



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 02:50 PM UTC

PDB ID : 4AAQ / pdb_00004aaq
EMDB ID : EMD-1998
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 : 8.00 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:

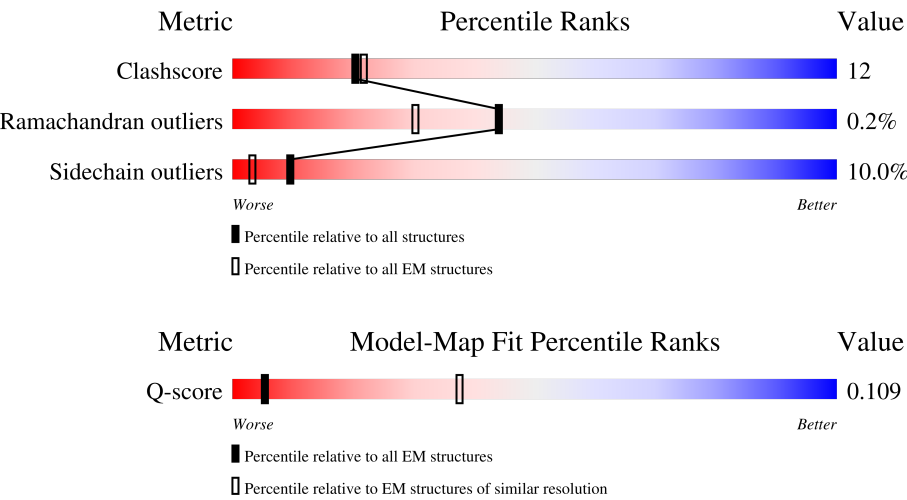
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 8.00 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	361 (7.50 - 8.50)

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	
1	B	548	
1	C	548	
1	D	548	

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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	1526	-	-	X	-
3	PO4	B	1526	-	-	X	-
3	PO4	C	1527	-	-	X	-
3	PO4	D	1526	-	-	X	-
3	PO4	E	1526	-	-	X	-
3	PO4	F	1525	-	-	X	-
3	PO4	G	1525	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 54159 atoms, of which 84 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:

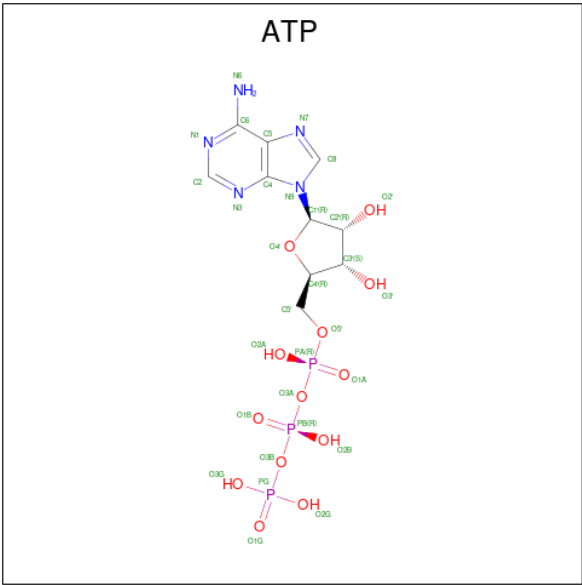
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	engineered mutation	UNP P0A6F5
B	398	ALA	ASP	engineered mutation	UNP P0A6F5

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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 ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



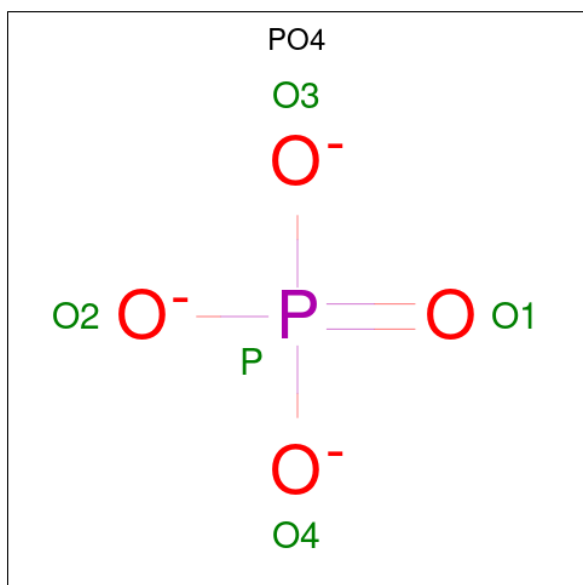
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	E	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

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Mol	Chain	Residues	Atoms						AltConf
2	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	G	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- 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	

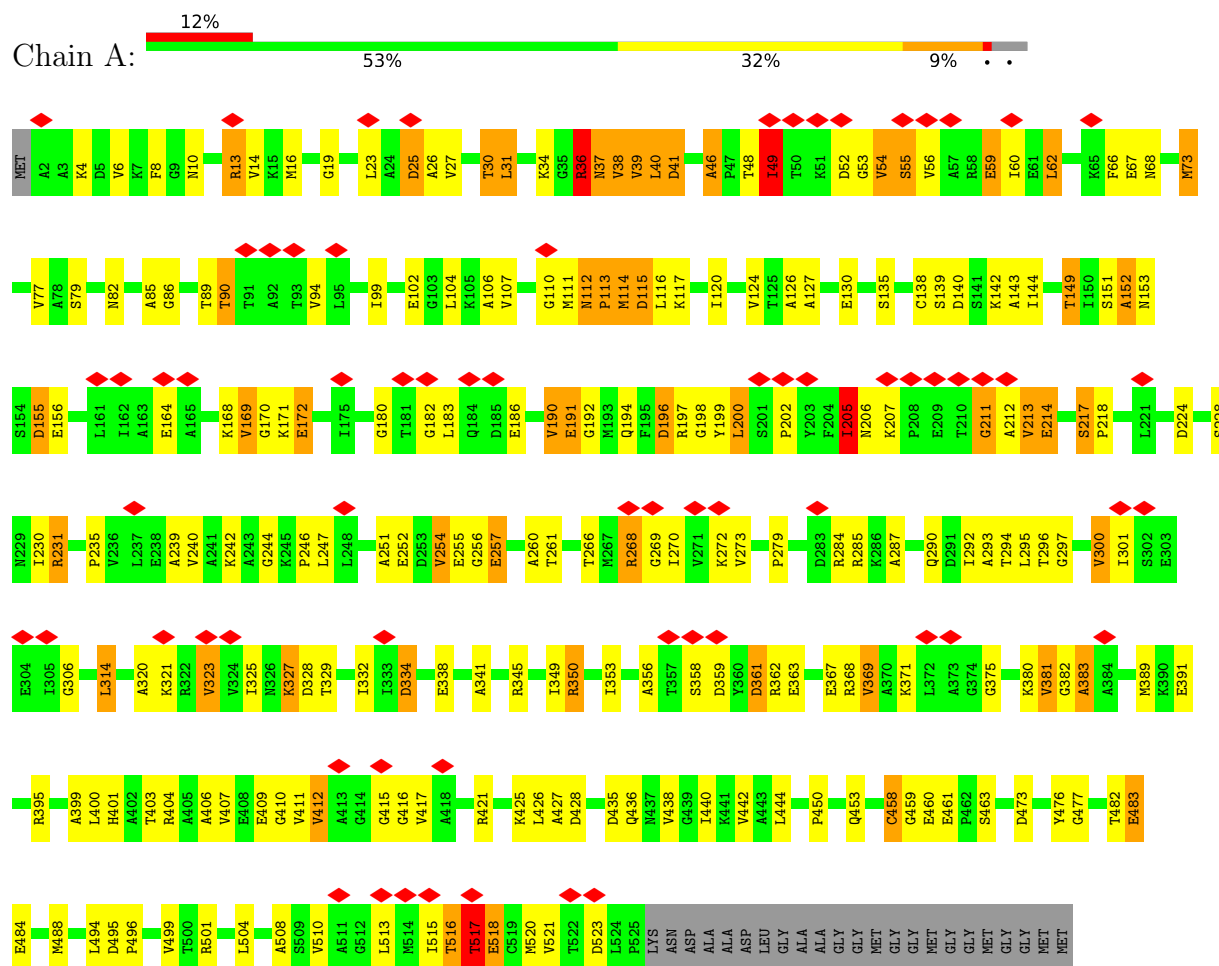
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0
4	B	1	Total 1	Mg 1	0
4	C	1	Total 1	Mg 1	0
4	D	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	0

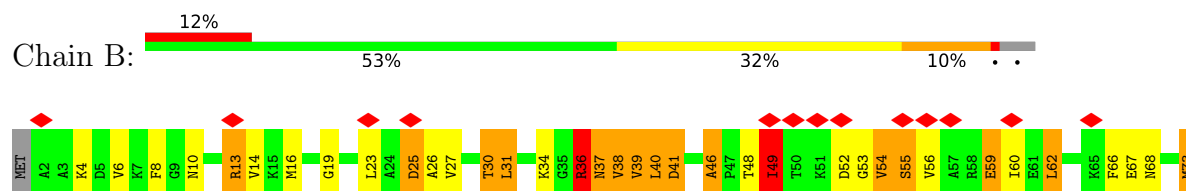
3 Residue-property plots [i](#)

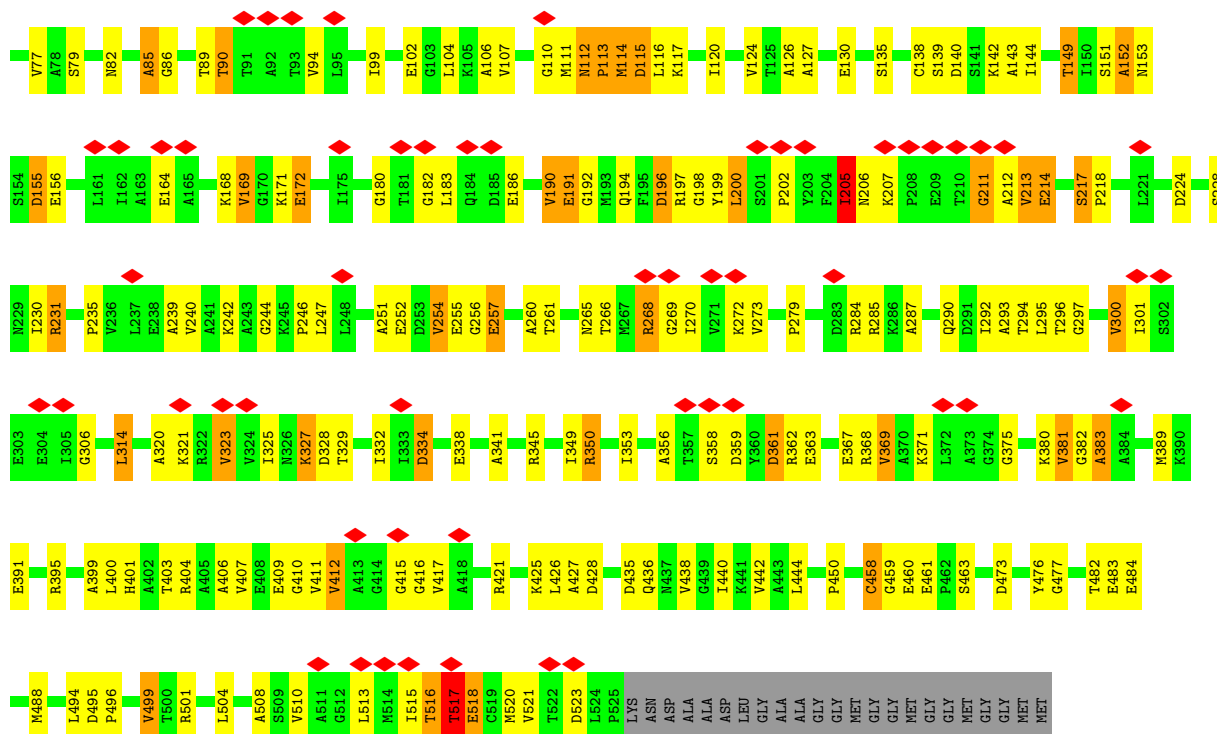
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

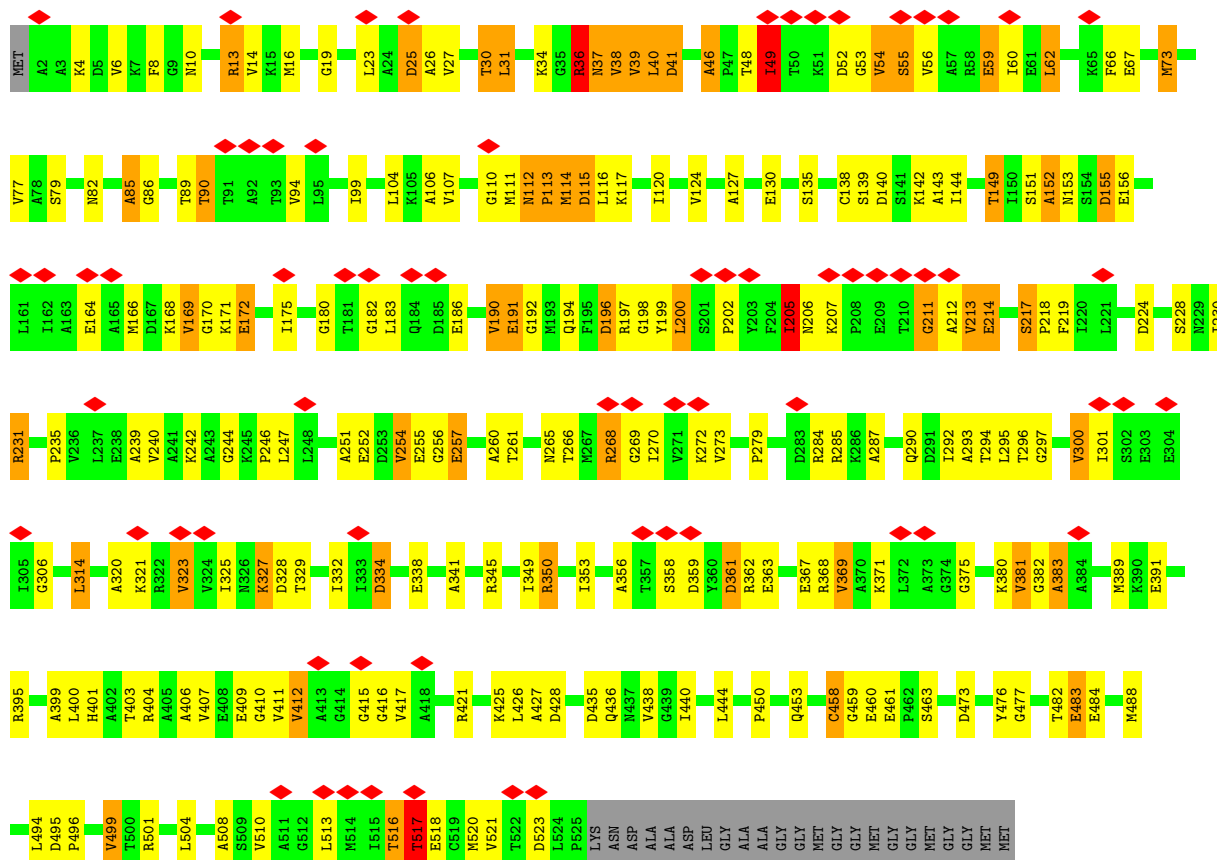


• Molecule 1: 60 KDA CHAPERONIN

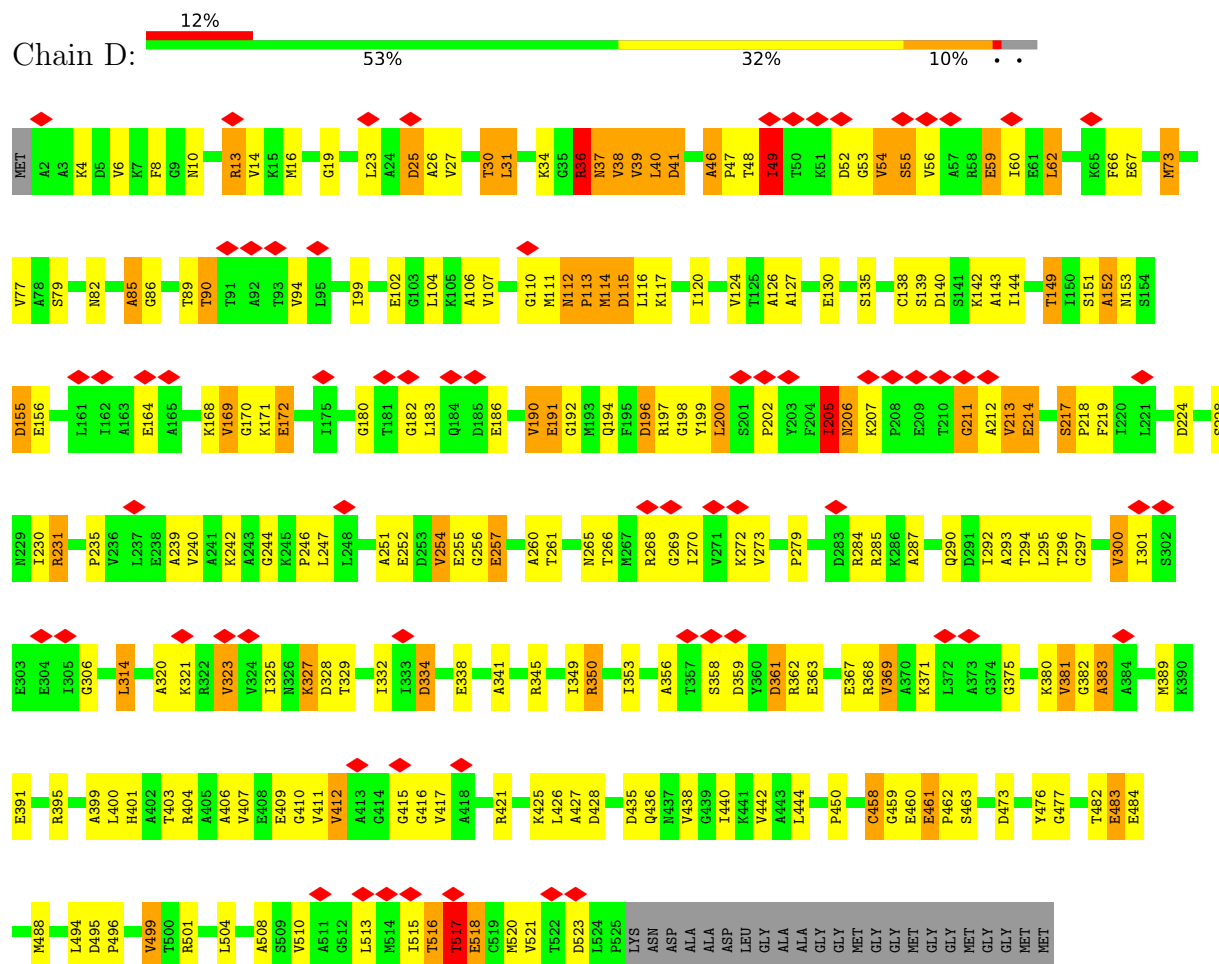




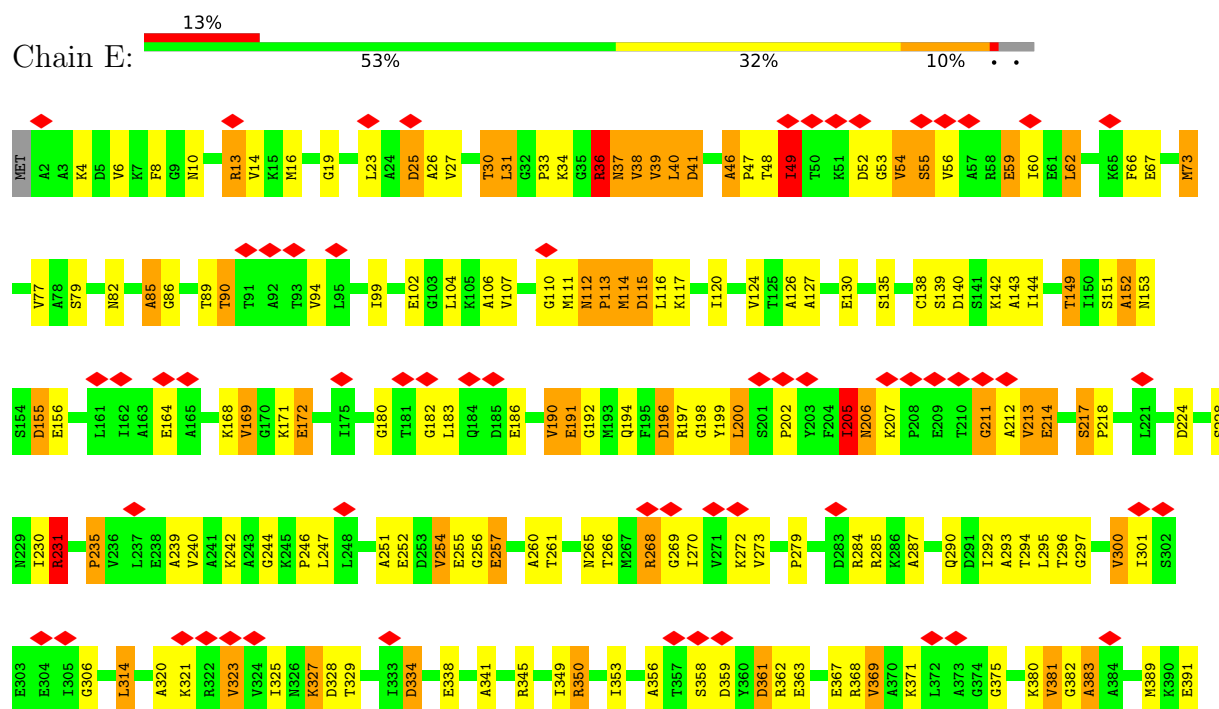
• Molecule 1: 60 KDA CHAPERONIN

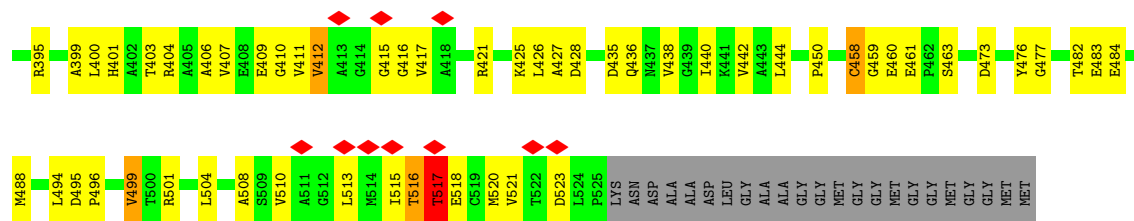


• Molecule 1: 60 KDA CHAPERONIN

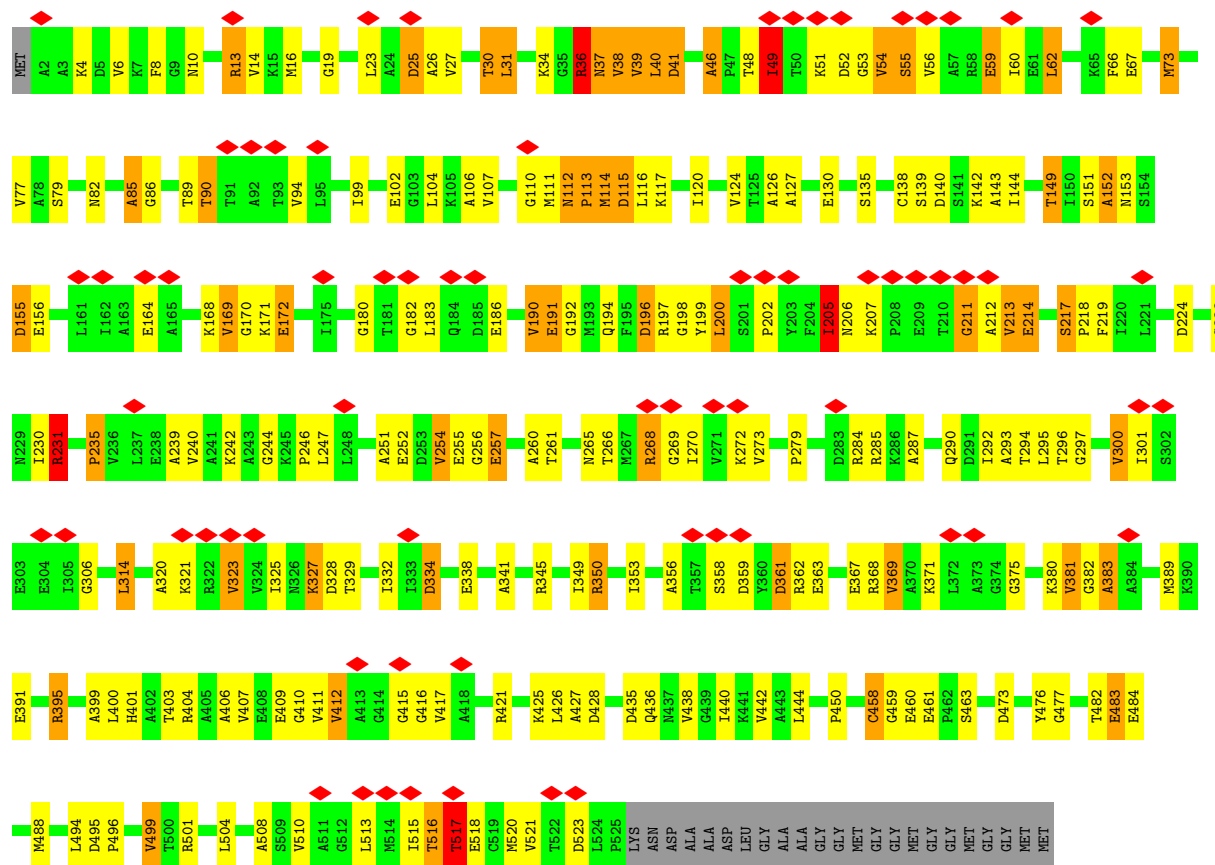


• Molecule 1: 60 KDA CHAPERONIN

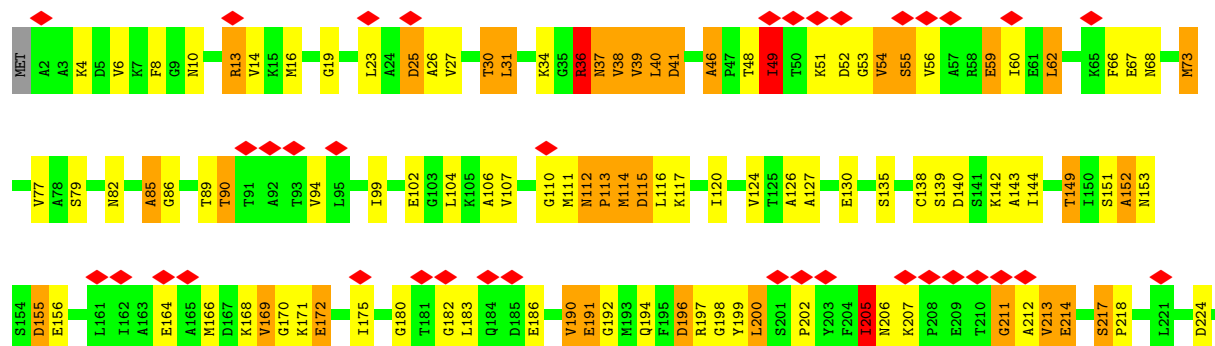


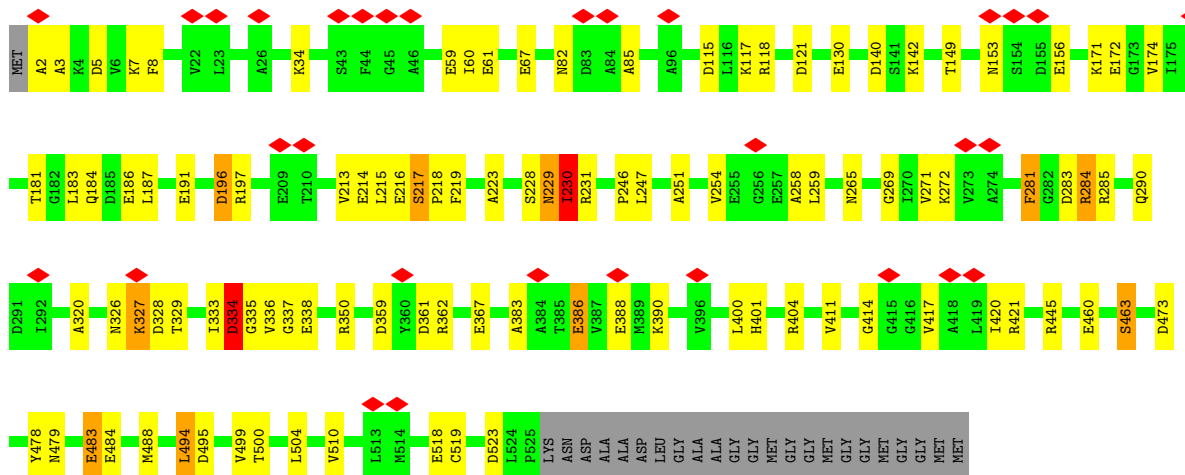


• Molecule 1: 60 KDA CHAPERONIN

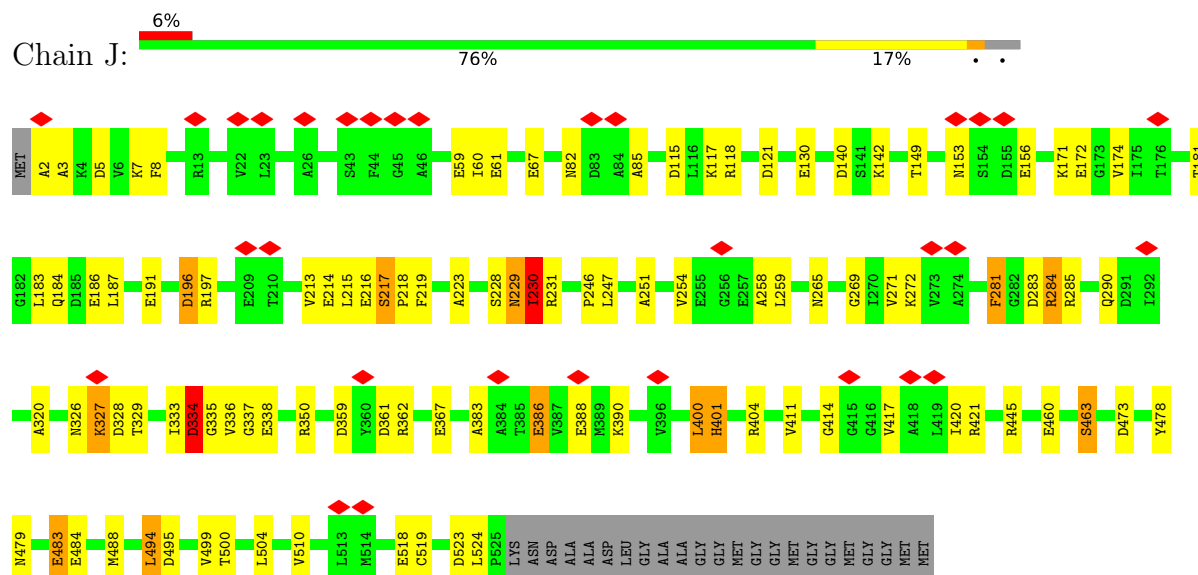


• Molecule 1: 60 KDA CHAPERONIN

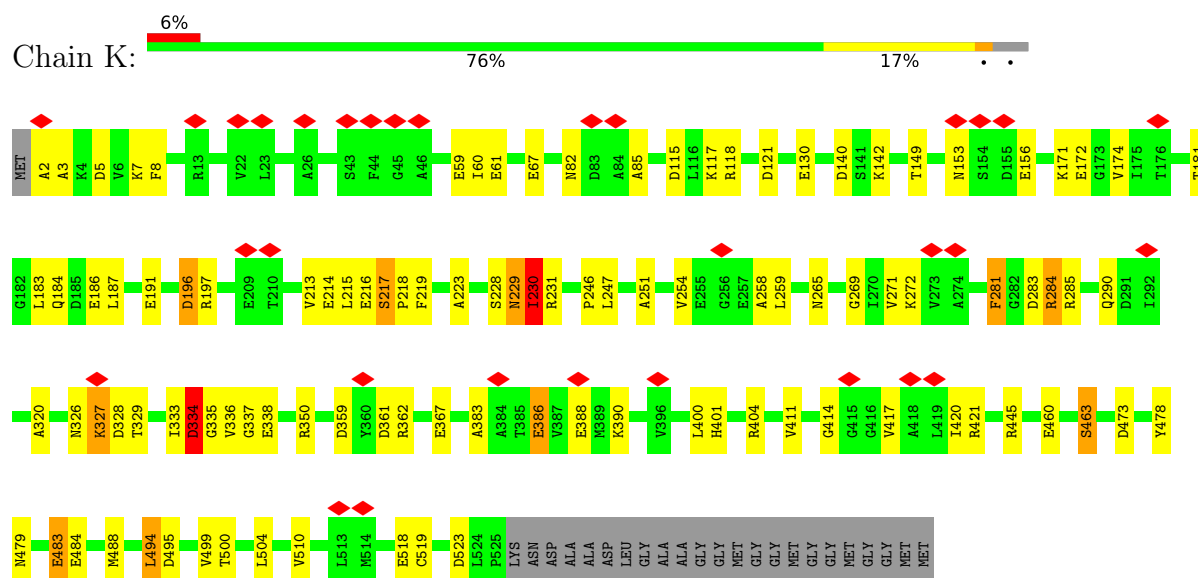




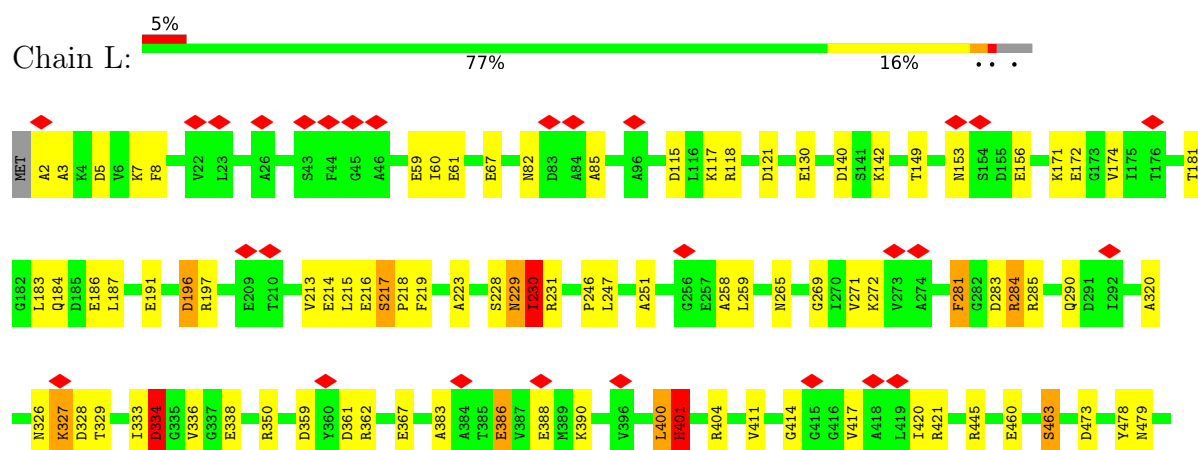
- Molecule 1: 60 KDA CHAPERONIN



- 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, C7	Depositor
Number of particles used	5500	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	3.488	Depositor
Minimum map value	-2.732	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.135	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: MG, PO4, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	2.05	7/3873 (0.2%)	1.95	132/5229 (2.5%)
1	B	2.05	7/3873 (0.2%)	1.95	132/5229 (2.5%)
1	C	2.05	7/3873 (0.2%)	1.95	132/5229 (2.5%)
1	D	2.05	7/3873 (0.2%)	1.95	133/5229 (2.5%)
1	E	2.05	7/3873 (0.2%)	1.95	132/5229 (2.5%)
1	F	2.05	7/3873 (0.2%)	1.95	132/5229 (2.5%)
1	G	2.05	7/3873 (0.2%)	1.95	132/5229 (2.5%)
1	H	0.85	2/3873 (0.1%)	1.29	24/5229 (0.5%)
1	I	0.81	2/3873 (0.1%)	1.29	26/5229 (0.5%)
1	J	0.91	3/3873 (0.1%)	1.30	27/5229 (0.5%)
1	K	0.84	2/3873 (0.1%)	1.29	25/5229 (0.5%)
1	L	0.94	2/3873 (0.1%)	1.34	30/5229 (0.6%)
1	M	0.79	2/3873 (0.1%)	1.33	28/5229 (0.5%)
1	N	1.05	3/3873 (0.1%)	1.29	24/5229 (0.5%)
All	All	1.58	65/54222 (0.1%)	1.66	1109/73206 (1.5%)

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	9
1	B	0	9
1	C	0	10
1	D	0	10
1	E	0	9
1	F	0	10
1	G	0	9
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	11
1	M	0	10
1	N	0	11
All	All	0	138

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	36	ARG	CZ-NH1	85.08	2.51	1.32
1	G	36	ARG	CZ-NH1	84.97	2.51	1.32
1	B	36	ARG	CZ-NH1	84.96	2.51	1.32
1	F	36	ARG	CZ-NH1	84.94	2.51	1.32
1	D	36	ARG	CZ-NH1	84.90	2.51	1.32
1	C	36	ARG	CZ-NH1	84.87	2.51	1.32
1	A	36	ARG	CZ-NH1	84.72	2.51	1.32
1	L	400	LEU	C-N	32.85	1.77	1.34
1	N	400	LEU	C-N	32.38	1.83	1.33
1	N	401	HIS	C-N	-29.77	0.90	1.33
1	J	400	LEU	C-N	25.89	1.72	1.33
1	H	401	HIS	C-N	19.23	1.60	1.33
1	K	401	HIS	C-N	-17.86	1.10	1.33
1	B	401	HIS	C-N	17.67	1.57	1.33
1	A	401	HIS	C-N	17.39	1.57	1.33
1	G	401	HIS	C-N	17.16	1.57	1.33
1	C	401	HIS	C-N	17.15	1.56	1.33
1	F	401	HIS	C-N	16.89	1.56	1.33
1	D	401	HIS	C-N	16.84	1.55	1.33
1	E	401	HIS	C-N	16.27	1.56	1.33
1	J	401	HIS	C-N	-13.85	1.14	1.33
1	F	36	ARG	CD-NE	11.19	1.61	1.46
1	C	36	ARG	CD-NE	11.18	1.61	1.46
1	A	36	ARG	CD-NE	11.12	1.61	1.46
1	B	36	ARG	CD-NE	11.09	1.61	1.46
1	D	36	ARG	CD-NE	11.07	1.61	1.46
1	E	36	ARG	CD-NE	11.07	1.61	1.46
1	G	36	ARG	CD-NE	11.02	1.61	1.46
1	H	400	LEU	C-N	10.08	1.47	1.33
1	I	400	LEU	C-N	9.95	1.47	1.33
1	I	401	HIS	C-N	9.85	1.47	1.33
1	M	400	LEU	C-N	8.52	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	517	THR	CA-CB	7.83	1.66	1.53
1	G	517	THR	CA-CB	7.82	1.66	1.53
1	C	517	THR	CA-CB	7.79	1.66	1.53
1	A	517	THR	CA-CB	7.79	1.66	1.53
1	E	517	THR	CA-CB	7.79	1.66	1.53
1	B	517	THR	CA-CB	7.77	1.66	1.53
1	D	517	THR	CA-CB	7.76	1.66	1.53
1	K	400	LEU	C-N	6.84	1.43	1.33
1	G	400	LEU	C-N	6.73	1.42	1.33
1	F	400	LEU	C-N	6.62	1.42	1.33
1	A	400	LEU	C-N	6.10	1.42	1.33
1	A	49	ILE	CA-CB	5.99	1.61	1.54
1	D	49	ILE	CA-CB	5.97	1.61	1.54
1	G	49	ILE	CA-CB	5.97	1.61	1.54
1	E	400	LEU	C-N	5.92	1.41	1.33
1	C	49	ILE	CA-CB	5.89	1.61	1.54
1	F	49	ILE	CA-CB	5.89	1.61	1.54
1	B	49	ILE	CA-CB	5.87	1.61	1.54
1	E	49	ILE	CA-CB	5.86	1.61	1.54
1	G	217	SER	CA-CB	5.51	1.56	1.52
1	B	217	SER	CA-CB	5.49	1.56	1.52
1	A	217	SER	CA-CB	5.44	1.56	1.52
1	F	217	SER	CA-CB	5.42	1.56	1.52
1	B	400	LEU	C-N	5.41	1.41	1.33
1	D	217	SER	CA-CB	5.40	1.56	1.52
1	E	217	SER	CA-CB	5.39	1.56	1.52
1	C	217	SER	CA-CB	5.30	1.56	1.52
1	D	400	LEU	C-N	5.23	1.40	1.33
1	J	524	LEU	C-N	-5.07	1.26	1.34
1	C	400	LEU	C-N	5.05	1.40	1.33
1	N	524	LEU	C-N	-5.02	1.26	1.34
1	M	524	LEU	C-N	-5.01	1.26	1.34
1	L	524	LEU	C-N	-5.01	1.26	1.34

All (1109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	401	HIS	O-C-N	-14.70	105.02	122.22
1	B	114	MET	N-CA-CB	14.67	131.69	110.12
1	D	114	MET	N-CA-CB	14.66	131.66	110.12
1	A	114	MET	N-CA-CB	14.64	131.64	110.12
1	C	49	ILE	CB-CA-C	-14.63	90.94	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	49	ILE	CB-CA-C	-14.62	90.94	110.98
1	F	114	MET	N-CA-CB	14.62	131.62	110.12
1	C	114	MET	N-CA-CB	14.62	131.61	110.12
1	G	114	MET	N-CA-CB	14.62	131.61	110.12
1	F	49	ILE	CB-CA-C	-14.62	90.95	110.98
1	B	49	ILE	CB-CA-C	-14.61	90.96	110.98
1	E	49	ILE	CB-CA-C	-14.61	90.96	110.98
1	E	114	MET	N-CA-CB	14.61	131.60	110.12
1	A	49	ILE	CB-CA-C	-14.61	90.97	110.98
1	G	49	ILE	CB-CA-C	-14.60	90.98	110.98
1	M	401	HIS	O-C-N	13.74	142.48	122.28
1	B	36	ARG	CD-NE-CZ	13.24	142.94	124.40
1	G	36	ARG	CD-NE-CZ	13.19	142.87	124.40
1	A	36	ARG	CD-NE-CZ	13.18	142.86	124.40
1	D	36	ARG	CD-NE-CZ	13.17	142.84	124.40
1	F	36	ARG	CD-NE-CZ	13.16	142.83	124.40
1	E	36	ARG	CD-NE-CZ	13.15	142.81	124.40
1	C	36	ARG	CD-NE-CZ	13.14	142.80	124.40
1	M	401	HIS	CA-C-N	-12.23	103.89	120.28
1	M	401	HIS	C-N-CA	-12.23	103.89	120.28
1	L	400	LEU	O-C-N	12.16	134.59	122.07
1	D	140	ASP	CA-CB-CG	12.10	124.70	112.60
1	F	140	ASP	CA-CB-CG	12.08	124.68	112.60
1	E	140	ASP	CA-CB-CG	12.06	124.66	112.60
1	C	140	ASP	CA-CB-CG	12.05	124.65	112.60
1	B	140	ASP	CA-CB-CG	12.02	124.62	112.60
1	G	140	ASP	CA-CB-CG	12.02	124.62	112.60
1	A	140	ASP	CA-CB-CG	12.02	124.61	112.60
1	C	517	THR	CA-CB-OG1	11.80	127.30	109.60
1	B	517	THR	CA-CB-OG1	11.73	127.20	109.60
1	F	517	THR	CA-CB-OG1	11.73	127.19	109.60
1	D	517	THR	CA-CB-OG1	11.72	127.18	109.60
1	G	517	THR	CA-CB-OG1	11.72	127.18	109.60
1	A	517	THR	CA-CB-OG1	11.70	127.16	109.60
1	E	517	THR	CA-CB-OG1	11.70	127.15	109.60
1	E	36	ARG	NH1-CZ-NH2	-11.63	104.18	119.30
1	F	36	ARG	NH1-CZ-NH2	-11.59	104.23	119.30
1	G	36	ARG	NH1-CZ-NH2	-11.58	104.24	119.30
1	D	36	ARG	NH1-CZ-NH2	-11.55	104.28	119.30
1	A	36	ARG	NH1-CZ-NH2	-11.55	104.28	119.30
1	B	36	ARG	NH1-CZ-NH2	-11.55	104.29	119.30
1	C	36	ARG	NH1-CZ-NH2	-11.52	104.32	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	461	GLU	CB-CA-C	11.13	127.31	109.51
1	A	461	GLU	CB-CA-C	11.12	127.30	109.51
1	F	461	GLU	CB-CA-C	11.12	127.30	109.51
1	C	461	GLU	CB-CA-C	11.10	127.28	109.51
1	B	461	GLU	CB-CA-C	11.10	127.27	109.51
1	E	461	GLU	CB-CA-C	11.09	127.25	109.51
1	G	461	GLU	CB-CA-C	11.08	127.23	109.51
1	A	41	ASP	N-CA-CB	11.04	126.07	110.17
1	E	41	ASP	N-CA-CB	11.04	126.06	110.17
1	B	41	ASP	N-CA-CB	11.03	126.05	110.17
1	F	41	ASP	N-CA-CB	11.01	126.03	110.17
1	C	41	ASP	N-CA-CB	11.01	126.02	110.17
1	G	41	ASP	N-CA-CB	10.99	126.00	110.17
1	D	41	ASP	N-CA-CB	10.96	125.96	110.17
1	A	231	ARG	CB-CA-C	-10.64	94.17	110.88
1	D	231	ARG	CB-CA-C	-10.63	94.19	110.88
1	E	231	ARG	CB-CA-C	-10.62	94.21	110.88
1	C	231	ARG	CB-CA-C	-10.61	94.23	110.88
1	F	231	ARG	CB-CA-C	-10.61	94.22	110.88
1	G	231	ARG	CB-CA-C	-10.60	94.24	110.88
1	G	112	ASN	CB-CA-C	10.58	126.44	109.51
1	B	231	ARG	CB-CA-C	-10.58	94.28	110.88
1	C	112	ASN	CB-CA-C	10.58	126.43	109.51
1	A	112	ASN	CB-CA-C	10.57	126.42	109.51
1	D	36	ARG	CB-CA-C	10.57	128.73	109.71
1	D	112	ASN	CB-CA-C	10.56	126.41	109.51
1	B	112	ASN	CB-CA-C	10.56	126.40	109.51
1	E	112	ASN	CB-CA-C	10.56	126.40	109.51
1	F	112	ASN	CB-CA-C	10.55	126.39	109.51
1	C	36	ARG	CB-CA-C	10.55	128.70	109.71
1	A	36	ARG	CB-CA-C	10.54	128.68	109.71
1	F	36	ARG	CB-CA-C	10.54	128.68	109.71
1	G	36	ARG	CB-CA-C	10.53	128.67	109.71
1	E	36	ARG	CB-CA-C	10.53	128.66	109.71
1	B	36	ARG	CB-CA-C	10.52	128.64	109.71
1	L	401	HIS	CA-C-N	10.46	138.47	120.58
1	L	401	HIS	C-N-CA	10.46	138.47	120.58
1	C	46	ALA	N-CA-CB	-10.31	94.46	110.03
1	A	46	ALA	N-CA-CB	-10.29	94.49	110.03
1	B	46	ALA	N-CA-CB	-10.29	94.49	110.03
1	G	46	ALA	N-CA-CB	-10.29	94.49	110.03
1	F	46	ALA	N-CA-CB	-10.28	94.51	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	46	ALA	N-CA-CB	-10.28	94.51	110.03
1	D	46	ALA	N-CA-CB	-10.26	94.53	110.03
1	B	39	VAL	CB-CA-C	10.18	126.28	110.81
1	E	39	VAL	CB-CA-C	10.15	126.24	110.81
1	F	39	VAL	CB-CA-C	10.13	126.20	110.81
1	F	36	ARG	NE-CZ-NH1	10.12	131.62	121.50
1	A	39	VAL	CB-CA-C	10.10	126.16	110.81
1	C	39	VAL	CB-CA-C	10.10	126.16	110.81
1	D	36	ARG	NE-CZ-NH1	10.09	131.59	121.50
1	G	36	ARG	NE-CZ-NH1	10.08	131.58	121.50
1	G	39	VAL	CB-CA-C	10.07	126.12	110.81
1	C	36	ARG	NE-CZ-NH1	10.06	131.56	121.50
1	D	39	VAL	CB-CA-C	10.06	126.10	110.81
1	A	36	ARG	NE-CZ-NH1	10.04	131.54	121.50
1	B	36	ARG	NE-CZ-NH1	10.02	131.52	121.50
1	E	36	ARG	NE-CZ-NH1	10.02	131.52	121.50
1	M	400	LEU	O-C-N	-9.83	110.72	122.22
1	F	391	GLU	CB-CA-C	-9.81	94.51	110.79
1	A	391	GLU	CB-CA-C	-9.80	94.53	110.79
1	A	383	ALA	N-CA-CB	9.78	126.72	111.56
1	B	473	ASP	N-CA-CB	9.78	125.28	110.42
1	E	391	GLU	CB-CA-C	-9.77	94.57	110.79
1	G	473	ASP	N-CA-CB	9.77	125.27	110.42
1	C	391	GLU	CB-CA-C	-9.77	94.58	110.79
1	D	391	GLU	CB-CA-C	-9.77	94.58	110.79
1	B	391	GLU	CB-CA-C	-9.76	94.58	110.79
1	C	383	ALA	N-CA-CB	9.76	126.69	111.56
1	F	383	ALA	N-CA-CB	9.76	126.69	111.56
1	E	473	ASP	N-CA-CB	9.76	125.25	110.42
1	D	473	ASP	N-CA-CB	9.76	125.25	110.42
1	G	391	GLU	CB-CA-C	-9.76	94.59	110.79
1	E	383	ALA	N-CA-CB	9.75	126.68	111.56
1	F	473	ASP	N-CA-CB	9.75	125.24	110.42
1	G	73	MET	CB-CA-C	-9.74	94.62	110.79
1	C	473	ASP	N-CA-CB	9.73	125.22	110.42
1	A	473	ASP	N-CA-CB	9.73	125.21	110.42
1	E	112	ASN	N-CA-CB	-9.73	94.72	109.90
1	G	383	ALA	N-CA-CB	9.73	126.64	111.56
1	D	112	ASN	N-CA-CB	-9.71	94.75	109.90
1	E	73	MET	CB-CA-C	-9.71	94.67	110.79
1	D	383	ALA	N-CA-CB	9.71	126.60	111.56
1	B	383	ALA	N-CA-CB	9.70	126.60	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	MET	CB-CA-C	-9.70	94.69	110.79
1	B	112	ASN	N-CA-CB	-9.70	94.77	109.90
1	A	112	ASN	N-CA-CB	-9.69	94.78	109.90
1	F	73	MET	CB-CA-C	-9.69	94.70	110.79
1	C	112	ASN	N-CA-CB	-9.69	94.78	109.90
1	B	73	MET	CB-CA-C	-9.69	94.71	110.79
1	F	112	ASN	N-CA-CB	-9.69	94.79	109.90
1	C	73	MET	CB-CA-C	-9.68	94.72	110.79
1	G	112	ASN	N-CA-CB	-9.67	94.82	109.90
1	A	73	MET	CB-CA-C	-9.66	94.75	110.79
1	E	510	VAL	CB-CA-C	-9.66	99.61	111.97
1	C	510	VAL	CB-CA-C	-9.64	99.63	111.97
1	A	510	VAL	CB-CA-C	-9.63	99.64	111.97
1	F	510	VAL	CB-CA-C	-9.63	99.64	111.97
1	D	510	VAL	CB-CA-C	-9.63	99.65	111.97
1	B	510	VAL	CB-CA-C	-9.62	99.65	111.97
1	G	510	VAL	CB-CA-C	-9.59	99.70	111.97
1	F	369	VAL	N-CA-CB	9.47	123.42	110.54
1	B	153	ASN	CB-CA-C	9.46	126.67	112.09
1	C	153	ASN	CB-CA-C	9.46	126.66	112.09
1	A	369	VAL	N-CA-CB	9.45	123.39	110.54
1	E	369	VAL	N-CA-CB	9.45	123.39	110.54
1	D	153	ASN	CB-CA-C	9.44	126.63	112.09
1	G	369	VAL	N-CA-CB	9.44	123.38	110.54
1	G	153	ASN	CB-CA-C	9.44	126.62	112.09
1	B	369	VAL	N-CA-CB	9.43	123.37	110.54
1	E	153	ASN	CB-CA-C	9.43	126.62	112.09
1	A	153	ASN	CB-CA-C	9.43	126.61	112.09
1	D	369	VAL	N-CA-CB	9.42	123.36	110.54
1	F	153	ASN	CB-CA-C	9.41	126.58	112.09
1	C	369	VAL	N-CA-CB	9.40	123.32	110.54
1	A	353	ILE	CB-CA-C	-9.16	100.25	111.97
1	D	353	ILE	CB-CA-C	-9.16	100.25	111.97
1	F	353	ILE	CB-CA-C	-9.15	100.26	111.97
1	C	353	ILE	CB-CA-C	-9.15	100.26	111.97
1	B	353	ILE	CB-CA-C	-9.14	100.28	111.97
1	G	353	ILE	CB-CA-C	-9.13	100.28	111.97
1	J	401	HIS	O-C-N	9.12	135.32	122.36
1	E	353	ILE	CB-CA-C	-9.12	100.30	111.97
1	B	115	ASP	N-CA-CB	8.85	123.12	110.12
1	A	115	ASP	N-CA-CB	8.84	123.12	110.12
1	G	115	ASP	N-CA-CB	8.83	123.10	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	359	ASP	CA-CB-CG	-8.83	103.77	112.60
1	I	359	ASP	CA-CB-CG	-8.82	103.78	112.60
1	L	359	ASP	CA-CB-CG	-8.82	103.78	112.60
1	D	115	ASP	N-CA-CB	8.81	123.08	110.12
1	E	115	ASP	N-CA-CB	8.81	123.08	110.12
1	M	359	ASP	CA-CB-CG	-8.81	103.79	112.60
1	J	359	ASP	CA-CB-CG	-8.81	103.79	112.60
1	K	359	ASP	CA-CB-CG	-8.80	103.80	112.60
1	C	115	ASP	N-CA-CB	8.79	123.04	110.12
1	N	359	ASP	CA-CB-CG	-8.79	103.81	112.60
1	F	115	ASP	N-CA-CB	8.78	123.02	110.12
1	F	52	ASP	CB-CA-C	8.39	124.89	109.70
1	G	52	ASP	CB-CA-C	8.38	124.86	109.70
1	C	52	ASP	CB-CA-C	8.37	124.84	109.70
1	A	52	ASP	CB-CA-C	8.35	124.82	109.70
1	B	52	ASP	CB-CA-C	8.33	124.78	109.70
1	D	52	ASP	CB-CA-C	8.33	124.78	109.70
1	E	52	ASP	CB-CA-C	8.33	124.78	109.70
1	L	400	LEU	CA-C-N	-8.22	108.44	120.28
1	L	400	LEU	C-N-CA	-8.22	108.44	120.28
1	E	285	ARG	CB-CA-C	-8.19	97.20	110.79
1	B	483	GLU	CB-CG-CD	8.19	126.52	112.60
1	D	483	GLU	CB-CG-CD	8.19	126.52	112.60
1	F	483	GLU	CB-CG-CD	8.18	126.51	112.60
1	A	285	ARG	CB-CA-C	-8.18	97.22	110.79
1	E	483	GLU	CB-CG-CD	8.17	126.50	112.60
1	G	285	ARG	CB-CA-C	-8.17	97.22	110.79
1	C	483	GLU	CB-CG-CD	8.17	126.49	112.60
1	A	483	GLU	CB-CG-CD	8.17	126.48	112.60
1	G	483	GLU	CB-CG-CD	8.16	126.48	112.60
1	D	285	ARG	CB-CA-C	-8.16	97.25	110.79
1	F	285	ARG	CB-CA-C	-8.14	97.27	110.79
1	C	285	ARG	CB-CA-C	-8.14	97.28	110.79
1	B	285	ARG	CB-CA-C	-8.14	97.28	110.79
1	A	482	THR	N-CA-CB	8.12	122.18	110.16
1	C	482	THR	N-CA-CB	8.10	122.15	110.16
1	C	140	ASP	N-CA-CB	-8.07	98.82	110.45
1	D	140	ASP	N-CA-CB	-8.07	98.82	110.45
1	A	140	ASP	N-CA-CB	-8.07	98.83	110.45
1	B	140	ASP	N-CA-CB	-8.07	98.83	110.45
1	E	140	ASP	N-CA-CB	-8.07	98.83	110.45
1	B	400	LEU	O-C-N	-8.07	113.76	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	482	THR	N-CA-CB	8.06	122.09	110.16
1	B	482	THR	N-CA-CB	8.04	122.07	110.16
1	F	140	ASP	N-CA-CB	-8.05	98.86	110.45
1	G	482	THR	N-CA-CB	8.04	122.07	110.16
1	E	482	THR	N-CA-CB	8.04	122.06	110.16
1	G	140	ASP	N-CA-CB	-8.04	98.87	110.45
1	F	482	THR	N-CA-CB	8.03	122.04	110.16
1	A	400	LEU	O-C-N	-8.01	113.82	122.07
1	E	371	LYS	CB-CA-C	7.98	123.41	110.88
1	B	371	LYS	CB-CA-C	7.97	123.39	110.88
1	C	371	LYS	CB-CA-C	7.96	123.38	110.88
1	A	371	LYS	CB-CA-C	7.92	123.31	110.88
1	D	371	LYS	CB-CA-C	7.88	123.26	110.88
1	G	371	LYS	CB-CA-C	7.88	123.25	110.88
1	F	371	LYS	CB-CA-C	7.88	123.24	110.88
1	G	400	LEU	O-C-N	-7.81	114.03	122.07
1	D	40	LEU	N-CA-CB	-7.72	98.46	110.57
1	G	40	LEU	N-CA-CB	-7.69	98.49	110.57
1	D	369	VAL	CB-CA-C	-7.68	101.77	112.14
1	A	40	LEU	N-CA-CB	-7.67	98.53	110.57
1	F	40	LEU	N-CA-CB	-7.67	98.53	110.57
1	D	112	ASN	CA-CB-CG	7.66	120.26	112.60
1	E	369	VAL	CB-CA-C	-7.66	101.79	112.14
1	C	369	VAL	CB-CA-C	-7.66	101.80	112.14
1	E	40	LEU	N-CA-CB	-7.66	98.55	110.57
1	G	112	ASN	CA-CB-CG	7.66	120.25	112.60
1	C	40	LEU	N-CA-CB	-7.65	98.55	110.57
1	B	40	LEU	N-CA-CB	-7.65	98.56	110.57
1	F	369	VAL	CB-CA-C	-7.65	101.81	112.14
1	B	112	ASN	CA-CB-CG	7.64	120.24	112.60
1	C	400	LEU	O-C-N	-7.64	114.20	122.07
1	N	367	GLU	CB-CA-C	-7.64	96.00	110.67
1	B	369	VAL	CB-CA-C	-7.63	101.83	112.14
1	J	367	GLU	CB-CA-C	-7.63	96.02	110.67
1	F	112	ASN	CA-CB-CG	7.63	120.23	112.60
1	L	367	GLU	CB-CA-C	-7.62	96.04	110.67
1	H	367	GLU	CB-CA-C	-7.62	96.04	110.67
1	I	367	GLU	CB-CA-C	-7.62	96.05	110.67
1	M	367	GLU	CB-CA-C	-7.61	96.05	110.67
1	G	369	VAL	CB-CA-C	-7.61	101.86	112.14
1	C	425	LYS	CB-CA-C	7.61	123.42	110.79
1	C	112	ASN	CA-CB-CG	7.61	120.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	367	GLU	CB-CA-C	-7.61	96.06	110.67
1	F	425	LYS	CB-CA-C	7.60	123.41	110.79
1	E	112	ASN	CA-CB-CG	7.60	120.20	112.60
1	G	425	LYS	CB-CA-C	7.60	123.41	110.79
1	A	369	VAL	CB-CA-C	-7.59	101.89	112.14
1	A	425	LYS	CB-CA-C	7.59	123.39	110.79
1	B	425	LYS	CB-CA-C	7.59	123.39	110.79
1	E	425	LYS	CB-CA-C	7.58	123.38	110.79
1	A	112	ASN	CA-CB-CG	7.57	120.17	112.60
1	E	149	THR	N-CA-CB	7.57	121.25	110.12
1	D	425	LYS	CB-CA-C	7.56	123.34	110.79
1	D	149	THR	N-CA-CB	7.56	121.23	110.12
1	G	149	THR	N-CA-CB	7.55	121.22	110.12
1	F	149	THR	N-CA-CB	7.55	121.22	110.12
1	L	196	ASP	N-CA-CB	-7.51	99.76	110.58
1	A	149	THR	N-CA-CB	7.51	121.15	110.12
1	C	149	THR	N-CA-CB	7.51	121.16	110.12
1	B	149	THR	N-CA-CB	7.50	121.14	110.12
1	M	196	ASP	N-CA-CB	-7.49	99.80	110.58
1	J	196	ASP	N-CA-CB	-7.49	99.80	110.58
1	N	196	ASP	N-CA-CB	-7.49	99.80	110.58
1	I	196	ASP	N-CA-CB	-7.48	99.81	110.58
1	K	196	ASP	N-CA-CB	-7.47	99.83	110.58
1	H	196	ASP	N-CA-CB	-7.46	99.83	110.58
1	G	461	GLU	CB-CG-CD	7.45	125.27	112.60
1	F	461	GLU	CB-CG-CD	7.44	125.25	112.60
1	F	400	LEU	O-C-N	-7.43	114.41	122.07
1	A	461	GLU	CB-CG-CD	7.43	125.23	112.60
1	A	517	THR	N-CA-CB	7.43	123.04	110.49
1	B	461	GLU	CB-CG-CD	7.42	125.21	112.60
1	E	461	GLU	CB-CG-CD	7.42	125.21	112.60
1	C	461	GLU	CB-CG-CD	7.41	125.20	112.60
1	D	461	GLU	CB-CG-CD	7.41	125.20	112.60
1	E	517	THR	N-CA-CB	7.40	123.00	110.49
1	F	517	THR	N-CA-CB	7.39	122.98	110.49
1	D	517	THR	N-CA-CB	7.39	122.98	110.49
1	B	517	THR	N-CA-CB	7.38	122.96	110.49
1	G	517	THR	N-CA-CB	7.37	122.95	110.49
1	E	41	ASP	CA-CB-CG	7.36	119.96	112.60
1	L	333	ILE	N-CA-C	7.36	118.15	110.72
1	C	517	THR	N-CA-CB	7.35	122.92	110.49
1	F	41	ASP	CA-CB-CG	7.35	119.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	ASP	CA-CB-CG	7.34	119.94	112.60
1	M	333	ILE	N-CA-C	7.34	118.13	110.72
1	B	41	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	41	ASP	CA-CB-CG	7.32	119.92	112.60
1	J	333	ILE	N-CA-C	7.32	118.11	110.72
1	H	333	ILE	N-CA-C	7.31	118.11	110.72
1	C	41	ASP	CA-CB-CG	7.29	119.89	112.60
1	K	333	ILE	N-CA-C	7.29	118.09	110.72
1	G	41	ASP	CA-CB-CG	7.28	119.88	112.60
1	I	333	ILE	N-CA-C	7.28	118.07	110.72
1	A	60	ILE	N-CA-CB	7.27	119.25	110.31
1	E	367	GLU	CB-CA-C	-7.26	98.73	110.79
1	D	367	GLU	CB-CA-C	-7.26	98.73	110.79
1	B	367	GLU	CB-CA-C	-7.25	98.76	110.79
1	A	367	GLU	CB-CA-C	-7.24	98.77	110.79
1	C	367	GLU	CB-CA-C	-7.24	98.77	110.79
1	B	60	ILE	N-CA-CB	7.23	119.21	110.31
1	N	333	ILE	N-CA-C	7.23	118.02	110.72
1	G	367	GLU	CB-CA-C	-7.23	98.79	110.79
1	F	367	GLU	CB-CA-C	-7.23	98.79	110.79
1	E	60	ILE	N-CA-CB	7.23	119.20	110.31
1	G	60	ILE	N-CA-CB	7.22	119.19	110.31
1	C	60	ILE	N-CA-CB	7.21	119.18	110.31
1	D	60	ILE	N-CA-CB	7.21	119.18	110.31
1	F	60	ILE	N-CA-CB	7.21	119.18	110.31
1	D	400	LEU	O-C-N	-7.21	114.64	122.07
1	A	269	GLY	N-CA-C	-7.18	104.83	114.95
1	A	89	THR	CB-CA-C	-7.16	99.64	110.88
1	D	89	THR	CB-CA-C	-7.16	99.64	110.88
1	E	89	THR	CB-CA-C	-7.16	99.64	110.88
1	B	269	GLY	N-CA-C	-7.15	104.87	114.95
1	B	89	THR	CB-CA-C	-7.15	99.66	110.88
1	D	269	GLY	N-CA-C	-7.14	104.88	114.95
1	C	89	THR	CB-CA-C	-7.14	99.67	110.88
1	E	412	VAL	CB-CA-C	-7.14	100.62	110.90
1	F	269	GLY	N-CA-C	-7.13	104.89	114.95
1	C	231	ARG	CA-CB-CG	7.13	128.35	114.10
1	C	412	VAL	CB-CA-C	-7.13	100.64	110.90
1	F	89	THR	CB-CA-C	-7.12	99.70	110.88
1	D	412	VAL	CB-CA-C	-7.12	100.65	110.90
1	B	231	ARG	CA-CB-CG	7.12	128.33	114.10
1	F	412	VAL	CB-CA-C	-7.12	100.65	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	412	VAL	CB-CA-C	-7.12	100.65	110.90
1	G	231	ARG	CA-CB-CG	7.11	128.32	114.10
1	B	412	VAL	CB-CA-C	-7.11	100.66	110.90
1	A	231	ARG	CA-CB-CG	7.11	128.32	114.10
1	G	89	THR	CB-CA-C	-7.10	99.73	110.88
1	D	231	ARG	CA-CB-CG	7.10	128.30	114.10
1	F	231	ARG	CA-CB-CG	7.09	128.28	114.10
1	E	400	LEU	O-C-N	-7.09	114.77	122.07
1	C	269	GLY	N-CA-C	-7.09	104.96	114.95
1	A	412	VAL	CB-CA-C	-7.08	100.71	110.90
1	E	269	GLY	N-CA-C	-7.08	104.97	114.95
1	G	269	GLY	N-CA-C	-7.08	104.97	114.95
1	E	231	ARG	CA-CB-CG	7.08	128.25	114.10
1	G	359	ASP	CA-CB-CG	-7.04	105.56	112.60
1	J	401	HIS	CA-C-N	-7.04	108.55	120.58
1	J	401	HIS	C-N-CA	-7.04	108.55	120.58
1	B	86	GLY	N-CA-C	-6.98	106.39	114.69
1	C	359	ASP	CA-CB-CG	-6.98	105.62	112.60
1	B	257	GLU	N-CA-CB	6.97	120.18	110.07
1	D	359	ASP	CA-CB-CG	-6.97	105.63	112.60
1	B	359	ASP	CA-CB-CG	-6.96	105.64	112.60
1	D	86	GLY	N-CA-C	-6.96	106.41	114.69
1	F	257	GLU	N-CA-CB	6.96	120.16	110.07
1	K	115	ASP	CB-CA-C	6.96	121.90	110.90
1	F	86	GLY	N-CA-C	-6.95	106.42	114.69
1	C	257	GLU	N-CA-CB	6.95	120.15	110.07
1	E	359	ASP	CA-CB-CG	-6.95	105.65	112.60
1	A	117	LYS	N-CA-CB	6.94	120.33	110.12
1	E	257	GLU	N-CA-CB	6.94	120.13	110.07
1	F	359	ASP	CA-CB-CG	-6.93	105.67	112.60
1	A	359	ASP	CA-CB-CG	-6.93	105.67	112.60
1	E	86	GLY	N-CA-C	-6.93	106.44	114.69
1	E	117	LYS	N-CA-CB	6.93	120.30	110.12
1	D	257	GLU	N-CA-CB	6.92	120.11	110.07
1	G	86	GLY	N-CA-C	-6.92	106.45	114.69
1	C	117	LYS	N-CA-CB	6.92	120.29	110.12
1	L	115	ASP	CB-CA-C	6.91	121.82	110.90
1	G	117	LYS	N-CA-CB	6.91	120.27	110.12
1	B	117	LYS	N-CA-CB	6.90	120.27	110.12
1	M	5	ASP	N-CA-CB	6.90	121.42	110.65
1	D	117	LYS	N-CA-CB	6.90	120.26	110.12
1	I	5	ASP	N-CA-CB	6.90	121.41	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	117	LYS	N-CA-CB	6.90	120.26	110.12
1	I	115	ASP	CB-CA-C	6.89	121.80	110.90
1	N	115	ASP	CB-CA-C	6.89	121.79	110.90
1	C	409	GLU	N-CA-CB	6.89	120.36	110.16
1	J	217	SER	CB-CA-C	-6.89	104.23	110.71
1	N	5	ASP	N-CA-CB	6.89	121.40	110.65
1	A	257	GLU	N-CA-CB	6.89	120.06	110.07
1	M	217	SER	CB-CA-C	-6.88	104.24	110.71
1	A	409	GLU	N-CA-CB	6.88	120.34	110.16
1	J	115	ASP	CB-CA-C	6.88	121.77	110.90
1	A	86	GLY	N-CA-C	-6.88	106.51	114.69
1	C	86	GLY	N-CA-C	-6.88	106.51	114.69
1	L	5	ASP	N-CA-CB	6.87	121.37	110.65
1	N	115	ASP	CA-CB-CG	-6.87	105.73	112.60
1	J	5	ASP	N-CA-CB	6.87	121.37	110.65
1	M	115	ASP	CB-CA-C	6.87	121.76	110.90
1	H	217	SER	CB-CA-C	-6.87	104.25	110.71
1	H	115	ASP	CB-CA-C	6.86	121.74	110.90
1	L	217	SER	CB-CA-C	-6.86	104.26	110.71
1	D	409	GLU	N-CA-CB	6.86	120.31	110.16
1	G	257	GLU	N-CA-CB	6.86	120.02	110.07
1	N	217	SER	CB-CA-C	-6.86	104.27	110.71
1	K	5	ASP	N-CA-CB	6.85	121.33	110.65
1	E	409	GLU	N-CA-CB	6.85	120.30	110.16
1	H	5	ASP	N-CA-CB	6.84	121.33	110.65
1	I	217	SER	CB-CA-C	-6.84	104.28	110.71
1	L	115	ASP	CA-CB-CG	-6.83	105.77	112.60
1	B	409	GLU	N-CA-CB	6.83	120.27	110.16
1	K	217	SER	CB-CA-C	-6.83	104.29	110.71
1	J	115	ASP	CA-CB-CG	-6.83	105.77	112.60
1	F	409	GLU	N-CA-CB	6.82	120.25	110.16
1	I	115	ASP	CA-CB-CG	-6.80	105.80	112.60
1	G	67	GLU	CB-CG-CD	6.80	124.16	112.60
1	F	67	GLU	CB-CG-CD	6.80	124.16	112.60
1	G	409	GLU	N-CA-CB	6.79	120.22	110.16
1	K	115	ASP	CA-CB-CG	-6.79	105.81	112.60
1	H	115	ASP	CA-CB-CG	-6.78	105.82	112.60
1	B	67	GLU	CB-CG-CD	6.77	124.11	112.60
1	D	67	GLU	CB-CG-CD	6.76	124.10	112.60
1	A	67	GLU	CB-CG-CD	6.76	124.10	112.60
1	F	517	THR	CB-CA-C	-6.76	96.96	110.42
1	G	517	THR	CB-CA-C	-6.76	96.96	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	517	THR	CB-CA-C	-6.76	96.97	110.42
1	M	115	ASP	CA-CB-CG	-6.76	105.84	112.60
1	C	435	ASP	CB-CA-C	-6.76	99.57	110.79
1	A	435	ASP	CB-CA-C	-6.76	99.57	110.79
1	G	435	ASP	CB-CA-C	-6.76	99.58	110.79
1	B	517	THR	CB-CA-C	-6.75	96.98	110.42
1	E	435	ASP	CB-CA-C	-6.75	99.58	110.79
1	F	435	ASP	CB-CA-C	-6.74	99.60	110.79
1	A	517	THR	CB-CA-C	-6.74	97.02	110.42
1	E	67	GLU	CB-CG-CD	6.74	124.05	112.60
1	D	435	ASP	CB-CA-C	-6.73	99.62	110.79
1	B	435	ASP	CB-CA-C	-6.73	99.62	110.79
1	C	67	GLU	CB-CG-CD	6.72	124.03	112.60
1	D	517	THR	CB-CA-C	-6.72	97.04	110.42
1	E	517	THR	CB-CA-C	-6.72	97.06	110.42
1	B	115	ASP	CA-CB-CG	-6.71	105.89	112.60
1	D	115	ASP	CA-CB-CG	-6.67	105.93	112.60
1	A	115	ASP	CA-CB-CG	-6.66	105.94	112.60
1	E	321	LYS	N-CA-CB	6.65	119.66	110.01
1	E	115	ASP	CA-CB-CG	-6.65	105.95	112.60
1	F	321	LYS	N-CA-CB	6.64	119.65	110.01
1	C	115	ASP	CA-CB-CG	-6.64	105.96	112.60
1	G	321	LYS	N-CA-CB	6.64	119.64	110.01
1	A	321	LYS	N-CA-CB	6.64	119.64	110.01
1	D	321	LYS	N-CA-CB	6.63	119.62	110.01
1	B	152	ALA	CB-CA-C	6.63	122.89	110.63
1	F	115	ASP	CA-CB-CG	-6.63	105.97	112.60
1	F	152	ALA	CB-CA-C	6.62	122.88	110.63
1	B	321	LYS	N-CA-CB	6.62	119.60	110.01
1	D	152	ALA	CB-CA-C	6.60	122.85	110.63
1	G	270	ILE	N-CA-C	-6.60	103.89	110.62
1	C	152	ALA	CB-CA-C	6.59	122.82	110.63
1	G	152	ALA	CB-CA-C	6.59	122.81	110.63
1	B	270	ILE	N-CA-C	-6.58	103.90	110.62
1	C	321	LYS	N-CA-CB	6.58	119.54	110.01
1	E	152	ALA	CB-CA-C	6.57	122.79	110.63
1	G	115	ASP	CA-CB-CG	-6.57	106.03	112.60
1	A	152	ALA	CB-CA-C	6.56	122.77	110.63
1	A	270	ILE	N-CA-C	-6.56	103.93	110.62
1	B	52	ASP	N-CA-CB	6.54	122.11	110.80
1	C	52	ASP	N-CA-CB	6.54	122.11	110.80
1	A	52	ASP	N-CA-CB	6.53	122.10	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	52	ASP	N-CA-CB	6.53	122.10	110.80
1	E	270	ILE	N-CA-C	-6.52	103.97	110.62
1	C	436	GLN	N-CA-CB	6.52	119.70	110.12
1	B	436	GLN	N-CA-CB	6.51	119.69	110.12
1	F	52	ASP	N-CA-CB	6.51	122.06	110.80
1	F	270	ILE	N-CA-C	-6.51	103.98	110.62
1	D	52	ASP	N-CA-CB	6.51	122.06	110.80
1	G	52	ASP	N-CA-CB	6.51	122.06	110.80
1	G	436	GLN	N-CA-CB	6.50	119.68	110.12
1	A	436	GLN	N-CA-CB	6.50	119.67	110.12
1	E	436	GLN	N-CA-CB	6.49	119.67	110.12
1	F	436	GLN	N-CA-CB	6.49	119.67	110.12
1	D	436	GLN	N-CA-CB	6.49	119.66	110.12
1	D	270	ILE	N-CA-C	-6.47	104.02	110.62
1	C	270	ILE	N-CA-C	-6.47	104.02	110.62
1	F	297	GLY	N-CA-C	-6.47	106.40	115.32
1	F	284	ARG	CB-CA-C	-6.44	100.10	110.79
1	A	284	ARG	CB-CA-C	-6.44	100.10	110.79
1	E	297	GLY	N-CA-C	-6.43	106.44	115.32
1	A	297	GLY	N-CA-C	-6.42	106.46	115.32
1	G	284	ARG	CB-CA-C	-6.41	100.14	110.79
1	B	284	ARG	CB-CA-C	-6.41	100.15	110.79
1	C	284	ARG	CB-CA-C	-6.41	100.15	110.79
1	D	284	ARG	CB-CA-C	-6.41	100.15	110.79
1	E	113	PRO	N-CA-CB	6.41	109.66	103.51
1	E	284	ARG	CB-CA-C	-6.39	100.18	110.79
1	B	297	GLY	N-CA-C	-6.37	106.53	115.32
1	C	113	PRO	N-CA-CB	6.37	109.62	103.51
1	D	297	GLY	N-CA-C	-6.37	106.53	115.32
1	C	297	GLY	N-CA-C	-6.35	106.55	115.32
1	F	113	PRO	N-CA-CB	6.34	109.60	103.51
1	F	77	VAL	CB-CA-C	6.34	120.69	112.14
1	F	196	ASP	N-CA-CB	-6.33	101.05	110.24
1	G	297	GLY	N-CA-C	-6.33	106.58	115.32
1	A	77	VAL	CB-CA-C	6.33	120.68	112.14
1	A	196	ASP	N-CA-CB	-6.32	101.08	110.24
1	D	196	ASP	N-CA-CB	-6.32	101.08	110.24
1	C	196	ASP	N-CA-CB	-6.32	101.08	110.24
1	E	196	ASP	N-CA-CB	-6.30	101.10	110.24
1	D	113	PRO	N-CA-CB	6.30	109.56	103.51
1	B	196	ASP	N-CA-CB	-6.30	101.10	110.24
1	G	113	PRO	N-CA-CB	6.30	109.56	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	PRO	N-CA-CB	6.30	109.55	103.51
1	D	77	VAL	CB-CA-C	6.29	120.63	112.14
1	B	113	PRO	N-CA-CB	6.29	109.55	103.51
1	D	39	VAL	CA-CB-CG1	6.29	121.08	110.40
1	G	196	ASP	N-CA-CB	-6.28	101.13	110.24
1	E	77	VAL	CB-CA-C	6.28	120.62	112.14
1	C	39	VAL	CA-CB-CG1	6.28	121.07	110.40
1	E	510	VAL	N-CA-CB	6.28	117.89	110.55
1	F	510	VAL	N-CA-CB	6.28	117.89	110.55
1	G	39	VAL	CA-CB-CG1	6.28	121.07	110.40
1	B	77	VAL	CB-CA-C	6.27	120.61	112.14
1	G	77	VAL	CB-CA-C	6.27	120.61	112.14
1	C	77	VAL	CB-CA-C	6.27	120.61	112.14
1	C	510	VAL	N-CA-CB	6.27	117.88	110.55
1	D	510	VAL	N-CA-CB	6.27	117.88	110.55
1	B	39	VAL	CA-CB-CG1	6.26	121.05	110.40
1	A	39	VAL	CA-CB-CG1	6.26	121.05	110.40
1	B	59	GLU	CB-CA-C	6.26	121.18	110.79
1	E	39	VAL	CA-CB-CG1	6.26	121.03	110.40
1	D	54	VAL	CB-CA-C	-6.25	103.71	112.14
1	D	59	GLU	CB-CA-C	6.24	121.16	110.79
1	F	39	VAL	CA-CB-CG1	6.24	121.01	110.40
1	A	54	VAL	CB-CA-C	-6.24	103.72	112.14
1	G	59	GLU	CB-CA-C	6.23	121.12	110.79
1	G	510	VAL	N-CA-CB	6.22	117.83	110.55
1	B	510	VAL	N-CA-CB	6.22	117.83	110.55
1	B	54	VAL	CB-CA-C	-6.22	103.75	112.14
1	G	54	VAL	CB-CA-C	-6.22	103.75	112.14
1	F	54	VAL	CB-CA-C	-6.21	103.75	112.14
1	E	54	VAL	CB-CA-C	-6.21	103.76	112.14
1	E	59	GLU	CB-CA-C	6.21	121.09	110.79
1	F	59	GLU	CB-CA-C	6.21	121.09	110.79
1	A	510	VAL	N-CA-CB	6.19	117.80	110.55
1	C	59	GLU	CB-CA-C	6.19	121.07	110.79
1	A	59	GLU	CB-CA-C	6.19	121.06	110.79
1	C	54	VAL	CB-CA-C	-6.16	103.82	112.14
1	B	435	ASP	CA-CB-CG	6.16	118.76	112.60
1	C	90	THR	N-CA-CB	6.15	119.17	110.12
1	G	82	ASN	N-CA-CB	6.15	118.92	110.01
1	C	82	ASN	N-CA-CB	6.14	118.91	110.01
1	M	67	GLU	CB-CG-CD	6.14	123.03	112.60
1	B	82	ASN	N-CA-CB	6.14	118.91	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	ASP	CA-CB-CG	6.13	118.73	112.60
1	D	381	VAL	N-CA-CB	-6.13	102.91	111.25
1	F	90	THR	N-CA-CB	6.13	119.13	110.12
1	G	90	THR	N-CA-CB	6.13	119.13	110.12
1	E	90	THR	N-CA-CB	6.13	119.13	110.12
1	F	435	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	90	THR	N-CA-CB	6.13	119.13	110.12
1	D	435	ASP	CA-CB-CG	6.12	118.72	112.60
1	E	82	ASN	N-CA-CB	6.12	118.88	110.01
1	J	67	GLU	CB-CG-CD	6.12	123.00	112.60
1	E	435	ASP	CA-CB-CG	6.11	118.71	112.60
1	L	67	GLU	CB-CG-CD	6.11	122.99	112.60
1	F	82	ASN	N-CA-CB	6.11	118.87	110.01
1	E	244	GLY	N-CA-C	-6.11	107.27	115.21
1	H	67	GLU	CB-CG-CD	6.11	122.98	112.60
1	F	381	VAL	N-CA-CB	-6.10	102.95	111.25
1	D	82	ASN	N-CA-CB	6.10	118.85	110.01
1	D	244	GLY	N-CA-C	-6.10	107.28	115.21
1	G	381	VAL	N-CA-CB	-6.10	102.96	111.25
1	I	67	GLU	CB-CG-CD	6.09	122.95	112.60
1	A	82	ASN	N-CA-CB	6.09	118.84	110.01
1	N	67	GLU	CB-CG-CD	6.09	122.95	112.60
1	E	381	VAL	N-CA-CB	-6.08	102.97	111.25
1	B	391	GLU	CA-CB-CG	6.08	126.27	114.10
1	D	391	GLU	CA-CB-CG	6.08	126.27	114.10
1	E	391	GLU	CA-CB-CG	6.08	126.27	114.10
1	B	90	THR	N-CA-CB	6.08	119.06	110.12
1	C	435	ASP	CA-CB-CG	6.08	118.68	112.60
1	C	381	VAL	N-CA-CB	-6.08	102.98	111.25
1	G	391	GLU	CA-CB-CG	6.08	126.26	114.10
1	D	90	THR	N-CA-CB	6.08	119.05	110.12
1	K	67	GLU	CB-CG-CD	6.08	122.93	112.60
1	G	244	GLY	N-CA-C	-6.07	107.32	115.21
1	A	381	VAL	N-CA-CB	-6.07	102.99	111.25
1	G	190	VAL	CB-CA-C	6.07	120.40	110.69
1	B	381	VAL	N-CA-CB	-6.07	103.00	111.25
1	F	459	GLY	N-CA-C	-6.07	107.03	114.92
1	B	190	VAL	CB-CA-C	6.06	120.39	110.69
1	E	190	VAL	CB-CA-C	6.06	120.39	110.69
1	F	211	GLY	N-CA-C	-6.06	107.04	114.92
1	F	244	GLY	N-CA-C	-6.06	107.33	115.21
1	G	435	ASP	CA-CB-CG	6.06	118.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	391	GLU	CA-CB-CG	6.06	126.22	114.10
1	A	391	GLU	CA-CB-CG	6.06	126.21	114.10
1	C	244	GLY	N-CA-C	-6.06	107.34	115.21
1	A	190	VAL	CB-CA-C	6.05	120.38	110.69
1	B	244	GLY	N-CA-C	-6.05	107.34	115.21
1	C	391	GLU	CA-CB-CG	6.05	126.20	114.10
1	F	60	ILE	CB-CA-C	-6.04	102.33	111.33
1	F	190	VAL	CB-CA-C	6.04	120.36	110.69
1	A	60	ILE	CB-CA-C	-6.04	102.33	111.33
1	C	190	VAL	CB-CA-C	6.04	120.35	110.69
1	C	459	GLY	N-CA-C	-6.03	107.08	114.92
1	E	60	ILE	CB-CA-C	-6.03	102.34	111.33
1	B	459	GLY	N-CA-C	-6.03	107.08	114.92
1	B	60	ILE	CB-CA-C	-6.03	102.35	111.33
1	C	60	ILE	CB-CA-C	-6.03	102.35	111.33
1	D	190	VAL	CB-CA-C	6.02	120.32	110.69
1	D	60	ILE	CB-CA-C	-6.02	102.36	111.33
1	A	244	GLY	N-CA-C	-6.01	107.40	115.21
1	G	459	GLY	N-CA-C	-6.00	107.12	114.92
1	G	60	ILE	CB-CA-C	-6.00	102.39	111.33
1	C	211	GLY	N-CA-C	-5.99	107.14	114.92
1	E	459	GLY	N-CA-C	-5.99	107.14	114.92
1	A	400	LEU	CA-C-N	5.98	128.30	120.28
1	A	400	LEU	C-N-CA	5.98	128.30	120.28
1	B	211	GLY	N-CA-C	-5.97	107.15	114.92
1	D	14	VAL	N-CA-CB	5.96	118.64	110.54
1	G	211	GLY	N-CA-C	-5.96	107.17	114.92
1	E	211	GLY	N-CA-C	-5.95	107.18	114.92
1	C	14	VAL	N-CA-CB	5.95	118.64	110.54
1	L	265	ASN	CA-CB-CG	-5.95	106.65	112.60
1	A	14	VAL	N-CA-CB	5.95	118.63	110.54
1	A	211	GLY	N-CA-C	-5.94	107.20	114.92
1	D	211	GLY	N-CA-C	-5.93	107.20	114.92
1	B	400	LEU	CA-C-N	5.93	128.23	120.28
1	B	400	LEU	C-N-CA	5.93	128.23	120.28
1	H	361	ASP	CA-CB-CG	-5.93	106.67	112.60
1	I	361	ASP	CA-CB-CG	-5.93	106.67	112.60
1	L	361	ASP	CA-CB-CG	-5.93	106.67	112.60
1	N	361	ASP	CA-CB-CG	-5.93	106.67	112.60
1	A	459	GLY	N-CA-C	-5.93	107.22	114.92
1	B	14	VAL	N-CA-CB	5.92	118.59	110.54
1	M	361	ASP	CA-CB-CG	-5.91	106.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	14	VAL	N-CA-CB	5.90	118.57	110.54
1	A	516	THR	N-CA-CB	5.90	118.79	110.12
1	I	265	ASN	CA-CB-CG	-5.90	106.70	112.60
1	G	14	VAL	N-CA-CB	5.90	118.56	110.54
1	D	459	GLY	N-CA-C	-5.89	107.26	114.92
1	C	46	ALA	CB-CA-C	-5.89	99.80	109.46
1	C	516	THR	N-CA-CB	5.89	118.78	110.12
1	D	516	THR	N-CA-CB	5.88	118.77	110.12
1	F	516	THR	N-CA-CB	5.88	118.77	110.12
1	G	46	ALA	CB-CA-C	-5.88	99.82	109.46
1	D	46	ALA	CB-CA-C	-5.88	99.82	109.46
1	K	265	ASN	CA-CB-CG	-5.88	106.72	112.60
1	G	516	THR	N-CA-CB	5.88	118.76	110.12
1	E	14	VAL	N-CA-CB	5.87	118.52	110.54
1	E	516	THR	N-CA-CB	5.87	118.74	110.12
1	J	361	ASP	CA-CB-CG	-5.87	106.73	112.60
1	M	265	ASN	CA-CB-CG	-5.86	106.74	112.60
1	J	265	ASN	CA-CB-CG	-5.86	106.74	112.60
1	N	265	ASN	CA-CB-CG	-5.86	106.74	112.60
1	B	46	ALA	CB-CA-C	-5.86	99.86	109.46
1	C	361	ASP	CB-CA-C	5.86	120.52	110.79
1	A	46	ALA	CB-CA-C	-5.85	99.86	109.46
1	E	501	ARG	N-CA-CB	-5.85	101.52	110.01
1	F	46	ALA	CB-CA-C	-5.85	99.86	109.46
1	K	361	ASP	CA-CB-CG	-5.85	106.75	112.60
1	B	361	ASP	CB-CA-C	5.85	120.50	110.79
1	E	46	ALA	CB-CA-C	-5.85	99.87	109.46
1	B	516	THR	N-CA-CB	5.85	118.72	110.12
1	D	200	LEU	N-CA-CB	5.85	118.49	110.01
1	F	501	ARG	N-CA-CB	-5.85	101.53	110.01
1	C	501	ARG	N-CA-CB	-5.85	101.53	110.01
1	G	361	ASP	CB-CA-C	5.84	120.49	110.79
1	D	62	LEU	CB-CA-C	5.84	119.29	109.48
1	A	200	LEU	N-CA-CB	5.84	118.47	110.01
1	A	361	ASP	CB-CA-C	5.84	120.48	110.79
1	H	265	ASN	CA-CB-CG	-5.84	106.76	112.60
1	B	501	ARG	N-CA-CB	-5.83	101.55	110.01
1	D	361	ASP	CB-CA-C	5.83	120.47	110.79
1	F	361	ASP	CB-CA-C	5.83	120.47	110.79
1	B	200	LEU	N-CA-CB	5.83	118.46	110.01
1	J	473	ASP	N-CA-CB	5.83	122.35	111.52
1	E	200	LEU	N-CA-CB	5.82	118.45	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	200	LEU	N-CA-CB	5.82	118.44	110.01
1	N	473	ASP	N-CA-CB	5.82	122.34	111.52
1	F	200	LEU	N-CA-CB	5.81	118.44	110.01
1	B	62	LEU	CB-CA-C	5.81	119.24	109.48
1	C	113	PRO	CA-N-CD	-5.81	103.87	112.00
1	D	501	ARG	N-CA-CB	-5.81	101.59	110.01
1	G	501	ARG	N-CA-CB	-5.81	101.59	110.01
1	E	361	ASP	CB-CA-C	5.80	120.43	110.79
1	I	473	ASP	N-CA-CB	5.80	122.31	111.52
1	C	200	LEU	N-CA-CB	5.80	118.42	110.01
1	A	501	ARG	N-CA-CB	-5.79	101.61	110.01
1	E	62	LEU	CB-CA-C	5.79	119.22	109.48
1	G	400	LEU	CA-C-N	5.79	128.05	120.28
1	G	400	LEU	C-N-CA	5.79	128.05	120.28
1	K	473	ASP	N-CA-CB	5.79	122.30	111.52
1	A	62	LEU	CB-CA-C	5.79	119.21	109.48
1	E	113	PRO	CA-N-CD	-5.79	103.89	112.00
1	D	41	ASP	CB-CA-C	5.79	120.19	109.54
1	C	41	ASP	CB-CA-C	5.78	120.18	109.54
1	M	473	ASP	N-CA-CB	5.78	122.27	111.52
1	F	41	ASP	CB-CA-C	5.78	120.17	109.54
1	H	473	ASP	N-CA-CB	5.78	122.27	111.52
1	G	41	ASP	CB-CA-C	5.77	120.17	109.54
1	B	41	ASP	CB-CA-C	5.77	120.16	109.54
1	E	41	ASP	CB-CA-C	5.77	120.15	109.54
1	F	499	VAL	N-CA-CB	5.77	118.38	110.54
1	L	473	ASP	N-CA-CB	5.76	122.24	111.52
1	A	41	ASP	CB-CA-C	5.76	120.14	109.54
1	A	499	VAL	N-CA-CB	5.76	118.38	110.54
1	C	62	LEU	CB-CA-C	5.76	119.16	109.48
1	G	62	LEU	CB-CA-C	5.76	119.16	109.48
1	F	113	PRO	CA-N-CD	-5.76	103.94	112.00
1	B	113	PRO	CA-N-CD	-5.75	103.94	112.00
1	A	113	PRO	CA-N-CD	-5.75	103.95	112.00
1	G	255	GLU	CB-CA-C	5.75	119.08	109.89
1	G	499	VAL	N-CA-CB	5.75	118.35	110.54
1	F	62	LEU	CB-CA-C	5.74	119.12	109.48
1	F	85	ALA	N-CA-CB	-5.74	101.67	110.16
1	C	391	GLU	N-CA-CB	5.74	118.55	110.12
1	G	391	GLU	N-CA-CB	5.73	118.55	110.12
1	A	391	GLU	N-CA-CB	5.72	118.53	110.12
1	D	499	VAL	N-CA-CB	5.72	118.32	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	391	GLU	N-CA-CB	5.72	118.53	110.12
1	E	255	GLU	CB-CA-C	5.72	119.04	109.89
1	B	499	VAL	N-CA-CB	5.71	118.31	110.54
1	D	113	PRO	CA-N-CD	-5.71	104.01	112.00
1	F	391	GLU	N-CA-CB	5.71	118.51	110.12
1	G	113	PRO	CA-N-CD	-5.70	104.02	112.00
1	C	499	VAL	N-CA-CB	5.70	118.29	110.54
1	A	255	GLU	CB-CA-C	5.70	119.01	109.89
1	E	85	ALA	N-CA-CB	-5.70	101.73	110.16
1	E	499	VAL	N-CA-CB	5.70	118.29	110.54
1	B	391	GLU	N-CA-CB	5.70	118.50	110.12
1	B	255	GLU	CB-CA-C	5.70	119.00	109.89
1	D	255	GLU	CB-CA-C	5.70	119.00	109.89
1	D	391	GLU	N-CA-CB	5.70	118.49	110.12
1	C	255	GLU	CB-CA-C	5.69	119.00	109.89
1	C	85	ALA	N-CA-CB	-5.69	101.74	110.16
1	G	85	ALA	N-CA-CB	-5.69	101.74	110.16
1	B	85	ALA	N-CA-CB	-5.68	101.75	110.16
1	D	85	ALA	N-CA-CB	-5.68	101.75	110.16
1	K	523	ASP	CB-CA-C	5.68	119.99	109.54
1	A	85	ALA	N-CA-CB	-5.68	101.76	110.16
1	C	400	LEU	CA-C-N	5.67	127.88	120.28
1	C	400	LEU	C-N-CA	5.67	127.88	120.28
1	F	255	GLU	CB-CA-C	5.67	118.96	109.89
1	G	60	ILE	CA-CB-CG1	5.66	120.01	110.40
1	C	60	ILE	CA-CB-CG1	5.65	120.00	110.40
1	F	60	ILE	CA-CB-CG1	5.64	119.98	110.40
1	E	60	ILE	CA-CB-CG1	5.63	119.97	110.40
1	B	60	ILE	CA-CB-CG1	5.63	119.97	110.40
1	A	60	ILE	CA-CB-CG1	5.62	119.96	110.40
1	M	59	GLU	CB-CA-C	5.62	120.52	109.72
1	E	428	ASP	CA-CB-CG	-5.62	106.98	112.60
1	G	428	ASP	CA-CB-CG	-5.62	106.98	112.60
1	A	428	ASP	CA-CB-CG	-5.62	106.98	112.60
1	D	60	ILE	CA-CB-CG1	5.62	119.95	110.40
1	F	30	THR	CA-CB-OG1	5.62	118.02	109.60
1	I	59	GLU	CB-CA-C	5.62	120.50	109.72
1	B	30	THR	CA-CB-OG1	5.61	118.01	109.60
1	C	30	THR	CA-CB-OG1	5.61	118.01	109.60
1	F	306	GLY	N-CA-C	-5.61	107.52	115.43
1	F	407	VAL	N-CA-CB	5.61	117.11	110.55
1	F	428	ASP	CA-CB-CG	-5.61	106.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	428	ASP	CA-CB-CG	-5.61	107.00	112.60
1	B	407	VAL	N-CA-CB	5.60	117.11	110.55
1	H	59	GLU	CB-CA-C	5.60	120.47	109.72
1	L	59	GLU	CB-CA-C	5.60	120.47	109.72
1	K	59	GLU	CB-CA-C	5.59	120.46	109.72
1	N	59	GLU	CB-CA-C	5.59	120.45	109.72
1	A	30	THR	CA-CB-OG1	5.58	117.98	109.60
1	D	30	THR	CA-CB-OG1	5.58	117.98	109.60
1	A	306	GLY	N-CA-C	-5.58	107.56	115.43
1	C	300	VAL	CB-CA-C	-5.58	101.96	110.95
1	E	300	VAL	CB-CA-C	-5.58	101.97	110.95
1	G	30	THR	CA-CB-OG1	5.58	117.97	109.60
1	G	300	VAL	CB-CA-C	-5.58	101.97	110.95
1	I	495	ASP	CB-CA-C	5.58	117.52	108.87
1	F	300	VAL	CB-CA-C	-5.58	101.97	110.95
1	G	306	GLY	N-CA-C	-5.58	107.56	115.43
1	B	296	THR	N-CA-CB	5.58	118.31	110.12
1	H	495	ASP	CB-CA-C	5.58	117.51	108.87
1	B	428	ASP	CA-CB-CG	-5.57	107.03	112.60
1	C	407	VAL	N-CA-CB	5.57	117.07	110.55
1	E	306	GLY	N-CA-C	-5.57	107.57	115.43
1	A	300	VAL	CB-CA-C	-5.57	101.98	110.95
1	B	306	GLY	N-CA-C	-5.57	107.58	115.43
1	D	428	ASP	CA-CB-CG	-5.57	107.03	112.60
1	E	407	VAL	N-CA-CB	5.57	117.06	110.55
1	M	495	ASP	CB-CA-C	5.57	117.50	108.87
1	B	300	VAL	CB-CA-C	-5.57	101.99	110.95
1	J	495	ASP	CB-CA-C	5.57	117.50	108.87
1	A	407	VAL	N-CA-CB	5.56	117.06	110.55
1	L	495	ASP	CB-CA-C	5.56	117.49	108.87
1	D	407	VAL	N-CA-CB	5.56	117.05	110.55
1	K	495	ASP	CB-CA-C	5.56	117.49	108.87
1	C	296	THR	N-CA-CB	5.56	118.29	110.12
1	E	296	THR	N-CA-CB	5.55	118.28	110.12
1	F	296	THR	N-CA-CB	5.55	118.28	110.12
1	D	300	VAL	CB-CA-C	-5.55	102.01	110.95
1	J	59	GLU	CB-CA-C	5.55	120.38	109.72
1	D	306	GLY	N-CA-C	-5.54	107.62	115.43
1	E	30	THR	CA-CB-OG1	5.54	117.91	109.60
1	G	407	VAL	N-CA-CB	5.54	117.03	110.55
1	C	306	GLY	N-CA-C	-5.54	107.62	115.43
1	N	495	ASP	CB-CA-C	5.54	117.45	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	THR	N-CA-CB	5.54	118.26	110.12
1	D	296	THR	N-CA-CB	5.54	118.26	110.12
1	B	473	ASP	CB-CA-C	5.53	120.97	110.51
1	D	473	ASP	CB-CA-C	5.53	120.97	110.51
1	G	473	ASP	CB-CA-C	5.53	120.96	110.51
1	B	415	GLY	N-CA-C	-5.52	107.63	115.30
1	E	473	ASP	CB-CA-C	5.52	120.94	110.51
1	B	99	ILE	N-CA-CB	5.51	117.00	110.55
1	G	296	THR	N-CA-CB	5.51	118.22	110.12
1	A	473	ASP	CB-CA-C	5.51	120.92	110.51
1	F	473	ASP	CB-CA-C	5.51	120.92	110.51
1	B	314	LEU	CB-CA-C	-5.51	101.65	110.79
1	C	473	ASP	CB-CA-C	5.51	120.92	110.51
1	E	99	ILE	N-CA-CB	5.50	116.98	110.55
1	G	415	GLY	N-CA-C	-5.50	107.66	115.30
1	C	415	GLY	N-CA-C	-5.50	107.66	115.30
1	C	242	LYS	CB-CA-C	-5.49	101.67	110.79
1	F	99	ILE	N-CA-CB	5.49	116.97	110.55
1	D	436	GLN	CB-CA-C	-5.49	101.68	110.79
1	F	314	LEU	CB-CA-C	-5.49	101.68	110.79
1	B	416	GLY	N-CA-C	-5.49	106.63	115.08
1	G	416	GLY	N-CA-C	-5.49	106.63	115.08
1	G	314	LEU	CB-CA-C	-5.48	101.69	110.79
1	D	415	GLY	N-CA-C	-5.48	107.68	115.30
1	F	242	LYS	CB-CA-C	-5.48	101.69	110.79
1	C	436	GLN	CB-CA-C	-5.47	101.71	110.79
1	E	242	LYS	CB-CA-C	-5.47	101.71	110.79
1	E	436	GLN	CB-CA-C	-5.47	101.72	110.79
1	E	416	GLY	N-CA-C	-5.46	106.67	115.08
1	A	436	GLN	CB-CA-C	-5.46	101.72	110.79
1	D	242	LYS	CB-CA-C	-5.46	101.72	110.79
1	D	314	LEU	CB-CA-C	-5.46	101.72	110.79
1	B	242	LYS	CB-CA-C	-5.46	101.72	110.79
1	D	99	ILE	N-CA-CB	5.46	116.94	110.55
1	E	314	LEU	CB-CA-C	-5.46	101.72	110.79
1	L	386	GLU	CB-CA-C	-5.46	100.53	110.63
1	F	400	LEU	CA-C-N	5.46	127.59	120.28
1	F	400	LEU	C-N-CA	5.46	127.59	120.28
1	A	314	LEU	CB-CA-C	-5.46	101.73	110.79
1	B	206	ASN	N-CA-CB	5.46	117.91	110.38
1	N	386	GLU	CB-CA-C	-5.46	100.54	110.63
1	A	242	LYS	CB-CA-C	-5.45	101.74	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	386	GLU	CB-CA-C	-5.45	100.54	110.63
1	A	415	GLY	N-CA-C	-5.45	107.72	115.30
1	B	436	GLN	CB-CA-C	-5.45	101.74	110.79
1	G	242	LYS	CB-CA-C	-5.45	101.74	110.79
1	A	99	ILE	N-CA-CB	5.45	116.93	110.55
1	C	25	ASP	CA-CB-CG	-5.45	107.15	112.60
1	F	206	ASN	N-CA-CB	5.45	117.90	110.38
1	F	436	GLN	CB-CA-C	-5.45	101.75	110.79
1	J	386	GLU	CB-CA-C	-5.45	100.55	110.63
1	G	266	THR	N-CA-CB	5.45	118.22	110.16
1	C	206	ASN	N-CA-CB	5.44	117.89	110.38
1	G	99	ILE	N-CA-CB	5.44	116.92	110.55
1	C	314	LEU	CB-CA-C	-5.44	101.76	110.79
1	D	104	LEU	CB-CA-C	5.44	119.82	110.79
1	D	266	THR	N-CA-CB	5.44	118.21	110.16
1	C	266	THR	N-CA-CB	5.44	118.21	110.16
1	F	266	THR	N-CA-CB	5.44	118.21	110.16
1	F	415	GLY	N-CA-C	-5.44	107.74	115.30
1	G	206	ASN	N-CA-CB	5.44	117.88	110.38
1	A	416	GLY	N-CA-C	-5.44	106.71	115.08
1	E	25	ASP	CA-CB-CG	-5.44	107.16	112.60
1	E	30	THR	N-CA-CB	5.44	118.11	110.12
1	G	436	GLN	CB-CA-C	-5.44	101.77	110.79
1	E	415	GLY	N-CA-C	-5.43	107.75	115.30
1	A	38	VAL	CB-CA-C	5.43	119.70	110.95
1	G	38	VAL	CB-CA-C	5.43	119.70	110.95
1	F	25	ASP	CA-CB-CG	-5.43	107.17	112.60
1	H	386	GLU	CB-CA-C	-5.43	100.58	110.63
1	A	266	THR	N-CA-CB	5.43	118.20	110.16
1	F	104	LEU	CB-CA-C	5.43	119.80	110.79
1	B	266	THR	N-CA-CB	5.43	118.19	110.16
1	E	266	THR	N-CA-CB	5.43	118.19	110.16
1	G	25	ASP	CA-CB-CG	-5.43	107.17	112.60
1	M	386	GLU	CB-CA-C	-5.43	100.59	110.63
1	C	99	ILE	N-CA-CB	5.42	116.90	110.55
1	I	386	GLU	CB-CA-C	-5.42	100.59	110.63
1	D	25	ASP	CA-CB-CG	-5.42	107.18	112.60
1	C	416	GLY	N-CA-C	-5.42	106.73	115.08
1	H	281	PHE	N-CA-CB	5.42	120.36	111.31
1	I	281	PHE	N-CA-CB	5.42	120.36	111.31
1	D	206	ASN	N-CA-CB	5.42	117.85	110.38
1	D	38	VAL	CB-CA-C	5.41	119.66	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	206	ASN	N-CA-CB	5.41	117.85	110.38
1	C	30	THR	N-CA-CB	5.41	118.07	110.12
1	B	38	VAL	CB-CA-C	5.41	119.66	110.95
1	B	104	LEU	CB-CA-C	5.40	119.76	110.79
1	F	416	GLY	N-CA-C	-5.40	106.76	115.08
1	L	281	PHE	N-CA-CB	5.40	120.33	111.31
1	M	281	PHE	N-CA-CB	5.40	120.33	111.31
1	A	104	LEU	CB-CA-C	5.40	119.76	110.79
1	B	25	ASP	CA-CB-CG	-5.40	107.20	112.60
1	E	104	LEU	CB-CA-C	5.40	119.75	110.79
1	A	25	ASP	CA-CB-CG	-5.40	107.20	112.60
1	D	416	GLY	N-CA-C	-5.40	106.77	115.08
1	J	281	PHE	N-CA-CB	5.39	120.32	111.31
1	F	38	VAL	CB-CA-C	5.39	119.63	110.95
1	F	30	THR	N-CA-CB	5.39	118.05	110.12
1	A	206	ASN	N-CA-CB	5.39	117.82	110.38
1	E	38	VAL	CB-CA-C	5.38	119.62	110.95
1	K	281	PHE	N-CA-CB	5.38	120.30	111.31
1	G	104	LEU	CB-CA-C	5.38	119.72	110.79
1	C	38	VAL	CB-CA-C	5.37	119.60	110.95
1	C	104	LEU	CB-CA-C	5.37	119.70	110.79
1	D	30	THR	N-CA-CB	5.37	118.01	110.12
1	A	30	THR	N-CA-CB	5.36	118.00	110.12
1	N	281	PHE	N-CA-CB	5.36	120.26	111.31
1	G	30	THR	N-CA-CB	5.36	117.99	110.12
1	I	523	ASP	CB-CA-C	5.36	119.39	109.54
1	F	252	GLU	N-CA-C	-5.35	105.35	111.07
1	B	30	THR	N-CA-CB	5.35	117.98	110.12
1	K	388	GLU	CB-CA-C	-5.34	102.49	110.88
1	H	388	GLU	CB-CA-C	-5.34	102.50	110.88
1	J	60	ILE	N-CA-C	5.33	116.04	107.98
1	N	388	GLU	CB-CA-C	-5.33	102.51	110.88
1	E	191	GLU	N-CA-CB	-5.33	102.50	110.17
1	I	60	ILE	N-CA-C	5.33	116.02	107.98
1	H	61	GLU	N-CA-CB	-5.33	101.86	110.81
1	L	60	ILE	N-CA-C	5.32	116.01	107.98
1	D	252	GLU	N-CA-C	-5.31	105.38	111.07
1	N	61	GLU	N-CA-CB	-5.31	101.88	110.81
1	K	60	ILE	N-CA-C	5.31	116.00	107.98
1	D	400	LEU	CA-C-N	5.31	127.40	120.28
1	D	400	LEU	C-N-CA	5.31	127.40	120.28
1	M	523	ASP	CB-CA-C	5.31	119.31	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	388	GLU	CB-CA-C	-5.31	102.55	110.88
1	I	61	GLU	N-CA-CB	-5.30	101.90	110.81
1	E	400	LEU	CA-C-N	5.30	127.39	120.28
1	E	400	LEU	C-N-CA	5.30	127.39	120.28
1	G	321	LYS	CB-CA-C	5.30	119.20	110.88
1	K	61	GLU	N-CA-CB	-5.30	101.90	110.81
1	L	61	GLU	N-CA-CB	-5.30	101.90	110.81
1	M	61	GLU	N-CA-CB	-5.30	101.90	110.81
1	M	388	GLU	CB-CA-C	-5.30	102.56	110.88
1	A	53	GLY	N-CA-C	-5.29	106.38	112.73
1	M	60	ILE	N-CA-C	5.29	115.97	107.98
1	E	205	ILE	CB-CA-C	5.29	119.97	111.29
1	G	252	GLU	N-CA-C	-5.29	105.41	111.07
1	E	37	ASN	N-CA-CB	5.29	117.79	110.17
1	H	523	ASP	CB-CA-C	5.29	119.27	109.54
1	A	321	LYS	CB-CA-C	5.29	119.18	110.88
1	J	388	GLU	CB-CA-C	-5.29	102.58	110.88
1	A	37	ASN	N-CA-CB	5.29	117.78	110.17
1	C	110	GLY	N-CA-C	-5.29	107.98	115.43
1	B	37	ASN	N-CA-CB	5.28	117.78	110.17
1	C	53	GLY	N-CA-C	-5.28	106.39	112.73
1	D	321	LYS	CB-CA-C	5.28	119.17	110.88
1	F	321	LYS	CB-CA-C	5.28	119.18	110.88
1	G	37	ASN	N-CA-CB	5.28	117.78	110.17
1	E	321	LYS	CB-CA-C	5.28	119.17	110.88
1	L	523	ASP	CB-CA-C	5.28	119.26	109.54
1	F	110	GLY	N-CA-C	-5.28	107.99	115.43
1	H	60	ILE	N-CA-C	5.28	115.95	107.98
1	J	523	ASP	CB-CA-C	5.28	119.25	109.54
1	C	235	PRO	N-CA-CB	5.27	109.09	103.39
1	B	53	GLY	N-CA-C	-5.27	106.40	112.73
1	C	205	ILE	CB-CA-C	5.27	119.94	111.29
1	A	205	ILE	CB-CA-C	5.27	119.94	111.29
1	B	205	ILE	CB-CA-C	5.27	119.93	111.29
1	D	37	ASN	N-CA-CB	5.27	117.76	110.17
1	G	205	ILE	CB-CA-C	5.27	119.93	111.29
1	N	523	ASP	CB-CA-C	5.27	119.23	109.54
1	F	205	ILE	CB-CA-C	5.27	119.93	111.29
1	G	410	GLY	N-CA-C	-5.26	105.96	112.33
1	A	252	GLU	N-CA-C	-5.26	105.44	111.07
1	C	37	ASN	N-CA-CB	5.26	117.75	110.17
1	L	388	GLU	CB-CA-C	-5.26	102.62	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	LYS	CB-CA-C	5.26	119.14	110.88
1	D	205	ILE	CB-CA-C	5.26	119.91	111.29
1	G	53	GLY	N-CA-C	-5.26	106.42	112.73
1	G	110	GLY	N-CA-C	-5.26	108.02	115.43
1	N	60	ILE	N-CA-C	5.26	115.92	107.98
1	C	252	GLU	N-CA-C	-5.25	105.45	111.07
1	F	410	GLY	N-CA-C	-5.25	105.97	112.33
1	D	53	GLY	N-CA-C	-5.24	106.44	112.73
1	G	458	CYS	N-CA-CB	5.24	117.83	110.12
1	A	235	PRO	N-CA-CB	5.24	109.05	103.39
1	B	321	LYS	CB-CA-C	5.24	119.11	110.88
1	E	252	GLU	N-CA-C	-5.24	105.47	111.07
1	B	252	GLU	N-CA-C	-5.24	105.47	111.07
1	F	37	ASN	N-CA-CB	5.24	117.71	110.17
1	D	410	GLY	N-CA-C	-5.24	105.99	112.33
1	D	458	CYS	N-CA-CB	5.23	117.81	110.12
1	A	110	GLY	N-CA-C	-5.23	108.06	115.43
1	E	235	PRO	N-CA-CB	5.23	109.04	103.39
1	E	458	CYS	N-CA-CB	5.23	117.81	110.12
1	C	458	CYS	N-CA-CB	5.22	117.80	110.12
1	B	458	CYS	N-CA-CB	5.22	117.80	110.12
1	D	235	PRO	N-CA-CB	5.22	109.03	103.39
1	C	410	GLY	N-CA-C	-5.21	106.02	112.33
1	A	458	CYS	N-CA-CB	5.21	117.78	110.12
1	F	235	PRO	N-CA-CB	5.21	109.02	103.39
1	B	110	GLY	N-CA-C	-5.20	108.10	115.43
1	G	194	GLN	N-CA-CB	-5.20	101.94	110.68
1	G	235	PRO	N-CA-CB	5.20	109.00	103.39
1	F	458	CYS	N-CA-CB	5.20	117.76	110.12
1	C	261	THR	N-CA-CB	5.20	117.54	110.01
1	F	53	GLY	N-CA-C	-5.20	106.50	112.73
1	E	110	GLY	N-CA-C	-5.19	108.11	115.43
1	A	410	GLY	N-CA-C	-5.19	106.05	112.33
1	K	400	LEU	O-C-N	5.19	127.62	122.12
1	B	261	THR	N-CA-CB	5.19	117.53	110.01
1	E	53	GLY	N-CA-C	-5.19	106.50	112.73
1	A	169	VAL	CB-CA-C	5.18	119.38	112.22
1	E	410	GLY	N-CA-C	-5.18	106.06	112.33
1	D	169	VAL	CB-CA-C	5.18	119.37	112.22
1	M	334	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	169	VAL	CB-CA-C	5.18	119.37	112.22
1	B	410	GLY	N-CA-C	-5.17	106.07	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	VAL	CB-CA-C	5.17	119.35	112.22
1	E	169	VAL	CB-CA-C	5.17	119.35	112.22
1	D	110	GLY	N-CA-C	-5.16	108.15	115.43
1	H	334	ASP	CA-CB-CG	5.16	117.76	112.60
1	D	224	ASP	N-CA-CB	5.16	117.80	110.16
1	F	169	VAL	CB-CA-C	5.16	119.34	112.22
1	A	191	GLU	N-CA-CB	-5.16	102.45	110.29
1	G	191	GLU	N-CA-CB	-5.16	102.45	110.29
1	B	235	PRO	N-CA-CB	5.16	108.96	103.39
1	D	191	GLU	N-CA-CB	-5.16	102.45	110.29
1	F	194	GLN	N-CA-CB	-5.16	102.02	110.68
1	C	194	GLN	N-CA-CB	-5.15	102.02	110.68
1	C	224	ASP	N-CA-CB	5.15	117.78	110.16
1	D	194	GLN	N-CA-CB	-5.15	102.03	110.68
1	E	194	GLN	N-CA-CB	-5.15	102.03	110.68
1	C	191	GLU	N-CA-CB	-5.14	102.47	110.29
1	L	334	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	194	GLN	N-CA-CB	-5.14	102.04	110.68
1	B	194	GLN	N-CA-CB	-5.14	102.04	110.68
1	I	334	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	191	GLU	N-CA-CB	-5.14	102.48	110.29
1	E	224	ASP	N-CA-CB	5.14	117.76	110.16
1	N	334	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	224	ASP	N-CA-CB	5.13	117.76	110.16
1	J	334	ASP	CA-CB-CG	5.13	117.73	112.60
1	G	169	VAL	CB-CA-C	5.13	119.30	112.22
1	L	328	ASP	N-CA-CB	-5.13	103.65	111.66
1	A	261	THR	N-CA-CB	5.13	117.45	110.01
1	G	224	ASP	N-CA-CB	5.13	117.75	110.16
1	J	61	GLU	N-CA-CB	-5.13	102.20	110.81
1	K	328	ASP	N-CA-CB	-5.12	103.67	111.66
1	E	261	THR	N-CA-CB	5.12	117.44	110.01
1	F	191	GLU	N-CA-CB	-5.12	102.51	110.29
1	F	224	ASP	N-CA-CB	5.12	117.74	110.16
1	G	261	THR	N-CA-CB	5.12	117.43	110.01
1	D	261	THR	N-CA-CB	5.11	117.42	110.01
1	E	265	ASN	CA-CB-CG	-5.10	107.50	112.60
1	I	328	ASP	N-CA-CB	-5.10	103.70	111.66
1	F	261	THR	N-CA-CB	5.10	117.40	110.01
1	K	334	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	224	ASP	N-CA-CB	5.09	117.70	110.16
1	J	230	ILE	CB-CA-C	-5.09	103.86	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	328	ASP	N-CA-CB	-5.09	103.72	111.66
1	A	438	VAL	N-CA-CB	5.08	117.45	110.54
1	E	438	VAL	N-CA-CB	5.08	117.45	110.54
1	H	463	SER	N-CA-CB	-5.08	102.12	110.40
1	N	230	ILE	CB-CA-C	-5.08	103.89	112.16
1	L	230	ILE	CB-CA-C	-5.07	103.90	112.16
1	C	438	VAL	N-CA-CB	5.07	117.43	110.54
1	C	265	ASN	CA-CB-CG	-5.07	107.53	112.60
1	J	463	SER	N-CA-CB	-5.07	102.14	110.40
1	H	230	ILE	CB-CA-C	-5.06	103.91	112.16
1	A	59	GLU	CB-CG-CD	5.06	121.21	112.60
1	J	328	ASP	N-CA-CB	-5.06	103.76	111.66
1	K	463	SER	N-CA-CB	-5.06	102.15	110.40
1	M	463	SER	N-CA-CB	-5.06	102.15	110.40
1	A	107	VAL	N-CA-CB	5.06	117.42	110.54
1	B	59	GLU	CB-CG-CD	5.06	121.20	112.60
1	I	463	SER	N-CA-CB	-5.06	102.15	110.40
1	M	230	ILE	CB-CA-C	-5.06	103.91	112.16
1	B	265	ASN	CA-CB-CG	-5.06	107.54	112.60
1	I	401	HIS	CA-C-N	5.06	127.47	120.29
1	I	401	HIS	C-N-CA	5.06	127.47	120.29
1	D	438	VAL	N-CA-CB	5.05	117.42	110.54
1	F	438	VAL	N-CA-CB	5.05	117.41	110.54
1	G	265	ASN	CA-CB-CG	-5.05	107.55	112.60
1	M	328	ASP	N-CA-CB	-5.05	103.77	111.66
1	E	59	GLU	CB-CG-CD	5.05	121.19	112.60
1	F	59	GLU	CB-CG-CD	5.05	121.19	112.60
1	K	230	ILE	CB-CA-C	-5.05	103.93	112.16
1	L	463	SER	N-CA-CB	-5.05	102.17	110.40
1	I	230	ILE	CB-CA-C	-5.05	103.93	112.16
1	N	328	ASP	N-CA-CB	-5.05	103.79	111.66
1	B	438	VAL	N-CA-CB	5.04	117.40	110.54
1	G	59	GLU	CB-CG-CD	5.04	121.17	112.60
1	G	107	VAL	N-CA-CB	5.04	117.40	110.54
1	D	59	GLU	CB-CG-CD	5.03	121.16	112.60
1	G	438	VAL	N-CA-CB	5.03	117.38	110.54
1	N	463	SER	N-CA-CB	-5.03	102.20	110.40
1	C	59	GLU	CB-CG-CD	5.03	121.15	112.60
1	A	170	GLY	N-CA-C	-5.03	105.45	112.18
1	C	107	VAL	N-CA-CB	5.03	117.37	110.54
1	F	170	GLY	N-CA-C	-5.03	105.45	112.18
1	D	518	GLU	N-CA-CB	5.02	117.59	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	170	GLY	N-CA-C	-5.02	105.45	112.18
1	E	107	VAL	N-CA-CB	5.02	117.37	110.54
1	F	107	VAL	N-CA-CB	5.02	117.36	110.54
1	D	107	VAL	N-CA-CB	5.01	117.36	110.54
1	D	265	ASN	CA-CB-CG	-5.01	107.59	112.60
1	B	107	VAL	N-CA-CB	5.01	117.35	110.54
1	B	518	GLU	N-CA-CB	5.01	117.57	110.16
1	E	33	PRO	N-CA-C	-5.01	107.33	113.84
1	A	518	GLU	N-CA-CB	5.00	117.56	110.16
1	C	170	GLY	N-CA-C	-5.00	105.48	112.18
1	F	265	ASN	CA-CB-CG	-5.00	107.60	112.60
1	G	170	GLY	N-CA-C	-5.00	105.47	112.18

There are no chirality outliers.

All (138) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	197	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	268	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	36	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	395	ARG	Sidechain
1	A	404	ARG	Sidechain
1	B	13	ARG	Sidechain
1	B	197	ARG	Sidechain
1	B	231	ARG	Sidechain
1	B	268	ARG	Sidechain
1	B	350	ARG	Sidechain
1	B	36	ARG	Sidechain
1	B	362	ARG	Sidechain
1	B	395	ARG	Sidechain
1	B	404	ARG	Sidechain
1	C	13	ARG	Sidechain
1	C	197	ARG	Sidechain
1	C	219	PHE	Sidechain
1	C	231	ARG	Sidechain
1	C	268	ARG	Sidechain
1	C	350	ARG	Sidechain
1	C	36	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	362	ARG	Sidechain
1	C	395	ARG	Sidechain
1	C	404	ARG	Sidechain
1	D	13	ARG	Sidechain
1	D	197	ARG	Sidechain
1	D	219	PHE	Sidechain
1	D	231	ARG	Sidechain
1	D	268	ARG	Sidechain
1	D	350	ARG	Sidechain
1	D	36	ARG	Sidechain
1	D	362	ARG	Sidechain
1	D	395	ARG	Sidechain
1	D	404	ARG	Sidechain
1	E	13	ARG	Sidechain
1	E	197	ARG	Sidechain
1	E	231	ARG	Sidechain
1	E	268	ARG	Sidechain
1	E	350	ARG	Sidechain
1	E	36	ARG	Sidechain
1	E	362	ARG	Sidechain
1	E	395	ARG	Sidechain
1	E	404	ARG	Sidechain
1	F	13	ARG	Sidechain
1	F	197	ARG	Sidechain
1	F	219	PHE	Sidechain
1	F	231	ARG	Sidechain
1	F	268	ARG	Sidechain
1	F	350	ARG	Sidechain
1	F	36	ARG	Sidechain
1	F	362	ARG	Sidechain
1	F	395	ARG	Sidechain
1	F	404	ARG	Sidechain
1	G	13	ARG	Sidechain
1	G	197	ARG	Sidechain
1	G	231	ARG	Sidechain
1	G	268	ARG	Sidechain
1	G	350	ARG	Sidechain
1	G	36	ARG	Sidechain
1	G	362	ARG	Sidechain
1	G	395	ARG	Sidechain
1	G	404	ARG	Sidechain
1	H	118	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	H	197	ARG	Sidechain
1	H	231	ARG	Sidechain
1	H	284	ARG	Sidechain
1	H	285	ARG	Sidechain
1	H	350	ARG	Sidechain
1	H	362	ARG	Sidechain
1	H	421	ARG	Sidechain
1	H	445	ARG	Sidechain
1	H	478	TYR	Sidechain
1	I	118	ARG	Sidechain
1	I	197	ARG	Sidechain
1	I	231	ARG	Sidechain
1	I	284	ARG	Sidechain
1	I	285	ARG	Sidechain
1	I	350	ARG	Sidechain
1	I	362	ARG	Sidechain
1	I	421	ARG	Sidechain
1	I	445	ARG	Sidechain
1	I	478	TYR	Sidechain
1	J	118	ARG	Sidechain
1	J	197	ARG	Sidechain
1	J	231	ARG	Sidechain
1	J	284	ARG	Sidechain
1	J	285	ARG	Sidechain
1	J	350	ARG	Sidechain
1	J	362	ARG	Sidechain
1	J	421	ARG	Sidechain
1	J	445	ARG	Sidechain
1	J	478	TYR	Sidechain
1	K	118	ARG	Sidechain
1	K	197	ARG	Sidechain
1	K	231	ARG	Sidechain
1	K	284	ARG	Sidechain
1	K	285	ARG	Sidechain
1	K	350	ARG	Sidechain
1	K	362	ARG	Sidechain
1	K	421	ARG	Sidechain
1	K	445	ARG	Sidechain
1	K	478	TYR	Sidechain
1	L	118	ARG	Sidechain
1	L	197	ARG	Sidechain
1	L	231	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	L	284	ARG	Sidechain
1	L	285	ARG	Sidechain
1	L	350	ARG	Sidechain
1	L	362	ARG	Sidechain
1	L	401	HIS	Mainchain
1	L	421	ARG	Sidechain
1	L	445	ARG	Sidechain
1	L	478	TYR	Sidechain
1	M	118	ARG	Sidechain
1	M	197	ARG	Sidechain
1	M	231	ARG	Sidechain
1	M	284	ARG	Sidechain
1	M	285	ARG	Sidechain
1	M	350	ARG	Sidechain
1	M	362	ARG	Sidechain
1	M	421	ARG	Sidechain
1	M	445	ARG	Sidechain
1	M	478	TYR	Sidechain
1	N	118	ARG	Sidechain
1	N	197	ARG	Sidechain
1	N	231	ARG	Sidechain
1	N	284	ARG	Sidechain
1	N	285	ARG	Sidechain
1	N	350	ARG	Sidechain
1	N	362	ARG	Sidechain
1	N	401	HIS	Mainchain
1	N	421	ARG	Sidechain
1	N	445	ARG	Sidechain
1	N	478	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3846	0	3970	209	0
1	B	3846	0	3970	209	0
1	C	3846	0	3970	209	0
1	D	3846	0	3970	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3846	0	3970	214	0
1	F	3846	0	3970	214	0
1	G	3846	0	3970	212	0
1	H	3846	0	3970	31	0
1	I	3846	0	3970	30	0
1	J	3846	0	3969	31	0
1	K	3846	0	3969	29	0
1	L	3846	0	3969	30	0
1	M	3846	0	3970	29	0
1	N	3846	0	3968	33	0
2	A	31	12	12	4	0
2	B	31	12	12	3	0
2	C	31	12	12	3	0
2	D	31	12	12	3	0
2	E	31	12	12	3	0
2	F	31	12	12	4	0
2	G	31	12	12	4	0
3	A	1	0	0	5	0
3	B	1	0	0	4	0
3	C	1	0	0	4	0
3	D	1	0	0	4	0
3	E	1	0	0	4	0
3	F	1	0	0	5	0
3	G	1	0	0	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
All	All	54075	84	55659	1336	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 12.

All (1336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:400:LEU:C	1:J:401:HIS:N	1.72	1.48
1:L:400:LEU:C	1:L:401:HIS:N	1.78	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASP:H	1:B:36:ARG:CZ	1.37	1.37
1:C:115:ASP:H	1:D:36:ARG:CZ	1.37	1.37
1:D:115:ASP:H	1:E:36:ARG:CZ	1.37	1.36
1:N:400:LEU:C	1:N:401:HIS:N	1.83	1.36
1:A:116:LEU:H	1:B:36:ARG:NH1	1.24	1.36
1:C:116:LEU:H	1:D:36:ARG:NH1	1.24	1.36
1:B:115:ASP:H	1:C:36:ARG:CZ	1.37	1.36
1:F:115:ASP:H	1:G:36:ARG:CZ	1.37	1.35
1:A:36:ARG:CZ	1:G:115:ASP:H	1.37	1.35
1:E:115:ASP:H	1:F:36:ARG:CZ	1.37	1.34
1:E:116:LEU:H	1:F:36:ARG:NH1	1.24	1.33
1:F:116:LEU:H	1:G:36:ARG:NH1	1.24	1.33
1:D:116:LEU:H	1:E:36:ARG:NH1	1.24	1.33
1:A:36:ARG:NH1	1:G:116:LEU:H	1.24	1.32
1:B:116:LEU:H	1:C:36:ARG:NH1	1.24	1.32
1:B:116:LEU:N	1:C:36:ARG:HH12	1.29	1.30
1:A:36:ARG:HH12	1:G:116:LEU:N	1.30	1.29
1:C:116:LEU:N	1:D:36:ARG:HH12	1.30	1.29
1:D:116:LEU:N	1:E:36:ARG:HH12	1.29	1.29
1:E:116:LEU:N	1:F:36:ARG:HH12	1.30	1.28
1:A:116:LEU:N	1:B:36:ARG:HH12	1.30	1.27
1:F:116:LEU:N	1:G:36:ARG:HH12	1.30	1.26
1:C:113:PRO:C	1:D:36:ARG:HH11	1.59	1.11
1:A:36:ARG:HH11	1:G:113:PRO:C	1.59	1.11
1:D:113:PRO:C	1:E:36:ARG:HH11	1.59	1.11
1:F:113:PRO:C	1:G:36:ARG:HH11	1.59	1.11
1:A:113:PRO:C	1:B:36:ARG:HH11	1.59	1.11
1:B:113:PRO:C	1:C:36:ARG:HH11	1.59	1.11
1:E:113:PRO:C	1:F:36:ARG:HH11	1.59	1.11
1:A:113:PRO:C	1:B:36:ARG:NH1	2.09	1.10
1:A:36:ARG:NH1	1:G:113:PRO:C	2.10	1.10
1:B:113:PRO:C	1:C:36:ARG:NH1	2.10	1.10
1:A:112:ASN:O	1:B:36:ARG:NH1	1.85	1.10
1:F:112:ASN:O	1:G:36:ARG:NH1	1.85	1.10
1:C:112:ASN:O	1:D:36:ARG:NH1	1.85	1.10
1:F:113:PRO:C	1:G:36:ARG:NH1	2.10	1.10
1:C:113:PRO:C	1:D:36:ARG:NH1	2.10	1.10
1:E:112:ASN:O	1:F:36:ARG:NH1	1.85	1.09
1:E:113:PRO:C	1:F:36:ARG:NH1	2.10	1.09
1:B:112:ASN:O	1:C:36:ARG:NH1	1.85	1.09
1:D:113:PRO:C	1:E:36:ARG:NH1	2.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:NH1	1:G:112:ASN:O	1.84	1.08
1:D:112:ASN:O	1:E:36:ARG:NH1	1.85	1.08
1:B:115:ASP:N	1:C:36:ARG:CZ	2.18	1.07
1:C:115:ASP:N	1:D:36:ARG:CZ	2.18	1.07
1:A:115:ASP:N	1:B:36:ARG:CZ	2.18	1.06
1:A:36:ARG:CZ	1:G:115:ASP:N	2.18	1.06
1:F:115:ASP:N	1:G:36:ARG:CZ	2.18	1.05
1:D:115:ASP:N	1:E:36:ARG:CZ	2.18	1.05
1:E:115:ASP:N	1:F:36:ARG:CZ	2.18	1.05
1:C:115:ASP:N	1:D:36:ARG:NH1	2.05	1.05
1:D:115:ASP:N	1:E:36:ARG:NH1	2.05	1.05
1:B:115:ASP:N	1:C:36:ARG:NH1	2.05	1.04
1:E:115:ASP:N	1:F:36:ARG:NH1	2.05	1.04
1:F:115:ASP:N	1:G:36:ARG:NH1	2.05	1.03
1:A:36:ARG:NH1	1:G:115:ASP:N	2.05	1.03
1:A:115:ASP:N	1:B:36:ARG:NH1	2.05	1.02
1:B:112:ASN:O	1:C:36:ARG:CZ	2.08	1.02
1:D:112:ASN:O	1:E:36:ARG:CZ	2.08	1.01
1:A:36:ARG:CZ	1:G:112:ASN:O	2.08	1.01
1:F:112:ASN:O	1:G:36:ARG:CZ	2.08	1.01
1:C:112:ASN:O	1:D:36:ARG:CZ	2.08	1.01
1:E:112:ASN:O	1:F:36:ARG:CZ	2.08	1.01
1:A:112:ASN:O	1:B:36:ARG:CZ	2.08	1.00
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.51	0.93
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.50	0.92
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.51	0.92
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.51	0.91
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.50	0.91
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.51	0.91
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.50	0.90
1:E:114:MET:N	1:F:36:ARG:CZ	2.38	0.87
1:D:114:MET:N	1:E:36:ARG:CZ	2.38	0.87
1:A:36:ARG:CZ	1:G:114:MET:N	2.38	0.87
1:F:114:MET:N	1:G:36:ARG:CZ	2.38	0.87
1:C:114:MET:N	1:D:36:ARG:CZ	2.38	0.86
1:B:114:MET:N	1:C:36:ARG:CZ	2.38	0.86
1:A:114:MET:N	1:B:36:ARG:CZ	2.38	0.86
1:B:112:ASN:C	1:C:36:ARG:CZ	2.49	0.86
1:C:112:ASN:C	1:D:36:ARG:CZ	2.49	0.86
1:E:112:ASN:C	1:F:36:ARG:CZ	2.49	0.86
1:F:112:ASN:C	1:G:36:ARG:CZ	2.49	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASN:C	1:B:36:ARG:CZ	2.49	0.85
1:D:112:ASN:C	1:E:36:ARG:CZ	2.49	0.85
1:A:36:ARG:CZ	1:G:112:ASN:C	2.49	0.84
1:A:49:ILE:HD11	1:G:513:LEU:HA	1.61	0.83
1:F:513:LEU:HA	1:G:49:ILE:HD11	1.61	0.83
1:E:513:LEU:HA	1:F:49:ILE:HD11	1.61	0.83
1:A:513:LEU:HA	1:B:49:ILE:HD11	1.61	0.82
1:D:513:LEU:HA	1:E:49:ILE:HD11	1.61	0.82
1:C:513:LEU:HA	1:D:49:ILE:HD11	1.61	0.82
1:B:513:LEU:HA	1:C:49:ILE:HD11	1.61	0.82
1:A:183:LEU:O	1:A:382:GLY:HA3	1.82	0.80
1:B:183:LEU:O	1:B:382:GLY:HA3	1.82	0.80
1:C:183:LEU:O	1:C:382:GLY:HA3	1.82	0.80
1:F:183:LEU:O	1:F:382:GLY:HA3	1.82	0.80
1:D:183:LEU:O	1:D:382:GLY:HA3	1.82	0.80
1:B:114:MET:H	1:C:36:ARG:NE	1.80	0.79
1:G:183:LEU:O	1:G:382:GLY:HA3	1.82	0.79
1:D:114:MET:H	1:E:36:ARG:NE	1.80	0.79
1:E:114:MET:H	1:F:36:ARG:NE	1.81	0.79
1:E:116:LEU:N	1:F:36:ARG:NH1	2.05	0.79
1:E:183:LEU:O	1:E:382:GLY:HA3	1.82	0.79
1:A:36:ARG:NE	1:G:114:MET:H	1.80	0.79
1:A:113:PRO:CA	1:B:36:ARG:HH11	1.96	0.79
1:C:114:MET:H	1:D:36:ARG:NE	1.80	0.78
1:A:114:MET:H	1:B:36:ARG:NE	1.80	0.78
1:F:114:MET:H	1:G:36:ARG:NE	1.80	0.78
1:E:199:TYR:CD2	1:E:205:ILE:HD11	2.19	0.78
1:F:199:TYR:CD2	1:F:205:ILE:HD11	2.19	0.78
1:A:199:TYR:CD2	1:A:205:ILE:HD11	2.19	0.78
1:A:135:SER:HA	1:A:412:VAL:HG12	1.66	0.78
1:B:199:TYR:CD2	1:B:205:ILE:HD11	2.19	0.78
1:C:113:PRO:CA	1:D:36:ARG:HH11	1.96	0.78
1:E:115:ASP:HB2	1:F:36:ARG:HH22	1.49	0.78
1:G:199:TYR:CD2	1:G:205:ILE:HD11	2.19	0.78
1:D:113:PRO:CA	1:E:36:ARG:HH11	1.96	0.78
1:D:115:ASP:HB2	1:E:36:ARG:HH22	1.49	0.78
1:F:113:PRO:CA	1:G:36:ARG:HH11	1.96	0.78
1:F:115:ASP:HB2	1:G:36:ARG:HH22	1.49	0.78
1:B:135:SER:HA	1:B:412:VAL:HG12	1.66	0.78
1:D:199:TYR:CD2	1:D:205:ILE:HD11	2.19	0.77
1:G:135:SER:HA	1:G:412:VAL:HG12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PRO:CA	1:C:36:ARG:HH11	1.96	0.77
1:A:36:ARG:HH22	1:G:115:ASP:HB2	1.49	0.77
1:A:36:ARG:HH11	1:G:113:PRO:CA	1.96	0.77
1:C:135:SER:HA	1:C:412:VAL:HG12	1.66	0.77
1:C:199:TYR:CD2	1:C:205:ILE:HD11	2.19	0.77
1:E:113:PRO:CA	1:F:36:ARG:HH11	1.96	0.77
1:D:198:GLY:HA2	1:D:327:LYS:O	1.86	0.76
1:F:198:GLY:HA2	1:F:327:LYS:O	1.86	0.76
1:B:115:ASP:HB2	1:C:36:ARG:HH22	1.49	0.76
1:F:135:SER:HA	1:F:412:VAL:HG12	1.66	0.76
1:G:198:GLY:HA2	1:G:327:LYS:O	1.86	0.76
1:C:115:ASP:HB2	1:D:36:ARG:HH22	1.49	0.76
1:D:135:SER:HA	1:D:412:VAL:HG12	1.66	0.76
1:C:198:GLY:HA2	1:C:327:LYS:O	1.86	0.75
1:D:115:ASP:H	1:E:36:ARG:NH1	1.84	0.75
1:D:116:LEU:N	1:E:36:ARG:NH1	2.05	0.75
1:E:135:SER:HA	1:E:412:VAL:HG12	1.66	0.75
1:A:115:ASP:HB2	1:B:36:ARG:HH22	1.49	0.75
1:A:198:GLY:HA2	1:A:327:LYS:O	1.86	0.75
1:C:115:ASP:H	1:D:36:ARG:NH1	1.84	0.75
1:B:115:ASP:H	1:C:36:ARG:NH1	1.84	0.75
1:B:198:GLY:HA2	1:B:327:LYS:O	1.86	0.74
1:E:198:GLY:HA2	1:E:327:LYS:O	1.86	0.74
1:A:30:THR:HG22	1:A:38:VAL:HG21	1.69	0.74
1:A:36:ARG:CZ	1:A:36:ARG:NH1	2.51	0.74
1:B:521:VAL:HG21	1:C:59:GLU:HB3	1.70	0.74
1:G:36:ARG:CZ	1:G:36:ARG:NH1	2.51	0.74
1:D:30:THR:HG22	1:D:38:VAL:HG21	1.69	0.74
1:A:36:ARG:NH1	1:G:115:ASP:H	1.84	0.73
1:F:521:VAL:HG21	1:G:59:GLU:HB3	1.70	0.73
1:G:30:THR:HG22	1:G:38:VAL:HG21	1.69	0.73
1:A:115:ASP:H	1:B:36:ARG:NH1	1.84	0.73
1:D:36:ARG:CZ	1:D:36:ARG:NH1	2.51	0.73
1:C:521:VAL:HG21	1:D:59:GLU:HB3	1.70	0.73
1:F:36:ARG:CZ	1:F:36:ARG:NH1	2.51	0.73
1:E:30:THR:HG22	1:E:38:VAL:HG21	1.69	0.73
1:A:36:ARG:NH1	1:G:116:LEU:N	2.05	0.73
1:B:30:THR:HG22	1:B:38:VAL:HG21	1.69	0.73
1:B:36:ARG:CZ	1:B:36:ARG:NH1	2.51	0.73
1:C:30:THR:HG22	1:C:38:VAL:HG21	1.69	0.73
1:E:521:VAL:HG21	1:F:59:GLU:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:VAL:HG21	1:B:59:GLU:HB3	1.70	0.73
1:C:36:ARG:CZ	1:C:36:ARG:NH1	2.51	0.73
1:D:521:VAL:HG21	1:E:59:GLU:HB3	1.70	0.72
1:F:30:THR:HG22	1:F:38:VAL:HG21	1.69	0.72
3:E:1526:PO4:P	2:E:1527:ATP:O1G	2.48	0.72
3:G:1525:PO4:P	2:G:1527:ATP:O1G	2.48	0.72
1:A:59:GLU:HB3	1:G:521:VAL:HG21	1.70	0.72
1:E:36:ARG:CZ	1:E:36:ARG:NH1	2.51	0.72
1:F:115:ASP:H	1:G:36:ARG:NH1	1.84	0.72
3:F:1525:PO4:P	2:F:1527:ATP:O1G	2.48	0.72
2:D:1525:ATP:O1G	3:D:1526:PO4:P	2.48	0.72
2:C:1526:ATP:O1G	3:C:1527:PO4:P	2.48	0.71
2:A:1525:ATP:O1G	3:A:1526:PO4:P	2.48	0.71
1:L:181:THR:O	1:M:283:ASP:N	2.24	0.71
1:M:181:THR:O	1:N:283:ASP:N	2.24	0.71
1:E:115:ASP:H	1:F:36:ARG:NH1	1.84	0.71
1:E:115:ASP:H	1:F:36:ARG:NH2	1.86	0.71
2:B:1525:ATP:O1G	3:B:1526:PO4:P	2.48	0.71
2:B:1525:ATP:O1A	3:B:1526:PO4:P	2.49	0.71
1:L:400:LEU:C	1:L:401:HIS:CA	2.63	0.71
1:D:115:ASP:H	1:E:36:ARG:NH2	1.86	0.71
2:D:1525:ATP:O1A	3:D:1526:PO4:P	2.49	0.71
1:I:181:THR:O	1:J:283:ASP:N	2.23	0.70
1:F:115:ASP:H	1:G:36:ARG:NH2	1.86	0.70
3:E:1526:PO4:P	2:E:1527:ATP:O1A	2.49	0.70
1:J:181:THR:O	1:K:283:ASP:N	2.24	0.70
3:G:1525:PO4:P	2:G:1527:ATP:O1A	2.49	0.70
2:C:1526:ATP:O1A	3:C:1527:PO4:P	2.49	0.70
3:F:1525:PO4:P	2:F:1527:ATP:O1A	2.49	0.70
1:K:181:THR:O	1:L:283:ASP:N	2.23	0.70
2:A:1525:ATP:O1A	3:A:1526:PO4:P	2.49	0.70
1:D:191:GLU:O	1:D:334:ASP:HA	1.92	0.70
1:C:115:ASP:H	1:D:36:ARG:NH2	1.86	0.70
1:C:191:GLU:O	1:C:334:ASP:HA	1.92	0.70
1:H:283:ASP:N	1:N:181:THR:O	2.24	0.70
1:A:36:ARG:NH2	1:G:115:ASP:H	1.86	0.69
1:B:116:LEU:N	1:C:36:ARG:NH1	2.05	0.69
1:E:191:GLU:O	1:E:334:ASP:HA	1.92	0.69
1:H:181:THR:O	1:I:283:ASP:N	2.24	0.69
1:C:116:LEU:N	1:D:36:ARG:NH1	2.05	0.69
1:B:115:ASP:H	1:C:36:ARG:NH2	1.86	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASP:H	1:B:36:ARG:NH2	1.86	0.69
1:F:191:GLU:O	1:F:334:ASP:HA	1.92	0.69
1:B:191:GLU:O	1:B:334:ASP:HA	1.92	0.69
1:G:191:GLU:O	1:G:334:ASP:HA	1.92	0.69
1:A:191:GLU:O	1:A:334:ASP:HA	1.92	0.68
1:E:517:THR:HB	1:F:39:VAL:HB	1.76	0.68
1:B:114:MET:H	1:C:36:ARG:CZ	2.05	0.68
1:F:517:THR:HB	1:G:39:VAL:HB	1.76	0.68
1:D:517:THR:HB	1:E:39:VAL:HB	1.76	0.68
1:F:114:MET:H	1:G:36:ARG:CZ	2.06	0.68
1:A:6:VAL:HG22	1:A:521:VAL:HG22	1.76	0.68
1:B:6:VAL:HG22	1:B:521:VAL:HG22	1.76	0.68
1:F:116:LEU:N	1:G:36:ARG:NH1	2.05	0.68
1:E:114:MET:H	1:F:36:ARG:CZ	2.05	0.67
1:C:6:VAL:HG22	1:C:521:VAL:HG22	1.76	0.67
1:A:36:ARG:CZ	1:G:114:MET:H	2.05	0.67
1:B:517:THR:HB	1:C:39:VAL:HB	1.76	0.67
1:G:6:VAL:HG22	1:G:521:VAL:HG22	1.76	0.67
1:A:517:THR:HB	1:B:39:VAL:HB	1.76	0.66
1:A:116:LEU:N	1:B:36:ARG:NH1	2.05	0.66
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.78	0.66
1:C:517:THR:HB	1:D:39:VAL:HB	1.76	0.66
1:D:6:VAL:HG22	1:D:521:VAL:HG22	1.76	0.66
1:F:6:VAL:HG22	1:F:521:VAL:HG22	1.76	0.66
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.78	0.66
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.78	0.66
1:K:223:ALA:O	1:K:251:ALA:HA	1.96	0.66
1:A:39:VAL:HB	1:G:517:THR:HB	1.76	0.66
1:G:40:LEU:HD21	1:G:55:SER:HB3	1.78	0.66
1:I:223:ALA:O	1:I:251:ALA:HA	1.96	0.66
1:C:114:MET:H	1:D:36:ARG:CZ	2.05	0.66
1:C:180:GLY:HA2	1:C:380:LYS:HB3	1.78	0.66
1:E:6:VAL:HG22	1:E:521:VAL:HG22	1.76	0.66
1:A:40:LEU:HD21	1:A:55:SER:HB3	1.78	0.65
1:F:73:MET:HA	1:G:46:ALA:CB	2.26	0.65
1:F:180:GLY:HA2	1:F:380:LYS:HB3	1.78	0.65
1:D:114:MET:H	1:E:36:ARG:CZ	2.05	0.65
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.78	0.65
1:B:73:MET:HA	1:C:46:ALA:HB2	1.78	0.65
1:C:39:VAL:HG13	1:C:48:THR:O	1.97	0.65
1:M:223:ALA:O	1:M:251:ALA:HA	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:MET:HA	1:C:46:ALA:CB	2.26	0.65
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.78	0.65
1:F:40:LEU:HD21	1:F:55:SER:HB3	1.78	0.65
1:L:223:ALA:O	1:L:251:ALA:HA	1.96	0.65
1:J:223:ALA:O	1:J:251:ALA:HA	1.96	0.65
1:C:73:MET:HA	1:D:46:ALA:HB2	1.79	0.65
1:F:39:VAL:HG13	1:F:48:THR:O	1.97	0.65
1:G:39:VAL:HG13	1:G:48:THR:O	1.97	0.65
1:A:27:VAL:HG12	1:A:90:THR:CG2	2.27	0.65
1:B:40:LEU:HD21	1:B:55:SER:HB3	1.78	0.65
1:A:46:ALA:CB	1:G:73:MET:HA	2.26	0.65
1:A:73:MET:HA	1:B:46:ALA:CB	2.26	0.65
1:D:73:MET:HA	1:E:46:ALA:CB	2.26	0.65
1:E:73:MET:HA	1:F:46:ALA:CB	2.26	0.65
1:N:223:ALA:O	1:N:251:ALA:HA	1.96	0.65
1:A:73:MET:HA	1:B:46:ALA:HB2	1.79	0.65
1:H:223:ALA:O	1:H:251:ALA:HA	1.96	0.65
1:F:114:MET:HB2	1:G:36:ARG:HD2	1.79	0.64
1:E:39:VAL:HG13	1:E:48:THR:O	1.97	0.64
1:A:39:VAL:HG13	1:A:48:THR:O	1.97	0.64
1:C:73:MET:HA	1:D:46:ALA:CB	2.26	0.64
1:B:27:VAL:HG12	1:B:90:THR:CG2	2.27	0.64
1:E:114:MET:HB2	1:F:36:ARG:HD2	1.79	0.64
1:A:46:ALA:HB2	1:G:73:MET:HA	1.78	0.64
1:A:36:ARG:HD2	1:G:114:MET:HB2	1.79	0.64
1:D:40:LEU:HD21	1:D:55:SER:HB3	1.78	0.64
1:D:73:MET:HA	1:E:46:ALA:HB2	1.79	0.64
1:E:40:LEU:HD21	1:E:55:SER:HB3	1.78	0.64
1:A:39:VAL:HB	1:G:517:THR:CB	2.28	0.64
1:A:517:THR:CB	1:B:39:VAL:HB	2.28	0.64
1:C:40:LEU:HD21	1:C:55:SER:HB3	1.78	0.64
1:D:39:VAL:HG13	1:D:48:THR:O	1.97	0.64
1:D:114:MET:HB2	1:E:36:ARG:HD2	1.79	0.64
1:E:73:MET:HA	1:F:46:ALA:HB2	1.79	0.63
1:E:517:THR:CB	1:F:39:VAL:HB	2.28	0.63
1:F:73:MET:HA	1:G:46:ALA:HB2	1.79	0.63
1:A:114:MET:HB2	1:B:36:ARG:HD2	1.79	0.63
1:B:114:MET:HB2	1:C:36:ARG:HD2	1.79	0.63
1:F:517:THR:CB	1:G:39:VAL:HB	2.28	0.63
1:C:27:VAL:HG12	1:C:90:THR:CG2	2.27	0.63
1:B:39:VAL:HG13	1:B:48:THR:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:THR:HA	1:D:39:VAL:HG23	1.81	0.63
1:C:114:MET:HB2	1:D:36:ARG:HD2	1.79	0.63
1:A:39:VAL:HG23	1:G:517:THR:HA	1.81	0.63
1:A:114:MET:H	1:B:36:ARG:CD	2.12	0.63
1:D:114:MET:H	1:E:36:ARG:CD	2.12	0.63
1:B:517:THR:HA	1:C:39:VAL:HG23	1.81	0.63
1:E:114:MET:H	1:F:36:ARG:CD	2.12	0.63
1:B:517:THR:CB	1:C:39:VAL:HB	2.29	0.62
1:F:114:MET:H	1:G:36:ARG:CD	2.12	0.62
1:A:517:THR:HA	1:B:39:VAL:HG23	1.81	0.62
1:D:517:THR:CB	1:E:39:VAL:HB	2.28	0.62
1:E:517:THR:HA	1:F:39:VAL:HG23	1.81	0.62
1:F:517:THR:HA	1:G:39:VAL:HG23	1.81	0.62
1:B:31:LEU:HB3	1:B:90:THR:HG21	1.82	0.62
1:B:114:MET:H	1:C:36:ARG:CD	2.12	0.62
1:C:114:MET:H	1:D:36:ARG:CD	2.12	0.62
1:D:517:THR:HA	1:E:39:VAL:HG23	1.81	0.62
1:A:114:MET:H	1:B:36:ARG:CZ	2.05	0.62
1:A:521:VAL:H	1:B:41:ASP:HB3	1.65	0.62
1:D:30:THR:HG21	1:D:56:VAL:HG21	1.82	0.62
1:E:30:THR:HG21	1:E:56:VAL:HG21	1.82	0.62
1:C:31:LEU:HB3	1:C:90:THR:HG21	1.82	0.62
1:F:30:THR:HG21	1:F:56:VAL:HG21	1.82	0.62
1:B:520:MET:HA	1:C:41:ASP:HB2	1.82	0.62
1:C:517:THR:CB	1:D:39:VAL:HB	2.28	0.62
1:D:521:VAL:H	1:E:41:ASP:HB3	1.65	0.62
1:A:41:ASP:HB3	1:G:521:VAL:H	1.65	0.62
1:B:521:VAL:H	1:C:41:ASP:HB3	1.65	0.62
1:D:27:VAL:HG12	1:D:90:THR:CG2	2.27	0.62
1:A:31:LEU:HB3	1:A:90:THR:HG21	1.82	0.61
1:A:520:MET:HA	1:B:41:ASP:HB2	1.82	0.61
1:G:30:THR:HG21	1:G:56:VAL:HG21	1.82	0.61
1:D:520:MET:HA	1:E:41:ASP:HB2	1.82	0.61
1:F:27:VAL:HG12	1:F:90:THR:CG2	2.27	0.61
1:A:36:ARG:CD	1:G:114:MET:H	2.12	0.61
1:C:30:THR:HG21	1:C:56:VAL:HG21	1.82	0.61
1:C:520:MET:HA	1:D:41:ASP:HB2	1.82	0.61
1:E:520:MET:HA	1:F:41:ASP:HB2	1.82	0.61
1:A:36:ARG:HH12	1:G:115:ASP:C	2.07	0.61
1:D:31:LEU:HB3	1:D:90:THR:HG21	1.82	0.61
1:E:214:GLU:HA	1:E:323:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:THR:HG21	1:A:56:VAL:HG21	1.82	0.61
1:D:214:GLU:HA	1:D:323:VAL:O	2.01	0.61
1:F:521:VAL:H	1:G:41:ASP:HB3	1.65	0.61
1:A:41:ASP:HB2	1:G:520:MET:HA	1.82	0.61
1:F:520:MET:HA	1:G:41:ASP:HB2	1.82	0.61
1:G:214:GLU:HA	1:G:323:VAL:O	2.01	0.61
1:A:115:ASP:C	1:B:36:ARG:HH12	2.07	0.61
1:F:115:ASP:C	1:G:36:ARG:HH12	2.07	0.61
1:C:112:ASN:C	1:D:36:ARG:NE	2.59	0.61
1:C:214:GLU:HA	1:C:323:VAL:O	2.01	0.61
1:E:521:VAL:H	1:F:41:ASP:HB3	1.65	0.61
1:G:31:LEU:HB3	1:G:90:THR:HG21	1.82	0.61
1:A:36:ARG:NH1	1:G:114:MET:N	2.49	0.61
1:A:214:GLU:HA	1:A:323:VAL:O	2.00	0.61
1:F:31:LEU:HB3	1:F:90:THR:HG21	1.82	0.61
1:F:214:GLU:HA	1:F:323:VAL:O	2.01	0.61
1:B:214:GLU:HA	1:B:323:VAL:O	2.01	0.60
1:C:521:VAL:H	1:D:41:ASP:HB3	1.65	0.60
1:E:31:LEU:HB3	1:E:90:THR:HG21	1.82	0.60
1:B:115:ASP:C	1:C:36:ARG:HH12	2.07	0.60
1:E:27:VAL:HG12	1:E:90:THR:CG2	2.27	0.60
1:B:30:THR:HG21	1:B:56:VAL:HG21	1.82	0.60
1:B:114:MET:N	1:C:36:ARG:NH1	2.49	0.60
1:F:112:ASN:C	1:G:36:ARG:NE	2.59	0.60
1:A:36:ARG:NE	1:G:112:ASN:C	2.59	0.60
1:D:114:MET:N	1:E:36:ARG:NH1	2.50	0.60
1:A:114:MET:N	1:B:36:ARG:NH1	2.49	0.60
1:B:112:ASN:C	1:C:36:ARG:NE	2.59	0.60
1:E:417:VAL:HG21	1:E:477:GLY:HA3	1.84	0.60
1:E:114:MET:N	1:F:36:ARG:NH1	2.50	0.60
1:E:115:ASP:C	1:F:36:ARG:HH12	2.07	0.60
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.84	0.60
1:G:417:VAL:HG21	1:G:477:GLY:HA3	1.84	0.60
1:C:114:MET:N	1:D:36:ARG:NH1	2.49	0.60
1:E:112:ASN:C	1:F:36:ARG:NE	2.59	0.60
1:G:40:LEU:HB3	1:G:59:GLU:HG3	1.84	0.60
1:A:112:ASN:C	1:B:36:ARG:NE	2.59	0.59
1:C:115:ASP:C	1:D:36:ARG:HH12	2.07	0.59
1:D:112:ASN:C	1:E:36:ARG:NE	2.59	0.59
1:D:115:ASP:C	1:E:36:ARG:HH12	2.06	0.59
1:E:40:LEU:HB3	1:E:59:GLU:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:VAL:HG12	1:G:90:THR:CG2	2.27	0.59
1:D:417:VAL:HG21	1:D:477:GLY:HA3	1.84	0.59
1:F:40:LEU:HB3	1:F:59:GLU:HG3	1.84	0.59
1:A:40:LEU:HB3	1:A:59:GLU:HG3	1.84	0.59
1:C:417:VAL:HG21	1:C:477:GLY:HA3	1.84	0.59
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.84	0.59
1:G:151:SER:HB3	1:G:399:ALA:HA	1.85	0.59
1:B:417:VAL:HG21	1:B:477:GLY:HA3	1.84	0.59
1:F:114:MET:N	1:G:36:ARG:NH1	2.49	0.59
1:B:40:LEU:HB3	1:B:59:GLU:HG3	1.84	0.59
1:D:40:LEU:HB3	1:D:59:GLU:HG3	1.84	0.59
1:C:240:VAL:HG11	1:C:247:LEU:HB2	1.85	0.58
1:L:400:LEU:CA	1:L:401:HIS:N	2.62	0.58
1:A:36:ARG:HH12	1:G:116:LEU:H	0.62	0.58
1:D:240:VAL:HG11	1:D:247:LEU:HB2	1.85	0.58
1:F:151:SER:HB3	1:F:399:ALA:HA	1.85	0.58
1:A:151:SER:HB3	1:A:399:ALA:HA	1.85	0.58
1:A:217:SER:HA	1:A:320:ALA:O	2.04	0.58
1:B:116:LEU:H	1:C:36:ARG:HH12	0.61	0.58
1:A:115:ASP:CB	1:B:36:ARG:HH22	2.15	0.58
1:B:217:SER:HA	1:B:320:ALA:O	2.04	0.58
1:C:40:LEU:HB3	1:C:59:GLU:HG3	1.84	0.58
1:C:217:SER:HA	1:C:320:ALA:O	2.04	0.58
1:G:217:SER:HA	1:G:320:ALA:O	2.04	0.58
1:D:116:LEU:H	1:E:36:ARG:HH12	0.61	0.58
1:E:151:SER:CB	1:E:399:ALA:HA	2.34	0.58
1:F:192:GLY:O	1:F:375:GLY:HA2	2.04	0.58
1:G:151:SER:CB	1:G:399:ALA:HA	2.34	0.58
1:B:240:VAL:HG11	1:B:247:LEU:HB2	1.85	0.58
1:D:151:SER:CB	1:D:399:ALA:HA	2.34	0.58
1:E:151:SER:HB3	1:E:399:ALA:HA	1.85	0.58
1:G:39:VAL:HG13	1:G:48:THR:C	2.29	0.58
1:F:217:SER:HA	1:F:320:ALA:O	2.04	0.58
1:A:151:SER:CB	1:A:399:ALA:HA	2.34	0.58
1:E:116:LEU:H	1:F:36:ARG:HH12	0.62	0.58
1:E:240:VAL:HG11	1:E:247:LEU:HB2	1.85	0.58
1:G:192:GLY:O	1:G:375:GLY:HA2	2.04	0.58
1:D:39:VAL:HG13	1:D:48:THR:C	2.29	0.57
1:D:217:SER:HA	1:D:320:ALA:O	2.04	0.57
1:E:217:SER:HA	1:E:320:ALA:O	2.04	0.57
1:F:240:VAL:HG11	1:F:247:LEU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.85	0.57
1:C:192:GLY:O	1:C:375:GLY:HA2	2.04	0.57
1:D:192:GLY:O	1:D:375:GLY:HA2	2.04	0.57
1:F:115:ASP:CB	1:G:36:ARG:HH22	2.15	0.57
1:B:151:SER:HB3	1:B:399:ALA:HA	1.85	0.57
1:G:127:ALA:HB2	1:G:426:LEU:HD11	1.86	0.57
1:A:39:VAL:HG13	1:A:48:THR:C	2.29	0.57
1:B:192:GLY:O	1:B:375:GLY:HA2	2.04	0.57
1:C:151:SER:CB	1:C:399:ALA:HA	2.34	0.57
1:E:39:VAL:HG13	1:E:48:THR:C	2.29	0.57
1:A:192:GLY:O	1:A:375:GLY:HA2	2.04	0.57
1:B:151:SER:CB	1:B:399:ALA:HA	2.34	0.57
1:D:151:SER:HB3	1:D:399:ALA:HA	1.85	0.57
1:E:115:ASP:CB	1:F:36:ARG:HH22	2.15	0.57
1:E:192:GLY:O	1:E:375:GLY:HA2	2.04	0.57
1:F:127:ALA:HB2	1:F:426:LEU:HD11	1.87	0.57
1:A:36:ARG:NH2	1:G:112:ASN:O	2.38	0.57
1:D:115:ASP:CB	1:E:36:ARG:HH22	2.15	0.57
1:D:127:ALA:HB2	1:D:426:LEU:HD11	1.86	0.57
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.86	0.57
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.86	0.57
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.85	0.57
1:C:151:SER:HB3	1:C:399:ALA:HA	1.85	0.57
1:F:151:SER:CB	1:F:399:ALA:HA	2.34	0.57
1:E:127:ALA:HB2	1:E:426:LEU:HD11	1.87	0.57
1:H:25:ASP:CG	1:H:28:LYS:HZ3	2.13	0.57
1:A:36:ARG:HH22	1:G:115:ASP:CB	2.15	0.57
1:C:39:VAL:HG13	1:C:48:THR:C	2.29	0.57
1:F:39:VAL:HG13	1:F:48:THR:C	2.29	0.57
1:A:112:ASN:O	1:B:36:ARG:NH2	2.38	0.57
1:F:39:VAL:HG21	1:F:49:ILE:CD1	2.35	0.57
1:B:39:VAL:HG13	1:B:48:THR:C	2.29	0.56
1:A:127:ALA:HB2	1:A:426:LEU:HD11	1.87	0.56
1:D:212:ALA:HA	1:D:325:ILE:O	2.06	0.56
1:E:39:VAL:HG21	1:E:49:ILE:CD1	2.35	0.56
1:E:112:ASN:O	1:F:36:ARG:NH2	2.38	0.56
1:K:229:ASN:HA	1:K:258:ALA:HB3	1.87	0.56
1:E:212:ALA:HA	1:E:325:ILE:O	2.06	0.56
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.86	0.56
1:M:229:ASN:HA	1:M:258:ALA:HB3	1.88	0.56
1:C:127:ALA:HB2	1:C:426:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:ALA:HA	1:F:325:ILE:O	2.06	0.56
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.86	0.56
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.86	0.56
1:L:229:ASN:HA	1:L:258:ALA:HB3	1.88	0.56
1:N:229:ASN:HA	1:N:258:ALA:HB3	1.88	0.56
1:E:152:ALA:HB1	1:E:155:ASP:HB2	1.87	0.56
1:F:112:ASN:O	1:G:36:ARG:NH2	2.38	0.56
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.86	0.56
1:B:39:VAL:HG21	1:B:49:ILE:CD1	2.35	0.56
1:B:112:ASN:O	1:C:36:ARG:NH2	2.38	0.56
1:C:112:ASN:O	1:D:36:ARG:NH2	2.38	0.56
1:D:152:ALA:HB1	1:D:155:ASP:HB2	1.87	0.56
1:G:152:ALA:HB1	1:G:155:ASP:HB2	1.87	0.56
1:J:229:ASN:HA	1:J:258:ALA:HB3	1.87	0.56
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.86	0.56
1:A:152:ALA:HB1	1:A:155:ASP:HB2	1.87	0.56
1:B:115:ASP:CB	1:C:36:ARG:HH22	2.15	0.56
1:B:127:ALA:HB2	1:B:426:LEU:HD11	1.86	0.56
1:C:115:ASP:CB	1:D:36:ARG:HH22	2.15	0.56
1:D:39:VAL:HG21	1:D:49:ILE:CD1	2.35	0.56
1:A:212:ALA:HA	1:A:325:ILE:O	2.06	0.56
1:B:212:ALA:HA	1:B:325:ILE:O	2.05	0.56
1:C:113:PRO:O	1:D:36:ARG:NH1	2.39	0.56
1:A:39:VAL:HG21	1:A:49:ILE:CD1	2.35	0.56
1:B:113:PRO:O	1:C:36:ARG:NH1	2.39	0.56
1:B:152:ALA:HB1	1:B:155:ASP:HB2	1.87	0.56
1:G:39:VAL:HG21	1:G:49:ILE:CD1	2.35	0.56
1:C:152:ALA:HB1	1:C:155:ASP:HB2	1.87	0.56
1:C:212:ALA:HA	1:C:325:ILE:O	2.05	0.56
1:A:36:ARG:NH1	1:G:113:PRO:O	2.39	0.55
1:E:113:PRO:O	1:F:36:ARG:NH1	2.39	0.55
1:H:229:ASN:HA	1:H:258:ALA:HB3	1.88	0.55
1:C:39:VAL:HG21	1:C:49:ILE:CD1	2.35	0.55
1:D:112:ASN:O	1:E:36:ARG:NH2	2.38	0.55
1:C:186:GLU:H	1:C:380:LYS:HB2	1.72	0.55
1:F:152:ALA:HB1	1:F:155:ASP:HB2	1.87	0.55
1:G:212:ALA:HA	1:G:325:ILE:O	2.06	0.55
1:C:116:LEU:H	1:D:36:ARG:HH12	0.62	0.55
1:A:26:ALA:O	1:A:30:THR:HG23	2.07	0.55
1:B:114:MET:CB	1:C:36:ARG:HD2	2.36	0.55
1:C:114:MET:CB	1:D:36:ARG:HD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:MET:CB	1:E:36:ARG:HD2	2.36	0.55
1:D:246:PRO:HB3	1:D:272:LYS:HB2	1.89	0.55
1:E:246:PRO:HB3	1:E:272:LYS:HB2	1.89	0.55
1:A:114:MET:CB	1:B:36:ARG:HD2	2.36	0.55
1:I:229:ASN:HA	1:I:258:ALA:HB3	1.88	0.55
1:F:246:PRO:HB3	1:F:272:LYS:HB2	1.89	0.55
1:G:26:ALA:O	1:G:30:THR:HG23	2.07	0.55
1:G:246:PRO:HB3	1:G:272:LYS:HB2	1.89	0.55
1:A:186:GLU:H	1:A:380:LYS:HB2	1.72	0.54
1:E:186:GLU:H	1:E:380:LYS:HB2	1.72	0.54
1:E:114:MET:CB	1:F:36:ARG:HD2	2.37	0.54
1:N:400:LEU:C	1:N:401:HIS:CA	2.77	0.54
1:B:26:ALA:O	1:B:30:THR:HG23	2.07	0.54
1:C:26:ALA:O	1:C:30:THR:HG23	2.07	0.54
1:D:26:ALA:O	1:D:30:THR:HG23	2.07	0.54
1:D:39:VAL:HG21	1:D:49:ILE:HG12	1.89	0.54
1:N:398:ALA:O	1:N:401:HIS:N	2.41	0.54
1:A:246:PRO:HB3	1:A:272:LYS:HB2	1.89	0.54
1:G:186:GLU:H	1:G:380:LYS:HB2	1.72	0.54
1:C:39:VAL:HG21	1:C:49:ILE:HG12	1.89	0.54
1:F:114:MET:CB	1:G:36:ARG:HD2	2.36	0.54
1:B:186:GLU:H	1:B:380:LYS:HB2	1.72	0.54
1:C:218:PRO:HG2	1:C:320:ALA:HB3	1.90	0.54
1:D:40:LEU:HD11	1:D:55:SER:HB3	1.90	0.54
1:D:172:GLU:CD	1:D:172:GLU:H	2.16	0.54
1:E:172:GLU:CD	1:E:172:GLU:H	2.16	0.54
1:G:39:VAL:HG21	1:G:49:ILE:HG12	1.89	0.54
1:A:36:ARG:HD2	1:G:114:MET:CB	2.36	0.54
1:C:246:PRO:HB3	1:C:272:LYS:HB2	1.89	0.54
1:E:26:ALA:O	1:E:30:THR:HG23	2.07	0.54
1:F:26:ALA:O	1:F:30:THR:HG23	2.07	0.54
1:F:39:VAL:HG21	1:F:49:ILE:HG12	1.89	0.54
1:A:218:PRO:HG2	1:A:320:ALA:HB3	1.90	0.54
1:G:218:PRO:HG2	1:G:320:ALA:HB3	1.90	0.54
1:B:39:VAL:HG21	1:B:49:ILE:HG12	1.89	0.54
1:B:218:PRO:HG2	1:B:320:ALA:HB3	1.90	0.54
1:E:39:VAL:HG21	1:E:49:ILE:HG12	1.89	0.54
1:F:186:GLU:H	1:F:380:LYS:HB2	1.72	0.54
1:B:246:PRO:HB3	1:B:272:LYS:HB2	1.89	0.54
1:C:40:LEU:HD11	1:C:55:SER:HB3	1.90	0.54
1:E:40:LEU:HD11	1:E:55:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:LEU:HD11	1:F:55:SER:HB3	1.90	0.54
1:B:40:LEU:HD11	1:B:55:SER:HB3	1.90	0.53
1:B:205:ILE:HD12	1:B:211:GLY:O	2.09	0.53
1:C:205:ILE:HD12	1:C:211:GLY:O	2.09	0.53
1:D:218:PRO:HG2	1:D:320:ALA:HB3	1.90	0.53
1:D:113:PRO:O	1:E:36:ARG:NH1	2.39	0.53
1:D:186:GLU:H	1:D:380:LYS:HB2	1.72	0.53
1:E:31:LEU:CB	1:E:90:THR:HG21	2.39	0.53
1:D:31:LEU:CB	1:D:90:THR:HG21	2.39	0.53
1:F:218:PRO:HG2	1:F:320:ALA:HB3	1.90	0.53
1:A:205:ILE:HD12	1:A:211:GLY:O	2.08	0.53
1:C:31:LEU:CB	1:C:90:THR:HG21	2.39	0.53
1:D:205:ILE:HD12	1:D:211:GLY:O	2.09	0.53
1:A:39:VAL:HG21	1:A:49:ILE:HG12	1.89	0.53
1:A:172:GLU:H	1:A:172:GLU:CD	2.16	0.53
1:F:31:LEU:CB	1:F:90:THR:HG21	2.39	0.53
1:F:205:ILE:HD12	1:F:211:GLY:O	2.09	0.53
1:G:40:LEU:HD11	1:G:55:SER:HB3	1.90	0.53
1:F:113:PRO:HA	1:G:36:ARG:HH11	1.73	0.53
1:A:113:PRO:O	1:B:36:ARG:NH1	2.39	0.53
1:B:31:LEU:CB	1:B:90:THR:HG21	2.39	0.53
1:B:239:ALA:HB1	1:B:314:LEU:HG	1.91	0.53
1:C:112:ASN:CG	1:D:36:ARG:HE	2.18	0.53
1:E:16:MET:HG2	1:E:520:MET:HE3	1.91	0.53
1:F:112:ASN:CB	1:G:36:ARG:HE	2.22	0.53
1:F:172:GLU:H	1:F:172:GLU:CD	2.16	0.53
1:A:36:ARG:HE	1:G:112:ASN:CB	2.22	0.52
1:B:411:VAL:HB	1:B:494:LEU:HB3	1.92	0.52
1:C:239:ALA:HB1	1:C:314:LEU:HG	1.91	0.52
1:E:218:PRO:HG2	1:E:320:ALA:HB3	1.90	0.52
1:G:31:LEU:CB	1:G:90:THR:HG21	2.39	0.52
1:A:239:ALA:HB1	1:A:314:LEU:HG	1.91	0.52
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.40	0.52
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.40	0.52
1:D:16:MET:HG2	1:D:520:MET:HE3	1.91	0.52
1:D:112:ASN:CG	1:E:36:ARG:HE	2.18	0.52
1:F:16:MET:HG2	1:F:520:MET:HE3	1.90	0.52
1:G:411:VAL:HB	1:G:494:LEU:HB3	1.92	0.52
1:A:36:ARG:HH11	1:G:113:PRO:HA	1.73	0.52
1:A:40:LEU:HD11	1:A:55:SER:HB3	1.90	0.52
1:A:112:ASN:CB	1:B:36:ARG:HE	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ASN:CG	1:C:36:ARG:HE	2.18	0.52
1:B:172:GLU:CD	1:B:172:GLU:H	2.16	0.52
1:E:113:PRO:HA	1:F:36:ARG:HH11	1.73	0.52
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.40	0.52
1:C:114:MET:C	1:D:36:ARG:NH1	2.67	0.52
1:C:142:LYS:H	1:C:142:LYS:HD2	1.75	0.52
1:C:172:GLU:CD	1:C:172:GLU:H	2.16	0.52
1:D:247:LEU:O	1:D:273:VAL:HA	2.10	0.52
1:E:112:ASN:CG	1:F:36:ARG:HE	2.17	0.52
1:F:411:VAL:HB	1:F:494:LEU:HB3	1.92	0.52
1:A:112:ASN:CG	1:B:36:ARG:HE	2.18	0.52
1:A:247:LEU:O	1:A:273:VAL:HA	2.10	0.52
1:G:142:LYS:H	1:G:142:LYS:HD2	1.75	0.52
1:E:205:ILE:HD12	1:E:211:GLY:O	2.09	0.52
1:F:113:PRO:O	1:G:36:ARG:NH1	2.39	0.52
1:G:172:GLU:CD	1:G:172:GLU:H	2.16	0.52
1:A:31:LEU:CB	1:A:90:THR:HG21	2.39	0.52
1:B:142:LYS:H	1:B:142:LYS:HD2	1.75	0.52
1:C:247:LEU:O	1:C:273:VAL:HA	2.10	0.52
1:E:142:LYS:H	1:E:142:LYS:HD2	1.75	0.52
1:G:239:ALA:HB1	1:G:314:LEU:HG	1.92	0.52
1:G:247:LEU:O	1:G:273:VAL:HA	2.10	0.52
1:A:36:ARG:HE	1:G:112:ASN:CG	2.17	0.52
1:B:247:LEU:O	1:B:273:VAL:HA	2.10	0.52
1:D:142:LYS:H	1:D:142:LYS:HD2	1.75	0.52
1:F:247:LEU:O	1:F:273:VAL:HA	2.10	0.52
1:G:205:ILE:HD12	1:G:211:GLY:O	2.09	0.52
1:A:142:LYS:HD2	1:A:142:LYS:H	1.75	0.52
2:A:1525:ATP:O3B	3:A:1526:PO4:P	2.68	0.52
1:B:114:MET:C	1:C:36:ARG:NH1	2.67	0.52
1:C:411:VAL:HB	1:C:494:LEU:HB3	1.92	0.52
2:C:1526:ATP:O3B	3:C:1527:PO4:P	2.68	0.52
1:D:144:ILE:HG23	1:D:403:THR:CG2	2.40	0.52
1:E:13:ARG:HG2	1:E:13:ARG:HH11	1.75	0.52
1:E:247:LEU:O	1:E:273:VAL:HA	2.10	0.52
1:F:112:ASN:CG	1:G:36:ARG:HE	2.18	0.52
1:A:36:ARG:NH1	1:G:114:MET:C	2.67	0.52
1:A:113:PRO:HA	1:B:36:ARG:HH11	1.73	0.52
1:E:112:ASN:CB	1:F:36:ARG:HE	2.22	0.52
3:E:1526:PO4:P	2:E:1527:ATP:O3B	2.68	0.52
1:B:16:MET:HG2	1:B:520:MET:HE3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ARG:HH11	1:D:13:ARG:HG2	1.75	0.51
1:D:113:PRO:HA	1:E:36:ARG:HH11	1.73	0.51
1:A:16:MET:HG2	1:A:520:MET:HE3	1.91	0.51
1:F:239:ALA:HB1	1:F:314:LEU:HG	1.91	0.51
1:G:16:MET:HG2	1:G:520:MET:HE3	1.91	0.51
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.40	0.51
1:A:13:ARG:HG2	1:A:13:ARG:HH11	1.75	0.51
1:A:411:VAL:HB	1:A:494:LEU:HB3	1.91	0.51
1:B:113:PRO:HA	1:C:36:ARG:HH11	1.73	0.51
1:D:106:ALA:HB3	1:D:116:LEU:HD21	1.92	0.51
1:D:239:ALA:HB1	1:D:314:LEU:HG	1.91	0.51
1:E:114:MET:C	1:F:36:ARG:NH1	2.67	0.51
1:F:251:ALA:HB3	1:F:254:VAL:HG23	1.93	0.51
1:A:149:THR:HA	1:A:152:ALA:HB3	1.92	0.51
1:B:251:ALA:HB3	1:B:254:VAL:HG23	1.92	0.51
1:D:251:ALA:HB3	1:D:254:VAL:HG23	1.92	0.51
1:E:106:ALA:HB3	1:E:116:LEU:HD21	1.93	0.51
1:F:13:ARG:HG2	1:F:13:ARG:HH11	1.75	0.51
3:F:1525:PO4:P	2:F:1527:ATP:O3B	2.68	0.51
1:B:112:ASN:CB	1:C:36:ARG:HE	2.22	0.51
1:C:13:ARG:HG2	1:C:13:ARG:HH11	1.75	0.51
1:C:112:ASN:CB	1:D:36:ARG:HE	2.22	0.51
1:J:400:LEU:C	1:J:401:HIS:CA	2.77	0.51
2:B:1525:ATP:O3B	3:B:1526:PO4:P	2.68	0.51
1:C:113:PRO:HA	1:D:36:ARG:HH11	1.74	0.51
1:D:112:ASN:CB	1:E:36:ARG:HE	2.22	0.51
1:E:144:ILE:HG23	1:E:403:THR:CG2	2.40	0.51
1:E:251:ALA:HB3	1:E:254:VAL:HG23	1.93	0.51
1:F:106:ALA:HB3	1:F:116:LEU:HD21	1.93	0.51
1:F:113:PRO:CA	1:G:36:ARG:NH1	2.66	0.51
1:A:106:ALA:HB3	1:A:116:LEU:HD21	1.93	0.51
1:B:149:THR:HA	1:B:152:ALA:HB3	1.93	0.51
1:C:16:MET:HG2	1:C:520:MET:HE3	1.91	0.51
1:E:239:ALA:HB1	1:E:314:LEU:HG	1.91	0.51
1:F:114:MET:C	1:G:36:ARG:NH1	2.67	0.51
1:G:106:ALA:HB3	1:G:116:LEU:HD21	1.93	0.51
1:G:251:ALA:HB3	1:G:254:VAL:HG23	1.92	0.51
3:G:1525:PO4:P	2:G:1527:ATP:O3B	2.68	0.51
1:E:213:VAL:HG13	1:E:325:ILE:HB	1.93	0.51
1:E:411:VAL:HB	1:E:494:LEU:HB3	1.92	0.51
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ALA:HB3	1:B:116:LEU:HD21	1.93	0.51
1:D:411:VAL:HB	1:D:494:LEU:HB3	1.92	0.51
2:D:1525:ATP:O3B	3:D:1526:PO4:P	2.68	0.51
1:E:39:VAL:CG2	1:E:49:ILE:HD13	2.41	0.51
1:F:142:LYS:H	1:F:142:LYS:HD2	1.75	0.51
1:A:39:VAL:CG2	1:A:49:ILE:HD13	2.41	0.50
1:C:213:VAL:HG13	1:C:325:ILE:HB	1.94	0.50
1:D:39:VAL:CG2	1:D:49:ILE:HD13	2.41	0.50
1:F:39:VAL:CG2	1:F:49:ILE:HD13	2.41	0.50
1:G:39:VAL:CG2	1:G:49:ILE:HD13	2.42	0.50
1:B:213:VAL:HG13	1:B:325:ILE:HB	1.93	0.50
1:E:34:LYS:HE2	1:E:458:CYS:HA	1.93	0.50
1:F:34:LYS:HE2	1:F:458:CYS:HA	1.94	0.50
1:F:213:VAL:HG13	1:F:325:ILE:HB	1.93	0.50
1:G:149:THR:HA	1:G:152:ALA:HB3	1.93	0.50
1:B:39:VAL:CG2	1:B:49:ILE:HD13	2.41	0.50
1:C:106:ALA:HB3	1:C:116:LEU:HD21	1.92	0.50
1:F:13:ARG:HH21	1:F:518:GLU:CD	2.20	0.50
1:C:39:VAL:CG2	1:C:49:ILE:HD13	2.42	0.50
1:D:114:MET:C	1:E:36:ARG:NH1	2.67	0.50
1:D:213:VAL:HG13	1:D:325:ILE:HB	1.94	0.50
1:G:34:LYS:HE2	1:G:458:CYS:HA	1.94	0.50
1:A:13:ARG:HH21	1:A:518:GLU:CD	2.20	0.50
1:C:149:THR:HA	1:C:152:ALA:HB3	1.93	0.50
1:D:13:ARG:HH21	1:D:518:GLU:CD	2.20	0.50
1:D:113:PRO:CA	1:E:36:ARG:NH1	2.66	0.50
1:E:149:THR:HA	1:E:152:ALA:HB3	1.93	0.50
1:A:114:MET:C	1:B:36:ARG:NH1	2.67	0.49
1:A:213:VAL:HG13	1:A:325:ILE:HB	1.94	0.49
1:C:13:ARG:HH21	1:C:518:GLU:CD	2.20	0.49
1:E:113:PRO:CA	1:F:36:ARG:NH1	2.66	0.49
1:G:213:VAL:HG13	1:G:325:ILE:HB	1.93	0.49
1:A:34:LYS:HE2	1:A:458:CYS:HA	1.94	0.49
1:E:13:ARG:HH21	1:E:518:GLU:CD	2.20	0.49
1:F:149:THR:HA	1:F:152:ALA:HB3	1.93	0.49
1:D:34:LYS:HE2	1:D:458:CYS:HA	1.94	0.49
1:D:149:THR:HA	1:D:152:ALA:HB3	1.93	0.49
1:G:13:ARG:HG2	1:G:13:ARG:HH11	1.75	0.49
1:B:13:ARG:HG2	1:B:13:ARG:HH11	1.75	0.49
1:C:251:ALA:HB3	1:C:254:VAL:HG23	1.93	0.49
1:E:138:CYS:HA	1:E:411:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:VAL:HG13	1:G:521:VAL:HG22	1.95	0.49
1:F:6:VAL:HG13	1:F:521:VAL:HG22	1.95	0.49
1:F:138:CYS:HA	1:F:411:VAL:HG22	1.95	0.49
1:A:36:ARG:NH1	1:G:113:PRO:CA	2.66	0.49
1:A:251:ALA:HB3	1:A:254:VAL:HG23	1.93	0.49
1:F:114:MET:CA	1:G:36:ARG:CZ	2.91	0.49
1:A:6:VAL:HG13	1:A:521:VAL:HG22	1.95	0.49
1:B:114:MET:CA	1:C:36:ARG:CZ	2.91	0.49
1:G:13:ARG:HH21	1:G:518:GLU:CD	2.20	0.49
1:A:36:ARG:CZ	1:G:114:MET:CA	2.91	0.49
1:F:39:VAL:HG21	1:F:49:ILE:HD13	1.95	0.49
1:G:39:VAL:HG21	1:G:49:ILE:HD13	1.95	0.49
1:B:13:ARG:HH21	1:B:518:GLU:CD	2.20	0.48
1:C:106:ALA:CB	1:C:116:LEU:HD21	2.43	0.48
1:E:517:THR:HA	1:F:39:VAL:CG2	2.43	0.48
1:G:138:CYS:HA	1:G:411:VAL:HG22	1.94	0.48
1:A:39:VAL:HG21	1:A:49:ILE:HD13	1.95	0.48
1:A:114:MET:CA	1:B:36:ARG:CZ	2.91	0.48
1:B:6:VAL:HG13	1:B:521:VAL:HG22	1.95	0.48
1:B:39:VAL:HG21	1:B:49:ILE:HD13	1.95	0.48
1:C:34:LYS:HE2	1:C:458:CYS:HA	1.94	0.48
1:D:517:THR:HA	1:E:39:VAL:CG2	2.43	0.48
1:B:34:LYS:HE2	1:B:458:CYS:HA	1.94	0.48
1:E:6:VAL:HG13	1:E:521:VAL:HG22	1.95	0.48
1:E:39:VAL:HG21	1:E:49:ILE:HD13	1.95	0.48
1:B:106:ALA:CB	1:B:116:LEU:HD21	2.43	0.48
1:L:117:LYS:HZ2	1:L:121:ASP:CG	2.21	0.48
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.35	0.48
1:B:517:THR:HA	1:C:39:VAL:CG2	2.43	0.48
1:C:39:VAL:HG21	1:C:49:ILE:HD13	1.95	0.48
1:D:106:ALA:CB	1:D:116:LEU:HD21	2.43	0.48
1:B:30:THR:CG2	1:B:38:VAL:HG21	2.42	0.48
1:B:138:CYS:HA	1:B:411:VAL:HG22	1.95	0.48
1:C:517:THR:HA	1:D:39:VAL:CG2	2.43	0.48
1:D:39:VAL:HG21	1:D:49:ILE:HD13	1.95	0.48
1:A:39:VAL:CG2	1:G:517:THR:HA	2.43	0.48
1:C:138:CYS:HA	1:C:411:VAL:HG22	1.94	0.48
1:F:106:ALA:CB	1:F:116:LEU:HD21	2.43	0.48
1:F:116:LEU:H	1:G:36:ARG:HH12	0.62	0.48
1:H:117:LYS:HZ2	1:H:121:ASP:CG	2.21	0.48
1:G:106:ALA:CB	1:G:116:LEU:HD21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:MET:CA	1:E:36:ARG:CZ	2.91	0.48
1:F:517:THR:HA	1:G:39:VAL:CG2	2.43	0.48
1:B:39:VAL:HG21	1:B:49:ILE:CG1	2.44	0.48
1:C:6:VAL:HG13	1:C:521:VAL:HG22	1.95	0.48
1:D:115:ASP:CA	1:E:36:ARG:NH1	2.77	0.47
1:A:138:CYS:HA	1:A:411:VAL:HG22	1.94	0.47
1:C:39:VAL:HG21	1:C:49:ILE:CG1	2.44	0.47
1:C:114:MET:CA	1:D:36:ARG:CZ	2.91	0.47
1:F:115:ASP:CA	1:G:36:ARG:NH1	2.77	0.47
1:L:326:ASN:HD22	1:L:327:LYS:HD2	1.80	0.47
1:A:240:VAL:HG21	1:A:247:LEU:HD13	1.97	0.47
1:D:6:VAL:HG13	1:D:521:VAL:HG22	1.95	0.47
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.97	0.47
1:E:106:ALA:CB	1:E:116:LEU:HD21	2.43	0.47
1:E:114:MET:CA	1:F:36:ARG:CZ	2.91	0.47
1:J:117:LYS:HZ2	1:J:121:ASP:CG	2.23	0.47
1:A:113:PRO:CA	1:B:36:ARG:NH1	2.66	0.47
1:D:138:CYS:HA	1:D:411:VAL:HG22	1.95	0.47
1:E:144:ILE:HG23	1:E:403:THR:HG21	1.97	0.47
1:H:326:ASN:HD22	1:H:327:LYS:HD2	1.80	0.47
1:A:106:ALA:CB	1:A:116:LEU:HD21	2.43	0.47
1:J:326:ASN:HD22	1:J:327:LYS:HD2	1.80	0.47
1:N:117:LYS:HZ2	1:N:121:ASP:CG	2.23	0.47
1:A:196:ASP:HA	1:A:329:THR:HA	1.97	0.47
1:B:240:VAL:HG21	1:B:247:LEU:HD13	1.97	0.47
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.35	0.47
1:C:196:ASP:HA	1:C:329:THR:HA	1.97	0.47
1:G:196:ASP:HA	1:G:329:THR:HA	1.97	0.47
1:I:117:LYS:HZ2	1:I:121:ASP:CG	2.23	0.47
1:I:326:ASN:HD22	1:I:327:LYS:HD2	1.80	0.47
1:J:320:ALA:HA	1:J:334:ASP:O	2.15	0.47
1:K:320:ALA:HA	1:K:334:ASP:O	2.15	0.47
1:M:320:ALA:HA	1:M:334:ASP:O	2.15	0.47
1:N:326:ASN:HD22	1:N:327:LYS:HD2	1.79	0.47
1:C:144:ILE:HG23	1:C:403:THR:HG21	1.97	0.47
1:E:427:ALA:HA	1:E:444:LEU:CD1	2.45	0.47
1:M:117:LYS:HZ2	1:M:121:ASP:CG	2.22	0.47
1:M:326:ASN:HD22	1:M:327:LYS:HD2	1.80	0.47
1:A:30:THR:CG2	1:A:38:VAL:HG21	2.42	0.47
1:B:196:ASP:HA	1:B:329:THR:HA	1.97	0.47
1:F:144:ILE:HG23	1:F:403:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:320:ALA:HA	1:I:334:ASP:O	2.15	0.47
1:L:320:ALA:HA	1:L:334:ASP:O	2.15	0.47
1:N:320:ALA:HA	1:N:334:ASP:O	2.15	0.47
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.45	0.47
1:F:196:ASP:HA	1:F:329:THR:HA	1.97	0.47
1:G:39:VAL:HG21	1:G:49:ILE:CG1	2.44	0.47
1:G:240:VAL:HG21	1:G:247:LEU:HD13	1.97	0.47
1:H:320:ALA:HA	1:H:334:ASP:O	2.15	0.47
1:D:356:ALA:HB1	1:D:361:ASP:HB2	1.97	0.46
1:D:427:ALA:HA	1:D:444:LEU:CD1	2.45	0.46
1:E:39:VAL:HG21	1:E:49:ILE:CG1	2.44	0.46
1:E:356:ALA:HB1	1:E:361:ASP:HB2	1.97	0.46
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.97	0.46
1:N:479:ASN:O	1:N:483:GLU:N	2.49	0.46
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.46	0.46
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.46	0.46
1:G:356:ALA:HB1	1:G:361:ASP:HB2	1.97	0.46
1:K:183:LEU:HA	1:K:383:ALA:O	2.15	0.46
1:L:183:LEU:HA	1:L:383:ALA:O	2.15	0.46
1:A:144:ILE:HG23	1:A:403:THR:HG21	1.97	0.46
1:A:152:ALA:HB1	1:A:155:ASP:CB	2.45	0.46
1:A:356:ALA:HB1	1:A:361:ASP:HB2	1.97	0.46
1:C:34:LYS:HZ1	1:C:483:GLU:CD	2.23	0.46
1:F:356:ALA:HB1	1:F:361:ASP:HB2	1.97	0.46
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.46	0.46
1:H:183:LEU:HA	1:H:383:ALA:O	2.15	0.46
1:A:39:VAL:HG21	1:A:49:ILE:CG1	2.44	0.46
1:A:120:ILE:O	1:A:124:VAL:HG23	2.16	0.46
1:B:120:ILE:O	1:B:124:VAL:HG23	2.16	0.46
1:B:427:ALA:HA	1:B:444:LEU:CD1	2.45	0.46
1:C:113:PRO:CA	1:D:36:ARG:NH1	2.66	0.46
1:D:39:VAL:HG21	1:D:49:ILE:CG1	2.44	0.46
1:E:120:ILE:O	1:E:124:VAL:HG23	2.16	0.46
1:G:152:ALA:HB1	1:G:155:ASP:CB	2.46	0.46
1:J:183:LEU:HA	1:J:383:ALA:O	2.15	0.46
1:M:183:LEU:HA	1:M:383:ALA:O	2.16	0.46
1:B:356:ALA:HB1	1:B:361:ASP:HB2	1.98	0.46
1:C:356:ALA:HB1	1:C:361:ASP:HB2	1.97	0.46
1:D:124:VAL:HG21	1:D:508:ALA:CB	2.45	0.46
1:D:196:ASP:HA	1:D:329:THR:HA	1.97	0.46
1:D:517:THR:HA	1:E:39:VAL:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:ILE:O	1:G:124:VAL:HG23	2.16	0.46
1:K:326:ASN:HD22	1:K:327:LYS:HD2	1.80	0.46
1:B:113:PRO:CA	1:C:36:ARG:NH1	2.66	0.46
1:D:139:SER:HB3	1:D:143:ALA:HB2	1.98	0.46
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.98	0.46
1:F:120:ILE:O	1:F:124:VAL:HG23	2.16	0.46
1:L:2:ALA:O	1:L:3:ALA:C	2.59	0.46
1:B:152:ALA:HB1	1:B:155:ASP:CB	2.45	0.46
1:C:240:VAL:HG21	1:C:247:LEU:HD13	1.97	0.46
1:C:383:ALA:HB3	1:C:389:MET:HB2	1.98	0.46
1:E:517:THR:HA	1:F:39:VAL:CB	2.46	0.46
1:F:39:VAL:HG21	1:F:49:ILE:CG1	2.44	0.46
1:J:246:PRO:HB3	1:J:272:LYS:HB2	1.98	0.46
1:K:414:GLY:N	1:K:494:LEU:HA	2.31	0.46
1:M:479:ASN:O	1:M:483:GLU:N	2.48	0.46
1:N:2:ALA:O	1:N:3:ALA:C	2.59	0.46
1:N:183:LEU:HA	1:N:383:ALA:O	2.16	0.46
1:B:144:ILE:HG23	1:B:403:THR:HG21	1.97	0.46
1:C:427:ALA:HA	1:C:444:LEU:CD1	2.45	0.46
1:E:124:VAL:HG21	1:E:508:ALA:CB	2.45	0.46
1:E:139:SER:HB3	1:E:143:ALA:HB2	1.98	0.46
1:H:2:ALA:O	1:H:3:ALA:C	2.59	0.46
1:H:246:PRO:HB3	1:H:272:LYS:HB2	1.98	0.46
1:I:246:PRO:HB3	1:I:272:LYS:HB2	1.98	0.46
1:A:517:THR:HA	1:B:39:VAL:CB	2.46	0.46
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.98	0.46
1:C:111:MET:O	1:C:113:PRO:HD3	2.16	0.46
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.35	0.46
1:E:196:ASP:HA	1:E:329:THR:HA	1.97	0.46
1:F:152:ALA:HB1	1:F:155:ASP:CB	2.45	0.46
1:F:240:VAL:HG21	1:F:247:LEU:HD13	1.97	0.46
1:F:517:THR:HA	1:G:39:VAL:CB	2.46	0.46
1:G:427:ALA:HA	1:G:444:LEU:CD1	2.45	0.46
1:K:117:LYS:HZ2	1:K:121:ASP:CG	2.23	0.46
1:K:246:PRO:HB3	1:K:272:LYS:HB2	1.98	0.46
1:A:36:ARG:NH1	1:G:115:ASP:CA	2.77	0.46
1:A:39:VAL:CB	1:G:517:THR:HA	2.46	0.46
1:A:115:ASP:CA	1:B:36:ARG:NH1	2.77	0.46
1:A:517:THR:HA	1:B:39:VAL:CG2	2.43	0.46
1:C:115:ASP:CA	1:D:36:ARG:NH1	2.77	0.46
1:C:517:THR:HA	1:D:39:VAL:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.46	0.46
1:G:287:ALA:HB1	1:G:368:ARG:CZ	2.46	0.46
1:M:246:PRO:HB3	1:M:272:LYS:HB2	1.98	0.46
1:N:246:PRO:HB3	1:N:272:LYS:HB2	1.98	0.46
1:C:139:SER:HB3	1:C:143:ALA:HB2	1.98	0.45
1:C:427:ALA:HA	1:C:444:LEU:HD11	1.98	0.45
1:D:120:ILE:O	1:D:124:VAL:HG23	2.16	0.45
1:F:111:MET:O	1:F:113:PRO:HD3	2.17	0.45
1:L:246:PRO:HB3	1:L:272:LYS:HB2	1.98	0.45
1:A:427:ALA:HA	1:A:444:LEU:CD1	2.45	0.45
1:B:427:ALA:HA	1:B:444:LEU:HD11	1.99	0.45
1:C:31:LEU:HA	3:C:1527:PO4:P	2.56	0.45
1:C:287:ALA:HB1	1:C:368:ARG:CZ	2.46	0.45
1:F:287:ALA:HB1	1:F:368:ARG:CZ	2.47	0.45
1:F:427:ALA:HA	1:F:444:LEU:CD1	2.45	0.45
1:G:30:THR:CG2	1:G:38:VAL:HG21	2.42	0.45
1:G:111:MET:O	1:G:113:PRO:HD3	2.16	0.45
1:I:414:GLY:N	1:I:494:LEU:HA	2.32	0.45
1:J:2:ALA:O	1:J:3:ALA:C	2.59	0.45
1:N:414:GLY:N	1:N:494:LEU:HA	2.31	0.45
1:A:34:LYS:HZ1	1:A:483:GLU:CD	2.24	0.45
1:A:287:ALA:HB1	1:A:368:ARG:CZ	2.46	0.45
1:B:139:SER:HB3	1:B:143:ALA:HB2	1.98	0.45
1:B:287:ALA:HB1	1:B:368:ARG:CZ	2.47	0.45
1:F:427:ALA:HA	1:F:444:LEU:HD11	1.99	0.45
1:H:414:GLY:N	1:H:494:LEU:HA	2.31	0.45
1:M:414:GLY:N	1:M:494:LEU:HA	2.31	0.45
1:A:31:LEU:HA	3:A:1526:PO4:P	2.57	0.45
1:C:120:ILE:O	1:C:124:VAL:HG23	2.16	0.45
1:D:111:MET:O	1:D:113:PRO:HD3	2.16	0.45
1:D:287:ALA:HB1	1:D:368:ARG:CZ	2.47	0.45
1:D:427:ALA:HA	1:D:444:LEU:HD11	1.99	0.45
1:E:287:ALA:HB1	1:E:368:ARG:CZ	2.46	0.45
1:E:427:ALA:HA	1:E:444:LEU:HD11	1.99	0.45
1:G:31:LEU:HA	3:G:1525:PO4:P	2.57	0.45
1:J:149:THR:CG2	1:J:156:GLU:HA	2.47	0.45
1:J:479:ASN:O	1:J:483:GLU:N	2.48	0.45
1:L:149:THR:CG2	1:L:156:GLU:HA	2.47	0.45
1:A:111:MET:O	1:A:113:PRO:HD3	2.16	0.45
1:A:112:ASN:HA	1:A:113:PRO:HD2	1.74	0.45
1:A:127:ALA:CB	1:A:426:LEU:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ALA:HA	1:A:444:LEU:HD11	1.99	0.45
1:B:115:ASP:CA	1:C:36:ARG:NH1	2.77	0.45
1:C:349:ILE:HG22	1:C:369:VAL:HG13	1.98	0.45
1:F:383:ALA:HB3	1:F:389:MET:HB2	1.98	0.45
1:I:2:ALA:O	1:I:3:ALA:C	2.59	0.45
1:K:149:THR:CG2	1:K:156:GLU:HA	2.47	0.45
1:M:217:SER:HA	1:M:320:ALA:O	2.17	0.45
1:M:284:ARG:HG3	1:M:284:ARG:HH11	1.81	0.45
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.98	0.45
1:E:115:ASP:CA	1:F:36:ARG:NH1	2.77	0.45
1:F:139:SER:HB3	1:F:143:ALA:HB2	1.98	0.45
1:G:127:ALA:CB	1:G:426:LEU:HD11	2.46	0.45
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.98	0.45
1:G:427:ALA:HA	1:G:444:LEU:HD11	1.99	0.45
1:I:284:ARG:HG3	1:I:284:ARG:HH11	1.81	0.45
1:I:479:ASN:O	1:I:483:GLU:N	2.48	0.45
1:B:31:LEU:HA	3:B:1526:PO4:P	2.56	0.45
1:D:31:LEU:HA	3:D:1526:PO4:P	2.56	0.45
1:D:152:ALA:HB1	1:D:155:ASP:CB	2.46	0.45
1:I:149:THR:CG2	1:I:156:GLU:HA	2.46	0.45
1:I:183:LEU:HA	1:I:383:ALA:O	2.15	0.45
1:J:284:ARG:HG3	1:J:284:ARG:HH11	1.81	0.45
1:K:479:ASN:O	1:K:483:GLU:N	2.49	0.45
1:N:217:SER:HA	1:N:320:ALA:O	2.17	0.45
1:N:284:ARG:HH11	1:N:284:ARG:HG3	1.81	0.45
1:E:127:ALA:CB	1:E:426:LEU:HD11	2.47	0.45
1:E:152:ALA:HB1	1:E:155:ASP:CB	2.45	0.45
1:F:30:THR:CG2	1:F:38:VAL:HG21	2.42	0.45
1:F:406:ALA:HB2	1:F:496:PRO:HG3	1.99	0.45
1:H:149:THR:CG2	1:H:156:GLU:HA	2.46	0.45
1:I:217:SER:HA	1:I:320:ALA:O	2.17	0.45
1:B:349:ILE:HG22	1:B:369:VAL:HG13	1.99	0.45
1:C:152:ALA:HB1	1:C:155:ASP:CB	2.45	0.45
1:D:240:VAL:HG21	1:D:247:LEU:HD13	1.97	0.45
1:D:349:ILE:HG22	1:D:369:VAL:HG13	1.99	0.45
1:J:217:SER:HA	1:J:320:ALA:O	2.17	0.45
1:B:127:ALA:CB	1:B:426:LEU:HD11	2.46	0.45
1:G:406:ALA:HB2	1:G:496:PRO:HG3	1.99	0.45
1:K:284:ARG:HG3	1:K:284:ARG:HH11	1.81	0.45
1:A:139:SER:HB3	1:A:143:ALA:HB2	1.98	0.44
1:B:111:MET:O	1:B:113:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:THR:HA	1:C:39:VAL:CB	2.46	0.44
1:E:240:VAL:HG21	1:E:247:LEU:HD13	1.97	0.44
1:A:349:ILE:HG22	1:A:369:VAL:HG13	1.99	0.44
1:F:256:GLY:O	1:F:260:ALA:HB3	2.18	0.44
1:H:217:SER:HA	1:H:320:ALA:O	2.17	0.44
1:J:414:GLY:N	1:J:494:LEU:HA	2.31	0.44
1:L:414:GLY:N	1:L:494:LEU:HA	2.31	0.44
1:M:149:THR:CG2	1:M:156:GLU:HA	2.46	0.44
1:A:256:GLY:O	1:A:260:ALA:HB3	2.18	0.44
1:E:349:ILE:HG22	1:E:369:VAL:HG13	1.98	0.44
1:E:417:VAL:HG13	1:E:476:TYR:O	2.18	0.44
1:J:191:GLU:O	1:J:334:ASP:HA	2.18	0.44
1:K:2:ALA:O	1:K:3:ALA:C	2.59	0.44
1:N:149:THR:CG2	1:N:156:GLU:HA	2.47	0.44
1:B:440:ILE:O	1:B:444:LEU:HG	2.18	0.44
1:D:521:VAL:HG21	1:E:59:GLU:CB	2.46	0.44
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.35	0.44
1:H:8:PHE:HA	1:H:518:GLU:O	2.18	0.44
1:K:230:ILE:HG23	1:K:259:LEU:HD12	2.00	0.44
1:L:8:PHE:HA	1:L:518:GLU:O	2.18	0.44
1:M:417:VAL:HA	1:M:420:ILE:HG22	2.00	0.44
1:N:417:VAL:HA	1:N:420:ILE:HG22	2.00	0.44
1:B:115:ASP:CA	1:C:36:ARG:HH12	2.30	0.44
1:C:440:ILE:O	1:C:444:LEU:HG	2.18	0.44
1:D:256:GLY:O	1:D:260:ALA:HB3	2.18	0.44
1:E:111:MET:O	1:E:113:PRO:HD3	2.17	0.44
1:F:127:ALA:CB	1:F:426:LEU:HD11	2.46	0.44
1:F:349:ILE:HG22	1:F:369:VAL:HG13	1.98	0.44
1:F:417:VAL:HG13	1:F:476:TYR:O	2.18	0.44
1:F:521:VAL:N	1:G:41:ASP:HB3	2.32	0.44
1:G:139:SER:HB3	1:G:143:ALA:HB2	1.98	0.44
1:G:417:VAL:HG13	1:G:476:TYR:O	2.18	0.44
1:H:284:ARG:HG3	1:H:284:ARG:HH11	1.81	0.44
1:H:479:ASN:O	1:H:483:GLU:N	2.48	0.44
1:L:230:ILE:HG23	1:L:259:LEU:HD12	2.00	0.44
1:L:284:ARG:HG3	1:L:284:ARG:HH11	1.81	0.44
1:M:8:PHE:HA	1:M:518:GLU:O	2.18	0.44
1:N:8:PHE:HA	1:N:518:GLU:O	2.18	0.44
1:N:230:ILE:HG23	1:N:259:LEU:HD12	2.00	0.44
1:A:440:ILE:O	1:A:444:LEU:HG	2.18	0.44
1:B:412:VAL:HG22	1:B:495:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:VAL:HG13	1:D:476:TYR:O	2.18	0.44
1:E:90:THR:HG22	1:E:94:VAL:HG23	2.00	0.44
1:E:406:ALA:HB2	1:E:496:PRO:HG3	1.99	0.44
1:F:31:LEU:HA	3:F:1525:PO4:P	2.56	0.44
1:G:349:ILE:HG22	1:G:369:VAL:HG13	1.99	0.44
1:I:191:GLU:O	1:I:334:ASP:HA	2.18	0.44
1:K:8:PHE:HA	1:K:518:GLU:O	2.18	0.44
1:A:90:THR:HG22	1:A:94:VAL:HG23	2.00	0.44
1:A:115:ASP:CA	1:B:36:ARG:HH12	2.31	0.44
1:A:412:VAL:HG22	1:A:495:ASP:O	2.18	0.44
1:B:90:THR:HG22	1:B:94:VAL:HG23	2.00	0.44
1:D:127:ALA:CB	1:D:426:LEU:HD11	2.47	0.44
1:D:279:PRO:HG3	1:D:292:ILE:HD11	2.00	0.44
1:E:30:THR:CG2	1:E:38:VAL:HG21	2.42	0.44
1:E:31:LEU:HA	3:E:1526:PO4:P	2.57	0.44
1:F:440:ILE:O	1:F:444:LEU:HG	2.18	0.44
1:I:8:PHE:HA	1:I:518:GLU:O	2.18	0.44
1:I:386:GLU:HA	1:J:281:PHE:CG	2.53	0.44
1:J:8:PHE:HA	1:J:518:GLU:O	2.18	0.44
1:L:479:ASN:O	1:L:483:GLU:N	2.48	0.44
1:A:36:ARG:HH12	1:G:115:ASP:CA	2.30	0.44
1:C:279:PRO:HG3	1:C:292:ILE:HD11	2.00	0.44
1:D:90:THR:HG22	1:D:94:VAL:HG23	2.00	0.44
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.98	0.44
1:E:412:VAL:HG22	1:E:495:ASP:O	2.18	0.44
1:G:34:LYS:HZ1	1:G:483:GLU:CD	2.26	0.44
1:H:230:ILE:HG23	1:H:259:LEU:HD12	2.00	0.44
1:H:386:GLU:HA	1:I:281:PHE:CG	2.53	0.44
1:J:230:ILE:HG23	1:J:259:LEU:HD12	2.00	0.44
1:K:217:SER:HA	1:K:320:ALA:O	2.17	0.44
1:L:217:SER:HA	1:L:320:ALA:O	2.17	0.44
1:B:417:VAL:HG13	1:B:476:TYR:O	2.18	0.44
1:C:412:VAL:HG22	1:C:495:ASP:O	2.18	0.44
1:C:521:VAL:HG21	1:D:59:GLU:CB	2.45	0.44
1:E:440:ILE:O	1:E:444:LEU:HG	2.18	0.44
1:F:34:LYS:HZ1	1:F:483:GLU:CD	2.26	0.44
1:F:412:VAL:HG22	1:F:495:ASP:O	2.18	0.44
1:M:230:ILE:HG23	1:M:259:LEU:HD12	2.00	0.44
1:C:417:VAL:HG13	1:C:476:TYR:O	2.18	0.43
1:D:66:PHE:O	1:D:520:MET:HE1	2.18	0.43
1:D:412:VAL:HG22	1:D:495:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:412:VAL:HG22	1:G:495:ASP:O	2.18	0.43
1:J:386:GLU:HA	1:K:281:PHE:CG	2.53	0.43
1:L:386:GLU:HA	1:M:281:PHE:CG	2.53	0.43
1:A:417:VAL:HG13	1:A:476:TYR:O	2.18	0.43
1:C:115:ASP:CA	1:D:36:ARG:HH12	2.31	0.43
1:E:256:GLY:O	1:E:260:ALA:HB3	2.18	0.43
1:E:279:PRO:HG3	1:E:292:ILE:HD11	2.00	0.43
1:F:90:THR:HG22	1:F:94:VAL:HG23	2.00	0.43
1:H:281:PHE:CG	1:N:386:GLU:HA	2.53	0.43
1:K:191:GLU:O	1:K:334:ASP:HA	2.18	0.43
1:L:215:LEU:O	1:L:218:PRO:HD3	2.18	0.43
1:L:417:VAL:HA	1:L:420:ILE:HG22	2.00	0.43
1:B:521:VAL:N	1:C:41:ASP:HB3	2.31	0.43
1:C:256:GLY:O	1:C:260:ALA:HB3	2.18	0.43
1:D:520:MET:CA	1:E:41:ASP:HB2	2.48	0.43
1:E:293:ALA:HB2	1:E:300:VAL:CG2	2.49	0.43
1:B:279:PRO:HG3	1:B:292:ILE:HD11	2.00	0.43
1:B:488:MET:HE2	1:B:488:MET:HA	2.01	0.43
1:B:520:MET:CA	1:C:41:ASP:HB2	2.48	0.43
1:C:90:THR:HG22	1:C:94:VAL:HG23	2.00	0.43
1:C:406:ALA:HB2	1:C:496:PRO:HG3	1.99	0.43
1:E:66:PHE:O	1:E:520:MET:HE1	2.18	0.43
1:F:115:ASP:CA	1:G:36:ARG:HH12	2.30	0.43
1:F:293:ALA:HB2	1:F:300:VAL:CG2	2.49	0.43
1:G:256:GLY:O	1:G:260:ALA:HB3	2.18	0.43
1:I:230:ILE:HG23	1:I:259:LEU:HD12	2.00	0.43
1:M:2:ALA:O	1:M:3:ALA:C	2.59	0.43
1:M:7:LYS:O	1:M:519:CYS:HA	2.18	0.43
1:A:66:PHE:O	1:A:520:MET:HE1	2.18	0.43
1:A:406:ALA:HB2	1:A:496:PRO:HG3	1.99	0.43
1:B:66:PHE:O	1:B:520:MET:HE1	2.19	0.43
1:C:488:MET:HE2	1:C:488:MET:HA	2.01	0.43
1:C:520:MET:CA	1:D:41:ASP:HB2	2.48	0.43
1:D:40:LEU:HD11	1:D:55:SER:CB	2.48	0.43
1:D:488:MET:HA	1:D:488:MET:HE2	2.01	0.43
1:E:112:ASN:C	1:F:36:ARG:NH1	2.72	0.43
1:H:191:GLU:O	1:H:334:ASP:HA	2.18	0.43
1:J:7:LYS:O	1:J:519:CYS:HA	2.18	0.43
1:M:215:LEU:O	1:M:218:PRO:HD3	2.18	0.43
1:A:10:ASN:HA	1:A:13:ARG:HD2	2.01	0.43
1:A:41:ASP:HB3	1:G:521:VAL:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:PRO:O	1:B:205:ILE:HB	2.19	0.43
1:B:256:GLY:O	1:B:260:ALA:HB3	2.18	0.43
1:B:406:ALA:HB2	1:B:496:PRO:HG3	1.99	0.43
1:B:513:LEU:CA	1:C:49:ILE:HD11	2.43	0.43
1:C:10:ASN:HA	1:C:13:ARG:HD2	2.01	0.43
1:C:180:GLY:HA3	1:C:381:VAL:O	2.19	0.43
1:F:10:ASN:HA	1:F:13:ARG:HD2	2.01	0.43
1:F:13:ARG:NH1	1:F:515:ILE:O	2.49	0.43
1:F:279:PRO:HG3	1:F:292:ILE:HD11	2.00	0.43
1:G:40:LEU:HD11	1:G:55:SER:CB	2.48	0.43
1:G:293:ALA:HB2	1:G:300:VAL:CG2	2.49	0.43
1:G:440:ILE:O	1:G:444:LEU:HG	2.18	0.43
1:H:417:VAL:HA	1:H:420:ILE:HG22	2.00	0.43
1:K:215:LEU:O	1:K:218:PRO:HD3	2.18	0.43
1:A:293:ALA:HB2	1:A:300:VAL:CG2	2.49	0.43
1:B:10:ASN:HA	1:B:13:ARG:HD2	2.01	0.43
1:C:182:GLY:O	1:C:382:GLY:HA2	2.19	0.43
1:D:115:ASP:CA	1:E:36:ARG:HH12	2.30	0.43
1:E:40:LEU:HD11	1:E:55:SER:CB	2.48	0.43
1:E:488:MET:HE2	1:E:488:MET:HA	2.01	0.43
1:F:180:GLY:HA3	1:F:381:VAL:O	2.19	0.43
1:I:215:LEU:O	1:I:218:PRO:HD3	2.18	0.43
1:I:417:VAL:HA	1:I:420:ILE:HG22	2.00	0.43
1:M:191:GLU:O	1:M:334:ASP:HA	2.18	0.43
1:M:386:GLU:HA	1:N:281:PHE:CG	2.53	0.43
1:A:40:LEU:HD11	1:A:55:SER:CB	2.48	0.43
1:D:182:GLY:O	1:D:382:GLY:HA2	2.18	0.43
1:D:293:ALA:HB2	1:D:300:VAL:CG2	2.49	0.43
1:E:10:ASN:HA	1:E:13:ARG:HD2	2.01	0.43
1:F:40:LEU:HD11	1:F:55:SER:CB	2.48	0.43
1:G:90:THR:HG22	1:G:94:VAL:HG23	2.00	0.43
1:H:7:LYS:O	1:H:519:CYS:HA	2.18	0.43
1:H:215:LEU:O	1:H:218:PRO:HD3	2.18	0.43
1:M:219:PHE:O	1:M:247:LEU:HD12	2.19	0.43
1:N:7:LYS:O	1:N:519:CYS:HA	2.18	0.43
1:N:215:LEU:O	1:N:218:PRO:HD3	2.18	0.43
1:A:279:PRO:HG3	1:A:292:ILE:HD11	2.00	0.43
1:A:520:MET:CA	1:B:41:ASP:HB2	2.48	0.43
1:B:30:THR:HG22	1:B:38:VAL:CG2	2.45	0.43
1:B:180:GLY:HA3	1:B:381:VAL:O	2.19	0.43
1:C:202:PRO:O	1:C:205:ILE:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:VAL:N	1:D:41:ASP:HB3	2.32	0.43
1:D:30:THR:CG2	1:D:38:VAL:HG21	2.42	0.43
1:D:440:ILE:O	1:D:444:LEU:HG	2.18	0.43
1:E:115:ASP:CA	1:F:36:ARG:HH12	2.31	0.43
1:F:39:VAL:HG13	1:F:49:ILE:HA	2.01	0.43
1:I:219:PHE:O	1:I:247:LEU:HD12	2.19	0.43
1:L:7:LYS:O	1:L:519:CYS:HA	2.18	0.43
1:L:219:PHE:O	1:L:247:LEU:HD12	2.19	0.43
1:A:30:THR:HG22	1:A:38:VAL:CG2	2.45	0.43
1:A:41:ASP:HB2	1:G:520:MET:CA	2.48	0.43
1:A:513:LEU:CA	1:B:49:ILE:HD11	2.43	0.43
1:C:40:LEU:HD11	1:C:55:SER:CB	2.48	0.43
1:C:513:LEU:CA	1:D:49:ILE:HD11	2.43	0.43
1:D:10:ASN:HA	1:D:13:ARG:HD2	2.01	0.43
1:E:39:VAL:HG13	1:E:49:ILE:HA	2.01	0.43
1:E:180:GLY:HA3	1:E:381:VAL:O	2.19	0.43
1:F:182:GLY:O	1:F:382:GLY:HA2	2.19	0.43
1:G:10:ASN:HA	1:G:13:ARG:HD2	2.01	0.43
1:G:13:ARG:NH1	1:G:515:ILE:O	2.49	0.43
1:G:182:GLY:O	1:G:382:GLY:HA2	2.19	0.43
1:J:417:VAL:HA	1:J:420:ILE:HG22	2.00	0.43
1:K:417:VAL:HA	1:K:420:ILE:HG22	2.00	0.43
1:A:202:PRO:O	1:A:205:ILE:HB	2.19	0.42
1:B:182:GLY:O	1:B:382:GLY:HA2	2.19	0.42
1:B:293:ALA:HB2	1:B:300:VAL:CG2	2.49	0.42
1:C:112:ASN:HA	1:C:113:PRO:HD2	1.74	0.42
1:C:127:ALA:CB	1:C:426:LEU:HD11	2.47	0.42
1:D:23:LEU:O	1:D:27:VAL:HG23	2.19	0.42
1:D:406:ALA:HB2	1:D:496:PRO:HG3	1.99	0.42
1:D:521:VAL:N	1:E:41:ASP:HB3	2.32	0.42
1:F:112:ASN:HA	1:F:113:PRO:HD2	1.74	0.42
1:G:279:PRO:HG3	1:G:292:ILE:HD11	2.00	0.42
1:K:386:GLU:HA	1:L:281:PHE:CG	2.54	0.42
1:L:191:GLU:O	1:L:334:ASP:HA	2.18	0.42
1:N:219:PHE:O	1:N:247:LEU:HD12	2.19	0.42
1:A:73:MET:HA	1:B:46:ALA:HB1	2.01	0.42
1:A:488:MET:HA	1:A:488:MET:HE2	2.01	0.42
1:D:39:VAL:HG13	1:D:49:ILE:HA	2.01	0.42
1:F:66:PHE:O	1:F:520:MET:HE1	2.18	0.42
1:G:180:GLY:HA3	1:G:381:VAL:O	2.19	0.42
1:H:219:PHE:O	1:H:247:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.35	0.42
1:C:66:PHE:O	1:C:520:MET:HE1	2.18	0.42
1:E:182:GLY:O	1:E:382:GLY:HA2	2.19	0.42
1:F:73:MET:HA	1:G:46:ALA:HB1	2.01	0.42
1:G:23:LEU:O	1:G:27:VAL:HG23	2.19	0.42
1:G:66:PHE:O	1:G:520:MET:HE1	2.18	0.42
1:J:219:PHE:O	1:J:247:LEU:HD12	2.19	0.42
1:K:219:PHE:O	1:K:247:LEU:HD12	2.19	0.42
1:N:271:VAL:HG12	1:N:272:LYS:H	1.85	0.42
1:A:19:GLY:HA2	1:A:62:LEU:CD1	2.50	0.42
1:A:182:GLY:O	1:A:382:GLY:HA2	2.19	0.42
1:A:517:THR:HA	1:B:39:VAL:HB	2.02	0.42
1:C:30:THR:HG22	1:C:38:VAL:CG2	2.45	0.42
1:E:23:LEU:O	1:E:27:VAL:HG23	2.19	0.42
1:E:521:VAL:N	1:F:41:ASP:HB3	2.32	0.42
1:H:271:VAL:HG12	1:H:272:LYS:H	1.85	0.42
1:I:271:VAL:HG12	1:I:272:LYS:H	1.85	0.42
1:J:215:LEU:O	1:J:218:PRO:HD3	2.18	0.42
1:K:488:MET:HA	1:K:488:MET:HE2	2.02	0.42
1:N:400:LEU:CA	1:N:401:HIS:N	2.76	0.42
1:A:46:ALA:HB1	1:G:73:MET:HA	2.01	0.42
1:D:180:GLY:HA3	1:D:381:VAL:O	2.19	0.42
1:E:520:MET:CA	1:F:41:ASP:HB2	2.48	0.42
1:F:294:THR:HG21	1:F:345:ARG:HG3	2.01	0.42
1:G:19:GLY:HA2	1:G:62:LEU:CD1	2.50	0.42
1:L:488:MET:HE2	1:L:488:MET:HA	2.02	0.42
1:M:271:VAL:HG12	1:M:272:LYS:H	1.85	0.42
1:A:13:ARG:NH1	1:A:515:ILE:O	2.49	0.42
1:A:23:LEU:O	1:A:27:VAL:HG23	2.19	0.42
1:A:39:VAL:HB	1:G:517:THR:HA	2.02	0.42
1:C:39:VAL:HG13	1:C:49:ILE:HA	2.01	0.42
1:D:338:GLU:CD	1:D:341:ALA:HB2	2.45	0.42
1:E:112:ASN:HA	1:E:113:PRO:HD2	1.74	0.42
1:G:39:VAL:HG13	1:G:49:ILE:HA	2.01	0.42
1:I:7:LYS:O	1:I:519:CYS:HA	2.18	0.42
1:J:271:VAL:HG12	1:J:272:LYS:H	1.85	0.42
1:N:488:MET:HE2	1:N:488:MET:HA	2.02	0.42
1:B:73:MET:HA	1:C:46:ALA:HB1	2.01	0.42
1:C:23:LEU:O	1:C:27:VAL:HG23	2.19	0.42
1:D:513:LEU:CA	1:E:49:ILE:HD11	2.43	0.42
1:E:19:GLY:HA2	1:E:62:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:MET:HA	1:F:46:ALA:HB1	2.01	0.42
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.35	0.42
1:G:294:THR:HG21	1:G:345:ARG:HG3	2.01	0.42
1:B:23:LEU:O	1:B:27:VAL:HG23	2.19	0.42
1:B:40:LEU:HD11	1:B:55:SER:CB	2.48	0.42
1:C:30:THR:CG2	1:C:38:VAL:HG21	2.42	0.42
1:C:338:GLU:CD	1:C:341:ALA:HB2	2.45	0.42
1:D:30:THR:HG22	1:D:38:VAL:CG2	2.45	0.42
1:D:46:ALA:HA	1:D:47:PRO:HD2	1.85	0.42
1:E:294:THR:HG21	1:E:345:ARG:HG3	2.02	0.42
1:F:19:GLY:HA2	1:F:62:LEU:CD1	2.50	0.42
1:F:488:MET:HA	1:F:488:MET:HE2	2.01	0.42
1:F:520:MET:CA	1:G:41:ASP:HB2	2.48	0.42
1:L:271:VAL:HG12	1:L:272:LYS:H	1.85	0.42
1:N:191:GLU:O	1:N:334:ASP:HA	2.18	0.42
1:A:521:VAL:N	1:B:41:ASP:HB3	2.32	0.42
1:C:19:GLY:HA2	1:C:62:LEU:CD1	2.50	0.42
1:F:202:PRO:O	1:F:205:ILE:HB	2.19	0.42
1:F:338:GLU:CD	1:F:341:ALA:HB2	2.45	0.42
1:K:7:LYS:O	1:K:519:CYS:HA	2.18	0.42
1:A:180:GLY:HA3	1:A:381:VAL:O	2.19	0.42
1:A:383:ALA:HB3	1:A:389:MET:N	2.35	0.42
1:B:39:VAL:HG13	1:B:49:ILE:HA	2.01	0.42
1:E:30:THR:HG22	1:E:38:VAL:CG2	2.45	0.42
1:F:30:THR:HG22	1:F:38:VAL:CG2	2.45	0.42
1:F:517:THR:HA	1:G:39:VAL:HB	2.02	0.42
1:G:30:THR:HG22	1:G:38:VAL:CG2	2.45	0.42
1:A:39:VAL:HG13	1:A:49:ILE:HA	2.01	0.41
1:C:293:ALA:HB2	1:C:300:VAL:CG2	2.49	0.41
1:D:73:MET:HA	1:E:46:ALA:HB1	2.01	0.41
1:E:202:PRO:O	1:E:205:ILE:HB	2.19	0.41
1:I:34:LYS:HZ3	1:I:483:GLU:CD	2.28	0.41
1:J:488:MET:HE2	1:J:488:MET:HA	2.02	0.41
1:K:254:VAL:CG1	1:K:259:LEU:HD23	2.50	0.41
1:B:517:THR:HA	1:C:39:VAL:HB	2.02	0.41
1:D:19:GLY:HA2	1:D:62:LEU:CD1	2.50	0.41
1:D:294:THR:HG21	1:D:345:ARG:HG3	2.02	0.41
1:E:102:GLU:HB2	1:E:442:VAL:HG13	2.02	0.41
1:G:112:ASN:HA	1:G:113:PRO:HD2	1.74	0.41
1:G:383:ALA:HB3	1:G:389:MET:N	2.35	0.41
1:J:254:VAL:CG1	1:J:259:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HD11	1:G:513:LEU:CA	2.43	0.41
1:B:323:VAL:HG22	1:B:332:ILE:HA	2.03	0.41
1:C:73:MET:HA	1:D:46:ALA:HB1	2.01	0.41
1:C:294:THR:HG21	1:C:345:ARG:HG3	2.01	0.41
1:E:338:GLU:CD	1:E:341:ALA:HB2	2.45	0.41
1:F:23:LEU:O	1:F:27:VAL:HG23	2.19	0.41
1:F:126:ALA:HB3	1:F:426:LEU:HD22	2.03	0.41
1:I:488:MET:HE2	1:I:488:MET:HA	2.02	0.41
1:K:335:GLY:C	1:K:337:GLY:H	2.29	0.41
1:N:254:VAL:CG1	1:N:259:LEU:HD23	2.50	0.41
1:A:323:VAL:HG22	1:A:332:ILE:HA	2.03	0.41
1:B:19:GLY:HA2	1:B:62:LEU:CD1	2.50	0.41
1:C:383:ALA:HB3	1:C:389:MET:N	2.35	0.41
1:G:126:ALA:HB3	1:G:426:LEU:HD22	2.03	0.41
1:H:335:GLY:C	1:H:337:GLY:H	2.29	0.41
1:A:294:THR:HG21	1:A:345:ARG:HG3	2.01	0.41
1:D:13:ARG:NH1	1:D:515:ILE:O	2.49	0.41
1:D:202:PRO:O	1:D:205:ILE:HB	2.19	0.41
1:G:488:MET:HE2	1:G:488:MET:HA	2.01	0.41
1:H:488:MET:HE2	1:H:488:MET:HA	2.02	0.41
1:I:254:VAL:CG1	1:I:259:LEU:HD23	2.50	0.41
1:I:335:GLY:C	1:I:337:GLY:H	2.29	0.41
1:A:268:ARG:CZ	1:A:268:ARG:HA	2.51	0.41
1:E:126:ALA:HB3	1:E:426:LEU:HD22	2.03	0.41
1:E:205:ILE:HG23	1:E:211:GLY:HA2	2.03	0.41
1:E:513:LEU:CA	1:F:49:ILE:HD11	2.43	0.41
1:E:517:THR:HA	1:F:39:VAL:HB	2.02	0.41
1:G:338:GLU:CD	1:G:341:ALA:HB2	2.45	0.41
1:M:254:VAL:CG1	1:M:259:LEU:HD23	2.50	0.41
1:A:102:GLU:HB2	1:A:442:VAL:HG13	2.02	0.41
1:A:126:ALA:HB3	1:A:426:LEU:HD22	2.03	0.41
1:C:135:SER:CA	1:C:412:VAL:HG12	2.45	0.41
1:D:517:THR:HA	1:E:39:VAL:HB	2.02	0.41
1:G:202:PRO:O	1:G:205:ILE:HB	2.19	0.41
1:G:323:VAL:HG22	1:G:332:ILE:HA	2.03	0.41
1:M:488:MET:HA	1:M:488:MET:HE2	2.02	0.41
1:A:112:ASN:C	1:B:36:ARG:NH1	2.72	0.41
1:B:294:THR:HG21	1:B:345:ARG:HG3	2.01	0.41
1:B:383:ALA:HB3	1:B:389:MET:N	2.35	0.41
1:C:323:VAL:HG22	1:C:332:ILE:HA	2.03	0.41
1:D:383:ALA:HB3	1:D:389:MET:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:GLU:HB2	1:F:442:VAL:HG13	2.02	0.41
1:H:34:LYS:HZ3	1:H:483:GLU:CD	2.29	0.41
1:B:13:ARG:NH1	1:B:515:ILE:O	2.49	0.41
1:B:268:ARG:CZ	1:B:268:ARG:HA	2.51	0.41
1:B:338:GLU:CD	1:B:341:ALA:HB2	2.45	0.41
1:D:102:GLU:HB2	1:D:442:VAL:HG13	2.02	0.41
1:E:46:ALA:HA	1:E:47:PRO:HD2	1.84	0.41
1:F:85:ALA:HB1	1:F:499:VAL:HA	2.03	0.41
1:F:383:ALA:HB3	1:F:389:MET:N	2.35	0.41
1:F:513:LEU:CA	1:G:49:ILE:HD11	2.43	0.41
1:K:271:VAL:HG12	1:K:272:LYS:H	1.85	0.41
1:N:335:GLY:C	1:N:337:GLY:H	2.28	0.41
1:C:152:ALA:HB1	1:C:155:ASP:CA	2.51	0.41
1:D:112:ASN:HA	1:D:113:PRO:HD2	1.74	0.41
1:F:51:LYS:HB2	1:F:395:ARG:HD3	2.03	0.41
1:F:205:ILE:HG23	1:F:211:GLY:HA2	2.03	0.41
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.35	0.41
1:G:268:ARG:CZ	1:G:268:ARG:HA	2.51	0.41
1:B:102:GLU:HB2	1:B:442:VAL:HG13	2.02	0.40
1:B:126:ALA:HB3	1:B:426:LEU:HD22	2.03	0.40
1:B:152:ALA:HB1	1:B:155:ASP:CA	2.51	0.40
1:D:34:LYS:HZ1	1:D:483:GLU:CD	2.29	0.40
1:G:102:GLU:HB2	1:G:442:VAL:HG13	2.02	0.40
1:A:338:GLU:CD	1:A:341:ALA:HB2	2.45	0.40
1:D:152:ALA:HB1	1:D:155:ASP:CA	2.51	0.40
1:D:461:GLU:HA	1:D:462:PRO:HD2	1.83	0.40
1:E:13:ARG:NH1	1:E:515:ILE:O	2.49	0.40
1:E:383:ALA:HB3	1:E:389:MET:N	2.35	0.40
3:G:1525:PO4:P	2:G:1527:ATP:PG	3.20	0.40
1:J:335:GLY:C	1:J:337:GLY:H	2.29	0.40
1:A:152:ALA:HB1	1:A:155:ASP:CA	2.51	0.40
1:D:126:ALA:HB3	1:D:426:LEU:HD22	2.03	0.40
1:D:205:ILE:HG23	1:D:211:GLY:HA2	2.03	0.40
1:D:206:ASN:HB2	1:D:213:VAL:CB	2.52	0.40
1:D:323:VAL:HG22	1:D:332:ILE:HA	2.03	0.40
1:E:85:ALA:HB1	1:E:499:VAL:HA	2.04	0.40
1:E:206:ASN:HB2	1:E:213:VAL:CB	2.51	0.40
1:F:231:ARG:O	1:F:235:PRO:HD2	2.22	0.40
3:F:1525:PO4:P	2:F:1527:ATP:PG	3.20	0.40
1:G:205:ILE:HG23	1:G:211:GLY:HA2	2.03	0.40
1:H:254:VAL:CG1	1:H:259:LEU:HD23	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1525:ATP:PG	3:A:1526:PO4:P	3.20	0.40
1:B:13:ARG:HH11	1:B:13:ARG:CG	2.34	0.40
1:B:85:ALA:HB1	1:B:499:VAL:HA	2.04	0.40
1:C:166:MET:HA	1:C:175:ILE:HD11	2.04	0.40
1:C:268:ARG:HA	1:C:268:ARG:CZ	2.51	0.40
1:C:517:THR:HA	1:D:39:VAL:HB	2.02	0.40
1:D:85:ALA:HB1	1:D:499:VAL:HA	2.03	0.40
1:D:517:THR:CA	1:E:39:VAL:HB	2.52	0.40
1:F:152:ALA:HB1	1:F:155:ASP:CA	2.51	0.40
1:F:323:VAL:HG22	1:F:332:ILE:HA	2.03	0.40
1:G:62:LEU:HB2	1:G:68:ASN:HA	2.04	0.40
1:G:166:MET:HA	1:G:175:ILE:HD11	2.04	0.40
1:A:62:LEU:HB2	1:A:68:ASN:HA	2.04	0.40
1:B:62:LEU:HB2	1:B:68:ASN:HA	2.04	0.40
1:C:85:ALA:HB1	1:C:499:VAL:HA	2.04	0.40
1:E:231:ARG:O	1:E:235:PRO:HD2	2.22	0.40
1:E:268:ARG:HA	1:E:268:ARG:CZ	2.51	0.40
1:E:517:THR:CA	1:F:39:VAL:HB	2.52	0.40
1:F:268:ARG:HA	1:F:268:ARG:NE	2.37	0.40
1:G:51:LYS:HB2	1:G:395:ARG:HD3	2.03	0.40
1:G:85:ALA:HB1	1:G:499:VAL:HA	2.04	0.40
1:M:335:GLY:C	1:M:337:GLY:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	B	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	C	522/548 (95%)	517 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	E	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	F	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	G	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	H	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	30	67
1	I	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	30	67
1	J	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	30	67
1	K	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	30	67
1	L	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	30	67
1	M	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	30	67
1	N	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	30	67
All	All	7308/7672 (95%)	7105 (97%)	189 (3%)	14 (0%)	44	78

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	269	GLY
1	I	269	GLY
1	J	269	GLY
1	K	269	GLY
1	L	269	GLY
1	M	269	GLY
1	N	269	GLY
1	H	336	VAL
1	I	336	VAL
1	J	336	VAL
1	K	336	VAL
1	L	336	VAL
1	M	336	VAL
1	N	336	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	355 (88%)	47 (12%)	5	18
1	B	402/414 (97%)	356 (89%)	46 (11%)	5	18
1	C	402/414 (97%)	355 (88%)	47 (12%)	5	18
1	D	402/414 (97%)	356 (89%)	46 (11%)	5	18
1	E	402/414 (97%)	356 (89%)	46 (11%)	5	18
1	F	402/414 (97%)	356 (89%)	46 (11%)	5	18
1	G	402/414 (97%)	356 (89%)	46 (11%)	5	18
1	H	402/414 (97%)	368 (92%)	34 (8%)	10	29
1	I	402/414 (97%)	368 (92%)	34 (8%)	10	29
1	J	402/414 (97%)	368 (92%)	34 (8%)	10	29
1	K	402/414 (97%)	368 (92%)	34 (8%)	10	29
1	L	402/414 (97%)	368 (92%)	34 (8%)	10	29
1	M	402/414 (97%)	368 (92%)	34 (8%)	10	29
1	N	402/414 (97%)	368 (92%)	34 (8%)	10	29
All	All	5628/5796 (97%)	5066 (90%)	562 (10%)	9	24

All (562) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	8	PHE
1	A	25	ASP
1	A	31	LEU
1	A	37	ASN
1	A	49	ILE
1	A	54	VAL
1	A	55	SER
1	A	79	SER
1	A	130	GLU
1	A	155	ASP
1	A	156	GLU
1	A	164	GLU
1	A	168	LYS
1	A	169	VAL
1	A	171	LYS
1	A	172	GLU

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Mol	Chain	Res	Type
1	A	190	VAL
1	A	200	LEU
1	A	205	ILE
1	A	207	LYS
1	A	213	VAL
1	A	214	GLU
1	A	228	SER
1	A	230	ILE
1	A	254	VAL
1	A	257	GLU
1	A	290	GLN
1	A	295	LEU
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	363	GLU
1	A	421	ARG
1	A	450	PRO
1	A	453	GLN
1	A	460	GLU
1	A	463	SER
1	A	484	GLU
1	A	504	LEU
1	A	516	THR
1	A	517	THR
1	A	523	ASP
1	B	4	LYS
1	B	8	PHE
1	B	25	ASP
1	B	31	LEU
1	B	37	ASN
1	B	49	ILE
1	B	54	VAL
1	B	55	SER
1	B	79	SER
1	B	130	GLU
1	B	155	ASP
1	B	156	GLU

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Mol	Chain	Res	Type
1	B	164	GLU
1	B	168	LYS
1	B	169	VAL
1	B	171	LYS
1	B	172	GLU
1	B	190	VAL
1	B	200	LEU
1	B	205	ILE
1	B	207	LYS
1	B	213	VAL
1	B	214	GLU
1	B	228	SER
1	B	230	ILE
1	B	254	VAL
1	B	257	GLU
1	B	290	GLN
1	B	295	LEU
1	B	301	ILE
1	B	323	VAL
1	B	327	LYS
1	B	328	ASP
1	B	334	ASP
1	B	350	ARG
1	B	358	SER
1	B	363	GLU
1	B	421	ARG
1	B	450	PRO
1	B	460	GLU
1	B	463	SER
1	B	484	GLU
1	B	504	LEU
1	B	516	THR
1	B	517	THR
1	B	523	ASP
1	C	4	LYS
1	C	8	PHE
1	C	25	ASP
1	C	31	LEU
1	C	37	ASN
1	C	49	ILE
1	C	54	VAL
1	C	55	SER

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Mol	Chain	Res	Type
1	C	79	SER
1	C	130	GLU
1	C	155	ASP
1	C	156	GLU
1	C	164	GLU
1	C	168	LYS
1	C	169	VAL
1	C	171	LYS
1	C	172	GLU
1	C	190	VAL
1	C	200	LEU
1	C	205	ILE
1	C	207	LYS
1	C	213	VAL
1	C	214	GLU
1	C	228	SER
1	C	230	ILE
1	C	254	VAL
1	C	257	GLU
1	C	290	GLN
1	C	295	LEU
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	363	GLU
1	C	421	ARG
1	C	450	PRO
1	C	453	GLN
1	C	460	GLU
1	C	463	SER
1	C	484	GLU
1	C	504	LEU
1	C	516	THR
1	C	517	THR
1	C	523	ASP
1	D	4	LYS
1	D	8	PHE
1	D	25	ASP

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Mol	Chain	Res	Type
1	D	31	LEU
1	D	37	ASN
1	D	49	ILE
1	D	54	VAL
1	D	55	SER
1	D	79	SER
1	D	130	GLU
1	D	155	ASP
1	D	156	GLU
1	D	164	GLU
1	D	168	LYS
1	D	169	VAL
1	D	171	LYS
1	D	172	GLU
1	D	190	VAL
1	D	200	LEU
1	D	205	ILE
1	D	207	LYS
1	D	213	VAL
1	D	214	GLU
1	D	228	SER
1	D	230	ILE
1	D	254	VAL
1	D	257	GLU
1	D	290	GLN
1	D	295	LEU
1	D	301	ILE
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	363	GLU
1	D	421	ARG
1	D	450	PRO
1	D	460	GLU
1	D	463	SER
1	D	484	GLU
1	D	504	LEU
1	D	516	THR
1	D	517	THR

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Mol	Chain	Res	Type
1	D	523	ASP
1	E	4	LYS
1	E	8	PHE
1	E	25	ASP
1	E	31	LEU
1	E	37	ASN
1	E	49	ILE
1	E	54	VAL
1	E	55	SER
1	E	79	SER
1	E	130	GLU
1	E	155	ASP
1	E	156	GLU
1	E	164	GLU
1	E	168	LYS
1	E	169	VAL
1	E	171	LYS
1	E	172	GLU
1	E	190	VAL
1	E	200	LEU
1	E	205	ILE
1	E	207	LYS
1	E	213	VAL
1	E	214	GLU
1	E	228	SER
1	E	230	ILE
1	E	254	VAL
1	E	257	GLU
1	E	290	GLN
1	E	295	LEU
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	363	GLU
1	E	421	ARG
1	E	450	PRO
1	E	460	GLU
1	E	463	SER

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Mol	Chain	Res	Type
1	E	484	GLU
1	E	504	LEU
1	E	516	THR
1	E	517	THR
1	E	523	ASP
1	F	4	LYS
1	F	8	PHE
1	F	25	ASP
1	F	31	LEU
1	F	37	ASN
1	F	49	ILE
1	F	54	VAL
1	F	55	SER
1	F	79	SER
1	F	130	GLU
1	F	155	ASP
1	F	156	GLU
1	F	164	GLU
1	F	168	LYS
1	F	169	VAL
1	F	171	LYS
1	F	172	GLU
1	F	190	VAL
1	F	200	LEU
1	F	205	ILE
1	F	207	LYS
1	F	213	VAL
1	F	214	GLU
1	F	228	SER
1	F	230	ILE
1	F	254	VAL
1	F	257	GLU
1	F	290	GLN
1	F	295	LEU
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	363	GLU

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Mol	Chain	Res	Type
1	F	421	ARG
1	F	450	PRO
1	F	460	GLU
1	F	463	SER
1	F	484	GLU
1	F	504	LEU
1	F	516	THR
1	F	517	THR
1	F	523	ASP
1	G	4	LYS
1	G	8	PHE
1	G	25	ASP
1	G	31	LEU
1	G	37	ASN
1	G	49	ILE
1	G	54	VAL
1	G	55	SER
1	G	79	SER
1	G	130	GLU
1	G	155	ASP
1	G	156	GLU
1	G	164	GLU
1	G	168	LYS
1	G	169	VAL
1	G	171	LYS
1	G	172	GLU
1	G	190	VAL
1	G	200	LEU
1	G	205	ILE
1	G	207	LYS
1	G	213	VAL
1	G	214	GLU
1	G	228	SER
1	G	230	ILE
1	G	254	VAL
1	G	257	GLU
1	G	290	GLN
1	G	295	LEU
1	G	301	ILE
1	G	323	VAL
1	G	327	LYS
1	G	328	ASP

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Mol	Chain	Res	Type
1	G	334	ASP
1	G	350	ARG
1	G	358	SER
1	G	363	GLU
1	G	421	ARG
1	G	450	PRO
1	G	460	GLU
1	G	463	SER
1	G	484	GLU
1	G	504	LEU
1	G	516	THR
1	G	517	THR
1	G	523	ASP
1	H	82	ASN
1	H	130	GLU
1	H	140	ASP
1	H	142	LYS
1	H	153	ASN
1	H	171	LYS
1	H	172	GLU
1	H	174	VAL
1	H	184	GLN
1	H	186	GLU
1	H	187	LEU
1	H	196	ASP
1	H	213	VAL
1	H	214	GLU
1	H	216	GLU
1	H	228	SER
1	H	229	ASN
1	H	230	ILE
1	H	290	GLN
1	H	327	LYS
1	H	329	THR
1	H	334	ASP
1	H	338	GLU
1	H	390	LYS
1	H	404	ARG
1	H	411	VAL
1	H	460	GLU
1	H	463	SER
1	H	483	GLU

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Mol	Chain	Res	Type
1	H	484	GLU
1	H	494	LEU
1	H	500	THR
1	H	504	LEU
1	H	510	VAL
1	I	82	ASN
1	I	130	GLU
1	I	140	ASP
1	I	142	LYS
1	I	153	ASN
1	I	171	LYS
1	I	172	GLU
1	I	174	VAL
1	I	184	GLN
1	I	186	GLU
1	I	187	LEU
1	I	196	ASP
1	I	213	VAL
1	I	214	GLU
1	I	216	GLU
1	I	228	SER
1	I	229	ASN
1	I	230	ILE
1	I	290	GLN
1	I	327	LYS
1	I	329	THR
1	I	334	ASP
1	I	338	GLU
1	I	390	LYS
1	I	404	ARG
1	I	411	VAL
1	I	460	GLU
1	I	463	SER
1	I	483	GLU
1	I	484	GLU
1	I	494	LEU
1	I	500	THR
1	I	504	LEU
1	I	510	VAL
1	J	82	ASN
1	J	130	GLU
1	J	140	ASP

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Mol	Chain	Res	Type
1	J	142	LYS
1	J	153	ASN
1	J	171	LYS
1	J	172	GLU
1	J	174	VAL
1	J	184	GLN
1	J	186	GLU
1	J	187	LEU
1	J	196	ASP
1	J	213	VAL
1	J	214	GLU
1	J	216	GLU
1	J	228	SER
1	J	229	ASN
1	J	230	ILE
1	J	290	GLN
1	J	327	LYS
1	J	329	THR
1	J	334	ASP
1	J	338	GLU
1	J	390	LYS
1	J	404	ARG
1	J	411	VAL
1	J	460	GLU
1	J	463	SER
1	J	483	GLU
1	J	484	GLU
1	J	494	LEU
1	J	500	THR
1	J	504	LEU
1	J	510	VAL
1	K	82	ASN
1	K	130	GLU
1	K	140	ASP
1	K	142	LYS
1	K	153	ASN
1	K	171	LYS
1	K	172	GLU
1	K	174	VAL
1	K	184	GLN
1	K	186	GLU
1	K	187	LEU

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Mol	Chain	Res	Type
1	K	196	ASP
1	K	213	VAL
1	K	214	GLU
1	K	216	GLU
1	K	228	SER
1	K	229	ASN
1	K	230	ILE
1	K	290	GLN
1	K	327	LYS
1	K	329	THR
1	K	334	ASP
1	K	338	GLU
1	K	390	LYS
1	K	404	ARG
1	K	411	VAL
1	K	460	GLU
1	K	463	SER
1	K	483	GLU
1	K	484	GLU
1	K	494	LEU
1	K	500	THR
1	K	504	LEU
1	K	510	VAL
1	L	82	ASN
1	L	130	GLU
1	L	140	ASP
1	L	142	LYS
1	L	153	ASN
1	L	171	LYS
1	L	172	GLU
1	L	174	VAL
1	L	184	GLN
1	L	186	GLU
1	L	187	LEU
1	L	196	ASP
1	L	213	VAL
1	L	214	GLU
1	L	216	GLU
1	L	228	SER
1	L	229	ASN
1	L	230	ILE
1	L	290	GLN

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Mol	Chain	Res	Type
1	L	327	LYS
1	L	329	THR
1	L	334	ASP
1	L	338	GLU
1	L	390	LYS
1	L	404	ARG
1	L	411	VAL
1	L	460	GLU
1	L	463	SER
1	L	483	GLU
1	L	484	GLU
1	L	494	LEU
1	L	500	THR
1	L	504	LEU
1	L	510	VAL
1	M	82	ASN
1	M	130	GLU
1	M	140	ASP
1	M	142	LYS
1	M	153	ASN
1	M	171	LYS
1	M	172	GLU
1	M	174	VAL
1	M	184	GLN
1	M	186	GLU
1	M	187	LEU
1	M	196	ASP
1	M	213	VAL
1	M	214	GLU
1	M	216	GLU
1	M	228	SER
1	M	229	ASN
1	M	230	ILE
1	M	290	GLN
1	M	327	LYS
1	M	329	THR
1	M	334	ASP
1	M	338	GLU
1	M	390	LYS
1	M	404	ARG
1	M	411	VAL
1	M	460	GLU

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Mol	Chain	Res	Type
1	M	463	SER
1	M	483	GLU
1	M	484	GLU
1	M	494	LEU
1	M	500	THR
1	M	504	LEU
1	M	510	VAL
1	N	82	ASN
1	N	130	GLU
1	N	140	ASP
1	N	142	LYS
1	N	153	ASN
1	N	171	LYS
1	N	172	GLU
1	N	174	VAL
1	N	184	GLN
1	N	186	GLU
1	N	187	LEU
1	N	196	ASP
1	N	213	VAL
1	N	214	GLU
1	N	216	GLU
1	N	228	SER
1	N	229	ASN
1	N	230	ILE
1	N	290	GLN
1	N	327	LYS
1	N	329	THR
1	N	334	ASP
1	N	338	GLU
1	N	390	LYS
1	N	404	ARG
1	N	411	VAL
1	N	460	GLU
1	N	463	SER
1	N	483	GLU
1	N	484	GLU
1	N	494	LEU
1	N	500	THR
1	N	504	LEU
1	N	510	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	366	GLN
1	B	229	ASN
1	B	366	GLN
1	C	366	GLN
1	D	366	GLN
1	E	366	GLN
1	F	366	GLN
1	G	366	GLN
1	H	326	ASN
1	H	352	GLN
1	I	326	ASN
1	I	352	GLN
1	J	326	ASN
1	J	352	GLN
1	K	326	ASN
1	K	352	GLN
1	L	326	ASN
1	L	352	GLN
1	M	326	ASN
1	M	352	GLN
1	N	326	ASN
1	N	352	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 21 ligands modelled in this entry, 7 are modelled with single atom and 7 are monoatomic - leaving 7 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	$\# Z > 2$
2	ATP	C	1526	4	32,33,33	1.61	2 (6%)	48,52,52	1.03	4 (8%)
2	ATP	B	1525	4	32,33,33	1.60	2 (6%)	48,52,52	1.04	4 (8%)
2	ATP	F	1527	4	32,33,33	1.60	2 (6%)	48,52,52	1.04	4 (8%)
2	ATP	E	1527	4	32,33,33	1.60	2 (6%)	48,52,52	1.04	4 (8%)
2	ATP	D	1525	4	32,33,33	1.61	2 (6%)	48,52,52	1.04	4 (8%)
2	ATP	G	1527	4	32,33,33	1.61	2 (6%)	48,52,52	1.04	4 (8%)
2	ATP	A	1525	4	32,33,33	1.59	2 (6%)	48,52,52	1.04	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	C	1526	4	-	1/22/38/38	0/3/3/3
2	ATP	B	1525	4	-	1/22/38/38	0/3/3/3
2	ATP	F	1527	4	-	1/22/38/38	0/3/3/3
2	ATP	E	1527	4	-	1/22/38/38	0/3/3/3
2	ATP	D	1525	4	-	1/22/38/38	0/3/3/3
2	ATP	G	1527	4	-	1/22/38/38	0/3/3/3
2	ATP	A	1525	4	-	1/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1525	ATP	PA-O3A	-7.98	1.50	1.59
2	G	1527	ATP	PA-O3A	-7.95	1.50	1.59
2	C	1526	ATP	PA-O3A	-7.89	1.51	1.59
2	F	1527	ATP	PA-O3A	-7.86	1.51	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1527	ATP	PA-O3A	-7.85	1.51	1.59
2	B	1525	ATP	PA-O3A	-7.84	1.51	1.59
2	A	1525	ATP	PA-O3A	-7.80	1.51	1.59
2	B	1525	ATP	PB-O3B	2.14	1.61	1.59
2	E	1527	ATP	PB-O3B	2.07	1.61	1.59
2	A	1525	ATP	PB-O3B	2.07	1.61	1.59
2	C	1526	ATP	PB-O3B	2.07	1.61	1.59
2	D	1525	ATP	PB-O3B	2.05	1.61	1.59
2	F	1527	ATP	PB-O3B	2.04	1.61	1.59
2	G	1527	ATP	PB-O3B	2.02	1.61	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1526	ATP	O2A-PA-O3A	2.82	114.90	107.27
2	D	1525	ATP	O2A-PA-O3A	2.82	114.88	107.27
2	E	1527	ATP	O2A-PA-O3A	2.81	114.87	107.27
2	G	1527	ATP	O2A-PA-O3A	2.81	114.86	107.27
2	A	1525	ATP	O2A-PA-O3A	2.81	114.86	107.27
2	B	1525	ATP	O2A-PA-O3A	2.80	114.85	107.27
2	F	1527	ATP	O2A-PA-O3A	2.80	114.83	107.27
2	F	1527	ATP	O3B-PG-O1G	-2.57	97.52	111.04
2	B	1525	ATP	O3B-PG-O1G	-2.56	97.59	111.04
2	C	1526	ATP	O3B-PG-O1G	-2.56	97.59	111.04
2	E	1527	ATP	O3B-PG-O1G	-2.55	97.60	111.04
2	D	1525	ATP	O3B-PG-O1G	-2.55	97.61	111.04
2	A	1525	ATP	O3B-PG-O1G	-2.55	97.62	111.04
2	G	1527	ATP	O3B-PG-O1G	-2.55	97.63	111.04
2	F	1527	ATP	O4'-C1'-N9	2.39	112.67	108.09
2	B	1525	ATP	O4'-C1'-N9	2.39	112.67	108.09
2	A	1525	ATP	O4'-C1'-N9	2.39	112.67	108.09
2	G	1527	ATP	O4'-C1'-N9	2.37	112.64	108.09
2	C	1526	ATP	O4'-C1'-N9	2.36	112.62	108.09
2	E	1527	ATP	O4'-C1'-N9	2.35	112.61	108.09
2	D	1525	ATP	O4'-C1'-N9	2.34	112.59	108.09
2	F	1527	ATP	O3G-PG-O2G	2.30	116.43	107.80
2	B	1525	ATP	O3G-PG-O2G	2.29	116.40	107.80
2	C	1526	ATP	O3G-PG-O2G	2.29	116.37	107.80
2	E	1527	ATP	O3G-PG-O2G	2.28	116.36	107.80
2	D	1525	ATP	O3G-PG-O2G	2.28	116.36	107.80
2	A	1525	ATP	O3G-PG-O2G	2.27	116.33	107.80
2	G	1527	ATP	O3G-PG-O2G	2.27	116.30	107.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

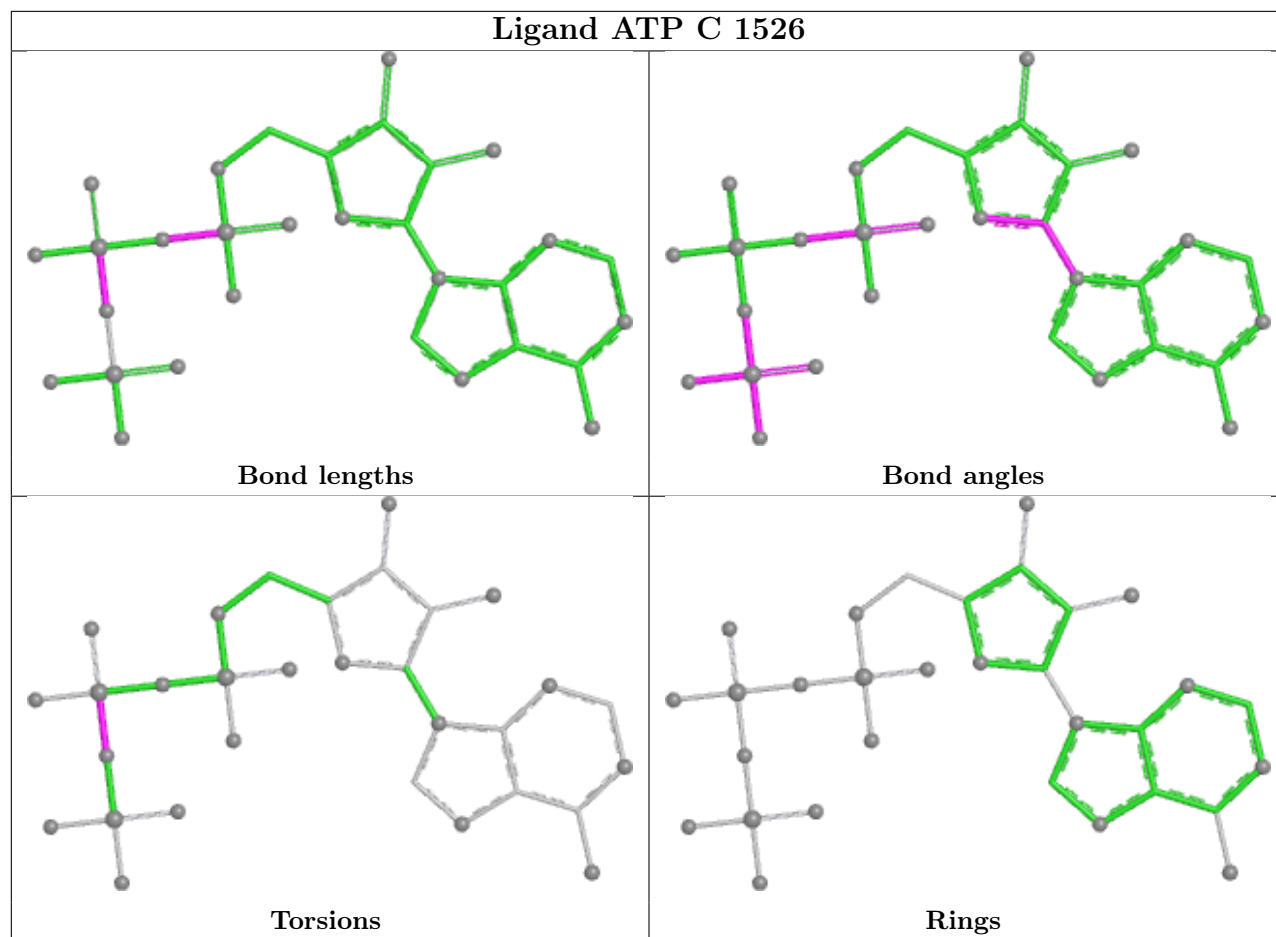
Mol	Chain	Res	Type	Atoms
2	A	1525	ATP	PG-O3B-PB-O2B
2	B	1525	ATP	PG-O3B-PB-O2B
2	C	1526	ATP	PG-O3B-PB-O2B
2	D	1525	ATP	PG-O3B-PB-O2B
2	E	1527	ATP	PG-O3B-PB-O2B
2	F	1527	ATP	PG-O3B-PB-O2B
2	G	1527	ATP	PG-O3B-PB-O2B

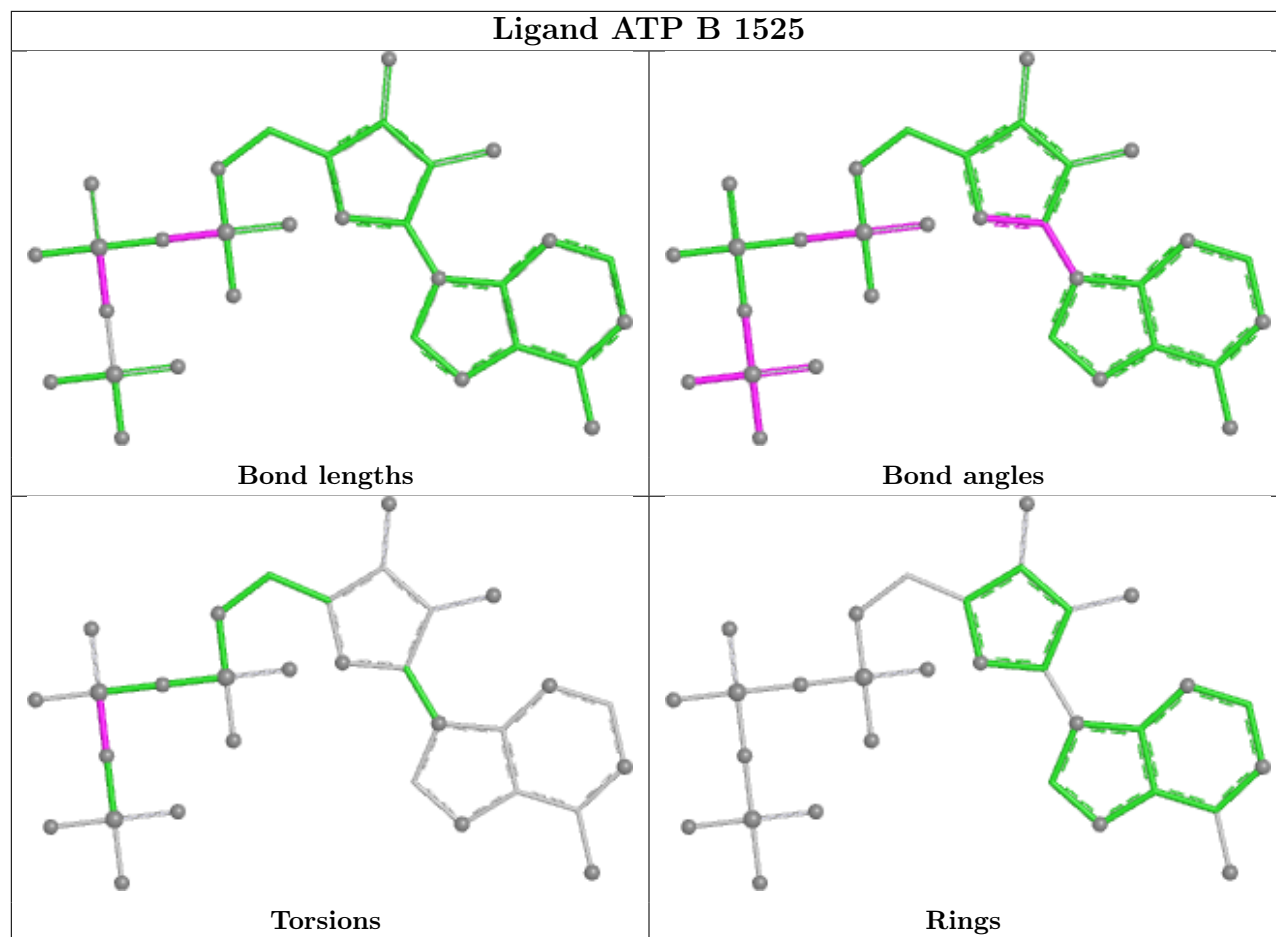
There are no ring outliers.

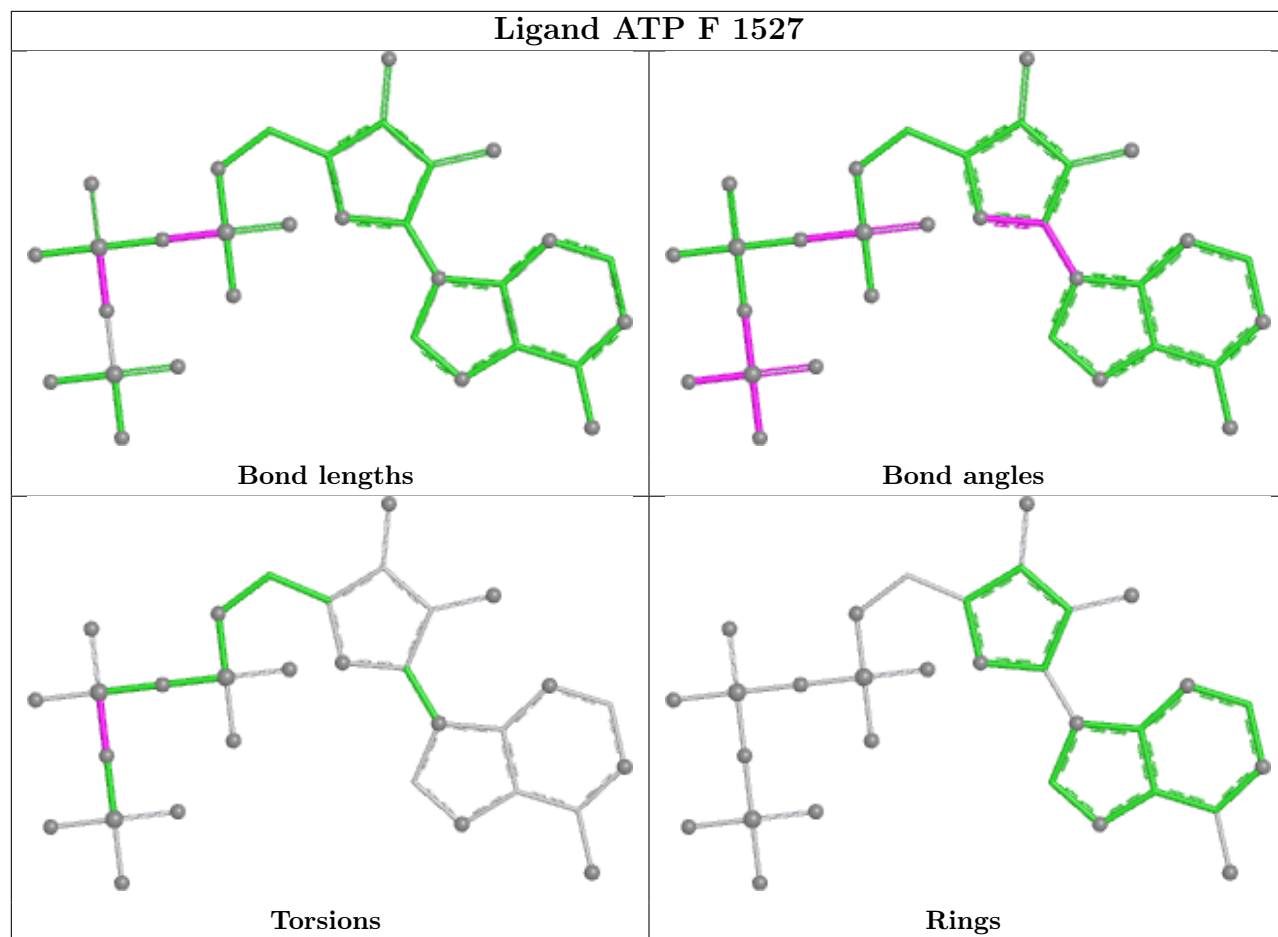
7 monomers are involved in 24 short contacts:

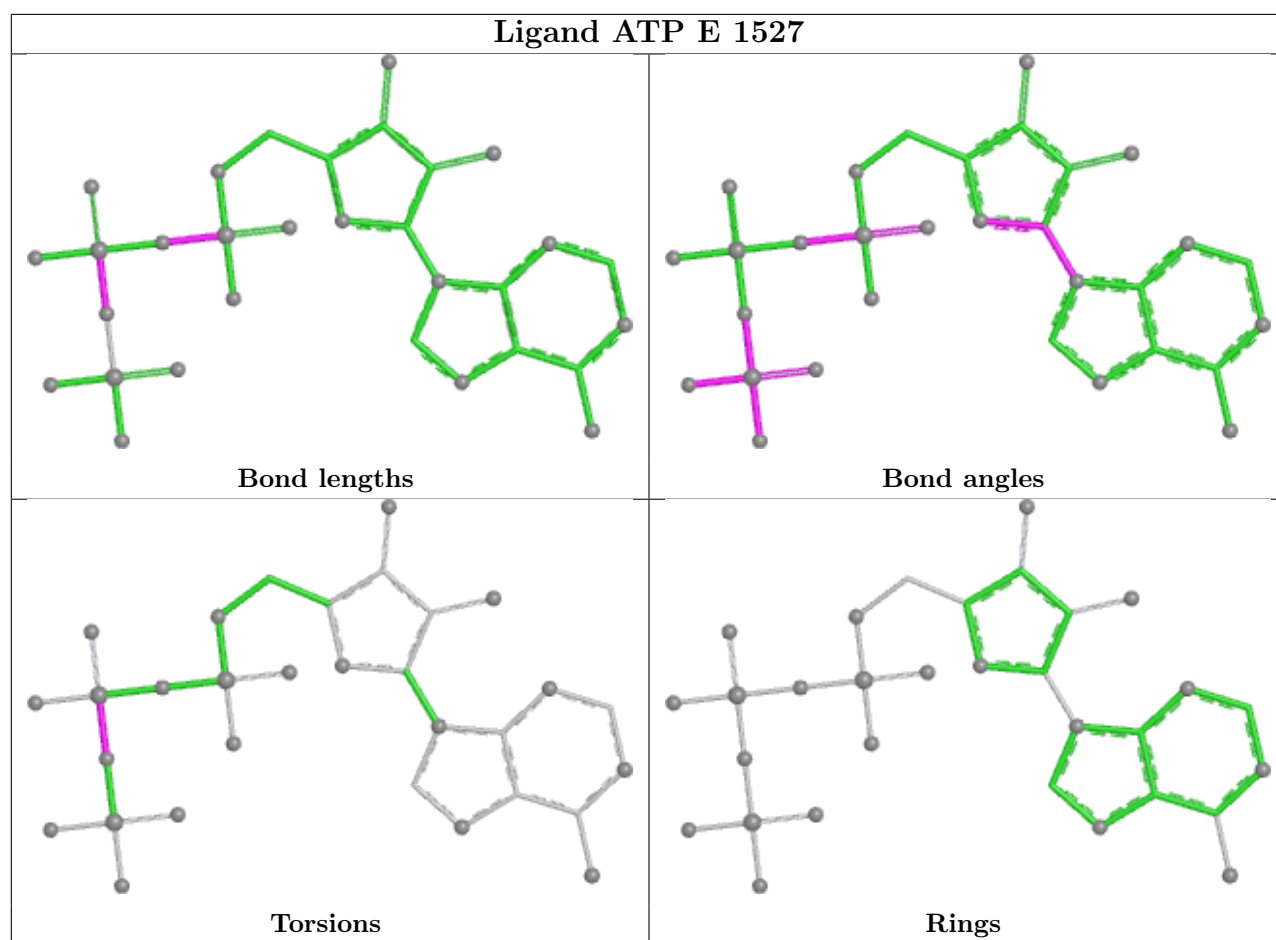
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1526	ATP	3	0
2	B	1525	ATP	3	0
2	F	1527	ATP	4	0
2	E	1527	ATP	3	0
2	D	1525	ATP	3	0
2	G	1527	ATP	4	0
2	A	1525	ATP	4	0

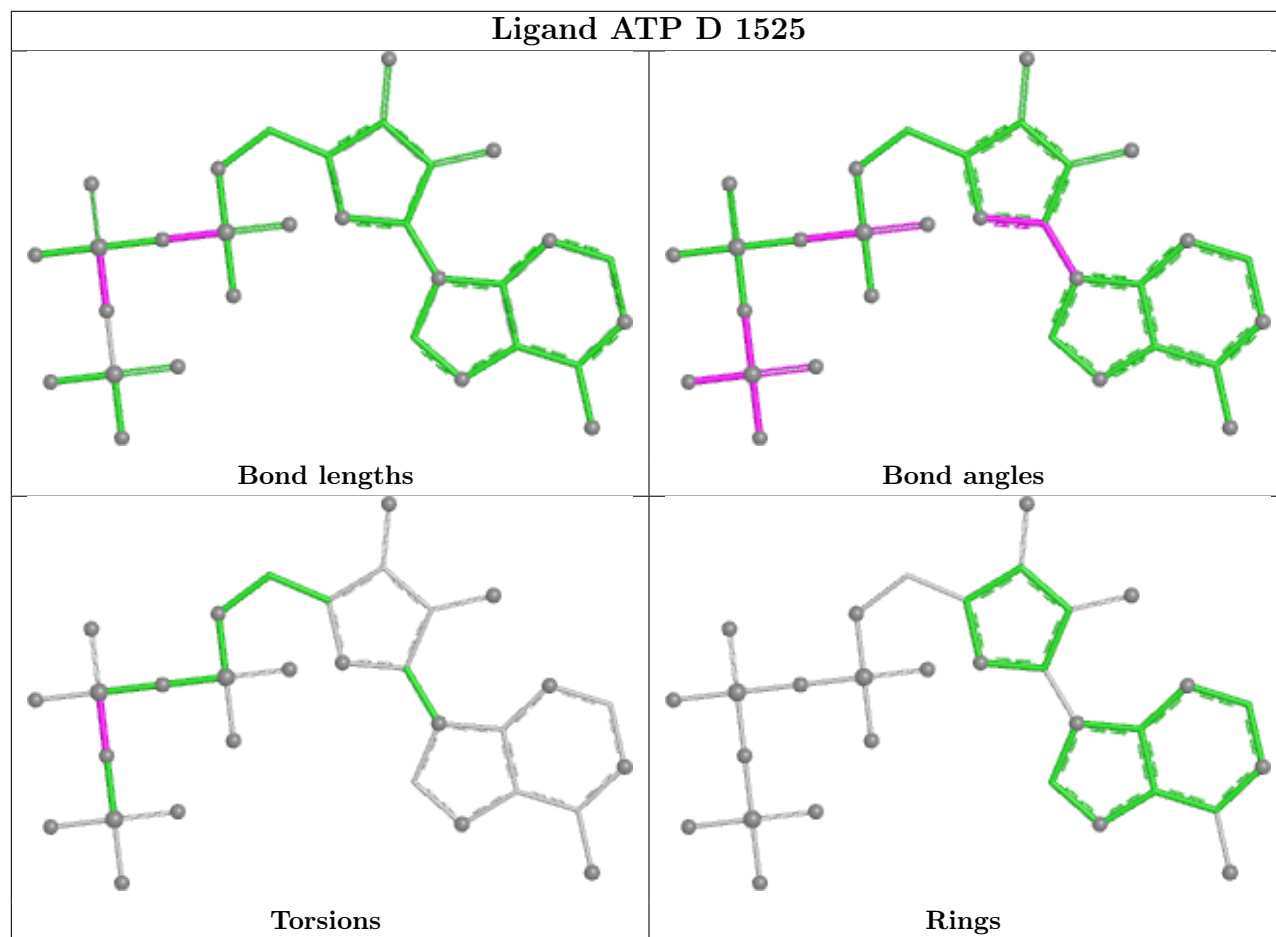
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

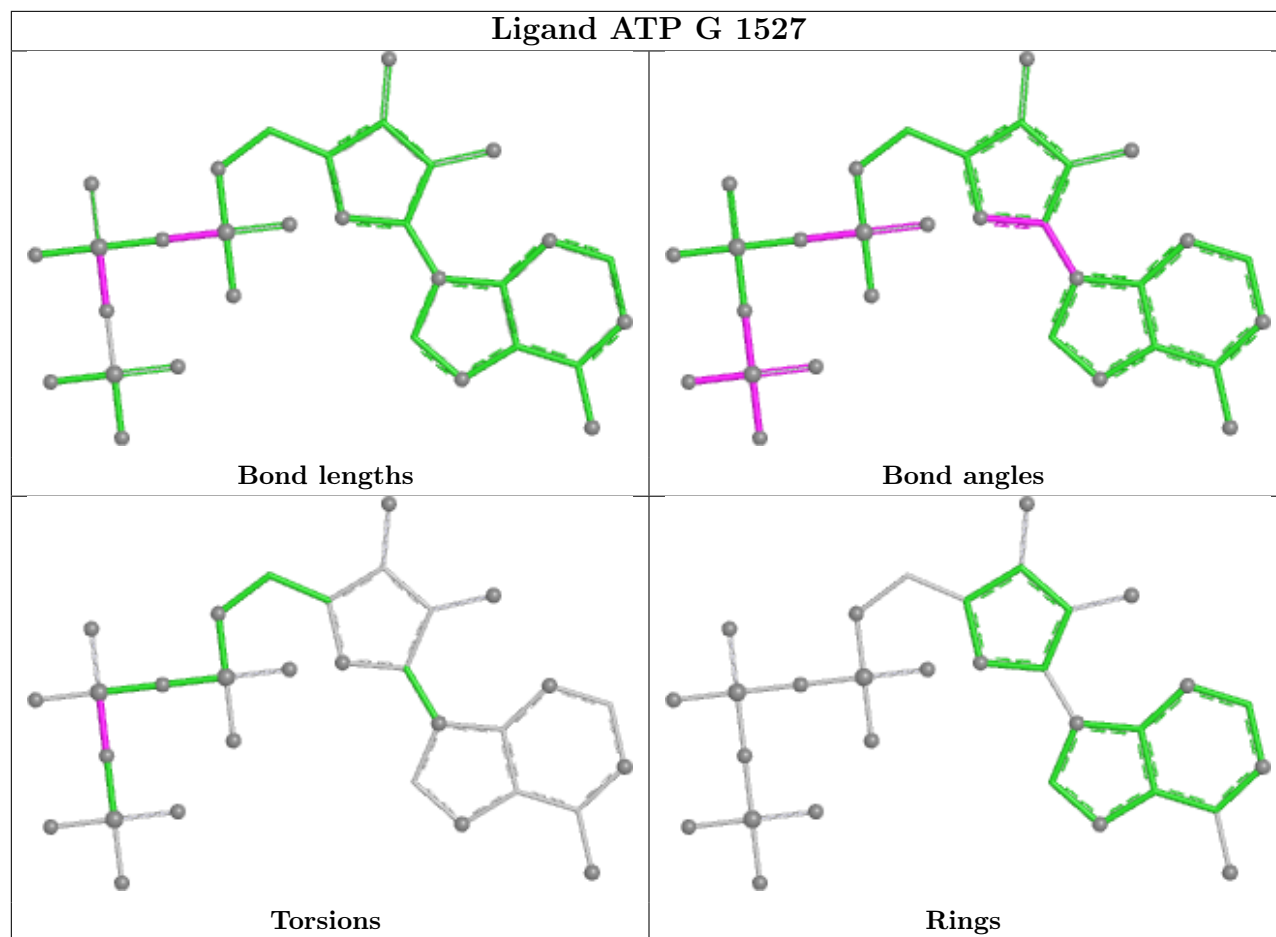


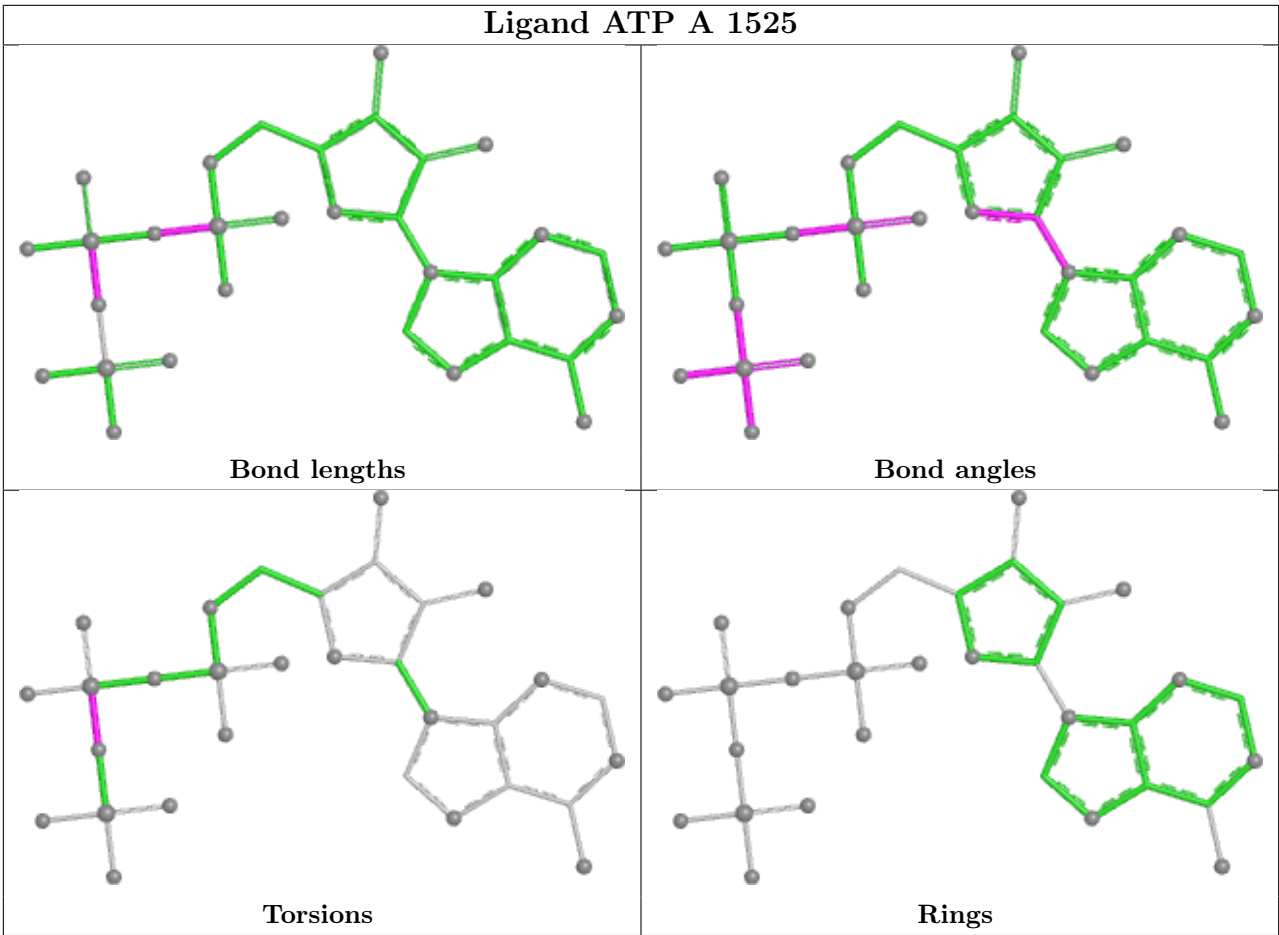












5.7 Other polymers [i](#)

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	N	2
1	J	2
1	L	1
1	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	400:LEU	C	401:HIS	N	1.83
1	L	400:LEU	C	401:HIS	N	1.78

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	400:LEU	C	401:HIS	N	1.72
1	J	401:HIS	C	402:ALA	N	1.14
1	K	401:HIS	C	402:ALA	N	1.10
1	N	401:HIS	C	402:ALA	N	0.90

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1998. 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](#)

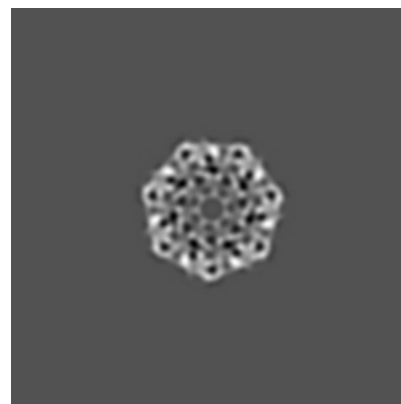
6.3.1 Primary map



X Index: 80



Y Index: 74

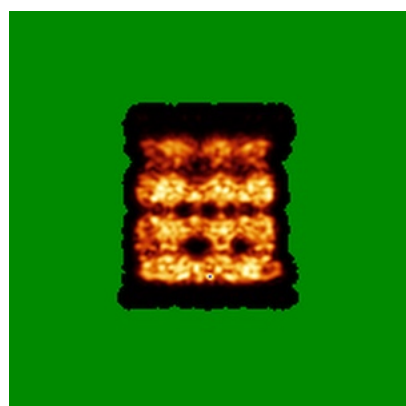


Z Index: 102

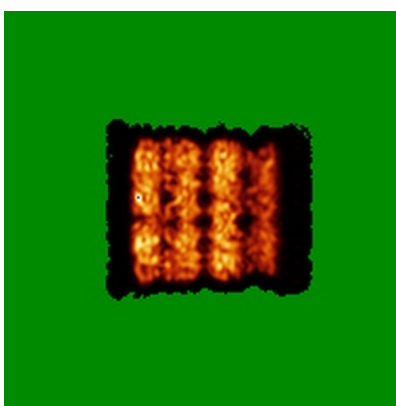
The images above show the largest variance slices of the map in three orthogonal directions.

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

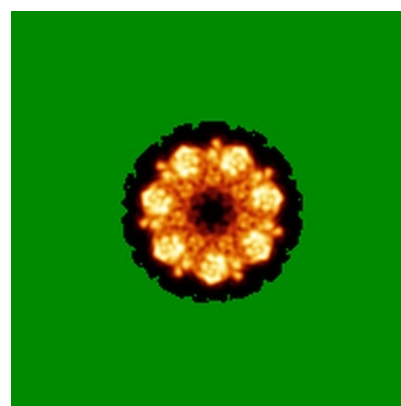
6.4.1 Primary map



X



Y

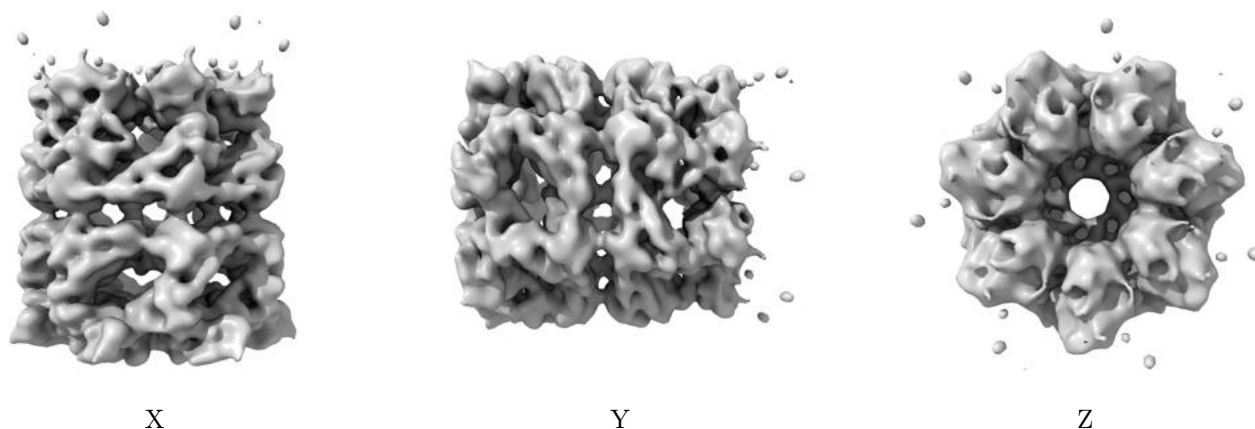


Z

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



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.

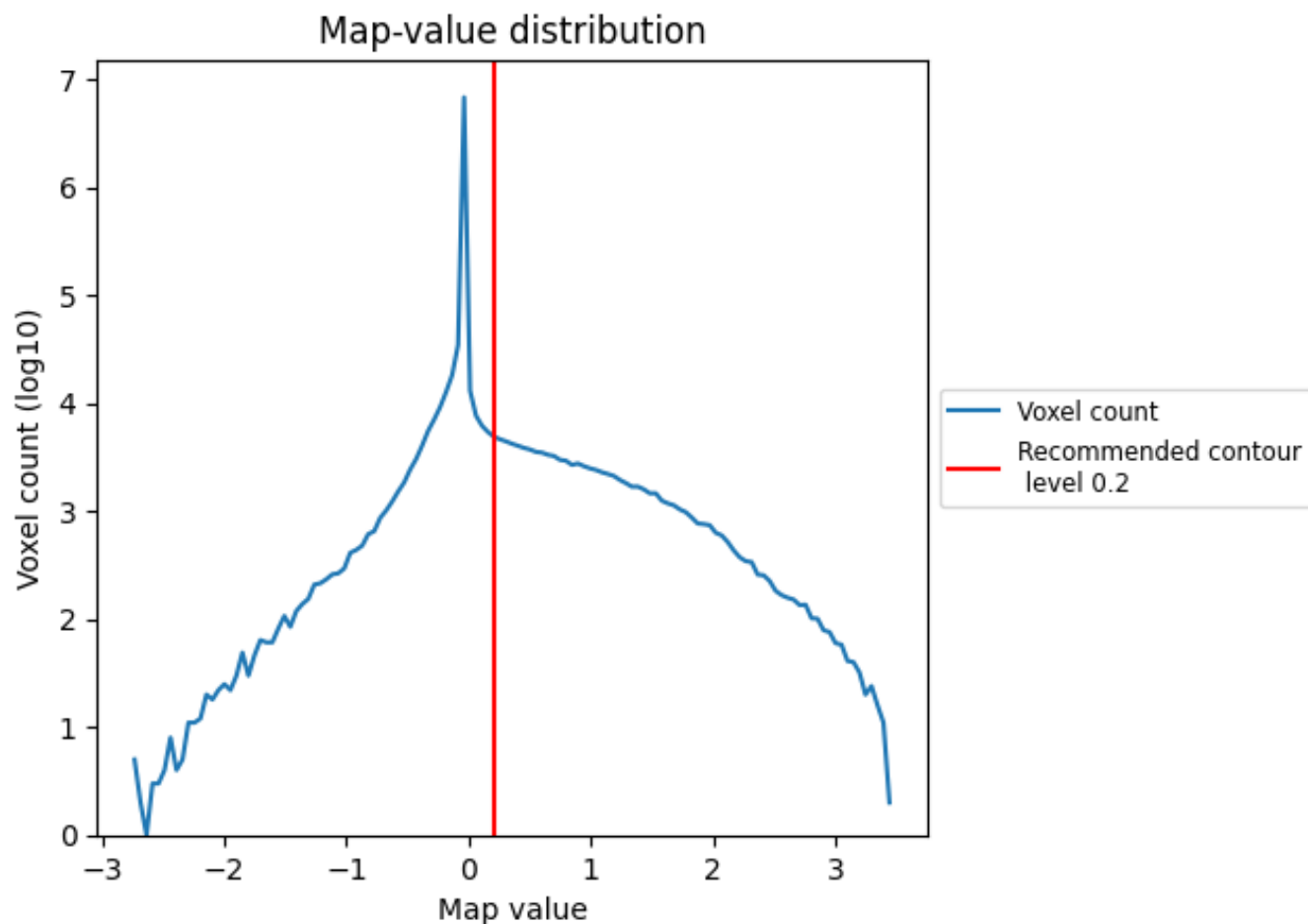
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

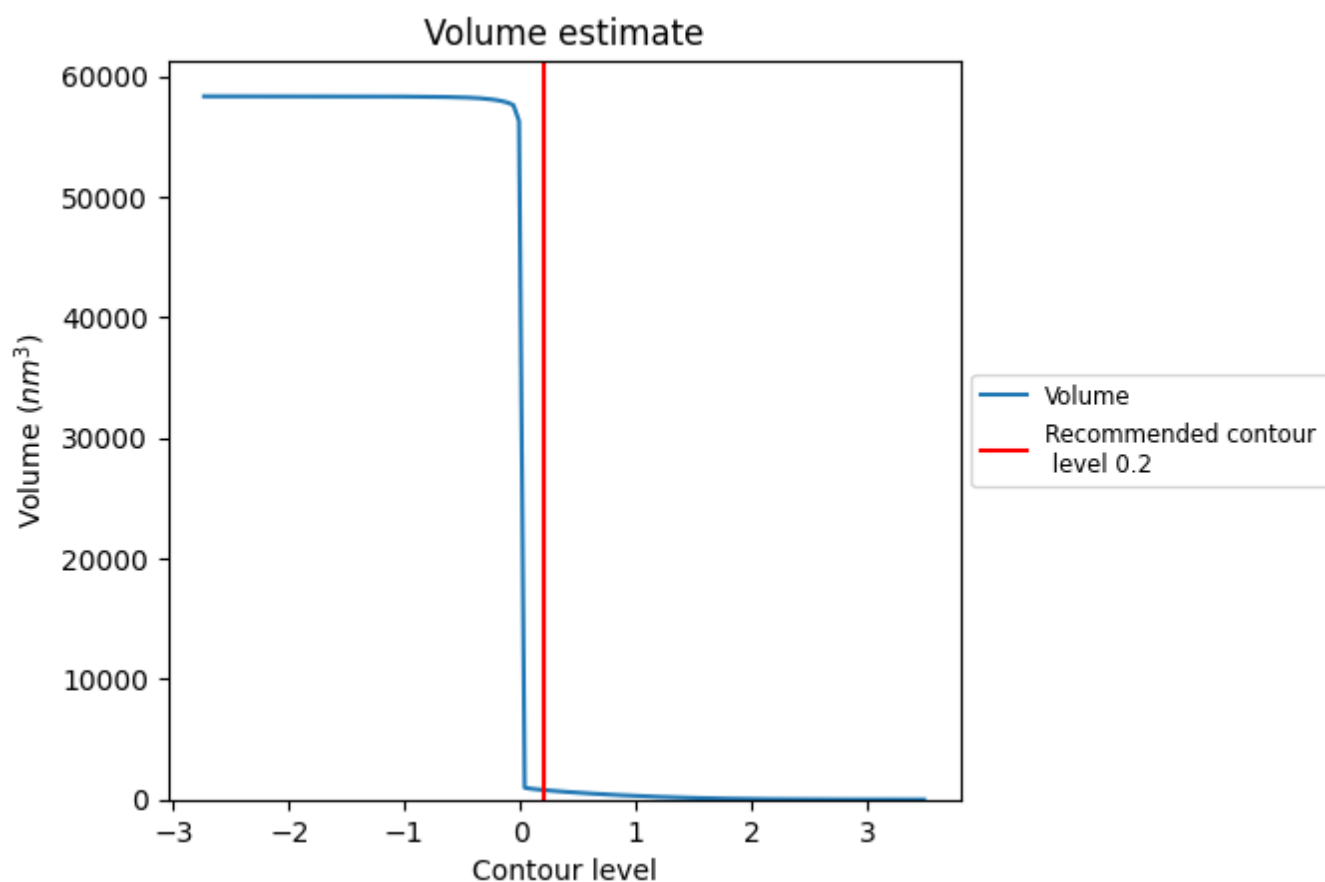
This section contains the results of statistical analysis of the map.

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.

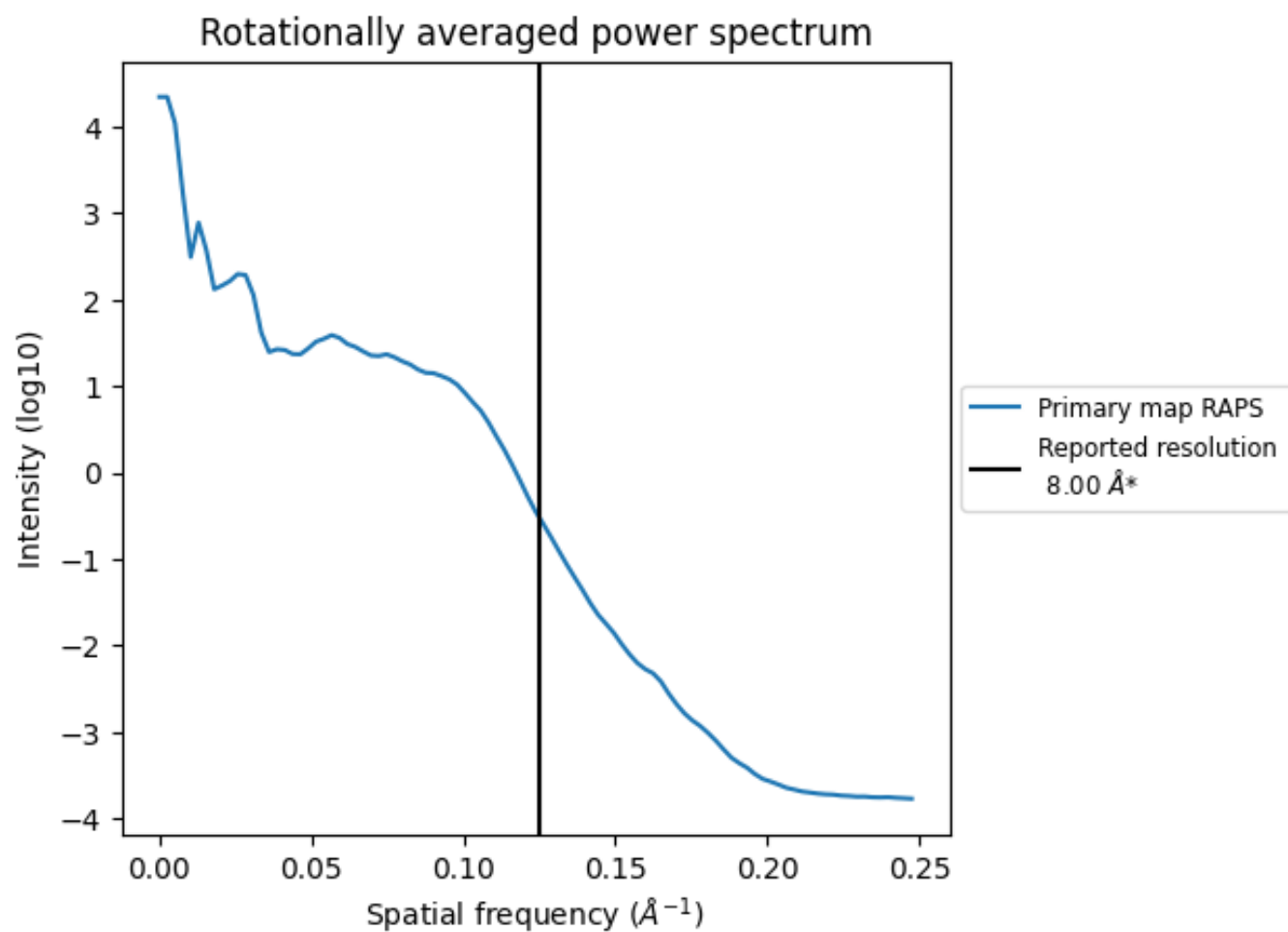
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 791 nm³; this corresponds to an approximate mass of 714 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 0.125 Å⁻¹

8 Fourier-Shell correlation

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

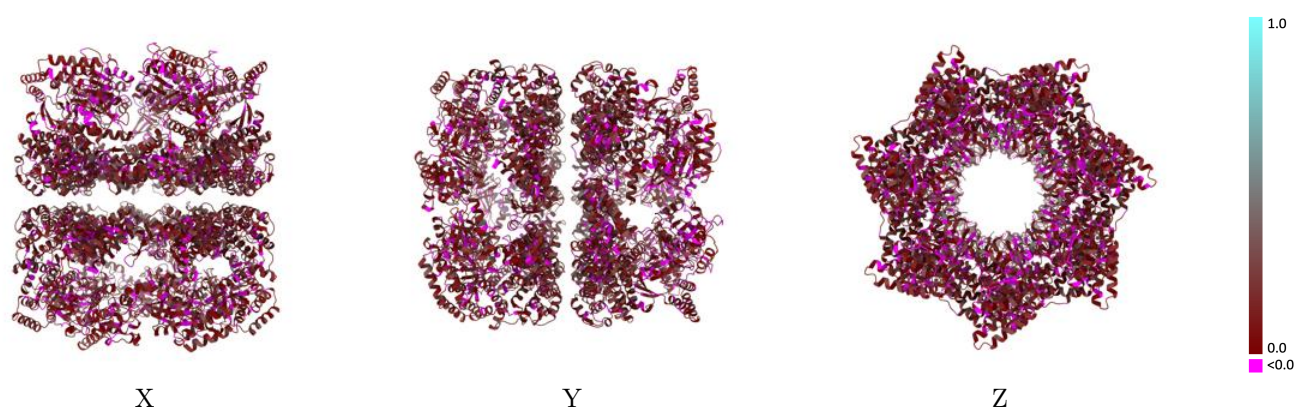
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1998 and PDB model 4AAQ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

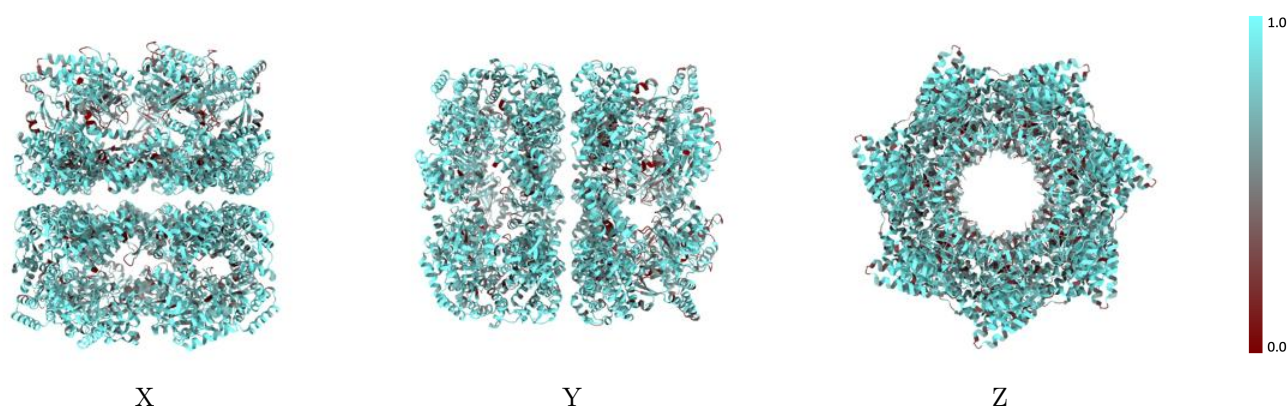
This section was not generated.

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



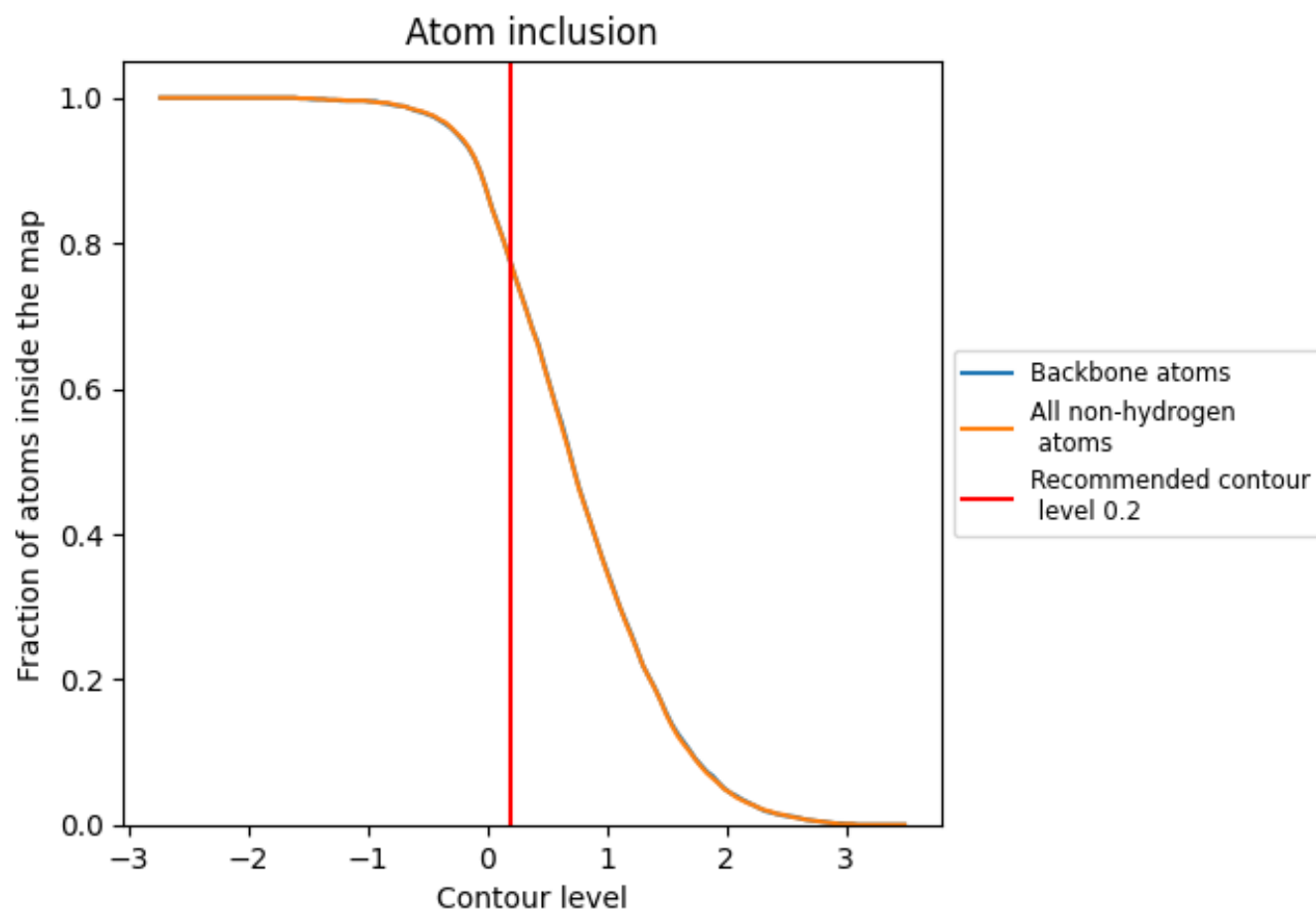
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 77% of all backbone atoms, 77% 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	0.7700	0.1090
A	0.7570	0.1030
B	0.7560	0.1030
C	0.7580	0.1030
D	0.7560	0.1030
E	0.7570	0.1040
F	0.7560	0.1050
G	0.7570	0.1040
H	0.7960	0.1160
I	0.7950	0.1160
J	0.7960	0.1150
K	0.7970	0.1140
L	0.7960	0.1140
M	0.7970	0.1140
N	0.7960	0.1130

