



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:25 PM UTC

PDB ID : 4AAR / pdb_00004aar
EMDB ID : EMD-1999
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

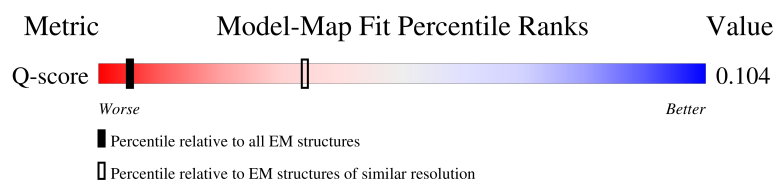
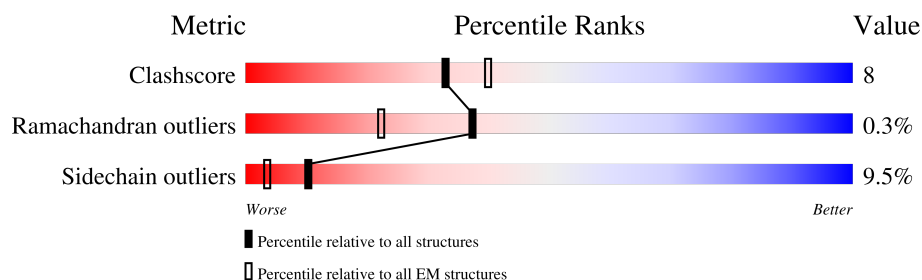
1 Overall quality at a glance

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	13% 54% 30% 10% ..
1	B	548	13% 55% 29% 11% ..
1	C	548	13% 55% 29% 11% ..
1	D	548	12% 55% 30% 10% ..

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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:

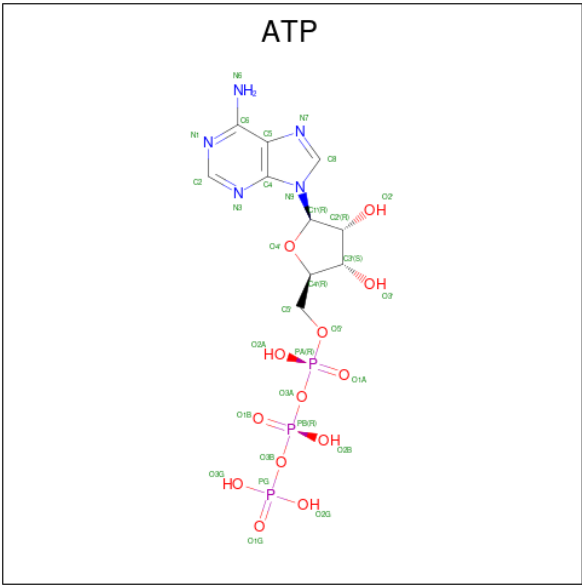
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	engineered mutation	UNP P0A6F5
B	398	ALA	ASP	engineered mutation	UNP P0A6F5

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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).



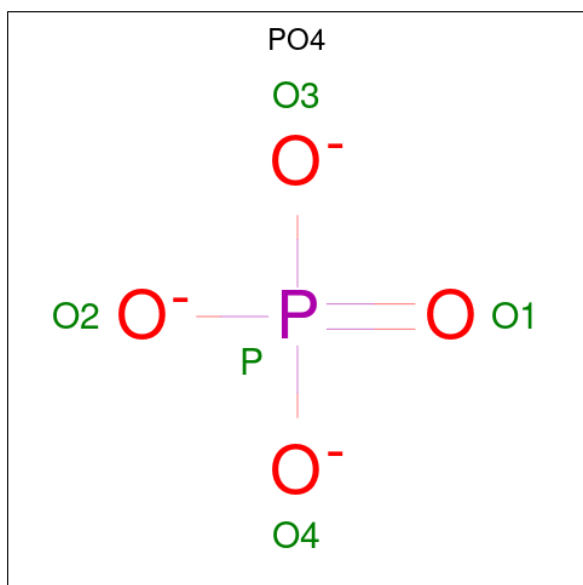
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	E	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

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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	

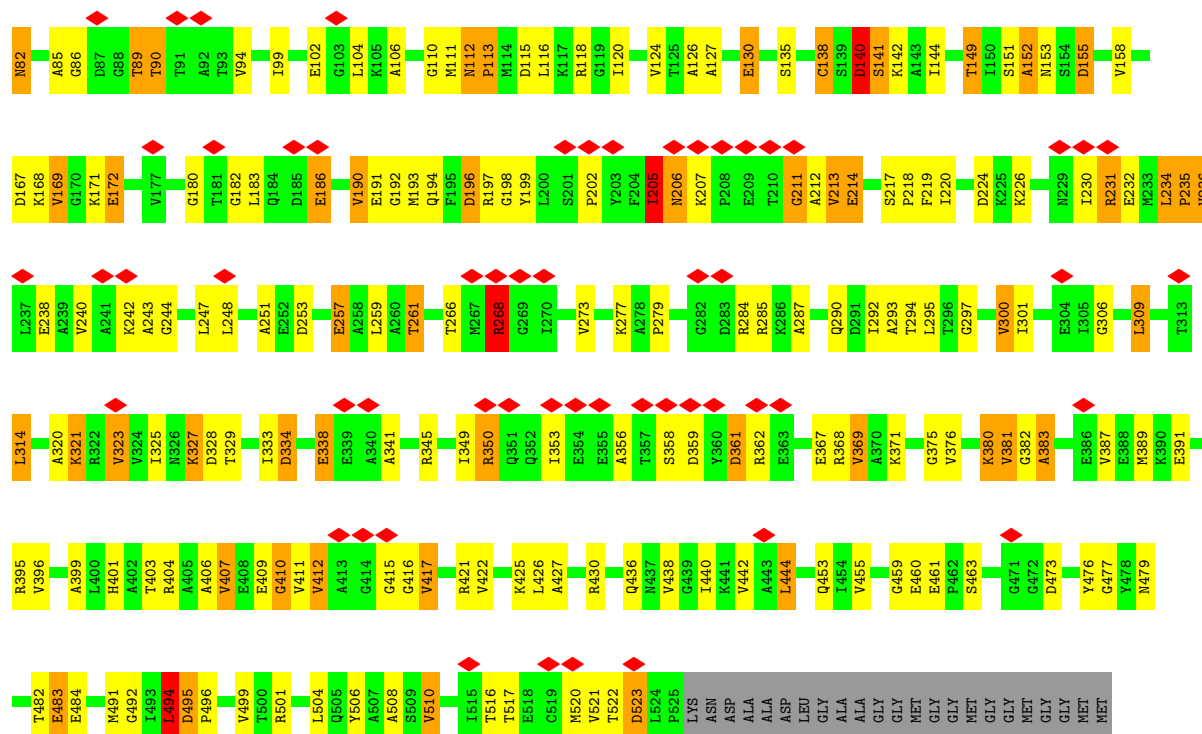
- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



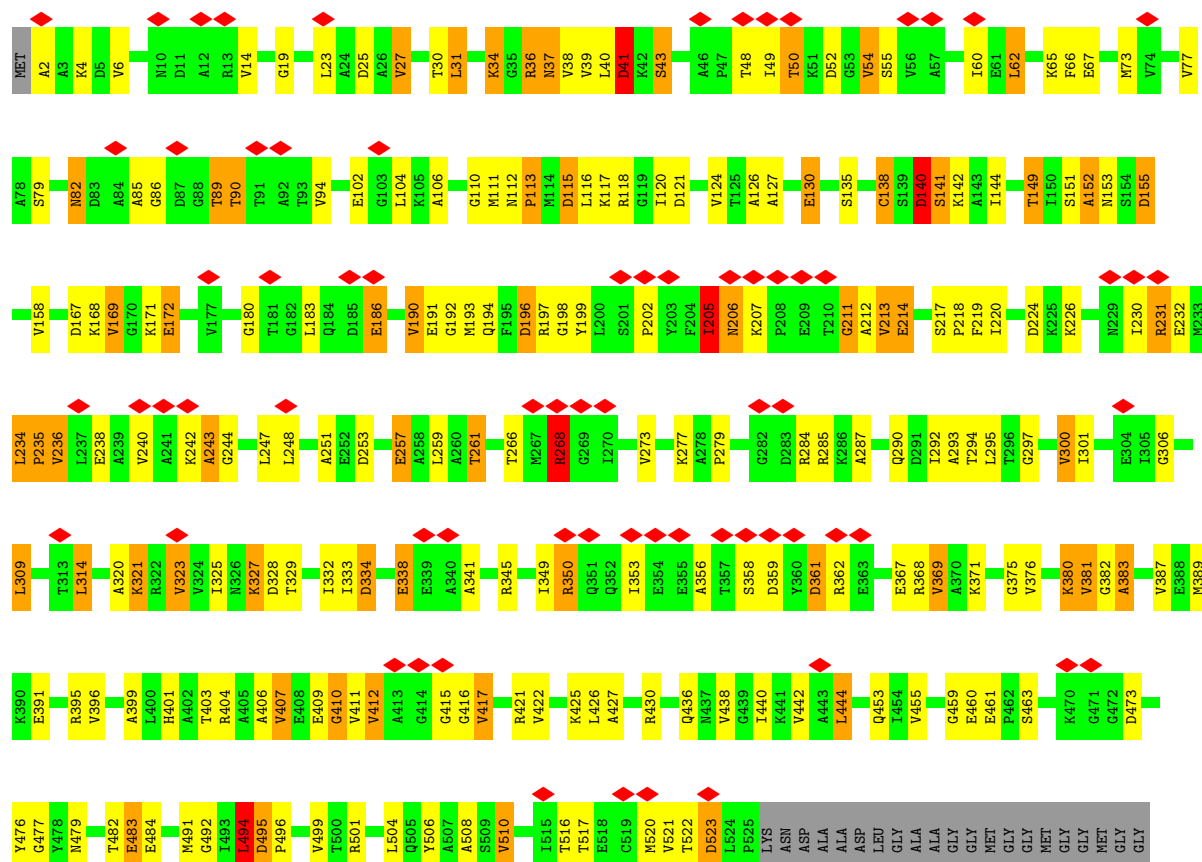
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	P	0
			1	1	
3	B	1	Total	P	0
			1	1	
3	C	1	Total	P	0
			1	1	
3	D	1	Total	P	0
			1	1	
3	E	1	Total	P	0
			1	1	
3	F	1	Total	P	0
			1	1	
3	G	1	Total	P	0
			1	1	

- 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



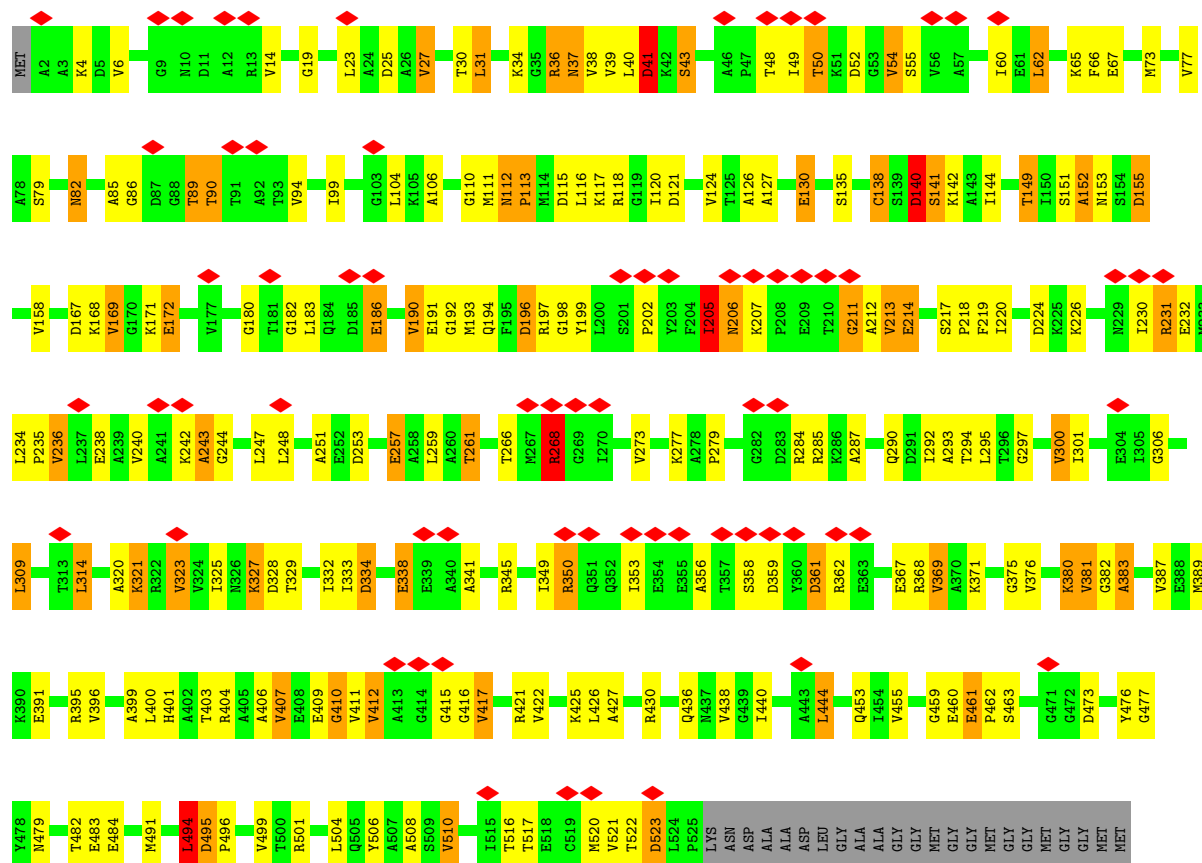
• Molecule 1: 60 KDA CHAPERONIN



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MET

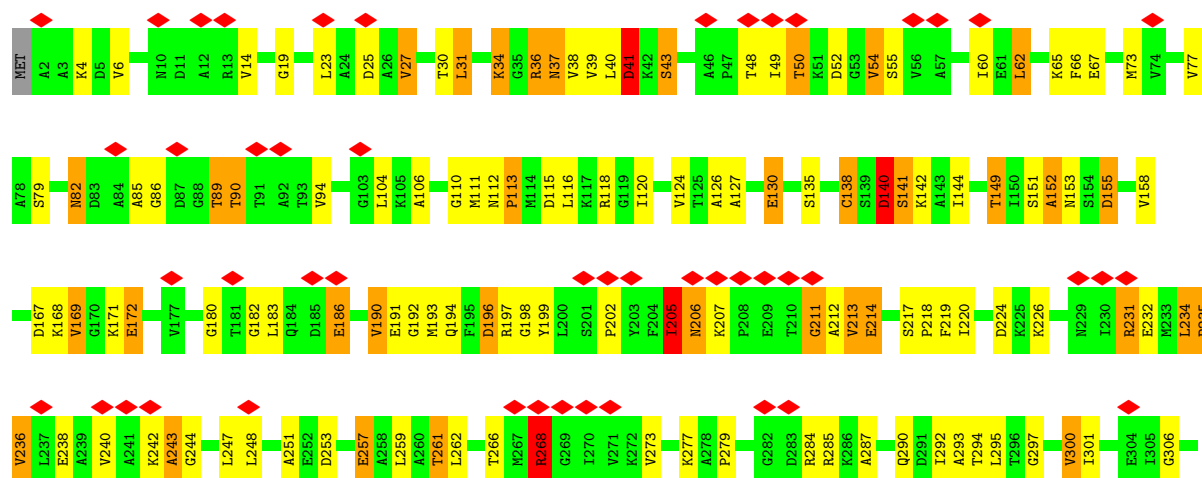
• Molecule 1: 60 KDA CHAPERONIN

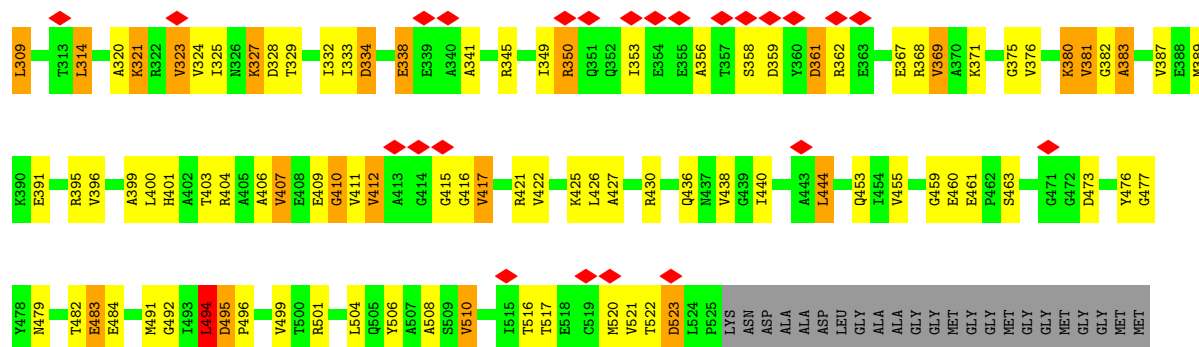
Chain D: 12% 55% 30% 10% . .



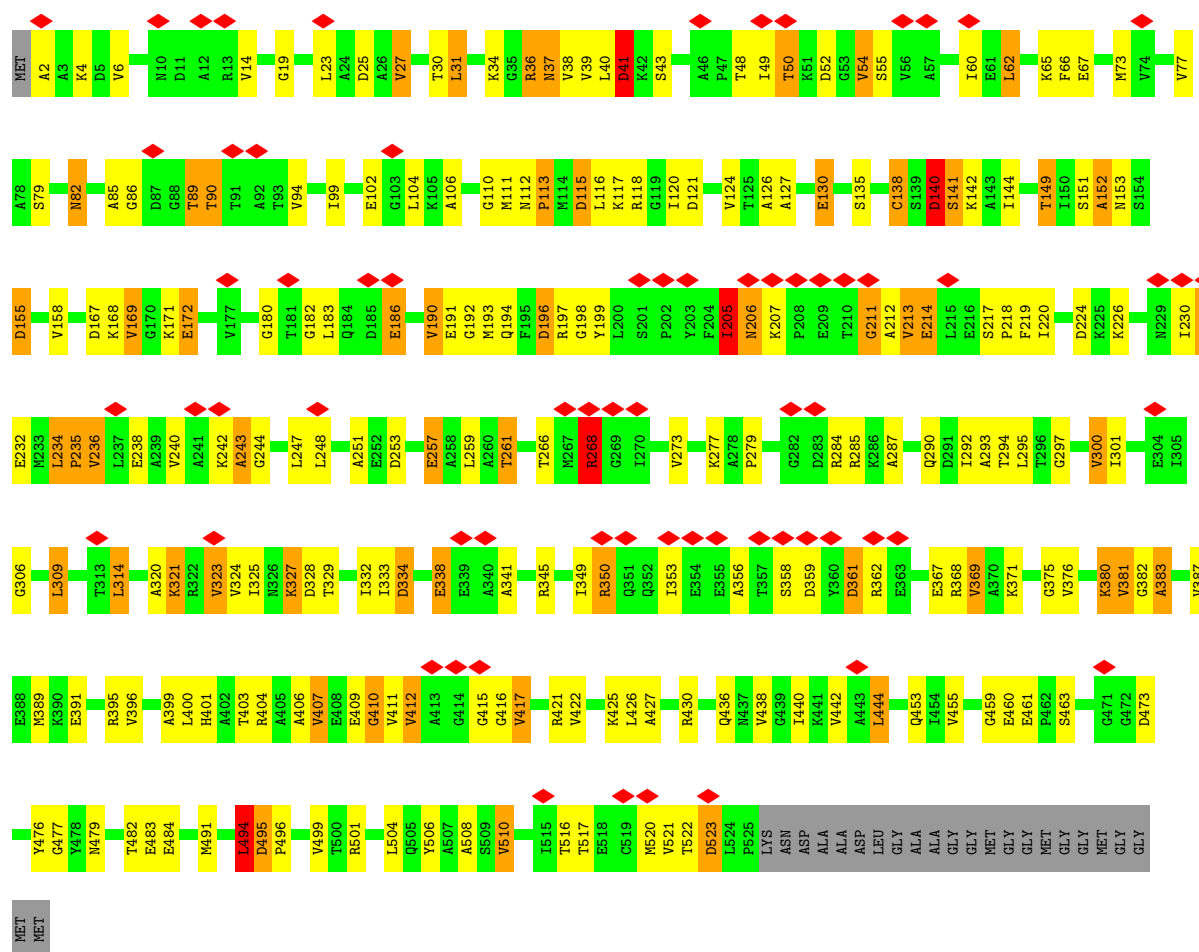
• Molecule 1: 60 KDA CHAPERONIN

Chain E: 13% 55% 29% 11% . .



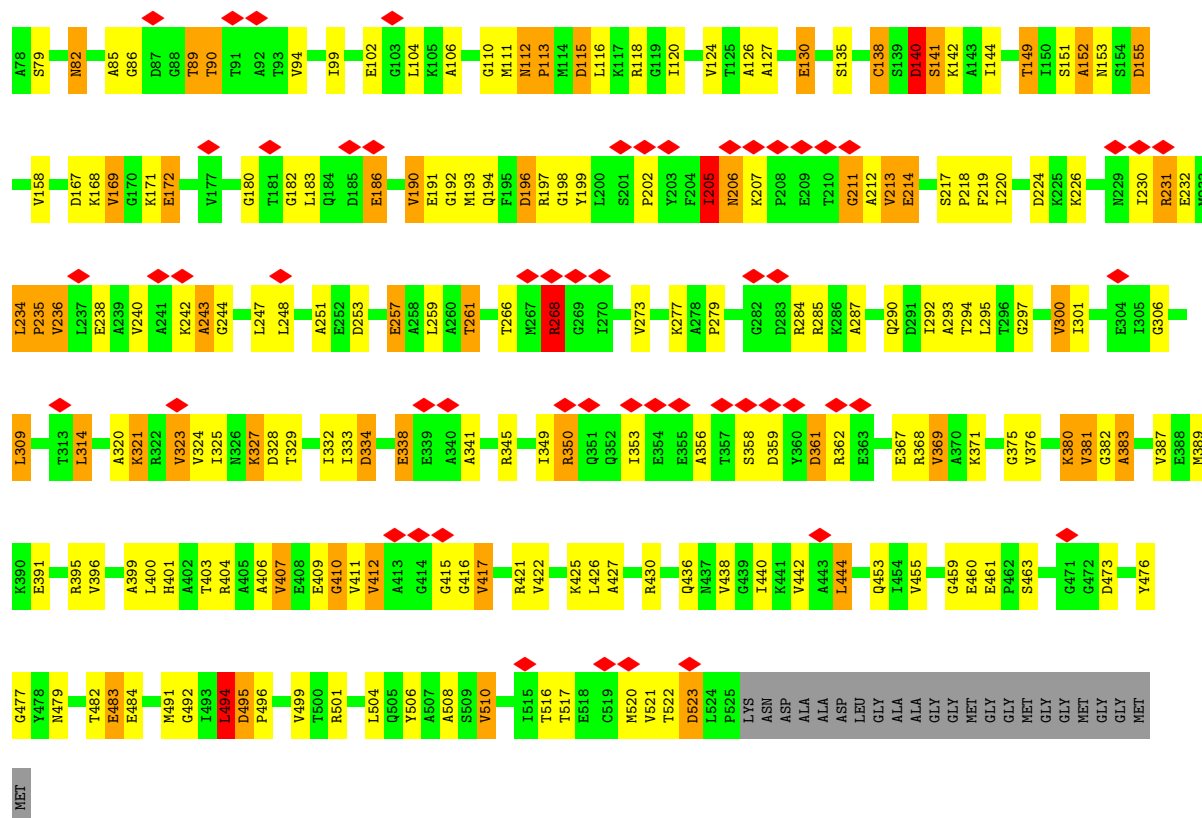


• Molecule 1: 60 KDA CHAPERONIN

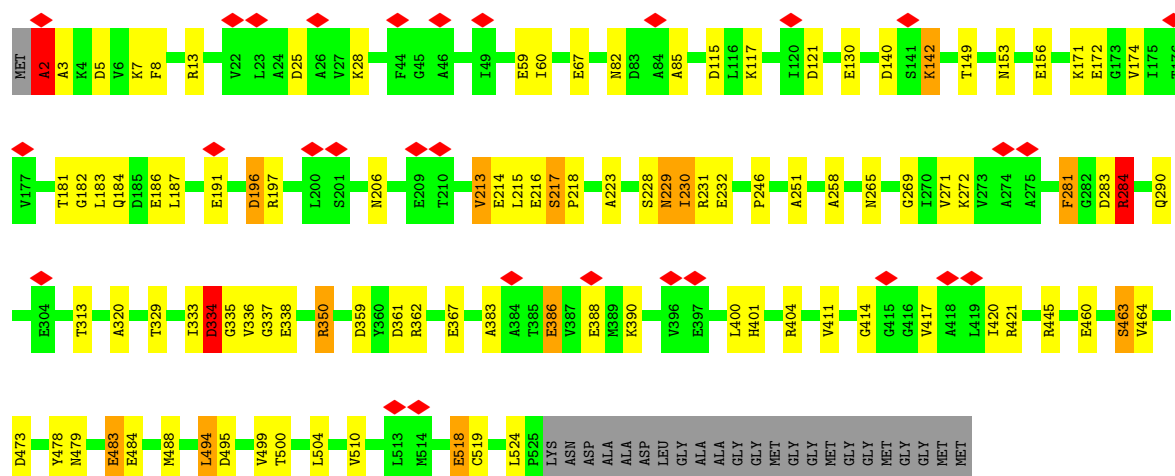


• Molecule 1: 60 KDA CHAPERONIN

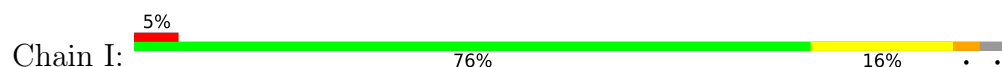


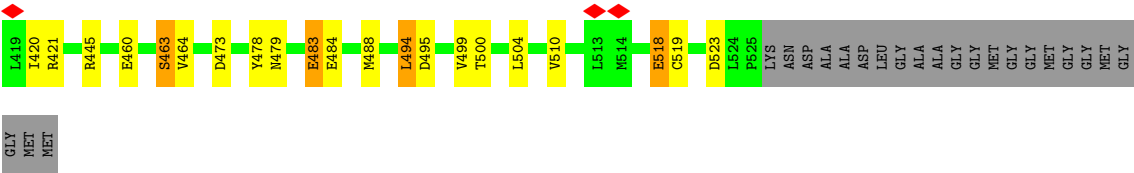


• Molecule 1: 60 KDA CHAPERONIN



• 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	4.100	Depositor
Minimum map value	-2.576	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	387.84, 387.84, 387.84	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.02, 2.02, 2.02	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.53	6/3873 (0.2%)	1.92	122/5229 (2.3%)
1	B	1.52	5/3873 (0.1%)	1.92	121/5229 (2.3%)
1	C	1.52	5/3873 (0.1%)	1.92	121/5229 (2.3%)
1	D	1.52	5/3873 (0.1%)	1.92	122/5229 (2.3%)
1	E	1.53	4/3873 (0.1%)	1.92	121/5229 (2.3%)
1	F	1.53	5/3873 (0.1%)	1.93	123/5229 (2.4%)
1	G	1.53	5/3873 (0.1%)	1.92	122/5229 (2.3%)
1	H	0.90	5/3873 (0.1%)	1.29	24/5229 (0.5%)
1	I	0.97	4/3873 (0.1%)	1.32	29/5229 (0.6%)
1	J	0.83	5/3873 (0.1%)	1.28	24/5229 (0.5%)
1	K	0.98	4/3873 (0.1%)	1.32	35/5229 (0.7%)
1	L	0.82	3/3873 (0.1%)	1.35	30/5229 (0.6%)
1	M	1.01	2/3873 (0.1%)	1.29	26/5229 (0.5%)
1	N	0.98	4/3873 (0.1%)	1.31	31/5229 (0.6%)
All	All	1.26	62/54222 (0.1%)	1.64	1051/73206 (1.4%)

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	1	10
1	B	1	10
1	C	1	10
1	D	1	10
1	E	1	10
1	F	1	10
1	G	1	10
1	H	0	11
1	I	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	9
1	K	0	10
1	L	0	9
1	M	0	10
1	N	0	9
All	All	7	137

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	400	LEU	C-N	35.10	1.81	1.34
1	M	400	LEU	C-N	33.80	1.86	1.33
1	I	400	LEU	C-N	29.53	1.77	1.33
1	N	401	HIS	C-N	26.90	1.70	1.33
1	M	401	HIS	C-N	-21.41	1.02	1.33
1	E	401	HIS	C-N	20.05	1.60	1.33
1	F	401	HIS	C-N	19.67	1.59	1.33
1	D	401	HIS	C-N	18.38	1.58	1.33
1	N	2	ALA	N-CA	18.13	1.80	1.46
1	G	401	HIS	C-N	17.70	1.57	1.33
1	I	2	ALA	N-CA	17.63	1.79	1.46
1	H	401	HIS	C-N	17.48	1.57	1.33
1	C	401	HIS	C-N	15.88	1.54	1.33
1	A	401	HIS	C-N	15.30	1.53	1.33
1	B	401	HIS	C-N	14.57	1.53	1.33
1	H	2	ALA	N-CA	14.35	1.73	1.46
1	N	400	LEU	C-N	13.96	1.52	1.33
1	L	400	LEU	C-N	13.54	1.53	1.33
1	H	400	LEU	C-N	12.93	1.50	1.33
1	H	2	ALA	CA-C	11.85	1.77	1.52
1	K	2	ALA	N-CA	-11.65	1.24	1.46
1	N	2	ALA	CA-C	-10.95	1.29	1.52
1	J	401	HIS	C-N	-10.31	1.20	1.33
1	J	400	LEU	C-N	9.87	1.48	1.33
1	A	2	ALA	N-CA	9.80	1.64	1.46
1	L	401	HIS	C-N	9.77	1.47	1.33
1	I	2	ALA	CA-C	9.51	1.73	1.52
1	A	37	ASN	C-N	9.44	1.45	1.33
1	F	37	ASN	C-N	9.43	1.45	1.33
1	C	37	ASN	C-N	9.41	1.45	1.33
1	D	37	ASN	C-N	9.37	1.45	1.33
1	E	37	ASN	C-N	9.28	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	ASN	C-N	9.28	1.44	1.33
1	G	37	ASN	C-N	9.28	1.44	1.33
1	J	2	ALA	CA-C	-9.24	1.33	1.52
1	G	2	ALA	N-CA	9.01	1.63	1.46
1	J	2	ALA	N-CA	8.91	1.63	1.46
1	B	2	ALA	N-CA	8.55	1.62	1.46
1	F	50	THR	C-N	6.94	1.50	1.34
1	B	50	THR	C-N	6.92	1.50	1.34
1	C	50	THR	C-N	6.90	1.50	1.34
1	A	50	THR	C-N	6.90	1.50	1.34
1	D	50	THR	C-N	6.90	1.50	1.34
1	G	50	THR	C-N	6.87	1.50	1.34
1	E	50	THR	C-N	6.83	1.50	1.34
1	F	2	ALA	N-CA	6.73	1.59	1.46
1	C	2	ALA	N-CA	6.06	1.57	1.46
1	A	400	LEU	C-N	-5.99	1.26	1.33
1	D	400	LEU	C-N	5.39	1.41	1.33
1	D	391	GLU	CA-CB	5.14	1.61	1.53
1	E	391	GLU	CA-CB	5.11	1.61	1.53
1	H	524	LEU	C-N	-5.11	1.26	1.34
1	C	391	GLU	CA-CB	5.11	1.61	1.53
1	A	391	GLU	CA-CB	5.11	1.61	1.53
1	G	391	GLU	CA-CB	5.10	1.61	1.53
1	B	391	GLU	CA-CB	5.09	1.61	1.53
1	L	524	LEU	C-N	-5.09	1.26	1.34
1	F	391	GLU	CA-CB	5.08	1.61	1.53
1	K	401	HIS	C-N	5.07	1.41	1.33
1	I	524	LEU	C-N	-5.05	1.26	1.34
1	K	524	LEU	C-N	-5.05	1.26	1.34
1	J	524	LEU	C-N	-5.01	1.26	1.34

All (1051) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	THR	O-C-N	-15.85	97.73	122.61
1	F	50	THR	O-C-N	-15.82	97.77	122.61
1	D	50	THR	O-C-N	-15.81	97.79	122.61
1	G	50	THR	O-C-N	-15.81	97.79	122.61
1	C	50	THR	O-C-N	-15.79	97.81	122.61
1	B	50	THR	O-C-N	-15.78	97.84	122.61
1	E	50	THR	O-C-N	-15.76	97.87	122.61
1	L	401	HIS	O-C-N	15.30	144.76	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASN	CA-C-N	-13.76	102.41	122.23
1	A	37	ASN	C-N-CA	-13.76	102.41	122.23
1	B	37	ASN	CA-C-N	-13.73	102.46	122.23
1	B	37	ASN	C-N-CA	-13.73	102.46	122.23
1	D	37	ASN	CA-C-N	-13.70	102.50	122.23
1	D	37	ASN	C-N-CA	-13.70	102.50	122.23
1	C	37	ASN	CA-C-N	-13.70	102.51	122.23
1	C	37	ASN	C-N-CA	-13.70	102.51	122.23
1	G	37	ASN	CA-C-N	-13.69	102.52	122.23
1	G	37	ASN	C-N-CA	-13.69	102.52	122.23
1	F	37	ASN	CA-C-N	-13.68	102.53	122.23
1	F	37	ASN	C-N-CA	-13.68	102.53	122.23
1	E	37	ASN	CA-C-N	-13.68	102.54	122.23
1	E	37	ASN	C-N-CA	-13.68	102.54	122.23
1	L	400	LEU	O-C-N	-13.65	106.25	122.22
1	A	391	GLU	CB-CA-C	-13.46	88.45	110.79
1	F	391	GLU	CB-CA-C	-13.45	88.47	110.79
1	C	391	GLU	CB-CA-C	-13.43	88.49	110.79
1	B	391	GLU	CB-CA-C	-13.42	88.52	110.79
1	E	391	GLU	CB-CA-C	-13.41	88.53	110.79
1	D	391	GLU	CB-CA-C	-13.41	88.53	110.79
1	L	401	HIS	CA-C-N	-13.40	101.27	120.29
1	L	401	HIS	C-N-CA	-13.40	101.27	120.29
1	G	391	GLU	CB-CA-C	-13.39	88.55	110.79
1	C	334	ASP	N-CA-CB	-11.89	92.52	110.71
1	E	334	ASP	N-CA-CB	-11.86	92.57	110.71
1	A	334	ASP	N-CA-CB	-11.85	92.58	110.71
1	F	334	ASP	N-CA-CB	-11.85	92.58	110.71
1	B	334	ASP	N-CA-CB	-11.85	92.58	110.71
1	G	334	ASP	N-CA-CB	-11.83	92.60	110.71
1	D	334	ASP	N-CA-CB	-11.81	92.64	110.71
1	I	401	HIS	O-C-N	11.52	137.77	122.33
1	K	401	HIS	O-C-N	-10.92	109.44	122.22
1	E	461	GLU	CB-CA-C	10.92	126.98	109.51
1	F	461	GLU	CB-CA-C	10.90	126.95	109.51
1	D	461	GLU	CB-CA-C	10.90	126.94	109.51
1	B	461	GLU	CB-CA-C	10.89	126.93	109.51
1	G	461	GLU	CB-CA-C	10.89	126.93	109.51
1	C	461	GLU	CB-CA-C	10.88	126.92	109.51
1	A	461	GLU	CB-CA-C	10.88	126.91	109.51
1	G	353	ILE	CB-CA-C	-9.95	99.24	111.97
1	A	353	ILE	CB-CA-C	-9.92	99.27	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	353	ILE	CB-CA-C	-9.92	99.27	111.97
1	E	353	ILE	CB-CA-C	-9.92	99.28	111.97
1	F	353	ILE	CB-CA-C	-9.91	99.28	111.97
1	B	353	ILE	CB-CA-C	-9.89	99.31	111.97
1	D	353	ILE	CB-CA-C	-9.89	99.32	111.97
1	B	50	THR	CA-C-N	9.85	140.16	122.92
1	B	50	THR	C-N-CA	9.85	140.16	122.92
1	A	50	THR	CA-C-N	9.84	140.14	122.92
1	A	50	THR	C-N-CA	9.84	140.14	122.92
1	E	50	THR	CA-C-N	9.83	140.12	122.92
1	E	50	THR	C-N-CA	9.83	140.12	122.92
1	D	50	THR	CA-C-N	9.80	140.08	122.92
1	D	50	THR	C-N-CA	9.80	140.08	122.92
1	C	50	THR	CA-C-N	9.80	140.06	122.92
1	C	50	THR	C-N-CA	9.80	140.06	122.92
1	G	50	THR	CA-C-N	9.79	140.06	122.92
1	G	50	THR	C-N-CA	9.79	140.06	122.92
1	F	50	THR	CA-C-N	9.78	140.03	122.92
1	F	50	THR	C-N-CA	9.78	140.03	122.92
1	D	369	VAL	N-CA-CB	9.75	123.79	110.54
1	E	369	VAL	N-CA-CB	9.73	123.77	110.54
1	A	369	VAL	N-CA-CB	9.70	123.72	110.54
1	F	369	VAL	N-CA-CB	9.68	123.71	110.54
1	B	369	VAL	N-CA-CB	9.68	123.70	110.54
1	C	257	GLU	N-CA-CB	9.66	124.08	110.07
1	C	369	VAL	N-CA-CB	9.65	123.66	110.54
1	D	257	GLU	N-CA-CB	9.64	124.05	110.07
1	A	257	GLU	N-CA-CB	9.63	124.04	110.07
1	E	257	GLU	N-CA-CB	9.63	124.03	110.07
1	G	257	GLU	N-CA-CB	9.62	124.02	110.07
1	G	369	VAL	N-CA-CB	9.62	123.62	110.54
1	B	257	GLU	N-CA-CB	9.60	123.99	110.07
1	D	383	ALA	N-CA-CB	9.60	126.44	111.56
1	F	383	ALA	N-CA-CB	9.59	126.42	111.56
1	B	383	ALA	N-CA-CB	9.58	126.41	111.56
1	A	383	ALA	N-CA-CB	9.56	126.38	111.56
1	G	383	ALA	N-CA-CB	9.56	126.38	111.56
1	E	383	ALA	N-CA-CB	9.54	126.35	111.56
1	C	383	ALA	N-CA-CB	9.52	126.32	111.56
1	F	257	GLU	N-CA-CB	9.51	123.87	110.07
1	F	257	GLU	CB-CA-C	9.50	125.91	110.90
1	B	257	GLU	CB-CA-C	9.39	125.74	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	GLU	CB-CA-C	9.37	125.71	110.90
1	G	257	GLU	CB-CA-C	9.36	125.69	110.90
1	D	257	GLU	CB-CA-C	9.36	125.69	110.90
1	C	257	GLU	CB-CA-C	9.34	125.65	110.90
1	B	510	VAL	CB-CA-C	-9.32	100.03	111.97
1	E	257	GLU	CB-CA-C	9.31	125.61	110.90
1	D	510	VAL	CB-CA-C	-9.28	100.09	111.97
1	C	510	VAL	CB-CA-C	-9.28	100.09	111.97
1	G	510	VAL	CB-CA-C	-9.28	100.10	111.97
1	E	510	VAL	CB-CA-C	-9.27	100.10	111.97
1	A	510	VAL	CB-CA-C	-9.27	100.11	111.97
1	C	115	ASP	CB-CA-C	9.25	126.15	110.79
1	F	510	VAL	CB-CA-C	-9.23	100.16	111.97
1	D	115	ASP	CB-CA-C	9.23	126.11	110.79
1	G	115	ASP	CB-CA-C	9.22	126.09	110.79
1	F	115	ASP	CB-CA-C	9.22	126.09	110.79
1	E	115	ASP	CB-CA-C	9.21	126.08	110.79
1	A	115	ASP	CB-CA-C	9.19	126.04	110.79
1	B	115	ASP	CB-CA-C	9.18	126.02	110.79
1	F	285	ARG	CB-CA-C	-9.04	95.78	110.79
1	G	285	ARG	CB-CA-C	-9.02	95.82	110.79
1	C	285	ARG	CB-CA-C	-9.02	95.83	110.79
1	B	285	ARG	CB-CA-C	-9.01	95.83	110.79
1	A	285	ARG	CB-CA-C	-8.99	95.86	110.79
1	D	285	ARG	CB-CA-C	-8.99	95.86	110.79
1	E	285	ARG	CB-CA-C	-8.99	95.87	110.79
1	F	391	GLU	CA-CB-CG	8.97	132.03	114.10
1	N	267	MET	CG-SD-CE	8.93	120.54	100.90
1	B	391	GLU	CA-CB-CG	8.91	131.93	114.10
1	C	391	GLU	CA-CB-CG	8.91	131.92	114.10
1	K	267	MET	CG-SD-CE	8.91	120.50	100.90
1	A	391	GLU	CA-CB-CG	8.90	131.90	114.10
1	E	391	GLU	CA-CB-CG	8.89	131.88	114.10
1	D	391	GLU	CA-CB-CG	8.89	131.88	114.10
1	G	391	GLU	CA-CB-CG	8.89	131.88	114.10
1	I	401	HIS	CA-C-N	-8.88	105.39	120.58
1	I	401	HIS	C-N-CA	-8.88	105.39	120.58
1	M	359	ASP	CA-CB-CG	-8.86	103.74	112.60
1	L	359	ASP	CA-CB-CG	-8.86	103.74	112.60
1	I	359	ASP	CA-CB-CG	-8.84	103.76	112.60
1	N	359	ASP	CA-CB-CG	-8.81	103.78	112.60
1	K	359	ASP	CA-CB-CG	-8.81	103.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	359	ASP	CA-CB-CG	-8.80	103.80	112.60
1	J	359	ASP	CA-CB-CG	-8.79	103.81	112.60
1	B	153	ASN	CB-CA-C	8.76	125.58	112.09
1	A	153	ASN	CB-CA-C	8.74	125.56	112.09
1	F	153	ASN	CB-CA-C	8.74	125.56	112.09
1	D	153	ASN	CB-CA-C	8.73	125.54	112.09
1	G	153	ASN	CB-CA-C	8.72	125.52	112.09
1	E	153	ASN	CB-CA-C	8.72	125.51	112.09
1	C	153	ASN	CB-CA-C	8.71	125.50	112.09
1	G	494	LEU	CB-CA-C	8.55	126.28	109.35
1	D	494	LEU	CB-CA-C	8.55	126.27	109.35
1	A	494	LEU	CB-CA-C	8.54	126.26	109.35
1	E	494	LEU	CB-CA-C	8.54	126.25	109.35
1	B	494	LEU	CB-CA-C	8.54	126.25	109.35
1	C	494	LEU	CB-CA-C	8.53	126.24	109.35
1	F	494	LEU	CB-CA-C	8.52	126.21	109.35
1	I	2	ALA	N-CA-C	-8.46	87.33	111.00
1	C	41	ASP	N-CA-CB	8.43	123.27	110.45
1	D	41	ASP	N-CA-CB	8.41	123.23	110.45
1	A	41	ASP	N-CA-CB	8.40	123.22	110.45
1	B	41	ASP	N-CA-CB	8.40	123.22	110.45
1	E	409	GLU	N-CA-CB	8.40	122.59	110.16
1	F	41	ASP	N-CA-CB	8.39	123.21	110.45
1	G	409	GLU	N-CA-CB	8.39	122.58	110.16
1	E	41	ASP	N-CA-CB	8.39	123.20	110.45
1	B	409	GLU	N-CA-CB	8.38	122.57	110.16
1	D	409	GLU	N-CA-CB	8.37	122.55	110.16
1	C	409	GLU	N-CA-CB	8.37	122.54	110.16
1	G	41	ASP	N-CA-CB	8.37	123.17	110.45
1	C	367	GLU	CB-CA-C	-8.36	96.92	110.79
1	F	409	GLU	N-CA-CB	8.35	122.52	110.16
1	A	409	GLU	N-CA-CB	8.34	122.51	110.16
1	E	367	GLU	CB-CA-C	-8.33	96.96	110.79
1	G	523	ASP	N-CA-CB	8.33	123.11	110.45
1	A	367	GLU	CB-CA-C	-8.32	96.98	110.79
1	H	2	ALA	N-CA-C	-8.31	87.74	111.00
1	B	367	GLU	CB-CA-C	-8.30	97.01	110.79
1	G	367	GLU	CB-CA-C	-8.30	97.01	110.79
1	D	367	GLU	CB-CA-C	-8.29	97.02	110.79
1	F	367	GLU	CB-CA-C	-8.29	97.03	110.79
1	D	482	THR	N-CA-CB	8.29	122.42	110.16
1	A	482	THR	N-CA-CB	8.28	122.42	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	482	THR	N-CA-CB	8.28	122.42	110.16
1	B	482	THR	N-CA-CB	8.27	122.41	110.16
1	F	482	THR	N-CA-CB	8.27	122.40	110.16
1	F	523	ASP	N-CA-CB	8.27	123.02	110.45
1	E	523	ASP	N-CA-CB	8.27	123.01	110.45
1	G	482	THR	N-CA-CB	8.26	122.38	110.16
1	C	482	THR	N-CA-CB	8.24	122.36	110.16
1	G	369	VAL	CB-CA-C	-8.23	101.03	112.14
1	F	369	VAL	CB-CA-C	-8.23	101.03	112.14
1	A	369	VAL	CB-CA-C	-8.21	101.05	112.14
1	B	369	VAL	CB-CA-C	-8.21	101.06	112.14
1	C	369	VAL	CB-CA-C	-8.20	101.08	112.14
1	D	369	VAL	CB-CA-C	-8.18	101.09	112.14
1	E	369	VAL	CB-CA-C	-8.18	101.10	112.14
1	H	2	ALA	CA-C-O	-8.09	107.05	120.80
1	G	412	VAL	CB-CA-C	-8.08	100.12	111.19
1	B	483	GLU	CB-CG-CD	8.05	126.29	112.60
1	D	483	GLU	CB-CG-CD	8.03	126.25	112.60
1	G	483	GLU	CB-CG-CD	8.03	126.24	112.60
1	E	483	GLU	CB-CG-CD	8.02	126.24	112.60
1	C	483	GLU	CB-CG-CD	8.01	126.22	112.60
1	F	483	GLU	CB-CG-CD	8.00	126.20	112.60
1	A	483	GLU	CB-CG-CD	8.00	126.19	112.60
1	D	510	VAL	N-CA-CB	7.93	119.82	110.55
1	F	510	VAL	N-CA-CB	7.92	119.81	110.55
1	G	510	VAL	N-CA-CB	7.92	119.81	110.55
1	A	510	VAL	N-CA-CB	7.89	119.78	110.55
1	G	115	ASP	CA-CB-CG	-7.89	104.71	112.60
1	F	400	LEU	O-C-N	-7.88	113.96	122.07
1	D	115	ASP	CA-CB-CG	-7.87	104.73	112.60
1	B	510	VAL	N-CA-CB	7.87	119.76	110.55
1	A	115	ASP	CA-CB-CG	-7.87	104.73	112.60
1	E	510	VAL	N-CA-CB	7.86	119.75	110.55
1	E	115	ASP	CA-CB-CG	-7.86	104.74	112.60
1	B	115	ASP	CA-CB-CG	-7.86	104.75	112.60
1	C	115	ASP	CA-CB-CG	-7.86	104.74	112.60
1	C	510	VAL	N-CA-CB	7.85	119.74	110.55
1	F	391	GLU	N-CA-CB	7.84	121.65	110.12
1	A	391	GLU	N-CA-CB	7.84	121.64	110.12
1	B	391	GLU	N-CA-CB	7.84	121.64	110.12
1	F	115	ASP	CA-CB-CG	-7.84	104.76	112.60
1	G	89	THR	CB-CA-C	-7.83	98.58	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	461	GLU	CB-CG-CD	7.83	125.90	112.60
1	F	235	PRO	CB-CA-C	7.82	122.96	111.85
1	G	235	PRO	CB-CA-C	7.82	122.96	111.85
1	B	89	THR	CB-CA-C	-7.82	98.61	110.88
1	C	391	GLU	N-CA-CB	7.82	121.61	110.12
1	E	235	PRO	CB-CA-C	7.81	122.94	111.85
1	E	391	GLU	N-CA-CB	7.81	121.60	110.12
1	E	461	GLU	CB-CG-CD	7.81	125.87	112.60
1	D	391	GLU	N-CA-CB	7.81	121.59	110.12
1	F	461	GLU	CB-CG-CD	7.81	125.87	112.60
1	C	89	THR	CB-CA-C	-7.80	98.63	110.88
1	D	461	GLU	CB-CG-CD	7.79	125.85	112.60
1	G	391	GLU	N-CA-CB	7.79	121.58	110.12
1	B	235	PRO	CB-CA-C	7.79	122.92	111.85
1	B	461	GLU	CB-CG-CD	7.79	125.84	112.60
1	A	235	PRO	CB-CA-C	7.79	122.91	111.85
1	C	235	PRO	CB-CA-C	7.79	122.91	111.85
1	G	461	GLU	CB-CG-CD	7.79	125.84	112.60
1	D	235	PRO	CB-CA-C	7.79	122.91	111.85
1	A	89	THR	CB-CA-C	-7.78	98.66	110.88
1	E	89	THR	CB-CA-C	-7.78	98.66	110.88
1	F	89	THR	CB-CA-C	-7.78	98.66	110.88
1	D	89	THR	CB-CA-C	-7.77	98.68	110.88
1	K	400	LEU	O-C-N	7.76	130.06	122.07
1	A	461	GLU	CB-CG-CD	7.76	125.78	112.60
1	A	86	GLY	N-CA-C	-7.73	105.88	115.08
1	E	149	THR	N-CA-CB	7.73	121.48	110.12
1	F	149	THR	N-CA-CB	7.72	121.47	110.12
1	A	149	THR	N-CA-CB	7.70	121.44	110.12
1	C	149	THR	N-CA-CB	7.70	121.44	110.12
1	D	149	THR	N-CA-CB	7.70	121.44	110.12
1	G	86	GLY	N-CA-C	-7.70	105.92	115.08
1	G	149	THR	N-CA-CB	7.70	121.44	110.12
1	J	367	GLU	CB-CA-C	-7.69	95.90	110.67
1	B	149	THR	N-CA-CB	7.69	121.42	110.12
1	E	86	GLY	N-CA-C	-7.69	105.93	115.08
1	F	86	GLY	N-CA-C	-7.69	105.93	115.08
1	M	367	GLU	CB-CA-C	-7.69	95.91	110.67
1	C	86	GLY	N-CA-C	-7.68	105.94	115.08
1	H	367	GLU	CB-CA-C	-7.68	95.93	110.67
1	L	367	GLU	CB-CA-C	-7.68	95.93	110.67
1	D	86	GLY	N-CA-C	-7.67	105.95	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	367	GLU	CB-CA-C	-7.66	95.96	110.67
1	K	367	GLU	CB-CA-C	-7.66	95.97	110.67
1	I	367	GLU	CB-CA-C	-7.65	95.97	110.67
1	B	86	GLY	N-CA-C	-7.65	105.97	115.08
1	D	138	CYS	N-CA-CB	7.54	121.03	110.17
1	G	138	CYS	N-CA-CB	7.53	121.02	110.17
1	E	138	CYS	N-CA-CB	7.51	120.98	110.17
1	B	138	CYS	N-CA-CB	7.50	120.97	110.17
1	F	138	CYS	N-CA-CB	7.50	120.97	110.17
1	K	401	HIS	CA-C-N	7.50	133.41	120.58
1	K	401	HIS	C-N-CA	7.50	133.41	120.58
1	A	138	CYS	N-CA-CB	7.49	120.96	110.17
1	I	196	ASP	N-CA-CB	-7.48	99.81	110.58
1	G	499	VAL	N-CA-CB	7.48	119.30	110.55
1	L	196	ASP	N-CA-CB	-7.47	99.83	110.58
1	M	196	ASP	N-CA-CB	-7.47	99.83	110.58
1	K	196	ASP	N-CA-CB	-7.46	99.84	110.58
1	J	196	ASP	N-CA-CB	-7.46	99.84	110.58
1	C	499	VAL	N-CA-CB	7.45	119.27	110.55
1	C	138	CYS	N-CA-CB	7.45	120.90	110.17
1	H	196	ASP	N-CA-CB	-7.45	99.85	110.58
1	F	499	VAL	N-CA-CB	7.45	119.26	110.55
1	B	412	VAL	CB-CA-C	-7.45	100.18	110.90
1	D	412	VAL	CB-CA-C	-7.45	100.18	110.90
1	N	196	ASP	N-CA-CB	-7.44	99.87	110.58
1	E	412	VAL	CB-CA-C	-7.44	100.19	110.90
1	F	412	VAL	CB-CA-C	-7.43	100.19	110.90
1	D	499	VAL	N-CA-CB	7.42	119.23	110.55
1	A	412	VAL	CB-CA-C	-7.42	100.22	110.90
1	C	412	VAL	CB-CA-C	-7.40	100.25	110.90
1	K	333	ILE	N-CA-C	7.38	118.18	110.72
1	C	36	ARG	N-CA-CB	-7.38	99.23	110.45
1	N	333	ILE	N-CA-C	7.35	118.14	110.72
1	I	333	ILE	N-CA-C	7.35	118.14	110.72
1	B	36	ARG	N-CA-CB	-7.35	99.28	110.45
1	G	36	ARG	N-CA-CB	-7.33	99.31	110.45
1	D	36	ARG	N-CA-CB	-7.33	99.31	110.45
1	F	36	ARG	N-CA-CB	-7.32	99.32	110.45
1	L	333	ILE	N-CA-C	7.32	118.11	110.72
1	A	36	ARG	N-CA-CB	-7.32	99.33	110.45
1	E	36	ARG	N-CA-CB	-7.29	99.36	110.45
1	M	333	ILE	N-CA-C	7.29	118.08	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	333	ILE	N-CA-C	7.27	118.06	110.72
1	N	400	LEU	O-C-N	-7.25	114.49	122.03
1	H	333	ILE	N-CA-C	7.22	118.01	110.72
1	C	168	LYS	N-CA-CB	-7.21	99.56	110.01
1	G	334	ASP	CA-CB-CG	7.19	119.79	112.60
1	B	334	ASP	CA-CB-CG	7.19	119.79	112.60
1	D	334	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	523	ASP	N-CA-CB	7.18	121.36	110.45
1	C	334	ASP	CA-CB-CG	7.16	119.76	112.60
1	A	334	ASP	CA-CB-CG	7.16	119.76	112.60
1	F	168	LYS	N-CA-CB	-7.16	99.63	110.01
1	B	168	LYS	N-CA-CB	-7.14	99.65	110.01
1	E	334	ASP	CA-CB-CG	7.14	119.74	112.60
1	E	168	LYS	N-CA-CB	-7.14	99.66	110.01
1	F	334	ASP	CA-CB-CG	7.14	119.74	112.60
1	D	523	ASP	N-CA-CB	7.13	121.29	110.45
1	A	168	LYS	N-CA-CB	-7.12	99.69	110.01
1	G	168	LYS	N-CA-CB	-7.12	99.69	110.01
1	B	523	ASP	N-CA-CB	7.11	121.26	110.45
1	D	168	LYS	N-CA-CB	-7.11	99.70	110.01
1	C	523	ASP	N-CA-CB	7.10	121.25	110.45
1	D	190	VAL	CB-CA-C	7.06	121.54	110.81
1	G	190	VAL	CB-CA-C	7.04	121.52	110.81
1	F	190	VAL	CB-CA-C	7.02	121.49	110.81
1	B	112	ASN	CA-CB-CG	-7.02	105.58	112.60
1	C	321	LYS	CB-CA-C	7.01	121.89	110.88
1	B	190	VAL	CB-CA-C	7.01	121.46	110.81
1	E	321	LYS	CB-CA-C	7.01	121.88	110.88
1	G	112	ASN	CA-CB-CG	-7.01	105.59	112.60
1	A	113	PRO	CA-N-CD	-7.00	102.19	112.00
1	G	321	LYS	CB-CA-C	7.00	121.88	110.88
1	C	190	VAL	CB-CA-C	7.00	121.45	110.81
1	D	321	LYS	CB-CA-C	7.00	121.87	110.88
1	F	112	ASN	CA-CB-CG	-7.00	105.60	112.60
1	H	5	ASP	N-CA-CB	7.00	121.57	110.65
1	C	112	ASN	CA-CB-CG	-7.00	105.60	112.60
1	E	113	PRO	CA-N-CD	-7.00	102.20	112.00
1	B	113	PRO	CA-N-CD	-6.99	102.21	112.00
1	A	321	LYS	CB-CA-C	6.99	121.85	110.88
1	F	113	PRO	CA-N-CD	-6.99	102.22	112.00
1	B	321	LYS	CB-CA-C	6.99	121.85	110.88
1	A	190	VAL	CB-CA-C	6.98	121.42	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ASN	CA-CB-CG	-6.98	105.62	112.60
1	G	113	PRO	CA-N-CD	-6.98	102.23	112.00
1	F	321	LYS	CB-CA-C	6.98	121.84	110.88
1	N	267	MET	N-CA-CB	-6.97	100.08	110.60
1	D	112	ASN	CA-CB-CG	-6.97	105.63	112.60
1	L	5	ASP	N-CA-CB	6.97	121.52	110.65
1	M	5	ASP	N-CA-CB	6.96	121.51	110.65
1	K	5	ASP	N-CA-CB	6.96	121.51	110.65
1	D	113	PRO	CA-N-CD	-6.96	102.25	112.00
1	E	190	VAL	CB-CA-C	6.96	121.39	110.81
1	N	5	ASP	N-CA-CB	6.96	121.51	110.65
1	E	112	ASN	CA-CB-CG	-6.96	105.64	112.60
1	A	371	LYS	CB-CA-C	6.95	121.80	110.88
1	C	113	PRO	CA-N-CD	-6.95	102.27	112.00
1	J	5	ASP	N-CA-CB	6.94	121.48	110.65
1	K	267	MET	N-CA-CB	-6.94	100.12	110.60
1	F	371	LYS	CB-CA-C	6.93	121.75	110.88
1	B	371	LYS	CB-CA-C	6.92	121.75	110.88
1	B	73	MET	CB-CA-C	-6.92	99.30	110.79
1	D	73	MET	CB-CA-C	-6.92	99.31	110.79
1	I	5	ASP	N-CA-CB	6.92	121.44	110.65
1	E	371	LYS	CB-CA-C	6.91	121.72	110.88
1	G	73	MET	CB-CA-C	-6.90	99.33	110.79
1	E	73	MET	CB-CA-C	-6.90	99.34	110.79
1	D	371	LYS	CB-CA-C	6.89	121.71	110.88
1	C	73	MET	CB-CA-C	-6.89	99.36	110.79
1	A	73	MET	CB-CA-C	-6.89	99.36	110.79
1	G	371	LYS	CB-CA-C	6.89	121.69	110.88
1	F	73	MET	CB-CA-C	-6.88	99.37	110.79
1	C	371	LYS	CB-CA-C	6.88	121.67	110.88
1	F	206	ASN	N-CA-CB	6.86	119.84	110.38
1	G	206	ASN	N-CA-CB	6.84	119.81	110.38
1	C	206	ASN	N-CA-CB	6.83	119.81	110.38
1	G	400	LEU	O-C-N	-6.83	115.03	122.07
1	E	206	ASN	N-CA-CB	6.83	119.81	110.38
1	A	206	ASN	N-CA-CB	6.82	119.80	110.38
1	B	206	ASN	N-CA-CB	6.80	119.77	110.38
1	D	206	ASN	N-CA-CB	6.77	119.72	110.38
1	G	381	VAL	N-CA-CB	-6.74	102.96	111.46
1	B	381	VAL	N-CA-CB	-6.72	102.99	111.46
1	F	381	VAL	N-CA-CB	-6.72	102.99	111.46
1	E	381	VAL	N-CA-CB	-6.70	103.01	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	VAL	N-CA-CB	-6.70	103.02	111.46
1	D	381	VAL	N-CA-CB	-6.69	103.03	111.46
1	C	381	VAL	N-CA-CB	-6.67	103.05	111.46
1	A	236	VAL	CB-CA-C	-6.65	103.16	112.14
1	N	2	ALA	CA-C-O	6.64	132.08	120.80
1	D	236	VAL	CB-CA-C	-6.63	103.19	112.14
1	G	236	VAL	CB-CA-C	-6.59	103.12	112.22
1	F	236	VAL	CB-CA-C	-6.57	103.15	112.22
1	E	236	VAL	CB-CA-C	-6.56	103.16	112.22
1	B	236	VAL	CB-CA-C	-6.55	103.19	112.22
1	B	41	ASP	CB-CA-C	6.54	122.78	109.76
1	E	41	ASP	CB-CA-C	6.54	122.78	109.76
1	F	41	ASP	CB-CA-C	6.54	122.78	109.76
1	G	297	GLY	N-CA-C	-6.53	106.43	114.92
1	G	41	ASP	CB-CA-C	6.53	122.75	109.76
1	C	236	VAL	CB-CA-C	-6.53	103.21	112.22
1	M	401	HIS	CA-C-N	-6.53	107.74	121.64
1	M	401	HIS	C-N-CA	-6.53	107.74	121.64
1	C	41	ASP	CB-CA-C	6.52	122.74	109.76
1	E	297	GLY	N-CA-C	-6.52	106.44	114.92
1	D	41	ASP	CB-CA-C	6.52	122.73	109.76
1	A	41	ASP	CB-CA-C	6.50	122.70	109.76
1	A	297	GLY	N-CA-C	-6.50	106.47	114.92
1	F	297	GLY	N-CA-C	-6.49	106.48	114.92
1	D	297	GLY	N-CA-C	-6.49	106.49	114.92
1	C	297	GLY	N-CA-C	-6.47	106.50	114.92
1	E	90	THR	N-CA-CB	6.47	119.63	110.12
1	D	284	ARG	CB-CA-C	-6.46	100.07	110.79
1	A	284	ARG	CB-CA-C	-6.46	100.07	110.79
1	F	284	ARG	CB-CA-C	-6.45	100.08	110.79
1	G	284	ARG	CB-CA-C	-6.45	100.08	110.79
1	D	90	THR	N-CA-CB	6.45	119.59	110.12
1	B	284	ARG	CB-CA-C	-6.44	100.09	110.79
1	A	141	SER	N-CA-CB	6.44	119.59	110.12
1	D	141	SER	N-CA-CB	6.44	119.58	110.12
1	C	284	ARG	CB-CA-C	-6.43	100.11	110.79
1	A	90	THR	N-CA-CB	6.43	119.57	110.12
1	E	400	LEU	O-C-N	-6.42	115.45	122.07
1	F	141	SER	N-CA-CB	6.42	119.56	110.12
1	B	297	GLY	N-CA-C	-6.42	106.57	114.92
1	B	141	SER	N-CA-CB	6.42	119.56	110.12
1	C	90	THR	N-CA-CB	6.41	119.54	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	141	SER	N-CA-CB	6.41	119.54	110.12
1	E	284	ARG	CB-CA-C	-6.41	100.16	110.79
1	B	90	THR	N-CA-CB	6.40	119.52	110.12
1	E	141	SER	N-CA-CB	6.40	119.53	110.12
1	D	67	GLU	CB-CG-CD	6.39	123.46	112.60
1	F	90	THR	N-CA-CB	6.39	119.51	110.12
1	E	67	GLU	CB-CG-CD	6.39	123.46	112.60
1	G	90	THR	N-CA-CB	6.39	119.51	110.12
1	C	67	GLU	CB-CG-CD	6.39	123.46	112.60
1	C	141	SER	N-CA-CB	6.38	119.50	110.12
1	B	499	VAL	N-CA-CB	6.38	119.22	110.54
1	A	499	VAL	N-CA-CB	6.38	119.21	110.54
1	E	499	VAL	N-CA-CB	6.37	119.20	110.54
1	A	67	GLU	CB-CG-CD	6.36	123.42	112.60
1	G	67	GLU	CB-CG-CD	6.36	123.41	112.60
1	B	67	GLU	CB-CG-CD	6.35	123.40	112.60
1	C	259	LEU	N-CA-CB	6.34	119.27	110.07
1	F	67	GLU	CB-CG-CD	6.34	123.38	112.60
1	D	196	ASP	N-CA-CB	-6.34	101.05	110.24
1	G	259	LEU	N-CA-CB	6.33	119.25	110.07
1	F	14	VAL	N-CA-CB	6.33	119.14	110.54
1	C	14	VAL	N-CA-CB	6.32	119.14	110.54
1	G	196	ASP	N-CA-CB	-6.32	101.08	110.24
1	B	259	LEU	N-CA-CB	6.32	119.23	110.07
1	A	196	ASP	N-CA-CB	-6.31	101.09	110.24
1	E	196	ASP	N-CA-CB	-6.31	101.10	110.24
1	K	217	SER	CB-CA-C	-6.31	104.78	110.71
1	F	196	ASP	N-CA-CB	-6.30	101.10	110.24
1	C	196	ASP	N-CA-CB	-6.30	101.10	110.24
1	B	196	ASP	N-CA-CB	-6.30	101.11	110.24
1	E	259	LEU	N-CA-CB	6.30	119.20	110.07
1	D	14	VAL	N-CA-CB	6.29	119.09	110.54
1	H	67	GLU	CB-CG-CD	6.29	123.29	112.60
1	A	259	LEU	N-CA-CB	6.28	119.18	110.07
1	M	217	SER	CB-CA-C	-6.28	104.81	110.71
1	N	217	SER	CB-CA-C	-6.28	104.81	110.71
1	J	59	GLU	CB-CA-C	6.27	121.76	109.72
1	L	67	GLU	CB-CG-CD	6.27	123.26	112.60
1	C	205	ILE	CB-CA-C	6.27	121.57	111.29
1	I	217	SER	CB-CA-C	-6.27	104.82	110.71
1	G	14	VAL	N-CA-CB	6.26	119.06	110.54
1	J	67	GLU	CB-CG-CD	6.26	123.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	14	VAL	N-CA-CB	6.26	119.06	110.54
1	L	217	SER	CB-CA-C	-6.26	104.82	110.71
1	A	14	VAL	N-CA-CB	6.26	119.05	110.54
1	G	155	ASP	CB-CA-C	6.26	121.82	111.31
1	L	59	GLU	CB-CA-C	6.25	121.73	109.72
1	M	67	GLU	CB-CG-CD	6.25	123.23	112.60
1	D	205	ILE	CB-CA-C	6.25	121.54	111.29
1	M	59	GLU	CB-CA-C	6.25	121.71	109.72
1	J	361	ASP	CA-CB-CG	-6.25	106.36	112.60
1	N	67	GLU	CB-CG-CD	6.25	123.22	112.60
1	B	14	VAL	N-CA-CB	6.24	119.03	110.54
1	G	205	ILE	CB-CA-C	6.24	121.53	111.29
1	H	59	GLU	CB-CA-C	6.24	121.71	109.72
1	H	217	SER	CB-CA-C	-6.24	104.84	110.71
1	J	217	SER	CB-CA-C	-6.24	104.84	110.71
1	K	67	GLU	CB-CG-CD	6.24	123.21	112.60
1	B	54	VAL	CB-CA-C	-6.24	103.72	112.14
1	I	67	GLU	CB-CG-CD	6.24	123.20	112.60
1	K	59	GLU	CB-CA-C	6.24	121.69	109.72
1	F	155	ASP	CB-CA-C	6.23	121.78	111.31
1	F	205	ILE	CB-CA-C	6.23	121.51	111.29
1	B	155	ASP	CB-CA-C	6.23	121.78	111.31
1	D	155	ASP	CB-CA-C	6.23	121.78	111.31
1	A	155	ASP	CB-CA-C	6.23	121.77	111.31
1	E	205	ILE	CB-CA-C	6.23	121.50	111.29
1	C	155	ASP	CB-CA-C	6.23	121.77	111.31
1	A	205	ILE	CB-CA-C	6.22	121.50	111.29
1	B	205	ILE	CB-CA-C	6.22	121.50	111.29
1	I	59	GLU	CB-CA-C	6.22	121.67	109.72
1	L	361	ASP	CA-CB-CG	-6.22	106.38	112.60
1	E	155	ASP	CB-CA-C	6.21	121.75	111.31
1	K	361	ASP	CA-CB-CG	-6.21	106.39	112.60
1	D	259	LEU	N-CA-CB	6.21	119.07	110.07
1	M	361	ASP	CA-CB-CG	-6.21	106.39	112.60
1	I	361	ASP	CA-CB-CG	-6.21	106.39	112.60
1	A	54	VAL	CB-CA-C	-6.20	103.77	112.14
1	C	54	VAL	CB-CA-C	-6.20	103.77	112.14
1	G	54	VAL	CB-CA-C	-6.19	103.78	112.14
1	D	54	VAL	CB-CA-C	-6.19	103.79	112.14
1	F	259	LEU	N-CA-CB	6.17	119.02	110.07
1	N	361	ASP	CA-CB-CG	-6.17	106.43	112.60
1	N	61	GLU	N-CA-CB	-6.16	100.46	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	361	ASP	CA-CB-CG	-6.15	106.45	112.60
1	E	54	VAL	CB-CA-C	-6.14	103.85	112.14
1	F	54	VAL	CB-CA-C	-6.14	103.85	112.14
1	D	167	ASP	CB-CA-C	6.14	120.51	110.88
1	E	153	ASN	CA-CB-CG	6.14	118.74	112.60
1	N	59	GLU	CB-CA-C	6.13	121.48	109.72
1	B	167	ASP	CB-CA-C	6.12	120.49	110.88
1	G	167	ASP	CB-CA-C	6.12	120.49	110.88
1	G	153	ASN	CA-CB-CG	6.12	118.72	112.60
1	F	167	ASP	CB-CA-C	6.11	120.47	110.88
1	B	268	ARG	CB-CA-C	6.10	120.92	110.79
1	C	167	ASP	CB-CA-C	6.10	120.45	110.88
1	E	167	ASP	CB-CA-C	6.09	120.45	110.88
1	A	167	ASP	CB-CA-C	6.09	120.44	110.88
1	D	459	GLY	N-CA-C	-6.08	107.01	114.92
1	B	153	ASN	CA-CB-CG	6.08	118.68	112.60
1	F	153	ASN	CA-CB-CG	6.08	118.68	112.60
1	A	153	ASN	CA-CB-CG	6.07	118.67	112.60
1	E	268	ARG	CB-CA-C	6.07	120.86	110.79
1	F	268	ARG	CB-CA-C	6.07	120.86	110.79
1	C	268	ARG	CB-CA-C	6.06	120.85	110.79
1	C	153	ASN	CA-CB-CG	6.06	118.66	112.60
1	D	153	ASN	CA-CB-CG	6.06	118.66	112.60
1	C	459	GLY	N-CA-C	-6.03	107.08	114.92
1	F	152	ALA	CB-CA-C	6.03	121.79	110.63
1	F	459	GLY	N-CA-C	-6.03	107.08	114.92
1	C	152	ALA	CB-CA-C	6.01	121.76	110.63
1	B	152	ALA	CB-CA-C	6.00	121.73	110.63
1	D	268	ARG	CB-CA-C	6.00	120.75	110.79
1	A	268	ARG	CB-CA-C	6.00	120.75	110.79
1	G	459	GLY	N-CA-C	-6.00	107.13	114.92
1	A	459	GLY	N-CA-C	-5.99	107.13	114.92
1	A	152	ALA	CB-CA-C	5.99	121.71	110.63
1	C	232	GLU	N-CA-CB	5.98	118.91	110.12
1	E	232	GLU	N-CA-CB	5.97	118.90	110.12
1	G	152	ALA	CB-CA-C	5.96	121.67	110.63
1	G	232	GLU	N-CA-CB	5.96	118.89	110.12
1	D	152	ALA	CB-CA-C	5.96	121.66	110.63
1	B	232	GLU	N-CA-CB	5.96	118.88	110.12
1	E	459	GLY	N-CA-C	-5.96	107.17	114.92
1	B	459	GLY	N-CA-C	-5.96	107.17	114.92
1	D	232	GLU	N-CA-CB	5.95	118.87	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	152	ALA	CB-CA-C	5.95	121.63	110.63
1	A	232	GLU	N-CA-CB	5.95	118.86	110.12
1	M	61	GLU	N-CA-CB	-5.94	100.83	110.81
1	F	361	ASP	CB-CA-C	5.92	120.62	110.79
1	D	361	ASP	CB-CA-C	5.91	120.60	110.79
1	F	232	GLU	N-CA-CB	5.91	118.80	110.12
1	B	62	LEU	CB-CA-C	5.91	119.40	109.48
1	D	62	LEU	CB-CA-C	5.91	119.40	109.48
1	E	261	THR	N-CA-CB	5.90	118.57	110.01
1	E	62	LEU	CB-CA-C	5.88	119.36	109.48
1	B	361	ASP	CB-CA-C	5.88	120.56	110.79
1	G	361	ASP	CB-CA-C	5.88	120.55	110.79
1	G	62	LEU	CB-CA-C	5.88	119.36	109.48
1	A	62	LEU	CB-CA-C	5.88	119.35	109.48
1	J	265	ASN	CA-CB-CG	-5.88	106.72	112.60
1	A	361	ASP	CB-CA-C	5.87	120.54	110.79
1	E	361	ASP	CB-CA-C	5.87	120.53	110.79
1	M	265	ASN	CA-CB-CG	-5.87	106.73	112.60
1	C	361	ASP	CB-CA-C	5.86	120.52	110.79
1	G	268	ARG	CB-CA-C	5.86	120.51	110.79
1	H	265	ASN	CA-CB-CG	-5.86	106.74	112.60
1	C	62	LEU	CB-CA-C	5.85	119.31	109.48
1	F	62	LEU	CB-CA-C	5.82	119.26	109.48
1	F	261	THR	N-CA-CB	5.82	118.45	110.01
1	F	300	VAL	CB-CA-C	-5.82	101.58	110.95
1	I	265	ASN	CA-CB-CG	-5.82	106.78	112.60
1	E	517	THR	CB-CA-C	-5.82	98.84	110.42
1	L	265	ASN	CA-CB-CG	-5.82	106.78	112.60
1	N	400	LEU	CA-C-N	5.82	128.07	120.28
1	N	400	LEU	C-N-CA	5.82	128.07	120.28
1	I	473	ASP	N-CA-CB	5.81	122.33	111.52
1	H	473	ASP	N-CA-CB	5.81	122.33	111.52
1	M	473	ASP	N-CA-CB	5.81	122.32	111.52
1	B	300	VAL	CB-CA-C	-5.81	101.60	110.95
1	G	517	THR	CB-CA-C	-5.80	98.87	110.42
1	J	473	ASP	N-CA-CB	5.80	122.31	111.52
1	L	473	ASP	N-CA-CB	5.80	122.31	111.52
1	A	261	THR	N-CA-CB	5.80	118.42	110.01
1	E	300	VAL	CB-CA-C	-5.80	101.62	110.95
1	D	517	THR	CB-CA-C	-5.79	98.89	110.42
1	G	300	VAL	CB-CA-C	-5.79	101.62	110.95
1	K	473	ASP	N-CA-CB	5.79	122.28	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	261	THR	N-CA-CB	5.78	118.40	110.01
1	C	517	THR	CB-CA-C	-5.78	98.92	110.42
1	A	517	THR	CB-CA-C	-5.78	98.92	110.42
1	F	517	THR	CB-CA-C	-5.78	98.92	110.42
1	A	211	GLY	N-CA-C	-5.78	107.41	114.92
1	B	261	THR	N-CA-CB	5.77	118.38	110.01
1	D	261	THR	N-CA-CB	5.77	118.38	110.01
1	N	473	ASP	N-CA-CB	5.77	122.26	111.52
1	A	300	VAL	CB-CA-C	-5.77	101.66	110.95
1	D	300	VAL	CB-CA-C	-5.77	101.66	110.95
1	C	300	VAL	CB-CA-C	-5.77	101.66	110.95
1	B	517	THR	CB-CA-C	-5.77	98.95	110.42
1	C	211	GLY	N-CA-C	-5.76	107.43	114.92
1	G	261	THR	N-CA-CB	5.76	118.36	110.01
1	D	211	GLY	N-CA-C	-5.75	107.44	114.92
1	H	230	ILE	CB-CA-C	-5.74	102.81	112.16
1	A	314	LEU	CB-CA-C	-5.73	101.28	110.79
1	B	314	LEU	CB-CA-C	-5.73	101.28	110.79
1	D	314	LEU	CB-CA-C	-5.73	101.28	110.79
1	C	407	VAL	N-CA-CB	5.72	117.24	110.55
1	C	314	LEU	CB-CA-C	-5.72	101.29	110.79
1	K	230	ILE	CB-CA-C	-5.71	102.84	112.16
1	B	407	VAL	N-CA-CB	5.71	117.23	110.55
1	D	407	VAL	N-CA-CB	5.71	117.23	110.55
1	E	314	LEU	CB-CA-C	-5.71	101.31	110.79
1	G	314	LEU	CB-CA-C	-5.71	101.31	110.79
1	B	211	GLY	N-CA-C	-5.71	107.50	114.92
1	F	234	LEU	N-CA-CB	5.71	118.80	110.30
1	K	265	ASN	CA-CB-CG	-5.71	106.89	112.60
1	N	265	ASN	CA-CB-CG	-5.71	106.89	112.60
1	F	407	VAL	N-CA-CB	5.71	117.22	110.55
1	A	407	VAL	N-CA-CB	5.70	117.22	110.55
1	A	516	THR	N-CA-CB	5.70	118.50	110.12
1	E	407	VAL	N-CA-CB	5.70	117.21	110.55
1	G	407	VAL	N-CA-CB	5.70	117.21	110.55
1	C	230	ILE	N-CA-CB	5.69	118.28	110.54
1	D	230	ILE	N-CA-CB	5.69	118.28	110.54
1	F	314	LEU	CB-CA-C	-5.68	101.36	110.79
1	G	516	THR	N-CA-CB	5.68	118.47	110.12
1	L	61	GLU	N-CA-CB	-5.68	101.27	110.81
1	C	516	THR	N-CA-CB	5.67	118.46	110.12
1	F	211	GLY	N-CA-C	-5.67	107.55	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	VAL	CB-CA-C	5.67	119.80	112.14
1	F	516	THR	N-CA-CB	5.67	118.46	110.12
1	C	77	VAL	CB-CA-C	5.67	119.79	112.14
1	G	211	GLY	N-CA-C	-5.67	107.55	114.92
1	D	516	THR	N-CA-CB	5.66	118.44	110.12
1	E	234	LEU	N-CA-CB	5.66	118.73	110.30
1	E	211	GLY	N-CA-C	-5.66	107.57	114.92
1	C	30	THR	N-CA-CB	5.65	118.43	110.12
1	B	516	THR	N-CA-CB	5.65	118.43	110.12
1	D	235	PRO	N-CA-CB	5.65	109.13	103.48
1	E	516	THR	N-CA-CB	5.65	118.42	110.12
1	G	230	ILE	N-CA-CB	5.65	118.22	110.54
1	A	30	THR	N-CA-CB	5.64	118.41	110.12
1	B	77	VAL	CB-CA-C	5.64	119.76	112.14
1	B	234	LEU	N-CA-CB	5.64	118.70	110.30
1	A	230	ILE	N-CA-CB	5.64	118.21	110.54
1	F	30	THR	N-CA-CB	5.63	118.40	110.12
1	C	235	PRO	N-CA-CB	5.63	109.11	103.48
1	G	77	VAL	CB-CA-C	5.63	119.74	112.14
1	E	77	VAL	CB-CA-C	5.63	119.74	112.14
1	F	235	PRO	N-CA-CB	5.63	109.11	103.48
1	C	306	GLY	N-CA-C	-5.63	107.49	115.43
1	E	82	ASN	N-CA-CB	5.63	118.39	110.12
1	I	2	ALA	CA-C-O	5.63	130.36	120.80
1	A	235	PRO	N-CA-CB	5.62	109.10	103.48
1	J	386	GLU	CB-CA-C	-5.62	100.23	110.63
1	A	82	ASN	N-CA-CB	5.62	118.38	110.12
1	E	30	THR	N-CA-CB	5.62	118.38	110.12
1	F	77	VAL	CB-CA-C	5.62	119.73	112.14
1	G	82	ASN	N-CA-CB	5.62	118.38	110.12
1	A	25	ASP	CA-CB-CG	-5.62	106.98	112.60
1	D	30	THR	N-CA-CB	5.61	118.37	110.12
1	N	495	ASP	CB-CA-C	5.61	117.57	108.87
1	C	82	ASN	N-CA-CB	5.61	118.36	110.12
1	D	82	ASN	N-CA-CB	5.61	118.36	110.12
1	E	235	PRO	N-CA-CB	5.61	109.08	103.48
1	M	495	ASP	CB-CA-C	5.61	117.56	108.87
1	D	77	VAL	CB-CA-C	5.60	119.70	112.14
1	M	386	GLU	CB-CA-C	-5.60	100.26	110.63
1	E	43	SER	N-CA-CB	5.60	118.97	110.28
1	K	386	GLU	CB-CA-C	-5.60	100.27	110.63
1	B	30	THR	N-CA-CB	5.60	118.35	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	LEU	N-CA-CB	5.60	118.64	110.30
1	B	82	ASN	N-CA-CB	5.60	118.35	110.12
1	F	27	VAL	CB-CA-C	5.60	119.70	112.14
1	D	104	LEU	CB-CA-C	5.60	120.08	110.79
1	F	82	ASN	N-CA-CB	5.60	118.35	110.12
1	B	235	PRO	N-CA-CB	5.59	109.07	103.48
1	E	104	LEU	CB-CA-C	5.59	120.07	110.79
1	G	30	THR	N-CA-CB	5.59	118.34	110.12
1	H	13	ARG	N-CA-CB	5.59	118.07	109.91
1	G	235	PRO	N-CA-CB	5.59	109.07	103.48
1	I	386	GLU	CB-CA-C	-5.59	100.30	110.63
1	D	25	ASP	CA-CB-CG	-5.58	107.02	112.60
1	E	193	MET	N-CA-CB	-5.58	101.21	111.37
1	G	306	GLY	N-CA-C	-5.58	107.56	115.43
1	H	386	GLU	CB-CA-C	-5.58	100.30	110.63
1	N	386	GLU	CB-CA-C	-5.58	100.30	110.63
1	A	27	VAL	CB-CA-C	5.58	119.67	112.14
1	B	230	ILE	N-CA-CB	5.58	118.13	110.54
1	I	495	ASP	CB-CA-C	5.58	117.52	108.87
1	M	13	ARG	N-CA-CB	5.58	118.06	109.91
1	E	25	ASP	CA-CB-CG	-5.58	107.02	112.60
1	K	495	ASP	CB-CA-C	5.58	117.51	108.87
1	E	306	GLY	N-CA-C	-5.57	107.57	115.43
1	A	104	LEU	CB-CA-C	5.57	120.03	110.79
1	B	25	ASP	CA-CB-CG	-5.57	107.03	112.60
1	L	495	ASP	CB-CA-C	5.57	117.50	108.87
1	B	306	GLY	N-CA-C	-5.56	107.58	115.43
1	H	495	ASP	CB-CA-C	5.56	117.49	108.87
1	B	193	MET	N-CA-CB	-5.56	101.25	111.37
1	C	25	ASP	CA-CB-CG	-5.56	107.04	112.60
1	L	523	ASP	CB-CA-C	5.56	119.78	109.54
1	I	61	GLU	N-CA-CB	-5.56	101.47	110.81
1	C	193	MET	N-CA-CB	-5.56	101.25	111.37
1	D	43	SER	N-CA-CB	5.56	118.90	110.28
1	E	266	THR	N-CA-CB	5.56	118.13	110.07
1	F	104	LEU	CB-CA-C	5.56	120.02	110.79
1	J	495	ASP	CB-CA-C	5.56	117.49	108.87
1	L	386	GLU	CB-CA-C	-5.56	100.35	110.63
1	B	104	LEU	CB-CA-C	5.56	120.02	110.79
1	F	25	ASP	CA-CB-CG	-5.56	107.04	112.60
1	G	27	VAL	CB-CA-C	5.56	119.64	112.14
1	D	306	GLY	N-CA-C	-5.56	107.60	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	GLY	N-CA-C	-5.55	107.60	115.43
1	B	380	LYS	N-CA-CB	-5.55	101.75	110.69
1	D	193	MET	N-CA-CB	-5.55	101.26	111.37
1	F	193	MET	N-CA-CB	-5.55	101.27	111.37
1	G	104	LEU	CB-CA-C	5.55	120.00	110.79
1	A	193	MET	N-CA-CB	-5.55	101.27	111.37
1	D	27	VAL	CB-CA-C	5.55	119.63	112.14
1	B	43	SER	N-CA-CB	5.55	118.88	110.28
1	C	27	VAL	CB-CA-C	5.54	119.62	112.14
1	N	267	MET	CB-CA-C	5.54	120.92	112.00
1	F	306	GLY	N-CA-C	-5.54	107.62	115.43
1	G	234	LEU	N-CA-CB	5.54	118.56	110.30
1	D	380	LYS	N-CA-CB	-5.54	101.77	110.69
1	C	104	LEU	CB-CA-C	5.54	119.98	110.79
1	G	193	MET	N-CA-CB	-5.54	101.30	111.37
1	F	99	ILE	N-CA-CB	5.53	117.02	110.55
1	G	25	ASP	CA-CB-CG	-5.53	107.07	112.60
1	C	43	SER	N-CA-CB	5.53	118.85	110.28
1	A	380	LYS	N-CA-CB	-5.53	101.79	110.69
1	I	13	ARG	N-CA-CB	5.53	117.98	109.91
1	A	234	LEU	N-CA-CB	5.53	118.53	110.30
1	B	285	ARG	N-CA-CB	5.52	118.24	110.12
1	K	267	MET	CB-CA-C	5.52	120.89	112.00
1	D	285	ARG	N-CA-CB	5.51	118.22	110.12
1	E	27	VAL	CB-CA-C	5.51	119.58	112.14
1	L	13	ARG	N-CA-CB	5.51	117.96	109.91
1	B	85	ALA	N-CA-CB	-5.51	102.00	110.16
1	C	85	ALA	N-CA-CB	-5.51	102.00	110.16
1	E	380	LYS	N-CA-CB	-5.51	101.82	110.69
1	G	380	LYS	N-CA-CB	-5.51	101.82	110.69
1	N	13	ARG	N-CA-CB	5.51	117.95	109.91
1	I	400	LEU	O-C-N	-5.51	115.78	122.22
1	B	27	VAL	CB-CA-C	5.50	119.57	112.14
1	G	285	ARG	N-CA-CB	5.50	118.21	110.12
1	B	410	GLY	N-CA-C	-5.50	105.68	112.33
1	C	285	ARG	N-CA-CB	5.50	118.20	110.12
1	J	13	ARG	N-CA-CB	5.50	117.94	109.91
1	E	85	ALA	N-CA-CB	-5.50	102.03	110.16
1	B	99	ILE	N-CA-CB	5.49	116.98	110.55
1	D	234	LEU	N-CA-CB	5.49	118.48	110.30
1	F	85	ALA	N-CA-CB	-5.49	102.04	110.16
1	A	85	ALA	N-CA-CB	-5.49	102.04	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99	ILE	N-CA-CB	5.49	116.97	110.55
1	A	99	ILE	N-CA-CB	5.48	116.96	110.55
1	D	85	ALA	N-CA-CB	-5.48	102.05	110.16
1	F	285	ARG	N-CA-CB	5.48	118.18	110.12
1	B	409	GLU	CB-CA-C	5.47	120.15	110.85
1	E	285	ARG	N-CA-CB	5.47	118.17	110.12
1	K	13	ARG	N-CA-CB	5.47	117.90	109.91
1	A	409	GLU	CB-CA-C	5.47	120.15	110.85
1	F	380	LYS	N-CA-CB	-5.47	101.89	110.69
1	L	400	LEU	CA-C-N	5.47	133.28	121.64
1	L	400	LEU	C-N-CA	5.47	133.28	121.64
1	E	409	GLU	CB-CA-C	5.46	120.13	110.85
1	G	99	ILE	N-CA-CB	5.46	116.94	110.55
1	C	380	LYS	N-CA-CB	-5.46	101.90	110.69
1	G	409	GLU	CB-CA-C	5.46	120.12	110.85
1	A	285	ARG	N-CA-CB	5.45	118.14	110.12
1	F	409	GLU	CB-CA-C	5.45	120.12	110.85
1	G	85	ALA	N-CA-CB	-5.45	102.09	110.16
1	B	309	LEU	N-CA-C	-5.45	105.34	111.28
1	C	224	ASP	N-CA-CB	5.45	118.22	110.16
1	D	48	THR	N-CA-CB	5.44	119.50	110.52
1	D	309	LEU	N-CA-C	-5.44	105.36	111.28
1	G	224	ASP	N-CA-CB	5.43	118.20	110.16
1	D	409	GLU	CB-CA-C	5.43	120.08	110.85
1	A	224	ASP	N-CA-CB	5.42	118.19	110.16
1	A	410	GLY	N-CA-C	-5.42	105.77	112.33
1	C	48	THR	N-CA-CB	5.42	119.47	110.52
1	C	409	GLU	CB-CA-C	5.42	120.07	110.85
1	E	48	THR	N-CA-CB	5.42	119.47	110.52
1	B	48	THR	N-CA-CB	5.42	119.46	110.52
1	B	34	LYS	N-CA-CB	5.42	118.08	110.12
1	F	34	LYS	N-CA-CB	5.41	118.08	110.12
1	A	48	THR	N-CA-CB	5.41	119.45	110.52
1	F	400	LEU	CA-C-N	5.41	127.84	120.54
1	F	400	LEU	C-N-CA	5.41	127.84	120.54
1	D	34	LYS	N-CA-CB	5.41	118.07	110.12
1	E	224	ASP	N-CA-CB	5.41	118.16	110.16
1	E	410	GLY	N-CA-C	-5.41	105.79	112.33
1	E	110	GLY	N-CA-C	-5.40	107.75	115.64
1	H	115	ASP	CA-CB-CG	-5.40	107.20	112.60
1	C	410	GLY	N-CA-C	-5.40	105.80	112.33
1	F	224	ASP	N-CA-CB	5.40	118.15	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	410	GLY	N-CA-C	-5.40	105.80	112.33
1	A	34	LYS	N-CA-CB	5.39	118.05	110.12
1	D	224	ASP	N-CA-CB	5.39	118.14	110.16
1	G	410	GLY	N-CA-C	-5.39	105.80	112.33
1	L	115	ASP	CA-CB-CG	-5.39	107.20	112.60
1	A	266	THR	N-CA-CB	5.39	117.89	110.07
1	N	115	ASP	CA-CB-CG	-5.39	107.21	112.60
1	C	309	LEU	N-CA-C	-5.39	105.40	111.28
1	D	266	THR	N-CA-CB	5.39	117.88	110.07
1	B	224	ASP	N-CA-CB	5.38	118.13	110.16
1	I	523	ASP	CB-CA-C	5.38	119.45	109.54
1	N	60	ILE	N-CA-C	5.38	116.11	107.98
1	J	115	ASP	CA-CB-CG	-5.38	107.22	112.60
1	K	115	ASP	CA-CB-CG	-5.38	107.22	112.60
1	I	60	ILE	N-CA-C	5.38	116.10	107.98
1	N	284	ARG	CB-CA-C	-5.37	101.87	110.79
1	C	34	LYS	N-CA-CB	5.37	118.01	110.12
1	E	479	ASN	CB-CA-C	5.37	118.89	110.19
1	G	309	LEU	N-CA-C	-5.37	105.43	111.28
1	F	410	GLY	N-CA-C	-5.37	105.84	112.33
1	G	48	THR	N-CA-CB	5.37	119.37	110.52
1	I	115	ASP	CA-CB-CG	-5.36	107.24	112.60
1	E	34	LYS	N-CA-CB	5.36	118.00	110.12
1	M	60	ILE	N-CA-C	5.36	116.08	107.98
1	H	284	ARG	CB-CA-C	-5.36	101.89	110.79
1	F	48	THR	N-CA-CB	5.36	119.36	110.52
1	F	110	GLY	N-CA-C	-5.36	107.82	115.64
1	J	284	ARG	CB-CA-C	-5.35	101.91	110.79
1	B	479	ASN	CB-CA-C	5.35	118.86	110.19
1	G	110	GLY	N-CA-C	-5.35	107.83	115.64
1	E	242	LYS	N-CA-CB	5.35	117.98	110.12
1	J	523	ASP	CB-CA-C	5.35	119.38	109.54
1	M	115	ASP	CA-CB-CG	-5.35	107.25	112.60
1	C	416	GLY	N-CA-C	-5.34	106.85	115.08
1	G	479	ASN	CB-CA-C	5.34	118.85	110.19
1	E	309	LEU	N-CA-C	-5.34	105.46	111.28
1	F	359	ASP	CA-CB-CG	-5.34	107.26	112.60
1	G	266	THR	N-CA-CB	5.34	117.81	110.07
1	M	284	ARG	CB-CA-C	-5.34	101.92	110.79
1	G	34	LYS	N-CA-CB	5.34	117.97	110.12
1	L	284	ARG	CB-CA-C	-5.34	101.93	110.79
1	A	479	ASN	CB-CA-C	5.34	118.83	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	309	LEU	N-CA-C	-5.34	105.46	111.28
1	K	284	ARG	CB-CA-C	-5.33	101.94	110.79
1	F	455	VAL	CB-CA-C	5.33	119.33	112.14
1	F	479	ASN	CB-CA-C	5.33	118.82	110.19
1	B	455	VAL	CB-CA-C	5.33	119.33	112.14
1	D	416	GLY	N-CA-C	-5.33	106.88	115.08
1	L	60	ILE	N-CA-C	5.33	116.03	107.98
1	C	359	ASP	CA-CB-CG	-5.33	107.27	112.60
1	F	230	ILE	N-CA-CB	5.33	117.78	110.54
1	K	60	ILE	N-CA-C	5.32	116.02	107.98
1	B	242	LYS	N-CA-CB	5.32	117.94	110.12
1	C	479	ASN	CB-CA-C	5.32	118.81	110.19
1	A	110	GLY	N-CA-C	-5.32	107.88	115.64
1	A	416	GLY	N-CA-C	-5.32	106.89	115.08
1	F	242	LYS	N-CA-CB	5.32	117.94	110.12
1	D	479	ASN	CB-CA-C	5.32	118.80	110.19
1	C	242	LYS	N-CA-CB	5.31	117.93	110.12
1	D	455	VAL	CB-CA-C	5.31	119.31	112.14
1	E	359	ASP	CA-CB-CG	-5.31	107.29	112.60
1	I	284	ARG	CB-CA-C	-5.31	101.97	110.79
1	B	110	GLY	N-CA-C	-5.31	107.89	115.64
1	B	359	ASP	CA-CB-CG	-5.31	107.29	112.60
1	F	416	GLY	N-CA-C	-5.31	106.91	115.08
1	C	110	GLY	N-CA-C	-5.31	107.89	115.64
1	E	416	GLY	N-CA-C	-5.31	106.91	115.08
1	G	416	GLY	N-CA-C	-5.30	106.91	115.08
1	A	359	ASP	CA-CB-CG	-5.30	107.30	112.60
1	B	266	THR	N-CA-CB	5.30	117.75	110.07
1	F	266	THR	N-CA-CB	5.30	117.75	110.07
1	D	242	LYS	N-CA-CB	5.29	117.90	110.12
1	C	455	VAL	CB-CA-C	5.29	119.29	112.14
1	D	110	GLY	N-CA-C	-5.29	107.91	115.64
1	B	416	GLY	N-CA-C	-5.29	106.93	115.08
1	C	501	ARG	N-CA-CB	-5.29	102.35	110.12
1	E	501	ARG	N-CA-CB	-5.29	102.35	110.12
1	G	455	VAL	CB-CA-C	5.29	119.28	112.14
1	E	140	ASP	CA-CB-CG	5.29	117.89	112.60
1	G	242	LYS	N-CA-CB	5.29	117.89	110.12
1	D	359	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	501	ARG	N-CA-CB	-5.28	102.36	110.12
1	D	113	PRO	N-CA-CB	5.28	108.76	103.48
1	A	242	LYS	N-CA-CB	5.28	117.88	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	PRO	N-CA-CB	5.28	108.75	103.48
1	D	140	ASP	CA-CB-CG	5.28	117.88	112.60
1	G	140	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	140	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	415	GLY	N-CA-C	-5.27	107.97	115.30
1	G	113	PRO	N-CA-CB	5.27	108.75	103.48
1	G	359	ASP	CA-CB-CG	-5.27	107.33	112.60
1	J	60	ILE	N-CA-C	5.27	115.94	107.98
1	H	60	ILE	N-CA-C	5.27	115.94	107.98
1	A	113	PRO	N-CA-CB	5.27	108.75	103.48
1	A	309	LEU	N-CA-C	-5.27	105.54	111.28
1	E	455	VAL	CB-CA-C	5.27	119.25	112.14
1	B	501	ARG	N-CA-CB	-5.26	102.39	110.12
1	F	113	PRO	N-CA-CB	5.26	108.74	103.48
1	A	455	VAL	CB-CA-C	5.25	119.23	112.14
1	G	501	ARG	N-CA-CB	-5.25	102.39	110.12
1	C	140	ASP	CA-CB-CG	5.25	117.85	112.60
1	E	113	PRO	N-CA-CB	5.25	108.73	103.48
1	F	140	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	266	THR	N-CA-CB	5.25	117.68	110.07
1	F	501	ARG	N-CA-CB	-5.24	102.41	110.12
1	D	415	GLY	N-CA-C	-5.24	108.02	115.30
1	D	501	ARG	N-CA-CB	-5.24	102.42	110.12
1	F	415	GLY	N-CA-C	-5.23	108.03	115.30
1	D	236	VAL	N-CA-CB	5.22	117.64	110.54
1	H	388	GLU	CB-CA-C	-5.22	102.69	110.88
1	M	523	ASP	CB-CA-C	5.22	119.14	109.54
1	N	388	GLU	CB-CA-C	-5.21	102.70	110.88
1	I	388	GLU	CB-CA-C	-5.21	102.70	110.88
1	M	388	GLU	CB-CA-C	-5.21	102.70	110.88
1	G	415	GLY	N-CA-C	-5.21	108.06	115.30
1	A	236	VAL	N-CA-CB	5.20	117.62	110.54
1	C	113	PRO	N-CA-CB	5.20	108.68	103.48
1	J	388	GLU	CB-CA-C	-5.20	102.72	110.88
1	C	169	VAL	N-CA-CB	5.20	118.37	110.58
1	K	388	GLU	CB-CA-C	-5.19	102.73	110.88
1	B	140	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	169	VAL	N-CA-CB	5.19	118.37	110.58
1	B	415	GLY	N-CA-C	-5.19	108.09	115.30
1	E	415	GLY	N-CA-C	-5.19	108.09	115.30
1	J	230	ILE	CB-CA-C	-5.19	103.70	112.16
1	L	388	GLU	CB-CA-C	-5.19	102.74	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	169	VAL	N-CA-CB	5.18	118.35	110.58
1	A	415	GLY	N-CA-C	-5.18	108.10	115.30
1	B	438	VAL	N-CA-CB	5.18	117.58	110.54
1	A	438	VAL	N-CA-CB	5.18	117.58	110.54
1	D	169	VAL	N-CA-CB	5.18	118.35	110.58
1	L	230	ILE	CB-CA-C	-5.17	103.73	112.16
1	N	334	ASP	CA-CB-CG	5.17	117.78	112.60
1	A	169	VAL	N-CA-CB	5.17	118.34	110.58
1	D	438	VAL	N-CA-CB	5.17	117.57	110.54
1	E	438	VAL	N-CA-CB	5.17	117.57	110.54
1	E	440	ILE	CB-CA-C	-5.17	105.17	112.14
1	K	334	ASP	CA-CB-CG	5.16	117.76	112.60
1	K	61	GLU	N-CA-CB	-5.16	102.14	110.81
1	M	334	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	438	VAL	N-CA-CB	5.16	117.55	110.54
1	F	438	VAL	N-CA-CB	5.16	117.55	110.54
1	F	169	VAL	N-CA-CB	5.15	118.31	110.58
1	C	417	VAL	CA-CB-CG2	-5.15	101.65	110.40
1	A	495	ASP	CB-CA-C	-5.15	100.74	108.61
1	I	334	ASP	CA-CB-CG	5.14	117.74	112.60
1	J	334	ASP	CA-CB-CG	5.14	117.74	112.60
1	M	230	ILE	CB-CA-C	-5.14	103.78	112.16
1	A	440	ILE	CB-CA-C	-5.14	105.20	112.14
1	B	367	GLU	CA-CB-CG	5.14	124.38	114.10
1	G	444	LEU	CB-CA-C	-5.14	102.26	110.79
1	G	417	VAL	CA-CB-CG2	-5.14	101.67	110.40
1	B	417	VAL	CA-CB-CG2	-5.14	101.67	110.40
1	F	491	MET	CB-CA-C	5.13	119.31	110.79
1	G	440	ILE	CB-CA-C	-5.13	105.21	112.14
1	C	440	ILE	CB-CA-C	-5.13	105.22	112.14
1	E	169	VAL	N-CA-CB	5.13	118.27	110.58
1	E	444	LEU	CB-CA-C	-5.13	102.28	110.79
1	F	367	GLU	CA-CB-CG	5.13	124.35	114.10
1	D	440	ILE	CB-CA-C	-5.12	105.22	112.14
1	G	491	MET	CB-CA-C	5.12	119.30	110.79
1	H	334	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	444	LEU	CB-CA-C	-5.12	102.29	110.79
1	A	491	MET	CB-CA-C	5.12	119.29	110.79
1	B	444	LEU	CB-CA-C	-5.12	102.29	110.79
1	D	444	LEU	CB-CA-C	-5.12	102.29	110.79
1	F	444	LEU	CB-CA-C	-5.12	102.29	110.79
1	G	438	VAL	N-CA-CB	5.12	117.50	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	GLU	CA-CB-CG	5.12	124.33	114.10
1	B	440	ILE	CB-CA-C	-5.12	105.23	112.14
1	C	444	LEU	CB-CA-C	-5.12	102.29	110.79
1	E	473	ASP	N-CA-CB	5.12	118.20	110.42
1	G	367	GLU	CA-CB-CG	5.12	124.34	114.10
1	E	495	ASP	CB-CA-C	-5.12	100.78	108.61
1	E	491	MET	CB-CA-C	5.12	119.28	110.79
1	C	495	ASP	CB-CA-C	-5.11	100.78	108.61
1	F	417	VAL	CA-CB-CG2	-5.11	101.71	110.40
1	F	440	ILE	CB-CA-C	-5.11	105.24	112.14
1	B	491	MET	CB-CA-C	5.11	119.28	110.79
1	F	436	GLN	N-CA-CB	5.11	117.63	110.12
1	A	417	VAL	CA-CB-CG2	-5.11	101.72	110.40
1	I	518	GLU	CB-CG-CD	5.11	121.28	112.60
1	D	417	VAL	CA-CB-CG2	-5.10	101.72	110.40
1	E	417	VAL	CA-CB-CG2	-5.10	101.73	110.40
1	F	473	ASP	N-CA-CB	5.10	118.17	110.42
1	C	436	GLN	N-CA-CB	5.10	117.61	110.12
1	D	436	GLN	N-CA-CB	5.09	117.61	110.12
1	D	367	GLU	CA-CB-CG	5.09	124.29	114.10
1	L	334	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	367	GLU	CA-CB-CG	5.09	124.28	114.10
1	B	436	GLN	N-CA-CB	5.09	117.60	110.12
1	M	518	GLU	CB-CG-CD	5.09	121.25	112.60
1	B	52	ASP	CB-CA-C	5.08	119.75	109.68
1	D	491	MET	CB-CA-C	5.08	119.23	110.79
1	B	495	ASP	CB-CA-C	-5.08	100.83	108.61
1	F	52	ASP	CB-CA-C	5.08	119.74	109.68
1	D	52	ASP	CB-CA-C	5.08	119.74	109.68
1	C	491	MET	CB-CA-C	5.08	119.22	110.79
1	L	463	SER	N-CA-CB	-5.08	102.12	110.40
1	B	473	ASP	N-CA-CB	5.08	118.13	110.42
1	K	518	GLU	CB-CG-CD	5.08	121.23	112.60
1	D	473	ASP	N-CA-CB	5.07	118.13	110.42
1	E	367	GLU	CA-CB-CG	5.07	124.24	114.10
1	J	463	SER	N-CA-CB	-5.07	102.14	110.40
1	A	473	ASP	N-CA-CB	5.07	118.12	110.42
1	G	473	ASP	N-CA-CB	5.07	118.12	110.42
1	G	492	GLY	N-CA-C	-5.07	108.29	115.43
1	F	495	ASP	CB-CA-C	-5.06	100.86	108.61
1	G	495	ASP	CB-CA-C	-5.06	100.86	108.61
1	N	518	GLU	CB-CG-CD	5.06	121.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	473	ASP	N-CA-CB	5.06	118.11	110.42
1	I	463	SER	N-CA-CB	-5.06	102.16	110.40
1	M	463	SER	N-CA-CB	-5.05	102.17	110.40
1	A	436	GLN	N-CA-CB	5.05	117.54	110.12
1	D	495	ASP	CB-CA-C	-5.05	100.89	108.61
1	N	463	SER	N-CA-CB	-5.05	102.17	110.40
1	A	52	ASP	CB-CA-C	5.04	119.67	109.68
1	H	463	SER	N-CA-CB	-5.04	102.18	110.40
1	F	243	ALA	N-CA-CB	5.04	119.01	110.49
1	C	52	ASP	CB-CA-C	5.04	119.66	109.68
1	E	52	ASP	CB-CA-C	5.04	119.66	109.68
1	K	25	ASP	CA-CB-CG	-5.04	107.56	112.60
1	G	436	GLN	N-CA-CB	5.04	117.52	110.12
1	K	463	SER	N-CA-CB	-5.04	102.19	110.40
1	H	518	GLU	CB-CG-CD	5.03	121.16	112.60
1	L	518	GLU	CB-CG-CD	5.03	121.16	112.60
1	N	25	ASP	CA-CB-CG	-5.03	107.57	112.60
1	G	52	ASP	CB-CA-C	5.03	119.64	109.68
1	N	523	ASP	CB-CA-C	5.03	118.79	109.54
1	J	518	GLU	CB-CG-CD	5.02	121.14	112.60
1	E	436	GLN	N-CA-CB	5.02	117.50	110.12
1	E	492	GLY	N-CA-C	-5.02	108.35	115.43
1	A	170	GLY	N-CA-C	-5.02	105.45	112.18
1	B	492	GLY	N-CA-C	-5.02	108.35	115.43
1	D	243	ALA	N-CA-CB	5.02	118.97	110.49
1	C	492	GLY	N-CA-C	-5.02	108.36	115.43
1	A	458	CYS	N-CA-CB	5.01	117.49	110.12
1	C	243	ALA	N-CA-CB	5.01	118.97	110.49
1	G	243	ALA	N-CA-CB	5.01	118.96	110.49
1	K	178	GLU	CB-CG-CD	5.01	121.12	112.60
1	K	400	LEU	CA-C-N	-5.01	113.07	120.28
1	K	400	LEU	C-N-CA	-5.01	113.07	120.28
1	K	523	ASP	CB-CA-C	5.01	118.75	109.54
1	E	243	ALA	N-CA-CB	5.00	118.95	110.49
1	J	25	ASP	CA-CB-CG	-5.00	107.60	112.60

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	257	GLU	CA
1	B	257	GLU	CA
1	C	257	GLU	CA

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Mol	Chain	Res	Type	Atom
1	D	257	GLU	CA
1	E	257	GLU	CA
1	F	257	GLU	CA
1	G	257	GLU	CA

All (137) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Sidechain
1	A	197	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	268	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	37	ASN	Mainchain
1	A	395	ARG	Sidechain
1	A	404	ARG	Sidechain
1	A	50	THR	Mainchain
1	B	118	ARG	Sidechain
1	B	197	ARG	Sidechain
1	B	231	ARG	Sidechain
1	B	268	ARG	Sidechain
1	B	350	ARG	Sidechain
1	B	362	ARG	Sidechain
1	B	37	ASN	Mainchain
1	B	395	ARG	Sidechain
1	B	404	ARG	Sidechain
1	B	50	THR	Mainchain
1	C	118	ARG	Sidechain
1	C	197	ARG	Sidechain
1	C	231	ARG	Sidechain
1	C	268	ARG	Sidechain
1	C	350	ARG	Sidechain
1	C	362	ARG	Sidechain
1	C	37	ASN	Mainchain
1	C	395	ARG	Sidechain
1	C	404	ARG	Sidechain
1	C	50	THR	Mainchain
1	D	118	ARG	Sidechain
1	D	197	ARG	Sidechain
1	D	231	ARG	Sidechain
1	D	268	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	350	ARG	Sidechain
1	D	362	ARG	Sidechain
1	D	37	ASN	Mainchain
1	D	395	ARG	Sidechain
1	D	404	ARG	Sidechain
1	D	50	THR	Mainchain
1	E	118	ARG	Sidechain
1	E	197	ARG	Sidechain
1	E	231	ARG	Sidechain
1	E	268	ARG	Sidechain
1	E	350	ARG	Sidechain
1	E	362	ARG	Sidechain
1	E	37	ASN	Mainchain
1	E	395	ARG	Sidechain
1	E	404	ARG	Sidechain
1	E	50	THR	Mainchain
1	F	118	ARG	Sidechain
1	F	197	ARG	Sidechain
1	F	231	ARG	Sidechain
1	F	268	ARG	Sidechain
1	F	350	ARG	Sidechain
1	F	362	ARG	Sidechain
1	F	37	ASN	Mainchain
1	F	395	ARG	Sidechain
1	F	404	ARG	Sidechain
1	F	50	THR	Mainchain
1	G	118	ARG	Sidechain
1	G	197	ARG	Sidechain
1	G	231	ARG	Sidechain
1	G	268	ARG	Sidechain
1	G	350	ARG	Sidechain
1	G	362	ARG	Sidechain
1	G	37	ASN	Mainchain
1	G	395	ARG	Sidechain
1	G	404	ARG	Sidechain
1	G	50	THR	Mainchain
1	H	197	ARG	Sidechain
1	H	2	ALA	Peptide,Mainchain
1	H	231	ARG	Sidechain
1	H	281	PHE	Sidechain
1	H	284	ARG	Sidechain
1	H	350	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	H	362	ARG	Sidechain
1	H	421	ARG	Sidechain
1	H	445	ARG	Sidechain
1	H	478	TYR	Sidechain
1	I	197	ARG	Sidechain
1	I	231	ARG	Sidechain
1	I	281	PHE	Sidechain
1	I	284	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	197	ARG	Sidechain
1	J	231	ARG	Sidechain
1	J	281	PHE	Sidechain
1	J	284	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	197	ARG	Sidechain
1	K	231	ARG	Sidechain
1	K	281	PHE	Sidechain
1	K	284	ARG	Sidechain
1	K	350	ARG	Sidechain
1	K	362	ARG	Sidechain
1	K	401	HIS	Mainchain
1	K	421	ARG	Sidechain
1	K	445	ARG	Sidechain
1	K	478	TYR	Sidechain
1	L	197	ARG	Sidechain
1	L	231	ARG	Sidechain
1	L	281	PHE	Sidechain
1	L	284	ARG	Sidechain
1	L	350	ARG	Sidechain
1	L	362	ARG	Sidechain
1	L	421	ARG	Sidechain
1	L	445	ARG	Sidechain
1	L	478	TYR	Sidechain
1	M	197	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	M	231	ARG	Sidechain
1	M	281	PHE	Sidechain
1	M	284	ARG	Sidechain
1	M	350	ARG	Sidechain
1	M	362	ARG	Sidechain
1	M	401	HIS	Mainchain
1	M	421	ARG	Sidechain
1	M	445	ARG	Sidechain
1	M	478	TYR	Sidechain
1	N	197	ARG	Sidechain
1	N	231	ARG	Sidechain
1	N	281	PHE	Sidechain
1	N	284	ARG	Sidechain
1	N	350	ARG	Sidechain
1	N	362	ARG	Sidechain
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	103	0
1	B	3846	0	3970	104	0
1	C	3846	0	3970	106	0
1	D	3846	0	3970	106	0
1	E	3846	0	3970	105	0
1	F	3846	0	3970	104	0
1	G	3846	0	3970	109	0
1	H	3846	0	3970	35	0
1	I	3846	0	3969	35	0
1	J	3846	0	3970	30	0
1	K	3846	0	3969	34	0
1	L	3846	0	3970	30	0
1	M	3846	0	3968	30	0
1	N	3846	0	3969	37	0
2	A	31	12	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	12	12	4	0
2	C	31	12	12	4	0
2	D	31	12	12	4	0
2	E	31	12	12	4	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	5	0
3	C	1	0	0	5	0
3	D	1	0	0	5	0
3	E	1	0	0	5	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	926	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 8.

All (926) 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:H:2:ALA:C	1:H:2:ALA:CA	1.77	1.52
1:H:2:ALA:CA	1:H:2:ALA:N	1.73	1.51
1:N:401:HIS:C	1:N:402:ALA:N	1.70	1.48
1:I:2:ALA:N	1:I:2:ALA:CA	1.79	1.45
1:N:2:ALA:CA	1:N:2:ALA:N	1.80	1.44
1:I:400:LEU:C	1:I:401:HIS:N	1.77	1.39
1:K:400:LEU:C	1:K:401:HIS:N	1.81	1.37
1:M:400:LEU:C	1:M:401:HIS:N	1.86	1.34
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.45	0.96
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.45	0.96
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.45	0.95
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.45	0.94
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.45	0.94
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.45	0.94
1:F:183:LEU:O	1:F:382:GLY:HA3	1.82	0.80
1:G:183:LEU:O	1:G:382:GLY:HA3	1.82	0.79
1:A:183:LEU:O	1:A:382:GLY:HA3	1.82	0.79
1:B:183:LEU:O	1:B:382:GLY:HA3	1.82	0.79
1:C:183:LEU:O	1:C:382:GLY:HA3	1.82	0.79
1:D:183:LEU:O	1:D:382:GLY:HA3	1.82	0.79
1:E:183:LEU:O	1:E:382:GLY:HA3	1.82	0.78
1:A:135:SER:HA	1:A:412:VAL:HG12	1.66	0.78
1:G:135:SER:HA	1:G:412:VAL:HG12	1.66	0.78
1:B:135:SER:HA	1:B:412:VAL:HG12	1.67	0.77
1:C:135:SER:HA	1:C:412:VAL:HG12	1.67	0.77
1:F:135:SER:HA	1:F:412:VAL:HG12	1.66	0.77
1:I:2:ALA:N	1:I:2:ALA:C	2.43	0.77
1:H:2:ALA:C	1:H:2:ALA:N	2.43	0.77
1:E:135:SER:HA	1:E:412:VAL:HG12	1.66	0.76
1:B:192:GLY:O	1:B:375:GLY:HA2	1.85	0.76
1:C:192:GLY:O	1:C:375:GLY:HA2	1.85	0.76
1:E:192:GLY:O	1:E:375:GLY:HA2	1.85	0.76
1:D:135:SER:HA	1:D:412:VAL:HG12	1.67	0.76
1:N:2:ALA:N	1:N:2:ALA:C	2.43	0.76
1:F:192:GLY:O	1:F:375:GLY:HA2	1.85	0.76
1:G:192:GLY:O	1:G:375:GLY:HA2	1.85	0.76
1:D:192:GLY:O	1:D:375:GLY:HA2	1.85	0.75
1:D:199:TYR:CD2	1:D:205:ILE:HD11	2.21	0.75
1:C:199:TYR:CD2	1:C:205:ILE:HD11	2.21	0.75
1:G:199:TYR:CD2	1:G:205:ILE:HD11	2.21	0.75
1:A:192:GLY:O	1:A:375:GLY:HA2	1.85	0.75
1:A:199:TYR:CD2	1:A:205:ILE:HD11	2.21	0.75
1:E:199:TYR:CD2	1:E:205:ILE:HD11	2.21	0.75
1:B:199:TYR:CD2	1:B:205:ILE:HD11	2.21	0.74
1:F:199:TYR:CD2	1:F:205:ILE:HD11	2.21	0.74
3:G:1525:PO4:P	2:G:1527:ATP:O1G	2.47	0.73
3:E:1526:PO4:P	2:E:1527:ATP:O1G	2.47	0.73
3:F:1525:PO4:P	2:F:1527:ATP:O1G	2.47	0.73
2:C:1526:ATP:O1G	3:C:1527:PO4:P	2.47	0.72
2:B:1525:ATP:O1G	3:B:1526:PO4:P	2.47	0.72
2:D:1525:ATP:O1G	3:D:1526:PO4:P	2.47	0.72
2:A:1525:ATP:O1G	3:A:1526:PO4:P	2.47	0.72
2:B:1525:ATP:O1A	3:B:1526:PO4:P	2.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1525:PO4:P	2:G:1527:ATP:O1A	2.50	0.70
2:D:1525:ATP:O1A	3:D:1526:PO4:P	2.50	0.70
3:E:1526:PO4:P	2:E:1527:ATP:O1A	2.50	0.70
2:C:1526:ATP:O1A	3:C:1527:PO4:P	2.50	0.69
1:B:198:GLY:HA2	1:B:327:LYS:O	1.93	0.69
3:F:1525:PO4:P	2:F:1527:ATP:O1A	2.49	0.69
1:A:198:GLY:HA2	1:A:327:LYS:O	1.93	0.69
2:A:1525:ATP:O1A	3:A:1526:PO4:P	2.50	0.69
1:E:198:GLY:HA2	1:E:327:LYS:O	1.93	0.69
1:G:198:GLY:HA2	1:G:327:LYS:O	1.93	0.69
1:C:198:GLY:HA2	1:C:327:LYS:O	1.93	0.69
1:E:127:ALA:HB2	1:E:426:LEU:HD11	1.75	0.69
1:L:181:THR:O	1:M:283:ASP:N	2.26	0.69
1:M:181:THR:O	1:N:283:ASP:N	2.26	0.69
1:D:198:GLY:HA2	1:D:327:LYS:O	1.93	0.68
1:F:127:ALA:HB2	1:F:426:LEU:HD11	1.75	0.68
1:C:127:ALA:HB2	1:C:426:LEU:HD11	1.75	0.68
1:F:138:CYS:N	1:F:410:GLY:HA2	2.09	0.68
1:G:138:CYS:N	1:G:410:GLY:HA2	2.09	0.68
1:E:138:CYS:N	1:E:410:GLY:HA2	2.08	0.68
1:I:181:THR:O	1:J:283:ASP:N	2.26	0.68
1:A:138:CYS:N	1:A:410:GLY:HA2	2.09	0.68
1:D:127:ALA:HB2	1:D:426:LEU:HD11	1.76	0.68
1:D:138:CYS:N	1:D:410:GLY:HA2	2.09	0.68
1:C:138:CYS:N	1:C:410:GLY:HA2	2.09	0.68
1:F:198:GLY:HA2	1:F:327:LYS:O	1.93	0.68
1:J:181:THR:O	1:K:283:ASP:N	2.26	0.68
1:B:138:CYS:N	1:B:410:GLY:HA2	2.08	0.68
1:G:127:ALA:HB2	1:G:426:LEU:HD11	1.75	0.67
1:E:191:GLU:O	1:E:334:ASP:HA	1.95	0.67
1:K:181:THR:O	1:L:283:ASP:N	2.26	0.67
1:D:191:GLU:O	1:D:334:ASP:HA	1.95	0.67
1:B:127:ALA:HB2	1:B:426:LEU:HD11	1.75	0.67
1:H:283:ASP:N	1:N:181:THR:O	2.26	0.67
1:A:127:ALA:HB2	1:A:426:LEU:HD11	1.75	0.67
1:F:191:GLU:O	1:F:334:ASP:HA	1.95	0.67
1:H:181:THR:O	1:I:283:ASP:N	2.26	0.67
1:C:191:GLU:O	1:C:334:ASP:HA	1.95	0.67
1:G:214:GLU:HA	1:G:323:VAL:O	1.95	0.66
1:E:214:GLU:HA	1:E:323:VAL:O	1.95	0.66
1:B:214:GLU:HA	1:B:323:VAL:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:GLU:O	1:G:334:ASP:HA	1.95	0.66
1:A:214:GLU:HA	1:A:323:VAL:O	1.95	0.66
1:D:27:VAL:HG12	1:D:90:THR:CG2	2.25	0.66
1:D:214:GLU:HA	1:D:323:VAL:O	1.95	0.66
1:K:223:ALA:O	1:K:251:ALA:HA	1.96	0.66
1:A:138:CYS:CB	1:A:407:VAL:HA	2.26	0.66
1:C:214:GLU:HA	1:C:323:VAL:O	1.95	0.66
1:I:223:ALA:O	1:I:251:ALA:HA	1.96	0.66
1:B:138:CYS:CB	1:B:407:VAL:HA	2.26	0.65
1:D:138:CYS:CB	1:D:407:VAL:HA	2.26	0.65
1:E:27:VAL:HG12	1:E:90:THR:CG2	2.25	0.65
1:F:138:CYS:CB	1:F:407:VAL:HA	2.26	0.65
1:L:223:ALA:O	1:L:251:ALA:HA	1.96	0.65
1:M:223:ALA:O	1:M:251:ALA:HA	1.96	0.65
1:J:223:ALA:O	1:J:251:ALA:HA	1.96	0.65
1:B:191:GLU:O	1:B:334:ASP:HA	1.95	0.65
1:E:138:CYS:CB	1:E:407:VAL:HA	2.26	0.65
1:A:191:GLU:O	1:A:334:ASP:HA	1.95	0.65
1:F:214:GLU:HA	1:F:323:VAL:O	1.95	0.65
1:C:138:CYS:CB	1:C:407:VAL:HA	2.26	0.65
1:F:27:VAL:HG12	1:F:90:THR:CG2	2.25	0.65
1:N:223:ALA:O	1:N:251:ALA:HA	1.96	0.65
1:H:223:ALA:O	1:H:251:ALA:HA	1.96	0.65
1:G:138:CYS:CB	1:G:407:VAL:HA	2.26	0.64
1:E:138:CYS:HB2	1:E:407:VAL:HA	1.81	0.63
1:D:138:CYS:HB2	1:D:407:VAL:HA	1.81	0.63
1:G:27:VAL:HG12	1:G:90:THR:CG2	2.25	0.63
1:B:31:LEU:HB3	1:B:90:THR:HG21	1.81	0.62
1:A:31:LEU:HB3	1:A:90:THR:HG21	1.81	0.62
1:C:31:LEU:HB3	1:C:90:THR:HG21	1.81	0.62
1:D:31:LEU:HB3	1:D:90:THR:HG21	1.81	0.62
1:F:138:CYS:HB2	1:F:407:VAL:HA	1.81	0.62
1:C:138:CYS:HB2	1:C:407:VAL:HA	1.81	0.62
1:B:138:CYS:HB2	1:B:407:VAL:HA	1.81	0.62
1:E:31:LEU:HB3	1:E:90:THR:HG21	1.81	0.62
1:G:31:LEU:HB3	1:G:90:THR:HG21	1.82	0.62
1:K:400:LEU:C	1:K:401:HIS:CA	2.73	0.62
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.82	0.62
1:F:31:LEU:HB3	1:F:90:THR:HG21	1.81	0.62
1:G:138:CYS:HB2	1:G:407:VAL:HA	1.81	0.61
1:H:2:ALA:CA	1:H:2:ALA:O	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.82	0.61
1:A:138:CYS:HB2	1:A:407:VAL:HA	1.81	0.61
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.82	0.61
1:A:27:VAL:HG12	1:A:90:THR:CG2	2.25	0.61
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.82	0.60
1:C:180:GLY:HA2	1:C:380:LYS:HB3	1.82	0.60
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.84	0.60
1:G:417:VAL:HG21	1:G:477:GLY:HA3	1.84	0.60
1:F:180:GLY:HA2	1:F:380:LYS:HB3	1.82	0.60
1:B:417:VAL:HG21	1:B:477:GLY:HA3	1.84	0.60
1:C:27:VAL:HG12	1:C:90:THR:CG2	2.25	0.60
1:D:417:VAL:HG21	1:D:477:GLY:HA3	1.84	0.59
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.82	0.59
1:A:60:ILE:HD12	1:G:6:VAL:HG11	1.85	0.59
1:F:6:VAL:HG11	1:G:60:ILE:HD12	1.85	0.59
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.84	0.59
1:E:6:VAL:HG11	1:F:60:ILE:HD12	1.85	0.59
1:E:417:VAL:HG21	1:E:477:GLY:HA3	1.84	0.59
1:B:27:VAL:HG12	1:B:90:THR:CG2	2.25	0.59
1:C:417:VAL:HG21	1:C:477:GLY:HA3	1.84	0.59
1:A:6:VAL:HG11	1:B:60:ILE:HD12	1.85	0.59
1:D:6:VAL:HG11	1:E:60:ILE:HD12	1.85	0.58
1:A:149:THR:HA	1:A:152:ALA:HB3	1.85	0.58
1:B:149:THR:HA	1:B:152:ALA:HB3	1.85	0.58
1:F:426:LEU:HB2	1:F:444:LEU:HD22	1.86	0.58
1:B:6:VAL:HG11	1:C:60:ILE:HD12	1.85	0.58
1:G:149:THR:HA	1:G:152:ALA:HB3	1.85	0.58
1:C:6:VAL:HG11	1:D:60:ILE:HD12	1.85	0.58
1:C:149:THR:HA	1:C:152:ALA:HB3	1.85	0.58
1:E:426:LEU:HB2	1:E:444:LEU:HD22	1.86	0.58
1:C:426:LEU:HB2	1:C:444:LEU:HD22	1.86	0.58
1:D:426:LEU:HB2	1:D:444:LEU:HD22	1.86	0.58
1:E:149:THR:HA	1:E:152:ALA:HB3	1.85	0.57
1:E:151:SER:HB3	1:E:399:ALA:HA	1.87	0.57
1:G:426:LEU:HB2	1:G:444:LEU:HD22	1.86	0.57
1:D:149:THR:HA	1:D:152:ALA:HB3	1.85	0.57
1:E:151:SER:CB	1:E:399:ALA:HA	2.34	0.57
1:F:149:THR:HA	1:F:152:ALA:HB3	1.85	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:D:151:SER:CB	1:D:399:ALA:HA	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:LEU:HB2	1:B:444:LEU:HD22	1.86	0.57
1:F:151:SER:CB	1:F:399:ALA:HA	2.35	0.57
1:G:151:SER:CB	1:G:399:ALA:HA	2.35	0.57
1:A:426:LEU:HB2	1:A:444:LEU:HD22	1.86	0.57
1:L:229:ASN:HA	1:L:258:ALA:HB3	1.87	0.57
1:D:151:SER:HB3	1:D:399:ALA:HA	1.87	0.57
1:F:151:SER:HB3	1:F:399:ALA:HA	1.87	0.57
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.86	0.56
1:C:151:SER:HB3	1:C:399:ALA:HA	1.87	0.56
1:G:151:SER:HB3	1:G:399:ALA:HA	1.87	0.56
1:A:151:SER:CB	1:A:399:ALA:HA	2.35	0.56
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.86	0.56
1:B:151:SER:HB3	1:B:399:ALA:HA	1.87	0.56
1:C:151:SER:CB	1:C:399:ALA:HA	2.35	0.56
1:J:229:ASN:HA	1:J:258:ALA:HB3	1.87	0.56
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.86	0.56
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.86	0.56
1:N:229:ASN:HA	1:N:258:ALA:HB3	1.88	0.56
1:A:151:SER:HB3	1:A:399:ALA:HA	1.87	0.56
1:B:212:ALA:HA	1:B:325:ILE:O	2.06	0.56
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.86	0.56
1:B:151:SER:CB	1:B:399:ALA:HA	2.35	0.56
1:D:172:GLU:CD	1:D:172:GLU:H	2.14	0.56
1:G:212:ALA:HA	1:G:325:ILE:O	2.07	0.55
1:E:172:GLU:CD	1:E:172:GLU:H	2.14	0.55
1:E:212:ALA:HA	1:E:325:ILE:O	2.06	0.55
1:D:212:ALA:HA	1:D:325:ILE:O	2.06	0.55
1:G:218:PRO:HG2	1:G:320:ALA:HB3	1.89	0.55
1:M:229:ASN:HA	1:M:258:ALA:HB3	1.89	0.55
1:A:427:ALA:HA	1:A:444:LEU:HD11	1.89	0.55
1:C:217:SER:HA	1:C:320:ALA:O	2.07	0.55
1:C:218:PRO:HG2	1:C:320:ALA:HB3	1.89	0.55
1:D:218:PRO:HG2	1:D:320:ALA:HB3	1.89	0.55
1:H:25:ASP:CG	1:H:28:LYS:HZ3	2.15	0.55
1:A:212:ALA:HA	1:A:325:ILE:O	2.06	0.55
1:F:212:ALA:HA	1:F:325:ILE:O	2.06	0.55
1:F:218:PRO:HG2	1:F:320:ALA:HB3	1.89	0.55
1:G:217:SER:HA	1:G:320:ALA:O	2.07	0.55
1:C:172:GLU:CD	1:C:172:GLU:H	2.14	0.55
2:A:1525:ATP:O3B	3:A:1526:PO4:P	2.66	0.55
1:C:212:ALA:HA	1:C:325:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:ALA:HA	1:D:444:LEU:HD11	1.89	0.55
1:D:31:LEU:CB	1:D:90:THR:HG21	2.37	0.54
1:E:427:ALA:HA	1:E:444:LEU:HD11	1.89	0.54
1:B:218:PRO:HG2	1:B:320:ALA:HB3	1.89	0.54
1:B:427:ALA:HA	1:B:444:LEU:HD11	1.89	0.54
1:D:217:SER:HA	1:D:320:ALA:O	2.07	0.54
1:E:31:LEU:CB	1:E:90:THR:HG21	2.37	0.54
1:E:247:LEU:O	1:E:273:VAL:HA	2.07	0.54
1:G:427:ALA:HA	1:G:444:LEU:HD11	1.89	0.54
1:A:218:PRO:HG2	1:A:320:ALA:HB3	1.89	0.54
1:E:218:PRO:HG2	1:E:320:ALA:HB3	1.89	0.54
3:F:1525:PO4:P	2:F:1527:ATP:O3B	2.66	0.54
1:K:229:ASN:HA	1:K:258:ALA:HB3	1.90	0.54
1:A:172:GLU:H	1:A:172:GLU:CD	2.14	0.54
2:B:1525:ATP:O3B	3:B:1526:PO4:P	2.66	0.54
1:C:31:LEU:CB	1:C:90:THR:HG21	2.38	0.54
1:D:523:ASP:H	1:E:43:SER:HB3	1.73	0.54
1:H:229:ASN:HA	1:H:258:ALA:HB3	1.89	0.54
1:A:247:LEU:O	1:A:273:VAL:HA	2.07	0.54
1:B:247:LEU:O	1:B:273:VAL:HA	2.08	0.54
2:C:1526:ATP:O3B	3:C:1527:PO4:P	2.66	0.54
3:E:1526:PO4:P	2:E:1527:ATP:O3B	2.66	0.54
1:F:31:LEU:CB	1:F:90:THR:HG21	2.37	0.54
1:I:229:ASN:HA	1:I:258:ALA:HB3	1.89	0.54
1:A:217:SER:HA	1:A:320:ALA:O	2.07	0.54
1:A:523:ASP:H	1:B:43:SER:HB3	1.73	0.54
1:B:172:GLU:CD	1:B:172:GLU:H	2.14	0.54
1:E:217:SER:HA	1:E:320:ALA:O	2.07	0.54
1:F:217:SER:HA	1:F:320:ALA:O	2.07	0.54
1:B:31:LEU:CB	1:B:90:THR:HG21	2.37	0.54
1:G:172:GLU:CD	1:G:172:GLU:H	2.14	0.54
1:B:523:ASP:H	1:C:43:SER:HB3	1.73	0.54
3:G:1525:PO4:P	2:G:1527:ATP:O3B	2.66	0.54
1:B:217:SER:HA	1:B:320:ALA:O	2.07	0.53
1:D:247:LEU:O	1:D:273:VAL:HA	2.08	0.53
1:F:247:LEU:O	1:F:273:VAL:HA	2.08	0.53
1:A:31:LEU:CB	1:A:90:THR:HG21	2.38	0.53
2:D:1525:ATP:O3B	3:D:1526:PO4:P	2.65	0.53
1:C:130:GLU:HB3	1:C:422:VAL:HG12	1.91	0.53
1:C:427:ALA:HA	1:C:444:LEU:HD11	1.89	0.53
1:F:427:ALA:HA	1:F:444:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:LEU:O	1:C:273:VAL:HA	2.07	0.53
1:G:31:LEU:CB	1:G:90:THR:HG21	2.38	0.53
1:D:130:GLU:HB3	1:D:422:VAL:HG12	1.91	0.53
1:E:523:ASP:H	1:F:43:SER:HB3	1.74	0.53
1:F:172:GLU:H	1:F:172:GLU:CD	2.14	0.53
1:G:247:LEU:O	1:G:273:VAL:HA	2.08	0.53
1:A:43:SER:HB3	1:G:523:ASP:H	1.74	0.53
1:A:411:VAL:HB	1:A:494:LEU:HB2	1.91	0.53
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:C:523:ASP:H	1:D:43:SER:HB3	1.73	0.52
1:B:130:GLU:HB3	1:B:422:VAL:HG12	1.91	0.52
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.40	0.52
1:E:130:GLU:HB3	1:E:422:VAL:HG12	1.91	0.52
1:B:6:VAL:HG13	1:B:521:VAL:HG22	1.92	0.52
1:F:411:VAL:HB	1:F:494:LEU:HB2	1.91	0.52
1:F:523:ASP:H	1:G:43:SER:HB3	1.74	0.52
1:D:6:VAL:HG13	1:D:521:VAL:HG22	1.92	0.52
1:C:31:LEU:HA	3:C:1527:PO4:P	2.50	0.52
1:D:144:ILE:HG23	1:D:403:THR:CG2	2.40	0.52
1:G:31:LEU:HA	3:G:1525:PO4:P	2.50	0.52
1:C:411:VAL:HB	1:C:494:LEU:HB2	1.91	0.52
1:D:411:VAL:HB	1:D:494:LEU:HB2	1.91	0.52
1:G:106:ALA:CB	1:G:116:LEU:HD21	2.40	0.52
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.40	0.52
1:A:31:LEU:HA	3:A:1526:PO4:P	2.50	0.52
1:A:130:GLU:HB3	1:A:422:VAL:HG12	1.91	0.52
1:E:406:ALA:HB2	1:E:496:PRO:HG3	1.92	0.52
1:A:6:VAL:HG13	1:A:521:VAL:HG22	1.92	0.51
1:C:186:GLU:H	1:C:380:LYS:HB2	1.75	0.51
1:D:31:LEU:HA	3:D:1526:PO4:P	2.50	0.51
1:F:130:GLU:HB3	1:F:422:VAL:HG12	1.91	0.51
1:G:411:VAL:HB	1:G:494:LEU:HB2	1.91	0.51
1:B:411:VAL:HB	1:B:494:LEU:HB2	1.91	0.51
1:E:144:ILE:HG23	1:E:403:THR:CG2	2.40	0.51
1:F:106:ALA:CB	1:F:116:LEU:HD21	2.40	0.51
1:F:406:ALA:HB2	1:F:496:PRO:HG3	1.93	0.51
1:G:130:GLU:HB3	1:G:422:VAL:HG12	1.91	0.51
1:A:106:ALA:CB	1:A:116:LEU:HD21	2.40	0.51
1:E:6:VAL:HG13	1:E:521:VAL:HG22	1.92	0.51
1:F:31:LEU:HA	3:F:1525:PO4:P	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HA	3:B:1526:PO4:P	2.50	0.51
1:B:186:GLU:H	1:B:380:LYS:HB2	1.75	0.51
1:G:406:ALA:HB2	1:G:496:PRO:HG3	1.92	0.51
1:E:411:VAL:HB	1:E:494:LEU:HB2	1.91	0.51
1:E:31:LEU:HA	3:E:1526:PO4:P	2.50	0.51
1:A:205:ILE:HD12	1:A:211:GLY:O	2.10	0.51
1:C:205:ILE:HD12	1:C:211:GLY:O	2.10	0.51
1:G:186:GLU:H	1:G:380:LYS:HB2	1.75	0.51
1:B:205:ILE:HD12	1:B:211:GLY:O	2.10	0.51
1:C:106:ALA:CB	1:C:116:LEU:HD21	2.40	0.51
1:E:106:ALA:CB	1:E:116:LEU:HD21	2.40	0.51
1:F:186:GLU:H	1:F:380:LYS:HB2	1.76	0.51
1:G:205:ILE:HD12	1:G:211:GLY:O	2.10	0.51
1:B:106:ALA:CB	1:B:116:LEU:HD21	2.40	0.51
1:B:406:ALA:HB2	1:B:496:PRO:HG3	1.93	0.51
1:C:463:SER:OG	1:J:464:VAL:HG22	2.11	0.51
1:D:106:ALA:CB	1:D:116:LEU:HD21	2.40	0.51
1:D:205:ILE:HD12	1:D:211:GLY:O	2.10	0.51
1:E:186:GLU:H	1:E:380:LYS:HB2	1.75	0.51
1:G:463:SER:OG	1:N:464:VAL:HG22	2.11	0.51
1:D:406:ALA:HB2	1:D:496:PRO:HG3	1.92	0.51
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.40	0.51
1:A:463:SER:OG	1:H:464:VAL:HG22	2.11	0.50
1:C:6:VAL:HG13	1:C:521:VAL:HG22	1.92	0.50
1:F:205:ILE:HD12	1:F:211:GLY:O	2.10	0.50
1:G:6:VAL:HG13	1:G:521:VAL:HG22	1.92	0.50
1:D:196:ASP:HA	1:D:329:THR:HA	1.94	0.50
1:D:463:SER:OG	1:K:464:VAL:HG22	2.11	0.50
1:E:196:ASP:HA	1:E:329:THR:HA	1.94	0.50
1:F:196:ASP:HA	1:F:329:THR:HA	1.93	0.50
1:F:6:VAL:HG13	1:F:521:VAL:HG22	1.92	0.50
1:G:152:ALA:HB1	1:G:155:ASP:HB3	1.94	0.50
1:A:152:ALA:HB1	1:A:155:ASP:HB3	1.94	0.50
1:C:196:ASP:HA	1:C:329:THR:HA	1.94	0.50
1:C:406:ALA:HB2	1:C:496:PRO:HG3	1.93	0.50
1:E:205:ILE:HD12	1:E:211:GLY:O	2.10	0.50
1:A:186:GLU:H	1:A:380:LYS:HB2	1.75	0.50
1:D:279:PRO:HG3	1:D:292:ILE:HD11	1.94	0.50
1:A:406:ALA:HB2	1:A:496:PRO:HG3	1.92	0.49
1:E:463:SER:OG	1:L:464:VAL:HG22	2.11	0.49
1:F:463:SER:OG	1:M:464:VAL:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:SER:OG	1:I:464:VAL:HG22	2.11	0.49
1:C:279:PRO:HG3	1:C:292:ILE:HD11	1.94	0.49
1:E:39:VAL:HG22	1:E:49:ILE:HG23	1.95	0.49
1:E:279:PRO:HG3	1:E:292:ILE:HD11	1.94	0.49
1:G:196:ASP:HA	1:G:329:THR:HA	1.94	0.49
1:D:186:GLU:H	1:D:380:LYS:HB2	1.75	0.49
1:B:152:ALA:HB1	1:B:155:ASP:HB3	1.94	0.49
1:C:383:ALA:HB3	1:C:389:MET:HB2	1.95	0.49
1:F:39:VAL:HG22	1:F:49:ILE:HG23	1.95	0.49
1:F:152:ALA:HB1	1:F:155:ASP:HB3	1.94	0.49
1:B:196:ASP:HA	1:B:329:THR:HA	1.94	0.49
1:H:2:ALA:C	1:H:2:ALA:CB	2.76	0.49
1:B:39:VAL:HG22	1:B:49:ILE:HG23	1.95	0.49
1:C:39:VAL:HG22	1:C:49:ILE:HG23	1.95	0.49
1:A:196:ASP:HA	1:A:329:THR:HA	1.94	0.49
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.95	0.49
1:E:124:VAL:HG21	1:E:508:ALA:CB	2.43	0.49
1:G:39:VAL:HG22	1:G:49:ILE:HG23	1.95	0.49
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.43	0.49
1:I:182:GLY:HA2	1:J:284:ARG:HH22	1.78	0.49
1:B:279:PRO:HG3	1:B:292:ILE:HD11	1.94	0.49
1:C:152:ALA:HB1	1:C:155:ASP:HB3	1.94	0.49
1:D:124:VAL:HG21	1:D:508:ALA:CB	2.43	0.49
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.95	0.49
1:G:279:PRO:HG3	1:G:292:ILE:HD11	1.94	0.49
1:K:386:GLU:HA	1:L:281:PHE:CG	2.48	0.49
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.43	0.48
1:E:152:ALA:HB1	1:E:155:ASP:HB3	1.94	0.48
1:D:152:ALA:HB1	1:D:155:ASP:HB3	1.94	0.48
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.43	0.48
1:M:386:GLU:HA	1:N:281:PHE:CG	2.48	0.48
1:A:213:VAL:HG13	1:A:325:ILE:HB	1.96	0.48
1:A:279:PRO:HG3	1:A:292:ILE:HD11	1.94	0.48
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.43	0.48
1:F:279:PRO:HG3	1:F:292:ILE:HD11	1.94	0.48
1:K:182:GLY:HA2	1:L:284:ARG:HH22	1.78	0.48
1:A:39:VAL:HG22	1:A:49:ILE:HG23	1.95	0.48
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.43	0.48
1:D:106:ALA:HB3	1:D:116:LEU:HD21	1.96	0.48
1:G:213:VAL:HG13	1:G:325:ILE:HB	1.96	0.48
1:H:117:LYS:HZ2	1:H:121:ASP:CG	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:182:GLY:HA2	1:N:284:ARG:HH22	1.78	0.48
1:C:106:ALA:HB3	1:C:116:LEU:HD21	1.96	0.48
1:H:386:GLU:HA	1:I:281:PHE:CG	2.49	0.48
1:D:39:VAL:HG22	1:D:49:ILE:HG23	1.95	0.48
1:E:144:ILE:HG23	1:E:403:THR:HG21	1.95	0.48
1:J:386:GLU:HA	1:K:281:PHE:CG	2.48	0.48
1:B:213:VAL:HG13	1:B:325:ILE:HB	1.96	0.48
1:I:386:GLU:HA	1:J:281:PHE:CG	2.49	0.48
1:J:182:GLY:HA2	1:K:284:ARG:HH22	1.78	0.48
1:I:140:ASP:CG	1:I:142:LYS:HZ3	2.22	0.48
1:L:182:GLY:HA2	1:M:284:ARG:HH22	1.78	0.48
1:C:240:VAL:HA	1:C:314:LEU:HD21	1.96	0.47
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.96	0.47
1:G:240:VAL:HA	1:G:314:LEU:HD21	1.96	0.47
1:H:182:GLY:HA2	1:I:284:ARG:HH22	1.78	0.47
1:H:281:PHE:CG	1:N:386:GLU:HA	2.49	0.47
1:H:284:ARG:HH22	1:N:182:GLY:HA2	1.78	0.47
1:A:240:VAL:HA	1:A:314:LEU:HD21	1.97	0.47
1:B:144:ILE:HG23	1:B:403:THR:HG21	1.95	0.47
1:C:40:LEU:HD11	1:C:55:SER:HB3	1.96	0.47
1:D:240:VAL:HA	1:D:314:LEU:HD21	1.96	0.47
1:F:144:ILE:HG23	1:F:403:THR:HG21	1.96	0.47
1:J:117:LYS:HZ2	1:J:121:ASP:CG	2.22	0.47
1:A:144:ILE:HG23	1:A:403:THR:HG21	1.96	0.47
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.95	0.47
1:B:240:VAL:HA	1:B:314:LEU:HD21	1.96	0.47
1:F:213:VAL:HG13	1:F:325:ILE:HB	1.96	0.47
1:F:383:ALA:HB3	1:F:389:MET:HB2	1.95	0.47
1:I:117:LYS:HZ2	1:I:121:ASP:CG	2.22	0.47
1:L:386:GLU:HA	1:M:281:PHE:CG	2.49	0.47
1:N:230:ILE:HG23	1:N:259:LEU:HD12	1.96	0.47
1:N:117:LYS:HZ2	1:N:121:ASP:CG	2.23	0.47
1:E:40:LEU:HD11	1:E:55:SER:HB3	1.96	0.47
1:E:106:ALA:HB3	1:E:116:LEU:HD21	1.96	0.47
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.95	0.47
1:D:40:LEU:HD11	1:D:55:SER:HB3	1.96	0.47
1:F:240:VAL:HA	1:F:314:LEU:HD21	1.97	0.47
1:C:213:VAL:HG13	1:C:325:ILE:HB	1.96	0.47
1:E:213:VAL:HG13	1:E:325:ILE:HB	1.96	0.47
1:E:240:VAL:HA	1:E:314:LEU:HD21	1.96	0.47
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:320:ALA:HA	1:K:334:ASP:O	2.15	0.47
1:M:117:LYS:HZ2	1:M:121:ASP:CG	2.22	0.47
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.95	0.47
1:J:320:ALA:HA	1:J:334:ASP:O	2.15	0.47
1:L:320:ALA:HA	1:L:334:ASP:O	2.15	0.47
1:M:320:ALA:HA	1:M:334:ASP:O	2.15	0.47
1:B:106:ALA:HB3	1:B:116:LEU:HD21	1.96	0.47
1:B:113:PRO:HD2	1:C:36:ARG:HD2	1.97	0.47
1:C:144:ILE:HG23	1:C:403:THR:HG21	1.96	0.47
1:D:213:VAL:HG13	1:D:325:ILE:HB	1.96	0.47
1:H:320:ALA:HA	1:H:334:ASP:O	2.15	0.47
1:I:320:ALA:HA	1:I:334:ASP:O	2.15	0.47
1:C:113:PRO:HD2	1:D:36:ARG:HD2	1.97	0.47
1:D:417:VAL:HG13	1:D:476:TYR:O	2.15	0.47
1:G:106:ALA:HB3	1:G:116:LEU:HD21	1.96	0.47
1:N:320:ALA:HA	1:N:334:ASP:O	2.15	0.47
1:N:479:ASN:O	1:N:483:GLU:N	2.48	0.47
1:B:40:LEU:HD11	1:B:55:SER:HB3	1.96	0.46
1:J:230:ILE:HG23	1:J:259:LEU:HD12	1.97	0.46
1:B:158:VAL:HG22	1:B:396:VAL:HG22	1.97	0.46
1:E:417:VAL:HG13	1:E:476:TYR:O	2.15	0.46
1:K:183:LEU:HA	1:K:383:ALA:O	2.15	0.46
1:K:400:LEU:CA	1:K:401:HIS:N	2.72	0.46
1:L:183:LEU:HA	1:L:383:ALA:O	2.15	0.46
1:L:230:ILE:HG23	1:L:259:LEU:HD12	1.97	0.46
1:A:113:PRO:HD2	1:B:36:ARG:HD2	1.97	0.46
1:C:226:LYS:HA	1:C:253:ASP:O	2.16	0.46
1:F:180:GLY:HA3	1:F:381:VAL:O	2.16	0.46
1:M:183:LEU:HA	1:M:383:ALA:O	2.15	0.46
1:A:66:PHE:CZ	1:A:522:THR:HG22	2.50	0.46
1:B:417:VAL:HG13	1:B:476:TYR:O	2.15	0.46
1:D:66:PHE:CZ	1:D:522:THR:HG22	2.51	0.46
1:D:113:PRO:HD2	1:E:36:ARG:HD2	1.97	0.46
1:J:183:LEU:HA	1:J:383:ALA:O	2.15	0.46
1:A:417:VAL:HG13	1:A:476:TYR:O	2.15	0.46
1:F:287:ALA:HB1	1:F:368:ARG:CZ	2.46	0.46
1:G:180:GLY:HA3	1:G:381:VAL:O	2.16	0.46
1:G:287:ALA:HB1	1:G:368:ARG:CZ	2.46	0.46
1:H:140:ASP:CG	1:H:142:LYS:HZ3	2.22	0.46
1:H:183:LEU:HA	1:H:383:ALA:O	2.16	0.46
1:M:398:ALA:O	1:M:401:HIS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:479:ASN:O	1:M:483:GLU:N	2.48	0.46
1:N:34:LYS:HZ3	1:N:483:GLU:CD	2.22	0.46
1:N:183:LEU:HA	1:N:383:ALA:O	2.15	0.46
1:E:66:PHE:CZ	1:E:522:THR:HG22	2.51	0.46
1:E:180:GLY:HA3	1:E:381:VAL:O	2.16	0.46
1:F:40:LEU:HD11	1:F:55:SER:HB3	1.97	0.46
1:F:417:VAL:HG13	1:F:476:TYR:O	2.15	0.46
1:F:520:MET:HA	1:G:41:ASP:HB2	1.97	0.46
1:H:2:ALA:O	1:H:3:ALA:C	2.58	0.46
1:N:2:ALA:O	1:N:3:ALA:C	2.59	0.46
1:A:180:GLY:HA3	1:A:381:VAL:O	2.16	0.46
1:C:158:VAL:HG22	1:C:396:VAL:HG22	1.97	0.46
1:C:520:MET:HA	1:D:41:ASP:HB2	1.97	0.46
1:E:356:ALA:HB1	1:E:361:ASP:HB2	1.98	0.46
1:F:106:ALA:HB3	1:F:116:LEU:HD21	1.96	0.46
1:G:356:ALA:HB1	1:G:361:ASP:HB2	1.98	0.46
1:K:117:LYS:HZ2	1:K:121:ASP:CG	2.23	0.46
1:L:2:ALA:O	1:L:3:ALA:C	2.59	0.46
1:A:158:VAL:HG22	1:A:396:VAL:HG22	1.97	0.46
1:A:287:ALA:HB1	1:A:368:ARG:CZ	2.46	0.46
1:C:180:GLY:HA3	1:C:381:VAL:O	2.16	0.46
1:C:287:ALA:HB1	1:C:368:ARG:CZ	2.46	0.46
1:C:417:VAL:HG13	1:C:476:TYR:O	2.15	0.46
1:F:158:VAL:HG22	1:F:396:VAL:HG22	1.97	0.46
1:A:106:ALA:HB3	1:A:116:LEU:HD21	1.96	0.46
1:A:356:ALA:HB1	1:A:361:ASP:HB2	1.98	0.46
1:D:356:ALA:HB1	1:D:361:ASP:HB2	1.98	0.46
1:K:414:GLY:N	1:K:494:LEU:HA	2.31	0.46
1:B:66:PHE:CZ	1:B:522:THR:HG22	2.50	0.46
1:B:226:LYS:HA	1:B:253:ASP:O	2.15	0.46
1:B:287:ALA:HB1	1:B:368:ARG:CZ	2.46	0.46
1:B:520:MET:HA	1:C:41:ASP:HB2	1.97	0.46
1:E:520:MET:HA	1:F:41:ASP:HB2	1.97	0.46
1:I:414:GLY:N	1:I:494:LEU:HA	2.31	0.46
1:L:117:LYS:HZ2	1:L:121:ASP:CG	2.24	0.46
1:A:226:LYS:HA	1:A:253:ASP:O	2.16	0.45
1:D:287:ALA:HB1	1:D:368:ARG:CZ	2.46	0.45
1:E:113:PRO:HD2	1:F:36:ARG:HD2	1.97	0.45
1:H:414:GLY:N	1:H:494:LEU:HA	2.31	0.45
1:I:246:PRO:HB3	1:I:272:LYS:HB2	1.99	0.45
1:A:36:ARG:HD2	1:G:113:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ILE:O	1:D:124:VAL:HG23	2.17	0.45
1:D:520:MET:HA	1:E:41:ASP:HB2	1.97	0.45
1:E:120:ILE:O	1:E:124:VAL:HG23	2.17	0.45
1:F:356:ALA:HB1	1:F:361:ASP:HB2	1.98	0.45
1:G:417:VAL:HG13	1:G:476:TYR:O	2.15	0.45
1:H:246:PRO:HB3	1:H:272:LYS:HB2	1.99	0.45
1:J:2:ALA:O	1:J:3:ALA:C	2.59	0.45
1:J:149:THR:CG2	1:J:156:GLU:HA	2.47	0.45
1:J:246:PRO:HB3	1:J:272:LYS:HB2	1.99	0.45
1:M:414:GLY:N	1:M:494:LEU:HA	2.31	0.45
1:B:120:ILE:O	1:B:124:VAL:HG23	2.17	0.45
1:B:206:ASN:HB2	1:B:213:VAL:HA	1.98	0.45
1:C:120:ILE:O	1:C:124:VAL:HG23	2.17	0.45
1:C:356:ALA:HB1	1:C:361:ASP:HB2	1.98	0.45
1:G:40:LEU:HD11	1:G:55:SER:HB3	1.96	0.45
1:N:246:PRO:HB3	1:N:272:LYS:HB2	1.99	0.45
1:N:414:GLY:N	1:N:494:LEU:HA	2.31	0.45
1:A:40:LEU:HD11	1:A:55:SER:HB3	1.96	0.45
1:A:41:ASP:HB2	1:G:520:MET:HA	1.97	0.45
1:B:356:ALA:HB1	1:B:361:ASP:HB2	1.98	0.45
1:C:206:ASN:HB2	1:C:213:VAL:HA	1.98	0.45
1:D:180:GLY:HA3	1:D:381:VAL:O	2.15	0.45
1:E:287:ALA:HB1	1:E:368:ARG:CZ	2.46	0.45
1:I:2:ALA:O	1:I:3:ALA:C	2.59	0.45
1:J:479:ASN:O	1:J:483:GLU:N	2.48	0.45
1:K:271:VAL:HG12	1:K:272:LYS:H	1.82	0.45
1:L:149:THR:CG2	1:L:156:GLU:HA	2.47	0.45
1:M:217:SER:HA	1:M:320:ALA:O	2.16	0.45
1:N:217:SER:HA	1:N:320:ALA:O	2.16	0.45
1:A:120:ILE:O	1:A:124:VAL:HG23	2.17	0.45
1:A:206:ASN:HB2	1:A:213:VAL:HA	1.99	0.45
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.33	0.45
1:E:158:VAL:HG22	1:E:396:VAL:HG22	1.97	0.45
1:F:66:PHE:CZ	1:F:522:THR:HG22	2.51	0.45
1:F:113:PRO:HD2	1:G:36:ARG:HD2	1.97	0.45
1:I:217:SER:HA	1:I:320:ALA:O	2.17	0.45
1:B:112:ASN:HA	1:B:113:PRO:HD2	1.88	0.45
1:F:226:LYS:HA	1:F:253:ASP:O	2.16	0.45
1:G:158:VAL:HG22	1:G:396:VAL:HG22	1.97	0.45
1:G:206:ASN:HB2	1:G:213:VAL:HA	1.98	0.45
1:I:183:LEU:HA	1:I:383:ALA:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:479:ASN:O	1:K:483:GLU:N	2.48	0.45
1:F:120:ILE:O	1:F:124:VAL:HG23	2.17	0.45
1:G:66:PHE:CZ	1:G:522:THR:HG22	2.51	0.45
1:I:479:ASN:O	1:I:483:GLU:N	2.49	0.45
1:J:217:SER:HA	1:J:320:ALA:O	2.16	0.45
1:K:149:THR:CG2	1:K:156:GLU:HA	2.47	0.45
1:B:180:GLY:HA3	1:B:381:VAL:O	2.16	0.45
1:C:34:LYS:HZ1	1:C:483:GLU:CD	2.25	0.45
1:C:66:PHE:CZ	1:C:522:THR:HG22	2.50	0.45
1:K:246:PRO:HB3	1:K:272:LYS:HB2	1.99	0.45
1:L:414:GLY:N	1:L:494:LEU:HA	2.31	0.45
1:M:246:PRO:HB3	1:M:272:LYS:HB2	1.99	0.45
1:N:271:VAL:HG12	1:N:272:LYS:H	1.82	0.45
1:A:244:GLY:O	1:G:257:GLU:HB3	2.17	0.45
1:A:257:GLU:HB3	1:B:244:GLY:O	2.17	0.45
1:B:257:GLU:HB3	1:C:244:GLY:O	2.17	0.45
1:D:257:GLU:HB3	1:E:244:GLY:O	2.17	0.45
1:G:120:ILE:O	1:G:124:VAL:HG23	2.17	0.45
1:G:183:LEU:C	1:G:382:GLY:HA3	2.42	0.45
1:G:226:LYS:HA	1:G:253:ASP:O	2.16	0.45
1:H:149:THR:CG2	1:H:156:GLU:HA	2.46	0.45
1:A:183:LEU:C	1:A:382:GLY:HA3	2.42	0.45
1:E:226:LYS:HA	1:E:253:ASP:O	2.16	0.45
1:E:257:GLU:HB3	1:F:244:GLY:O	2.17	0.45
1:H:217:SER:HA	1:H:320:ALA:O	2.16	0.45
1:I:149:THR:CG2	1:I:156:GLU:HA	2.47	0.45
1:M:271:VAL:HG12	1:M:272:LYS:H	1.82	0.45
1:A:190:VAL:HG11	1:A:333:ILE:HG23	2.00	0.44
1:A:520:MET:HA	1:B:41:ASP:HB2	1.97	0.44
1:B:190:VAL:HG11	1:B:333:ILE:HG23	2.00	0.44
1:D:226:LYS:HA	1:D:253:ASP:O	2.16	0.44
1:D:293:ALA:HB2	1:D:300:VAL:CG2	2.47	0.44
1:D:461:GLU:HA	1:D:462:PRO:HD2	1.78	0.44
1:E:293:ALA:HB2	1:E:300:VAL:CG2	2.48	0.44
1:F:206:ASN:HB2	1:F:213:VAL:HA	1.98	0.44
1:F:257:GLU:HB3	1:G:244:GLY:O	2.17	0.44
1:F:293:ALA:HB2	1:F:300:VAL:CG2	2.47	0.44
1:K:2:ALA:O	1:K:3:ALA:C	2.58	0.44
1:L:246:PRO:HB3	1:L:272:LYS:HB2	1.99	0.44
1:M:149:THR:CG2	1:M:156:GLU:HA	2.46	0.44
1:M:417:VAL:HA	1:M:420:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:8:PHE:HA	1:N:518:GLU:O	2.18	0.44
1:A:293:ALA:HB2	1:A:300:VAL:CG2	2.47	0.44
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.33	0.44
1:G:293:ALA:HB2	1:G:300:VAL:CG2	2.48	0.44
1:J:414:GLY:N	1:J:494:LEU:HA	2.31	0.44
1:J:8:PHE:HA	1:J:518:GLU:O	2.18	0.44
1:K:8:PHE:HA	1:K:518:GLU:O	2.18	0.44
1:N:417:VAL:HA	1:N:420:ILE:HG22	2.00	0.44
1:C:190:VAL:HG11	1:C:333:ILE:HG23	2.00	0.44
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.33	0.44
1:D:206:ASN:HB2	1:D:213:VAL:HA	1.99	0.44
1:D:349:ILE:HG22	1:D:369:VAL:HG13	1.99	0.44
1:G:338:GLU:CD	1:G:341:ALA:HB2	2.43	0.44
1:H:8:PHE:HA	1:H:518:GLU:O	2.18	0.44
1:H:479:ASN:O	1:H:483:GLU:N	2.48	0.44
1:J:191:GLU:O	1:J:334:ASP:HA	2.18	0.44
1:L:8:PHE:HA	1:L:518:GLU:O	2.18	0.44
1:M:8:PHE:HA	1:M:518:GLU:O	2.18	0.44
1:N:149:THR:CG2	1:N:156:GLU:HA	2.47	0.44
1:A:338:GLU:CD	1:A:341:ALA:HB2	2.43	0.44
1:C:412:VAL:HG22	1:C:495:ASP:O	2.18	0.44
1:D:158:VAL:HG22	1:D:396:VAL:HG22	1.97	0.44
1:E:206:ASN:HB2	1:E:213:VAL:HA	1.98	0.44
1:K:217:SER:HA	1:K:320:ALA:O	2.16	0.44
1:B:338:GLU:CD	1:B:341:ALA:HB2	2.43	0.44
1:D:190:VAL:HG11	1:D:333:ILE:HG23	1.99	0.44
1:F:338:GLU:CD	1:F:341:ALA:HB2	2.43	0.44
1:G:190:VAL:HG11	1:G:333:ILE:HG23	2.00	0.44
1:I:8:PHE:HA	1:I:518:GLU:O	2.18	0.44
1:I:191:GLU:O	1:I:334:ASP:HA	2.18	0.44
1:B:293:ALA:HB2	1:B:300:VAL:CG2	2.48	0.44
1:C:152:ALA:HB1	1:C:155:ASP:CA	2.48	0.44
1:D:23:LEU:O	1:D:27:VAL:HG23	2.18	0.44
1:D:111:MET:O	1:D:113:PRO:HD3	2.18	0.44
1:D:152:ALA:HB1	1:D:155:ASP:CA	2.48	0.44
1:D:412:VAL:HG22	1:D:495:ASP:O	2.18	0.44
1:E:199:TYR:CE2	1:E:327:LYS:HB3	2.53	0.44
1:L:217:SER:HA	1:L:320:ALA:O	2.17	0.44
1:N:2:ALA:N	1:N:2:ALA:CB	2.74	0.44
1:C:23:LEU:O	1:C:27:VAL:HG23	2.18	0.44
1:C:338:GLU:CD	1:C:341:ALA:HB2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:VAL:HG22	1:E:495:ASP:O	2.18	0.44
1:F:349:ILE:HG22	1:F:369:VAL:HG13	1.99	0.44
1:G:199:TYR:CE2	1:G:327:LYS:HB3	2.53	0.44
1:I:34:LYS:HZ3	1:I:483:GLU:CD	2.25	0.44
1:L:417:VAL:HA	1:L:420:ILE:HG22	2.00	0.44
1:L:479:ASN:O	1:L:483:GLU:N	2.49	0.44
1:B:6:VAL:HG11	1:C:60:ILE:CD1	2.48	0.43
1:B:111:MET:O	1:B:113:PRO:HD3	2.18	0.43
1:B:183:LEU:C	1:B:382:GLY:HA3	2.42	0.43
1:B:412:VAL:HG22	1:B:495:ASP:O	2.18	0.43
1:C:183:LEU:C	1:C:382:GLY:HA3	2.42	0.43
1:E:34:LYS:HZ1	1:E:483:GLU:CD	2.26	0.43
1:E:111:MET:O	1:E:113:PRO:HD3	2.18	0.43
1:E:294:THR:HG21	1:E:345:ARG:HG3	2.00	0.43
1:F:111:MET:O	1:F:113:PRO:HD3	2.18	0.43
1:G:349:ILE:HG22	1:G:369:VAL:HG13	1.99	0.43
1:D:127:ALA:CB	1:D:426:LEU:HD11	2.47	0.43
1:E:6:VAL:HG11	1:F:60:ILE:CD1	2.49	0.43
1:E:190:VAL:HG11	1:E:333:ILE:HG23	1.99	0.43
1:K:191:GLU:O	1:K:334:ASP:HA	2.18	0.43
1:A:126:ALA:HB3	1:A:426:LEU:HD22	2.01	0.43
1:C:135:SER:CA	1:C:412:VAL:HG12	2.45	0.43
1:C:199:TYR:CE2	1:C:327:LYS:HB3	2.53	0.43
1:F:23:LEU:O	1:F:27:VAL:HG23	2.18	0.43
1:G:34:LYS:HZ1	1:G:483:GLU:CD	2.26	0.43
1:L:215:LEU:O	1:L:218:PRO:HD3	2.18	0.43
1:A:60:ILE:CD1	1:G:6:VAL:HG11	2.49	0.43
1:B:23:LEU:O	1:B:27:VAL:HG23	2.18	0.43
1:B:152:ALA:HB1	1:B:155:ASP:CA	2.48	0.43
1:C:257:GLU:HB3	1:D:244:GLY:O	2.17	0.43
1:C:349:ILE:HG22	1:C:369:VAL:HG13	2.00	0.43
1:E:152:ALA:HB1	1:E:155:ASP:CA	2.48	0.43
1:E:338:GLU:CD	1:E:341:ALA:HB2	2.43	0.43
1:H:417:VAL:HA	1:H:420:ILE:HG22	2.00	0.43
1:M:2:ALA:O	1:M:3:ALA:C	2.59	0.43
1:M:215:LEU:O	1:M:218:PRO:HD3	2.18	0.43
1:B:126:ALA:HB3	1:B:426:LEU:HD22	2.01	0.43
1:C:82:ASN:HB2	1:C:89:THR:HG23	2.01	0.43
1:C:293:ALA:HB2	1:C:300:VAL:CG2	2.47	0.43
1:D:199:TYR:CE2	1:D:327:LYS:HB3	2.53	0.43
1:D:338:GLU:CD	1:D:341:ALA:HB2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:VAL:HG11	1:F:333:ILE:HG23	2.00	0.43
1:F:412:VAL:HG22	1:F:495:ASP:O	2.18	0.43
1:G:82:ASN:HB2	1:G:89:THR:HG23	2.01	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:K:34:LYS:HZ3	1:K:483:GLU:CD	2.25	0.43
1:M:7:LYS:O	1:M:519:CYS:HA	2.18	0.43
1:A:294:THR:HG21	1:A:345:ARG:HG3	2.00	0.43
1:A:412:VAL:HG22	1:A:495:ASP:O	2.18	0.43
1:D:117:LYS:HZ2	1:D:121:ASP:CG	2.27	0.43
1:E:23:LEU:O	1:E:27:VAL:HG23	2.18	0.43
1:F:294:THR:HG21	1:F:345:ARG:HG3	2.00	0.43
1:G:111:MET:O	1:G:113:PRO:HD3	2.18	0.43
1:G:126:ALA:HB3	1:G:426:LEU:HD22	2.01	0.43
1:A:199:TYR:CE2	1:A:327:LYS:HB3	2.53	0.43
1:A:349:ILE:HG22	1:A:369:VAL:HG13	1.99	0.43
1:D:112:ASN:HA	1:D:113:PRO:HD2	1.88	0.43
1:D:183:LEU:C	1:D:382:GLY:HA3	2.42	0.43
1:F:152:ALA:HB1	1:F:155:ASP:CA	2.48	0.43
1:G:152:ALA:HB1	1:G:155:ASP:CA	2.48	0.43
1:J:417:VAL:HA	1:J:420:ILE:HG22	1.99	0.43
1:K:215:LEU:O	1:K:218:PRO:HD3	2.18	0.43
1:B:82:ASN:HB2	1:B:89:THR:HG23	2.01	0.43
1:B:294:THR:HG21	1:B:345:ARG:HG3	2.00	0.43
1:B:349:ILE:HG22	1:B:369:VAL:HG13	1.99	0.43
1:D:506:TYR:O	1:D:510:VAL:HG23	2.19	0.43
1:E:126:ALA:HB3	1:E:426:LEU:HD22	2.01	0.43
1:E:183:LEU:C	1:E:382:GLY:HA3	2.42	0.43
1:E:349:ILE:HG22	1:E:369:VAL:HG13	1.99	0.43
1:F:117:LYS:HZ2	1:F:121:ASP:CG	2.27	0.43
1:F:126:ALA:HB3	1:F:426:LEU:HD22	2.01	0.43
1:I:215:LEU:O	1:I:218:PRO:HD3	2.18	0.43
1:L:219:PHE:O	1:L:247:LEU:HD12	2.19	0.43
1:M:191:GLU:O	1:M:334:ASP:HA	2.18	0.43
1:N:7:LYS:O	1:N:519:CYS:HA	2.18	0.43
1:A:90:THR:HG22	1:A:94:VAL:HG23	2.01	0.43
1:A:127:ALA:CB	1:A:426:LEU:HD11	2.47	0.43
1:B:199:TYR:CE2	1:B:327:LYS:HB3	2.53	0.43
1:C:251:ALA:O	1:C:277:LYS:HA	2.19	0.43
1:D:294:THR:HG21	1:D:345:ARG:HG3	2.00	0.43
1:G:23:LEU:O	1:G:27:VAL:HG23	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:H:7:LYS:O	1:H:519:CYS:HA	2.18	0.43
1:H:215:LEU:O	1:H:218:PRO:HD3	2.19	0.43
1:I:417:VAL:HA	1:I:420:ILE:HG22	2.00	0.43
1:J:206:ASN:HB2	1:J:213:VAL:HG23	2.01	0.43
1:A:82:ASN:HB2	1:A:89:THR:HG23	2.01	0.43
1:A:111:MET:O	1:A:113:PRO:HD3	2.18	0.43
1:A:152:ALA:HB1	1:A:155:ASP:CA	2.48	0.43
1:C:111:MET:O	1:C:113:PRO:HD3	2.18	0.43
1:D:194:GLN:HE21	1:D:329:THR:HG21	1.84	0.43
1:D:251:ALA:O	1:D:277:LYS:HA	2.19	0.43
1:F:506:TYR:O	1:F:510:VAL:HG23	2.19	0.43
1:J:219:PHE:O	1:J:247:LEU:HD12	2.19	0.43
1:K:417:VAL:HA	1:K:420:ILE:HG22	2.00	0.43
1:L:7:LYS:O	1:L:519:CYS:HA	2.18	0.43
1:L:191:GLU:O	1:L:334:ASP:HA	2.18	0.43
1:N:215:LEU:O	1:N:218:PRO:HD3	2.18	0.43
1:B:19:GLY:HA2	1:B:62:LEU:CD1	2.49	0.42
1:E:19:GLY:HA2	1:E:62:LEU:CD1	2.49	0.42
1:F:383:ALA:HB3	1:F:389:MET:N	2.34	0.42
1:G:127:ALA:CB	1:G:426:LEU:HD11	2.47	0.42
1:H:271:VAL:HG12	1:H:272:LYS:H	1.85	0.42
1:N:401:HIS:C	1:N:402:ALA:CA	2.77	0.42
1:A:23:LEU:O	1:A:27:VAL:HG23	2.18	0.42
1:B:90:THR:HG22	1:B:94:VAL:HG23	2.01	0.42
1:C:190:VAL:HG12	1:C:376:VAL:O	2.19	0.42
1:C:294:THR:HG21	1:C:345:ARG:HG3	2.00	0.42
1:D:6:VAL:HG11	1:E:60:ILE:CD1	2.49	0.42
1:E:190:VAL:HG12	1:E:376:VAL:O	2.19	0.42
1:F:19:GLY:HA2	1:F:62:LEU:CD1	2.49	0.42
1:G:383:ALA:HB3	1:G:389:MET:N	2.34	0.42
1:I:206:ASN:HB2	1:I:213:VAL:HG23	2.01	0.42
1:L:34:LYS:HZ3	1:L:483:GLU:CD	2.25	0.42
1:A:383:ALA:HB3	1:A:389:MET:N	2.34	0.42
1:A:506:TYR:O	1:A:510:VAL:HG23	2.19	0.42
1:B:194:GLN:HE21	1:B:329:THR:HG21	1.84	0.42
1:C:19:GLY:HA2	1:C:62:LEU:CD1	2.49	0.42
1:C:90:THR:HG22	1:C:94:VAL:HG23	2.01	0.42
1:C:126:ALA:HB3	1:C:426:LEU:HD22	2.01	0.42
1:C:194:GLN:HE21	1:C:329:THR:HG21	1.84	0.42
1:D:190:VAL:HG12	1:D:376:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:VAL:HG12	1:F:376:VAL:O	2.20	0.42
1:G:251:ALA:O	1:G:277:LYS:HA	2.19	0.42
1:G:506:TYR:O	1:G:510:VAL:HG23	2.19	0.42
1:L:488:MET:HE2	1:L:488:MET:HA	2.01	0.42
1:B:506:TYR:O	1:B:510:VAL:HG23	2.19	0.42
1:D:90:THR:HG22	1:D:94:VAL:HG23	2.01	0.42
1:E:194:GLN:HE21	1:E:329:THR:HG21	1.85	0.42
1:E:383:ALA:HB3	1:E:389:MET:N	2.35	0.42
1:F:199:TYR:CE2	1:F:327:LYS:HB3	2.53	0.42
1:G:90:THR:HG22	1:G:94:VAL:HG23	2.01	0.42
1:G:294:THR:HG21	1:G:345:ARG:HG3	2.00	0.42
1:K:206:ASN:HB2	1:K:213:VAL:HG23	2.01	0.42
1:B:34:LYS:HZ1	1:B:483:GLU:CD	2.26	0.42
1:B:190:VAL:HG12	1:B:376:VAL:O	2.19	0.42
1:F:82:ASN:HB2	1:F:89:THR:HG23	2.01	0.42
1:F:183:LEU:C	1:F:382:GLY:HA3	2.42	0.42
1:G:190:VAL:HG12	1:G:376:VAL:O	2.19	0.42
1:I:7:LYS:O	1:I:519:CYS:HA	2.18	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:488:MET:HE2	1:N:488:MET:HA	2.02	0.42
1:D:19:GLY:HA2	1:D:62:LEU:CD1	2.49	0.42
1:E:90:THR:HG22	1:E:94:VAL:HG23	2.01	0.42
1:F:194:GLN:HE21	1:F:329:THR:HG21	1.85	0.42
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.33	0.42
1:G:194:GLN:HE21	1:G:329:THR:HG21	1.85	0.42
1:H:206:ASN:HB2	1:H:213:VAL:HG23	2.01	0.42
1:A:19:GLY:HA2	1:A:62:LEU:CD1	2.49	0.42
1:A:236:VAL:HG22	1:A:309:LEU:O	2.20	0.42
1:C:117:LYS:HZ2	1:C:121:ASP:CG	2.27	0.42
1:D:383:ALA:HB3	1:D:389:MET:N	2.34	0.42
1:G:112:ASN:HA	1:G:113:PRO:HD2	1.88	0.42
1:A:6:VAL:HG11	1:B:60:ILE:CD1	2.49	0.42
1:B:383:ALA:HB3	1:B:389:MET:N	2.34	0.42
1:C:234:LEU:HB2	1:C:235:PRO:HD3	2.01	0.42
1:E:82:ASN:HB2	1:E:89:THR:HG23	2.01	0.42
1:E:506:TYR:O	1:E:510:VAL:HG23	2.19	0.42
1:G:19:GLY:HA2	1:G:62:LEU:CD1	2.49	0.42
1:K:7:LYS:O	1:K:519:CYS:HA	2.18	0.42
1:A:251:ALA:O	1:A:277:LYS:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ALA:CB	1:B:426:LEU:HD11	2.47	0.42
1:B:234:LEU:HB2	1:B:235:PRO:HD3	2.02	0.42
1:F:127:ALA:CB	1:F:426:LEU:HD11	2.47	0.42
1:J:488:MET:HE2	1:J:488:MET:HA	2.02	0.42
1:K:219:PHE:O	1:K:247:LEU:HD12	2.20	0.42
1:A:213:VAL:CG1	1:A:325:ILE:HB	2.50	0.42
1:D:126:ALA:HB3	1:D:426:LEU:HD22	2.01	0.42
1:F:6:VAL:HG11	1:G:60:ILE:CD1	2.49	0.42
1:F:251:ALA:O	1:F:277:LYS:HA	2.19	0.42
1:M:206:ASN:HB2	1:M:213:VAL:HG23	2.01	0.42
1:N:206:ASN:HB2	1:N:213:VAL:HG23	2.00	0.42
1:C:506:TYR:O	1:C:510:VAL:HG23	2.19	0.41
1:D:82:ASN:HB2	1:D:89:THR:HG23	2.01	0.41
1:F:234:LEU:HB2	1:F:235:PRO:HD3	2.01	0.41
1:G:213:VAL:CG1	1:G:325:ILE:HB	2.50	0.41
1:I:488:MET:HE2	1:I:488:MET:HA	2.02	0.41
1:J:271:VAL:HG12	1:J:272:LYS:H	1.85	0.41
1:N:191:GLU:O	1:N:334:ASP:HA	2.18	0.41
1:N:219:PHE:O	1:N:247:LEU:HD12	2.20	0.41
1:A:190:VAL:HG12	1:A:376:VAL:O	2.20	0.41
1:A:194:GLN:HE21	1:A:329:THR:HG21	1.84	0.41
1:C:236:VAL:HG22	1:C:309:LEU:O	2.20	0.41
1:C:383:ALA:HB3	1:C:389:MET:N	2.34	0.41
1:E:236:VAL:HG22	1:E:309:LEU:O	2.20	0.41
1:G:220:ILE:HD12	1:G:248:LEU:HD23	2.03	0.41
1:L:271:VAL:HG12	1:L:272:LYS:H	1.85	0.41
1:A:182:GLY:O	1:A:382:GLY:HA2	2.21	0.41
1:B:213:VAL:CG1	1:B:325:ILE:HB	2.50	0.41
1:B:251:ALA:O	1:B:277:LYS:HA	2.19	0.41
1:D:140:ASP:CG	1:D:141:SER:N	2.78	0.41
1:E:251:ALA:O	1:E:277:LYS:HA	2.19	0.41
1:F:220:ILE:HD12	1:F:248:LEU:HD23	2.03	0.41
1:K:335:GLY:C	1:K:337:GLY:H	2.28	0.41
1:M:488:MET:HA	1:M:488:MET:HE2	2.01	0.41
1:A:140:ASP:CG	1:A:141:SER:N	2.79	0.41
1:D:236:VAL:HG22	1:D:309:LEU:O	2.20	0.41
1:D:383:ALA:HB3	1:D:389:MET:CA	2.51	0.41
1:E:220:ILE:HD12	1:E:248:LEU:HD23	2.03	0.41
1:F:213:VAL:CG1	1:F:325:ILE:HB	2.50	0.41
1:F:323:VAL:HG22	1:F:332:ILE:HA	2.03	0.41
1:H:488:MET:HE2	1:H:488:MET:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:219:PHE:O	1:I:247:LEU:HD12	2.20	0.41
1:B:135:SER:CA	1:B:412:VAL:HG12	2.45	0.41
1:E:140:ASP:CG	1:E:141:SER:N	2.78	0.41
1:E:182:GLY:O	1:E:382:GLY:HA2	2.21	0.41
1:E:323:VAL:HG22	1:E:332:ILE:HA	2.03	0.41
1:F:90:THR:HG22	1:F:94:VAL:HG23	2.01	0.41
1:I:335:GLY:C	1:I:337:GLY:H	2.29	0.41
1:A:461:GLU:HA	1:A:462:PRO:HD2	1.78	0.41
1:B:140:ASP:CG	1:B:141:SER:N	2.79	0.41
1:D:323:VAL:HG22	1:D:332:ILE:HA	2.03	0.41
1:E:383:ALA:HB3	1:E:389:MET:CA	2.51	0.41
1:G:182:GLY:O	1:G:382:GLY:HA2	2.21	0.41
1:G:323:VAL:HG22	1:G:332:ILE:HA	2.03	0.41
1:H:335:GLY:C	1:H:337:GLY:H	2.29	0.41
1:A:102:GLU:HB2	1:A:442:VAL:HG13	2.03	0.41
1:A:202:PRO:O	1:A:205:ILE:HB	2.21	0.41
1:A:383:ALA:HB3	1:A:389:MET:CA	2.51	0.41
1:B:102:GLU:HB2	1:B:442:VAL:HG13	2.03	0.41
1:C:202:PRO:O	1:C:205:ILE:HB	2.21	0.41
1:D:220:ILE:HD12	1:D:248:LEU:HD23	2.02	0.41
2:D:1525:ATP:PG	3:D:1526:PO4:P	3.19	0.41
1:E:127:ALA:CB	1:E:426:LEU:HD11	2.47	0.41
1:F:140:ASP:CG	1:F:141:SER:N	2.78	0.41
1:F:236:VAL:HG22	1:F:309:LEU:O	2.20	0.41
1:F:383:ALA:HB3	1:F:389:MET:CA	2.51	0.41
1:G:140:ASP:CG	1:G:141:SER:N	2.78	0.41
1:G:205:ILE:HG23	1:G:211:GLY:HA2	2.03	0.41
1:G:236:VAL:HG22	1:G:309:LEU:O	2.20	0.41
1:A:220:ILE:HD12	1:A:248:LEU:HD23	2.03	0.41
1:A:234:LEU:HB2	1:A:235:PRO:HD3	2.03	0.41
1:B:182:GLY:O	1:B:382:GLY:HA2	2.21	0.41
1:B:202:PRO:O	1:B:205:ILE:HB	2.21	0.41
2:C:1526:ATP:PG	3:C:1527:PO4:P	3.19	0.41
1:D:205:ILE:HG23	1:D:211:GLY:HA2	2.03	0.41
1:D:213:VAL:CG1	1:D:325:ILE:HB	2.50	0.41
1:G:102:GLU:HB2	1:G:442:VAL:HG13	2.03	0.41
1:L:206:ASN:HB2	1:L:213:VAL:HG23	2.01	0.41
2:A:1525:ATP:PG	3:A:1526:PO4:P	3.19	0.41
1:B:236:VAL:HG22	1:B:309:LEU:O	2.20	0.41
1:C:127:ALA:N	1:C:426:LEU:HD21	2.36	0.41
1:C:213:VAL:CG1	1:C:325:ILE:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LYS:HA	1:D:522:THR:O	2.21	0.41
1:D:182:GLY:O	1:D:382:GLY:HA2	2.21	0.41
1:D:202:PRO:O	1:D:205:ILE:HB	2.21	0.41
1:E:205:ILE:HG23	1:E:211:GLY:HA2	2.03	0.41
1:E:234:LEU:HB2	1:E:235:PRO:HD3	2.02	0.41
3:E:1526:PO4:P	2:E:1527:ATP:PG	3.19	0.41
1:F:182:GLY:O	1:F:382:GLY:HA2	2.21	0.41
1:F:205:ILE:HG23	1:F:211:GLY:HA2	2.03	0.41
1:G:202:PRO:O	1:G:205:ILE:HB	2.21	0.41
1:G:383:ALA:HB3	1:G:389:MET:CA	2.51	0.41
1:N:263:VAL:O	1:N:267:MET:HB3	2.21	0.41
1:B:127:ALA:N	1:B:426:LEU:HD21	2.36	0.41
1:B:383:ALA:HB3	1:B:389:MET:CA	2.51	0.41
1:C:140:ASP:CG	1:C:141:SER:N	2.78	0.41
1:C:383:ALA:HB3	1:C:389:MET:CA	2.51	0.41
1:E:127:ALA:N	1:E:426:LEU:HD21	2.36	0.41
1:F:4:LYS:HA	1:F:522:THR:O	2.21	0.41
3:F:1525:PO4:P	2:F:1527:ATP:PG	3.19	0.41
3:G:1525:PO4:P	2:G:1527:ATP:PG	3.19	0.41
1:I:230:ILE:HG23	1:I:259:LEU:HD12	2.02	0.41
1:M:230:ILE:HG23	1:M:259:LEU:HD12	2.03	0.41
1:A:152:ALA:HB1	1:A:155:ASP:O	2.21	0.40
1:G:4:LYS:HA	1:G:522:THR:O	2.22	0.40
1:K:263:VAL:O	1:K:267:MET:HB3	2.21	0.40
1:A:323:VAL:HG22	1:A:332:ILE:HA	2.03	0.40
1:B:220:ILE:HD12	1:B:248:LEU:HD23	2.03	0.40
2:B:1525:ATP:PG	3:B:1526:PO4:P	3.19	0.40
1:C:6:VAL:HG11	1:D:60:ILE:CD1	2.48	0.40
1:C:205:ILE:HG23	1:C:211:GLY:HA2	2.03	0.40
1:C:220:ILE:HD12	1:C:248:LEU:HD23	2.03	0.40
1:D:152:ALA:HB1	1:D:155:ASP:O	2.22	0.40
1:E:213:VAL:CG1	1:E:325:ILE:HB	2.51	0.40
1:G:127:ALA:N	1:G:426:LEU:HD21	2.36	0.40
1:G:140:ASP:CG	1:G:141:SER:H	2.30	0.40
1:G:234:LEU:HB2	1:G:235:PRO:HD3	2.02	0.40
1:A:205:ILE:HG23	1:A:211:GLY:HA2	2.03	0.40
1:C:206:ASN:HB2	1:C:213:VAL:CB	2.52	0.40
1:C:323:VAL:HG22	1:C:332:ILE:HA	2.03	0.40
1:D:206:ASN:HB2	1:D:213:VAL:CB	2.52	0.40
1:E:4:LYS:HA	1:E:522:THR:O	2.21	0.40
1:E:206:ASN:HB2	1:E:213:VAL:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:VAL:O	1:F:324:VAL:HA	2.22	0.40
1:G:213:VAL:O	1:G:324:VAL:HA	2.22	0.40
1:N:335:GLY:C	1:N:337:GLY:H	2.29	0.40
1:C:102:GLU:HB2	1:C:442:VAL:HG13	2.03	0.40
1:F:102:GLU:HB2	1:F:442:VAL:HG13	2.03	0.40
1:F:140:ASP:CG	1:F:141:SER:H	2.30	0.40
1:G:152:ALA:HB1	1:G:155:ASP:O	2.22	0.40
1:C:4:LYS:HA	1:C:522:THR:O	2.21	0.40
1:E:202:PRO:O	1:E:205:ILE:HB	2.21	0.40
1:E:213:VAL:O	1:E:324:VAL:HA	2.22	0.40
1:J:335:GLY:C	1:J: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%)	516 (99%)	5 (1%)	1 (0%)	43	78
1	B	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	43	78
1	C	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	43	78
1	D	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	43	78
1	E	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	43	78
1	F	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	43	78
1	G	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	43	78
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	7098 (97%)	189 (3%)	21 (0%)	37	72

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ALA
1	B	243	ALA
1	C	243	ALA
1	D	243	ALA
1	E	243	ALA
1	F	243	ALA
1	G	243	ALA
1	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%)	361 (90%)	41 (10%)	7	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	402/414 (97%)	361 (90%)	41 (10%)	7	23
1	C	402/414 (97%)	360 (90%)	42 (10%)	7	22
1	D	402/414 (97%)	361 (90%)	41 (10%)	7	23
1	E	402/414 (97%)	360 (90%)	42 (10%)	7	22
1	F	402/414 (97%)	360 (90%)	42 (10%)	7	22
1	G	402/414 (97%)	360 (90%)	42 (10%)	7	22
1	H	402/414 (97%)	367 (91%)	35 (9%)	9	29
1	I	402/414 (97%)	367 (91%)	35 (9%)	9	29
1	J	402/414 (97%)	368 (92%)	34 (8%)	10	29
1	K	402/414 (97%)	366 (91%)	36 (9%)	9	27
1	L	402/414 (97%)	367 (91%)	35 (9%)	9	29
1	M	402/414 (97%)	367 (91%)	35 (9%)	9	29
1	N	402/414 (97%)	366 (91%)	36 (9%)	9	27
All	All	5628/5796 (97%)	5091 (90%)	537 (10%)	10	25

All (537) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	38	VAL
1	A	41	ASP
1	A	54	VAL
1	A	65	LYS
1	A	79	SER
1	A	130	GLU
1	A	140	ASP
1	A	142	LYS
1	A	169	VAL
1	A	171	LYS
1	A	172	GLU
1	A	186	GLU
1	A	205	ILE
1	A	207	LYS
1	A	213	VAL
1	A	214	GLU
1	A	219	PHE
1	A	231	ARG

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Mol	Chain	Res	Type
1	A	238	GLU
1	A	261	THR
1	A	268	ARG
1	A	290	GLN
1	A	295	LEU
1	A	301	ILE
1	A	321	LYS
1	A	323	VAL
1	A	327	LYS
1	A	328	ASP
1	A	338	GLU
1	A	350	ARG
1	A	358	SER
1	A	387	VAL
1	A	421	ARG
1	A	425	LYS
1	A	430	ARG
1	A	453	GLN
1	A	460	GLU
1	A	484	GLU
1	A	494	LEU
1	A	504	LEU
1	B	31	LEU
1	B	38	VAL
1	B	41	ASP
1	B	54	VAL
1	B	65	LYS
1	B	79	SER
1	B	130	GLU
1	B	140	ASP
1	B	142	LYS
1	B	169	VAL
1	B	171	LYS
1	B	172	GLU
1	B	186	GLU
1	B	205	ILE
1	B	207	LYS
1	B	213	VAL
1	B	214	GLU
1	B	219	PHE
1	B	231	ARG
1	B	238	GLU

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Mol	Chain	Res	Type
1	B	261	THR
1	B	268	ARG
1	B	290	GLN
1	B	295	LEU
1	B	301	ILE
1	B	321	LYS
1	B	323	VAL
1	B	327	LYS
1	B	328	ASP
1	B	338	GLU
1	B	350	ARG
1	B	358	SER
1	B	387	VAL
1	B	421	ARG
1	B	425	LYS
1	B	430	ARG
1	B	453	GLN
1	B	460	GLU
1	B	484	GLU
1	B	494	LEU
1	B	504	LEU
1	C	31	LEU
1	C	38	VAL
1	C	41	ASP
1	C	54	VAL
1	C	65	LYS
1	C	79	SER
1	C	115	ASP
1	C	130	GLU
1	C	140	ASP
1	C	142	LYS
1	C	169	VAL
1	C	171	LYS
1	C	172	GLU
1	C	186	GLU
1	C	205	ILE
1	C	207	LYS
1	C	213	VAL
1	C	214	GLU
1	C	219	PHE
1	C	231	ARG
1	C	238	GLU

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Mol	Chain	Res	Type
1	C	261	THR
1	C	268	ARG
1	C	290	GLN
1	C	295	LEU
1	C	301	ILE
1	C	321	LYS
1	C	323	VAL
1	C	327	LYS
1	C	328	ASP
1	C	338	GLU
1	C	350	ARG
1	C	358	SER
1	C	387	VAL
1	C	421	ARG
1	C	425	LYS
1	C	430	ARG
1	C	453	GLN
1	C	460	GLU
1	C	484	GLU
1	C	494	LEU
1	C	504	LEU
1	D	31	LEU
1	D	38	VAL
1	D	41	ASP
1	D	54	VAL
1	D	65	LYS
1	D	79	SER
1	D	130	GLU
1	D	140	ASP
1	D	142	LYS
1	D	169	VAL
1	D	171	LYS
1	D	172	GLU
1	D	186	GLU
1	D	205	ILE
1	D	207	LYS
1	D	213	VAL
1	D	214	GLU
1	D	219	PHE
1	D	231	ARG
1	D	238	GLU
1	D	261	THR

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Mol	Chain	Res	Type
1	D	268	ARG
1	D	290	GLN
1	D	295	LEU
1	D	301	ILE
1	D	321	LYS
1	D	323	VAL
1	D	327	LYS
1	D	328	ASP
1	D	338	GLU
1	D	350	ARG
1	D	358	SER
1	D	387	VAL
1	D	421	ARG
1	D	425	LYS
1	D	430	ARG
1	D	453	GLN
1	D	460	GLU
1	D	484	GLU
1	D	494	LEU
1	D	504	LEU
1	E	31	LEU
1	E	38	VAL
1	E	41	ASP
1	E	54	VAL
1	E	65	LYS
1	E	79	SER
1	E	130	GLU
1	E	140	ASP
1	E	142	LYS
1	E	169	VAL
1	E	171	LYS
1	E	172	GLU
1	E	186	GLU
1	E	205	ILE
1	E	207	LYS
1	E	213	VAL
1	E	214	GLU
1	E	219	PHE
1	E	231	ARG
1	E	238	GLU
1	E	261	THR
1	E	262	LEU

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Mol	Chain	Res	Type
1	E	268	ARG
1	E	290	GLN
1	E	295	LEU
1	E	301	ILE
1	E	321	LYS
1	E	323	VAL
1	E	327	LYS
1	E	328	ASP
1	E	338	GLU
1	E	350	ARG
1	E	358	SER
1	E	387	VAL
1	E	421	ARG
1	E	425	LYS
1	E	430	ARG
1	E	453	GLN
1	E	460	GLU
1	E	484	GLU
1	E	494	LEU
1	E	504	LEU
1	F	31	LEU
1	F	38	VAL
1	F	41	ASP
1	F	54	VAL
1	F	65	LYS
1	F	79	SER
1	F	115	ASP
1	F	130	GLU
1	F	140	ASP
1	F	142	LYS
1	F	169	VAL
1	F	171	LYS
1	F	172	GLU
1	F	186	GLU
1	F	205	ILE
1	F	207	LYS
1	F	213	VAL
1	F	214	GLU
1	F	219	PHE
1	F	231	ARG
1	F	238	GLU
1	F	261	THR

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Mol	Chain	Res	Type
1	F	268	ARG
1	F	290	GLN
1	F	295	LEU
1	F	301	ILE
1	F	321	LYS
1	F	323	VAL
1	F	327	LYS
1	F	328	ASP
1	F	338	GLU
1	F	350	ARG
1	F	358	SER
1	F	387	VAL
1	F	421	ARG
1	F	425	LYS
1	F	430	ARG
1	F	453	GLN
1	F	460	GLU
1	F	484	GLU
1	F	494	LEU
1	F	504	LEU
1	G	31	LEU
1	G	38	VAL
1	G	41	ASP
1	G	54	VAL
1	G	65	LYS
1	G	79	SER
1	G	115	ASP
1	G	130	GLU
1	G	140	ASP
1	G	142	LYS
1	G	169	VAL
1	G	171	LYS
1	G	172	GLU
1	G	186	GLU
1	G	205	ILE
1	G	207	LYS
1	G	213	VAL
1	G	214	GLU
1	G	219	PHE
1	G	231	ARG
1	G	238	GLU
1	G	261	THR

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Mol	Chain	Res	Type
1	G	268	ARG
1	G	290	GLN
1	G	295	LEU
1	G	301	ILE
1	G	321	LYS
1	G	323	VAL
1	G	327	LYS
1	G	328	ASP
1	G	338	GLU
1	G	350	ARG
1	G	358	SER
1	G	387	VAL
1	G	421	ARG
1	G	425	LYS
1	G	430	ARG
1	G	453	GLN
1	G	460	GLU
1	G	484	GLU
1	G	494	LEU
1	G	504	LEU
1	H	82	ASN
1	H	130	GLU
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	232	GLU
1	H	290	GLN
1	H	313	THR
1	H	329	THR
1	H	334	ASP

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Mol	Chain	Res	Type
1	H	338	GLU
1	H	350	ARG
1	H	390	LYS
1	H	404	ARG
1	H	411	VAL
1	H	460	GLU
1	H	463	SER
1	H	483	GLU
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	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	232	GLU
1	I	290	GLN
1	I	313	THR
1	I	329	THR
1	I	334	ASP
1	I	338	GLU
1	I	350	ARG
1	I	390	LYS
1	I	404	ARG
1	I	411	VAL
1	I	460	GLU
1	I	463	SER

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Mol	Chain	Res	Type
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	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	313	THR
1	J	329	THR
1	J	334	ASP
1	J	338	GLU
1	J	350	ARG
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

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Mol	Chain	Res	Type
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
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	232	GLU
1	K	271	VAL
1	K	290	GLN
1	K	313	THR
1	K	329	THR
1	K	334	ASP
1	K	338	GLU
1	K	350	ARG
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	142	LYS
1	L	153	ASN
1	L	171	LYS
1	L	172	GLU
1	L	174	VAL
1	L	184	GLN

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Mol	Chain	Res	Type
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	232	GLU
1	L	290	GLN
1	L	313	THR
1	L	329	THR
1	L	334	ASP
1	L	338	GLU
1	L	350	ARG
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	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

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Mol	Chain	Res	Type
1	M	229	ASN
1	M	230	ILE
1	M	232	GLU
1	M	290	GLN
1	M	313	THR
1	M	329	THR
1	M	334	ASP
1	M	338	GLU
1	M	350	ARG
1	M	390	LYS
1	M	404	ARG
1	M	411	VAL
1	M	460	GLU
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	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	232	GLU
1	N	271	VAL
1	N	290	GLN
1	N	313	THR
1	N	329	THR

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Mol	Chain	Res	Type
1	N	334	ASP
1	N	338	GLU
1	N	350	ARG
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	453	GLN
1	B	453	GLN
1	C	453	GLN
1	D	453	GLN
1	E	453	GLN
1	F	453	GLN
1	G	453	GLN
1	H	352	GLN
1	I	352	GLN
1	J	352	GLN
1	K	352	GLN
1	L	352	GLN
1	M	352	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	G	1527	4	32,33,33	1.61	2 (6%)	48,52,52	1.04	4 (8%)
2	ATP	E	1527	4	32,33,33	1.60	2 (6%)	48,52,52	1.03	4 (8%)
2	ATP	D	1525	4	32,33,33	1.61	2 (6%)	48,52,52	1.04	4 (8%)
2	ATP	B	1525	4	32,33,33	1.59	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%)
2	ATP	C	1526	4	32,33,33	1.60	2 (6%)	48,52,52	1.04	4 (8%)
2	ATP	F	1527	4	32,33,33	1.57	2 (6%)	48,52,52	1.03	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	G	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	B	1525	4	-	1/22/38/38	0/3/3/3
2	ATP	A	1525	4	-	1/22/38/38	0/3/3/3
2	ATP	C	1526	4	-	1/22/38/38	0/3/3/3
2	ATP	F	1527	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	G	1527	ATP	PA-O3A	-7.95	1.50	1.59
2	D	1525	ATP	PA-O3A	-7.91	1.51	1.59
2	E	1527	ATP	PA-O3A	-7.86	1.51	1.59
2	C	1526	ATP	PA-O3A	-7.85	1.51	1.59
2	B	1525	ATP	PA-O3A	-7.83	1.51	1.59
2	A	1525	ATP	PA-O3A	-7.79	1.51	1.59
2	F	1527	ATP	PA-O3A	-7.69	1.51	1.59
2	A	1525	ATP	PB-O3B	2.17	1.61	1.59
2	F	1527	ATP	PB-O3B	2.14	1.61	1.59
2	D	1525	ATP	PB-O3B	2.13	1.61	1.59
2	E	1527	ATP	PB-O3B	2.09	1.61	1.59
2	B	1525	ATP	PB-O3B	2.09	1.61	1.59
2	G	1527	ATP	PB-O3B	2.08	1.61	1.59
2	C	1526	ATP	PB-O3B	2.06	1.61	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1527	ATP	O2A-PA-O3A	2.85	114.98	107.27
2	G	1527	ATP	O2A-PA-O3A	2.85	114.98	107.27
2	B	1525	ATP	O2A-PA-O3A	2.84	114.96	107.27
2	D	1525	ATP	O2A-PA-O3A	2.84	114.95	107.27
2	A	1525	ATP	O2A-PA-O3A	2.84	114.95	107.27
2	C	1526	ATP	O2A-PA-O3A	2.84	114.94	107.27
2	F	1527	ATP	O2A-PA-O3A	2.82	114.91	107.27
2	A	1525	ATP	O3B-PG-O1G	-2.50	97.89	111.04
2	D	1525	ATP	O3B-PG-O1G	-2.49	97.91	111.04
2	G	1527	ATP	O3B-PG-O1G	-2.49	97.92	111.04
2	C	1526	ATP	O3B-PG-O1G	-2.49	97.92	111.04
2	E	1527	ATP	O3B-PG-O1G	-2.49	97.93	111.04
2	B	1525	ATP	O3B-PG-O1G	-2.49	97.96	111.04
2	F	1527	ATP	O3B-PG-O1G	-2.48	97.97	111.04
2	F	1527	ATP	O4'-C1'-N9	2.37	112.64	108.09
2	G	1527	ATP	O4'-C1'-N9	2.37	112.64	108.09
2	C	1526	ATP	O4'-C1'-N9	2.37	112.64	108.09
2	D	1525	ATP	O4'-C1'-N9	2.36	112.63	108.09
2	A	1525	ATP	O4'-C1'-N9	2.36	112.62	108.09
2	E	1527	ATP	O4'-C1'-N9	2.35	112.61	108.09
2	B	1525	ATP	O4'-C1'-N9	2.35	112.60	108.09
2	G	1527	ATP	O3G-PG-O2G	2.32	116.49	107.80
2	D	1525	ATP	O3G-PG-O2G	2.31	116.47	107.80
2	C	1526	ATP	O3G-PG-O2G	2.30	116.44	107.80
2	F	1527	ATP	O3G-PG-O2G	2.30	116.44	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1525	ATP	O3G-PG-O2G	2.30	116.43	107.80
2	E	1527	ATP	O3G-PG-O2G	2.30	116.41	107.80
2	B	1525	ATP	O3G-PG-O2G	2.29	116.41	107.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

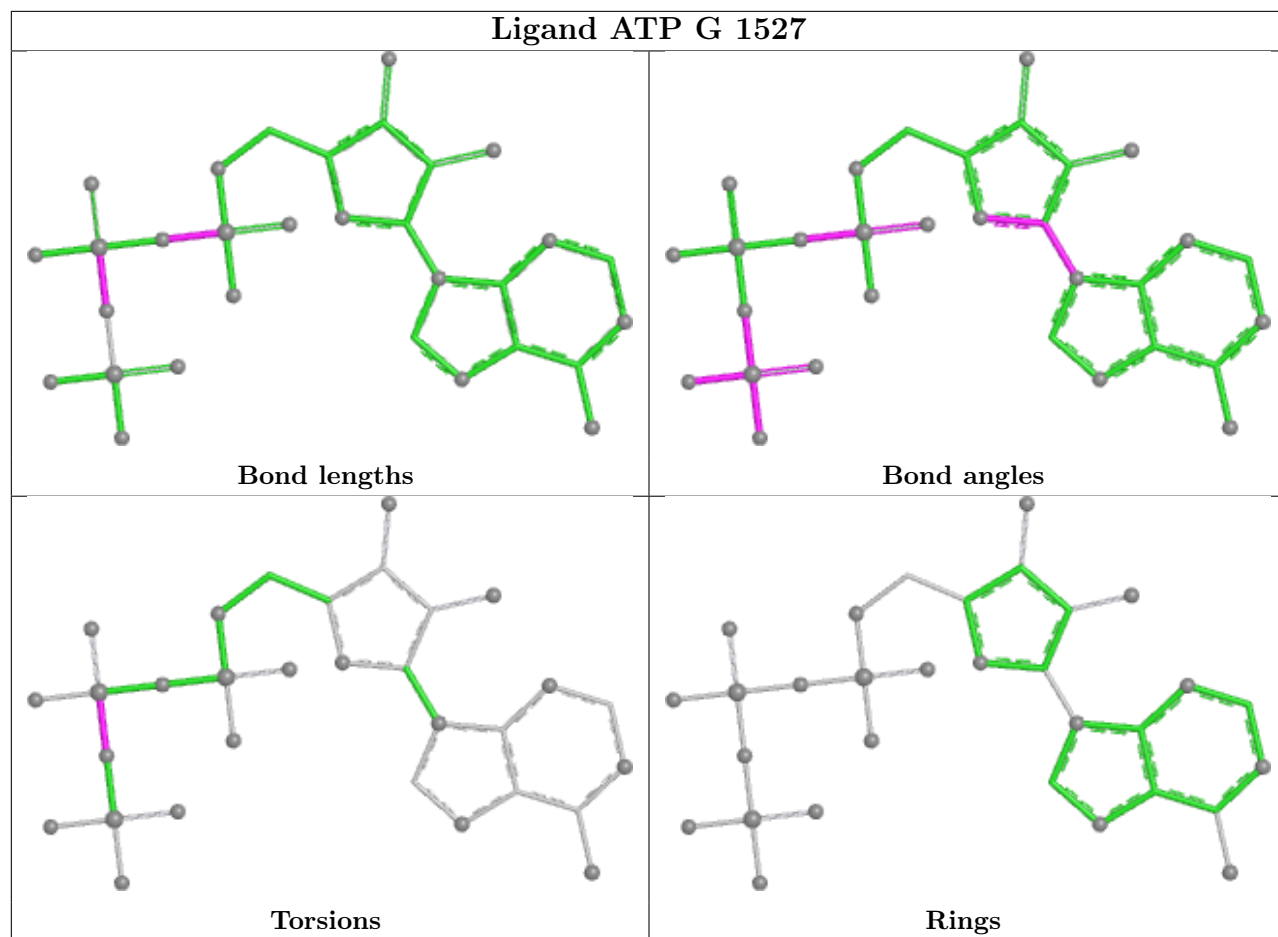
Mol	Chain	Res	Type	Atoms
2	A	1525	ATP	PG-O3B-PB-O2B
2	B	1525	ATP	PG-O3B-PB-O2B
2	C	1526	ATP	PG-O3B-PB-O2B
2	D	1525	ATP	PG-O3B-PB-O2B
2	E	1527	ATP	PG-O3B-PB-O2B
2	F	1527	ATP	PG-O3B-PB-O2B
2	G	1527	ATP	PG-O3B-PB-O2B

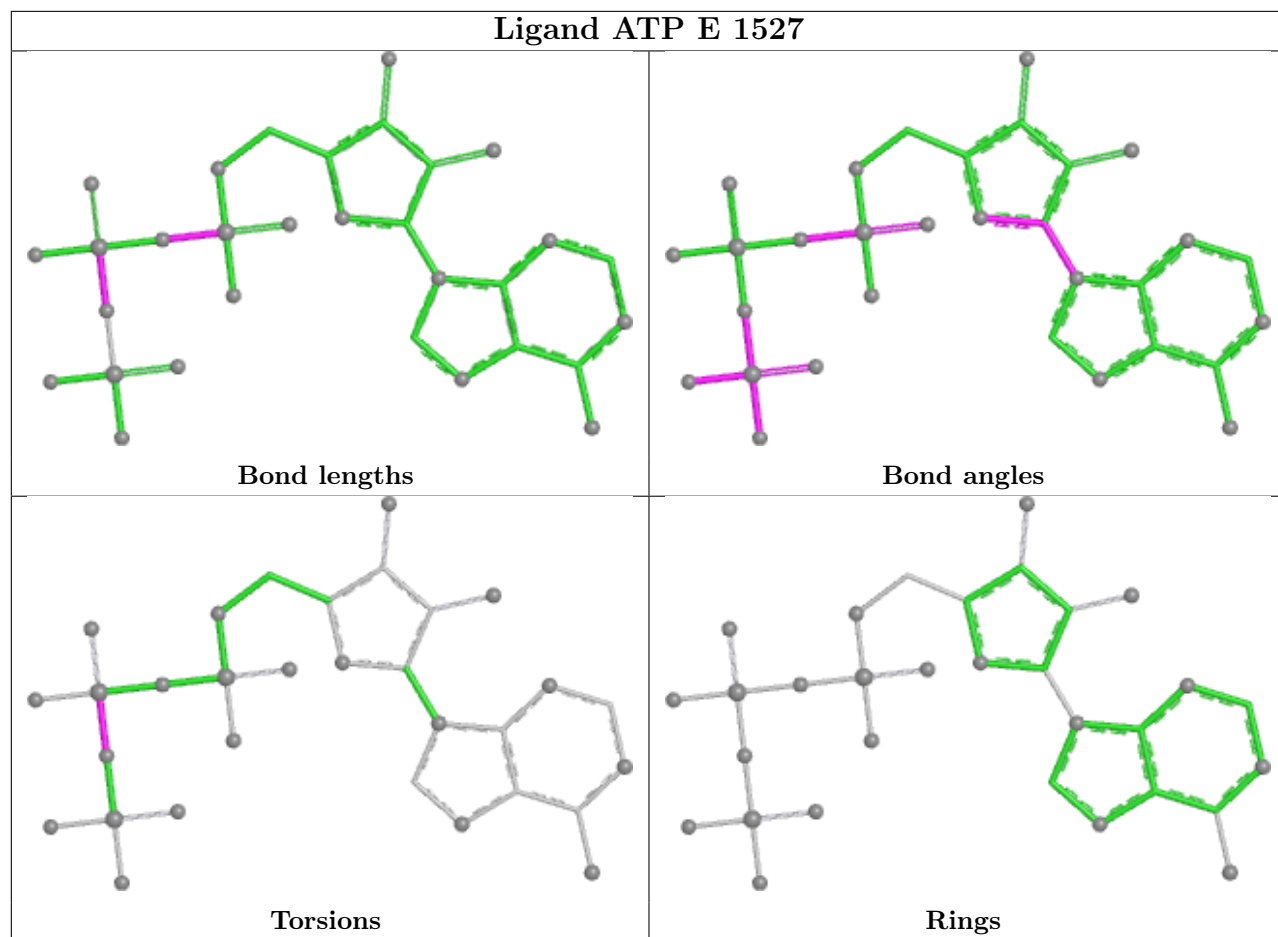
There are no ring outliers.

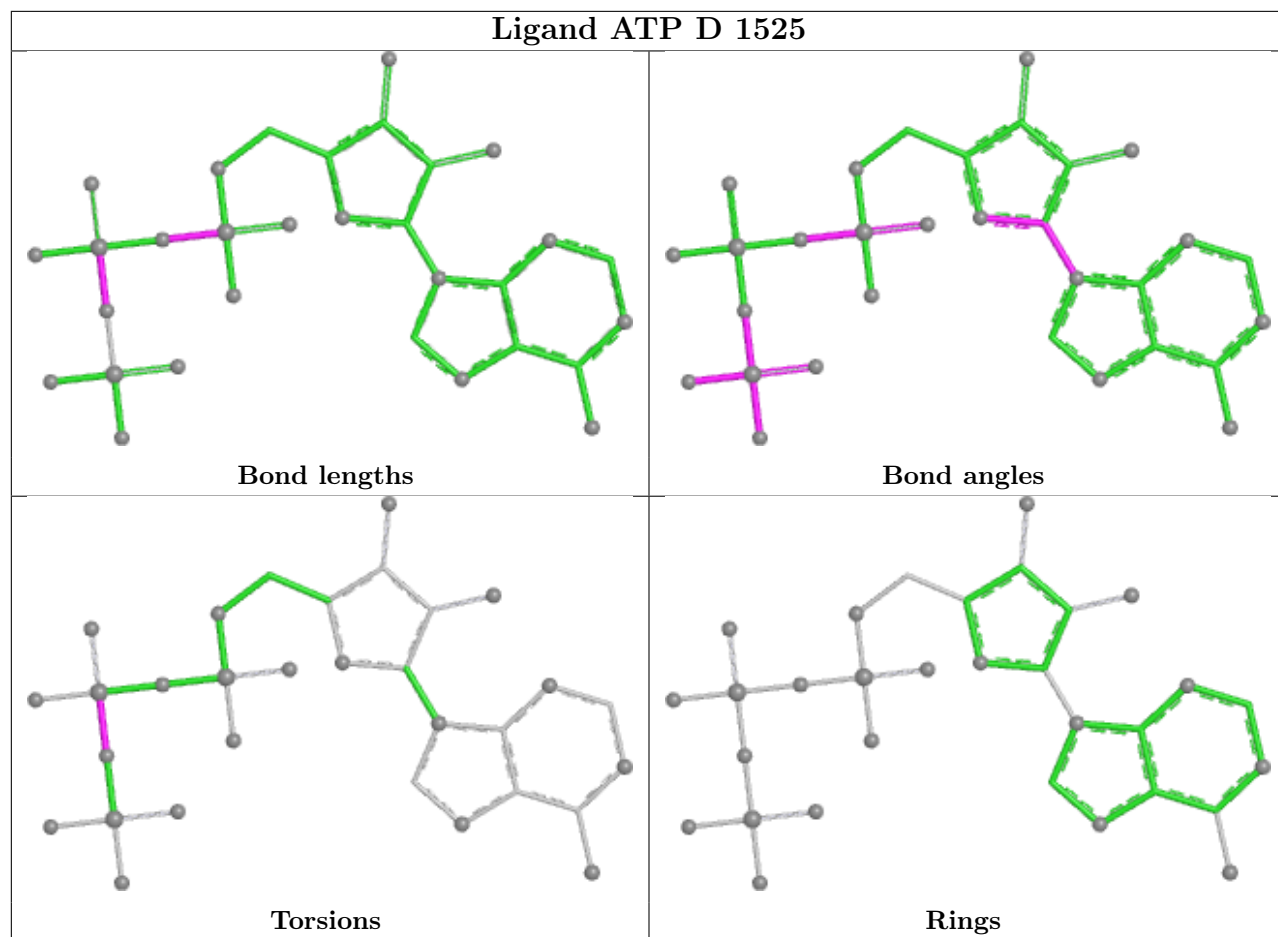
7 monomers are involved in 28 short contacts:

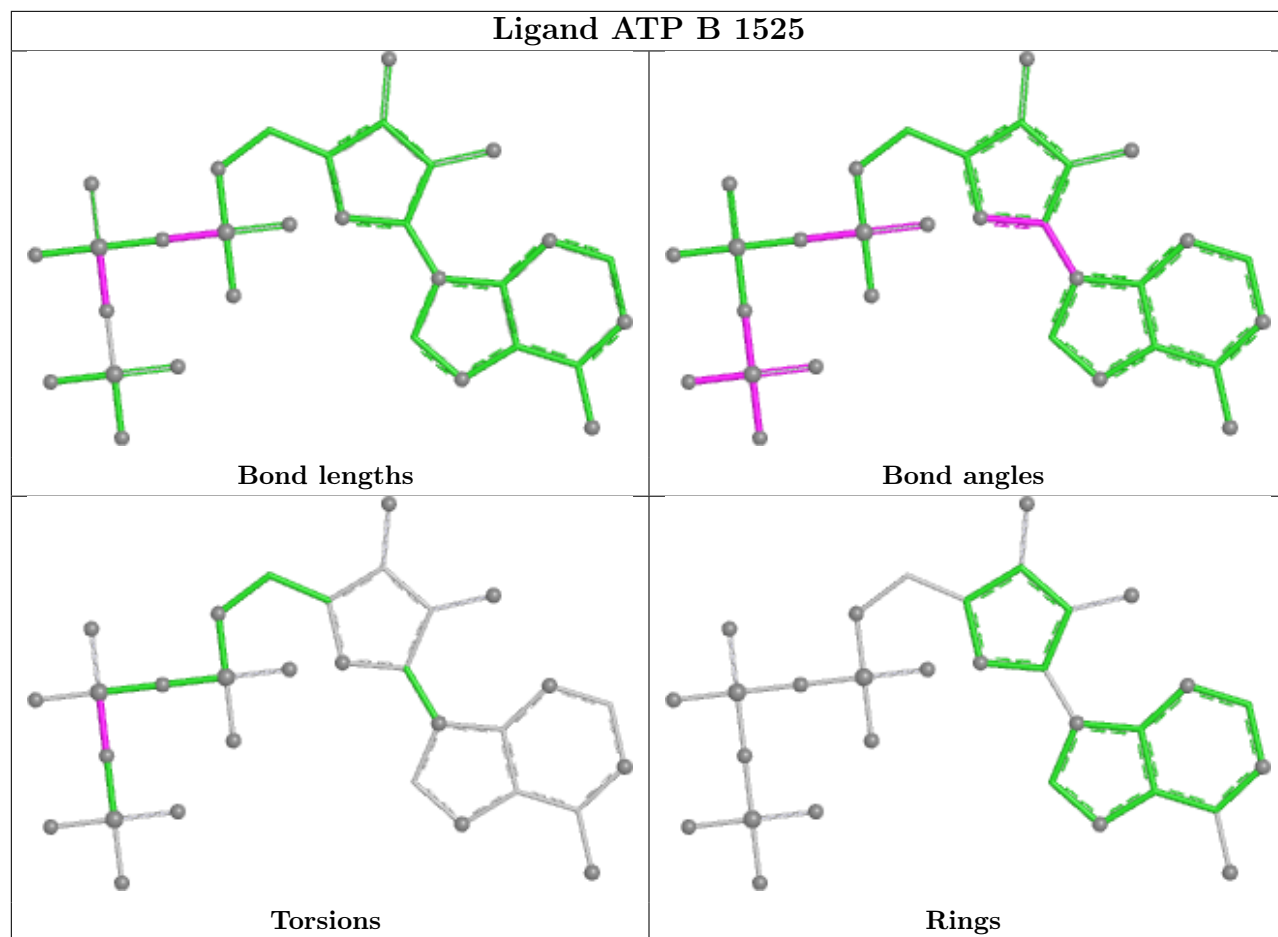
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1527	ATP	4	0
2	E	1527	ATP	4	0
2	D	1525	ATP	4	0
2	B	1525	ATP	4	0
2	A	1525	ATP	4	0
2	C	1526	ATP	4	0
2	F	1527	ATP	4	0

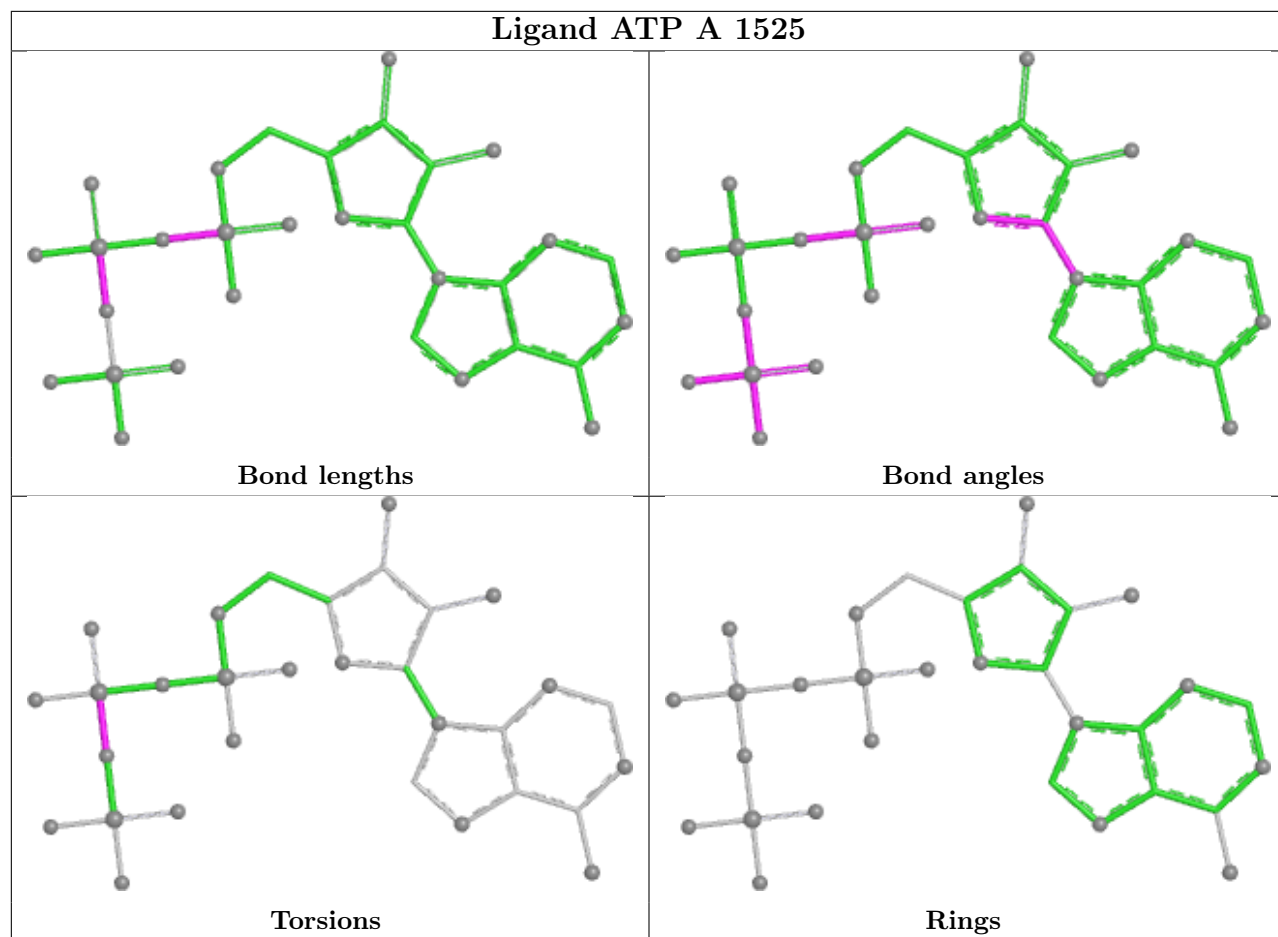
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

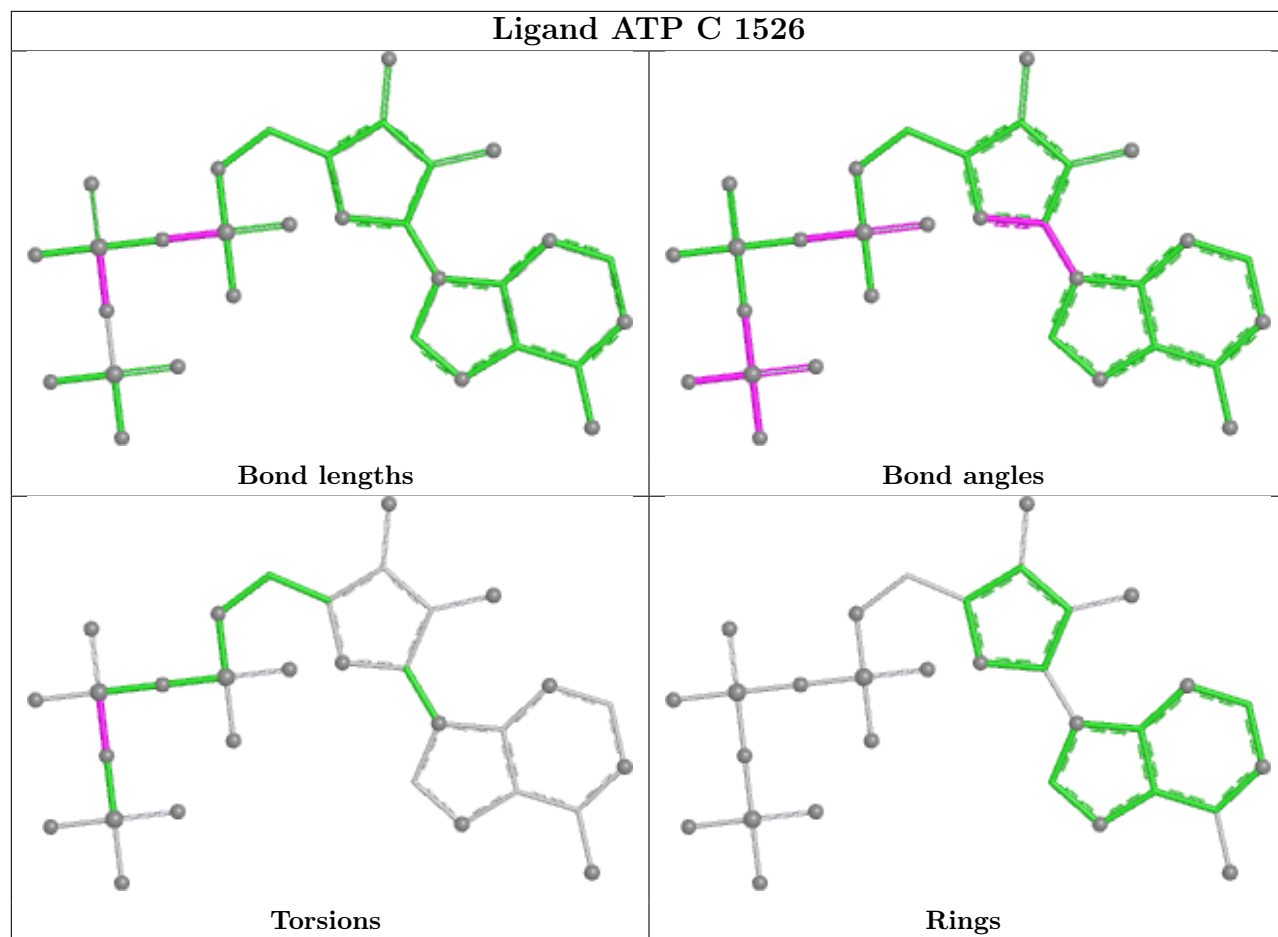


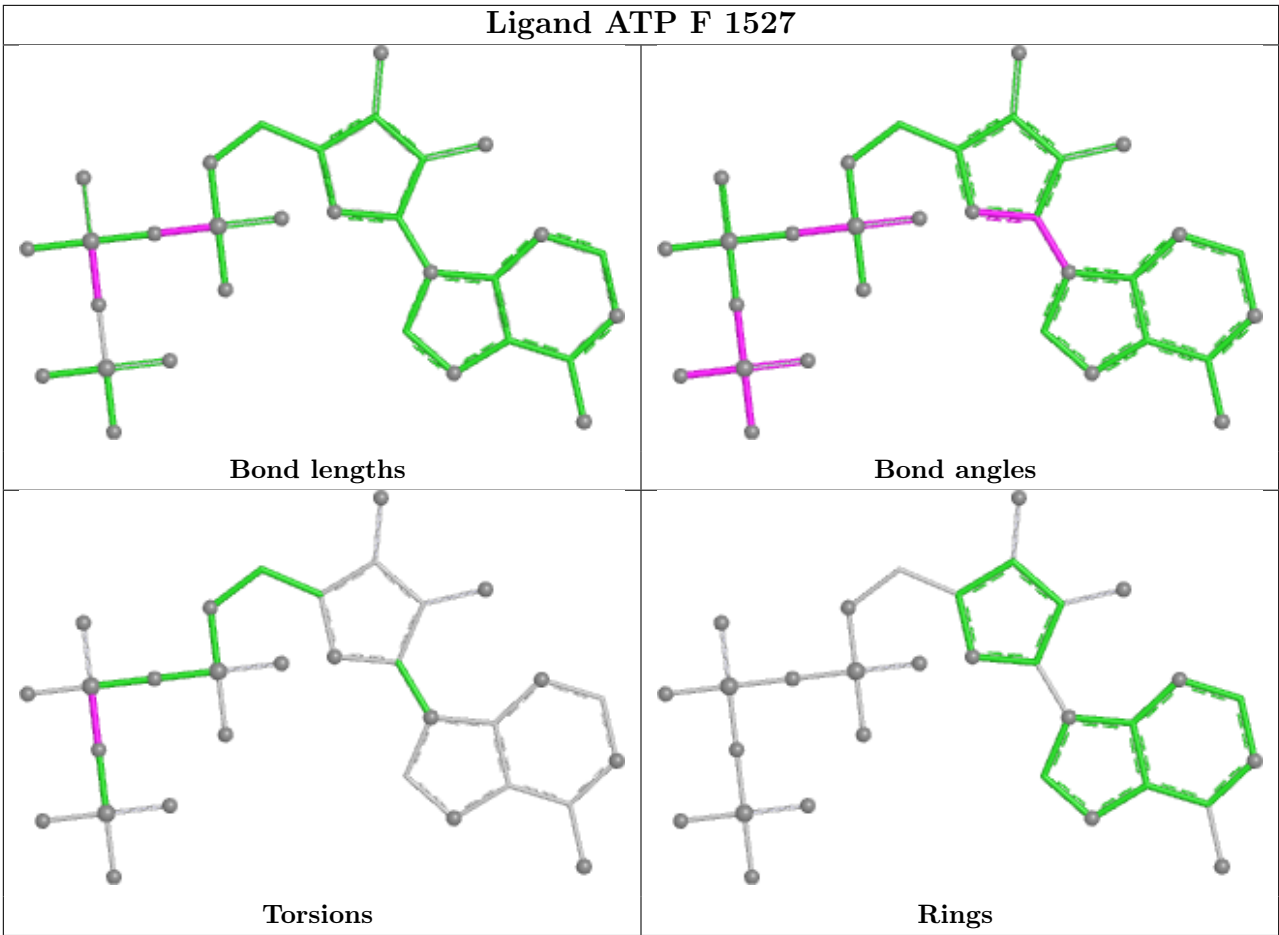












5.7 Other polymers [i](#)

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	M	2
1	K	1
1	I	1
1	N	1
1	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	400:LEU	C	401:HIS	N	1.86

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	400:LEU	C	401:HIS	N	1.81
1	I	400:LEU	C	401:HIS	N	1.77
1	N	401:HIS	C	402:ALA	N	1.70
1	J	401:HIS	C	402:ALA	N	1.19
1	M	401:HIS	C	402:ALA	N	1.02

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1999. 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

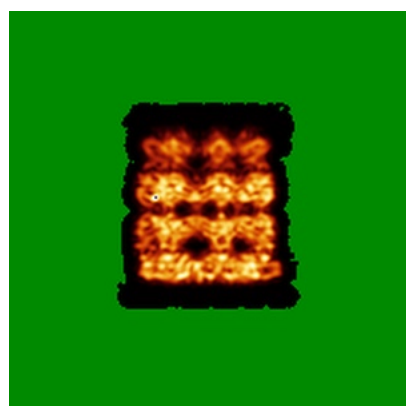


Z Index: 102

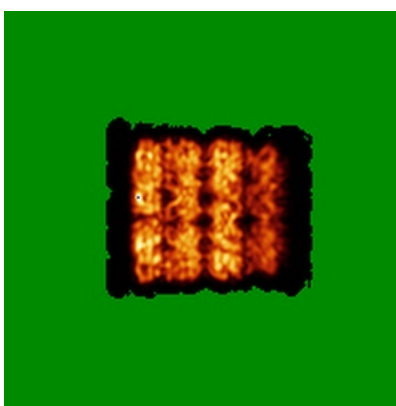
The images above show the largest variance slices of the map in three orthogonal directions.

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

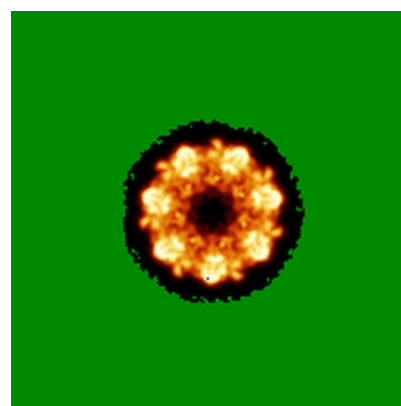
6.4.1 Primary map



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

This section was not generated.

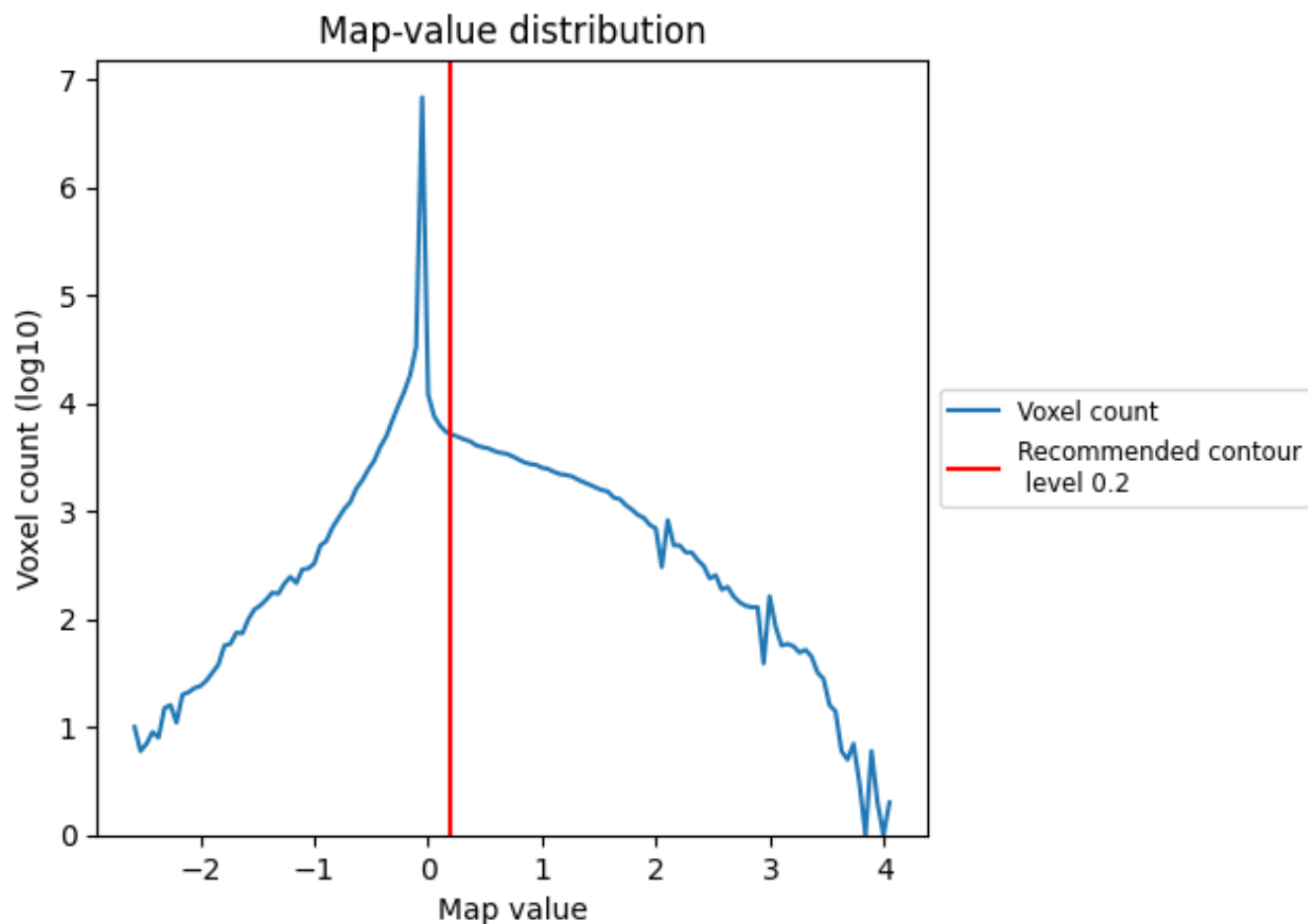
6.6 Mask visualisation

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

7 Map analysis [i](#)

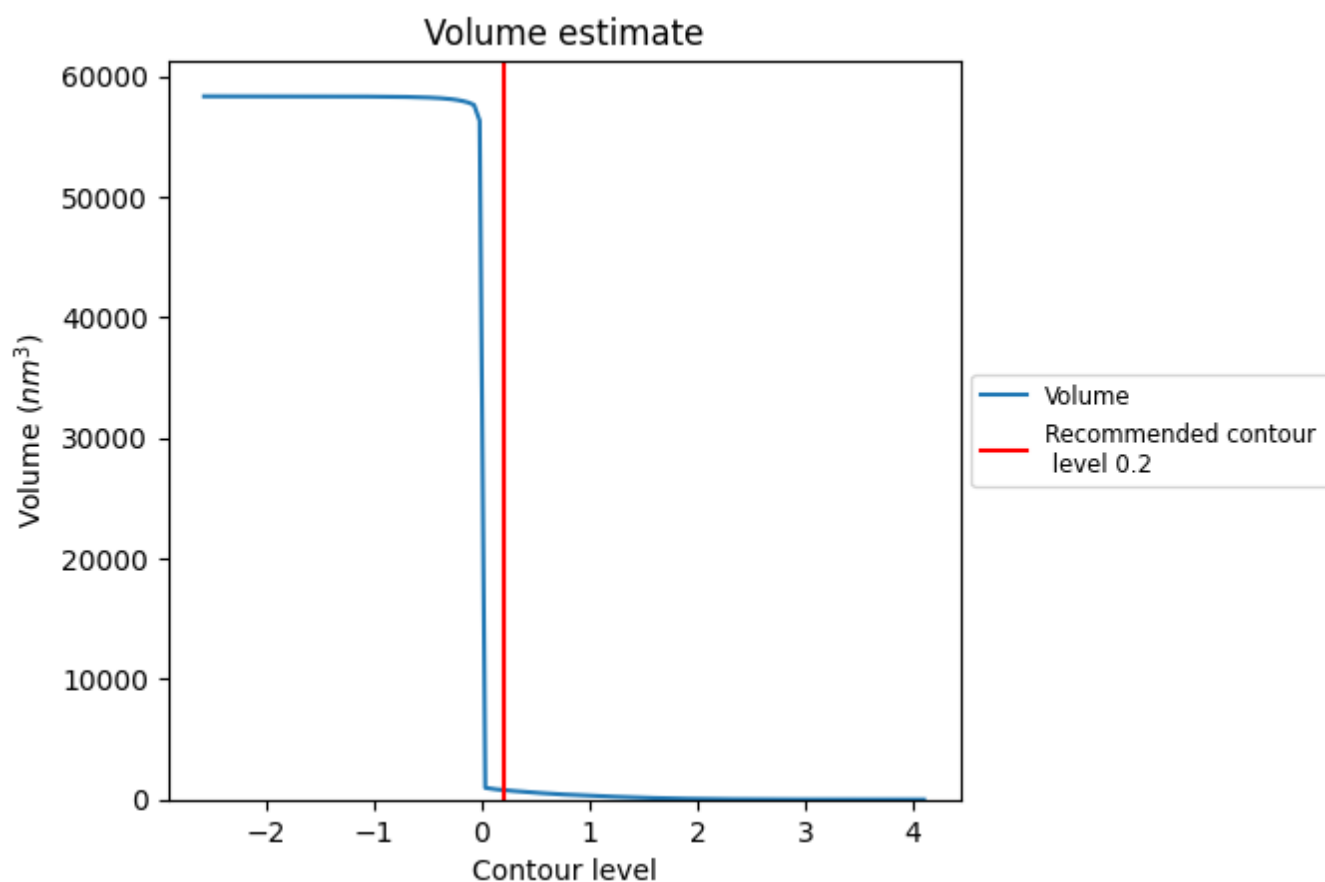
This section contains the results of statistical analysis of the map.

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.

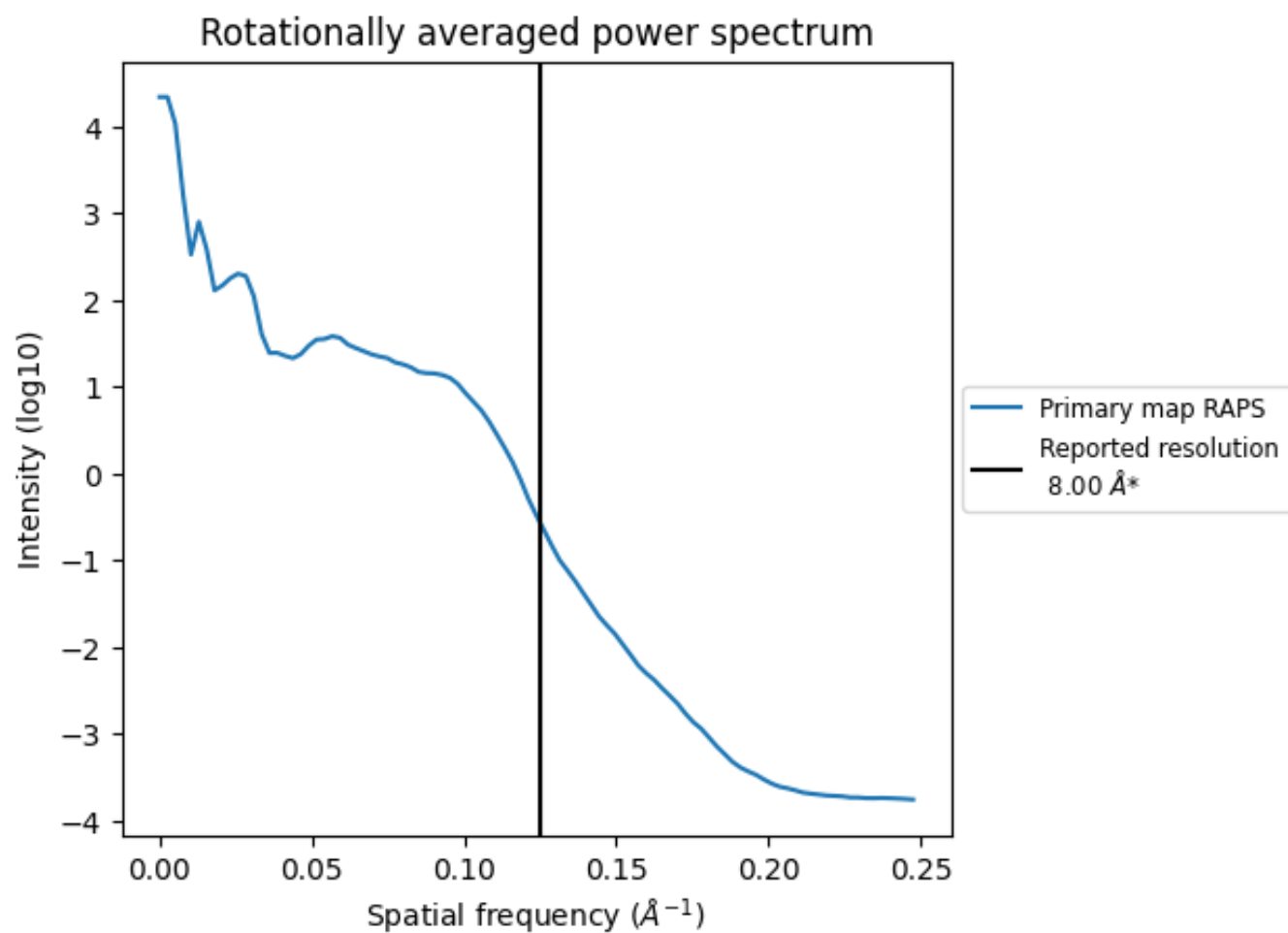
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 788 nm³; this corresponds to an approximate mass of 712 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

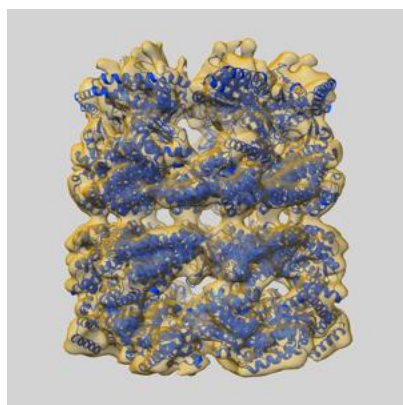
8 Fourier-Shell correlation

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

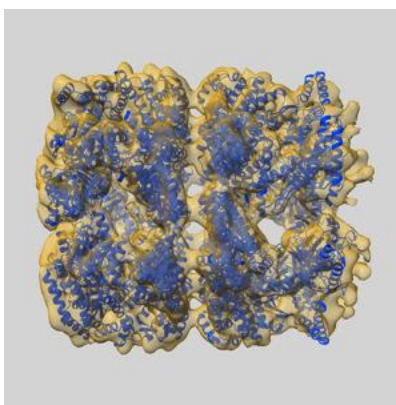
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1999 and PDB model 4AAR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

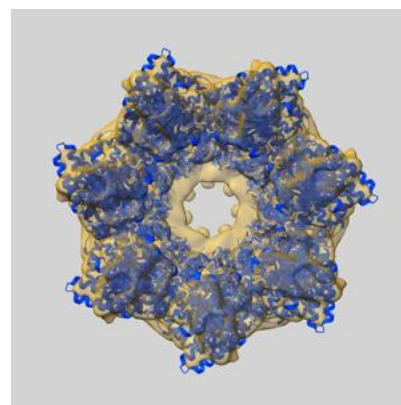
9.1 Map-model overlay [i](#)



X



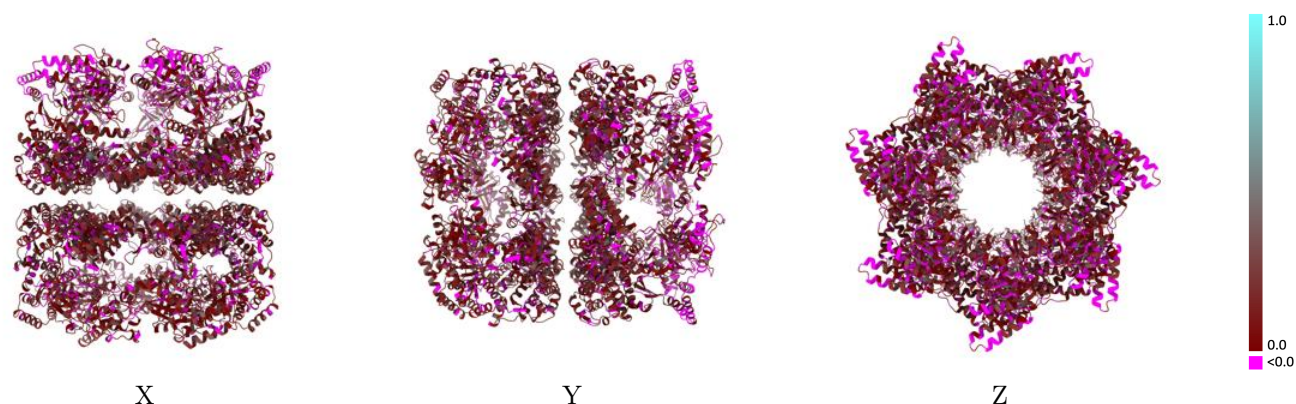
Y



Z

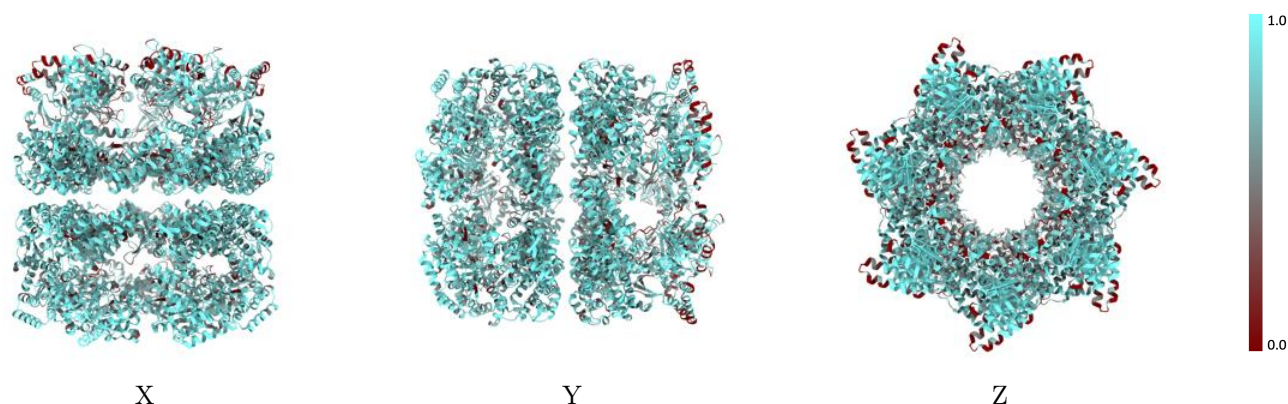
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



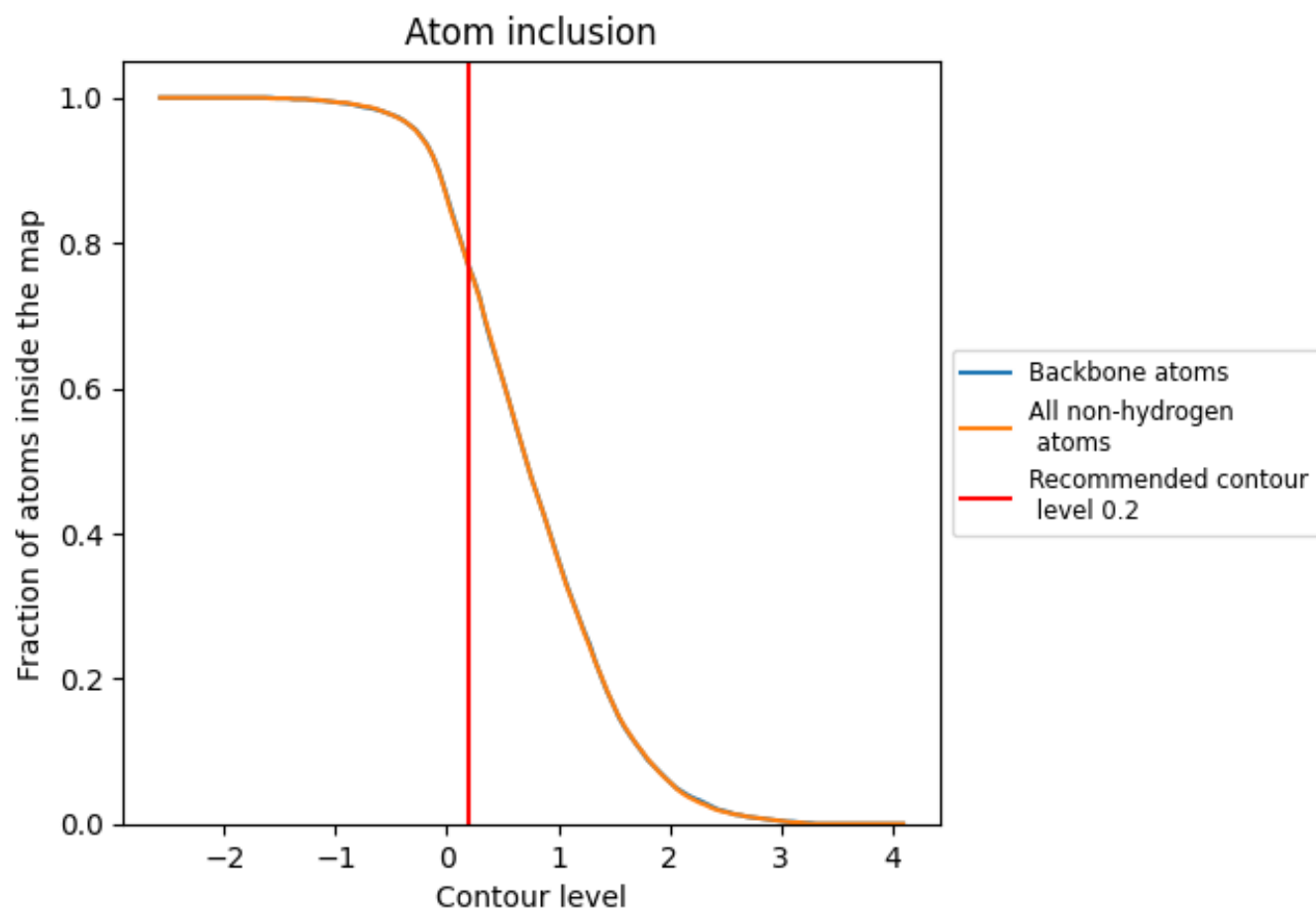
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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	 0.7650	 0.1040
A	 0.7470	 0.0920
B	 0.7460	 0.0920
C	 0.7470	 0.0920
D	 0.7460	 0.0900
E	 0.7480	 0.0890
F	 0.7470	 0.0900
G	 0.7470	 0.0910
H	 0.7920	 0.1180
I	 0.7920	 0.1190
J	 0.7910	 0.1170
K	 0.7930	 0.1170
L	 0.7920	 0.1160
M	 0.7920	 0.1160
N	 0.7930	 0.1160

