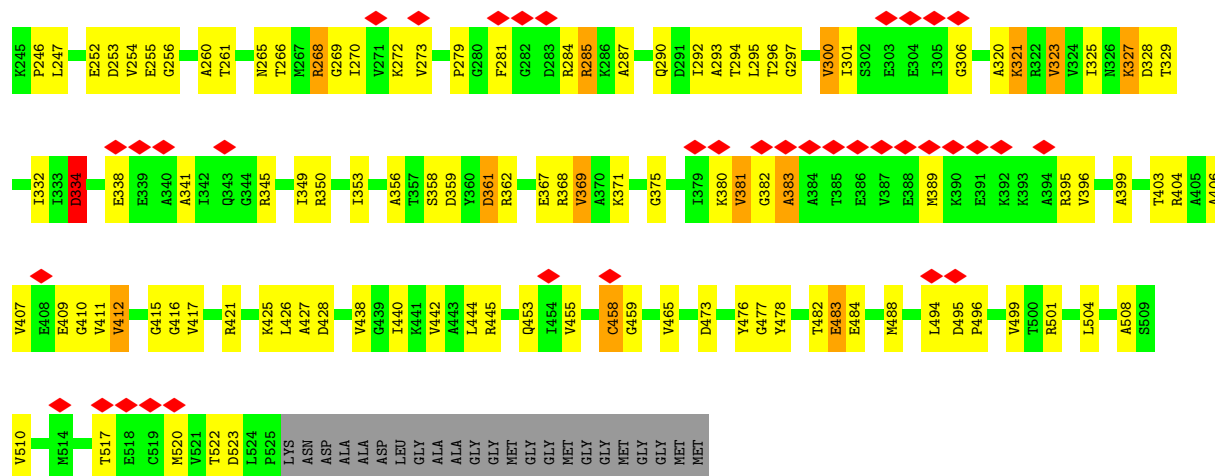


• Molecule 1: 60 KDA CHAPERONIN

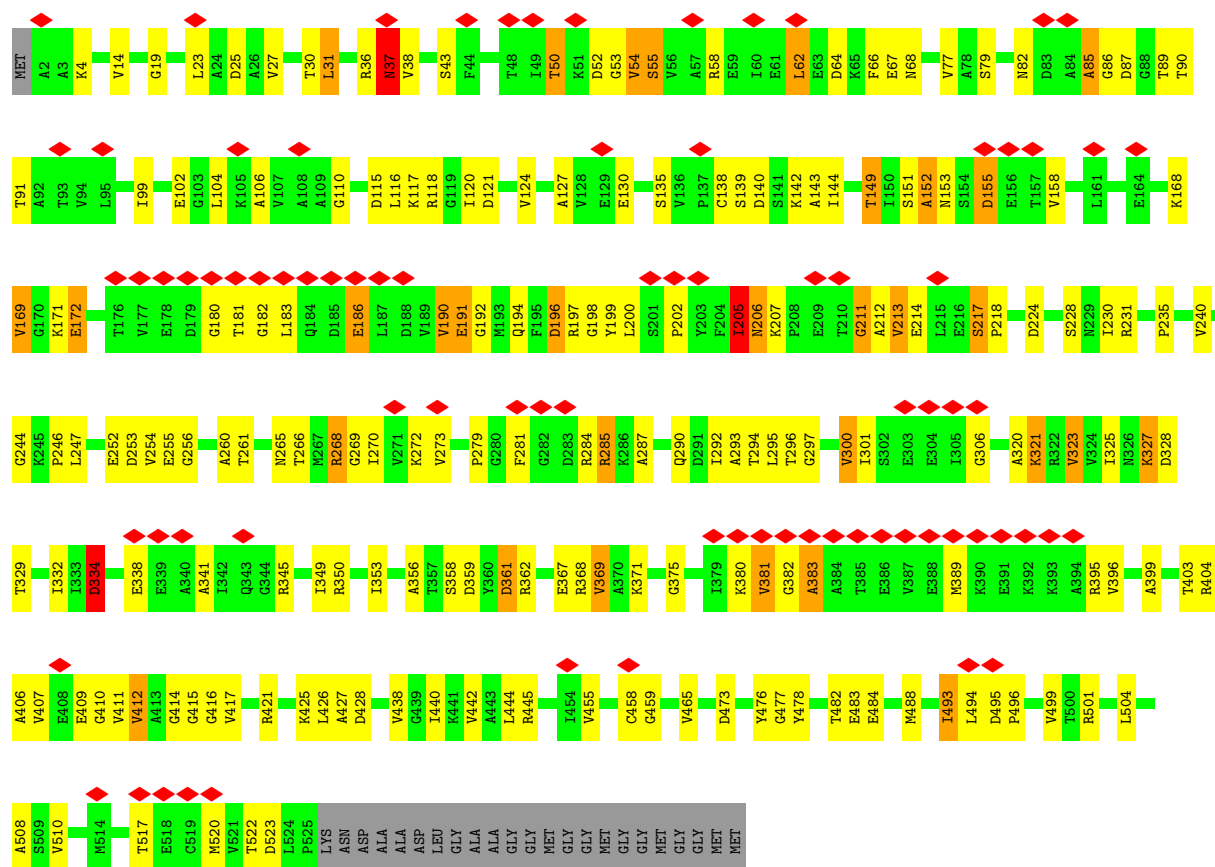


• Molecule 1: 60 KDA CHAPERONIN

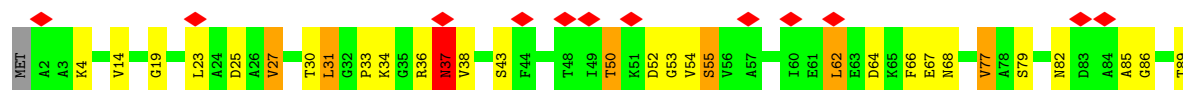




• Molecule 1: 60 KDA CHAPERONIN



• Molecule 1: 60 KDA CHAPERONIN





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	6500	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE WAS PHASE FLIPPED	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	148500	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	2.984	Depositor
Minimum map value	-1.957	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.117	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	387.84, 387.84, 387.84	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.02, 2.02, 2.02	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.48	3/3873 (0.1%)	1.88	112/5229 (2.1%)
1	B	1.48	3/3873 (0.1%)	1.88	113/5229 (2.2%)
1	C	1.48	3/3873 (0.1%)	1.88	112/5229 (2.1%)
1	D	1.48	2/3873 (0.1%)	1.88	113/5229 (2.2%)
1	E	1.48	3/3873 (0.1%)	1.87	112/5229 (2.1%)
1	F	1.48	3/3873 (0.1%)	1.88	113/5229 (2.2%)
1	G	1.48	2/3873 (0.1%)	1.88	112/5229 (2.1%)
1	H	1.47	0/3871	1.80	91/5223 (1.7%)
1	I	1.47	0/3871	1.80	92/5223 (1.8%)
1	J	1.47	0/3871	1.80	90/5223 (1.7%)
1	K	1.47	0/3871	1.81	89/5223 (1.7%)
1	L	1.47	0/3871	1.80	90/5223 (1.7%)
1	M	1.65	1/3871 (0.0%)	1.82	89/5223 (1.7%)
1	N	1.47	0/3871	1.80	93/5223 (1.8%)
All	All	1.49	20/54208 (0.0%)	1.84	1421/73164 (1.9%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	493	ILE	CG1-CD1	46.59	3.33	1.51
1	B	63	GLU	CA-CB	6.73	1.63	1.53
1	F	63	GLU	CA-CB	6.73	1.63	1.53
1	C	63	GLU	CA-CB	6.72	1.63	1.53
1	G	63	GLU	CA-CB	6.72	1.63	1.53
1	D	63	GLU	CA-CB	6.67	1.63	1.53
1	E	63	GLU	CA-CB	6.67	1.63	1.53
1	A	63	GLU	CA-CB	6.64	1.63	1.53
1	G	217	SER	CA-CB	5.43	1.56	1.52
1	D	217	SER	CA-CB	5.39	1.56	1.52
1	A	217	SER	CA-CB	5.38	1.56	1.52
1	F	217	SER	CA-CB	5.38	1.56	1.52
1	C	217	SER	CA-CB	5.37	1.56	1.52
1	E	217	SER	CA-CB	5.35	1.56	1.52
1	B	217	SER	CA-CB	5.35	1.56	1.52
1	C	524	LEU	C-N	-5.05	1.26	1.34
1	F	524	LEU	C-N	-5.05	1.26	1.34
1	A	524	LEU	C-N	-5.03	1.26	1.34
1	B	524	LEU	C-N	-5.03	1.26	1.34
1	E	524	LEU	C-N	-5.02	1.26	1.34

All (1421) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	GLU	N-CA-CB	-16.25	86.22	110.12
1	C	63	GLU	N-CA-CB	-16.24	86.24	110.12
1	G	63	GLU	N-CA-CB	-16.23	86.25	110.12
1	F	63	GLU	N-CA-CB	-16.22	86.27	110.12
1	A	63	GLU	N-CA-CB	-16.20	86.30	110.12
1	D	63	GLU	N-CA-CB	-16.19	86.31	110.12
1	E	63	GLU	N-CA-CB	-16.18	86.34	110.12
1	F	245	LYS	N-CA-CB	-15.74	85.26	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	LYS	N-CA-CB	-15.72	85.30	109.98
1	B	245	LYS	N-CA-CB	-15.71	85.31	109.98
1	A	245	LYS	N-CA-CB	-15.71	85.31	109.98
1	G	245	LYS	N-CA-CB	-15.70	85.33	109.98
1	C	245	LYS	N-CA-CB	-15.70	85.33	109.98
1	E	245	LYS	N-CA-CB	-15.68	85.37	109.98
1	M	493	ILE	N-CA-CB	15.31	130.54	111.41
1	G	206	ASN	CA-CB-CG	14.26	126.86	112.60
1	B	206	ASN	CA-CB-CG	14.25	126.85	112.60
1	D	206	ASN	CA-CB-CG	14.25	126.85	112.60
1	F	206	ASN	CA-CB-CG	14.22	126.82	112.60
1	E	206	ASN	CA-CB-CG	14.21	126.81	112.60
1	C	206	ASN	CA-CB-CG	14.19	126.79	112.60
1	A	206	ASN	CA-CB-CG	14.16	126.76	112.60
1	H	140	ASP	CA-CB-CG	12.25	124.85	112.60
1	L	140	ASP	CA-CB-CG	12.18	124.78	112.60
1	K	140	ASP	CA-CB-CG	12.14	124.74	112.60
1	M	140	ASP	CA-CB-CG	12.14	124.74	112.60
1	D	483	GLU	CB-CG-CD	11.95	132.91	112.60
1	E	483	GLU	CB-CG-CD	11.94	132.91	112.60
1	F	483	GLU	CB-CG-CD	11.94	132.89	112.60
1	A	483	GLU	CB-CG-CD	11.93	132.89	112.60
1	B	483	GLU	CB-CG-CD	11.93	132.88	112.60
1	C	483	GLU	CB-CG-CD	11.92	132.87	112.60
1	G	483	GLU	CB-CG-CD	11.91	132.85	112.60
1	I	140	ASP	CA-CB-CG	11.46	124.06	112.60
1	N	140	ASP	CA-CB-CG	11.33	123.93	112.60
1	J	140	ASP	CA-CB-CG	11.31	123.91	112.60
1	M	206	ASN	CA-CB-CG	11.07	123.67	112.60
1	J	206	ASN	CA-CB-CG	11.05	123.65	112.60
1	I	206	ASN	CA-CB-CG	11.04	123.64	112.60
1	K	206	ASN	CA-CB-CG	11.03	123.63	112.60
1	N	206	ASN	CA-CB-CG	11.03	123.63	112.60
1	H	206	ASN	CA-CB-CG	11.03	123.63	112.60
1	L	206	ASN	CA-CB-CG	11.02	123.62	112.60
1	E	82	ASN	CA-CB-CG	10.90	123.50	112.60
1	L	231	ARG	CB-CA-C	-10.89	93.79	110.88
1	M	231	ARG	CB-CA-C	-10.89	93.79	110.88
1	N	231	ARG	CB-CA-C	-10.88	93.79	110.88
1	K	231	ARG	CB-CA-C	-10.88	93.80	110.88
1	F	82	ASN	CA-CB-CG	10.87	123.47	112.60
1	J	231	ARG	CB-CA-C	-10.87	93.81	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	231	ARG	CB-CA-C	-10.87	93.82	110.88
1	H	231	ARG	CB-CA-C	-10.87	93.82	110.88
1	A	82	ASN	CA-CB-CG	10.85	123.45	112.60
1	D	82	ASN	CA-CB-CG	10.83	123.43	112.60
1	G	82	ASN	CA-CB-CG	10.83	123.43	112.60
1	B	82	ASN	CA-CB-CG	10.81	123.41	112.60
1	C	82	ASN	CA-CB-CG	10.81	123.41	112.60
1	K	153	ASN	CB-CA-C	10.80	128.73	112.09
1	B	140	ASP	CA-CB-CG	10.36	122.96	112.60
1	A	140	ASP	CA-CB-CG	10.36	122.96	112.60
1	E	140	ASP	CA-CB-CG	10.31	122.91	112.60
1	G	140	ASP	CA-CB-CG	10.31	122.91	112.60
1	D	140	ASP	CA-CB-CG	10.31	122.91	112.60
1	C	140	ASP	CA-CB-CG	10.29	122.89	112.60
1	F	140	ASP	CA-CB-CG	10.29	122.89	112.60
1	J	153	ASN	CB-CA-C	10.24	127.87	112.09
1	M	89	THR	CB-CA-C	-10.24	94.80	110.88
1	N	153	ASN	CB-CA-C	10.24	127.86	112.09
1	I	153	ASN	CB-CA-C	10.22	127.83	112.09
1	L	153	ASN	CB-CA-C	10.22	127.83	112.09
1	H	153	ASN	CB-CA-C	10.19	127.78	112.09
1	F	353	ILE	CB-CA-C	-10.17	98.96	111.97
1	C	353	ILE	CB-CA-C	-10.16	98.97	111.97
1	E	115	ASP	CB-CA-C	10.14	127.63	110.79
1	B	353	ILE	CB-CA-C	-10.14	98.99	111.97
1	E	353	ILE	CB-CA-C	-10.14	98.99	111.97
1	G	115	ASP	CB-CA-C	10.14	127.62	110.79
1	D	115	ASP	CB-CA-C	10.13	127.61	110.79
1	B	115	ASP	CB-CA-C	10.13	127.61	110.79
1	G	353	ILE	CB-CA-C	-10.13	99.00	111.97
1	A	115	ASP	CB-CA-C	10.13	127.60	110.79
1	C	115	ASP	CB-CA-C	10.13	127.61	110.79
1	D	353	ILE	CB-CA-C	-10.13	99.01	111.97
1	F	115	ASP	CB-CA-C	10.12	127.59	110.79
1	A	353	ILE	CB-CA-C	-10.12	99.02	111.97
1	E	285	ARG	CB-CA-C	-10.01	94.17	110.79
1	C	285	ARG	CB-CA-C	-10.00	94.19	110.79
1	D	285	ARG	CB-CA-C	-10.00	94.19	110.79
1	G	285	ARG	CB-CA-C	-10.00	94.20	110.79
1	B	285	ARG	CB-CA-C	-9.99	94.20	110.79
1	A	285	ARG	CB-CA-C	-9.99	94.21	110.79
1	F	285	ARG	CB-CA-C	-9.95	94.27	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	CYS	N-CA-CB	9.91	124.44	110.17
1	K	89	THR	CB-CA-C	-9.91	95.32	110.88
1	B	138	CYS	N-CA-CB	9.90	124.43	110.17
1	G	138	CYS	N-CA-CB	9.90	124.42	110.17
1	A	138	CYS	N-CA-CB	9.89	124.41	110.17
1	D	138	CYS	N-CA-CB	9.89	124.41	110.17
1	E	138	CYS	N-CA-CB	9.88	124.40	110.17
1	F	138	CYS	N-CA-CB	9.85	124.36	110.17
1	L	473	ASP	N-CA-CB	9.82	125.34	110.42
1	N	473	ASP	N-CA-CB	9.81	125.34	110.42
1	I	473	ASP	N-CA-CB	9.81	125.33	110.42
1	J	473	ASP	N-CA-CB	9.79	125.29	110.42
1	K	473	ASP	N-CA-CB	9.79	125.30	110.42
1	H	473	ASP	N-CA-CB	9.78	125.28	110.42
1	K	510	VAL	CB-CA-C	-9.78	99.46	111.97
1	H	383	ALA	N-CA-CB	9.77	126.69	111.56
1	L	510	VAL	CB-CA-C	-9.77	99.47	111.97
1	M	473	ASP	N-CA-CB	9.77	125.27	110.42
1	N	383	ALA	N-CA-CB	9.77	126.70	111.56
1	M	383	ALA	N-CA-CB	9.76	126.69	111.56
1	L	383	ALA	N-CA-CB	9.75	126.67	111.56
1	I	383	ALA	N-CA-CB	9.74	126.67	111.56
1	M	510	VAL	CB-CA-C	-9.74	99.50	111.97
1	K	383	ALA	N-CA-CB	9.73	126.64	111.56
1	J	383	ALA	N-CA-CB	9.70	126.60	111.56
1	H	510	VAL	CB-CA-C	-9.68	99.58	111.97
1	I	510	VAL	CB-CA-C	-9.68	99.58	111.97
1	J	510	VAL	CB-CA-C	-9.68	99.58	111.97
1	N	510	VAL	CB-CA-C	-9.66	99.60	111.97
1	N	369	VAL	N-CA-CB	9.59	123.58	110.54
1	H	369	VAL	N-CA-CB	9.56	123.55	110.54
1	M	369	VAL	N-CA-CB	9.55	123.53	110.54
1	L	369	VAL	N-CA-CB	9.54	123.51	110.54
1	J	353	ILE	CB-CA-C	-9.53	99.77	111.97
1	J	369	VAL	N-CA-CB	9.53	123.50	110.54
1	I	369	VAL	N-CA-CB	9.52	123.49	110.54
1	K	369	VAL	N-CA-CB	9.52	123.48	110.54
1	F	510	VAL	CB-CA-C	-9.51	99.80	111.97
1	K	353	ILE	CB-CA-C	-9.50	99.81	111.97
1	G	510	VAL	CB-CA-C	-9.50	99.81	111.97
1	M	353	ILE	CB-CA-C	-9.49	99.82	111.97
1	B	510	VAL	CB-CA-C	-9.49	99.82	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	353	ILE	CB-CA-C	-9.48	99.83	111.97
1	E	510	VAL	CB-CA-C	-9.48	99.84	111.97
1	M	153	ASN	CB-CA-C	9.48	126.69	112.09
1	C	510	VAL	CB-CA-C	-9.48	99.84	111.97
1	I	353	ILE	CB-CA-C	-9.48	99.84	111.97
1	A	510	VAL	CB-CA-C	-9.48	99.84	111.97
1	L	353	ILE	CB-CA-C	-9.47	99.84	111.97
1	H	353	ILE	CB-CA-C	-9.46	99.86	111.97
1	D	510	VAL	CB-CA-C	-9.45	99.88	111.97
1	A	369	VAL	N-CA-CB	9.28	123.16	110.54
1	G	369	VAL	N-CA-CB	9.27	123.15	110.54
1	D	369	VAL	N-CA-CB	9.26	123.13	110.54
1	E	369	VAL	N-CA-CB	9.24	123.11	110.54
1	B	369	VAL	N-CA-CB	9.23	123.10	110.54
1	C	369	VAL	N-CA-CB	9.23	123.09	110.54
1	F	369	VAL	N-CA-CB	9.22	123.08	110.54
1	B	383	ALA	N-CA-CB	9.21	125.83	111.56
1	C	383	ALA	N-CA-CB	9.21	125.83	111.56
1	A	383	ALA	N-CA-CB	9.20	125.82	111.56
1	F	383	ALA	N-CA-CB	9.20	125.82	111.56
1	G	383	ALA	N-CA-CB	9.18	125.78	111.56
1	D	383	ALA	N-CA-CB	9.15	125.74	111.56
1	E	383	ALA	N-CA-CB	9.13	125.71	111.56
1	K	482	THR	N-CA-CB	9.06	123.56	110.16
1	C	59	GLU	CB-CA-C	9.03	125.05	110.88
1	A	59	GLU	CB-CA-C	9.02	125.05	110.88
1	F	59	GLU	CB-CA-C	9.02	125.04	110.88
1	B	59	GLU	CB-CA-C	9.01	125.03	110.88
1	D	59	GLU	CB-CA-C	9.01	125.03	110.88
1	C	37	ASN	N-CA-CB	-8.99	96.73	110.49
1	E	37	ASN	N-CA-CB	-8.99	96.74	110.49
1	G	37	ASN	N-CA-CB	-8.98	96.75	110.49
1	A	37	ASN	N-CA-CB	-8.97	96.76	110.49
1	D	37	ASN	N-CA-CB	-8.97	96.77	110.49
1	B	37	ASN	N-CA-CB	-8.96	96.78	110.49
1	F	37	ASN	N-CA-CB	-8.94	96.81	110.49
1	J	482	THR	N-CA-CB	8.91	123.34	110.16
1	J	115	ASP	CB-CA-C	8.72	125.27	110.79
1	H	115	ASP	CB-CA-C	8.69	125.22	110.79
1	K	115	ASP	CB-CA-C	8.69	125.21	110.79
1	M	115	ASP	CB-CA-C	8.69	125.21	110.79
1	L	115	ASP	CB-CA-C	8.68	125.20	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	115	ASP	CB-CA-C	8.67	125.19	110.79
1	N	115	ASP	CB-CA-C	8.67	125.19	110.79
1	H	55	SER	CB-CA-C	-8.66	96.41	110.79
1	N	55	SER	CB-CA-C	-8.66	96.42	110.79
1	K	55	SER	CB-CA-C	-8.65	96.43	110.79
1	L	55	SER	CB-CA-C	-8.63	96.47	110.79
1	I	55	SER	CB-CA-C	-8.62	96.48	110.79
1	J	55	SER	CB-CA-C	-8.57	96.57	110.79
1	G	59	GLU	CB-CA-C	8.56	125.00	110.79
1	G	482	THR	N-CA-CB	8.56	122.82	110.16
1	E	59	GLU	CB-CA-C	8.55	124.98	110.79
1	E	482	THR	N-CA-CB	8.55	122.81	110.16
1	D	482	THR	N-CA-CB	8.54	122.80	110.16
1	F	482	THR	N-CA-CB	8.54	122.80	110.16
1	C	482	THR	N-CA-CB	8.53	122.79	110.16
1	B	482	THR	N-CA-CB	8.53	122.79	110.16
1	A	482	THR	N-CA-CB	8.53	122.78	110.16
1	N	479	ASN	CB-CA-C	8.42	123.83	110.19
1	A	411	VAL	CB-CA-C	-8.40	100.04	111.63
1	M	493	ILE	CB-CG1-CD1	8.40	131.43	113.80
1	F	411	VAL	CB-CA-C	-8.39	100.05	111.63
1	E	411	VAL	CB-CA-C	-8.38	100.07	111.63
1	D	411	VAL	CB-CA-C	-8.38	100.07	111.63
1	C	411	VAL	CB-CA-C	-8.37	100.08	111.63
1	C	412	VAL	CB-CA-C	-8.37	98.85	110.90
1	B	411	VAL	CB-CA-C	-8.36	100.09	111.63
1	H	115	ASP	CA-CB-CG	-8.36	104.24	112.60
1	G	411	VAL	CB-CA-C	-8.35	100.11	111.63
1	G	412	VAL	CB-CA-C	-8.35	98.88	110.90
1	B	412	VAL	CB-CA-C	-8.34	98.89	110.90
1	M	115	ASP	CA-CB-CG	-8.34	104.26	112.60
1	E	412	VAL	CB-CA-C	-8.33	98.90	110.90
1	A	412	VAL	CB-CA-C	-8.33	98.91	110.90
1	F	412	VAL	CB-CA-C	-8.33	98.91	110.90
1	N	115	ASP	CA-CB-CG	-8.32	104.28	112.60
1	K	115	ASP	CA-CB-CG	-8.32	104.28	112.60
1	D	412	VAL	CB-CA-C	-8.32	98.92	110.90
1	L	115	ASP	CA-CB-CG	-8.31	104.29	112.60
1	I	115	ASP	CA-CB-CG	-8.31	104.29	112.60
1	E	367	GLU	CB-CA-C	-8.30	97.02	110.79
1	C	367	GLU	CB-CA-C	-8.29	97.03	110.79
1	A	367	GLU	CB-CA-C	-8.29	97.03	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	GLU	CB-CA-C	-8.29	97.03	110.79
1	J	115	ASP	CA-CB-CG	-8.28	104.32	112.60
1	F	367	GLU	CB-CA-C	-8.28	97.05	110.79
1	L	482	THR	N-CA-CB	8.27	122.39	110.16
1	D	367	GLU	CB-CA-C	-8.26	97.08	110.79
1	G	367	GLU	CB-CA-C	-8.26	97.08	110.79
1	I	482	THR	N-CA-CB	8.21	122.31	110.16
1	L	285	ARG	CB-CA-C	-8.19	97.20	110.79
1	I	285	ARG	CB-CA-C	-8.19	97.20	110.79
1	M	285	ARG	CB-CA-C	-8.17	97.22	110.79
1	H	285	ARG	CB-CA-C	-8.17	97.23	110.79
1	N	285	ARG	CB-CA-C	-8.16	97.25	110.79
1	K	285	ARG	CB-CA-C	-8.15	97.25	110.79
1	H	482	THR	N-CA-CB	8.15	122.22	110.16
1	J	285	ARG	CB-CA-C	-8.14	97.27	110.79
1	M	482	THR	N-CA-CB	8.12	122.17	110.16
1	H	367	GLU	CB-CA-C	-8.06	97.42	110.79
1	L	367	GLU	CB-CA-C	-8.04	97.44	110.79
1	I	367	GLU	CB-CA-C	-8.04	97.44	110.79
1	L	140	ASP	N-CA-CB	-8.04	98.88	110.45
1	M	140	ASP	N-CA-CB	-8.04	98.88	110.45
1	J	367	GLU	CB-CA-C	-8.03	97.46	110.79
1	N	367	GLU	CB-CA-C	-8.03	97.46	110.79
1	K	367	GLU	CB-CA-C	-8.03	97.47	110.79
1	H	140	ASP	N-CA-CB	-8.02	98.90	110.45
1	K	140	ASP	N-CA-CB	-8.02	98.91	110.45
1	M	367	GLU	CB-CA-C	-8.01	97.49	110.79
1	N	140	ASP	N-CA-CB	-8.01	98.92	110.45
1	I	140	ASP	N-CA-CB	-8.00	98.93	110.45
1	J	140	ASP	N-CA-CB	-8.00	98.93	110.45
1	M	52	ASP	CB-CA-C	8.00	124.18	109.70
1	F	261	THR	N-CA-CB	7.98	121.59	110.01
1	M	55	SER	CB-CA-C	-7.98	97.54	110.79
1	C	261	THR	N-CA-CB	7.96	121.56	110.01
1	G	261	THR	N-CA-CB	7.95	121.54	110.01
1	D	261	THR	N-CA-CB	7.95	121.54	110.01
1	B	261	THR	N-CA-CB	7.92	121.49	110.01
1	A	261	THR	N-CA-CB	7.92	121.49	110.01
1	E	261	THR	N-CA-CB	7.91	121.48	110.01
1	E	216	GLU	N-CA-CB	-7.85	97.63	110.43
1	M	371	LYS	CB-CA-C	7.85	123.20	110.88
1	F	216	GLU	N-CA-CB	-7.84	97.65	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	371	LYS	CB-CA-C	7.84	123.19	110.88
1	J	181	THR	N-CA-CB	7.84	121.76	110.16
1	N	181	THR	N-CA-CB	7.84	121.76	110.16
1	K	181	THR	N-CA-CB	7.84	121.76	110.16
1	N	371	LYS	CB-CA-C	7.83	123.18	110.88
1	C	216	GLU	N-CA-CB	-7.83	97.67	110.43
1	B	216	GLU	N-CA-CB	-7.82	97.68	110.43
1	H	181	THR	N-CA-CB	7.82	121.73	110.16
1	I	371	LYS	CB-CA-C	7.82	123.16	110.88
1	H	371	LYS	CB-CA-C	7.82	123.16	110.88
1	G	216	GLU	N-CA-CB	-7.82	97.69	110.43
1	J	371	LYS	CB-CA-C	7.81	123.14	110.88
1	L	181	THR	N-CA-CB	7.81	121.72	110.16
1	L	371	LYS	CB-CA-C	7.81	123.15	110.88
1	A	216	GLU	N-CA-CB	-7.81	97.70	110.43
1	D	216	GLU	N-CA-CB	-7.80	97.72	110.43
1	F	235	PRO	CB-CA-C	7.79	124.36	112.21
1	M	181	THR	N-CA-CB	7.78	121.68	110.16
1	I	181	THR	N-CA-CB	7.78	121.67	110.16
1	A	235	PRO	CB-CA-C	7.77	124.33	112.21
1	C	235	PRO	CB-CA-C	7.76	124.32	112.21
1	E	235	PRO	CB-CA-C	7.75	124.30	112.21
1	B	235	PRO	CB-CA-C	7.75	124.29	112.21
1	D	235	PRO	CB-CA-C	7.74	124.29	112.21
1	G	235	PRO	CB-CA-C	7.73	124.28	112.21
1	N	30	THR	N-CA-CB	7.71	121.46	110.12
1	L	30	THR	N-CA-CB	7.69	121.42	110.12
1	H	30	THR	N-CA-CB	7.68	121.41	110.12
1	N	369	VAL	CB-CA-C	-7.68	101.77	112.14
1	I	369	VAL	CB-CA-C	-7.67	101.78	112.14
1	I	30	THR	N-CA-CB	7.67	121.39	110.12
1	K	369	VAL	CB-CA-C	-7.65	101.82	112.14
1	F	444	LEU	CB-CA-C	-7.64	98.10	110.79
1	L	369	VAL	CB-CA-C	-7.64	101.83	112.14
1	M	369	VAL	CB-CA-C	-7.64	101.83	112.14
1	C	444	LEU	CB-CA-C	-7.63	98.12	110.79
1	G	444	LEU	CB-CA-C	-7.63	98.12	110.79
1	H	369	VAL	CB-CA-C	-7.63	101.83	112.14
1	B	86	GLY	N-CA-C	-7.63	106.00	115.08
1	D	444	LEU	CB-CA-C	-7.63	98.13	110.79
1	E	444	LEU	CB-CA-C	-7.62	98.13	110.79
1	B	444	LEU	CB-CA-C	-7.62	98.14	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	369	VAL	CB-CA-C	-7.62	101.85	112.14
1	I	149	THR	N-CA-CB	7.62	121.32	110.12
1	D	149	THR	N-CA-CB	7.62	121.32	110.12
1	A	444	LEU	CB-CA-C	-7.62	98.15	110.79
1	C	86	GLY	N-CA-C	-7.61	106.03	115.08
1	F	115	ASP	CA-CB-CG	-7.60	105.00	112.60
1	F	149	THR	N-CA-CB	7.60	121.30	110.12
1	F	86	GLY	N-CA-C	-7.60	106.04	115.08
1	K	425	LYS	CB-CA-C	7.59	123.40	110.79
1	L	149	THR	N-CA-CB	7.59	121.28	110.12
1	G	86	GLY	N-CA-C	-7.59	106.05	115.08
1	G	115	ASP	CA-CB-CG	-7.59	105.01	112.60
1	D	86	GLY	N-CA-C	-7.58	106.06	115.08
1	E	115	ASP	CA-CB-CG	-7.58	105.03	112.60
1	G	149	THR	N-CA-CB	7.58	121.26	110.12
1	A	149	THR	N-CA-CB	7.57	121.25	110.12
1	B	115	ASP	CA-CB-CG	-7.57	105.03	112.60
1	D	55	SER	N-CA-CB	7.57	121.25	110.12
1	E	86	GLY	N-CA-C	-7.57	106.07	115.08
1	G	140	ASP	N-CA-CB	-7.57	99.54	110.45
1	E	140	ASP	N-CA-CB	-7.57	99.55	110.45
1	A	86	GLY	N-CA-C	-7.57	106.07	115.08
1	N	149	THR	N-CA-CB	7.57	121.24	110.12
1	M	425	LYS	CB-CA-C	7.57	123.35	110.79
1	B	149	THR	N-CA-CB	7.56	121.24	110.12
1	F	140	ASP	N-CA-CB	-7.56	99.56	110.45
1	B	55	SER	N-CA-CB	7.56	121.23	110.12
1	C	115	ASP	CA-CB-CG	-7.56	105.04	112.60
1	D	140	ASP	N-CA-CB	-7.56	99.57	110.45
1	L	425	LYS	CB-CA-C	7.56	123.33	110.79
1	C	149	THR	N-CA-CB	7.55	121.22	110.12
1	B	140	ASP	N-CA-CB	-7.55	99.58	110.45
1	D	115	ASP	CA-CB-CG	-7.55	105.05	112.60
1	H	149	THR	N-CA-CB	7.55	121.22	110.12
1	C	140	ASP	N-CA-CB	-7.55	99.58	110.45
1	A	140	ASP	N-CA-CB	-7.54	99.58	110.45
1	A	115	ASP	CA-CB-CG	-7.54	105.06	112.60
1	J	425	LYS	CB-CA-C	7.54	123.31	110.79
1	E	149	THR	N-CA-CB	7.54	121.21	110.12
1	I	425	LYS	CB-CA-C	7.54	123.31	110.79
1	H	425	LYS	CB-CA-C	7.54	123.31	110.79
1	A	55	SER	N-CA-CB	7.54	121.20	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	425	LYS	CB-CA-C	7.54	123.30	110.79
1	G	55	SER	N-CA-CB	7.53	121.19	110.12
1	E	55	SER	N-CA-CB	7.52	121.17	110.12
1	C	55	SER	N-CA-CB	7.51	121.16	110.12
1	G	235	PRO	N-CA-CB	7.50	111.49	103.39
1	B	235	PRO	N-CA-CB	7.49	111.48	103.39
1	C	235	PRO	N-CA-CB	7.49	111.48	103.39
1	E	235	PRO	N-CA-CB	7.49	111.48	103.39
1	F	55	SER	N-CA-CB	7.49	121.13	110.12
1	D	235	PRO	N-CA-CB	7.49	111.47	103.39
1	H	231	ARG	CA-CB-CG	7.47	129.05	114.10
1	H	483	GLU	CB-CG-CD	7.46	125.29	112.60
1	A	235	PRO	N-CA-CB	7.46	111.45	103.39
1	I	231	ARG	CA-CB-CG	7.46	129.01	114.10
1	M	231	ARG	CA-CB-CG	7.46	129.01	114.10
1	N	231	ARG	CA-CB-CG	7.46	129.01	114.10
1	L	231	ARG	CA-CB-CG	7.45	129.01	114.10
1	K	231	ARG	CA-CB-CG	7.45	129.00	114.10
1	J	231	ARG	CA-CB-CG	7.45	128.99	114.10
1	F	235	PRO	N-CA-CB	7.44	111.43	103.39
1	C	369	VAL	CB-CA-C	-7.40	102.14	112.14
1	E	369	VAL	CB-CA-C	-7.40	102.14	112.14
1	A	369	VAL	CB-CA-C	-7.39	102.16	112.14
1	B	369	VAL	CB-CA-C	-7.38	102.17	112.14
1	G	369	VAL	CB-CA-C	-7.38	102.17	112.14
1	D	369	VAL	CB-CA-C	-7.38	102.17	112.14
1	F	369	VAL	CB-CA-C	-7.38	102.18	112.14
1	K	217	SER	CB-CA-C	-7.36	104.59	111.00
1	M	30	THR	N-CA-CB	7.35	120.92	110.12
1	N	217	SER	CB-CA-C	-7.33	104.62	111.00
1	M	217	SER	CB-CA-C	-7.32	104.63	111.00
1	L	217	SER	CB-CA-C	-7.31	104.64	111.00
1	K	483	GLU	CB-CG-CD	7.31	125.03	112.60
1	I	217	SER	CB-CA-C	-7.30	104.64	111.00
1	J	217	SER	CB-CA-C	-7.30	104.64	111.00
1	N	483	GLU	CB-CG-CD	7.30	125.01	112.60
1	H	217	SER	CB-CA-C	-7.30	104.65	111.00
1	B	381	VAL	N-CA-CB	-7.30	101.33	111.25
1	A	381	VAL	N-CA-CB	-7.29	101.33	111.25
1	D	381	VAL	N-CA-CB	-7.28	101.35	111.25
1	F	381	VAL	N-CA-CB	-7.27	101.36	111.25
1	E	381	VAL	N-CA-CB	-7.27	101.37	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	381	VAL	N-CA-CB	-7.26	101.37	111.25
1	C	381	VAL	N-CA-CB	-7.26	101.38	111.25
1	I	483	GLU	CB-CG-CD	7.21	124.86	112.60
1	M	269	GLY	N-CA-C	-7.21	104.79	114.95
1	L	334	ASP	CA-CB-CG	7.20	119.80	112.60
1	I	269	GLY	N-CA-C	-7.19	104.81	114.95
1	J	483	GLU	CB-CG-CD	7.19	124.82	112.60
1	H	269	GLY	N-CA-C	-7.18	104.82	114.95
1	J	269	GLY	N-CA-C	-7.18	104.83	114.95
1	L	483	GLU	CB-CG-CD	7.18	124.81	112.60
1	K	334	ASP	CA-CB-CG	7.17	119.77	112.60
1	J	334	ASP	CA-CB-CG	7.17	119.77	112.60
1	L	269	GLY	N-CA-C	-7.17	104.85	114.95
1	L	89	THR	CB-CA-C	-7.16	99.63	110.88
1	N	334	ASP	CA-CB-CG	7.16	119.76	112.60
1	H	334	ASP	CA-CB-CG	7.16	119.76	112.60
1	K	269	GLY	N-CA-C	-7.16	104.85	114.95
1	I	334	ASP	CA-CB-CG	7.15	119.75	112.60
1	N	89	THR	CB-CA-C	-7.14	99.66	110.88
1	N	269	GLY	N-CA-C	-7.14	104.88	114.95
1	D	334	ASP	CA-CB-CG	7.14	119.74	112.60
1	F	68	ASN	CA-CB-CG	7.14	119.74	112.60
1	M	334	ASP	CA-CB-CG	7.14	119.74	112.60
1	I	89	THR	CB-CA-C	-7.13	99.69	110.88
1	C	334	ASP	CA-CB-CG	7.12	119.72	112.60
1	H	89	THR	CB-CA-C	-7.12	99.71	110.88
1	G	334	ASP	CA-CB-CG	7.12	119.72	112.60
1	D	11	ASP	CB-CA-C	7.11	122.60	110.79
1	L	412	VAL	CB-CA-C	-7.11	100.67	110.90
1	F	334	ASP	CA-CB-CG	7.10	119.70	112.60
1	I	412	VAL	CB-CA-C	-7.10	100.67	110.90
1	K	412	VAL	CB-CA-C	-7.10	100.68	110.90
1	A	68	ASN	CA-CB-CG	7.10	119.70	112.60
1	E	11	ASP	CB-CA-C	7.10	122.57	110.79
1	F	499	VAL	N-CA-CB	7.10	118.85	110.55
1	J	412	VAL	CB-CA-C	-7.10	100.68	110.90
1	N	412	VAL	CB-CA-C	-7.10	100.68	110.90
1	C	11	ASP	CB-CA-C	7.09	122.56	110.79
1	B	11	ASP	CB-CA-C	7.09	122.55	110.79
1	H	412	VAL	CB-CA-C	-7.09	100.69	110.90
1	B	68	ASN	CA-CB-CG	7.08	119.69	112.60
1	G	11	ASP	CB-CA-C	7.08	122.54	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	14	VAL	N-CA-CB	7.08	120.16	110.54
1	A	334	ASP	CA-CB-CG	7.07	119.67	112.60
1	D	68	ASN	CA-CB-CG	7.07	119.67	112.60
1	B	499	VAL	N-CA-CB	7.07	118.82	110.55
1	J	89	THR	CB-CA-C	-7.07	99.78	110.88
1	A	11	ASP	CB-CA-C	7.07	122.52	110.79
1	E	334	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	334	ASP	CA-CB-CG	7.06	119.66	112.60
1	G	68	ASN	CA-CB-CG	7.06	119.66	112.60
1	E	14	VAL	N-CA-CB	7.06	120.14	110.54
1	M	412	VAL	CB-CA-C	-7.06	100.74	110.90
1	D	14	VAL	N-CA-CB	7.05	120.13	110.54
1	F	11	ASP	CB-CA-C	7.05	122.50	110.79
1	E	68	ASN	CA-CB-CG	7.05	119.65	112.60
1	K	52	ASP	CB-CA-C	7.04	122.45	109.70
1	C	68	ASN	CA-CB-CG	7.03	119.63	112.60
1	A	14	VAL	N-CA-CB	7.03	120.10	110.54
1	J	52	ASP	CB-CA-C	7.03	122.42	109.70
1	I	52	ASP	CB-CA-C	7.03	122.42	109.70
1	B	14	VAL	N-CA-CB	7.02	120.09	110.54
1	C	14	VAL	N-CA-CB	7.02	120.09	110.54
1	G	155	ASP	CB-CA-C	7.02	123.10	111.31
1	G	14	VAL	N-CA-CB	7.02	120.08	110.54
1	L	52	ASP	CB-CA-C	7.01	122.38	109.70
1	C	155	ASP	CB-CA-C	7.00	123.06	111.31
1	D	155	ASP	CB-CA-C	6.99	123.06	111.31
1	F	155	ASP	CB-CA-C	6.98	123.04	111.31
1	H	52	ASP	CB-CA-C	6.98	122.34	109.70
1	A	155	ASP	CB-CA-C	6.98	123.03	111.31
1	B	155	ASP	CB-CA-C	6.97	123.03	111.31
1	J	86	GLY	N-CA-C	-6.97	106.40	114.69
1	N	52	ASP	CB-CA-C	6.97	122.31	109.70
1	L	86	GLY	N-CA-C	-6.96	106.40	114.69
1	E	155	ASP	CB-CA-C	6.96	123.01	111.31
1	N	86	GLY	N-CA-C	-6.96	106.41	114.69
1	H	86	GLY	N-CA-C	-6.95	106.42	114.69
1	K	86	GLY	N-CA-C	-6.95	106.42	114.69
1	M	86	GLY	N-CA-C	-6.95	106.43	114.69
1	I	86	GLY	N-CA-C	-6.93	106.44	114.69
1	H	409	GLU	N-CA-CB	6.88	120.35	110.16
1	J	409	GLU	N-CA-CB	6.88	120.34	110.16
1	L	409	GLU	N-CA-CB	6.88	120.33	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	499	VAL	N-CA-CB	6.87	118.59	110.55
1	N	409	GLU	N-CA-CB	6.86	120.31	110.16
1	F	34	LYS	CB-CA-C	6.85	122.50	110.85
1	A	34	LYS	CB-CA-C	6.84	122.49	110.85
1	G	34	LYS	CB-CA-C	6.84	122.48	110.85
1	I	409	GLU	N-CA-CB	6.84	120.29	110.16
1	K	409	GLU	N-CA-CB	6.84	120.28	110.16
1	A	499	VAL	N-CA-CB	6.84	118.55	110.55
1	C	34	LYS	CB-CA-C	6.83	122.47	110.85
1	D	34	LYS	CB-CA-C	6.83	122.46	110.85
1	M	409	GLU	N-CA-CB	6.82	120.26	110.16
1	B	34	LYS	CB-CA-C	6.82	122.44	110.85
1	D	501	ARG	N-CA-CB	-6.81	100.11	110.12
1	G	501	ARG	N-CA-CB	-6.81	100.11	110.12
1	F	501	ARG	N-CA-CB	-6.80	100.12	110.12
1	E	34	LYS	CB-CA-C	6.80	122.42	110.85
1	B	501	ARG	N-CA-CB	-6.78	100.15	110.12
1	B	218	PRO	N-CA-CB	6.78	109.63	103.33
1	A	218	PRO	N-CA-CB	6.78	109.63	103.33
1	N	67	GLU	CB-CG-CD	6.78	124.12	112.60
1	E	501	ARG	N-CA-CB	-6.77	100.16	110.12
1	A	501	ARG	N-CA-CB	-6.77	100.17	110.12
1	C	501	ARG	N-CA-CB	-6.76	100.18	110.12
1	C	218	PRO	N-CA-CB	6.76	109.62	103.33
1	J	67	GLU	CB-CG-CD	6.75	124.08	112.60
1	M	67	GLU	CB-CG-CD	6.75	124.08	112.60
1	D	218	PRO	N-CA-CB	6.74	109.60	103.33
1	H	190	VAL	CB-CA-C	6.74	121.47	110.69
1	E	218	PRO	N-CA-CB	6.74	109.59	103.33
1	F	218	PRO	N-CA-CB	6.73	109.59	103.33
1	I	67	GLU	CB-CG-CD	6.73	124.04	112.60
1	K	67	GLU	CB-CG-CD	6.73	124.04	112.60
1	L	67	GLU	CB-CG-CD	6.73	124.04	112.60
1	G	218	PRO	N-CA-CB	6.72	109.58	103.33
1	N	479	ASN	N-CA-CB	6.72	121.38	110.42
1	H	67	GLU	CB-CG-CD	6.72	124.02	112.60
1	M	190	VAL	CB-CA-C	6.71	121.42	110.69
1	I	190	VAL	CB-CA-C	6.70	121.42	110.69
1	M	54	VAL	CB-CA-C	-6.70	103.09	112.14
1	L	190	VAL	CB-CA-C	6.70	121.41	110.69
1	N	190	VAL	CB-CA-C	6.70	121.41	110.69
1	J	190	VAL	CB-CA-C	6.70	121.40	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	190	VAL	CB-CA-C	6.69	121.39	110.69
1	J	54	VAL	CB-CA-C	-6.67	103.13	112.14
1	H	54	VAL	CB-CA-C	-6.67	103.13	112.14
1	F	257	GLU	N-CA-CB	-6.65	100.37	110.01
1	L	54	VAL	CB-CA-C	-6.65	103.17	112.14
1	C	257	GLU	N-CA-CB	-6.64	100.38	110.01
1	E	257	GLU	N-CA-CB	-6.64	100.38	110.01
1	I	54	VAL	CB-CA-C	-6.64	103.18	112.14
1	B	257	GLU	N-CA-CB	-6.63	100.39	110.01
1	A	257	GLU	N-CA-CB	-6.63	100.40	110.01
1	D	257	GLU	N-CA-CB	-6.62	100.41	110.01
1	G	257	GLU	N-CA-CB	-6.62	100.41	110.01
1	N	54	VAL	CB-CA-C	-6.62	103.20	112.14
1	K	54	VAL	CB-CA-C	-6.57	103.26	112.14
1	I	270	ILE	N-CA-C	-6.57	103.92	110.62
1	J	30	THR	N-CA-CB	6.56	119.77	110.12
1	M	270	ILE	N-CA-C	-6.55	103.94	110.62
1	J	270	ILE	N-CA-C	-6.54	103.95	110.62
1	L	284	ARG	CB-CA-C	-6.54	99.94	110.79
1	I	284	ARG	CB-CA-C	-6.53	99.94	110.79
1	H	284	ARG	CB-CA-C	-6.53	99.95	110.79
1	K	284	ARG	CB-CA-C	-6.53	99.95	110.79
1	N	270	ILE	N-CA-C	-6.52	103.97	110.62
1	C	510	VAL	N-CA-CB	6.52	118.18	110.55
1	M	284	ARG	CB-CA-C	-6.52	99.97	110.79
1	N	284	ARG	CB-CA-C	-6.52	99.97	110.79
1	D	510	VAL	N-CA-CB	6.51	118.17	110.55
1	J	284	ARG	CB-CA-C	-6.51	99.98	110.79
1	G	510	VAL	N-CA-CB	6.51	118.16	110.55
1	H	270	ILE	N-CA-C	-6.50	103.99	110.62
1	M	155	ASP	CB-CA-C	6.50	122.23	111.31
1	F	510	VAL	N-CA-CB	6.50	118.15	110.55
1	A	284	ARG	CB-CA-C	-6.49	100.02	110.79
1	A	510	VAL	N-CA-CB	6.48	118.13	110.55
1	G	54	VAL	CB-CA-C	-6.48	103.68	111.97
1	K	270	ILE	N-CA-C	-6.48	104.01	110.62
1	D	54	VAL	CB-CA-C	-6.48	103.68	111.97
1	C	54	VAL	CB-CA-C	-6.48	103.68	111.97
1	C	284	ARG	CB-CA-C	-6.48	100.04	110.79
1	I	297	GLY	N-CA-C	-6.48	106.38	115.32
1	F	284	ARG	CB-CA-C	-6.47	100.04	110.79
1	A	54	VAL	CB-CA-C	-6.47	103.69	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ILE	CB-CA-C	6.47	121.90	111.29
1	B	510	VAL	N-CA-CB	6.47	118.12	110.55
1	E	510	VAL	N-CA-CB	6.47	118.12	110.55
1	C	226	LYS	N-CA-CB	-6.47	100.86	110.17
1	D	284	ARG	CB-CA-C	-6.47	100.06	110.79
1	E	226	LYS	N-CA-CB	-6.47	100.86	110.17
1	G	284	ARG	CB-CA-C	-6.47	100.06	110.79
1	E	284	ARG	CB-CA-C	-6.46	100.06	110.79
1	L	270	ILE	N-CA-C	-6.46	104.03	110.62
1	B	54	VAL	CB-CA-C	-6.45	103.71	111.97
1	C	205	ILE	CB-CA-C	6.45	121.86	111.29
1	F	205	ILE	CB-CA-C	6.45	121.86	111.29
1	F	54	VAL	CB-CA-C	-6.44	103.72	111.97
1	G	226	LYS	N-CA-CB	-6.44	100.89	110.17
1	B	205	ILE	CB-CA-C	6.44	121.89	111.71
1	B	284	ARG	CB-CA-C	-6.44	100.10	110.79
1	K	297	GLY	N-CA-C	-6.44	106.43	115.32
1	E	27	VAL	CB-CA-C	6.43	120.83	112.14
1	E	205	ILE	CB-CA-C	6.43	121.87	111.71
1	G	205	ILE	CB-CA-C	6.43	121.86	111.71
1	E	54	VAL	CB-CA-C	-6.42	103.75	111.97
1	F	226	LYS	N-CA-CB	-6.42	100.93	110.17
1	C	27	VAL	CB-CA-C	6.42	120.80	112.14
1	J	297	GLY	N-CA-C	-6.41	106.47	115.32
1	D	205	ILE	CB-CA-C	6.41	121.84	111.71
1	H	297	GLY	N-CA-C	-6.41	106.48	115.32
1	G	27	VAL	CB-CA-C	6.41	120.79	112.14
1	A	226	LYS	N-CA-CB	-6.40	100.95	110.17
1	D	27	VAL	CB-CA-C	6.40	120.78	112.14
1	C	63	GLU	CA-CB-CG	6.40	126.89	114.10
1	L	297	GLY	N-CA-C	-6.40	106.49	115.32
1	F	27	VAL	CB-CA-C	6.39	120.77	112.14
1	A	27	VAL	CB-CA-C	6.39	120.77	112.14
1	M	297	GLY	N-CA-C	-6.38	106.51	115.32
1	G	196	ASP	N-CA-CB	-6.38	100.07	110.21
1	E	196	ASP	N-CA-CB	-6.38	100.07	110.21
1	C	196	ASP	N-CA-CB	-6.37	100.08	110.21
1	G	63	GLU	CA-CB-CG	6.37	126.84	114.10
1	N	297	GLY	N-CA-C	-6.37	106.53	115.32
1	A	196	ASP	N-CA-CB	-6.37	100.09	110.21
1	F	196	ASP	N-CA-CB	-6.37	100.09	110.21
1	I	155	ASP	CB-CA-C	6.37	122.00	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	297	GLY	N-CA-C	-6.36	106.54	115.32
1	K	43	SER	N-CA-CB	6.36	119.58	110.16
1	J	43	SER	N-CA-CB	6.36	119.58	110.16
1	I	43	SER	N-CA-CB	6.36	119.57	110.16
1	L	155	ASP	CB-CA-C	6.36	121.99	111.31
1	B	27	VAL	CB-CA-C	6.36	120.72	112.14
1	B	63	GLU	CA-CB-CG	6.36	126.81	114.10
1	B	196	ASP	N-CA-CB	-6.36	100.11	110.21
1	H	43	SER	N-CA-CB	6.35	119.56	110.16
1	A	297	GLY	N-CA-C	-6.35	106.56	115.32
1	F	63	GLU	CA-CB-CG	6.35	126.80	114.10
1	D	63	GLU	CA-CB-CG	6.34	126.78	114.10
1	J	155	ASP	CB-CA-C	6.34	121.95	111.31
1	D	196	ASP	N-CA-CB	-6.33	100.14	110.21
1	D	297	GLY	N-CA-C	-6.33	106.58	115.32
1	B	226	LYS	N-CA-CB	-6.33	101.06	110.17
1	M	43	SER	N-CA-CB	6.33	119.52	110.16
1	A	63	GLU	CA-CB-CG	6.33	126.75	114.10
1	N	43	SER	N-CA-CB	6.32	119.52	110.16
1	L	43	SER	N-CA-CB	6.32	119.51	110.16
1	F	297	GLY	N-CA-C	-6.31	106.61	115.32
1	C	297	GLY	N-CA-C	-6.31	106.61	115.32
1	H	152	ALA	CB-CA-C	6.31	122.30	110.63
1	L	196	ASP	N-CA-CB	-6.31	101.09	110.24
1	N	196	ASP	N-CA-CB	-6.30	101.10	110.24
1	K	196	ASP	N-CA-CB	-6.30	101.11	110.24
1	L	152	ALA	CB-CA-C	6.29	122.28	110.63
1	B	297	GLY	N-CA-C	-6.29	106.63	115.32
1	H	196	ASP	N-CA-CB	-6.29	101.12	110.24
1	N	152	ALA	CB-CA-C	6.29	122.27	110.63
1	B	85	ALA	N-CA-CB	-6.29	100.86	110.16
1	J	149	THR	N-CA-CB	6.28	119.36	110.12
1	J	196	ASP	N-CA-CB	-6.28	101.13	110.24
1	I	152	ALA	CB-CA-C	6.28	122.25	110.63
1	K	30	THR	N-CA-CB	6.28	119.35	110.12
1	E	63	GLU	CA-CB-CG	6.28	126.65	114.10
1	M	196	ASP	N-CA-CB	-6.28	101.14	110.24
1	E	85	ALA	N-CA-CB	-6.27	100.88	110.16
1	D	226	LYS	N-CA-CB	-6.27	101.14	110.17
1	J	152	ALA	CB-CA-C	6.27	122.23	110.63
1	I	196	ASP	N-CA-CB	-6.27	101.15	110.24
1	H	155	ASP	CB-CA-C	6.27	121.84	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	152	ALA	CB-CA-C	6.27	122.22	110.63
1	E	297	GLY	N-CA-C	-6.26	106.69	115.32
1	N	155	ASP	CB-CA-C	6.26	121.82	111.31
1	G	85	ALA	N-CA-CB	-6.25	100.91	110.16
1	K	149	THR	N-CA-CB	6.24	119.29	110.12
1	F	85	ALA	N-CA-CB	-6.23	100.94	110.16
1	A	380	LYS	N-CA-CB	-6.22	100.25	110.52
1	C	380	LYS	N-CA-CB	-6.22	100.25	110.52
1	B	380	LYS	N-CA-CB	-6.22	100.26	110.52
1	K	152	ALA	CB-CA-C	6.22	122.14	110.63
1	E	380	LYS	N-CA-CB	-6.20	100.29	110.52
1	D	380	LYS	N-CA-CB	-6.19	100.30	110.52
1	J	37	ASN	CA-CB-CG	6.19	118.79	112.60
1	G	380	LYS	N-CA-CB	-6.18	100.32	110.52
1	F	380	LYS	N-CA-CB	-6.17	100.34	110.52
1	K	77	VAL	CB-CA-C	6.17	120.47	112.14
1	N	381	VAL	N-CA-CB	-6.16	102.88	111.25
1	M	77	VAL	CB-CA-C	6.16	120.45	112.14
1	I	37	ASN	CA-CB-CG	6.15	118.75	112.60
1	L	77	VAL	CB-CA-C	6.15	120.44	112.14
1	I	381	VAL	N-CA-CB	-6.14	102.90	111.25
1	J	381	VAL	N-CA-CB	-6.14	102.90	111.25
1	M	381	VAL	N-CA-CB	-6.14	102.90	111.25
1	B	300	VAL	CB-CA-C	-6.13	101.08	110.95
1	L	37	ASN	CA-CB-CG	6.13	118.73	112.60
1	L	244	GLY	N-CA-C	-6.12	107.25	115.21
1	L	381	VAL	N-CA-CB	-6.12	102.93	111.25
1	E	300	VAL	CB-CA-C	-6.12	101.10	110.95
1	F	300	VAL	CB-CA-C	-6.12	101.10	110.95
1	H	37	ASN	CA-CB-CG	6.12	118.72	112.60
1	K	37	ASN	CA-CB-CG	6.11	118.71	112.60
1	K	381	VAL	N-CA-CB	-6.11	102.94	111.25
1	J	244	GLY	N-CA-C	-6.11	107.27	115.21
1	D	300	VAL	CB-CA-C	-6.11	101.12	110.95
1	N	37	ASN	CA-CB-CG	6.11	118.71	112.60
1	A	300	VAL	CB-CA-C	-6.10	101.13	110.95
1	G	300	VAL	CB-CA-C	-6.10	101.13	110.95
1	C	300	VAL	CB-CA-C	-6.09	101.14	110.95
1	N	244	GLY	N-CA-C	-6.09	107.29	115.21
1	M	244	GLY	N-CA-C	-6.09	107.30	115.21
1	H	244	GLY	N-CA-C	-6.08	107.30	115.21
1	H	381	VAL	N-CA-CB	-6.08	102.98	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	GLY	N-CA-C	-6.07	107.03	114.92
1	K	244	GLY	N-CA-C	-6.07	107.32	115.21
1	M	149	THR	N-CA-CB	6.07	119.04	110.12
1	I	244	GLY	N-CA-C	-6.06	107.33	115.21
1	M	37	ASN	CA-CB-CG	6.03	118.63	112.60
1	G	499	VAL	N-CA-CB	6.03	118.74	110.54
1	K	211	GLY	N-CA-C	-6.03	107.09	114.92
1	E	499	VAL	N-CA-CB	6.02	118.73	110.54
1	G	459	GLY	N-CA-C	-6.02	107.10	114.92
1	J	90	THR	N-CA-CB	6.01	118.96	110.12
1	M	211	GLY	N-CA-C	-6.01	107.11	114.92
1	A	85	ALA	N-CA-CB	-6.00	101.29	110.16
1	A	459	GLY	N-CA-C	-6.00	107.13	114.92
1	C	85	ALA	N-CA-CB	-6.00	101.29	110.16
1	D	459	GLY	N-CA-C	-5.99	107.13	114.92
1	D	85	ALA	N-CA-CB	-5.99	101.30	110.16
1	L	211	GLY	N-CA-C	-5.99	107.14	114.92
1	E	459	GLY	N-CA-C	-5.98	107.14	114.92
1	J	459	GLY	N-CA-C	-5.98	107.14	114.92
1	M	82	ASN	N-CA-CB	5.98	118.69	110.01
1	H	459	GLY	N-CA-C	-5.98	107.15	114.92
1	K	155	ASP	CB-CA-C	5.97	121.35	111.31
1	K	459	GLY	N-CA-C	-5.97	107.16	114.92
1	F	459	GLY	N-CA-C	-5.97	107.16	114.92
1	I	459	GLY	N-CA-C	-5.97	107.16	114.92
1	M	459	GLY	N-CA-C	-5.97	107.16	114.92
1	J	62	LEU	CB-CA-C	5.97	119.51	109.48
1	C	459	GLY	N-CA-C	-5.97	107.16	114.92
1	L	361	ASP	CB-CA-C	5.97	120.69	110.79
1	M	361	ASP	CB-CA-C	5.97	120.69	110.79
1	J	361	ASP	CB-CA-C	5.96	120.69	110.79
1	J	211	GLY	N-CA-C	-5.96	107.17	114.92
1	K	361	ASP	CB-CA-C	5.96	120.69	110.79
1	H	211	GLY	N-CA-C	-5.96	107.18	114.92
1	A	64	ASP	CB-CA-C	5.95	119.83	109.65
1	N	211	GLY	N-CA-C	-5.95	107.19	114.92
1	N	361	ASP	CB-CA-C	5.95	120.66	110.79
1	M	62	LEU	CB-CA-C	5.94	119.46	109.48
1	H	361	ASP	CB-CA-C	5.94	120.65	110.79
1	I	211	GLY	N-CA-C	-5.94	107.20	114.92
1	I	62	LEU	CB-CA-C	5.93	119.45	109.48
1	I	361	ASP	CB-CA-C	5.93	120.64	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	62	LEU	CB-CA-C	5.93	119.44	109.48
1	N	459	GLY	N-CA-C	-5.93	107.22	114.92
1	D	64	ASP	CB-CA-C	5.92	119.78	109.65
1	E	64	ASP	CB-CA-C	5.92	119.78	109.65
1	H	62	LEU	CB-CA-C	5.92	119.43	109.48
1	H	82	ASN	N-CA-CB	5.92	118.60	110.01
1	K	82	ASN	N-CA-CB	5.92	118.60	110.01
1	K	62	LEU	CB-CA-C	5.92	119.42	109.48
1	L	82	ASN	N-CA-CB	5.92	118.59	110.01
1	L	14	VAL	N-CA-CB	5.91	118.58	110.54
1	G	64	ASP	CB-CA-C	5.91	119.76	109.65
1	L	90	THR	N-CA-CB	5.91	118.81	110.12
1	H	90	THR	N-CA-CB	5.91	118.80	110.12
1	B	64	ASP	CB-CA-C	5.90	119.74	109.65
1	I	90	THR	N-CA-CB	5.90	118.80	110.12
1	L	459	GLY	N-CA-C	-5.90	107.25	114.92
1	D	285	ARG	N-CA-CB	5.90	118.80	110.12
1	N	14	VAL	N-CA-CB	5.90	118.56	110.54
1	C	518	GLU	CB-CA-C	5.90	120.22	110.90
1	F	64	ASP	CB-CA-C	5.90	119.73	109.65
1	I	82	ASN	N-CA-CB	5.90	118.56	110.01
1	K	14	VAL	N-CA-CB	5.90	118.56	110.54
1	D	518	GLU	CB-CA-C	5.89	120.21	110.90
1	C	285	ARG	N-CA-CB	5.89	118.78	110.12
1	F	407	VAL	N-CA-CB	5.89	117.44	110.55
1	N	62	LEU	CB-CA-C	5.89	119.37	109.48
1	B	175	ILE	CB-CA-C	-5.89	101.85	110.62
1	G	518	GLU	CB-CA-C	5.89	120.20	110.90
1	E	285	ARG	N-CA-CB	5.88	118.77	110.12
1	N	90	THR	N-CA-CB	5.88	118.77	110.12
1	C	64	ASP	CB-CA-C	5.88	119.70	109.65
1	G	285	ARG	N-CA-CB	5.88	118.76	110.12
1	M	14	VAL	N-CA-CB	5.88	118.53	110.54
1	E	518	GLU	CB-CA-C	5.87	120.18	110.90
1	F	518	GLU	CB-CA-C	5.87	120.18	110.90
1	J	14	VAL	N-CA-CB	5.87	118.53	110.54
1	B	518	GLU	CB-CA-C	5.87	120.17	110.90
1	A	153	ASN	CA-CB-CG	5.87	118.47	112.60
1	C	499	VAL	N-CA-CB	5.87	118.52	110.54
1	B	285	ARG	N-CA-CB	5.87	118.74	110.12
1	C	41	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	153	ASN	CA-CB-CG	5.86	118.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	14	VAL	N-CA-CB	5.86	118.51	110.54
1	F	294	THR	N-CA-CB	5.86	118.73	110.12
1	E	153	ASN	CA-CB-CG	5.86	118.46	112.60
1	A	285	ARG	N-CA-CB	5.86	118.73	110.12
1	E	152	ALA	CB-CA-C	5.86	121.46	110.63
1	I	14	VAL	N-CA-CB	5.86	118.50	110.54
1	A	90	THR	N-CA-CB	5.85	118.73	110.12
1	D	175	ILE	CB-CA-C	-5.85	101.90	110.62
1	E	175	ILE	CB-CA-C	-5.85	101.90	110.62
1	G	41	ASP	CA-CB-CG	5.85	118.45	112.60
1	E	41	ASP	CA-CB-CG	5.85	118.45	112.60
1	F	175	ILE	CB-CA-C	-5.85	101.90	110.62
1	G	407	VAL	N-CA-CB	5.85	117.39	110.55
1	G	90	THR	N-CA-CB	5.85	118.72	110.12
1	G	294	THR	N-CA-CB	5.85	118.72	110.12
1	D	153	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	407	VAL	N-CA-CB	5.85	117.39	110.55
1	B	90	THR	N-CA-CB	5.84	118.71	110.12
1	G	152	ALA	CB-CA-C	5.84	121.44	110.63
1	C	90	THR	N-CA-CB	5.84	118.71	110.12
1	C	175	ILE	CB-CA-C	-5.84	101.92	110.62
1	D	90	THR	N-CA-CB	5.84	118.71	110.12
1	G	175	ILE	CB-CA-C	-5.84	101.92	110.62
1	A	175	ILE	CB-CA-C	-5.84	101.92	110.62
1	A	518	GLU	CB-CA-C	5.84	120.13	110.90
1	A	294	THR	N-CA-CB	5.84	118.70	110.12
1	D	407	VAL	N-CA-CB	5.84	117.38	110.55
1	G	153	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	152	ALA	CB-CA-C	5.83	121.42	110.63
1	E	294	THR	N-CA-CB	5.83	118.70	110.12
1	D	152	ALA	CB-CA-C	5.83	121.42	110.63
1	F	90	THR	N-CA-CB	5.83	118.69	110.12
1	M	501	ARG	N-CA-CB	-5.83	101.55	110.01
1	B	294	THR	N-CA-CB	5.83	118.69	110.12
1	L	501	ARG	N-CA-CB	-5.83	101.56	110.01
1	C	407	VAL	N-CA-CB	5.83	117.37	110.55
1	B	153	ASN	CA-CB-CG	5.83	118.43	112.60
1	F	285	ARG	N-CA-CB	5.83	118.69	110.12
1	B	152	ALA	CB-CA-C	5.83	121.41	110.63
1	C	294	THR	N-CA-CB	5.83	118.68	110.12
1	J	82	ASN	N-CA-CB	5.83	118.46	110.01
1	F	153	ASN	CA-CB-CG	5.82	118.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	ASP	CA-CB-CG	5.82	118.42	112.60
1	F	152	ALA	CB-CA-C	5.82	121.39	110.63
1	N	82	ASN	N-CA-CB	5.82	118.44	110.01
1	N	501	ARG	N-CA-CB	-5.81	101.58	110.01
1	B	41	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	152	ALA	CB-CA-C	5.81	121.38	110.63
1	D	294	THR	N-CA-CB	5.81	118.67	110.12
1	E	211	GLY	N-CA-C	-5.81	107.37	114.92
1	B	361	ASP	CB-CA-C	5.81	120.43	110.79
1	F	41	ASP	CA-CB-CG	5.81	118.41	112.60
1	F	211	GLY	N-CA-C	-5.80	107.38	114.92
1	K	501	ARG	N-CA-CB	-5.80	101.60	110.01
1	C	479	ASN	CB-CA-C	5.80	119.59	110.19
1	A	361	ASP	CB-CA-C	5.80	120.42	110.79
1	B	407	VAL	N-CA-CB	5.80	117.33	110.55
1	B	479	ASN	CB-CA-C	5.80	119.58	110.19
1	G	361	ASP	CB-CA-C	5.80	120.41	110.79
1	D	361	ASP	CB-CA-C	5.79	120.41	110.79
1	F	361	ASP	CB-CA-C	5.79	120.41	110.79
1	E	90	THR	N-CA-CB	5.79	118.64	110.12
1	G	479	ASN	CB-CA-C	5.79	119.58	110.19
1	C	361	ASP	CB-CA-C	5.79	120.40	110.79
1	E	479	ASN	CB-CA-C	5.79	119.57	110.19
1	A	211	GLY	N-CA-C	-5.79	107.40	114.92
1	A	479	ASN	CB-CA-C	5.79	119.57	110.19
1	E	407	VAL	N-CA-CB	5.79	117.32	110.55
1	H	499	VAL	N-CA-CB	5.78	118.40	110.54
1	A	41	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	211	GLY	N-CA-C	-5.78	107.41	114.92
1	D	211	GLY	N-CA-C	-5.77	107.42	114.92
1	G	211	GLY	N-CA-C	-5.77	107.42	114.92
1	H	501	ARG	N-CA-CB	-5.77	101.64	110.01
1	J	501	ARG	N-CA-CB	-5.77	101.64	110.01
1	E	361	ASP	CB-CA-C	5.77	120.36	110.79
1	F	479	ASN	CB-CA-C	5.77	119.53	110.19
1	I	501	ARG	N-CA-CB	-5.77	101.65	110.01
1	I	499	VAL	N-CA-CB	5.76	118.38	110.54
1	N	499	VAL	N-CA-CB	5.76	118.37	110.54
1	L	499	VAL	N-CA-CB	5.75	118.36	110.54
1	C	306	GLY	N-CA-C	-5.75	107.39	115.32
1	D	479	ASN	CB-CA-C	5.74	119.49	110.19
1	D	306	GLY	N-CA-C	-5.74	107.40	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	205	ILE	CB-CA-C	5.74	120.70	111.29
1	J	499	VAL	N-CA-CB	5.74	118.34	110.54
1	C	211	GLY	N-CA-C	-5.73	107.47	114.92
1	H	458	CYS	N-CA-CB	5.73	118.54	110.12
1	H	205	ILE	CB-CA-C	5.72	120.68	111.29
1	K	205	ILE	CB-CA-C	5.72	120.67	111.29
1	E	306	GLY	N-CA-C	-5.72	107.43	115.32
1	I	205	ILE	CB-CA-C	5.72	120.67	111.29
1	L	205	ILE	CB-CA-C	5.72	120.67	111.29
1	K	458	CYS	N-CA-CB	5.71	118.52	110.12
1	M	205	ILE	CB-CA-C	5.71	120.66	111.29
1	G	306	GLY	N-CA-C	-5.71	107.44	115.32
1	B	306	GLY	N-CA-C	-5.70	107.45	115.32
1	J	205	ILE	CB-CA-C	5.70	120.64	111.29
1	K	85	ALA	N-CA-CB	-5.70	101.72	110.16
1	N	458	CYS	N-CA-CB	5.70	118.51	110.12
1	L	458	CYS	N-CA-CB	5.70	118.50	110.12
1	F	345	ARG	N-CA-CB	5.70	118.50	110.12
1	J	85	ALA	N-CA-CB	-5.70	101.73	110.16
1	N	85	ALA	N-CA-CB	-5.70	101.73	110.16
1	K	499	VAL	N-CA-CB	5.69	118.28	110.54
1	F	306	GLY	N-CA-C	-5.69	107.47	115.32
1	G	314	LEU	CB-CA-C	-5.69	101.34	110.79
1	A	306	GLY	N-CA-C	-5.69	107.47	115.32
1	E	62	LEU	CB-CA-C	5.69	119.62	109.38
1	A	345	ARG	N-CA-CB	5.69	118.48	110.12
1	B	153	ASN	CB-CA-C	5.69	120.41	112.11
1	F	314	LEU	CB-CA-C	-5.69	101.35	110.79
1	D	62	LEU	CB-CA-C	5.69	119.61	109.38
1	G	62	LEU	CB-CA-C	5.69	119.62	109.38
1	C	314	LEU	CB-CA-C	-5.68	101.35	110.79
1	B	345	ARG	N-CA-CB	5.68	118.47	110.12
1	E	314	LEU	CB-CA-C	-5.68	101.36	110.79
1	L	85	ALA	N-CA-CB	-5.68	101.75	110.16
1	G	345	ARG	N-CA-CB	5.68	118.47	110.12
1	M	458	CYS	N-CA-CB	5.68	118.47	110.12
1	H	85	ALA	N-CA-CB	-5.68	101.76	110.16
1	J	458	CYS	N-CA-CB	5.67	118.46	110.12
1	N	296	THR	N-CA-CB	5.67	118.46	110.12
1	C	345	ARG	N-CA-CB	5.67	118.46	110.12
1	H	296	THR	N-CA-CB	5.67	118.46	110.12
1	I	296	THR	N-CA-CB	5.67	118.46	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	458	CYS	N-CA-CB	5.67	118.46	110.12
1	C	62	LEU	CB-CA-C	5.67	119.58	109.38
1	E	89	THR	CB-CA-C	-5.67	101.98	110.88
1	L	296	THR	N-CA-CB	5.67	118.45	110.12
1	D	345	ARG	N-CA-CB	5.67	118.45	110.12
1	G	25	ASP	CA-CB-CG	-5.67	106.93	112.60
1	I	85	ALA	N-CA-CB	-5.67	101.78	110.16
1	M	296	THR	N-CA-CB	5.67	118.45	110.12
1	B	314	LEU	CB-CA-C	-5.67	101.39	110.79
1	E	25	ASP	CA-CB-CG	-5.67	106.94	112.60
1	G	153	ASN	CB-CA-C	5.67	120.38	112.11
1	D	314	LEU	CB-CA-C	-5.66	101.39	110.79
1	N	473	ASP	CB-CA-C	5.66	121.21	110.51
1	C	153	ASN	CB-CA-C	5.66	120.38	112.11
1	D	89	THR	CB-CA-C	-5.66	101.99	110.88
1	A	254	VAL	N-CA-CB	-5.66	103.60	111.41
1	A	62	LEU	CB-CA-C	5.66	119.57	109.38
1	K	296	THR	N-CA-CB	5.66	118.44	110.12
1	F	89	THR	CB-CA-C	-5.66	102.00	110.88
1	F	153	ASN	CB-CA-C	5.66	120.37	112.11
1	K	153	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	25	ASP	CA-CB-CG	-5.65	106.95	112.60
1	C	254	VAL	N-CA-CB	-5.65	103.61	111.41
1	A	89	THR	CB-CA-C	-5.65	102.01	110.88
1	E	345	ARG	N-CA-CB	5.65	118.43	110.12
1	K	473	ASP	CB-CA-C	5.65	121.19	110.51
1	B	62	LEU	CB-CA-C	5.65	119.55	109.38
1	L	473	ASP	CB-CA-C	5.65	121.19	110.51
1	F	254	VAL	N-CA-CB	-5.65	103.62	111.41
1	G	89	THR	CB-CA-C	-5.65	102.02	110.88
1	F	25	ASP	CA-CB-CG	-5.64	106.96	112.60
1	I	473	ASP	CB-CA-C	5.64	121.18	110.51
1	B	254	VAL	N-CA-CB	-5.64	103.62	111.41
1	C	89	THR	CB-CA-C	-5.64	102.02	110.88
1	D	25	ASP	CA-CB-CG	-5.64	106.96	112.60
1	H	473	ASP	CB-CA-C	5.64	121.17	110.51
1	C	25	ASP	CA-CB-CG	-5.64	106.96	112.60
1	E	153	ASN	CB-CA-C	5.64	120.34	112.11
1	A	314	LEU	CB-CA-C	-5.63	101.44	110.79
1	D	153	ASN	CB-CA-C	5.63	120.34	112.11
1	J	77	VAL	CB-CA-C	5.63	119.75	112.14
1	M	473	ASP	CB-CA-C	5.63	121.16	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	254	VAL	N-CA-CB	-5.63	103.64	111.41
1	J	473	ASP	CB-CA-C	5.63	121.15	110.51
1	B	330	THR	CB-CA-C	-5.63	99.41	109.71
1	E	330	THR	CB-CA-C	-5.63	99.41	109.71
1	G	254	VAL	N-CA-CB	-5.63	103.64	111.41
1	J	306	GLY	N-CA-C	-5.63	107.50	115.43
1	A	153	ASN	CB-CA-C	5.63	120.33	112.11
1	A	330	THR	CB-CA-C	-5.63	99.41	109.71
1	F	62	LEU	CB-CA-C	5.63	119.51	109.38
1	B	89	THR	CB-CA-C	-5.62	102.06	110.88
1	I	77	VAL	CB-CA-C	5.62	119.72	112.14
1	J	25	ASP	CA-CB-CG	-5.62	106.98	112.60
1	N	495	ASP	CB-CA-C	-5.62	100.01	108.61
1	N	300	VAL	CB-CA-C	-5.62	101.91	110.95
1	B	25	ASP	CA-CB-CG	-5.62	106.98	112.60
1	E	254	VAL	N-CA-CB	-5.62	103.66	111.41
1	C	330	THR	CB-CA-C	-5.61	99.44	109.71
1	J	300	VAL	CB-CA-C	-5.61	101.92	110.95
1	F	330	THR	CB-CA-C	-5.61	99.45	109.71
1	H	77	VAL	CB-CA-C	5.60	119.70	112.14
1	M	87	ASP	CA-CB-CG	5.60	118.20	112.60
1	G	330	THR	CB-CA-C	-5.60	99.46	109.71
1	J	296	THR	N-CA-CB	5.60	118.35	110.12
1	L	300	VAL	CB-CA-C	-5.60	101.94	110.95
1	M	300	VAL	CB-CA-C	-5.60	101.94	110.95
1	D	330	THR	CB-CA-C	-5.59	99.47	109.71
1	K	300	VAL	CB-CA-C	-5.59	101.94	110.95
1	H	306	GLY	N-CA-C	-5.59	107.55	115.43
1	I	300	VAL	CB-CA-C	-5.59	101.95	110.95
1	I	306	GLY	N-CA-C	-5.59	107.55	115.43
1	E	491	MET	CB-CA-C	5.59	120.07	110.79
1	G	491	MET	CB-CA-C	5.59	120.07	110.79
1	H	300	VAL	CB-CA-C	-5.59	101.95	110.95
1	M	306	GLY	N-CA-C	-5.59	107.55	115.43
1	K	306	GLY	N-CA-C	-5.59	107.55	115.43
1	N	77	VAL	CB-CA-C	5.58	119.68	112.14
1	D	491	MET	CB-CA-C	5.58	120.05	110.79
1	F	491	MET	CB-CA-C	5.58	120.05	110.79
1	N	306	GLY	N-CA-C	-5.58	107.56	115.43
1	L	306	GLY	N-CA-C	-5.57	107.57	115.43
1	B	491	MET	CB-CA-C	5.57	120.04	110.79
1	C	491	MET	CB-CA-C	5.56	120.02	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	407	VAL	N-CA-CB	5.56	117.06	110.55
1	E	77	VAL	CB-CA-C	5.56	119.64	112.14
1	G	412	VAL	N-CA-CB	5.55	121.80	112.47
1	K	407	VAL	N-CA-CB	5.55	117.05	110.55
1	F	234	LEU	N-CA-CB	5.55	118.57	110.30
1	J	407	VAL	N-CA-CB	5.55	117.04	110.55
1	B	417	VAL	CA-CB-CG2	-5.55	100.97	110.40
1	H	407	VAL	N-CA-CB	5.55	117.04	110.55
1	F	77	VAL	CB-CA-C	5.54	119.62	112.14
1	D	417	VAL	CA-CB-CG2	-5.54	100.98	110.40
1	M	407	VAL	N-CA-CB	5.54	117.03	110.55
1	A	491	MET	CB-CA-C	5.53	119.97	110.79
1	G	234	LEU	N-CA-CB	5.53	118.55	110.30
1	A	373	ALA	N-CA-C	-5.53	105.15	111.07
1	B	77	VAL	CB-CA-C	5.53	119.61	112.14
1	F	338	GLU	N-CA-CB	5.53	120.45	110.83
1	F	417	VAL	CA-CB-CG2	-5.53	101.00	110.40
1	N	407	VAL	N-CA-CB	5.53	117.02	110.55
1	A	234	LEU	N-CA-CB	5.53	118.54	110.30
1	H	200	LEU	N-CA-CB	5.53	118.03	110.01
1	F	412	VAL	N-CA-CB	5.53	121.75	112.47
1	I	407	VAL	N-CA-CB	5.53	117.02	110.55
1	N	200	LEU	N-CA-CB	5.53	118.02	110.01
1	A	77	VAL	CB-CA-C	5.52	119.60	112.14
1	A	412	VAL	N-CA-CB	5.52	121.75	112.47
1	E	234	LEU	N-CA-CB	5.52	118.53	110.30
1	G	77	VAL	CB-CA-C	5.52	119.60	112.14
1	I	415	GLY	N-CA-C	-5.52	107.62	115.30
1	K	200	LEU	N-CA-CB	5.52	118.01	110.01
1	C	417	VAL	CA-CB-CG2	-5.52	101.02	110.40
1	D	412	VAL	N-CA-CB	5.52	121.74	112.47
1	G	417	VAL	CA-CB-CG2	-5.52	101.02	110.40
1	C	77	VAL	CB-CA-C	5.51	119.58	112.14
1	E	417	VAL	CA-CB-CG2	-5.51	101.02	110.40
1	B	234	LEU	N-CA-CB	5.51	118.51	110.30
1	B	412	VAL	N-CA-CB	5.51	121.73	112.47
1	C	412	VAL	N-CA-CB	5.51	121.73	112.47
1	A	338	GLU	N-CA-CB	5.51	120.42	110.83
1	F	420	ILE	CB-CA-C	5.51	119.82	112.22
1	M	200	LEU	N-CA-CB	5.51	118.00	110.01
1	C	338	GLU	N-CA-CB	5.51	120.41	110.83
1	G	338	GLU	N-CA-CB	5.51	120.41	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	200	LEU	N-CA-CB	5.51	118.00	110.01
1	L	415	GLY	N-CA-C	-5.51	107.65	115.30
1	D	77	VAL	CB-CA-C	5.50	119.57	112.14
1	J	415	GLY	N-CA-C	-5.50	107.65	115.30
1	K	415	GLY	N-CA-C	-5.50	107.65	115.30
1	C	455	VAL	CB-CA-C	5.50	119.57	112.14
1	D	234	LEU	N-CA-CB	5.50	118.50	110.30
1	E	412	VAL	N-CA-CB	5.50	121.71	112.47
1	E	72	GLN	N-CA-CB	5.50	118.20	110.12
1	J	416	GLY	N-CA-C	-5.50	106.61	115.08
1	D	338	GLU	N-CA-CB	5.50	120.40	110.83
1	N	25	ASP	CA-CB-CG	-5.50	107.10	112.60
1	B	338	GLU	N-CA-CB	5.50	120.39	110.83
1	M	104	LEU	CB-CA-C	5.50	119.91	110.79
1	E	338	GLU	N-CA-CB	5.49	120.39	110.83
1	L	255	GLU	CB-CA-C	5.49	118.68	109.89
1	A	420	ILE	CB-CA-C	5.49	119.80	112.22
1	C	234	LEU	N-CA-CB	5.49	118.48	110.30
1	M	255	GLU	CB-CA-C	5.49	118.68	109.89
1	E	216	GLU	CB-CG-CD	5.49	121.93	112.60
1	G	216	GLU	CB-CG-CD	5.49	121.93	112.60
1	I	99	ILE	N-CA-CB	5.49	116.97	110.55
1	I	200	LEU	N-CA-CB	5.49	117.97	110.01
1	L	104	LEU	CB-CA-C	5.49	119.90	110.79
1	F	373	ALA	N-CA-C	-5.49	105.20	111.07
1	H	415	GLY	N-CA-C	-5.49	107.67	115.30
1	K	255	GLU	CB-CA-C	5.49	118.67	109.89
1	E	455	VAL	CB-CA-C	5.49	119.55	112.14
1	C	196	ASP	CB-CA-C	5.48	119.86	110.81
1	I	265	ASN	CA-CB-CG	-5.48	107.12	112.60
1	N	416	GLY	N-CA-C	-5.48	106.64	115.08
1	E	420	ILE	CB-CA-C	5.48	119.78	112.22
1	F	216	GLU	CB-CG-CD	5.48	121.92	112.60
1	J	200	LEU	N-CA-CB	5.48	117.96	110.01
1	B	373	ALA	N-CA-C	-5.48	105.21	111.07
1	G	455	VAL	CB-CA-C	5.48	119.53	112.14
1	M	415	GLY	N-CA-C	-5.48	107.69	115.30
1	B	455	VAL	CB-CA-C	5.47	119.53	112.14
1	K	99	ILE	N-CA-CB	5.47	116.96	110.55
1	C	216	GLU	CB-CG-CD	5.47	121.90	112.60
1	F	455	VAL	CB-CA-C	5.47	119.53	112.14
1	G	196	ASP	CB-CA-C	5.47	119.84	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	25	ASP	CA-CB-CG	-5.47	107.13	112.60
1	J	255	GLU	CB-CA-C	5.47	118.64	109.89
1	A	417	VAL	CA-CB-CG2	-5.47	101.10	110.40
1	G	72	GLN	N-CA-CB	5.47	118.16	110.12
1	J	99	ILE	N-CA-CB	5.47	116.95	110.55
1	E	373	ALA	N-CA-C	-5.47	105.22	111.07
1	G	420	ILE	CB-CA-C	5.47	119.77	112.22
1	L	99	ILE	N-CA-CB	5.47	116.95	110.55
1	N	359	ASP	CA-CB-CG	-5.47	107.13	112.60
1	D	420	ILE	CB-CA-C	5.47	119.76	112.22
1	E	196	ASP	CB-CA-C	5.47	119.83	110.81
1	L	416	GLY	N-CA-C	-5.47	106.66	115.08
1	N	255	GLU	CB-CA-C	5.47	118.64	109.89
1	B	196	ASP	CB-CA-C	5.46	119.83	110.81
1	K	104	LEU	CB-CA-C	5.46	119.86	110.79
1	N	99	ILE	N-CA-CB	5.46	116.94	110.55
1	F	72	GLN	N-CA-CB	5.46	118.15	110.12
1	L	359	ASP	CA-CB-CG	-5.46	107.14	112.60
1	N	104	LEU	CB-CA-C	5.46	119.86	110.79
1	N	415	GLY	N-CA-C	-5.46	107.71	115.30
1	D	216	GLU	CB-CG-CD	5.46	121.88	112.60
1	F	196	ASP	CB-CA-C	5.46	119.82	110.81
1	J	104	LEU	CB-CA-C	5.46	119.85	110.79
1	B	216	GLU	CB-CG-CD	5.46	121.88	112.60
1	I	104	LEU	CB-CA-C	5.46	119.85	110.79
1	I	255	GLU	CB-CA-C	5.46	118.62	109.89
1	K	25	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	455	VAL	CB-CA-C	5.46	119.51	112.14
1	H	99	ILE	N-CA-CB	5.46	116.93	110.55
1	H	255	GLU	CB-CA-C	5.46	118.62	109.89
1	A	216	GLU	CB-CG-CD	5.46	121.87	112.60
1	M	416	GLY	N-CA-C	-5.46	106.68	115.08
1	D	72	GLN	N-CA-CB	5.45	118.14	110.12
1	C	416	GLY	N-CA-C	-5.45	106.68	115.08
1	G	415	GLY	N-CA-C	-5.45	107.72	115.30
1	D	455	VAL	CB-CA-C	5.45	119.49	112.14
1	B	415	GLY	N-CA-C	-5.45	107.73	115.30
1	F	416	GLY	N-CA-C	-5.45	106.69	115.08
1	H	104	LEU	CB-CA-C	5.45	119.83	110.79
1	M	359	ASP	CA-CB-CG	-5.45	107.16	112.60
1	A	72	GLN	N-CA-CB	5.44	118.12	110.12
1	A	416	GLY	N-CA-C	-5.44	106.70	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	GLN	N-CA-CB	5.44	118.12	110.12
1	D	196	ASP	CB-CA-C	5.44	119.79	110.81
1	H	416	GLY	N-CA-C	-5.44	106.70	115.08
1	G	373	ALA	N-CA-C	-5.44	105.25	111.07
1	C	420	ILE	CB-CA-C	5.44	119.73	112.22
1	C	373	ALA	N-CA-C	-5.44	105.25	111.07
1	I	25	ASP	CA-CB-CG	-5.44	107.16	112.60
1	M	99	ILE	N-CA-CB	5.43	116.91	110.55
1	B	420	ILE	CB-CA-C	5.43	119.72	112.22
1	A	196	ASP	CB-CA-C	5.43	119.77	110.81
1	H	265	ASN	CA-CB-CG	-5.43	107.17	112.60
1	K	359	ASP	CA-CB-CG	-5.43	107.17	112.60
1	A	415	GLY	N-CA-C	-5.43	107.75	115.30
1	M	25	ASP	CA-CB-CG	-5.43	107.17	112.60
1	J	510	VAL	N-CA-CB	5.42	116.90	110.55
1	J	359	ASP	CA-CB-CG	-5.42	107.18	112.60
1	C	72	GLN	N-CA-CB	5.42	118.09	110.12
1	I	266	THR	N-CA-CB	5.42	118.18	110.16
1	N	265	ASN	CA-CB-CG	-5.42	107.18	112.60
1	C	415	GLY	N-CA-C	-5.42	107.77	115.30
1	D	373	ALA	N-CA-C	-5.42	105.27	111.07
1	D	415	GLY	N-CA-C	-5.42	107.77	115.30
1	I	359	ASP	CA-CB-CG	-5.42	107.18	112.60
1	L	265	ASN	CA-CB-CG	-5.42	107.18	112.60
1	N	510	VAL	N-CA-CB	5.42	116.89	110.55
1	I	510	VAL	N-CA-CB	5.41	116.88	110.55
1	K	416	GLY	N-CA-C	-5.41	106.75	115.08
1	L	266	THR	N-CA-CB	5.41	118.17	110.16
1	B	416	GLY	N-CA-C	-5.41	106.75	115.08
1	L	25	ASP	CA-CB-CG	-5.41	107.19	112.60
1	M	265	ASN	CA-CB-CG	-5.41	107.19	112.60
1	K	265	ASN	CA-CB-CG	-5.41	107.19	112.60
1	E	415	GLY	N-CA-C	-5.41	107.78	115.30
1	I	416	GLY	N-CA-C	-5.41	106.75	115.08
1	J	265	ASN	CA-CB-CG	-5.40	107.20	112.60
1	E	416	GLY	N-CA-C	-5.40	106.77	115.08
1	H	359	ASP	CA-CB-CG	-5.40	107.20	112.60
1	K	510	VAL	N-CA-CB	5.40	116.87	110.55
1	M	510	VAL	N-CA-CB	5.40	116.86	110.55
1	K	266	THR	N-CA-CB	5.39	118.14	110.16
1	N	266	THR	N-CA-CB	5.39	118.14	110.16
1	H	510	VAL	N-CA-CB	5.39	116.85	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	416	GLY	N-CA-C	-5.39	106.78	115.08
1	J	266	THR	N-CA-CB	5.38	118.13	110.16
1	G	416	GLY	N-CA-C	-5.38	106.79	115.08
1	I	153	ASN	CA-CB-CG	5.38	117.98	112.60
1	I	321	LYS	N-CA-CB	5.38	117.81	110.01
1	H	321	LYS	N-CA-CB	5.38	117.80	110.01
1	H	266	THR	N-CA-CB	5.37	118.11	110.16
1	G	63	GLU	CB-CA-C	-5.37	101.87	110.79
1	M	85	ALA	N-CA-CB	-5.37	102.21	110.16
1	C	63	GLU	CB-CA-C	-5.37	101.88	110.79
1	H	261	THR	N-CA-CB	5.37	117.79	110.01
1	K	321	LYS	N-CA-CB	5.37	117.80	110.01
1	E	63	GLU	CB-CA-C	-5.37	101.88	110.79
1	N	261	THR	N-CA-CB	5.37	117.79	110.01
1	A	63	GLU	CB-CA-C	-5.36	101.89	110.79
1	E	266	THR	N-CA-CB	5.36	118.10	110.16
1	F	63	GLU	CB-CA-C	-5.36	101.89	110.79
1	J	261	THR	N-CA-CB	5.36	117.78	110.01
1	L	261	THR	N-CA-CB	5.36	117.78	110.01
1	F	415	GLY	N-CA-C	-5.36	107.85	115.30
1	N	321	LYS	N-CA-CB	5.36	117.78	110.01
1	A	126	ALA	CB-CA-C	5.36	119.68	110.79
1	B	63	GLU	CB-CA-C	-5.36	101.90	110.79
1	D	63	GLU	CB-CA-C	-5.36	101.90	110.79
1	J	153	ASN	CA-CB-CG	5.36	117.96	112.60
1	K	261	THR	N-CA-CB	5.36	117.78	110.01
1	L	321	LYS	N-CA-CB	5.36	117.78	110.01
1	M	266	THR	N-CA-CB	5.36	118.08	110.16
1	L	153	ASN	CA-CB-CG	5.35	117.95	112.60
1	D	411	VAL	CA-CB-CG2	5.35	119.49	110.40
1	L	510	VAL	N-CA-CB	5.35	116.81	110.55
1	K	52	ASP	CA-CB-CG	5.34	117.94	112.60
1	C	266	THR	N-CA-CB	5.34	118.07	110.16
1	K	252	GLU	N-CA-C	-5.34	105.35	111.07
1	I	261	THR	N-CA-CB	5.34	117.76	110.01
1	C	126	ALA	CB-CA-C	5.34	119.65	110.79
1	B	126	ALA	CB-CA-C	5.34	119.65	110.79
1	E	126	ALA	CB-CA-C	5.34	119.65	110.79
1	A	266	THR	N-CA-CB	5.33	118.05	110.16
1	B	266	THR	N-CA-CB	5.33	118.05	110.16
1	D	266	THR	N-CA-CB	5.33	118.05	110.16
1	F	266	THR	N-CA-CB	5.33	118.05	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	517	THR	N-CA-CB	5.33	119.50	110.49
1	C	411	VAL	CA-CB-CG2	5.33	119.46	110.40
1	M	261	THR	N-CA-CB	5.33	117.73	110.01
1	M	321	LYS	N-CA-CB	5.33	117.73	110.01
1	E	270	ILE	N-CA-CB	5.32	117.78	110.54
1	D	422	VAL	N-CA-CB	5.32	117.78	110.54
1	G	266	THR	N-CA-CB	5.32	118.03	110.16
1	J	321	LYS	N-CA-CB	5.32	117.72	110.01
1	A	411	VAL	CA-CB-CG2	5.32	119.44	110.40
1	A	270	ILE	N-CA-CB	5.32	117.77	110.54
1	B	104	LEU	CB-CA-C	5.32	119.61	110.79
1	B	224	ASP	N-CA-C	-5.32	105.49	111.28
1	E	104	LEU	CB-CA-C	5.32	119.61	110.79
1	F	126	ALA	CB-CA-C	5.31	119.61	110.79
1	F	411	VAL	CA-CB-CG2	5.31	119.43	110.40
1	I	252	GLU	N-CA-C	-5.31	105.39	111.07
1	G	126	ALA	CB-CA-C	5.31	119.61	110.79
1	C	422	VAL	N-CA-CB	5.31	117.76	110.54
1	D	126	ALA	CB-CA-C	5.31	119.60	110.79
1	D	270	ILE	N-CA-CB	5.31	117.76	110.54
1	I	517	THR	N-CA-CB	5.31	119.46	110.49
1	L	517	THR	N-CA-CB	5.31	119.46	110.49
1	F	270	ILE	N-CA-CB	5.31	117.76	110.54
1	F	422	VAL	N-CA-CB	5.30	117.75	110.54
1	B	422	VAL	N-CA-CB	5.30	117.75	110.54
1	G	409	GLU	N-CA-CB	5.30	117.91	110.12
1	N	517	THR	N-CA-CB	5.30	119.44	110.49
1	A	422	VAL	N-CA-CB	5.30	117.74	110.54
1	G	411	VAL	CA-CB-CG2	5.30	119.40	110.40
1	N	53	GLY	N-CA-C	-5.30	106.37	112.73
1	G	104	LEU	CB-CA-C	5.29	119.58	110.79
1	G	270	ILE	N-CA-CB	5.29	117.74	110.54
1	J	428	ASP	CA-CB-CG	-5.29	107.31	112.60
1	F	104	LEU	CB-CA-C	5.29	119.57	110.79
1	B	411	VAL	CA-CB-CG2	5.29	119.39	110.40
1	E	411	VAL	CA-CB-CG2	5.29	119.39	110.40
1	K	517	THR	N-CA-CB	5.29	119.42	110.49
1	C	104	LEU	CB-CA-C	5.28	119.56	110.79
1	D	440	ILE	CB-CA-C	-5.28	105.01	112.14
1	E	409	GLU	N-CA-CB	5.28	117.89	110.12
1	G	422	VAL	N-CA-CB	5.28	117.72	110.54
1	C	409	GLU	N-CA-CB	5.28	117.88	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	428	ASP	CA-CB-CG	-5.28	107.32	112.60
1	E	224	ASP	N-CA-C	-5.28	105.53	111.28
1	C	270	ILE	N-CA-CB	5.28	117.72	110.54
1	D	104	LEU	CB-CA-C	5.28	119.55	110.79
1	H	517	THR	N-CA-CB	5.28	119.41	110.49
1	A	440	ILE	CB-CA-C	-5.28	105.02	112.14
1	M	53	GLY	N-CA-C	-5.28	106.40	112.73
1	M	410	GLY	N-CA-C	-5.28	105.95	112.33
1	A	359	ASP	CA-CB-CG	-5.27	107.33	112.60
1	A	104	LEU	CB-CA-C	5.27	119.54	110.79
1	D	359	ASP	CA-CB-CG	-5.27	107.33	112.60
1	H	428	ASP	CA-CB-CG	-5.27	107.33	112.60
1	B	409	GLU	N-CA-CB	5.27	117.87	110.12
1	D	409	GLU	N-CA-CB	5.27	117.87	110.12
1	B	440	ILE	CB-CA-C	-5.27	105.03	112.14
1	C	224	ASP	N-CA-C	-5.27	105.54	111.28
1	L	53	GLY	N-CA-C	-5.27	106.41	112.73
1	B	270	ILE	N-CA-CB	5.27	117.70	110.54
1	E	440	ILE	CB-CA-C	-5.27	105.03	112.14
1	E	422	VAL	N-CA-CB	5.27	117.70	110.54
1	C	359	ASP	CA-CB-CG	-5.26	107.34	112.60
1	J	110	GLY	N-CA-C	-5.26	108.01	115.43
1	M	252	GLU	N-CA-C	-5.26	105.44	111.07
1	N	110	GLY	N-CA-C	-5.26	108.01	115.43
1	A	409	GLU	N-CA-CB	5.26	117.85	110.12
1	M	428	ASP	CA-CB-CG	-5.26	107.34	112.60
1	G	440	ILE	CB-CA-C	-5.26	105.04	112.14
1	N	252	GLU	N-CA-C	-5.26	105.44	111.07
1	F	359	ASP	CA-CB-CG	-5.26	107.34	112.60
1	I	53	GLY	N-CA-C	-5.26	106.42	112.73
1	F	440	ILE	CB-CA-C	-5.25	105.05	112.14
1	L	252	GLU	N-CA-C	-5.25	105.45	111.07
1	F	409	GLU	N-CA-CB	5.25	117.84	110.12
1	M	517	THR	N-CA-CB	5.25	119.37	110.49
1	H	53	GLY	N-CA-C	-5.25	106.43	112.73
1	J	235	PRO	N-CA-CB	5.25	109.06	103.39
1	I	428	ASP	CA-CB-CG	-5.25	107.35	112.60
1	K	428	ASP	CA-CB-CG	-5.25	107.35	112.60
1	L	235	PRO	N-CA-CB	5.25	109.06	103.39
1	J	53	GLY	N-CA-C	-5.24	106.44	112.73
1	G	224	ASP	N-CA-C	-5.24	105.57	111.28
1	L	410	GLY	N-CA-C	-5.24	105.99	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	440	ILE	CB-CA-C	-5.24	105.07	112.14
1	G	359	ASP	CA-CB-CG	-5.24	107.36	112.60
1	F	224	ASP	N-CA-C	-5.24	105.57	111.28
1	L	191	GLU	N-CA-CB	-5.24	102.63	110.17
1	M	483	GLU	CB-CG-CD	5.24	121.50	112.60
1	H	110	GLY	N-CA-C	-5.24	108.05	115.43
1	J	252	GLU	N-CA-C	-5.24	105.47	111.07
1	D	224	ASP	N-CA-C	-5.23	105.58	111.28
1	I	235	PRO	N-CA-CB	5.23	109.04	103.39
1	M	110	GLY	N-CA-C	-5.23	108.05	115.43
1	N	410	GLY	N-CA-C	-5.23	106.00	112.33
1	K	53	GLY	N-CA-C	-5.23	106.45	112.73
1	K	110	GLY	N-CA-C	-5.23	108.05	115.43
1	N	191	GLU	N-CA-CB	-5.23	102.63	110.17
1	M	235	PRO	N-CA-CB	5.23	109.04	103.39
1	D	438	VAL	N-CA-CB	5.23	117.65	110.54
1	E	438	VAL	N-CA-CB	5.23	117.65	110.54
1	J	410	GLY	N-CA-C	-5.23	106.00	112.33
1	N	153	ASN	CA-CB-CG	5.23	117.83	112.60
1	N	235	PRO	N-CA-CB	5.23	109.04	103.39
1	N	438	VAL	N-CA-CB	5.23	117.65	110.54
1	G	438	VAL	N-CA-CB	5.22	117.64	110.54
1	A	438	VAL	N-CA-CB	5.22	117.64	110.54
1	H	235	PRO	N-CA-CB	5.22	109.03	103.39
1	E	359	ASP	CA-CB-CG	-5.22	107.38	112.60
1	F	438	VAL	N-CA-CB	5.22	117.64	110.54
1	M	169	VAL	CB-CA-C	5.22	119.42	112.22
1	I	110	GLY	N-CA-C	-5.22	108.07	115.43
1	K	235	PRO	N-CA-CB	5.22	109.03	103.39
1	B	359	ASP	CA-CB-CG	-5.21	107.39	112.60
1	H	252	GLU	N-CA-C	-5.21	105.49	111.07
1	N	428	ASP	CA-CB-CG	-5.21	107.39	112.60
1	L	110	GLY	N-CA-C	-5.21	108.08	115.43
1	L	438	VAL	N-CA-CB	5.21	117.62	110.54
1	M	438	VAL	N-CA-CB	5.21	117.62	110.54
1	A	224	ASP	N-CA-C	-5.21	105.60	111.28
1	H	153	ASN	CA-CB-CG	5.21	117.81	112.60
1	K	410	GLY	N-CA-C	-5.21	106.03	112.33
1	H	438	VAL	N-CA-CB	5.20	117.62	110.54
1	B	438	VAL	N-CA-CB	5.20	117.61	110.54
1	I	410	GLY	N-CA-C	-5.20	106.04	112.33
1	C	438	VAL	N-CA-CB	5.19	117.60	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	GLY	N-CA-C	-5.18	108.07	115.64
1	H	169	VAL	CB-CA-C	5.18	119.37	112.22
1	I	438	VAL	N-CA-CB	5.18	117.59	110.54
1	J	438	VAL	N-CA-CB	5.18	117.58	110.54
1	G	110	GLY	N-CA-C	-5.17	108.10	115.64
1	H	410	GLY	N-CA-C	-5.16	106.08	112.33
1	N	169	VAL	CB-CA-C	5.16	119.34	112.22
1	K	169	VAL	CB-CA-C	5.16	119.34	112.22
1	E	179	ASP	N-CA-CB	-5.16	102.74	110.17
1	A	179	ASP	N-CA-CB	-5.16	102.75	110.17
1	K	438	VAL	N-CA-CB	5.16	117.55	110.54
1	D	110	GLY	N-CA-C	-5.14	108.13	115.64
1	F	179	ASP	N-CA-CB	-5.13	102.78	110.17
1	C	292	ILE	N-CA-CB	5.13	117.52	110.54
1	D	179	ASP	N-CA-CB	-5.13	102.78	110.17
1	A	492	GLY	N-CA-C	-5.13	108.20	115.43
1	C	110	GLY	N-CA-C	-5.13	108.15	115.64
1	A	110	GLY	N-CA-C	-5.13	108.16	115.64
1	B	292	ILE	N-CA-CB	5.13	117.51	110.54
1	A	292	ILE	N-CA-CB	5.12	117.51	110.54
1	N	224	ASP	N-CA-CB	5.12	117.75	110.16
1	D	492	GLY	N-CA-C	-5.12	108.20	115.43
1	J	169	VAL	CB-CA-C	5.12	119.29	112.22
1	K	224	ASP	N-CA-CB	5.12	117.74	110.16
1	F	492	GLY	N-CA-C	-5.12	108.21	115.43
1	I	224	ASP	N-CA-CB	5.12	117.73	110.16
1	B	492	GLY	N-CA-C	-5.12	108.21	115.43
1	J	224	ASP	N-CA-CB	5.12	117.73	110.16
1	G	179	ASP	N-CA-CB	-5.11	102.81	110.17
1	A	479	ASN	CA-CB-CG	5.11	117.71	112.60
1	C	179	ASP	N-CA-CB	-5.11	102.81	110.17
1	E	110	GLY	N-CA-C	-5.11	108.18	115.64
1	F	110	GLY	N-CA-C	-5.11	108.19	115.64
1	I	194	GLN	N-CA-CB	-5.10	102.11	110.68
1	M	224	ASP	N-CA-CB	5.10	117.72	110.16
1	B	179	ASP	N-CA-CB	-5.10	102.82	110.17
1	F	437	ASN	N-CA-CB	5.10	117.41	110.01
1	G	492	GLY	N-CA-C	-5.10	108.23	115.43
1	L	169	VAL	CB-CA-C	5.10	119.26	112.22
1	G	292	ILE	N-CA-CB	5.10	117.48	110.54
1	D	506	TYR	CB-CA-C	5.10	119.25	110.79
1	A	437	ASN	N-CA-CB	5.10	117.40	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	LYS	N-CA-CB	5.10	117.61	110.12
1	L	194	GLN	N-CA-CB	-5.10	102.11	110.68
1	F	506	TYR	CB-CA-C	5.10	119.25	110.79
1	D	292	ILE	N-CA-CB	5.09	117.47	110.54
1	H	224	ASP	N-CA-CB	5.09	117.70	110.16
1	I	169	VAL	CB-CA-C	5.09	119.25	112.22
1	F	292	ILE	N-CA-CB	5.09	117.46	110.54
1	B	437	ASN	N-CA-CB	5.09	117.39	110.01
1	H	194	GLN	N-CA-CB	-5.09	102.13	110.68
1	E	492	GLY	N-CA-C	-5.08	108.26	115.43
1	C	492	GLY	N-CA-C	-5.08	108.26	115.43
1	K	194	GLN	N-CA-CB	-5.08	102.14	110.68
1	L	224	ASP	N-CA-CB	5.08	117.68	110.16
1	G	437	ASN	N-CA-CB	5.08	117.38	110.01
1	G	506	TYR	CB-CA-C	5.08	119.23	110.79
1	D	479	ASN	CA-CB-CG	5.08	117.68	112.60
1	G	367	GLU	CA-CB-CG	5.08	124.25	114.10
1	M	194	GLN	N-CA-CB	-5.08	102.15	110.68
1	H	506	TYR	CB-CA-C	5.07	119.21	110.79
1	E	292	ILE	N-CA-CB	5.07	117.43	110.54
1	I	506	TYR	CB-CA-C	5.07	119.20	110.79
1	N	194	GLN	N-CA-CB	-5.06	102.18	110.68
1	C	506	TYR	CB-CA-C	5.06	119.19	110.79
1	A	506	TYR	CB-CA-C	5.06	119.18	110.79
1	B	479	ASN	CA-CB-CG	5.06	117.66	112.60
1	B	506	TYR	CB-CA-C	5.06	119.19	110.79
1	J	194	GLN	N-CA-CB	-5.06	102.18	110.68
1	J	506	TYR	CB-CA-C	5.06	119.19	110.79
1	E	506	TYR	CB-CA-C	5.05	119.18	110.79
1	F	367	GLU	CA-CB-CG	5.05	124.21	114.10
1	J	191	GLU	N-CA-CB	-5.05	102.61	110.29
1	A	367	GLU	CA-CB-CG	5.05	124.21	114.10
1	D	410	GLY	N-CA-C	-5.05	106.63	112.29
1	E	437	ASN	N-CA-CB	5.05	117.33	110.01
1	C	367	GLU	CA-CB-CG	5.05	124.20	114.10
1	C	437	ASN	N-CA-CB	5.05	117.33	110.01
1	D	367	GLU	CA-CB-CG	5.05	124.20	114.10
1	B	367	GLU	CA-CB-CG	5.05	124.20	114.10
1	B	311	LYS	N-CA-CB	5.04	117.53	110.12
1	D	437	ASN	N-CA-CB	5.04	117.32	110.01
1	G	479	ASN	CA-CB-CG	5.04	117.64	112.60
1	N	506	TYR	CB-CA-C	5.04	119.16	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	367	GLU	CA-CB-CG	5.04	124.18	114.10
1	H	27	VAL	CB-CA-C	5.04	118.94	112.14
1	C	467	ASN	CA-CB-CG	-5.04	107.56	112.60
1	H	191	GLU	N-CA-CB	-5.04	102.63	110.29
1	N	27	VAL	CB-CA-C	5.04	118.94	112.14
1	C	479	ASN	CA-CB-CG	5.03	117.63	112.60
1	E	479	ASN	CA-CB-CG	5.03	117.63	112.60
1	G	436	GLN	N-CA-CB	5.03	117.51	110.12
1	B	467	ASN	CA-CB-CG	-5.02	107.58	112.60
1	F	473	ASP	N-CA-CB	5.02	118.06	110.42
1	I	27	VAL	CB-CA-C	5.02	118.92	112.14
1	A	467	ASN	CA-CB-CG	-5.02	107.58	112.60
1	D	467	ASN	CA-CB-CG	-5.02	107.58	112.60
1	M	191	GLU	N-CA-CB	-5.02	102.66	110.29
1	E	369	VAL	CA-CB-CG2	5.02	118.93	110.40
1	F	479	ASN	CA-CB-CG	5.02	117.62	112.60
1	K	191	GLU	N-CA-CB	-5.02	102.66	110.29
1	L	27	VAL	CB-CA-C	5.02	118.92	112.14
1	A	410	GLY	N-CA-C	-5.02	106.67	112.29
1	I	191	GLU	N-CA-CB	-5.02	102.67	110.29
1	C	436	GLN	N-CA-CB	5.01	117.49	110.12
1	E	467	ASN	CA-CB-CG	-5.01	107.59	112.60
1	B	369	VAL	CA-CB-CG2	5.01	118.92	110.40
1	F	369	VAL	CA-CB-CG2	5.01	118.91	110.40
1	G	369	VAL	CA-CB-CG2	5.00	118.91	110.40
1	I	170	GLY	N-CA-C	-5.00	105.48	112.18
1	F	467	ASN	CA-CB-CG	-5.00	107.60	112.60

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	128	0
1	B	3846	0	3970	127	0
1	C	3846	0	3970	127	0
1	D	3846	0	3970	125	0
1	E	3846	0	3970	125	0
1	F	3846	0	3970	125	0
1	G	3846	0	3970	124	0
1	H	3846	0	3968	86	0
1	I	3846	0	3968	89	0
1	J	3846	0	3968	89	0
1	K	3846	0	3968	89	0
1	L	3846	0	3968	89	0
1	M	3846	0	3968	110	0
1	N	3846	0	3968	89	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1554	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 (1554) 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:C5	4:M:1527:ATP:C4	1.93	1.55
4:M:1527:ATP:C8	4:M:1527:ATP:N7	1.72	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:1527:ATP:C5	4:M:1527:ATP:N7	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:D:27:VAL:HG12	1:D:90:THR:HG23	1.42	1.01
1:G:27:VAL:HG12	1:G: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:H:37:ASN:C	1:H:50:THR:O	2.13	0.92
1:I:37:ASN:C	1:I:50:THR:O	2.13	0.92
1:N:37:ASN:C	1:N:50:THR:O	2.13	0.92
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:K:37:ASN:C	1:K:50:THR:O	2.13	0.91
1:L:37:ASN:C	1:L:50:THR:O	2.13	0.91
1:M:37:ASN:C	1:M:50:THR:O	2.13	0.91
1:J:37:ASN:C	1:J:50:THR:O	2.13	0.90
1:B:4:LYS:H	1:C:63:GLU:HB2	1.38	0.89
1:A:63:GLU:HB2	1:G:4:LYS:H	1.38	0.88
1:D:4:LYS:H	1:E:63:GLU:HB2	1.38	0.88
1:M:493:ILE:CG1	4:M:1527:ATP:N9	2.37	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:A:4:LYS:H	1:B:63:GLU:HB2	1.37	0.86
1:F:4:LYS:H	1:G:63:GLU:HB2	1.38	0.86
1:M:493:ILE:HD12	4:M:1527:ATP:C4	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:I:183:LEU:O	1:I:382:GLY:HA3	1.82	0.78
1:K:135:SER:HA	1:K:412:VAL:HG12	1.66	0.78
1:M:135:SER:HA	1:M:412:VAL:HG12	1.66	0.78
1:N:135:SER:HA	1:N:412:VAL:HG12	1.66	0.77
3:D:1527:PO4:P	4:D:1528:ATP:O1G	2.43	0.77
3:F:1527:PO4:P	4:F: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: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
1:M:198:GLY:HA2	1:M:327:LYS:O	1.86	0.76
3:B:1527:PO4:P	4:B:1528:ATP:O1G	2.43	0.76
3:C:1527:PO4:P	4:C: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
1:H:199:TYR:CD2	1:H:205:ILE:HD11	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:138:CYS:N	1:A:410:GLY:HA2	2.01	0.75
1:H:37:ASN:C	1:H:50:THR:C	2.55	0.75
1:J:198:GLY:HA2	1:J:327:LYS:O	1.86	0.75
1:M:37:ASN:C	1:M:50:THR:C	2.55	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:J:37:ASN:C	1:J:50:THR:C	2.55	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:F:138:CYS:N	1:F:410:GLY:HA2	2.01	0.74
1:N:37:ASN:C	1:N:50:THR:C	2.55	0.74
1:N:198:GLY:HA2	1:N:327:LYS:O	1.86	0.74
1:I:37:ASN:C	1:I:50:THR:C	2.55	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:K:37:ASN:C	1:K:50:THR:C	2.55	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: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:E:147:VAL:HG22	1:E:494:LEU:HD11	1.71	0.73
1:E:127:ALA:HB2	1:E:426:LEU:HD11	1.69	0.73
1:F:147:VAL:HG22	1:F:494:LEU:HD11	1.71	0.73
1:L:37:ASN:C	1:L:50:THR:C	2.55	0.73
1:C:147:VAL:HG22	1:C:494:LEU:HD11	1.71	0.73
3:J:1526:PO4:P	4:J:1527:ATP:O1G	2.47	0.73
1:A:147:VAL:HG22	1:A:494:LEU:HD11	1.71	0.73
1:D:147:VAL:HG22	1:D: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
1:A:214:GLU:HA	1:A:323:VAL:O	1.90	0.72
1:D:214:GLU:HA	1:D:323:VAL:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1526:PO4:P	4:I:1527:ATP:O1G	2.48	0.72
1:G:214:GLU:HA	1:G:323:VAL:O	1.90	0.72
1:D:29:VAL:O	1:D:35:GLY:HA3	1.90	0.71
1:F:138:CYS:HA	1:F:411:VAL:HG13	1.72	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
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:C:29:VAL:O	1:C:35:GLY:HA3	1.90	0.70
1:L:191:GLU:O	1:L:334:ASP:HA	1.92	0.70
1:K:191:GLU:O	1:K:334:ASP:HA	1.92	0.70
3:N:1526:PO4:P	4:N:1527:ATP:O1A	2.50	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:A:29:VAL:O	1:A:35:GLY:HA3	1.90	0.69
1:E:198:GLY:HA2	1:E:327:LYS:O	1.92	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:M:493:ILE:HG13	4:M:1527:ATP:C4	2.26	0.69
1:G:199:TYR:CD2	1:G:205:ILE:HD11	2.28	0.69
1:A:199:TYR:CD2	1:A:205:ILE:HD11	2.28	0.69
1:C:198:GLY:HA2	1:C:327:LYS:O	1.92	0.69
1:M:31:LEU:CB	1:M:90:THR:HG21	2.22	0.69
1:D:138:CYS:HA	1:D:411:VAL:HG13	1.73	0.69
1:E:31:LEU:HA	3:E:1527:PO4:P	2.32	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
1:N:191:GLU:O	1:N:334:ASP:HA	1.92	0.69
3:N:1526:PO4:P	4:N:1527:ATP:O1G	2.50	0.69
1:F:198:GLY:HA2	1:F:327:LYS:O	1.92	0.69
1:G:198:GLY:HA2	1:G:327:LYS:O	1.92	0.69
1:B:31:LEU:HA	3:B:1527:PO4:P	2.32	0.69
1:B:199:TYR:CD2	1:B:205:ILE:HD11	2.28	0.69
1:D:31:LEU:HA	3:D:1527:PO4:P	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLY:HA2	1:B:327:LYS:O	1.92	0.69
1:C:138:CYS:HA	1:C:411:VAL:HG13	1.73	0.69
1:F:31:LEU:HA	3:F:1527:PO4:P	2.32	0.69
1:A:198:GLY:HA2	1:A:327:LYS:O	1.92	0.68
3:M:1526:PO4:P	4:M:1527:ATP:O3G	2.51	0.68
1:C:31:LEU:HA	3:C:1527:PO4:P	2.32	0.68
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
1:C:199:TYR:CD2	1:C:205:ILE:HD11	2.28	0.68
3:J:1526:PO4:P	4:J:1527:ATP:O1A	2.52	0.68
3:L:1526:PO4:P	4:L:1527:ATP:O1A	2.52	0.68
3:I:1526:PO4:P	4:I:1527:ATP:O1A	2.52	0.67
1:M:493:ILE:HG12	4:M:1527:ATP:C8	2.27	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:C:180:GLY:HA2	1:C:380:LYS:HB3	1.77	0.66
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.77	0.66
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.78	0.66
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.77	0.66
3:K:1526:PO4:P	4:K:1527:ATP:O1G	2.53	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:B:135:SER:HA	1:B:412:VAL:HG12	1.77	0.65
1:B:138:CYS:CB	1:B:407:VAL:HA	2.26	0.65
1:C:138:CYS:CB	1:C:407:VAL:HA	2.27	0.65
1:E:135:SER:HA	1:E:412:VAL:HG12	1.77	0.65
1:L:180:GLY:HA2	1:L:380:LYS:HB3	1.78	0.65
1:A:135:SER:HA	1:A:412:VAL:HG12	1.77	0.65
1:G:138:CYS:CB	1:G:407:VAL:HA	2.27	0.65
3:M:1526:PO4:P	4:M:1527:ATP:O1A	2.54	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:C:135:SER:HA	1:C:412:VAL:HG12	1.77	0.65
1:E:138:CYS:CB	1:E:407:VAL:HA	2.26	0.65
1:N:180:GLY:HA2	1:N:380:LYS:HB3	1.78	0.65
1:F:135:SER:HA	1:F:412:VAL:HG12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:206:ASN:HB2	1:C:213:VAL:HA	1.79	0.64
1:D:138:CYS:CB	1:D:407:VAL:HA	2.26	0.64
1:J:180:GLY:HA2	1:J:380:LYS:HB3	1.78	0.64
1:N:27:VAL:HG12	1:N:90:THR:CG2	2.26	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
1:D:206:ASN:HB2	1:D:213:VAL:HA	1.79	0.63
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
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:M:493:ILE:HG12	4:M:1527:ATP:N7	2.11	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:A:1527:PO4:P	4:A:1528:ATP:O1A	2.57	0.62
3:F:1527:PO4:P	4:F: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: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:E:27:VAL:HG12	1:E:90:THR:CG2	2.24	0.62
1:C:149:THR:HA	1:C:152:ALA:HB3	1.82	0.62
1:D:411:VAL:HG12	1:D:494:LEU:HD13	1.81	0.62
1:J:31:LEU:HB3	1:J:90:THR:HG21	1.82	0.62
1:E:149:THR:HA	1:E:152:ALA:HB3	1.82	0.62
1:G:149:THR:HA	1:G:152:ALA:HB3	1.82	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:F:411:VAL:HG12	1:F:494:LEU:HD13	1.81	0.62
1:L:37:ASN:O	1:L:38:VAL:N	2.33	0.62
1:F:3:ALA:HA	1:G:63:GLU:CA	2.31	0.61
1:I:37:ASN:O	1:I:38:VAL:N	2.33	0.61

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:31:LEU:HB3	1:N:90:THR:HG21	1.82	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:A:30:THR:HG22	1:A:36:ARG:O	2.03	0.59
1:G:30:THR:HG22	1:G:36:ARG:O	2.03	0.59
1:A:3:ALA:HA	1:B:63:GLU:HA	1.84	0.59
1:A:279:PRO:HG3	1:A:292:ILE:HD11	1.85	0.59
1:L:417:VAL:HG21	1:L:477:GLY:HA3	1.84	0.59
1:D:30:THR:HG22	1:D:36:ARG:O	2.03	0.59
1:G:279:PRO:HG3	1:G:292:ILE:HD11	1.85	0.59
1:I:151:SER:HB3	1:I:399:ALA:HA	1.85	0.59
1:B:279:PRO:HG3	1:B:292:ILE:HD11	1.85	0.59
1:F:30:THR:HG22	1:F:36:ARG:O	2.03	0.59
1:F:31:LEU:HB3	1:F:90:THR:HG21	1.85	0.59
1:M:151:SER:HB3	1:M:399:ALA:HA	1.84	0.59
1:C:130:GLU:HB3	1:C:422:VAL:HG12	1.83	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:G:31:LEU:HB3	1:G:90:THR:HG21	1.85	0.59
1:D:130:GLU:HB3	1:D:422:VAL:HG12	1.84	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: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:B:3:ALA:HA	1:C:63:GLU:HA	1.84	0.59
1:K:31:LEU:CB	1:K:90:THR:HG21	2.33	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:B:130:GLU:HB3	1:B:422:VAL:HG12	1.84	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:H:151:SER:HB3	1:H:399:ALA:HA	1.85	0.58
1:J:151:SER:CB	1:J:399:ALA:HA	2.34	0.58
1:L:151:SER:HB3	1:L:399:ALA:HA	1.85	0.58
1:B:30:THR:HG22	1:B:36:ARG:O	2.02	0.58
1:B:31:LEU:HB3	1:B:90:THR:HG21	1.85	0.58
1:L:151:SER:CB	1:L:399:ALA:HA	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:246:PRO:HB3	1:N:272:LYS:HB2	1.84	0.58
1:C:279:PRO:HG3	1:C:292:ILE:HD11	1.85	0.58
1:D:279:PRO:HG3	1:D:292:ILE:HD11	1.85	0.58
1:I:246:PRO:HB3	1:I:272:LYS:HB2	1.84	0.58
3:K:1526:PO4:P	4:K:1527:ATP:O1A	2.61	0.58
1:I:151:SER:CB	1:I:399:ALA:HA	2.34	0.58
1:H:192:GLY:O	1:H:375:GLY:HA2	2.04	0.58
1:J:151:SER:HB3	1:J:399:ALA:HA	1.85	0.58
1:C:3:ALA:HA	1:D:63:GLU:HA	1.84	0.57
1:K:214:GLU:HA	1:K:323:VAL:O	2.04	0.57
1:M:214:GLU:HA	1:M:323:VAL:O	2.04	0.57
1:C:172:GLU:CD	1:C:172:GLU:H	2.12	0.57
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.86	0.57
1:D:3:ALA:HA	1:E:63:GLU:HA	1.84	0.57
1:H:151:SER:CB	1:H:399:ALA:HA	2.34	0.57
1:J:214:GLU:HA	1:J:323:VAL:O	2.04	0.57
1:K:127:ALA:HB2	1:K:426:LEU:HD11	1.86	0.57
1:L:127:ALA:HB2	1:L:426:LEU:HD11	1.87	0.57
1:M:151:SER:CB	1:M:399:ALA:HA	2.34	0.57
1:N:151:SER:HB3	1:N:399:ALA:HA	1.85	0.57
1:B:172:GLU:CD	1:B:172:GLU:H	2.13	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:E:212:ALA:HA	1:E:325:ILE:O	2.05	0.57
1:G:417:VAL:HG21	1:G:477:GLY:HA3	1.86	0.57
1:K:192:GLY:O	1:K:375:GLY:HA2	2.04	0.57
3:K:1526:PO4:P	4:K:1527:ATP:O3B	2.63	0.57
1:L:192:GLY:O	1:L:375:GLY:HA2	2.04	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:I:192:GLY:O	1:I:375:GLY:HA2	2.04	0.57
1:N:151:SER:CB	1:N:399:ALA:HA	2.34	0.57
1:D:217:SER:HA	1:D:320:ALA:O	2.05	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: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:E:169:VAL:HB	1:E:377:ALA:HB2	1.87	0.57
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:SER:HA	1:G:320:ALA:O	2.05	0.57
1:N:192:GLY:O	1:N:375:GLY:HA2	2.04	0.57
1:B:217:SER:HA	1:B:320:ALA:O	2.05	0.57
1:D:172:GLU:CD	1:D:172:GLU:H	2.12	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:F:169:VAL:HB	1:F:377:ALA:HB2	1.87	0.56
1:F:172:GLU:H	1:F:172:GLU:CD	2.12	0.56
1:H:214:GLU:HA	1:H:323:VAL:O	2.04	0.56
1:I:217:SER:HA	1:I:320:ALA:O	2.05	0.56
1:J:192:GLY:O	1:J:375:GLY:HA2	2.04	0.56
1:C:169:VAL:HB	1:C:377:ALA:HB2	1.87	0.56
1:F:138:CYS:HB2	1:F:407:VAL:HA	1.87	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:N:214:GLU:HA	1:N:323:VAL:O	2.04	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:169:VAL:HB	1:D:377:ALA:HB2	1.87	0.56
1:D:417:VAL:HG21	1:D:477:GLY:HA3	1.86	0.56
1:J:217:SER:HA	1:J:320:ALA:O	2.05	0.56
1:A:172:GLU:H	1:A:172:GLU:CD	2.12	0.56
1:B:138:CYS:HB2	1:B:407:VAL:HA	1.87	0.56
1:E:138:CYS:HB2	1:E: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:E:172:GLU:CD	1:E:172:GLU:H	2.13	0.56
1:E:417:VAL:HG21	1:E:477:GLY:HA3	1.86	0.56
1:H:127:ALA:HB2	1:H:426:LEU:HD11	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: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:N:127:ALA:HB2	1:N:426:LEU:HD11	1.87	0.56
1:N:217:SER:HA	1:N:320:ALA:O	2.05	0.56
1:F:212:ALA:HA	1:F:325:ILE:O	2.05	0.56
1:G:138:CYS:HB2	1:G:407:VAL:HA	1.87	0.56
1:I:127:ALA:HB2	1:I:426:LEU:HD11	1.87	0.56
1:M:217:SER:HA	1:M:320:ALA:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:172:GLU:CD	1:N:172:GLU:H	2.14	0.56
1:B:169:VAL:HB	1:B:377:ALA:HB2	1.87	0.56
1:B:212:ALA:HA	1:B:325:ILE:O	2.05	0.56
1:G:169:VAL:HB	1:G:377:ALA:HB2	1.87	0.56
1:K:212:ALA:HA	1:K:325:ILE:O	2.05	0.56
1:M:212:ALA:HA	1:M:325:ILE:O	2.05	0.56
4:M:1527:ATP:C5	4:M:1527:ATP:C8	2.94	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:G:172:GLU:CD	1:G:172:GLU:H	2.13	0.55
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:A:169:VAL:HB	1:A:377:ALA:HB2	1.88	0.55
1:H:212:ALA:HA	1:H:325:ILE:O	2.06	0.55
1:L:212:ALA:HA	1:L:325:ILE:O	2.06	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
1:G:186:GLU:H	1:G:380:LYS:HB2	1.71	0.55
1:E:151:SER:CB	1:E:399:ALA:HA	2.37	0.55
1:G:151:SER:CB	1:G: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: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: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:J:172:GLU:CD	1:J:172:GLU:H	2.14	0.55
1:L:206:ASN:HB2	1:L:213:VAL:HA	1.88	0.55
1:B:151:SER:CB	1:B:399:ALA:HA	2.37	0.55
1:D:235:PRO:HB2	1:D:310:GLU:HA	1.89	0.55
1:M:186:GLU:H	1:M:380:LYS:HB2	1.72	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
1:C:151:SER:CB	1:C:399:ALA:HA	2.37	0.54
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:E:31:LEU:CB	1:E:90:THR:HG21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:PRO:HB2	1:F:310:GLU:HA	1.89	0.54
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.37	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
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:A:144:ILE:HG23	1:A:403:THR:CG2	2.37	0.54
1:B:186:GLU:H	1:B:380:LYS:HB2	1.71	0.54
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:I:172:GLU:CD	1:I:172:GLU:H	2.14	0.54
1:K:218:PRO:HG2	1:K:320:ALA:HB3	1.90	0.54
1:H:218:PRO:HG2	1:H:320:ALA:HB3	1.90	0.54
1:L:186:GLU:H	1:L:380:LYS:HB2	1.72	0.54
1:M:218:PRO:HG2	1:M:320:ALA:HB3	1.90	0.54
1:A:31:LEU:CB	1:A:90:THR:HG21	2.37	0.54
1:B:31:LEU:CB	1:B: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: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
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: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
3:N:1526:PO4:P	4:N:1527:ATP:O3B	2.65	0.54
1:A:239:ALA:HB1	1:A:314:LEU:HG	1.90	0.54
1:I:186:GLU:H	1:I:380:LYS:HB2	1.72	0.54
1:L:172:GLU:CD	1:L:172:GLU:H	2.16	0.54
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.37	0.53
1:D:147:VAL:CG2	1:D:494:LEU:HD11	2.38	0.53
1:G:235:PRO:HB2	1:G:310:GLU:HA	1.89	0.53
3:H:1526:PO4:P	4:H:1527:ATP:O3B	2.66	0.53
1:K:172:GLU:H	1:K:172:GLU:CD	2.16	0.53
3:J:1526:PO4:P	4:J:1527:ATP:O3B	2.67	0.53
1:N:31:LEU:CB	1:N:90:THR:HG21	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:SER:HB3	1:F:399:ALA:HA	1.91	0.53
1:A:235:PRO:HB2	1:A:310:GLU:HA	1.89	0.53
1:N:186:GLU:H	1:N:380:LYS:HB2	1.72	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:H:172:GLU:H	1:H:172:GLU:CD	2.16	0.53
1:J:411:VAL:HB	1:J:494:LEU:HB3	1.91	0.53
1:B:106:ALA:CB	1:B:116:LEU:HD21	2.39	0.53
1:B:206:ASN:CB	1:B:213:VAL:HA	2.38	0.53
1:E:147:VAL:CG2	1:E:494:LEU:HD11	2.38	0.53
1:F:239:ALA:HB1	1:F:314:LEU:HG	1.90	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:K:411:VAL:HB	1:K:494:LEU:HB3	1.91	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:M:172:GLU:H	1:M:172:GLU:CD	2.16	0.53
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:H:31:LEU:CB	1:H: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:L:31:LEU:CB	1:L:90:THR:HG21	2.38	0.52
1:A:251:ALA:O	1:A:277:LYS:HA	2.09	0.52
1:H:144:ILE:HG23	1:H:403:THR:CG2	2.40	0.52
1:M:205:ILE:HD12	1:M:211:GLY:O	2.10	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: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:I:411:VAL:HB	1:I:494:LEU:HB3	1.91	0.52
1:J:31:LEU:CB	1:J:90:THR:HG21	2.39	0.52
1:L:144:ILE:HG23	1:L:403:THR:CG2	2.39	0.52
1:L:205:ILE:HD12	1:L:211:GLY:O	2.09	0.52
1:M:152:ALA:HB1	1:M:155:ASP:HB3	1.92	0.52
1:N:205:ILE:HD12	1:N:211:GLY:O	2.09	0.52
3:B:1527:PO4:P	4:B:1528:ATP:O3B	2.68	0.52

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:THR:HA	1:H:152:ALA:HB3	1.93	0.51
1:M:493:ILE:CG2	4:M:1527:ATP:H2'	2.40	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:D:169:VAL:HG13	1:D:170:GLY:O	2.11	0.51
1:G:180:GLY:HA3	1:G:381:VAL:O	2.11	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
1:M:149:THR:HA	1:M:152:ALA:HB3	1.93	0.51
1:G:127:ALA:N	1:G:426:LEU:HD21	2.26	0.50
3:K:1526:PO4:P	4:K:1527:ATP:PG	3.09	0.50
1:A:169:VAL:HG13	1:A:170:GLY:O	2.11	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:L:149:THR:HA	1:L:152:ALA:HB3	1.93	0.50
3:M:1526:PO4:P	4:M:1527:ATP:O2A	2.69	0.50
1:N:149:THR:HA	1:N:152:ALA:HB3	1.93	0.50
1:A:218:PRO:HG2	1:A:320:ALA:HB3	1.92	0.50
1:B:169:VAL:HG13	1:B:170:GLY:O	2.11	0.50
1:B:411:VAL:HB	1:B:494:LEU:HB2	1.93	0.50
1:D:180:GLY:HA3	1:D:381:VAL:O	2.11	0.50
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.40	0.50
1:G:411:VAL:HB	1:G:494:LEU:HB2	1.93	0.50
1:A:135:SER:HA	1:A:412:VAL:CG1	2.42	0.50
1:C:180:GLY:HA3	1:C:381:VAL:O	2.11	0.50
1:J:152:ALA:HB1	1:J:155:ASP:HB3	1.92	0.50
1:K:142:LYS:H	1:K:142:LYS:HD2	1.75	0.50
1:E:169:VAL:HG13	1:E:170:GLY:O	2.11	0.50
1:E:180:GLY:HA3	1:E:381:VAL:O	2.11	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:B:135:SER:HA	1:B:412:VAL:CG1	2.42	0.50
1:B:218:PRO:HG2	1:B:320:ALA:HB3	1.92	0.50
1:J:149:THR:HA	1:J:152:ALA:HB3	1.94	0.50
1:A:206:ASN:HB2	1:A:213:VAL:HB	1.94	0.50
1:A:411:VAL:HB	1:A:494:LEU:HB2	1.93	0.50
1:C:206:ASN:HB2	1:C:213:VAL:HB	1.94	0.50
1:E:206:ASN:HB2	1:E:213:VAL:HB	1.94	0.50
1:B:142:LYS:H	1:B:142:LYS:HD2	1.76	0.50
1:B:206:ASN:HB2	1:B:213:VAL:HB	1.94	0.50
1:D:517:THR:HG23	1:E:39:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:THR:HG23	1:F:39:VAL:HB	1.94	0.50
1:F:180:GLY:HA3	1:F:381:VAL:O	2.11	0.50
1:D:206:ASN:HB2	1:D:213:VAL:HB	1.94	0.50
1:F:293:ALA:HB2	1:F:300:VAL:CG2	2.42	0.50
1:G:169:VAL:HG13	1:G:170:GLY:O	2.11	0.50
1:I:152:ALA:HB1	1:I:155:ASP:HB3	1.92	0.50
1:K:138:CYS:HA	1:K:411:VAL:HG22	1.94	0.50
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:N:33:PRO:HG3	4:N:1527:ATP:C5	2.47	0.49
1:A:90:THR:HG22	1:A:94:VAL:HG23	1.95	0.49
1:A:142:LYS:HD2	1:A:142:LYS:H	1.76	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:G:293:ALA:HB2	1:G:300:VAL:CG2	2.42	0.49
1:K:149:THR:HA	1:K:152:ALA:HB3	1.94	0.49
1:B:169:VAL:HG11	1:B:175:ILE:CG1	2.43	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:C:349:ILE:HG22	1:C:369:VAL:HG13	1.95	0.49
1:C:517:THR:HG23	1:D:39:VAL:HB	1.94	0.49
1:D:169:VAL:HG11	1:D:175:ILE:CG1	2.42	0.49
1:D:224:ASP:HA	1:D:289:LEU:CD1	2.43	0.49
1:E:90:THR:HG22	1:E:94:VAL:HG23	1.95	0.49
1:F:90:THR:HG22	1:F:94:VAL:HG23	1.95	0.49
1:F:142:LYS:H	1:F:142:LYS:HD2	1.77	0.49
1:F:517:THR:HG23	1:G:39:VAL:HB	1.94	0.49
1:N:138:CYS:HA	1:N:411:VAL:HG22	1.94	0.49
1:A:224:ASP:HA	1:A:289:LEU:CD1	2.43	0.49
1:E:142:LYS:H	1:E:142:LYS:HD2	1.76	0.49
1:E:349:ILE:HG22	1:E:369:VAL:HG13	1.94	0.49
1:F:224:ASP:HA	1:F:289:LEU:CD1	2.43	0.49
1:G:90:THR:HG22	1:G:94:VAL:HG23	1.95	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: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: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
1:G:169:VAL:HG11	1:G:175:ILE:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:106:ALA:HB3	1:I:116:LEU:HD21	1.95	0.49
1:I:138:CYS:HA	1:I:411:VAL:HG22	1.94	0.49
1:M:106:ALA:HB3	1:M:116:LEU:HD21	1.95	0.49
1:A:180:GLY:HA3	1:A:381:VAL:O	2.11	0.49
1:D:90:THR:HG22	1:D:94:VAL:HG23	1.95	0.49
1:D:142:LYS:H	1:D:142:LYS:HD2	1.77	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:C:293:ALA:HB2	1:C:300:VAL:CG2	2.42	0.49
1:E:169:VAL:HG11	1:E:175:ILE:CG1	2.43	0.49
1:K:106:ALA:HB3	1:K:116:LEU:HD21	1.95	0.49
1:E:293:ALA:HB2	1:E:300:VAL:CG2	2.42	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:A:169:VAL:HG11	1:A:175:ILE:CG1	2.42	0.48
1:B:90:THR:HG22	1:B:94:VAL:HG23	1.95	0.48
1:D:293:ALA:HB2	1:D:300:VAL:CG2	2.42	0.48
1:G:135:SER:HA	1:G:412:VAL:CG1	2.42	0.48
1:G:142:LYS:H	1:G:142:LYS:HD2	1.76	0.48
1:J:106:ALA:HB3	1:J:116:LEU:HD21	1.95	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:F:183:LEU:C	1:F:382:GLY:HA3	2.38	0.48
1:N:142:LYS:H	1:N:142:LYS:HD2	1.78	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:E:135:SER:HA	1:E:412:VAL:CG1	2.42	0.48
1:C:142:LYS:H	1:C:142:LYS:HD2	1.76	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:H:138:CYS:HA	1:H:411:VAL:HG22	1.94	0.48
1:I:142:LYS:H	1:I:142:LYS:HD2	1.78	0.48
1:M:138:CYS:HA	1:M:411:VAL:HG22	1.94	0.48
1:G:224:ASP:HA	1:G:289:LEU:CD1	2.43	0.48
1:M:206:ASN:HB2	1:M:213:VAL:CB	2.44	0.48
1:A:158:VAL:HG22	1:A:396:VAL:HG22	1.96	0.48
1:A:293:ALA:HB2	1:A:300:VAL:CG2	2.42	0.48
1:D:135:SER:HA	1:D:412:VAL:CG1	2.42	0.48
1:G:183:LEU:C	1:G:382:GLY:HA3	2.38	0.48
1:L:206:ASN:HB2	1:L: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:J:206:ASN:HB2	1:J:213:VAL:CB	2.44	0.48
1:D:158:VAL:HG22	1:D:396:VAL:HG22	1.96	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: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: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: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:M:496:PRO:HB2	1:M:499:VAL:HG13	1.94	0.48
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:H:206:ASN:HB2	1:H:213:VAL:CB	2.44	0.47
1:K:27:VAL:CG1	1:K:90:THR:HG23	2.34	0.47
1:B:158:VAL:HG22	1:B:396:VAL:HG22	1.96	0.47
1:D:183:LEU:C	1:D:382:GLY:HA3	2.38	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:F:205:ILE:HD12	1:F:211:GLY:O	2.14	0.47
1:G:158:VAL:HG22	1:G:396:VAL:HG22	1.96	0.47
1:K:206:ASN:HB2	1:K:213:VAL:CB	2.43	0.47
1:B:205:ILE:HD12	1:B:211:GLY:O	2.14	0.47
1:C:90:THR:HG22	1:C:94:VAL:HG23	1.95	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:144:ILE:HG23	1:G:403:THR:HG21	1.96	0.47
1:G:406:ALA:HB2	1:G:496:PRO:HG3	1.95	0.47
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.97	0.47
1:C:406:ALA:HB2	1:C:496:PRO:HG3	1.95	0.47
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.97	0.47
1:K:158:VAL:HG22	1:K:396:VAL:HG22	1.96	0.47
1:A:126:ALA:HB3	1:A:426:LEU:HD22	1.97	0.47
1:A:183:LEU:C	1:A:382:GLY:HA3	2.38	0.47
1:C:183:LEU:C	1:C:382:GLY:HA3	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.97	0.47
1:B:126:ALA:HB3	1:B:426:LEU:HD22	1.97	0.47
1:B:406:ALA:HB2	1:B:496:PRO:HG3	1.95	0.47
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.96	0.47
1:F:158:VAL:HG22	1:F:396:VAL:HG22	1.96	0.47
1:H:158:VAL:HG22	1:H:396:VAL:HG22	1.97	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:E:136:VAL:O	1:E:410:GLY:HA3	2.15	0.47
1:M:493:ILE:CB	4:M:1527:ATP:N9	2.77	0.47
1:C:135:SER:HA	1:C:412:VAL:CG1	2.42	0.47
1:C:426:LEU:HB2	1:C:444:LEU:HD22	1.97	0.47
1:D:126:ALA:HB3	1:D:426:LEU:HD22	1.97	0.47
1:F:426:LEU:HB2	1:F:444:LEU:HD22	1.97	0.47
1:G:126:ALA:HB3	1:G:426:LEU:HD22	1.97	0.47
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.34	0.47
1:L:427:ALA:HA	1:L:444:LEU:CD1	2.45	0.47
1:A:199:TYR:CE2	1:A:327:LYS:HB3	2.50	0.47
1:A:371:LYS:O	1:A:374:GLY:HA3	2.15	0.47
1:B:199:TYR:CE2	1:B:327:LYS:HB3	2.50	0.47
1:D:199:TYR:CE2	1:D:327:LYS:HB3	2.50	0.47
1:D:426:LEU:HB2	1:D:444:LEU:HD22	1.97	0.47
1:E:158:VAL:HG22	1:E:396:VAL:HG22	1.96	0.47
1:E:183:LEU:C	1:E:382:GLY:HA3	2.38	0.47
1:E:426:LEU:HB2	1:E:444:LEU:HD22	1.97	0.47
1:F:199:TYR:CE2	1:F:327:LYS:HB3	2.50	0.47
1:I:158:VAL:HG22	1:I:396:VAL:HG22	1.97	0.47
1:J:158:VAL:HG22	1:J:396:VAL:HG22	1.97	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:N:158:VAL:HG22	1:N:396:VAL:HG22	1.97	0.47
1:A:406:ALA:HB2	1:A:496:PRO:HG3	1.95	0.46
1:B:34:LYS:HB2	1:B:457:ASN:HB3	1.97	0.46
1:B:183:LEU:C	1:B:382:GLY:HA3	2.38	0.46
1:B:371:LYS:O	1:B:374:GLY:HA3	2.15	0.46
1:C:126:ALA:HB3	1:C:426:LEU:HD22	1.97	0.46
1:C:371:LYS:O	1:C:374:GLY:HA3	2.15	0.46
1:D:136:VAL:O	1:D:410:GLY:HA3	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:VAL:O	1:F:410:GLY:HA3	2.15	0.46
1:I:106:ALA:CB	1:I:116:LEU:HD21	2.45	0.46
1:K:196:ASP:HA	1:K:329:THR:HA	1.97	0.46
1:C:136:VAL:O	1:C:410:GLY:HA3	2.15	0.46
1:D:371:LYS:O	1:D:374:GLY:HA3	2.15	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:G:136:VAL:O	1:G:410:GLY:HA3	2.15	0.46
1:G:199:TYR:CE2	1:G:327:LYS:HB3	2.50	0.46
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.34	0.46
1:K:106:ALA:CB	1:K:116:LEU:HD21	2.45	0.46
1:L:106:ALA:CB	1:L:116:LEU:HD21	2.45	0.46
1:L:158:VAL:HG22	1:L:396:VAL:HG22	1.97	0.46
1:L:196:ASP:HA	1:L:329:THR:HA	1.97	0.46
1:N:427:ALA:HA	1:N:444:LEU:CD1	2.45	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:J:27:VAL:CG1	1:J:90:THR:HG23	2.35	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:A:120:ILE:O	1:A:124:VAL:HG23	2.16	0.46
1:C:205:ILE:HD12	1:C:211:GLY:O	2.14	0.46
1:G:120:ILE:O	1:G:124:VAL:HG23	2.16	0.46
1:G:371:LYS:O	1:G:374:GLY:HA3	2.15	0.46
1:G:426:LEU:HB2	1:G:444:LEU:HD22	1.97	0.46
1:H:240:VAL:HG11	1:H:247:LEU:HB2	1.96	0.46
1:H:287:ALA:HB1	1:H:368:ARG:CZ	2.45	0.46
1:H:427:ALA:HA	1:H:444:LEU:CD1	2.45	0.46
1:L:120:ILE:O	1:L:124:VAL:HG23	2.16	0.46
1:N:124:VAL:HG21	1:N:508:ALA:CB	2.46	0.46
1:N:139:SER:HB3	1:N:143:ALA:HB2	1.98	0.46
1:N:196:ASP:HA	1:N:329:THR:HA	1.97	0.46
1:N:240:VAL:HG11	1:N:247:LEU:HB2	1.97	0.46
1:N:287:ALA:HB1	1:N:368:ARG:CZ	2.45	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:D:219:PHE:CE2	1:D:314:LEU:HD22	2.51	0.46
1:E:371:LYS:O	1:E:374:GLY:HA3	2.15	0.46
1:F:120:ILE:O	1:F:124:VAL:HG23	2.15	0.46
1:H:120:ILE:O	1:H:124:VAL:HG23	2.16	0.46
1:J:106:ALA:CB	1:J:116:LEU:HD21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:124:VAL:HG21	1:K:508:ALA:CB	2.46	0.46
1:M:240:VAL:HG11	1:M:247:LEU:HB2	1.97	0.46
1:M:493:ILE:HD11	4:M:1527:ATP:N7	2.29	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
1:C:219:PHE:CE2	1:C:314:LEU:HD22	2.51	0.46
1:I:427:ALA:HA	1:I:444:LEU:CD1	2.45	0.46
1:J:120:ILE:O	1:J:124:VAL:HG23	2.16	0.46
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.97	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:M:406:ALA:HB2	1:M:496:PRO:HG3	1.98	0.46
1:N:106:ALA:CB	1:N:116:LEU:HD21	2.45	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: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:51:LYS:O	3:K:1526:PO4:P	2.74	0.46
1:K:427:ALA:HA	1:K:444:LEU:CD1	2.45	0.46
1:L:139:SER:HB3	1:L:143:ALA:HB2	1.98	0.46
1:A:34:LYS:HB2	1:A:457:ASN:HB3	1.98	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: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:K:240:VAL:HG11	1:K:247:LEU:HB2	1.97	0.46
1:M:139:SER:HB3	1:M:143:ALA:HB2	1.98	0.46
1:A:345:ARG:HD3	1:A:345:ARG:HA	1.96	0.46
1:B:120:ILE:O	1:B:124:VAL:HG23	2.15	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:H:27:VAL:CG1	1:H:90:THR:HG23	2.34	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:H:356:ALA:HB1	1:H:361:ASP:HB2	1.97	0.46
1:K:356:ALA:HB1	1:K:361:ASP:HB2	1.98	0.46
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.98	0.46
1:L:240:VAL:HG21	1:L:247:LEU:HD13	1.98	0.46
1:L:356:ALA:HB1	1:L:361:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:124:VAL:HG21	1:M:508:ALA:CB	2.46	0.46
1:M:144:ILE:HG23	1:M:403:THR:HG21	1.98	0.46
1:N:27:VAL:CG1	1:N:90:THR:HG23	2.34	0.46
1:N:356:ALA:HB1	1:N:361:ASP:HB2	1.97	0.46
1:E:345:ARG:HD3	1:E:345:ARG:HA	1.96	0.46
1:E:411:VAL:CG1	1:E:494:LEU:HD22	2.46	0.46
1:F:34:LYS:HB2	1:F:457:ASN:HB3	1.97	0.46
1:F:126:ALA:HB3	1:F:426:LEU:HD22	1.97	0.46
1:I:117:LYS:HZ2	1:I:121:ASP:CG	2.24	0.46
1:L:383:ALA:HB3	1:L:389:MET:HB2	1.98	0.46
1:M:240:VAL:HG21	1:M:247:LEU:HD13	1.98	0.46
1:M:287:ALA:HB1	1:M:368:ARG:CZ	2.45	0.46
1:E:34:LYS:HB2	1:E:457:ASN:HB3	1.97	0.45
1:E:120:ILE:O	1:E:124:VAL:HG23	2.16	0.45
1:I:287:ALA:HB1	1:I:368:ARG:CZ	2.45	0.45
1:J:124:VAL:HG21	1:J:508:ALA:CB	2.46	0.45
1:K:349:ILE:HG22	1:K:369:VAL:HG13	1.99	0.45
1:L:124:VAL:HG21	1:L:508:ALA:CB	2.46	0.45
1:N:127:ALA:CB	1:N:426:LEU:HD11	2.47	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:F:383:ALA:HB3	1:F:389:MET:HB2	1.97	0.45
1:H:127:ALA:CB	1:H:426:LEU:HD11	2.46	0.45
1:I:124:VAL:HG21	1:I:508:ALA:CB	2.46	0.45
1:I:427:ALA:HA	1:I:444:LEU:HD11	1.98	0.45
1:J:139:SER:HB3	1:J:143:ALA:HB2	1.97	0.45
1:J:349:ILE:HG22	1:J:369:VAL:HG13	1.99	0.45
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.98	0.45
1:L:240:VAL:HG11	1:L:247:LEU:HB2	1.96	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: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:H:144:ILE:HG23	1:H:403:THR:HG21	1.97	0.45
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.98	0.45
1:K:150:ILE:HA	4:K:1527:ATP:C8	2.52	0.45
1:B:287:ALA:HB1	1:B:368:ARG:CZ	2.47	0.45
1:D:34:LYS:HB2	1:D:457:ASN:HB3	1.97	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:I:196:ASP:HA	1:I:329:THR:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:356:ALA:HB1	1:I:361:ASP:HB2	1.97	0.45
1:K:240:VAL:HG21	1:K:247:LEU:HD13	1.98	0.45
1:L:127:ALA:CB	1:L:426:LEU:HD11	2.47	0.45
1:D:411:VAL:CG1	1:D:494:LEU:HD22	2.46	0.45
1:F:345:ARG:HD3	1:F:345:ARG:HA	1.96	0.45
1:G:169:VAL:HG11	1:G:175:ILE:HG13	1.99	0.45
1:G:411:VAL:HG11	1:G:494:LEU:HD22	1.99	0.45
1:H:240:VAL:HG21	1:H:247:LEU:HD13	1.98	0.45
1:I:120:ILE:O	1:I:124:VAL:HG23	2.16	0.45
1:I:139:SER:HB3	1:I:143:ALA:HB2	1.98	0.45
1:I:240:VAL:HG21	1:I:247:LEU:HD13	1.98	0.45
1:I:349:ILE:HG22	1:I:369:VAL:HG13	1.99	0.45
1:J:427:ALA:HA	1:J:444:LEU:HD11	1.99	0.45
1:K:406:ALA:HB2	1:K:496:PRO:HG3	1.99	0.45
1:L:349:ILE:HG22	1:L:369:VAL:HG13	1.99	0.45
1:N:144:ILE:HG23	1:N:403:THR:HG21	1.97	0.45
1:A:287:ALA:HB1	1:A:368:ARG:CZ	2.47	0.45
1:C:417:VAL:HG13	1:C:476:TYR:O	2.17	0.45
1:G:34:LYS:HB2	1:G:457:ASN:HB3	1.97	0.45
1:K:127:ALA:CB	1:K:426:LEU:HD11	2.46	0.45
1:M:117:LYS:HZ2	1:M:121:ASP:CG	2.25	0.45
1:M:120:ILE:O	1:M:124:VAL:HG23	2.16	0.45
1:N:120:ILE:O	1:N:124:VAL:HG23	2.16	0.45
1:B:417:VAL:HG13	1:B:476:TYR:O	2.17	0.45
1:C:287:ALA:HB1	1:C:368:ARG:CZ	2.47	0.45
1:D:120:ILE:O	1:D:124:VAL:HG23	2.16	0.45
1:J:127:ALA:CB	1:J:426:LEU:HD11	2.46	0.45
1:A:411:VAL:HG11	1:A:494:LEU:HD22	1.99	0.45
1:C:51:LYS:O	1:C:55:SER:HB2	2.17	0.45
1:D:127:ALA:CB	1:D:426:LEU:HD11	2.44	0.45
1:F:219:PHE:CE2	1:F:314:LEU:HD22	2.51	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:F:417:VAL:HG13	1:F:476:TYR:O	2.17	0.45
1:G:417:VAL:HG13	1:G:476:TYR:O	2.17	0.45
1:J:406:ALA:HB2	1:J:496:PRO:HG3	1.99	0.45
1:K:117:LYS:HZ2	1:K:121:ASP:CG	2.25	0.45
1:L:406:ALA:HB2	1:L:496:PRO:HG3	1.99	0.45
1:M:349:ILE:HG22	1:M:369:VAL:HG13	1.99	0.45
1:B:127:ALA:CB	1:B:426:LEU:HD11	2.44	0.45
1:C:23:LEU:O	1:C:27:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:LEU:O	1:E:27:VAL:HG23	2.17	0.45
1:E:287:ALA:HB1	1:E:368:ARG:CZ	2.47	0.45
1:G:411:VAL:CG1	1:G:494:LEU:HD22	2.46	0.45
1:H:34:LYS:HE2	1:H:458:CYS:HA	1.99	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: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
1:D:51:LYS:O	1:D:55:SER:HB2	2.17	0.45
1:E:217:SER:O	1:E:245:LYS:HG2	2.17	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:M:356:ALA:HB1	1:M:361:ASP:HB2	1.98	0.45
1:N:240:VAL:HG21	1:N:247:LEU:HD13	1.98	0.45
1:B:411:VAL:HG11	1:B:494:LEU:HD22	1.99	0.44
1:F:37:ASN:HB2	1:F:50:THR:O	2.18	0.44
1:G:287:ALA:HB1	1:G:368:ARG:CZ	2.47	0.44
1:H:349:ILE:HG22	1:H:369:VAL:HG13	1.99	0.44
1:L:117:LYS:HZ2	1:L:121:ASP:CG	2.25	0.44
1:A:417:VAL:HG13	1:A:476:TYR:O	2.17	0.44
1:D:23:LEU:O	1:D:27:VAL:HG23	2.17	0.44
1:D:287:ALA:HB1	1:D:368:ARG:CZ	2.47	0.44
1:H:383:ALA:HB3	1:H:389:MET:HB2	1.98	0.44
1:J:31:LEU:HA	3:J:1526:PO4:P	2.57	0.44
1:J:356:ALA:HB1	1:J:361:ASP:HB2	1.97	0.44
1:C:217:SER:O	1:C:245:LYS:HG2	2.17	0.44
1:D:54:VAL:HG13	1:D:89:THR:HG21	1.99	0.44
1:D:217:SER:O	1:D:245:LYS:HG2	2.17	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:G:37:ASN:HB2	1:G:50:THR:O	2.18	0.44
1:G:106:ALA:HB3	1:G:116:LEU:HD21	1.99	0.44
1:G:217:SER:O	1:G:245:LYS:HG2	2.17	0.44
1:J:144:ILE:HG23	1:J:403:THR:HG21	1.98	0.44
1:K:206:ASN:CB	1:K:213:VAL:HA	2.48	0.44
1:M:27:VAL:CG1	1:M:90:THR:HG23	2.25	0.44
1:N:349:ILE:HG22	1:N:369:VAL:HG13	1.99	0.44
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.98	0.44
1:A:217:SER:O	1:A:245:LYS:HG2	2.17	0.44
1:B:51:LYS:O	1:B:55:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ALA:CB	1:E:426:LEU:HD11	2.44	0.44
1:E:417:VAL:HG13	1:E:476:TYR:O	2.17	0.44
1:F:23:LEU:O	1:F:27:VAL:HG23	2.17	0.44
1:H:427:ALA:HA	1:H:444:LEU:HD11	1.98	0.44
1:J:240:VAL:HG21	1:J:247:LEU:HD13	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:L:427:ALA:HA	1:L:444:LEU:HD11	1.99	0.44
1:M:127:ALA:CB	1:M:426:LEU:HD11	2.47	0.44
1:M:279:PRO:HG3	1:M:292:ILE:HD11	2.00	0.44
1:N:417:VAL:HG13	1:N:476:TYR:O	2.18	0.44
1:C:37:ASN:HB2	1:C:50:THR:O	2.18	0.44
1:C:106:ALA:HB3	1:C:116:LEU:HD21	1.99	0.44
1:D:102:GLU:HB2	1:D:442:VAL:HG13	1.99	0.44
1:E:411:VAL:HG11	1:E:494:LEU:HD22	1.99	0.44
1:F:54:VAL:HG13	1:F:89:THR:HG21	1.99	0.44
1:K:427:ALA:HA	1:K:444:LEU:HD11	1.98	0.44
1:L:206:ASN:CB	1:L:213:VAL:HA	2.48	0.44
1:M:427:ALA:HA	1:M:444:LEU:HD11	1.98	0.44
1:N:279:PRO:HG3	1:N:292:ILE:HD11	2.00	0.44
1:B:37:ASN:HB2	1:B:50:THR:O	2.18	0.44
1:C:169:VAL:HG11	1:C:175:ILE:HG13	1.99	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:B:217:SER:O	1:B:245:LYS:HG2	2.17	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:J:117:LYS:HZ2	1:J:121:ASP:CG	2.26	0.44
1:K:440:ILE:O	1:K:444:LEU:HG	2.18	0.44
1:L:412:VAL:HG22	1:L:495:ASP:O	2.18	0.44
1:A:51:LYS:O	1:A:55:SER:HB2	2.17	0.44
1:C:54:VAL:HG13	1:C:89:THR:HG21	1.99	0.44
1:C:213:VAL:O	1:C:324:VAL:HA	2.18	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:G:152:ALA:HB1	1:G:155:ASP:O	2.18	0.44
1:H:417:VAL:HG13	1:H:476:TYR:O	2.18	0.44
1:H:455:VAL:HG11	1:H:465:VAL:HG21	2.00	0.44
1:I:440:ILE:O	1:I:444:LEU:HG	2.18	0.44
1:J:206:ASN:CB	1:J:213:VAL:HA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:417:VAL:HG13	1:M:476:TYR:O	2.18	0.44
1:N:406:ALA:HB2	1:N:496:PRO:HG3	1.99	0.44
1:A:169:VAL:HG11	1:A:175:ILE:HG13	1.99	0.44
1:B:213:VAL:O	1:B:324:VAL:HA	2.18	0.44
1:B:356:ALA:HB1	1:B:361:ASP:HB2	2.00	0.44
1:E:37:ASN:HB2	1:E:50:THR:O	2.18	0.44
1:H:117:LYS:HZ2	1:H:121:ASP:CG	2.26	0.44
1:H:256:GLY:O	1:H:260:ALA:HB3	2.18	0.44
1:H:440:ILE:O	1:H:444:LEU:HG	2.18	0.44
1:I:406:ALA:HB2	1:I:496:PRO:HG3	1.99	0.44
1:I:455:VAL:HG11	1:I:465:VAL:HG21	2.00	0.44
1:J:90:THR:HG22	1:J:94:VAL:HG23	2.00	0.44
1:J:417:VAL:HG13	1:J:476:TYR:O	2.18	0.44
1:K:279:PRO:HG3	1:K:292:ILE:HD11	2.00	0.44
1:M:412:VAL:HG22	1:M:495:ASP:O	2.18	0.44
1:N:455:VAL:HG11	1:N:465:VAL:HG21	2.00	0.44
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:F:152:ALA:HB1	1:F:155:ASP:O	2.18	0.43
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:J:440:ILE:O	1:J:444:LEU:HG	2.18	0.43
1:L:440:ILE:O	1:L:444:LEU:HG	2.18	0.43
1:M:64:ASP:O	1:M:68:ASN:HB2	2.18	0.43
1:M:206:ASN:HB2	1:M:213:VAL:HB	2.00	0.43
1:M:206:ASN:CB	1:M:213:VAL:HA	2.48	0.43
1:M:256:GLY:O	1:M:260:ALA:HB3	2.18	0.43
1:B:23:LEU:O	1:B:27:VAL:HG23	2.17	0.43
1:B:169:VAL:HG11	1:B:175:ILE:HG13	1.99	0.43
1:D:411:VAL:HG11	1:D:494:LEU:HD22	1.99	0.43
1:F:196:ASP:HA	1:F:329:THR:HA	2.00	0.43
1:H:412:VAL:HG22	1:H:495:ASP:O	2.18	0.43
1:I:256:GLY:O	1:I:260:ALA:HB3	2.18	0.43
1:I:412:VAL:HG22	1:I:495:ASP:O	2.18	0.43
1:J:412:VAL:HG22	1:J:495:ASP:O	2.18	0.43
3:M:1526:PO4:P	4:M:1527:ATP:O1B	2.76	0.43
1:N:412:VAL:HG22	1:N:495:ASP:O	2.18	0.43
1:A:102:GLU:HB2	1:A:442:VAL:HG13	1.99	0.43
1:D:488:MET:HA	1:D:488:MET:HE2	2.00	0.43
1:E:51:LYS:O	1:E:55:SER:HB2	2.17	0.43
1:E:196:ASP:HA	1:E:329:THR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:ALA:CB	1:G:426:LEU:HD11	2.44	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:K:417:VAL:HG13	1:K:476:TYR:O	2.18	0.43
1:A:213:VAL:O	1:A:324:VAL:HA	2.18	0.43
1:D:196:ASP:HA	1:D:329:THR:HA	2.01	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
3:L:1526:PO4:P	4:L:1527:ATP:PG	3.17	0.43
1:N:34:LYS:HE2	1:N:458:CYS:HA	2.01	0.43
1:A:152:ALA:HB1	1:A:155:ASP:O	2.18	0.43
1:C:356:ALA:HB1	1:C:361:ASP:HB2	2.00	0.43
1:G:488:MET:HE2	1:G:488:MET:HA	2.00	0.43
1:I:383:ALA:HB3	1:I:389:MET:N	2.34	0.43
1:J:102:GLU:HB2	1:J:442:VAL:HG13	2.01	0.43
1:J:279:PRO:HG3	1:J:292:ILE:HD11	2.00	0.43
3:J:1526:PO4:P	4:J:1527:ATP:PG	3.16	0.43
1:L:455:VAL:HG11	1:L:465:VAL:HG21	2.00	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: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:A:37:ASN:HB2	1:A:50:THR:O	2.18	0.43
1:A:488:MET:HA	1:A:488:MET:HE2	2.00	0.43
1:G:54:VAL:HG13	1:G:89:THR:HG21	1.99	0.43
1:H:102:GLU:HB2	1:H:442:VAL:HG13	2.01	0.43
1:H:206:ASN:CB	1:H:213:VAL:HA	2.48	0.43
1:I:279:PRO:HG3	1:I:292:ILE:HD11	2.00	0.43
1:J:34:LYS:HE2	1:J:458:CYS:HA	2.01	0.43
1:K:64:ASP:O	1:K:68:ASN:HB2	2.18	0.43
1:L:206:ASN:HB2	1:L:213:VAL:HB	2.00	0.43
1:L:417:VAL:HG13	1:L:476:TYR:O	2.18	0.43
1:N:180:GLY:HA3	1:N:381:VAL:O	2.19	0.43
1:A:106:ALA:HB3	1:A:116:LEU:HD21	1.99	0.43
1:A:356:ALA:HB1	1:A:361:ASP:HB2	2.00	0.43
1:C:488:MET:HE2	1:C:488:MET:HA	2.00	0.43
1:D:106:ALA:HB3	1:D:116:LEU:HD21	1.99	0.43
1:D:356:ALA:HB1	1:D:361:ASP:HB2	2.00	0.43
1:E:227:ILE:H	1:E:251:ALA:HB1	1.84	0.43
1:G:213:VAL:O	1:G:324:VAL:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:ILE:H	1:G:251:ALA:HB1	1.84	0.43
1:G:345:ARG:HD3	1:G:345:ARG:HA	1.96	0.43
1:I:34:LYS:HE2	1:I:458:CYS:HA	2.01	0.43
1:I:182:GLY:O	1:I:382:GLY:HA2	2.19	0.43
1:J:383:ALA:HB3	1:J:389:MET:N	2.34	0.43
1:M:493:ILE:HG21	4:M:1527:ATP:C8	2.52	0.43
1:N:206:ASN:HB2	1:N:213:VAL:HB	2.00	0.43
1:C:117:LYS:HZ2	1:C:121:ASP:CG	2.27	0.43
1:C:220:ILE:HD12	1:C:248:LEU:HD23	2.01	0.43
1:F:152:ALA:HB1	1:F:155:ASP:CA	2.49	0.43
1:F:356:ALA:HB1	1:F:361:ASP:HB2	2.00	0.43
1:G:102:GLU:HB2	1:G:442:VAL:HG13	1.99	0.43
1:G:152:ALA:HB1	1:G:155:ASP:CA	2.49	0.43
1:H:182:GLY:O	1:H:382:GLY:HA2	2.19	0.43
1:H:488:MET:HE2	1:H:488:MET:HA	2.01	0.43
1:I:90:THR:HG22	1:I:94:VAL:HG23	2.01	0.43
1:I:102:GLU:HB2	1:I:442:VAL:HG13	2.01	0.43
1:I:417:VAL:HG13	1:I:476:TYR:O	2.18	0.43
1:K:102:GLU:HB2	1:K:442:VAL:HG13	2.01	0.43
1:K:182:GLY:O	1:K:382:GLY:HA2	2.19	0.43
1:K:213:VAL:HG13	1:K:325:ILE:HB	2.01	0.43
1:K:455:VAL:HG11	1:K:465:VAL:HG21	2.01	0.43
1:L:90:THR:HG22	1:L:94:VAL:HG23	2.01	0.43
1:L:102:GLU:HB2	1:L:442:VAL:HG13	2.01	0.43
1:M:180:GLY:HA3	1:M:381:VAL:O	2.19	0.43
1:M:440:ILE:O	1:M:444:LEU:HG	2.18	0.43
1:N:102:GLU:HB2	1:N:442:VAL:HG13	2.01	0.43
1:B:54:VAL:HG13	1:B:89:THR:HG21	1.99	0.43
1:D:213:VAL:O	1:D:324:VAL:HA	2.18	0.43
1:D:227:ILE:H	1:D:251:ALA:HB1	1.84	0.43
1:E:488:MET:HE2	1:E:488:MET:HA	2.00	0.43
1:G:196:ASP:HA	1:G:329:THR:HA	2.00	0.43
1:H:180:GLY:HA3	1:H:381:VAL:O	2.19	0.43
1:I:206:ASN:HB2	1:I:213:VAL:HB	2.00	0.43
1:J:180:GLY:HA3	1:J:381:VAL:O	2.19	0.43
1:J:206:ASN:HB2	1:J:213:VAL:HB	2.00	0.43
1:K:31:LEU:HB3	1:K:90:THR:HG21	2.00	0.43
1:K:180:GLY:HA3	1:K:381:VAL:O	2.19	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:L:383:ALA:HB3	1:L:389:MET:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:213:VAL:HG13	1:M:325:ILE:HB	2.01	0.43
1:M:488:MET:HA	1:M:488:MET:HE2	2.00	0.43
1:N:182:GLY:O	1:N:382:GLY:HA2	2.19	0.43
1:N:206:ASN:CB	1:N:213:VAL:HA	2.48	0.43
1:E:152:ALA:HB1	1:E:155:ASP:CA	2.49	0.43
1:E:356:ALA:HB1	1:E:361:ASP:HB2	2.00	0.43
1:F:117:LYS:HZ2	1:F:121:ASP:CG	2.27	0.43
1:I:64:ASP:O	1:I:68:ASN:HB2	2.19	0.43
1:I:180:GLY:HA3	1:I:381:VAL:O	2.19	0.43
1:K:206:ASN:HB2	1:K:213:VAL:HB	2.00	0.43
1:L:213:VAL:HG13	1:L:325:ILE:HB	2.01	0.43
1:M:182:GLY:O	1:M:382:GLY:HA2	2.19	0.43
1:N:117:LYS:HZ2	1:N:121:ASP:CG	2.26	0.43
1:A:480:ALA:O	1:A:483:GLU:CG	2.67	0.42
1:B:102:GLU:HB2	1:B:442:VAL:HG13	2.00	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:C:480:ALA:O	1:C:483:GLU:CG	2.67	0.42
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:J:293:ALA:HB2	1:J:300:VAL:CG2	2.49	0.42
1:K:256:GLY:O	1:K:260:ALA:HB3	2.18	0.42
1:K:383:ALA:HB3	1:K:389:MET:N	2.34	0.42
1:M:102:GLU:HB2	1:M:442:VAL:HG13	2.01	0.42
1:N:293:ALA:HB2	1:N:300:VAL:CG2	2.49	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:B:488:MET:HE2	1:B:488:MET:HA	2.00	0.42
1:D:106:ALA:HB1	1:D:116:LEU:HD21	2.01	0.42
1:D:349:ILE:HB	1:D:369:VAL:HG12	2.02	0.42
1:F:227:ILE:H	1:F:251:ALA:HB1	1.84	0.42
1:H:64:ASP:O	1:H:68:ASN:HB2	2.19	0.42
1:H:90:THR:HG22	1:H:94:VAL:HG23	2.01	0.42
1:I:293:ALA:HB2	1:I:300:VAL:CG2	2.49	0.42
1:J:256:GLY:O	1:J:260:ALA:HB3	2.18	0.42
1:K:144:ILE:HG23	1:K:403:THR:HG21	2.01	0.42
1:L:34:LYS:HE2	1:L:458:CYS:HA	2.01	0.42
1:L:182:GLY:O	1:L:382:GLY:HA2	2.19	0.42
1:L:294:THR:HG21	1:L:345:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ALA:HB1	1:C:116:LEU:HD21	2.01	0.42
1:C:152:ALA:HB1	1:C:155:ASP:O	2.18	0.42
1:C:152:ALA:HB1	1:C:155:ASP:CA	2.49	0.42
1:D:152:ALA:HB1	1:D:155:ASP:O	2.18	0.42
1:D:220:ILE:HD12	1:D:248:LEU:HD23	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:K:23:LEU:O	1:K:27:VAL:HG23	2.20	0.42
1:K:294:THR:HG21	1:K:345:ARG:HG3	2.01	0.42
1:K:412:VAL:HG22	1:K:495:ASP:O	2.18	0.42
1:M:455:VAL:HG11	1:M:465:VAL:HG21	2.01	0.42
1:N:213:VAL:HG13	1:N:325:ILE:HB	2.01	0.42
1:N:256:GLY:O	1:N:260:ALA:HB3	2.18	0.42
1:B:15:LYS:HB3	1:B:66:PHE:HB3	2.02	0.42
1:B:106:ALA:HB3	1:B:116:LEU:HD21	1.99	0.42
1:B:227:ILE:H	1:B:251:ALA:HB1	1.84	0.42
1:C:349:ILE:HB	1:C:369:VAL:HG12	2.01	0.42
1:C:349:ILE:HG23	1:C:365:LEU:CD1	2.50	0.42
1:E:213:VAL:O	1:E:324:VAL:HA	2.18	0.42
1:E:349:ILE:HG23	1:E:365:LEU:CD1	2.50	0.42
1:F:488:MET:HA	1:F:488:MET:HE2	2.00	0.42
1:G:356:ALA:HB1	1:G:361:ASP:HB2	2.00	0.42
3:I:1526:PO4:P	4:I:1527:ATP:PG	3.17	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:A:117:LYS:HZ2	1:A:121:ASP:CG	2.27	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:C:285:ARG:HG3	1:C:285:ARG:HH11	1.85	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:M:293:ALA:HB2	1:M:300:VAL:CG2	2.49	0.42
1:N:90:THR:HG22	1:N:94:VAL:HG23	2.01	0.42
1:A:147:VAL:HG22	1:A:494:LEU:CD1	2.46	0.42
1:A:349:ILE:HB	1:A:369:VAL:HG12	2.02	0.42
1:C:227:ILE:H	1:C:251:ALA:HB1	1.84	0.42
1:D:152:ALA:HB1	1:D:155:ASP:CA	2.49	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:F:138:CYS:SG	1:F:407:VAL:HA	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:ASN:ND2	1:F:214:GLU:H	2.18	0.42
1:I:383:ALA:HB3	1:I:389:MET:CA	2.50	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:B:19:GLY:HA2	1:B:62:LEU:CD1	2.50	0.42
1:B:480:ALA:O	1:B:483:GLU:CG	2.67	0.42
1:C:19:GLY:HA2	1:C:62:LEU:CD1	2.50	0.42
1:C:206:ASN:ND2	1:C:214:GLU:H	2.18	0.42
1:D:138:CYS:SG	1:D:407:VAL:HA	2.60	0.42
1:E:7:LYS:HB2	1:E:11:ASP:HB3	2.01	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:G:220:ILE:HD12	1:G:248:LEU:HD23	2.01	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:J:268:ARG:HA	1:J:268:ARG:NE	2.35	0.42
1:K:19:GLY:HA2	1:K:62:LEU:CD1	2.50	0.42
1:L:180:GLY:HA3	1:L:381:VAL:O	2.19	0.42
1:M:135:SER:CA	1:M:412:VAL:HG12	2.45	0.42
1:M:414:GLY:HA2	1:M:495:ASP:CG	2.44	0.42
1:N:23:LEU:O	1:N:27:VAL:HG23	2.20	0.42
1:N:64:ASP:O	1:N:68:ASN:HB2	2.19	0.42
1:N:488:MET:HE2	1:N:488:MET:HA	2.02	0.42
1:A:50:THR:HG21	1:A:59:GLU:HB2	2.01	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:C:138:CYS:SG	1:C:407:VAL:HA	2.60	0.42
1:D:213:VAL:CG1	1:D:325:ILE:HB	2.50	0.42
1:F:7:LYS:HB2	1:F:11:ASP:HB3	2.02	0.42
1:G:19:GLY:HA2	1:G:62:LEU:CD1	2.50	0.42
1:G:213:VAL:CG1	1:G:325:ILE:HB	2.50	0.42
1:H:293:ALA:HB2	1:H:300:VAL:CG2	2.49	0.42
1:H:383:ALA:HB3	1:H:389:MET:CA	2.50	0.42
1:I:66:PHE:CZ	1:I:522:THR:HG22	2.55	0.42
1:J:202:PRO:O	1:J:205:ILE:HB	2.20	0.42
1:K:268:ARG:NE	1:K:268:ARG:HA	2.35	0.42
1:K:488:MET:HA	1:K:488:MET:HE2	2.01	0.42
1:L:23:LEU:O	1:L:27:VAL:HG23	2.20	0.42
1:A:227:ILE:H	1:A:251:ALA:HB1	1.84	0.42
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.85	0.42
1:B:196:ASP:HA	1:B:329:THR:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:LYS:HB3	1:D:66:PHE:HB3	2.02	0.42
1:E:106:ALA:HB1	1:E:116:LEU:HD21	2.01	0.42
1:E:213:VAL:CG1	1:E:325:ILE:HB	2.50	0.42
1:F:220:ILE:HD12	1:F:248:LEU:HD23	2.01	0.42
1:G:50:THR:HG21	1:G:59:GLU:HB2	2.01	0.42
1:G:349:ILE:HG23	1:G:365:LEU:CD1	2.50	0.42
1:G:480:ALA:O	1:G:483:GLU:CG	2.67	0.42
1:J:294:THR:HG21	1:J:345:ARG:HG3	2.01	0.42
1:J:383:ALA:HB3	1:J:389:MET:CA	2.50	0.42
1:L:202:PRO:O	1:L:205:ILE:HB	2.20	0.42
1:M:23:LEU:O	1:M:27:VAL:HG23	2.20	0.42
4:M:1527:ATP:C4	4:M:1527:ATP:C8	3.07	0.42
1:A:15:LYS:HB3	1:A:66:PHE:HB3	2.02	0.42
1:A:19:GLY:HA2	1:A:62:LEU:CD1	2.50	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:B:349:ILE:HG23	1:B:365:LEU:CD1	2.49	0.42
1:E:480:ALA:O	1:E:483:GLU:CG	2.67	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:H:66:PHE:CZ	1:H:522:THR:HG22	2.55	0.42
1:H:152:ALA:HB1	1:H:155:ASP:CA	2.50	0.42
1:I:33:PRO:HG3	4:I:1527:ATP:C4	2.55	0.42
1:I:268:ARG:HA	1:I:268:ARG:NE	2.35	0.42
1:J:19:GLY:HA2	1:J:62:LEU:CD1	2.50	0.42
1:J:23:LEU:O	1:J:27:VAL:HG23	2.20	0.42
1:J:66:PHE:CZ	1:J:522:THR:HG22	2.55	0.42
1:M:152:ALA:HB1	1:M:155:ASP:CA	2.50	0.42
1:N:486:GLY:HA3	1:N:491:MET:HE3	2.02	0.42
1:B:106:ALA:HB1	1:B:116:LEU:HD21	2.01	0.41
1:B:294:THR:HG21	1:B:345:ARG:HG3	2.02	0.41
1:E:117:LYS:HZ2	1:E:121:ASP:CG	2.28	0.41
1:F:77:VAL:HG12	1:F:506:TYR:HB3	2.02	0.41
1:F:218:PRO:HG2	1:F:323:VAL:HG23	2.02	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:G:285:ARG:HG3	1:G:285:ARG:HH11	1.85	0.41
1:H:323:VAL:HG22	1:H:332:ILE:HA	2.02	0.41
1:J:488:MET:HE2	1:J:488:MET:HA	2.01	0.41
1:L:268:ARG:HA	1:L:268:ARG:NE	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:GLY:HA2	1:N:62:LEU:CD1	2.50	0.41
1:N:152:ALA:HB1	1:N:155:ASP:CA	2.50	0.41
1:N:294:THR:HG21	1:N:345:ARG:HG3	2.02	0.41
1:N:323:VAL:HG22	1:N:332:ILE:HA	2.02	0.41
1:B:50:THR:HG21	1:B:59:GLU:HB2	2.01	0.41
1:B:285:ARG:HG3	1:B:285:ARG:HH11	1.85	0.41
1:C:218:PRO:HG2	1:C:323:VAL:HG23	2.02	0.41
1:D:19:GLY:HA2	1:D:62:LEU:CD1	2.50	0.41
1:D:218:PRO:HG2	1:D:323:VAL:HG23	2.02	0.41
1:E:199:TYR:CD2	1:E:327:LYS:HA	2.56	0.41
1:F:19:GLY:HA2	1:F:62:LEU:CD1	2.50	0.41
1:F:50:THR:HG21	1:F:59:GLU:HB2	2.01	0.41
1:F:480:ALA:O	1:F:483:GLU:CG	2.67	0.41
1:G:349:ILE:HB	1:G:369:VAL:HG12	2.02	0.41
1:G:383:ALA:HB3	1:G:389:MET:N	2.35	0.41
1:I:323:VAL:HG22	1:I:332:ILE:HA	2.02	0.41
1:K:383:ALA:HB3	1:K:389:MET:CA	2.50	0.41
1:L:152:ALA:HB1	1:L:155:ASP:CA	2.50	0.41
1:A:106:ALA:HB1	1:A:116:LEU:HD21	2.01	0.41
1:A:294:THR:HG21	1:A:345:ARG:HG3	2.03	0.41
1:A:349:ILE:HG23	1:A:365:LEU:CD1	2.49	0.41
1:B:51:LYS:HG2	1:B:52:ASP:H	1.85	0.41
1:B:147:VAL:HG22	1:B:494:LEU:CD1	2.46	0.41
1:D:13:ARG:CG	1:D:104:LEU:HD22	2.51	0.41
1:D:77:VAL:HG12	1:D:506:TYR:HB3	2.02	0.41
1:D:199:TYR:CD2	1:D:327:LYS:HA	2.56	0.41
1:E:138:CYS:SG	1:E:407:VAL:HA	2.60	0.41
1:F:199:TYR:CD2	1:F:327:LYS:HA	2.55	0.41
1:F:240:VAL:HA	1:F:243:ALA:HB3	2.02	0.41
1:G:7:LYS:HB2	1:G:11:ASP:HB3	2.01	0.41
1:G:106:ALA:HB1	1:G:116:LEU:HD21	2.01	0.41
1:K:152:ALA:HB1	1:K:155:ASP:CA	2.50	0.41
1:L:488:MET:HE2	1:L:488:MET:HA	2.01	0.41
1:M:268:ARG:HA	1:M:268:ARG:NE	2.35	0.41
1:M:383:ALA:HB3	1:M:389:MET:CA	2.50	0.41
1:N:338:GLU:CD	1:N:341:ALA:HB2	2.45	0.41
1:N:383:ALA:HB3	1:N:389:MET:CA	2.50	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:A:240:VAL:HA	1:A:243:ALA:HB3	2.02	0.41
1:B:117:LYS:HZ2	1:B:121:ASP:CG	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ARG:CG	1:C:104:LEU:HD22	2.51	0.41
1:C:199:TYR:CD2	1:C:327:LYS:HA	2.56	0.41
1:C:294:THR:HG21	1:C:345:ARG:HG3	2.02	0.41
1:C:383:ALA:HB3	1:C:389:MET:N	2.35	0.41
1:D:285:ARG:HG3	1:D:285:ARG:HH11	1.85	0.41
1:E:218:PRO:HG2	1:E:323:VAL:HG23	2.03	0.41
1:F:13:ARG:CG	1:F:104:LEU:HD22	2.51	0.41
1:F:294:THR:HG21	1:F:345:ARG:HG3	2.03	0.41
1:G:13:ARG:CG	1:G:104:LEU:HD22	2.51	0.41
1:H:19:GLY:HA2	1:H:62:LEU:CD1	2.50	0.41
1:I:152:ALA:HB1	1:I:155:ASP:CA	2.51	0.41
1:I:488:MET:HE2	1:I:488:MET:HA	2.01	0.41
1:L:33:PRO:HG3	4:L:1527:ATP:C4	2.55	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:B:218:PRO:HG2	1:B:323:VAL:HG23	2.03	0.41
1:C:50:THR:HG21	1:C:59:GLU:HB2	2.01	0.41
1:C:51:LYS:HG2	1:C:52:ASP:H	1.85	0.41
1:C:77:VAL:HG12	1:C:506:TYR:HB3	2.02	0.41
1:D:7:LYS:HB2	1:D:11:ASP:HB3	2.02	0.41
1:D:50:THR:HG21	1:D:59:GLU:HB2	2.01	0.41
1:D:65:LYS:HZ1	1:E:41:ASP:CG	2.27	0.41
1:D:206:ASN:ND2	1:D:214:GLU:H	2.18	0.41
1:E:50:THR:HG21	1:E:59:GLU:HB2	2.01	0.41
1:E:77:VAL:HG12	1:E:506:TYR:HB3	2.03	0.41
1:E:220:ILE:HD12	1:E:248:LEU:HD23	2.01	0.41
1:E:285:ARG:HG3	1:E:285:ARG:HH11	1.85	0.41
1:G:77:VAL:HG12	1:G:506:TYR:HB3	2.02	0.41
1:G:206:ASN:ND2	1:G:214:GLU:H	2.18	0.41
1:G:218:PRO:HG2	1:G:323:VAL:HG23	2.03	0.41
1:H:268:ARG:HA	1:H:268:ARG:NE	2.35	0.41
1:I:205:ILE:HD13	1:I:205:ILE:HA	1.91	0.41
1:K:338:GLU:CD	1:K:341:ALA:HB2	2.46	0.41
1:L:383:ALA:HB3	1:L:389:MET:CA	2.50	0.41
1:B:213:VAL:CG1	1:B:325:ILE:HB	2.50	0.41
1:B:383:ALA:HB3	1:B:389:MET:N	2.35	0.41
1:C:213:VAL:CG1	1:C:325:ILE:HB	2.50	0.41
1:D:51:LYS:HG2	1:D:52:ASP:H	1.85	0.41
1:E:13:ARG:CG	1:E:104:LEU:HD22	2.51	0.41
1:G:15:LYS:HB3	1:G:66:PHE:HB3	2.01	0.41
1:G:147:VAL:HG22	1:G:494:LEU:CD1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:PRO:O	1:H:205:ILE:HB	2.20	0.41
1:J:126:ALA:HB3	1:J:426:LEU:HD22	2.03	0.41
1:M:66:PHE:CZ	1:M:522:THR:HG22	2.55	0.41
1:M:202:PRO:O	1:M:205:ILE:HB	2.20	0.41
1:A:51:LYS:HG2	1:A:52:ASP:H	1.85	0.41
1:A:218:PRO:HG2	1:A:323:VAL:HG23	2.03	0.41
1:B:349:ILE:HB	1:B:369:VAL:HG12	2.01	0.41
1:C:65:LYS:HZ1	1:D:41:ASP:CG	2.27	0.41
1:C:85:ALA:HB1	1:C:499:VAL:HA	2.03	0.41
1:D:117:LYS:HZ2	1:D:121:ASP:CG	2.27	0.41
1:F:106:ALA:HB1	1:F:116:LEU:HD21	2.01	0.41
1:G:383:ALA:HB3	1:G:389:MET:CA	2.51	0.41
1:I:19:GLY:HA2	1:I:62:LEU:CD1	2.50	0.41
1:I:294:THR:HG21	1:I:345:ARG:HG3	2.02	0.41
1:J:152:ALA:HB1	1:J:155:ASP:CA	2.50	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:M:323:VAL:HG22	1:M:332:ILE:HA	2.02	0.41
1:N:66:PHE:CZ	1:N:522:THR:HG22	2.55	0.41
3:N:1526:PO4:P	4:N:1527:ATP:PG	3.19	0.41
1:A:166:MET:HA	1:A:175:ILE:HD11	2.03	0.41
1:A:383:ALA:HB3	1:A:389:MET:CA	2.51	0.41
1:B:199:TYR:CD2	1:B:327:LYS:HA	2.55	0.41
1:B:383:ALA:HB3	1:B:389:MET:CA	2.51	0.41
1:D:85:ALA:HB1	1:D:499:VAL:HA	2.03	0.41
1:D:294:THR:HG21	1:D:345:ARG:HG3	2.02	0.41
1:E:147:VAL:HG22	1:E:494:LEU:CD1	2.46	0.41
1:E:206:ASN:ND2	1:E:214:GLU:H	2.18	0.41
1:E:294:THR:HG21	1:E:345:ARG:HG3	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:F:383:ALA:HB3	1:F:389:MET:CA	2.51	0.41
1:G:138:CYS:SG	1:G:407:VAL:HA	2.60	0.41
1:H:23:LEU:O	1:H:27:VAL:HG23	2.20	0.41
1:H:281:PHE:HA	1:H:285:ARG:HB2	2.03	0.41
1:I:77:VAL:HG12	1:I:506:TYR:HB3	2.03	0.41
1:A:206:ASN:HB2	1:A:213:VAL:CA	2.49	0.41
1:B:13:ARG:CG	1:B:104:LEU:HD22	2.51	0.41
1:B:166:MET:HA	1:B:175:ILE:HD11	2.03	0.41
1:B:206:ASN:ND2	1:B:214:GLU:H	2.18	0.41
1:E:19:GLY:HA2	1:E:62:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:LYS:HG2	1:E:52:ASP:H	1.85	0.41
1:E:85:ALA:O	1:E:499:VAL:HG12	2.21	0.41
1:E:383:ALA:HB3	1:E:389:MET:N	2.36	0.41
3:F:1527:PO4:P	4:F:1528:ATP:PG	3.19	0.41
1:G:199:TYR:CD2	1:G:327:LYS:HA	2.56	0.41
1:H:294:THR:HG21	1:H:345:ARG:HG3	2.02	0.41
3:H:1526:PO4:P	4:H:1527:ATP:PG	3.19	0.41
1:I:126:ALA:HB3	1:I:426:LEU:HD22	2.03	0.41
1:I:202:PRO:O	1:I:205:ILE:HB	2.20	0.41
1:J:77:VAL:HG12	1:J:506:TYR:HB3	2.03	0.41
1:L:281:PHE:HA	1:L:285:ARG:HB2	2.03	0.41
1:L:338:GLU:CD	1:L:341:ALA:HB2	2.46	0.41
1:M:281:PHE:HA	1:M:285:ARG:HB2	2.03	0.41
1:M:338:GLU:CD	1:M:341:ALA:HB2	2.46	0.41
1:N:268:ARG:HA	1:N:268:ARG:NE	2.35	0.41
1:N:281:PHE:HA	1:N:285:ARG:HB2	2.03	0.41
1:A:13:ARG:CG	1:A:104:LEU:HD22	2.51	0.41
1:A:197:ARG:HD2	1:A:277:LYS:HB2	2.03	0.41
1:B:7:LYS:HB2	1:B:11:ASP:HB3	2.01	0.41
1:B:206:ASN:HB2	1:B:213:VAL:CA	2.49	0.41
1:B:240:VAL:HA	1:B:243:ALA:HB3	2.02	0.41
1:B:426:LEU:HB2	1:B:444:LEU:CD2	2.51	0.41
3:B:1527:PO4:P	4:B:1528:ATP:PG	3.19	0.41
1:C:166:MET:HA	1:C:175:ILE:HD11	2.03	0.41
1:D:197:ARG:HD2	1:D:277:LYS:HB2	2.03	0.41
1:E:197:ARG:HD2	1:E:277:LYS:HB2	2.03	0.41
1:F:285:ARG:HH11	1:F:285:ARG:HG3	1.85	0.41
1:G:197:ARG:HD2	1:G:277:LYS:HB2	2.03	0.41
1:H:77:VAL:HG12	1:H:506:TYR:HB3	2.03	0.41
1:L:66:PHE:CZ	1:L:522:THR:HG22	2.55	0.41
1:L:126:ALA:HB3	1:L:426:LEU:HD22	2.03	0.41
1:M:205:ILE:HG23	1:M:211:GLY:HA2	2.03	0.41
1:N:77:VAL:HG12	1:N:506:TYR:HB3	2.03	0.41
1:B:77:VAL:HG12	1:B:506:TYR:HB3	2.03	0.40
1:B:85:ALA:O	1:B:499:VAL:HG12	2.21	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:C:226:LYS:HA	1:C:252:GLU:H	1.86	0.40
3:C:1527:PO4:P	4:C:1528:ATP:PG	3.19	0.40
1:G:117:LYS:HZ2	1:G:121:ASP:CG	2.29	0.40
1:I:281:PHE:HA	1:I:285:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:323:VAL:HG22	1:L:332:ILE:HA	2.02	0.40
1:A:199:TYR:CD2	1:A:327:LYS:HA	2.56	0.40
3:A:1527:PO4:P	4:A:1528:ATP:PG	3.19	0.40
1:E:15:LYS:HB3	1:E:66:PHE:HB3	2.02	0.40
1:F:197:ARG:HD2	1:F:277:LYS:HB2	2.03	0.40
1:K:66:PHE:CZ	1:K:522:THR:HG22	2.55	0.40
1:K:323:VAL:HG22	1:K:332:ILE:HA	2.02	0.40
1:N:197:ARG:HD3	1:N:197:ARG:HA	1.95	0.40
1:A:7:LYS:HB2	1:A:11:ASP:HB3	2.01	0.40
1:C:7:LYS:HB2	1:C:11:ASP:HB3	2.02	0.40
1:C:383:ALA:HB3	1:C:389:MET:CA	2.51	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
3:D:1527:PO4:P	4:D:1528:ATP:PG	3.19	0.40
1:E:383:ALA:HB3	1:E:389:MET:CA	2.51	0.40
1:F:426:LEU:HB2	1:F:444:LEU:CD2	2.52	0.40
1:G:51:LYS:HG2	1:G:52:ASP:H	1.85	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:A:77:VAL:HG12	1:A:506:TYR:HB3	2.03	0.40
1:H:205:ILE:HG23	1:H:211:GLY:HA2	2.03	0.40
1:I:205:ILE:HG23	1:I:211:GLY:HA2	2.03	0.40
1:J:33:PRO:HG3	4:J:1527:ATP:C4	2.57	0.40
1:J:338:GLU:CD	1:J:341:ALA:HB2	2.46	0.40
1:K:205:ILE:HG23	1:K:211:GLY:HA2	2.03	0.40
1:K:281:PHE:HA	1:K:285:ARG:HB2	2.03	0.40
1:L:206:ASN:HD22	1:L:214:GLU:H	1.70	0.40
1:M:206:ASN:HD22	1:M:214:GLU:H	1.70	0.40
1:A:19:GLY:HA2	1:A:62:LEU:HD13	2.04	0.40
1:J:166:MET:HA	1:J:175:ILE:HD11	2.04	0.40
1:K:166:MET:HA	1:K:175:ILE:HD11	2.04	0.40
1:L:231:ARG:O	1:L:235:PRO:HD2	2.22	0.40
1:M:85:ALA:HB1	1:M:499:VAL:HA	2.02	0.40
1:N:206:ASN:HD22	1:N:214:GLU:H	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	30	67
1	B	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	C	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	D	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	E	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	F	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	G	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
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%)	44	78

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

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Mol	Chain	Res	Type
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%)	353 (88%)	49 (12%)	5	17
1	B	402/414 (97%)	353 (88%)	49 (12%)	5	17
1	C	402/414 (97%)	353 (88%)	49 (12%)	5	17
1	D	402/414 (97%)	353 (88%)	49 (12%)	5	17
1	E	402/414 (97%)	353 (88%)	49 (12%)	5	17
1	F	402/414 (97%)	353 (88%)	49 (12%)	5	17
1	G	402/414 (97%)	353 (88%)	49 (12%)	5	17
1	H	402/414 (97%)	365 (91%)	37 (9%)	8	27
1	I	402/414 (97%)	365 (91%)	37 (9%)	8	27
1	J	402/414 (97%)	365 (91%)	37 (9%)	8	27
1	K	402/414 (97%)	366 (91%)	36 (9%)	9	27
1	L	402/414 (97%)	365 (91%)	37 (9%)	8	27
1	M	402/414 (97%)	365 (91%)	37 (9%)	8	27
1	N	402/414 (97%)	365 (91%)	37 (9%)	8	27
All	All	5628/5796 (97%)	5027 (89%)	601 (11%)	8	21

All (601) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	31	LEU

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Mol	Chain	Res	Type
1	A	40	LEU
1	A	52	ASP
1	A	54	VAL
1	A	63	GLU
1	A	65	LYS
1	A	79	SER
1	A	82	ASN
1	A	89	THR
1	A	107	VAL
1	A	130	GLU
1	A	136	VAL
1	A	168	LYS
1	A	171	LYS
1	A	172	GLU
1	A	193	MET
1	A	205	ILE
1	A	207	LYS
1	A	213	VAL
1	A	214	GLU
1	A	219	PHE
1	A	230	ILE
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	270	ILE
1	A	272	LYS
1	A	285	ARG
1	A	294	THR
1	A	301	ILE
1	A	323	VAL
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	425	LYS
1	A	430	ARG
1	A	453	GLN

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Mol	Chain	Res	Type
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	31	LEU
1	B	40	LEU
1	B	52	ASP
1	B	54	VAL
1	B	63	GLU
1	B	65	LYS
1	B	79	SER
1	B	82	ASN
1	B	89	THR
1	B	107	VAL
1	B	130	GLU
1	B	136	VAL
1	B	168	LYS
1	B	171	LYS
1	B	172	GLU
1	B	193	MET
1	B	205	ILE
1	B	207	LYS
1	B	213	VAL
1	B	214	GLU
1	B	219	PHE
1	B	230	ILE
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	270	ILE
1	B	272	LYS
1	B	294	THR
1	B	301	ILE
1	B	303	GLU
1	B	323	VAL
1	B	327	LYS
1	B	328	ASP

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Mol	Chain	Res	Type
1	B	334	ASP
1	B	350	ARG
1	B	358	SER
1	B	421	ARG
1	B	425	LYS
1	B	430	ARG
1	B	453	GLN
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	31	LEU
1	C	40	LEU
1	C	52	ASP
1	C	54	VAL
1	C	63	GLU
1	C	65	LYS
1	C	79	SER
1	C	82	ASN
1	C	89	THR
1	C	107	VAL
1	C	130	GLU
1	C	136	VAL
1	C	168	LYS
1	C	171	LYS
1	C	172	GLU
1	C	193	MET
1	C	205	ILE
1	C	207	LYS
1	C	213	VAL
1	C	214	GLU
1	C	219	PHE
1	C	230	ILE
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	270	ILE

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Mol	Chain	Res	Type
1	C	272	LYS
1	C	285	ARG
1	C	294	THR
1	C	301	ILE
1	C	323	VAL
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	425	LYS
1	C	430	ARG
1	C	453	GLN
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	31	LEU
1	D	40	LEU
1	D	52	ASP
1	D	54	VAL
1	D	63	GLU
1	D	65	LYS
1	D	79	SER
1	D	82	ASN
1	D	89	THR
1	D	107	VAL
1	D	130	GLU
1	D	136	VAL
1	D	168	LYS
1	D	171	LYS
1	D	172	GLU
1	D	193	MET
1	D	205	ILE
1	D	207	LYS
1	D	213	VAL
1	D	214	GLU
1	D	219	PHE
1	D	230	ILE

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Mol	Chain	Res	Type
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	270	ILE
1	D	272	LYS
1	D	294	THR
1	D	301	ILE
1	D	303	GLU
1	D	323	VAL
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	425	LYS
1	D	430	ARG
1	D	453	GLN
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	31	LEU
1	E	40	LEU
1	E	52	ASP
1	E	54	VAL
1	E	63	GLU
1	E	65	LYS
1	E	79	SER
1	E	82	ASN
1	E	89	THR
1	E	107	VAL
1	E	130	GLU
1	E	136	VAL
1	E	168	LYS
1	E	171	LYS
1	E	172	GLU

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Mol	Chain	Res	Type
1	E	193	MET
1	E	205	ILE
1	E	207	LYS
1	E	213	VAL
1	E	214	GLU
1	E	219	PHE
1	E	230	ILE
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	270	ILE
1	E	272	LYS
1	E	285	ARG
1	E	294	THR
1	E	301	ILE
1	E	323	VAL
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	425	LYS
1	E	430	ARG
1	E	453	GLN
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	31	LEU
1	F	40	LEU
1	F	52	ASP
1	F	54	VAL
1	F	63	GLU
1	F	65	LYS
1	F	79	SER
1	F	82	ASN

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Mol	Chain	Res	Type
1	F	89	THR
1	F	107	VAL
1	F	130	GLU
1	F	136	VAL
1	F	168	LYS
1	F	171	LYS
1	F	172	GLU
1	F	193	MET
1	F	205	ILE
1	F	207	LYS
1	F	213	VAL
1	F	214	GLU
1	F	219	PHE
1	F	230	ILE
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	270	ILE
1	F	272	LYS
1	F	285	ARG
1	F	294	THR
1	F	301	ILE
1	F	323	VAL
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	425	LYS
1	F	430	ARG
1	F	453	GLN
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	31	LEU

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Mol	Chain	Res	Type
1	G	40	LEU
1	G	52	ASP
1	G	54	VAL
1	G	63	GLU
1	G	65	LYS
1	G	79	SER
1	G	82	ASN
1	G	89	THR
1	G	107	VAL
1	G	130	GLU
1	G	136	VAL
1	G	168	LYS
1	G	171	LYS
1	G	172	GLU
1	G	193	MET
1	G	205	ILE
1	G	207	LYS
1	G	213	VAL
1	G	214	GLU
1	G	219	PHE
1	G	230	ILE
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	270	ILE
1	G	272	LYS
1	G	285	ARG
1	G	294	THR
1	G	301	ILE
1	G	323	VAL
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	425	LYS
1	G	430	ARG
1	G	453	GLN

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Mol	Chain	Res	Type
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	31	LEU
1	H	37	ASN
1	H	50	THR
1	H	54	VAL
1	H	55	SER
1	H	79	SER
1	H	130	GLU
1	H	168	LYS
1	H	169	VAL
1	H	171	LYS
1	H	172	GLU
1	H	186	GLU
1	H	190	VAL
1	H	205	ILE
1	H	207	LYS
1	H	213	VAL
1	H	228	SER
1	H	230	ILE
1	H	253	ASP
1	H	254	VAL
1	H	290	GLN
1	H	295	LEU
1	H	301	ILE
1	H	321	LYS
1	H	323	VAL
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	453	GLN
1	H	484	GLU
1	H	504	LEU
1	H	520	MET
1	H	523	ASP

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Mol	Chain	Res	Type
1	I	4	LYS
1	I	31	LEU
1	I	37	ASN
1	I	50	THR
1	I	54	VAL
1	I	55	SER
1	I	79	SER
1	I	130	GLU
1	I	168	LYS
1	I	169	VAL
1	I	171	LYS
1	I	172	GLU
1	I	186	GLU
1	I	190	VAL
1	I	205	ILE
1	I	207	LYS
1	I	213	VAL
1	I	228	SER
1	I	230	ILE
1	I	253	ASP
1	I	254	VAL
1	I	290	GLN
1	I	295	LEU
1	I	301	ILE
1	I	321	LYS
1	I	323	VAL
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	453	GLN
1	I	484	GLU
1	I	504	LEU
1	I	520	MET
1	I	523	ASP
1	J	4	LYS
1	J	31	LEU
1	J	37	ASN
1	J	50	THR
1	J	54	VAL

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Mol	Chain	Res	Type
1	J	55	SER
1	J	79	SER
1	J	130	GLU
1	J	168	LYS
1	J	169	VAL
1	J	171	LYS
1	J	172	GLU
1	J	186	GLU
1	J	190	VAL
1	J	205	ILE
1	J	207	LYS
1	J	213	VAL
1	J	228	SER
1	J	230	ILE
1	J	253	ASP
1	J	254	VAL
1	J	290	GLN
1	J	295	LEU
1	J	301	ILE
1	J	321	LYS
1	J	323	VAL
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	453	GLN
1	J	484	GLU
1	J	504	LEU
1	J	520	MET
1	J	523	ASP
1	K	4	LYS
1	K	31	LEU
1	K	37	ASN
1	K	50	THR
1	K	54	VAL
1	K	55	SER
1	K	130	GLU
1	K	168	LYS
1	K	169	VAL
1	K	171	LYS

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Mol	Chain	Res	Type
1	K	172	GLU
1	K	186	GLU
1	K	190	VAL
1	K	205	ILE
1	K	207	LYS
1	K	213	VAL
1	K	228	SER
1	K	230	ILE
1	K	253	ASP
1	K	254	VAL
1	K	290	GLN
1	K	295	LEU
1	K	301	ILE
1	K	321	LYS
1	K	323	VAL
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	453	GLN
1	K	484	GLU
1	K	504	LEU
1	K	520	MET
1	K	523	ASP
1	L	4	LYS
1	L	31	LEU
1	L	37	ASN
1	L	50	THR
1	L	54	VAL
1	L	55	SER
1	L	79	SER
1	L	130	GLU
1	L	168	LYS
1	L	169	VAL
1	L	171	LYS
1	L	172	GLU
1	L	186	GLU
1	L	190	VAL
1	L	205	ILE
1	L	207	LYS

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Mol	Chain	Res	Type
1	L	213	VAL
1	L	228	SER
1	L	230	ILE
1	L	253	ASP
1	L	254	VAL
1	L	290	GLN
1	L	295	LEU
1	L	301	ILE
1	L	321	LYS
1	L	323	VAL
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	453	GLN
1	L	484	GLU
1	L	504	LEU
1	L	520	MET
1	L	523	ASP
1	M	4	LYS
1	M	31	LEU
1	M	37	ASN
1	M	50	THR
1	M	54	VAL
1	M	55	SER
1	M	79	SER
1	M	91	THR
1	M	130	GLU
1	M	168	LYS
1	M	169	VAL
1	M	171	LYS
1	M	172	GLU
1	M	186	GLU
1	M	190	VAL
1	M	205	ILE
1	M	207	LYS
1	M	213	VAL
1	M	228	SER
1	M	230	ILE
1	M	253	ASP

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Mol	Chain	Res	Type
1	M	254	VAL
1	M	290	GLN
1	M	295	LEU
1	M	301	ILE
1	M	321	LYS
1	M	323	VAL
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	484	GLU
1	M	504	LEU
1	M	520	MET
1	M	523	ASP
1	N	4	LYS
1	N	31	LEU
1	N	37	ASN
1	N	50	THR
1	N	55	SER
1	N	79	SER
1	N	130	GLU
1	N	168	LYS
1	N	169	VAL
1	N	171	LYS
1	N	172	GLU
1	N	186	GLU
1	N	190	VAL
1	N	205	ILE
1	N	207	LYS
1	N	213	VAL
1	N	228	SER
1	N	230	ILE
1	N	253	ASP
1	N	254	VAL
1	N	290	GLN
1	N	295	LEU
1	N	301	ILE
1	N	321	LYS
1	N	323	VAL
1	N	327	LYS

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Mol	Chain	Res	Type
1	N	328	ASP
1	N	334	ASP
1	N	350	ARG
1	N	358	SER
1	N	421	ARG
1	N	453	GLN
1	N	479	ASN
1	N	484	GLU
1	N	504	LEU
1	N	520	MET
1	N	523	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	GLN
1	A	453	GLN
1	A	475	ASN
1	B	319	GLN
1	B	453	GLN
1	B	475	ASN
1	C	319	GLN
1	C	453	GLN
1	C	475	ASN
1	D	319	GLN
1	D	453	GLN
1	D	475	ASN
1	E	319	GLN
1	E	453	GLN
1	E	475	ASN
1	F	319	GLN
1	F	453	GLN
1	F	475	ASN
1	G	319	GLN
1	G	453	GLN
1	G	475	ASN
1	H	453	GLN
1	I	453	GLN
1	J	453	GLN
1	K	453	GLN
1	L	453	GLN
1	M	453	GLN

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Mol	Chain	Res	Type
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 14 are monoatomic and 14 are modelled with single atom - 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	E	1528	2	32,33,33	1.59	2 (6%)	48,52,52	1.00	4 (8%)
4	ATP	B	1528	2	32,33,33	1.60	2 (6%)	48,52,52	1.00	4 (8%)
4	ATP	A	1528	2	32,33,33	1.60	2 (6%)	48,52,52	1.00	4 (8%)
4	ATP	G	1528	2	32,33,33	1.59	2 (6%)	48,52,52	1.00	4 (8%)
4	ATP	M	1527	2	32,33,33	11.74	8 (25%)	48,52,52	2.17	17 (35%)
4	ATP	N	1527	2	32,33,33	1.62	1 (3%)	48,52,52	1.08	5 (10%)
4	ATP	I	1527	2	32,33,33	1.54	2 (6%)	48,52,52	0.92	3 (6%)
4	ATP	C	1528	2	32,33,33	1.58	2 (6%)	48,52,52	1.00	4 (8%)
4	ATP	H	1527	2	32,33,33	1.60	1 (3%)	48,52,52	1.04	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	F	1528	2	32,33,33	1.60	2 (6%)	48,52,52	1.00	4 (8%)
4	ATP	K	1527	2	32,33,33	1.56	1 (3%)	48,52,52	1.11	5 (10%)
4	ATP	D	1528	2	32,33,33	1.58	2 (6%)	48,52,52	1.00	4 (8%)
4	ATP	J	1527	2	32,33,33	1.55	2 (6%)	48,52,52	0.94	3 (6%)
4	ATP	L	1527	2	32,33,33	1.56	2 (6%)	48,52,52	0.92	3 (6%)

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	E	1528	2	-	1/22/38/38	0/3/3/3
4	ATP	B	1528	2	-	1/22/38/38	0/3/3/3
4	ATP	A	1528	2	-	1/22/38/38	0/3/3/3
4	ATP	G	1528	2	-	1/22/38/38	0/3/3/3
4	ATP	M	1527	2	-	5/22/38/38	0/3/3/3
4	ATP	N	1527	2	-	0/22/38/38	0/3/3/3
4	ATP	I	1527	2	-	1/22/38/38	0/3/3/3
4	ATP	C	1528	2	-	1/22/38/38	0/3/3/3
4	ATP	H	1527	2	-	1/22/38/38	0/3/3/3
4	ATP	F	1528	2	-	1/22/38/38	0/3/3/3
4	ATP	K	1527	2	-	2/22/38/38	0/3/3/3
4	ATP	D	1528	2	-	1/22/38/38	0/3/3/3
4	ATP	J	1527	2	-	1/22/38/38	0/3/3/3
4	ATP	L	1527	2	-	1/22/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1527	ATP	C8-N9	33.20	1.94	1.37
4	M	1527	ATP	C4-N9	30.96	2.02	1.37
4	M	1527	ATP	C5-C4	30.21	1.93	1.39
4	M	1527	ATP	C5-N7	29.60	1.93	1.39
4	M	1527	ATP	C8-N7	21.37	1.72	1.31
4	M	1527	ATP	PA-O3A	-8.04	1.50	1.59
4	N	1527	ATP	PA-O3A	-7.94	1.50	1.59
4	K	1527	ATP	PA-O3A	-7.94	1.50	1.59
4	A	1528	ATP	PA-O3A	-7.93	1.50	1.59
4	H	1527	ATP	PA-O3A	-7.92	1.51	1.59
4	F	1528	ATP	PA-O3A	-7.88	1.51	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1528	ATP	PA-O3A	-7.87	1.51	1.59
4	E	1528	ATP	PA-O3A	-7.87	1.51	1.59
4	G	1528	ATP	PA-O3A	-7.86	1.51	1.59
4	L	1527	ATP	PA-O3A	-7.86	1.51	1.59
4	D	1528	ATP	PA-O3A	-7.82	1.51	1.59
4	J	1527	ATP	PA-O3A	-7.80	1.51	1.59
4	C	1528	ATP	PA-O3A	-7.80	1.51	1.59
4	I	1527	ATP	PA-O3A	-7.80	1.51	1.59
4	M	1527	ATP	PB-O3B	2.88	1.62	1.59
4	B	1528	ATP	PB-O3B	2.48	1.62	1.59
4	F	1528	ATP	PB-O3B	2.44	1.62	1.59
4	C	1528	ATP	PB-O3B	2.42	1.62	1.59
4	D	1528	ATP	PB-O3B	2.41	1.62	1.59
4	G	1528	ATP	PB-O3B	2.41	1.62	1.59
4	E	1528	ATP	PB-O3B	2.39	1.62	1.59
4	A	1528	ATP	PB-O3B	2.38	1.62	1.59
4	M	1527	ATP	C5'-C4'	2.26	1.58	1.51
4	L	1527	ATP	PB-O3B	2.22	1.61	1.59
4	J	1527	ATP	PB-O3B	2.17	1.61	1.59
4	I	1527	ATP	PB-O3B	2.10	1.61	1.59

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1527	ATP	N3-C2-N1	5.53	136.95	128.58
4	M	1527	ATP	C5-C4-N3	-5.36	119.33	126.72
4	M	1527	ATP	N3-C4-N9	4.75	135.25	127.17
4	M	1527	ATP	C4-N9-C1'	3.91	135.77	126.63
4	M	1527	ATP	C2-N1-C6	3.90	125.13	118.73
4	M	1527	ATP	O3G-PG-O2G	-3.81	93.53	107.80
4	M	1527	ATP	C4-N9-C8	-3.41	102.16	105.74
4	K	1527	ATP	O2A-PA-O3A	3.14	115.75	107.27
4	N	1527	ATP	O2A-PA-O3A	3.06	115.55	107.27
4	M	1527	ATP	C1'-N9-C8	-3.00	120.43	127.09
4	H	1527	ATP	O2A-PA-O3A	2.93	115.20	107.27
4	M	1527	ATP	O3B-PB-O1B	-2.91	101.96	110.70
4	J	1527	ATP	O2A-PA-O3A	2.78	114.80	107.27
4	F	1528	ATP	O2A-PA-O3A	2.76	114.72	107.27
4	E	1528	ATP	O2A-PA-O3A	2.75	114.72	107.27
4	G	1528	ATP	O2A-PA-O3A	2.75	114.71	107.27
4	A	1528	ATP	O2A-PA-O3A	2.75	114.70	107.27
4	D	1528	ATP	O2A-PA-O3A	2.74	114.69	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1528	ATP	O2A-PA-O3A	2.74	114.67	107.27
4	B	1528	ATP	O2A-PA-O3A	2.73	114.65	107.27
4	I	1527	ATP	O2A-PA-O3A	2.72	114.63	107.27
4	L	1527	ATP	O2A-PA-O3A	2.71	114.59	107.27
4	N	1527	ATP	O3B-PG-O1G	-2.68	96.95	111.04
4	M	1527	ATP	O2A-PA-O3A	2.61	114.34	107.27
4	H	1527	ATP	O3B-PG-O1G	-2.60	97.34	111.04
4	M	1527	ATP	C6-C5-C4	-2.60	113.63	117.18
4	K	1527	ATP	O3B-PG-O1G	-2.57	97.53	111.04
4	K	1527	ATP	C2'-C1'-N9	2.53	119.58	113.30
4	M	1527	ATP	C6-C5-N7	2.50	136.91	132.09
4	L	1527	ATP	O3B-PG-O1G	-2.49	97.94	111.04
4	I	1527	ATP	O3B-PG-O1G	-2.49	97.94	111.04
4	J	1527	ATP	O3B-PG-O1G	-2.48	97.97	111.04
4	D	1528	ATP	O3B-PG-O1G	-2.43	98.27	111.04
4	C	1528	ATP	O3B-PG-O1G	-2.42	98.28	111.04
4	A	1528	ATP	O3B-PG-O1G	-2.42	98.30	111.04
4	B	1528	ATP	O3B-PG-O1G	-2.42	98.30	111.04
4	E	1528	ATP	O3B-PG-O1G	-2.42	98.32	111.04
4	F	1528	ATP	O3B-PG-O1G	-2.42	98.33	111.04
4	G	1528	ATP	O3B-PG-O1G	-2.41	98.36	111.04
4	I	1527	ATP	O3G-PG-O2G	2.40	116.81	107.80
4	L	1527	ATP	O3G-PG-O2G	2.40	116.79	107.80
4	J	1527	ATP	O3G-PG-O2G	2.39	116.76	107.80
4	M	1527	ATP	O3G-PG-O1G	2.31	119.83	110.83
4	M	1527	ATP	O3A-PB-O1B	2.31	117.64	110.70
4	K	1527	ATP	O3G-PG-O2G	2.30	116.43	107.80
4	H	1527	ATP	O4'-C1'-N9	2.29	112.49	108.09
4	N	1527	ATP	O4'-C1'-N9	2.28	112.47	108.09
4	H	1527	ATP	O3G-PG-O2G	2.28	116.34	107.80
4	K	1527	ATP	O4'-C1'-N9	2.28	112.46	108.09
4	M	1527	ATP	C5-N7-C8	2.24	106.97	103.45
4	C	1528	ATP	O3G-PG-O2G	2.22	116.12	107.80
4	M	1527	ATP	O2G-PG-O3B	2.22	112.07	104.64
4	B	1528	ATP	O3G-PG-O2G	2.22	116.11	107.80
4	E	1528	ATP	O3G-PG-O2G	2.22	116.11	107.80
4	N	1527	ATP	O3G-PG-O2G	2.21	116.09	107.80
4	F	1528	ATP	O3G-PG-O2G	2.21	116.07	107.80
4	D	1528	ATP	O3G-PG-O2G	2.20	116.05	107.80
4	A	1528	ATP	O3G-PG-O2G	2.20	116.04	107.80
4	G	1528	ATP	O3G-PG-O2G	2.20	116.03	107.80
4	N	1527	ATP	O3'-C3'-C4'	2.10	117.11	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1528	ATP	O4'-C1'-N9	2.07	112.06	108.09
4	A	1528	ATP	O4'-C1'-N9	2.06	112.05	108.09
4	G	1528	ATP	O4'-C1'-N9	2.05	112.03	108.09
4	B	1528	ATP	O4'-C1'-N9	2.05	112.03	108.09
4	F	1528	ATP	O4'-C1'-N9	2.05	112.02	108.09
4	C	1528	ATP	O4'-C1'-N9	2.03	111.98	108.09
4	E	1528	ATP	O4'-C1'-N9	2.02	111.97	108.09
4	M	1527	ATP	C2'-C1'-N9	2.01	118.31	113.30

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1527	ATP	C5'-O5'-PA-O1A
4	M	1527	ATP	C5'-O5'-PA-O2A
4	M	1527	ATP	C5'-O5'-PA-O3A
4	M	1527	ATP	O4'-C4'-C5'-O5'
4	M	1527	ATP	C3'-C4'-C5'-O5'
4	K	1527	ATP	PB-O3A-PA-O1A
4	K	1527	ATP	PB-O3A-PA-O2A
4	A	1528	ATP	PG-O3B-PB-O2B
4	B	1528	ATP	PG-O3B-PB-O2B
4	C	1528	ATP	PG-O3B-PB-O2B
4	D	1528	ATP	PG-O3B-PB-O2B
4	E	1528	ATP	PG-O3B-PB-O2B
4	F	1528	ATP	PG-O3B-PB-O2B
4	G	1528	ATP	PG-O3B-PB-O2B
4	H	1527	ATP	PG-O3B-PB-O2B
4	I	1527	ATP	PG-O3B-PB-O2B
4	J	1527	ATP	PG-O3B-PB-O2B
4	L	1527	ATP	PG-O3B-PB-O2B

There are no ring outliers.

14 monomers are involved in 89 short contacts:

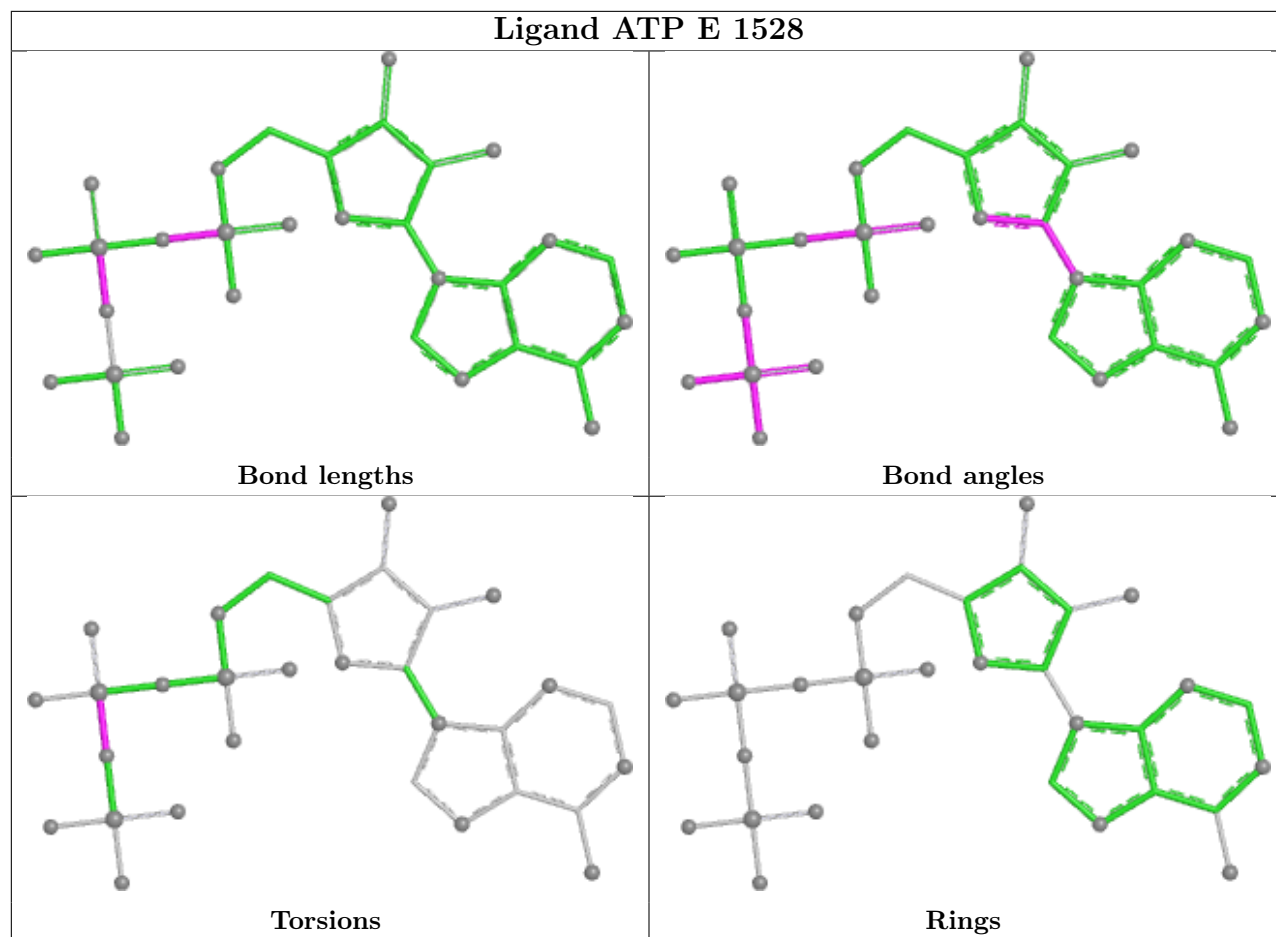
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1528	ATP	3	0
4	B	1528	ATP	4	0
4	A	1528	ATP	4	0
4	G	1528	ATP	3	0
4	M	1527	ATP	34	0

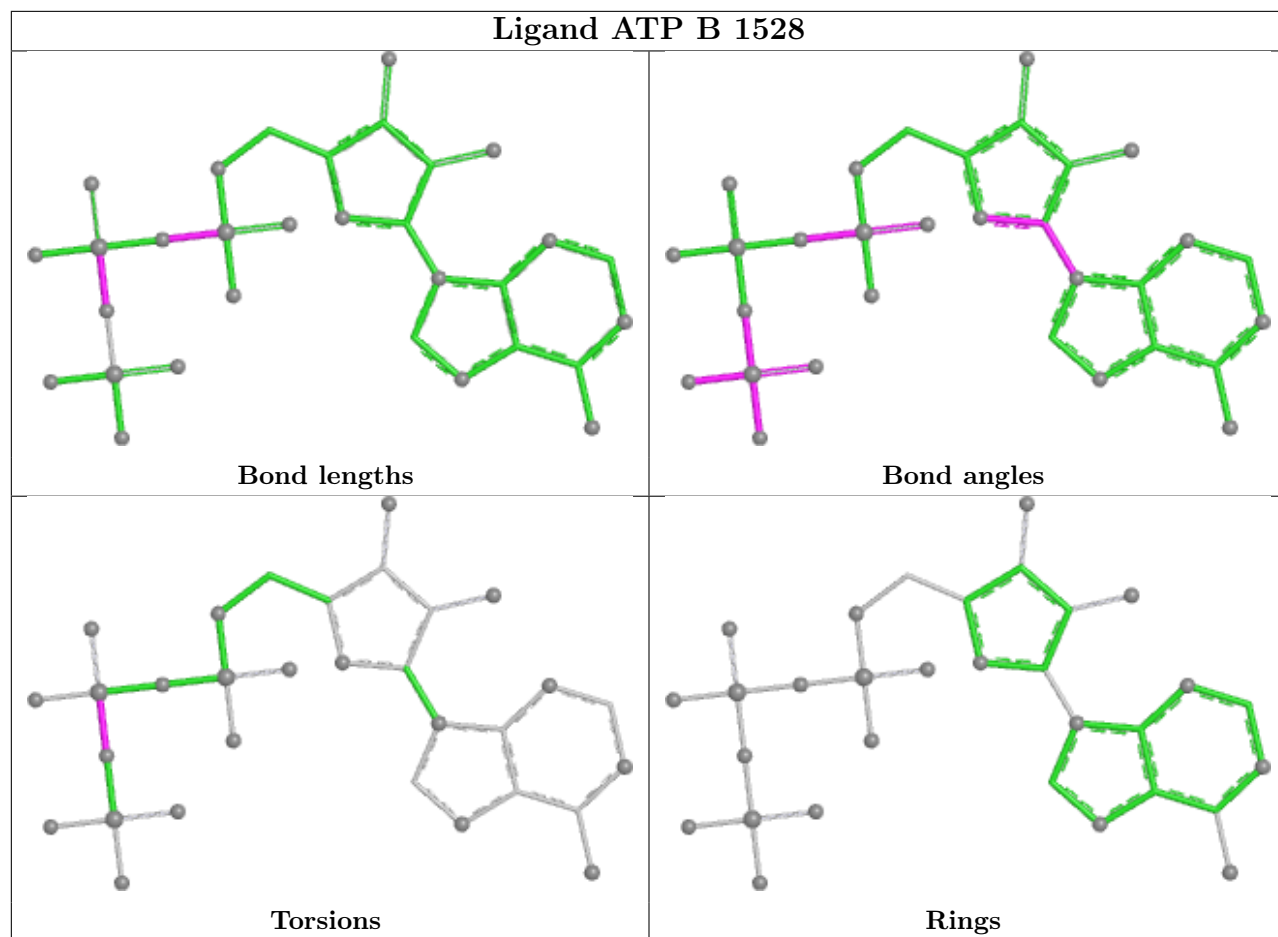
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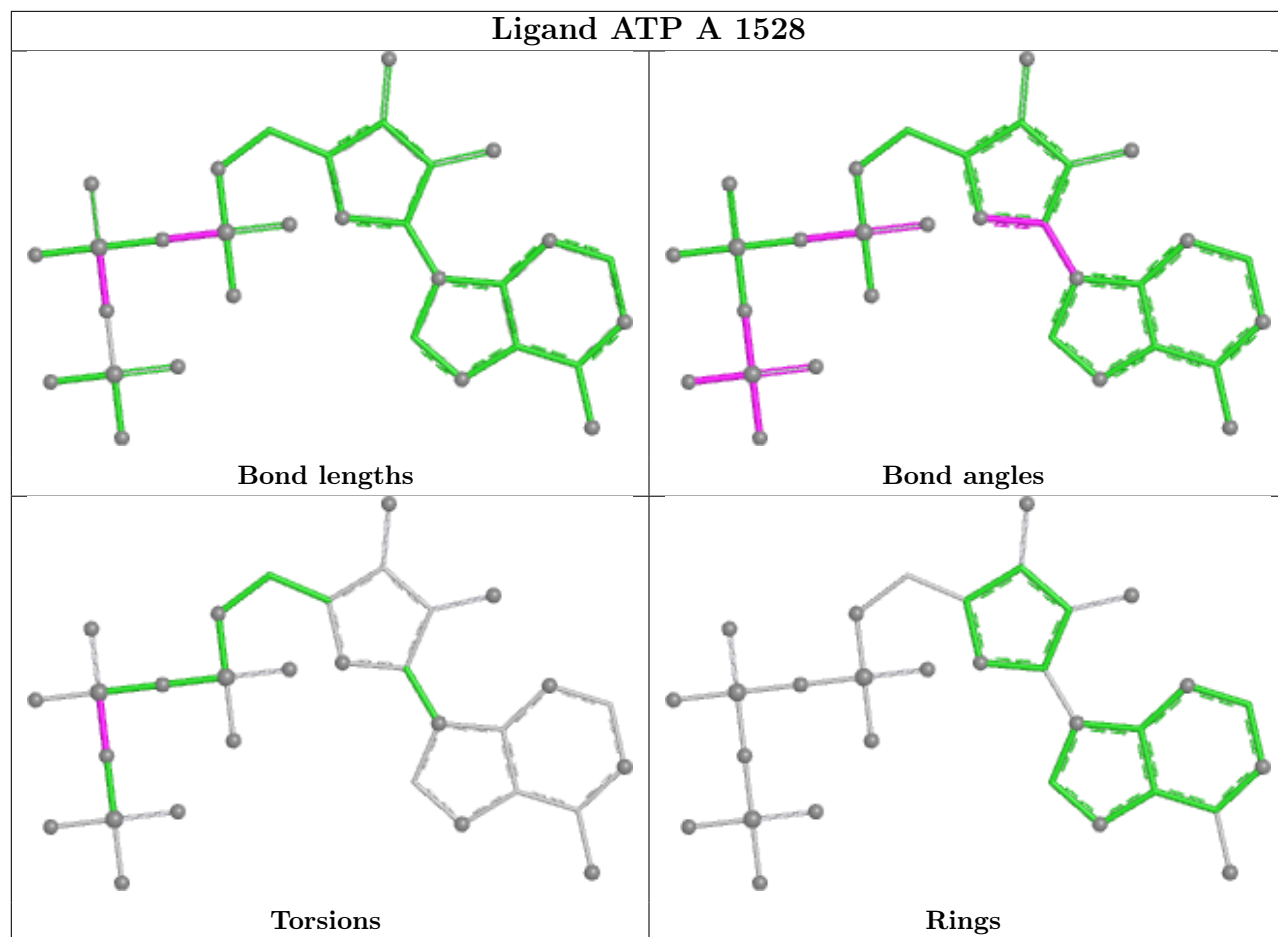
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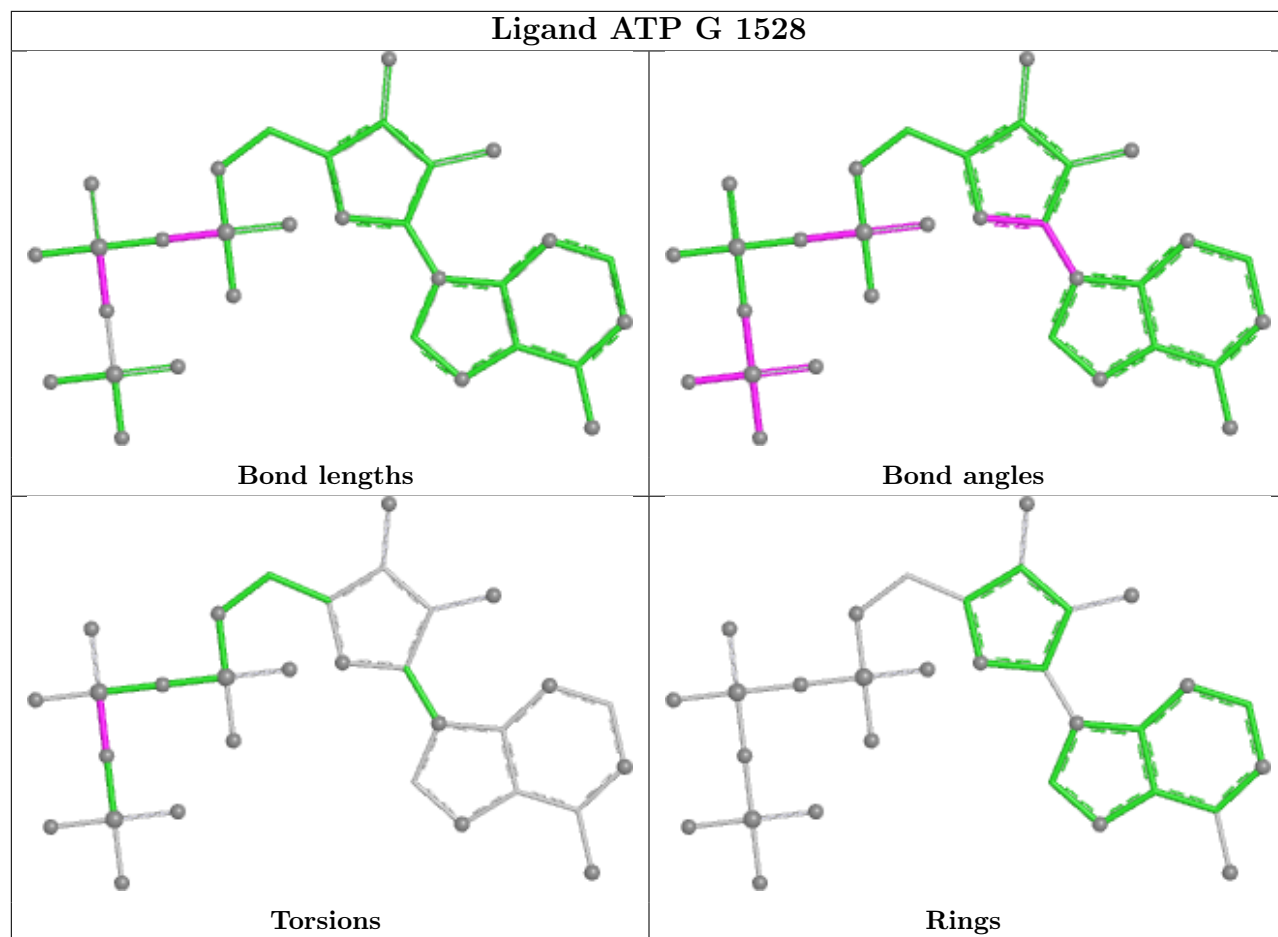
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1527	ATP	5	0
4	I	1527	ATP	5	0
4	C	1528	ATP	4	0
4	H	1527	ATP	4	0
4	F	1528	ATP	4	0
4	K	1527	ATP	5	0
4	D	1528	ATP	4	0
4	J	1527	ATP	5	0
4	L	1527	ATP	5	0

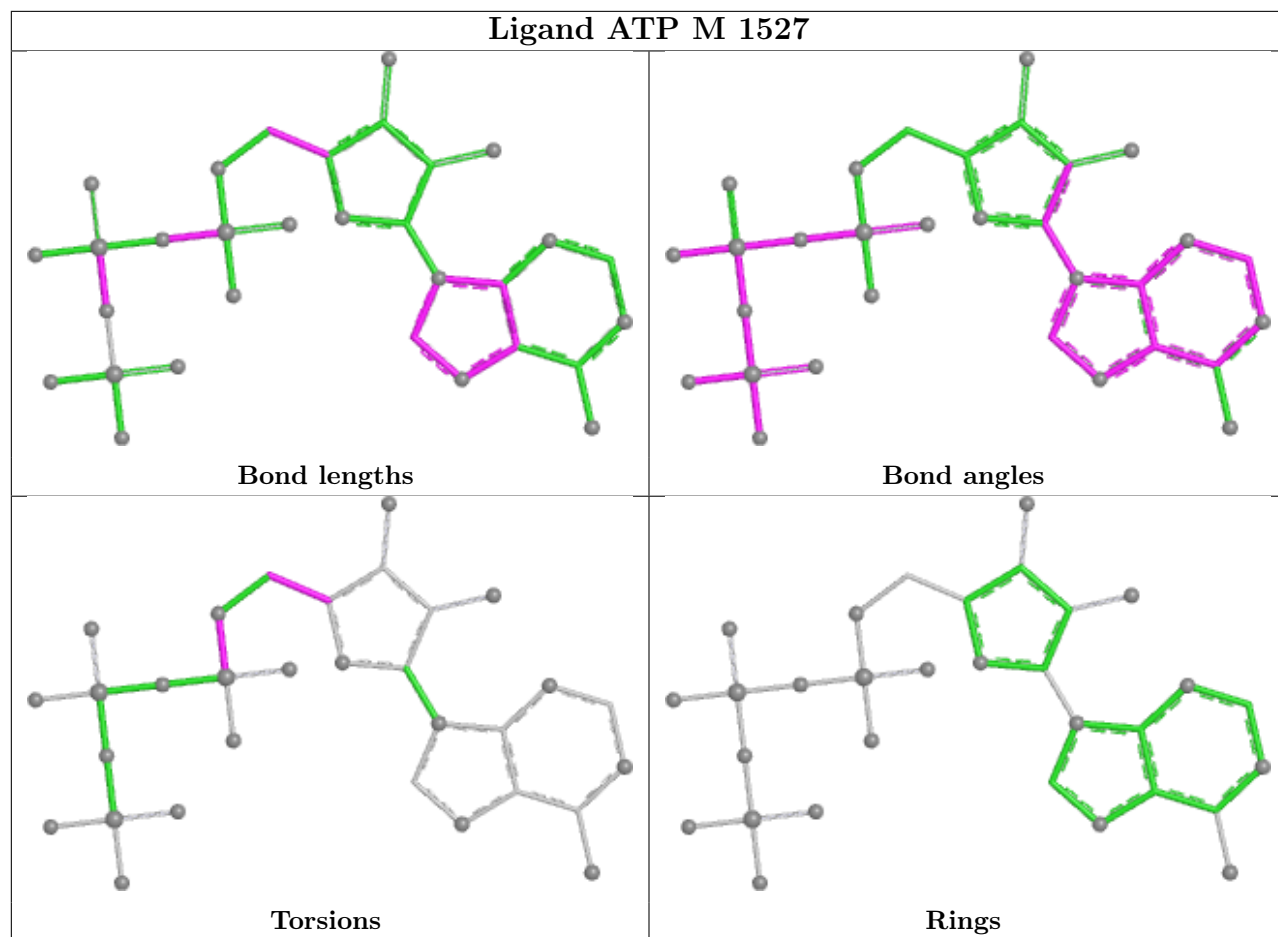
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

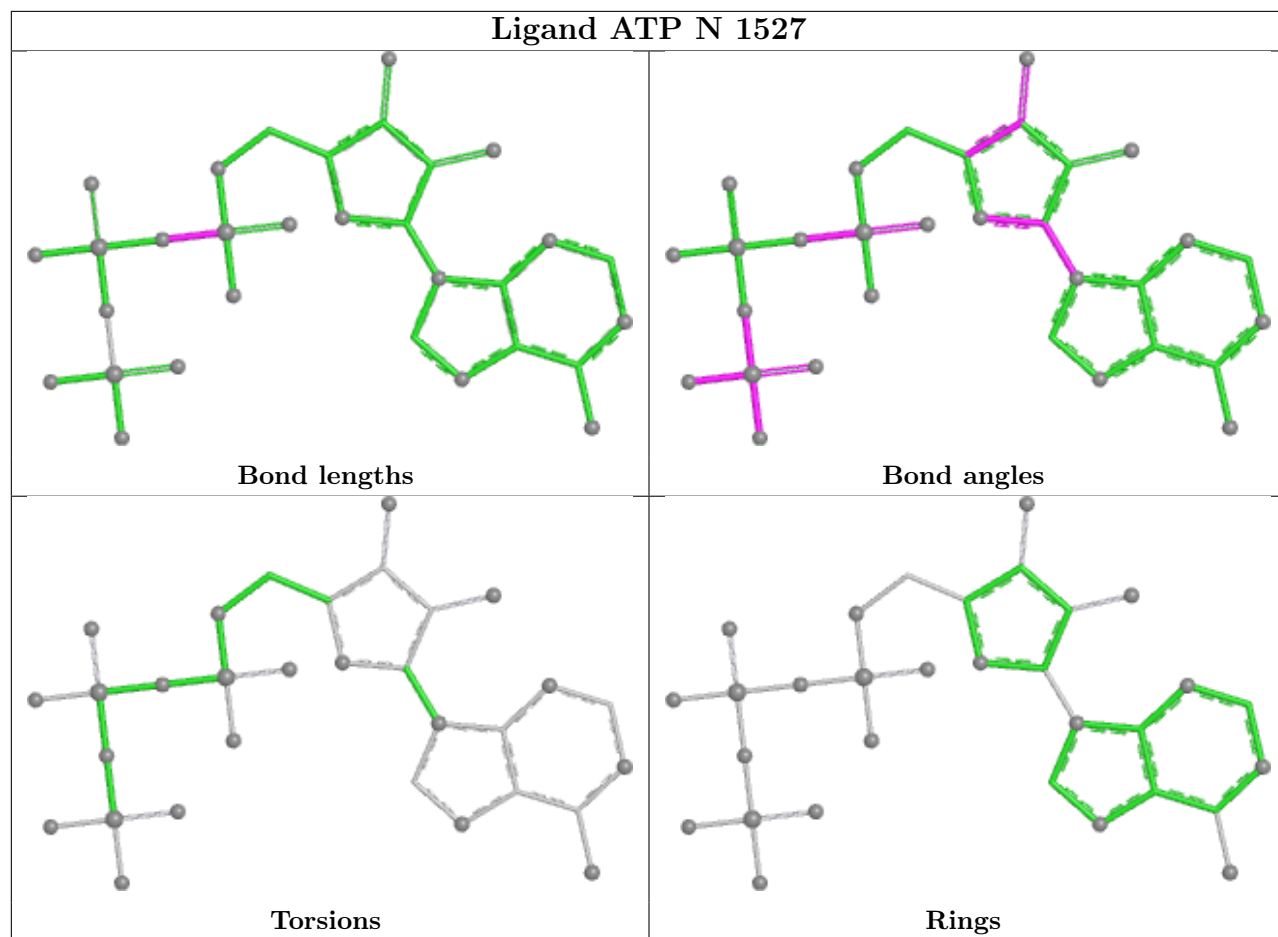


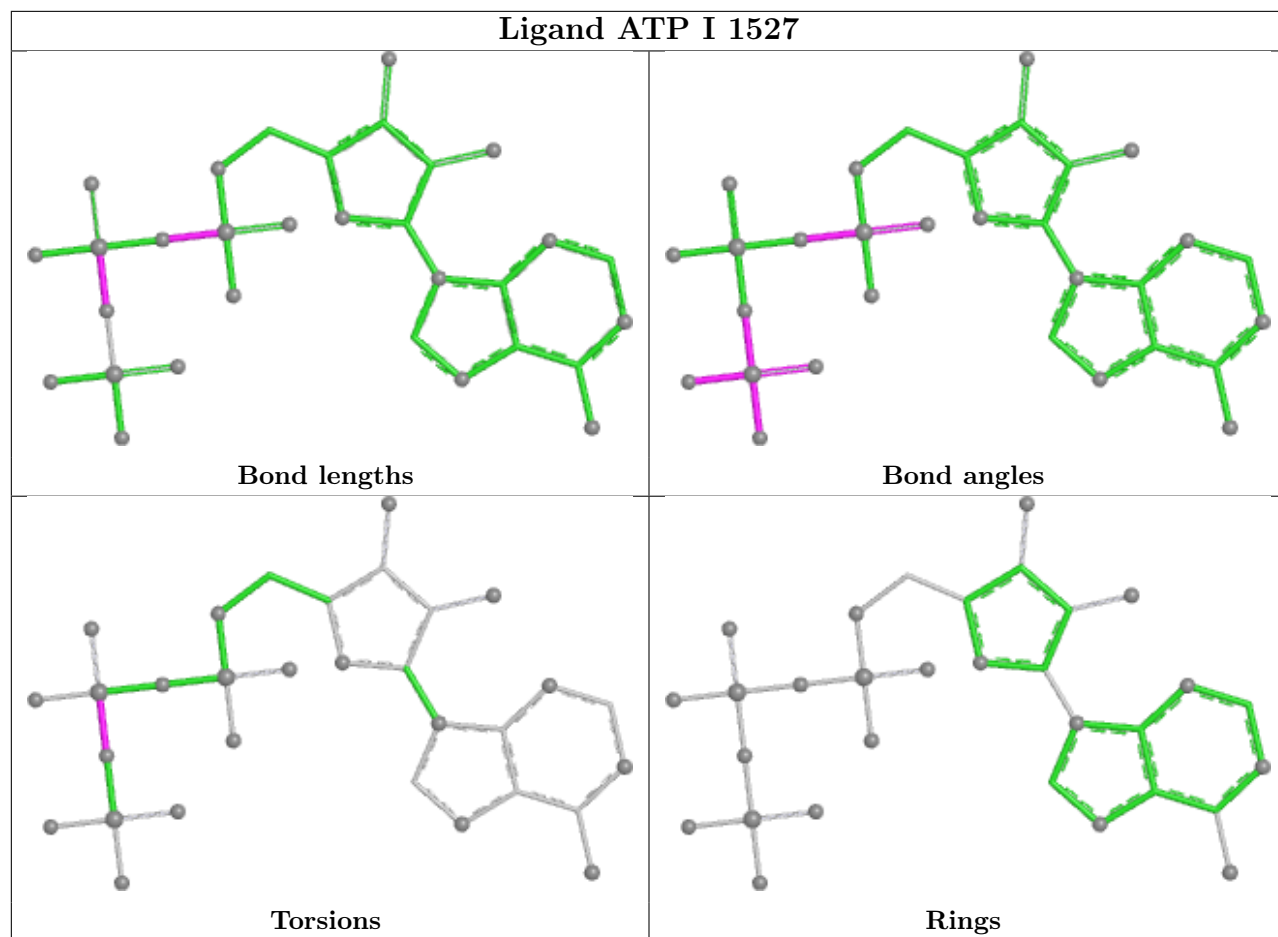


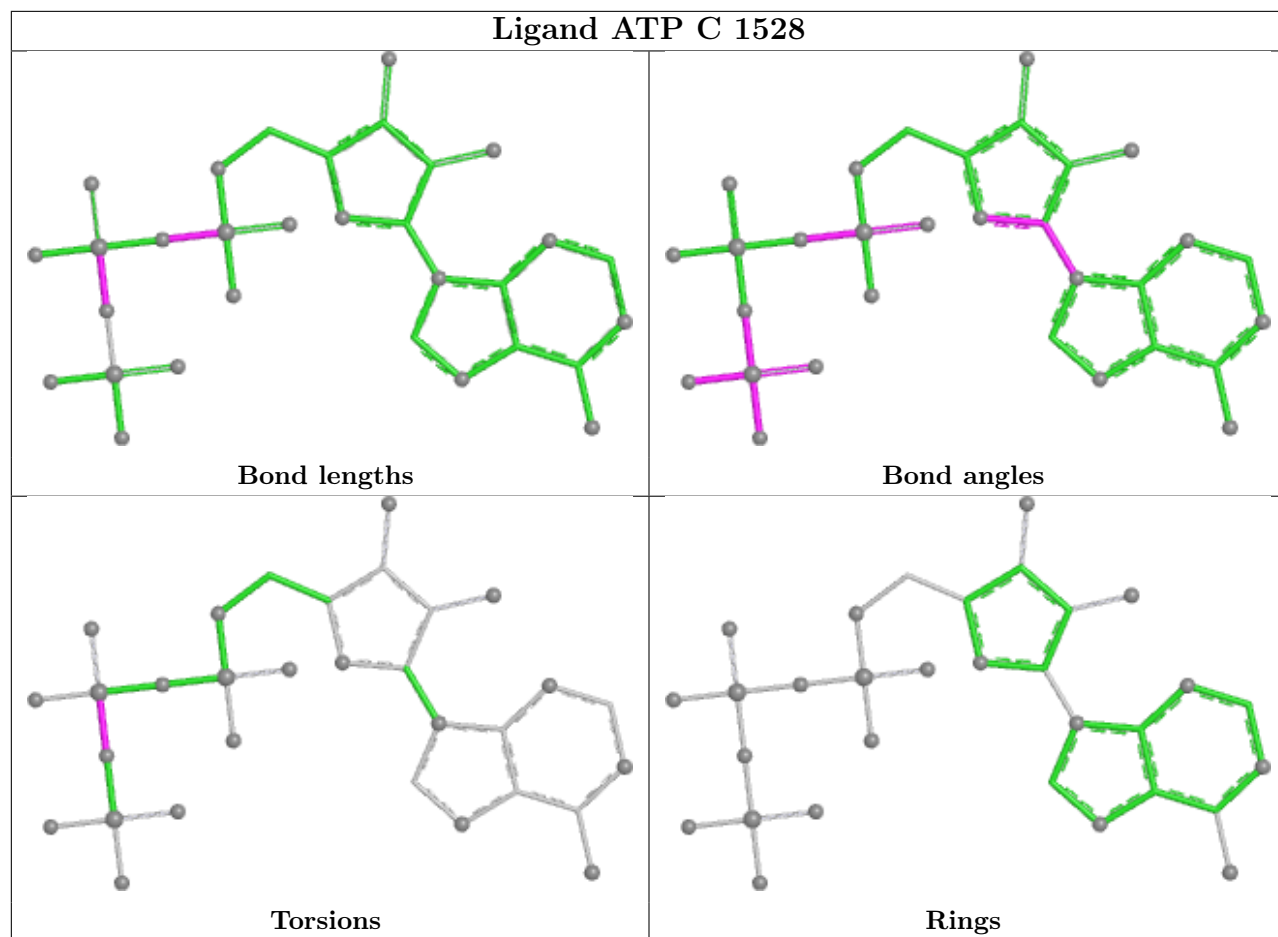


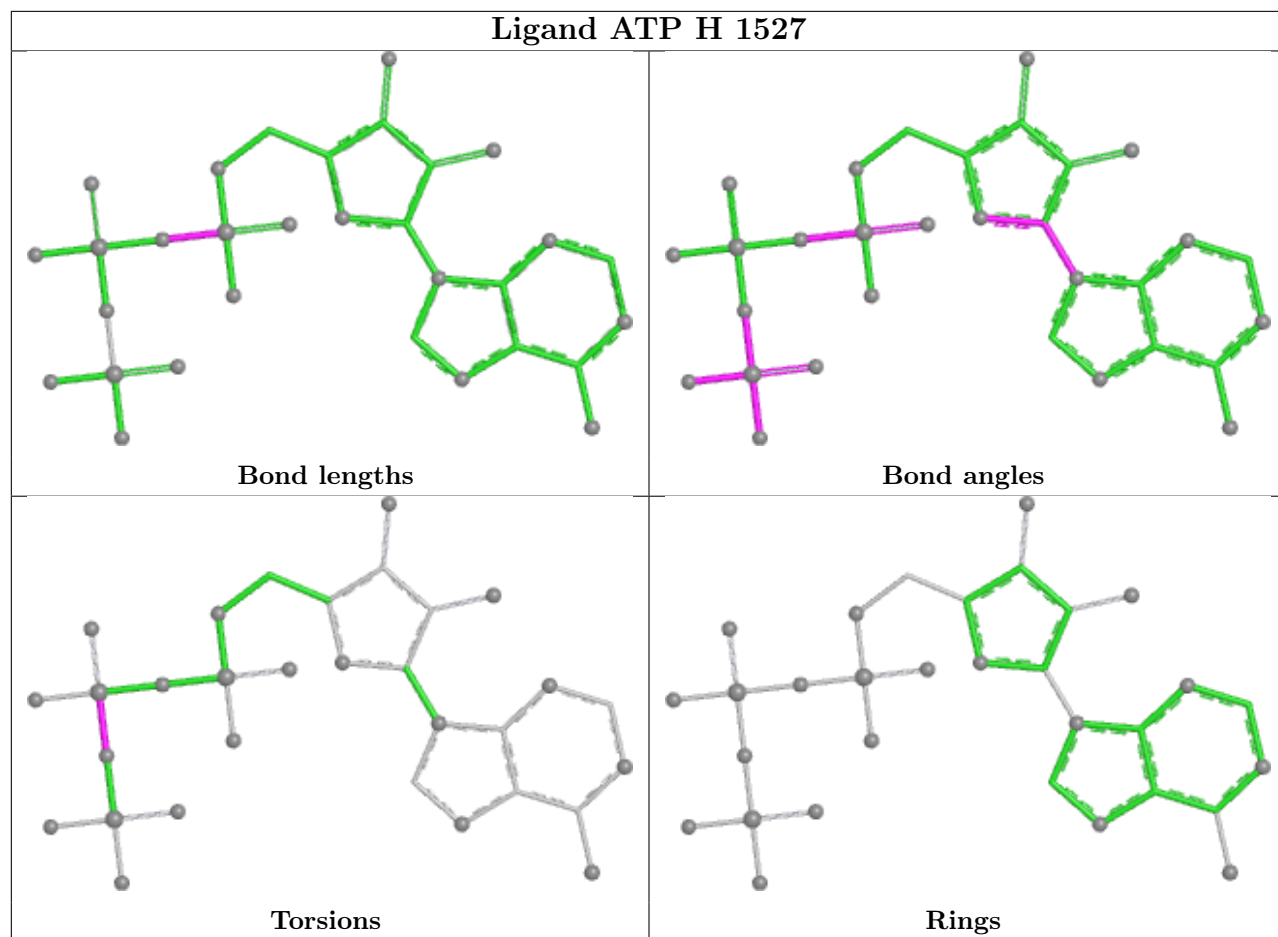


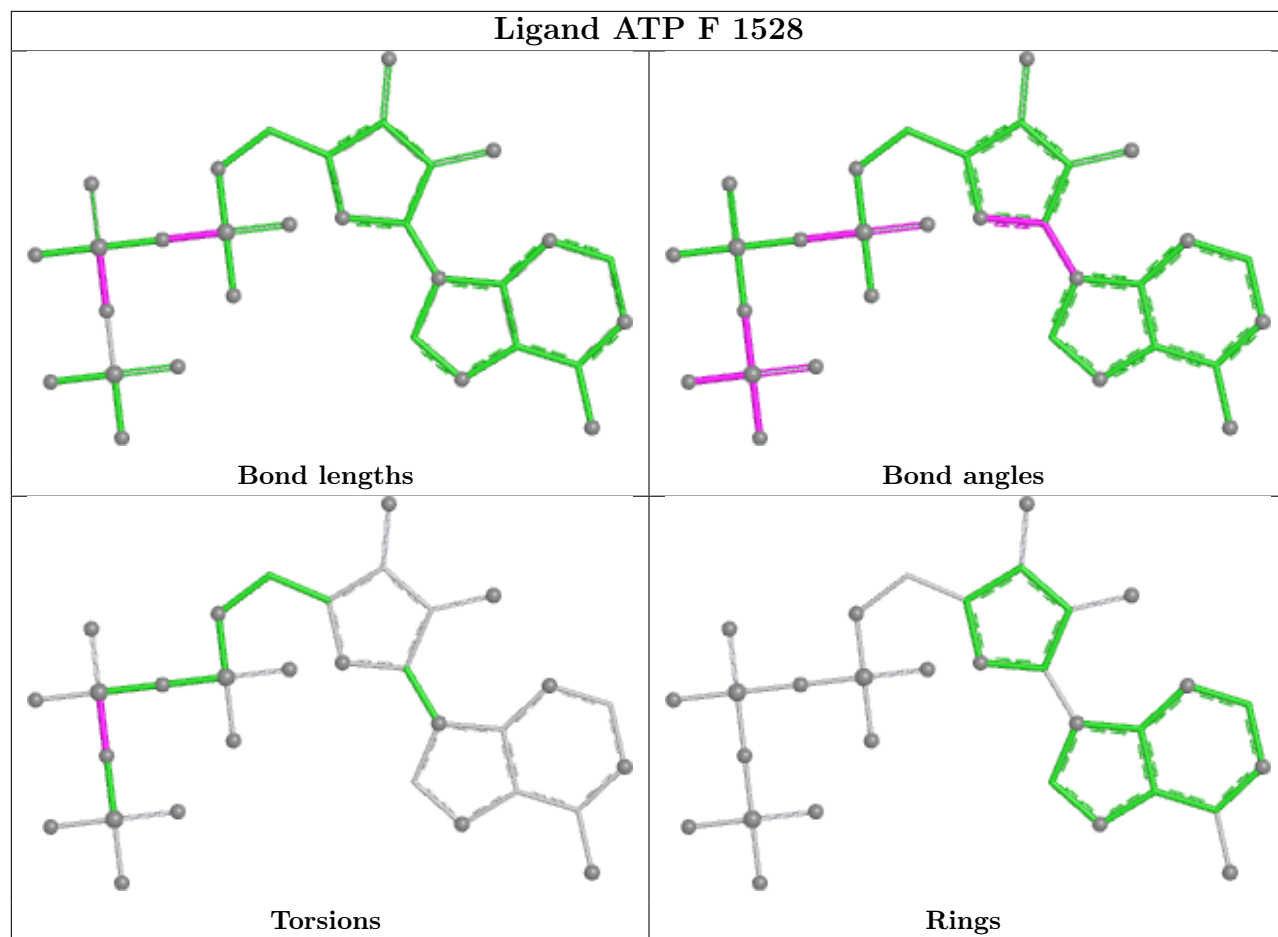


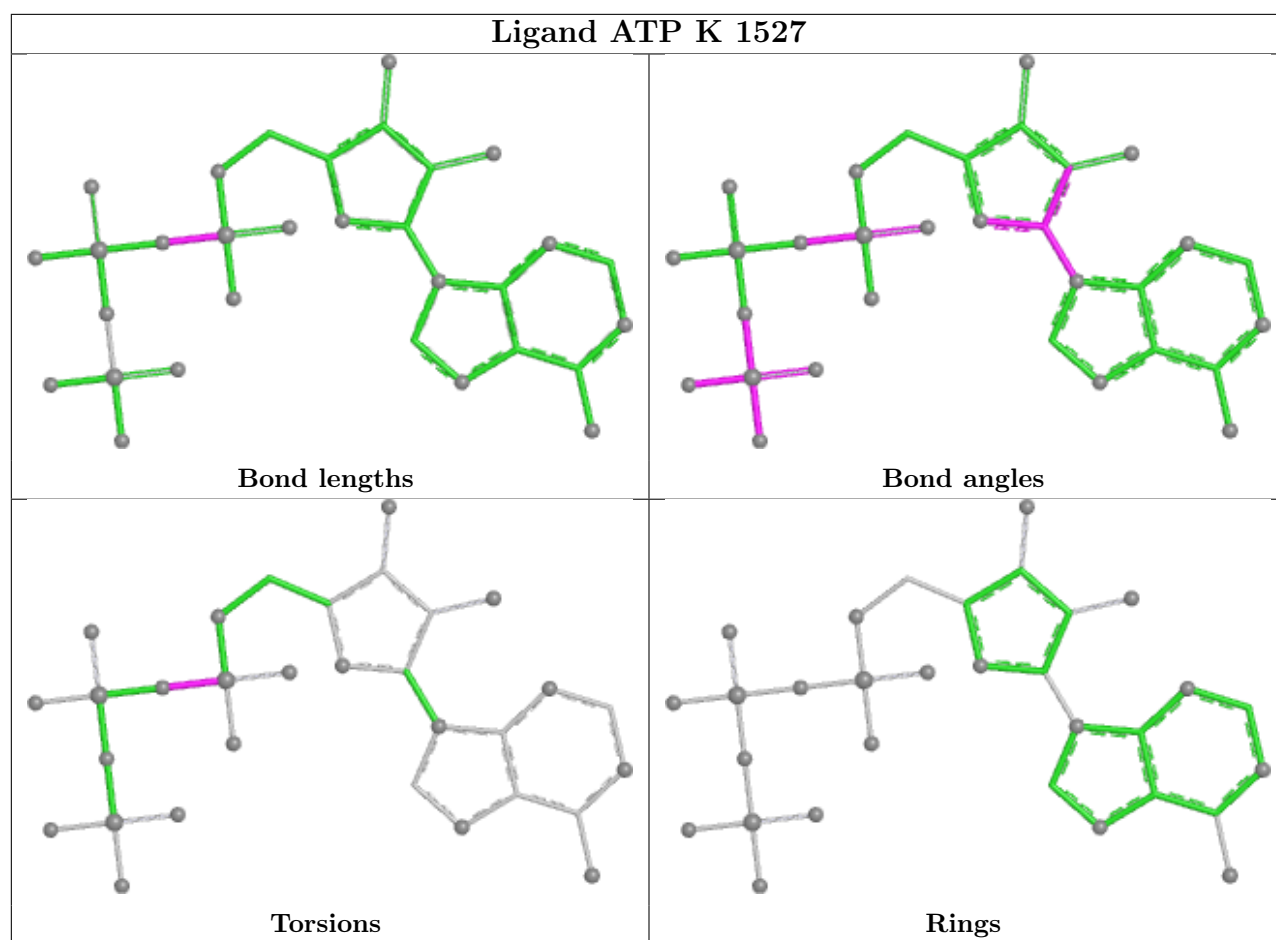


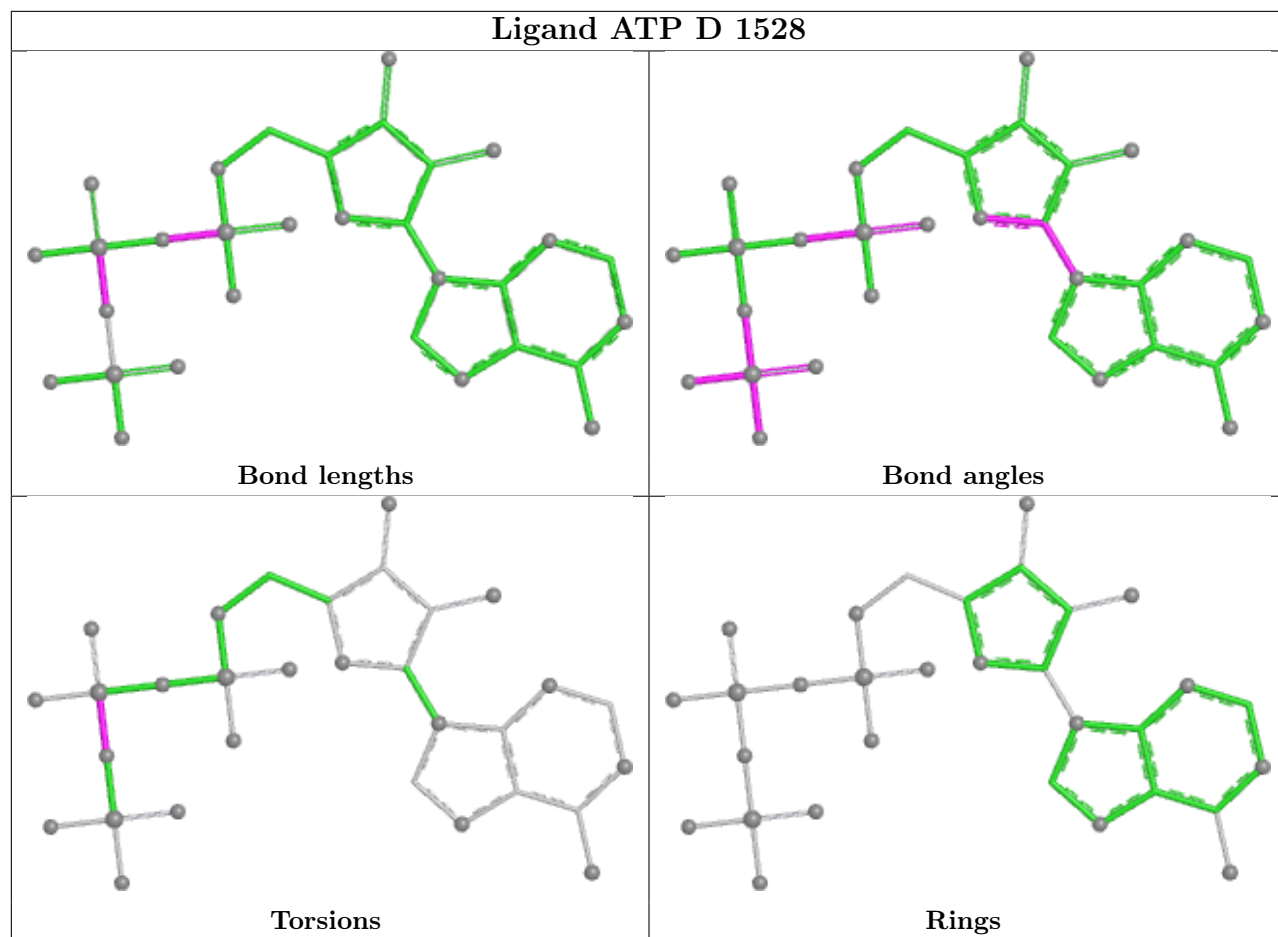


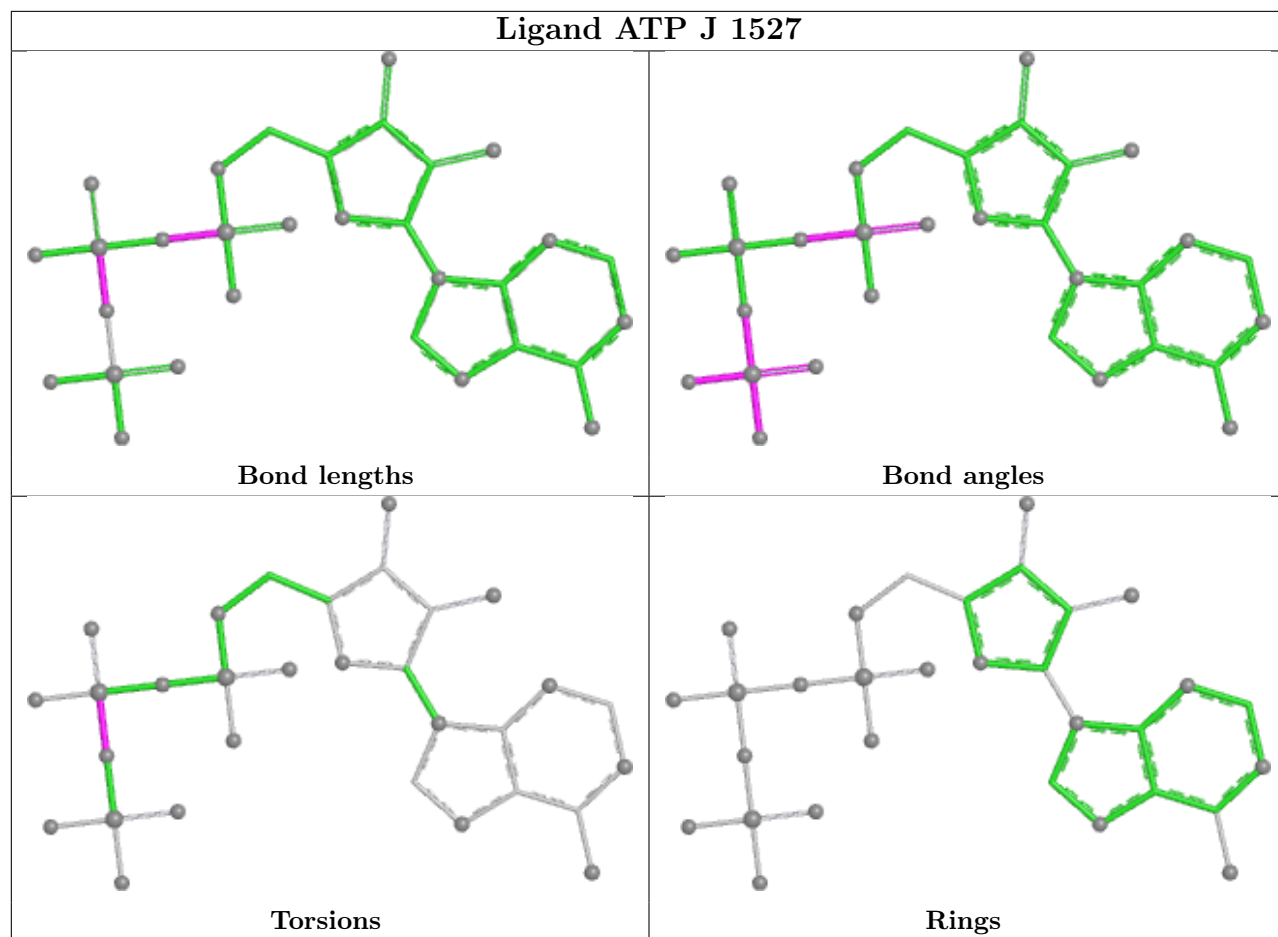


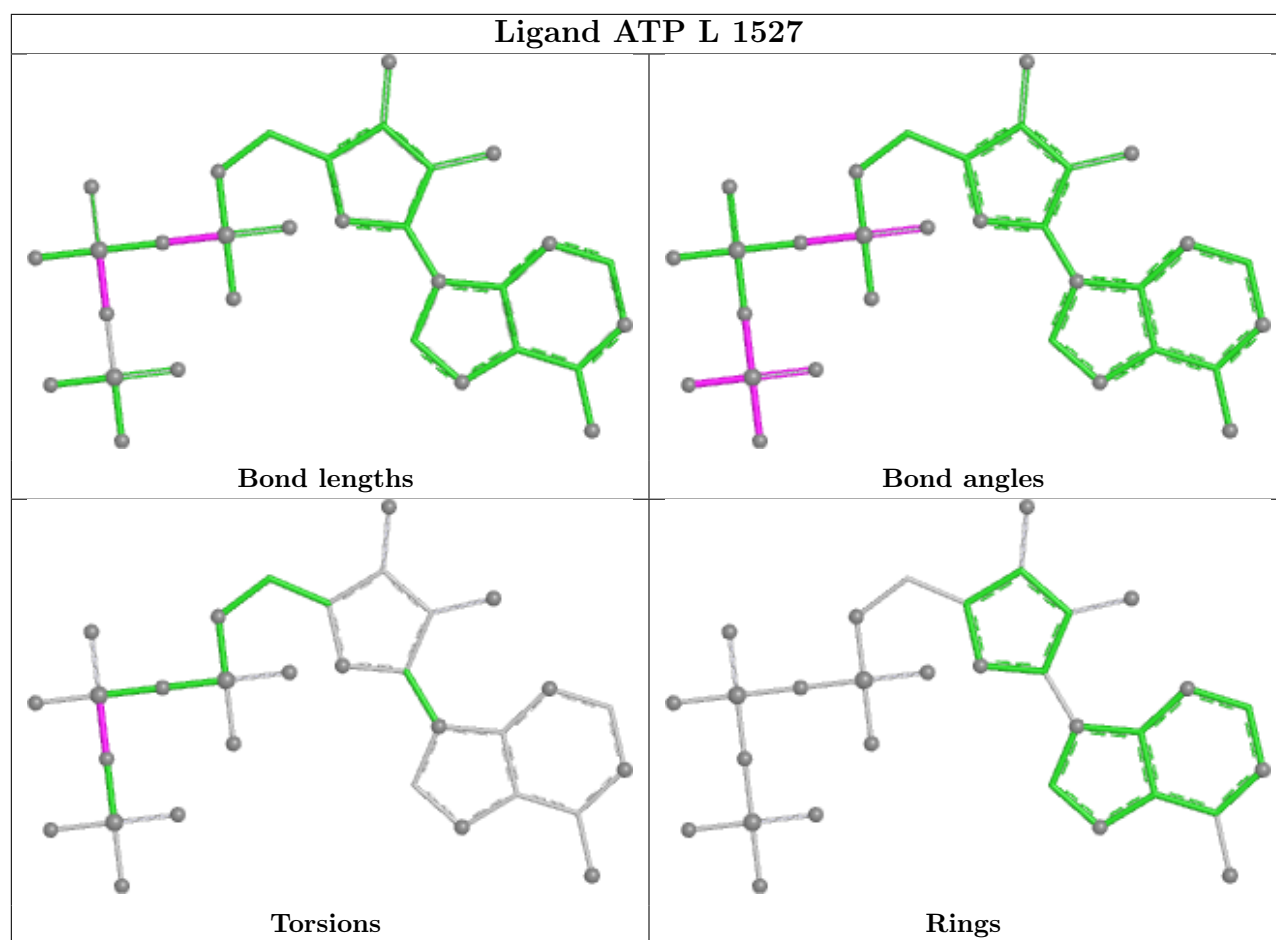












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	2
1	I	2
1	L	2
1	N	2
1	J	2
1	K	2
1	M	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	50:THR	C	51:LYS	N	4.25
1	I	50:THR	C	51:LYS	N	4.25
1	L	50:THR	C	51:LYS	N	4.25
1	N	50:THR	C	51:LYS	N	4.25
1	J	50:THR	C	51:LYS	N	4.24
1	K	50:THR	C	51:LYS	N	4.24
1	M	50:THR	C	51:LYS	N	4.24
1	H	37:ASN	C	38:VAL	N	3.11
1	I	37:ASN	C	38:VAL	N	3.11
1	J	37:ASN	C	38:VAL	N	3.11
1	K	37:ASN	C	38:VAL	N	3.11
1	L	37:ASN	C	38:VAL	N	3.11
1	M	37:ASN	C	38:VAL	N	3.11
1	N	37:ASN	C	38:VAL	N	3.11

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2001. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 96



Y Index: 96



Z Index: 96

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 73



Y Index: 79

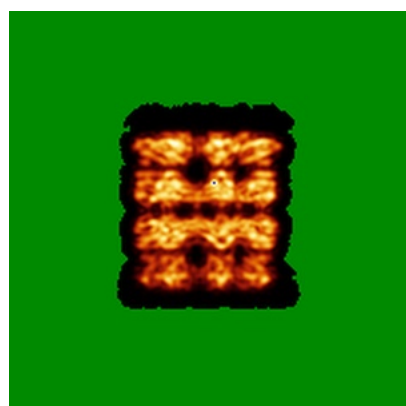


Z Index: 128

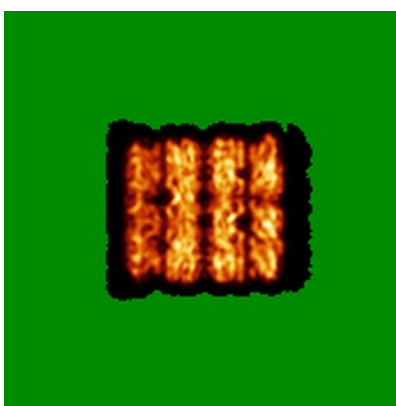
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

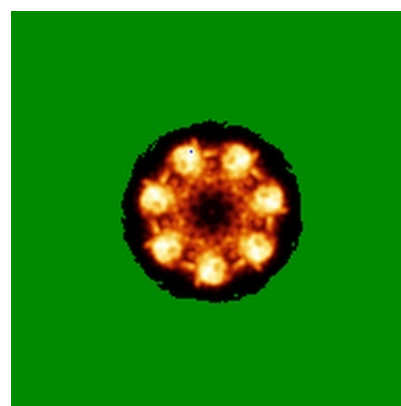
6.4.1 Primary map



X



Y

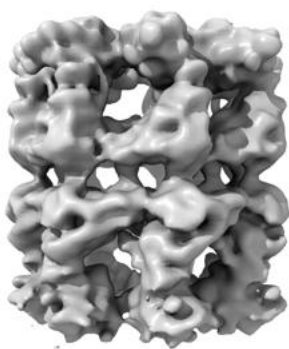


Z

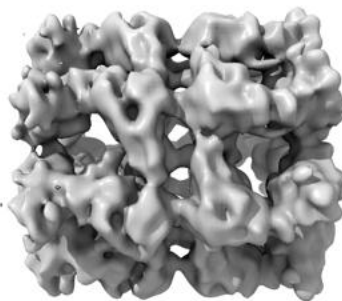
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

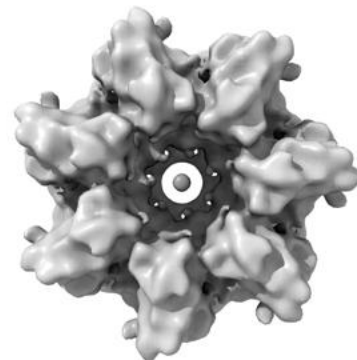
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

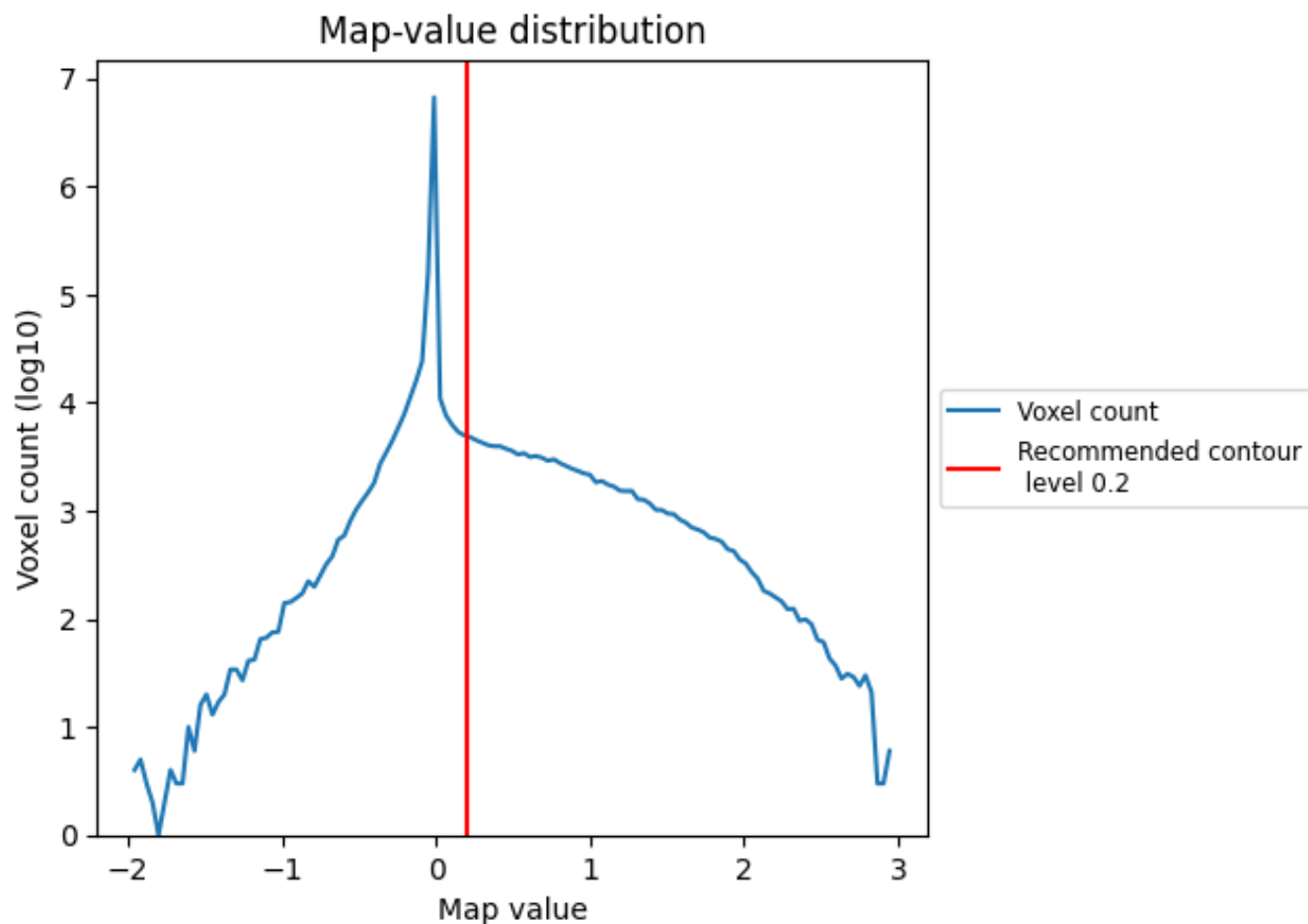
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

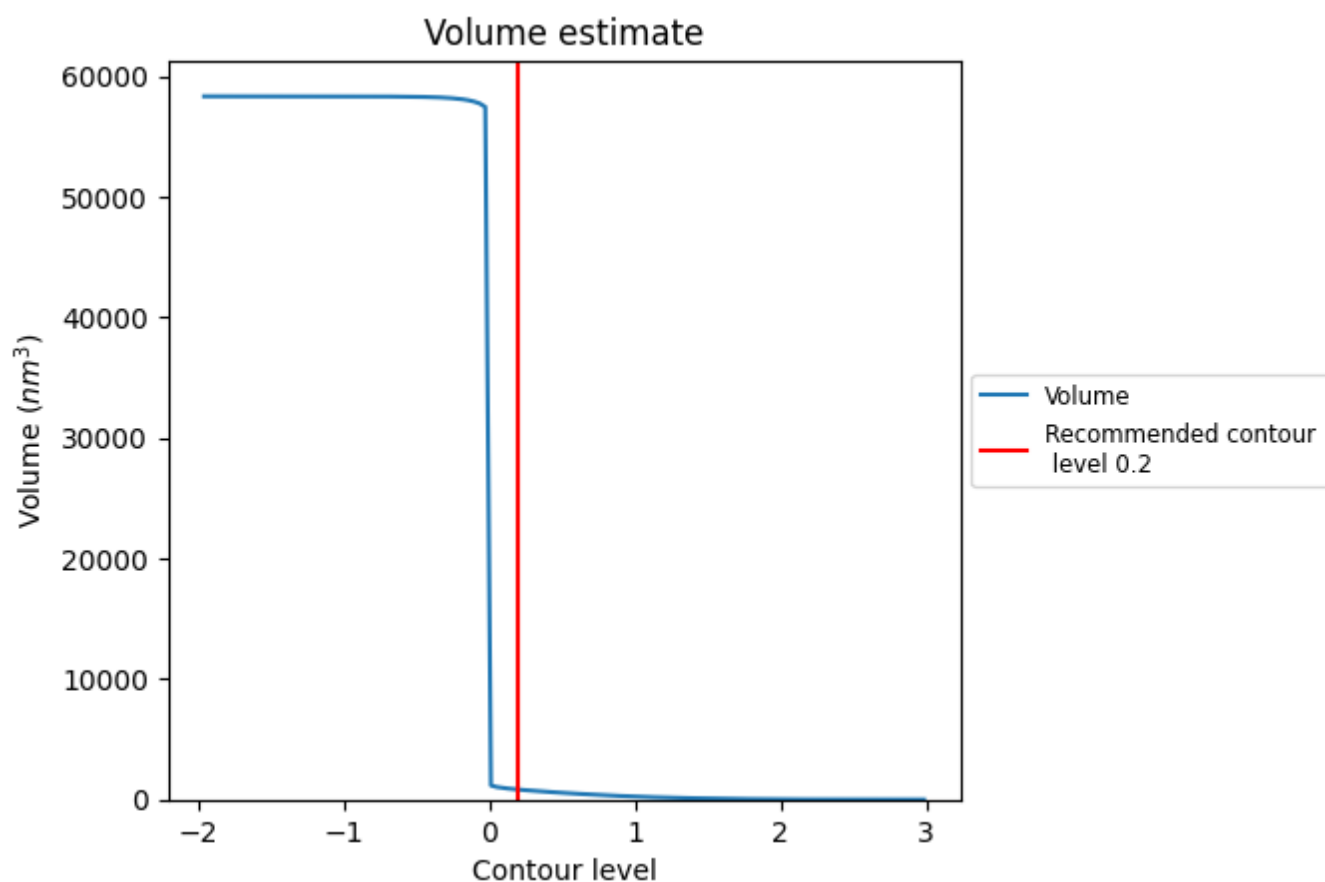
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

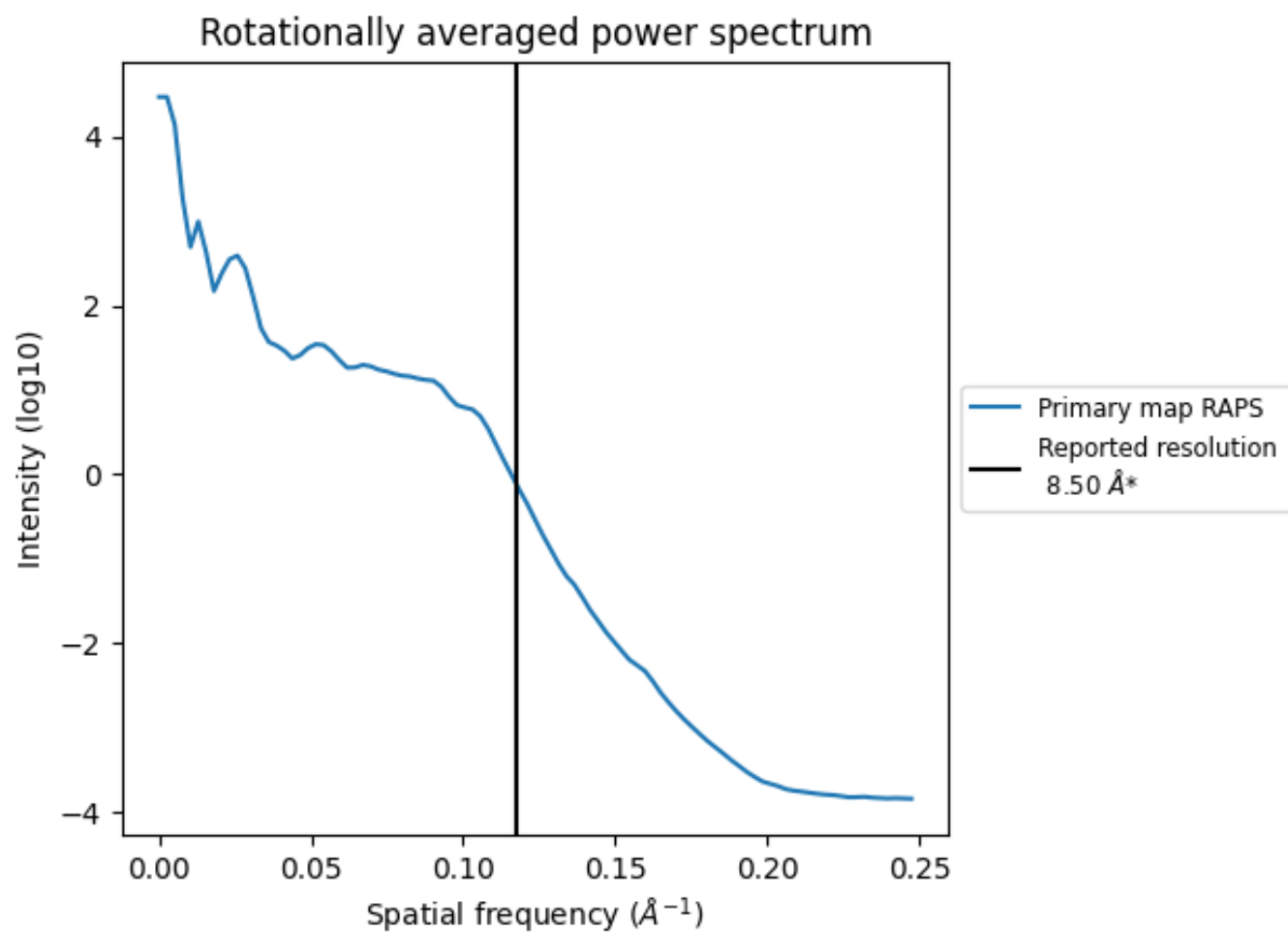
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 831 nm³; this corresponds to an approximate mass of 751 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.118 Å⁻¹

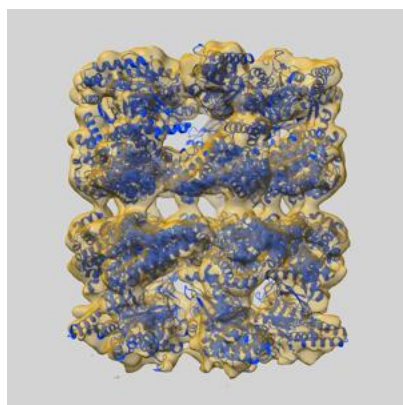
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

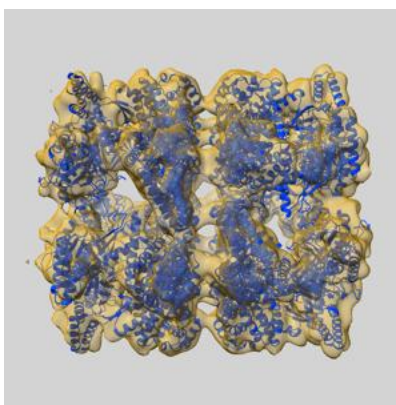
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2001 and PDB model 4AAU. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

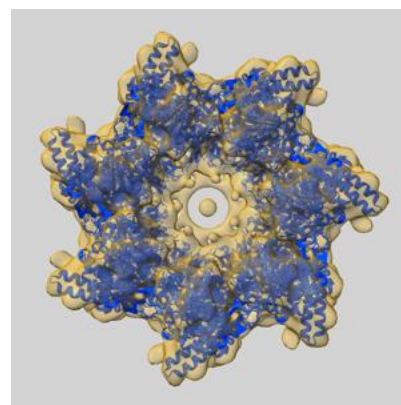
9.1 Map-model overlay [i](#)



X



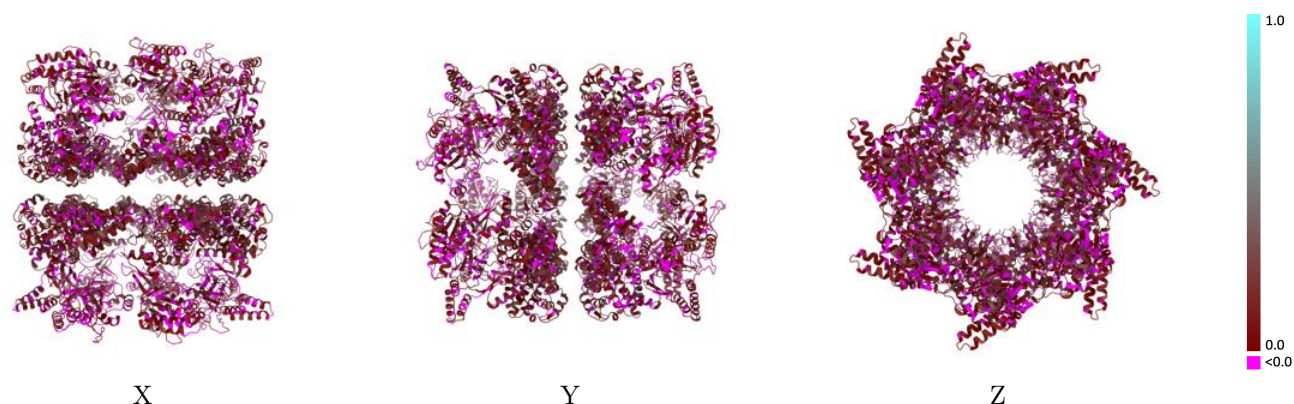
Y



Z

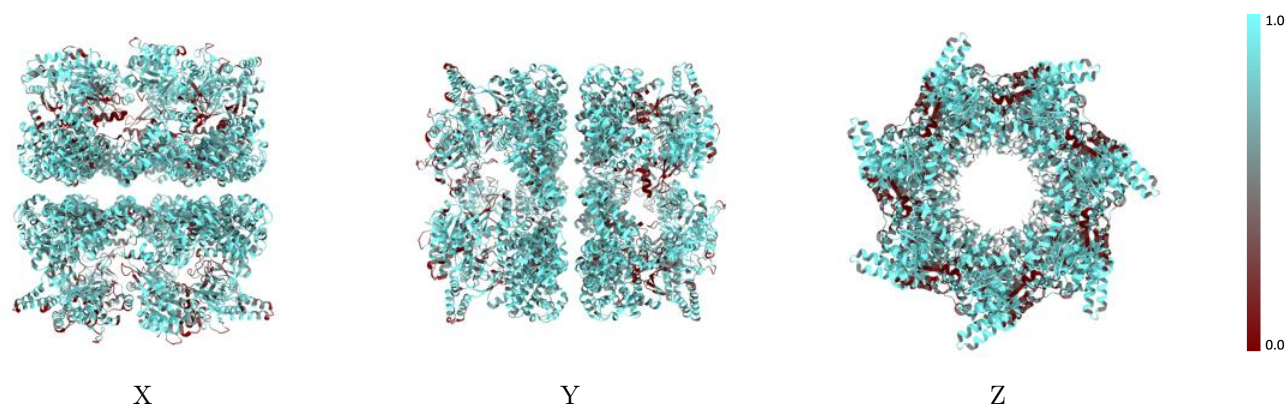
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



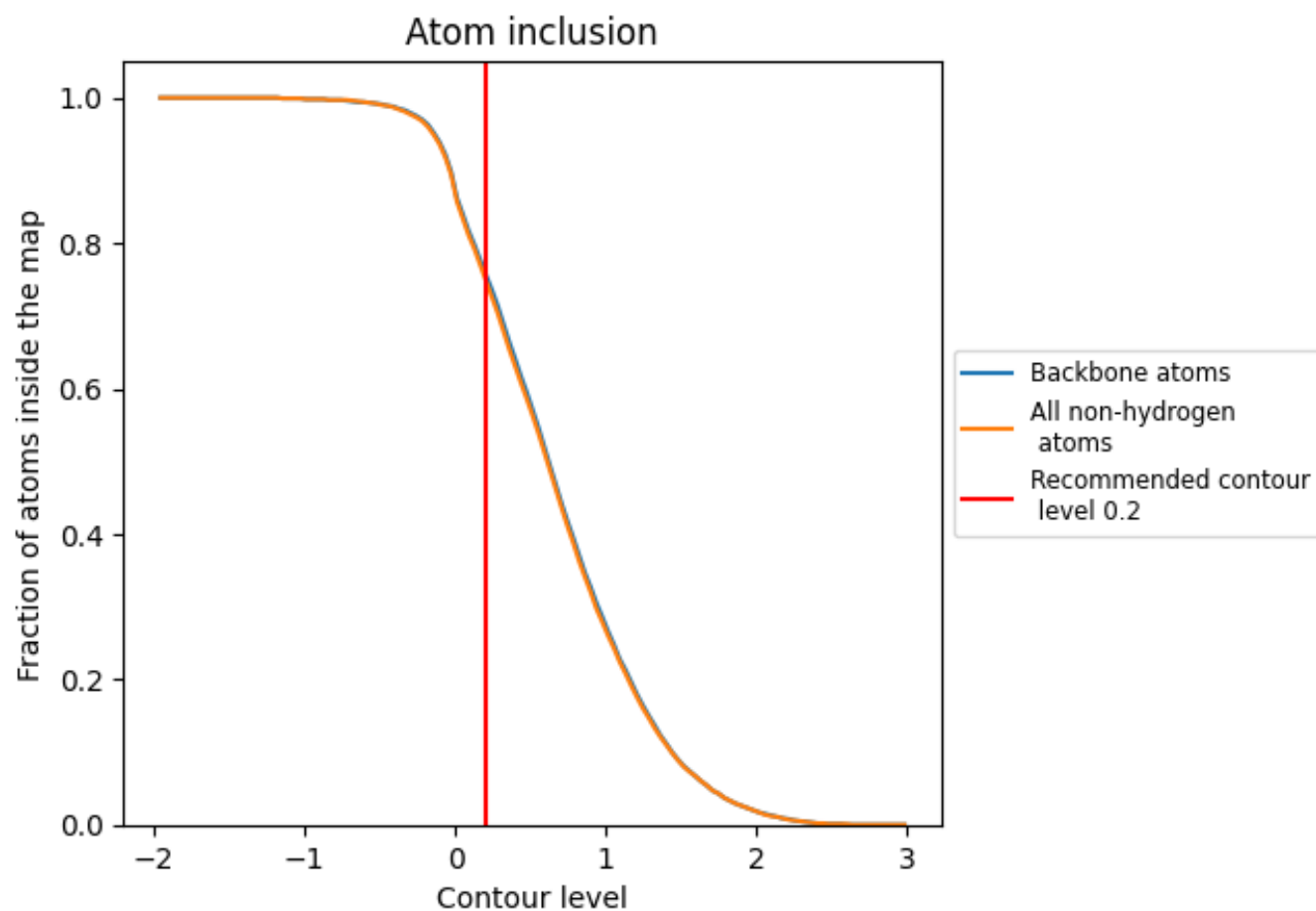
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.0880
A	0.7550	0.0840
B	0.7510	0.0840
C	0.7540	0.0830
D	0.7540	0.0840
E	0.7530	0.0840
F	0.7530	0.0850
G	0.7520	0.0850
H	0.7560	0.0920
I	0.7590	0.0920
J	0.7560	0.0910
K	0.7540	0.0900
L	0.7570	0.0910
M	0.7540	0.0910
N	0.7550	0.0910

1.0

0.0

<0.0