



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 11:19 AM UTC

PDB ID : 3J3S / pdb_00003j3s
EMDB ID : EMD-5608
Title : Structural dynamics of the MecA-ClpC complex revealed by cryo-EM
Authors : Liu, J.; Mei, Z.; Li, N.; Qi, Y.; Xu, Y.; Shi, Y.; Wang, F.; Lei, J.; Gao, N.
Deposited on : 2013-04-18
Resolution : 11.00 Å(reported)
Based on initial model : 3PXI

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
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

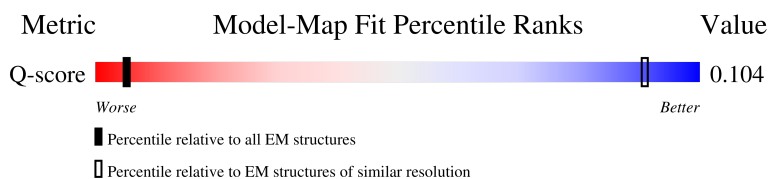
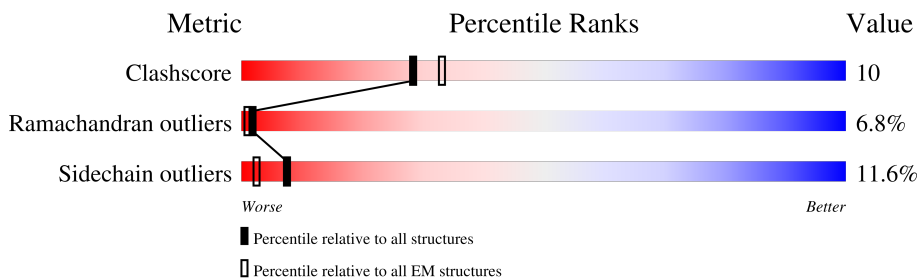
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.00 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	97 (10.50 - 11.50)

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	1	218	
1	2	218	
1	3	218	
1	4	218	

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Mol	Chain	Length	Quality of chain
1	5	218	24%16%57%
1	6	218	27%12%57%
2	A	810	7%57%31%8%
2	B	810	7%57%31%8%
2	C	810	6%59%31%7%
2	D	810	6%55%33%9%
2	E	810	7%59%28%9%
2	F	810	7%58%30%8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41862 atoms, of which 0 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 Adapter protein MecA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	2	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	3	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	4	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	5	94	Total	C	N	O	S	0	0
			777	498	123	154	2		
1	6	94	Total	C	N	O	S	0	0
			777	498	123	154	2		

- Molecule 2 is a protein called Negative regulator of genetic competence ClpC/MecB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	B	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	C	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	D	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	E	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		
2	F	798	Total	C	N	O	S	0	0
			6200	3850	1120	1215	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	618	ALA	GLU	engineered mutation	UNP P37571
B	618	ALA	GLU	engineered mutation	UNP P37571

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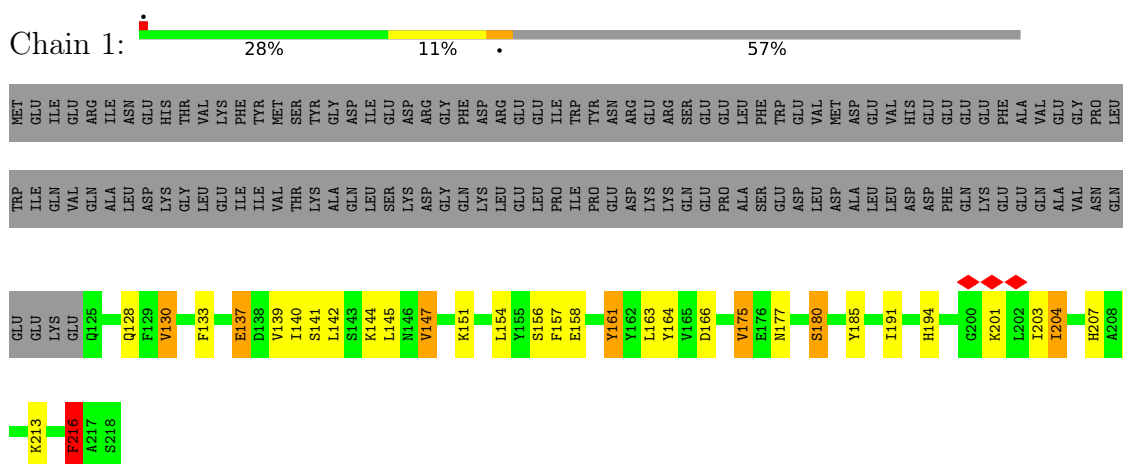
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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	ALA	GLU	engineered mutation	UNP P37571
D	618	ALA	GLU	engineered mutation	UNP P37571
E	618	ALA	GLU	engineered mutation	UNP P37571
F	618	ALA	GLU	engineered mutation	UNP P37571

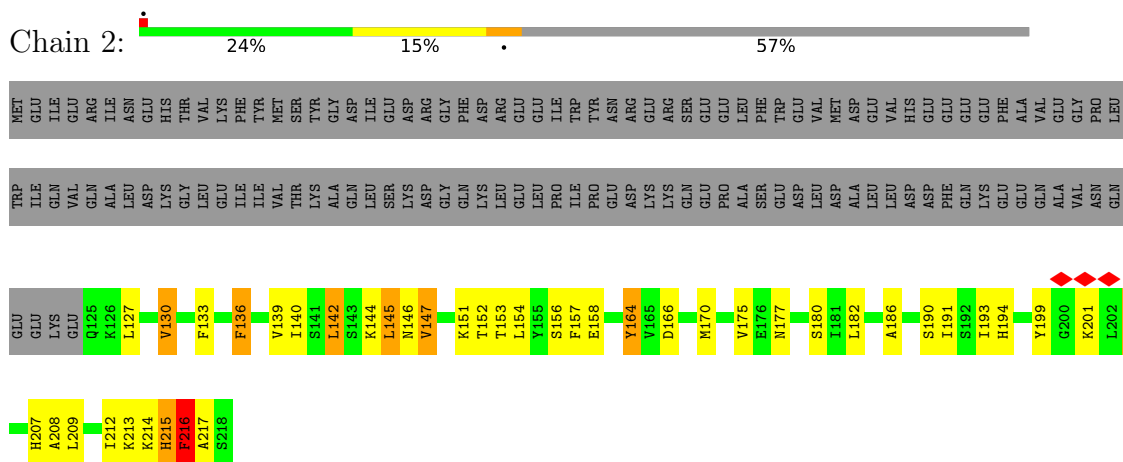
3 Residue-property plots

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

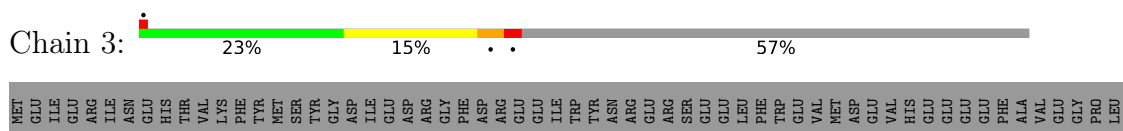
• Molecule 1: Adapter protein MecA 1

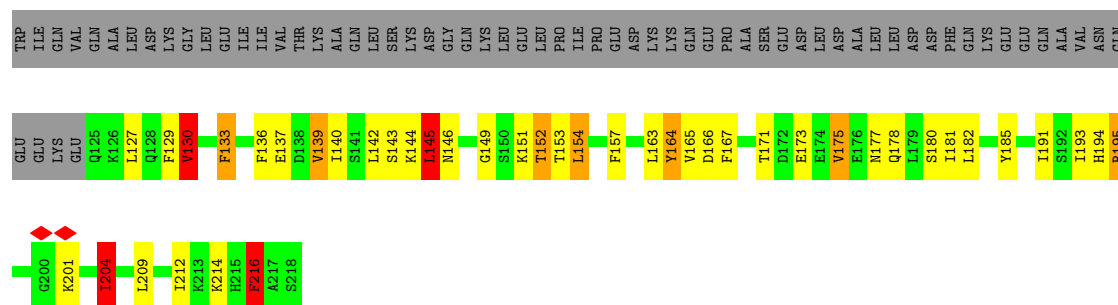


• Molecule 1: Adapter protein MecA 1



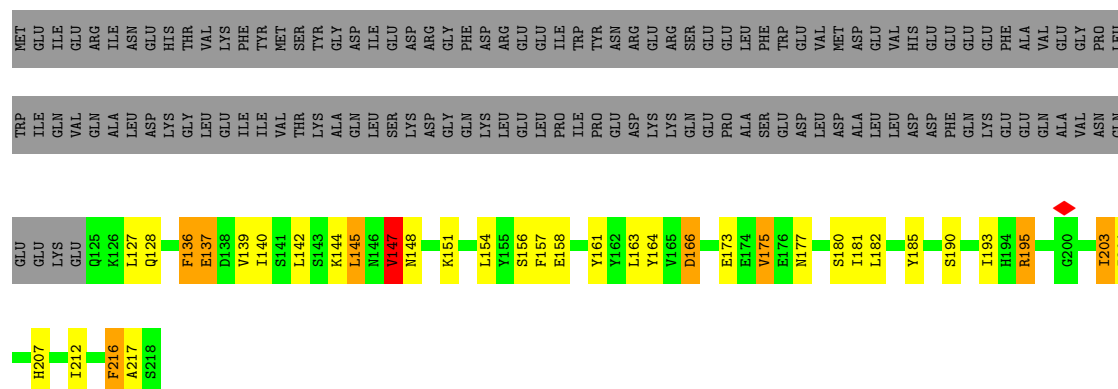
• Molecule 1: Adapter protein MecA 1





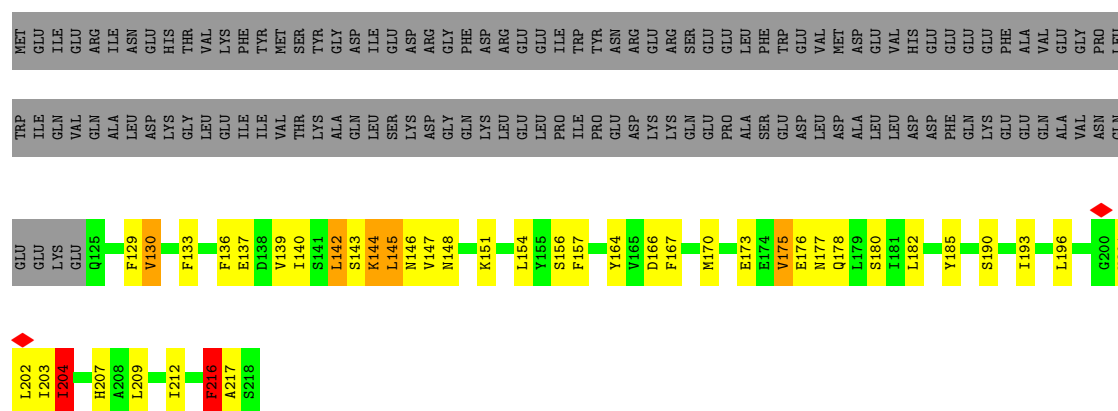
• Molecule 1: Adapter protein MecA 1

Chain 4: 27% 12% 57%



• Molecule 1: Adapter protein MecA 1

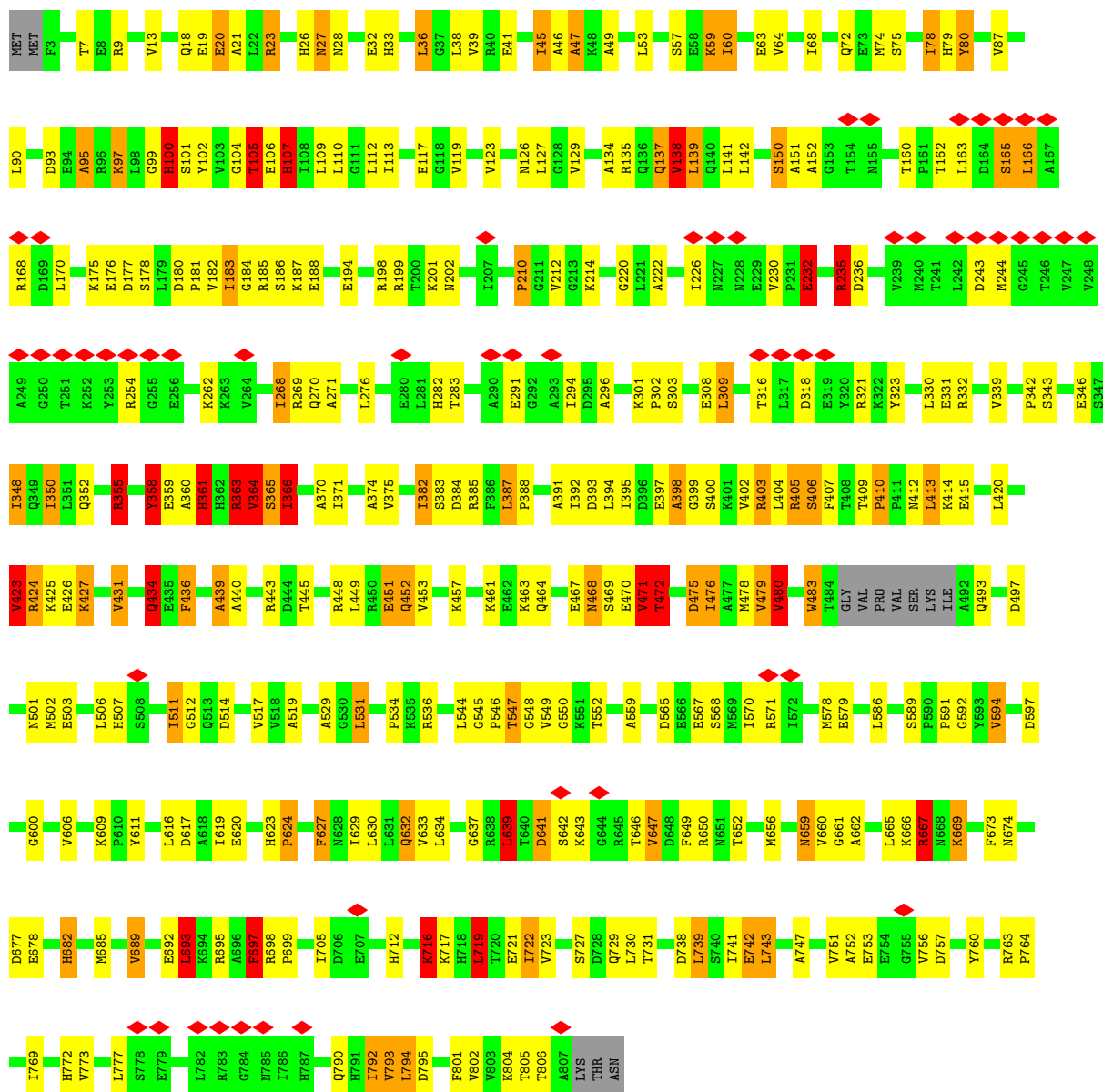
Chain 5: 24% 16% 57%

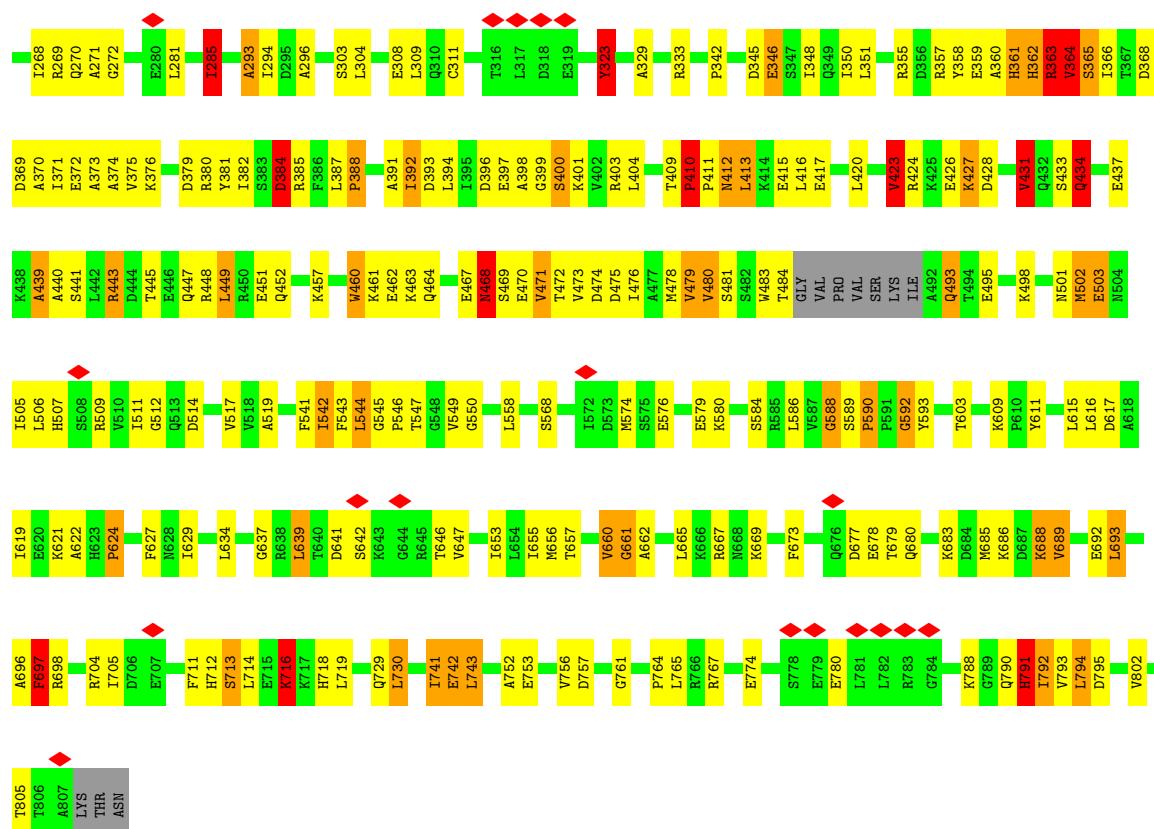


• Molecule 1: Adapter protein MecA 1

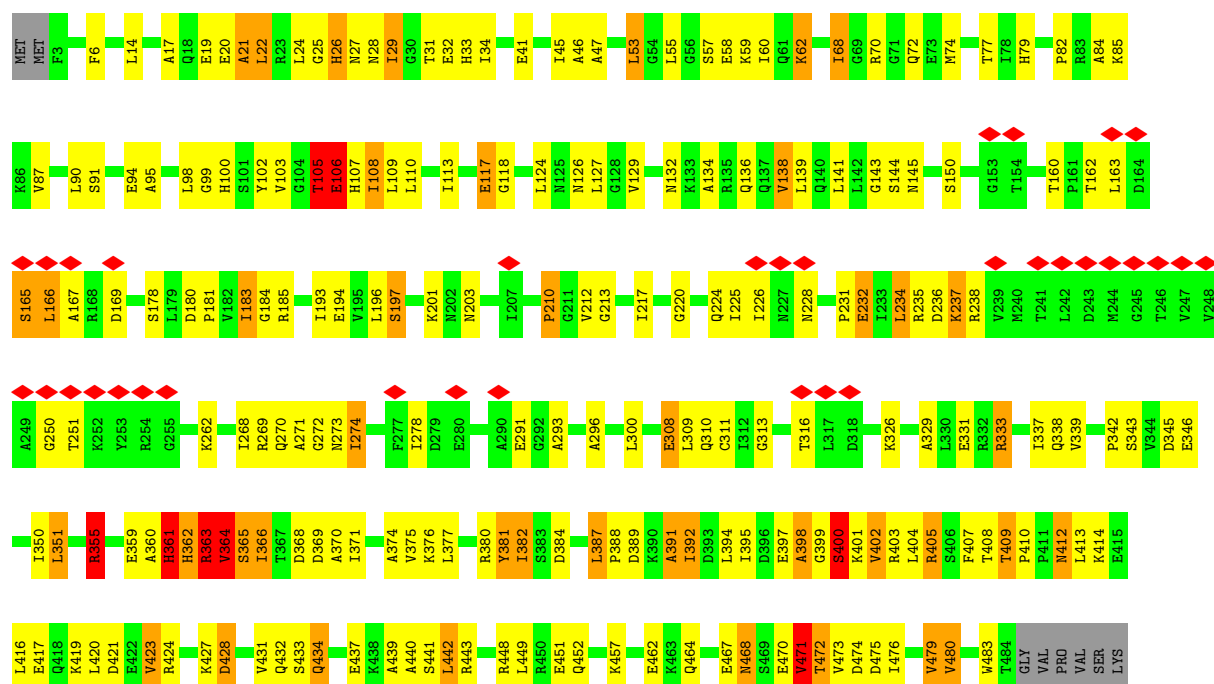
Chain 6: 27% 12% 57%

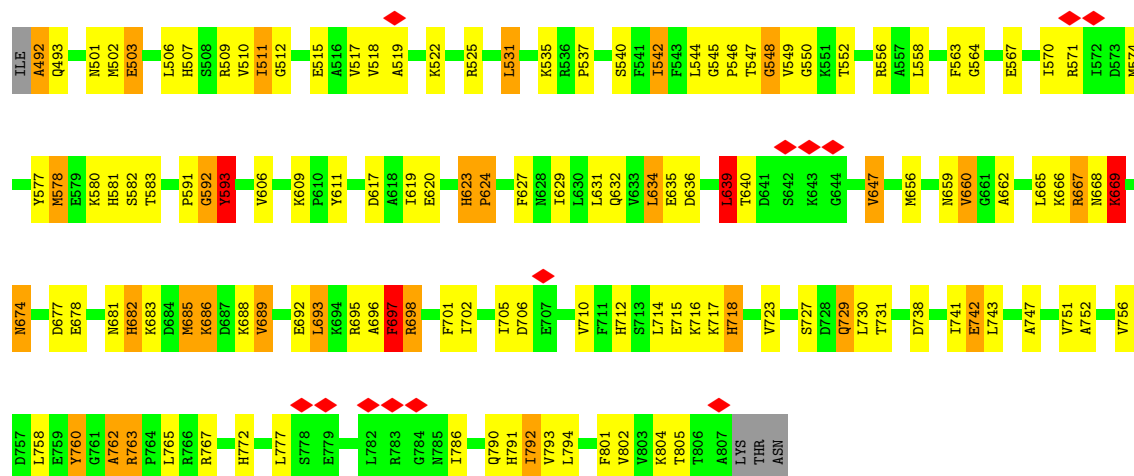




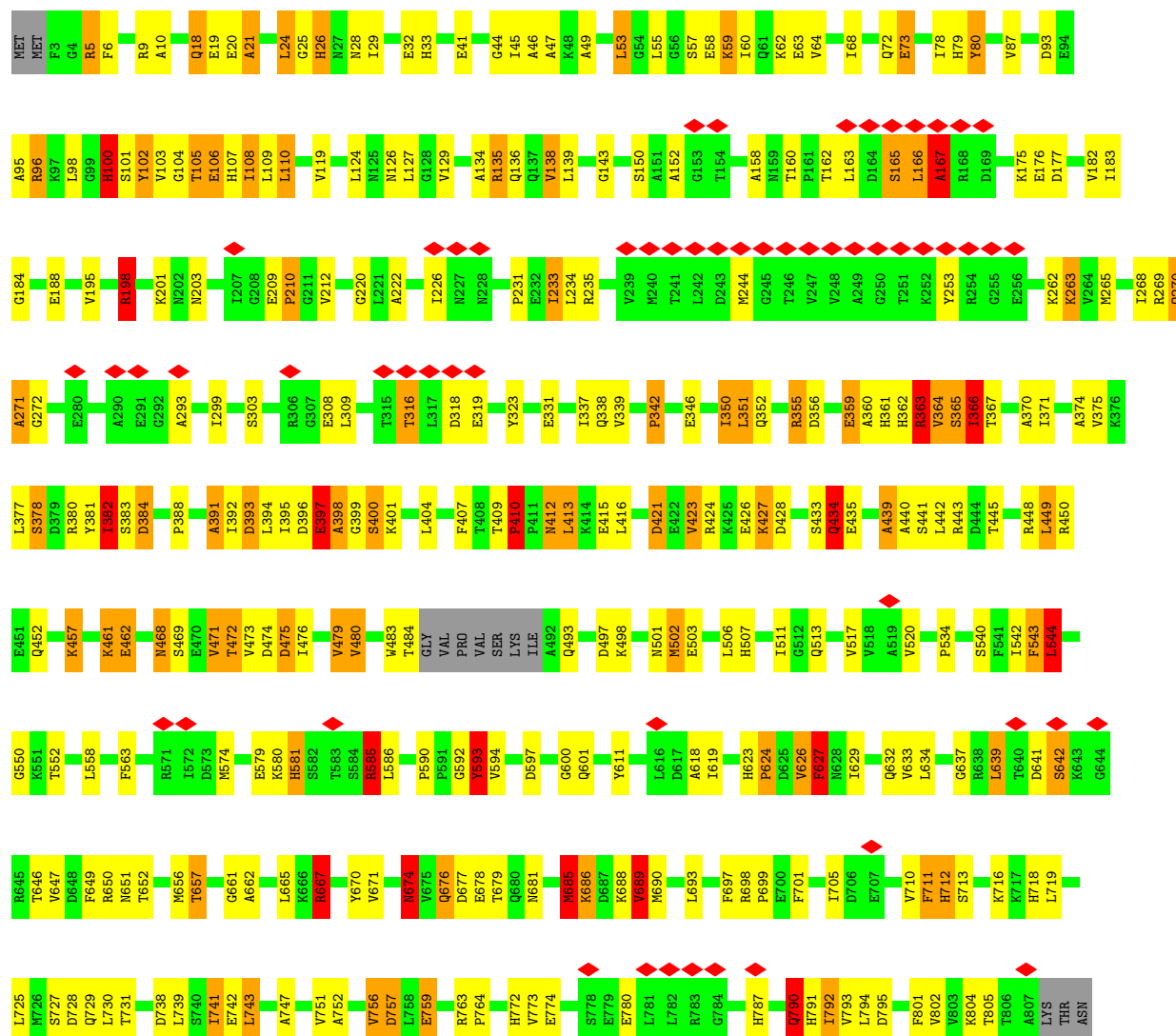


• Molecule 2: Negative regulator of genetic competence ClpC/MecB



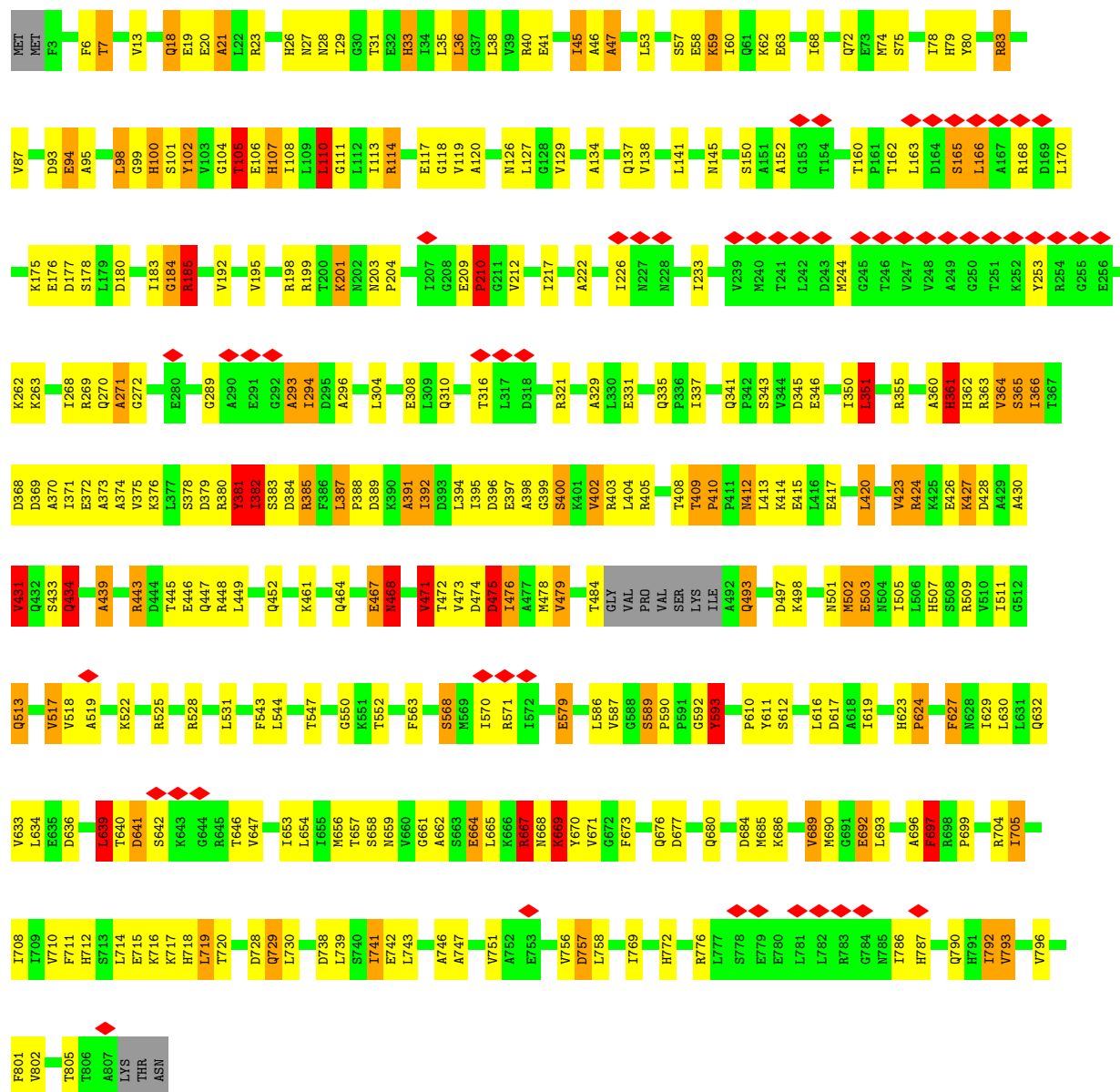


• Molecule 2: Negative regulator of genetic competence ClpC/MecB



● Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain F: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	41902	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each defocus group on 3D level	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	7.059	Depositor
Minimum map value	-4.200	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.997	Depositor
Recommended contour level	1.5	Depositor
Map size ($\text{\AA}$)	225.0, 225.0, 225.0	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.5, 1.5, 1.5	Depositor

5 Model quality

5.1 Standard geometry

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	1	1.40	0/791	1.79	18/1064 (1.7%)
1	2	1.38	2/791 (0.3%)	1.90	23/1064 (2.2%)
1	3	1.39	0/791	1.89	28/1064 (2.6%)
1	4	1.41	2/791 (0.3%)	1.77	19/1064 (1.8%)
1	5	1.38	1/791 (0.1%)	1.89	26/1064 (2.4%)
1	6	1.43	1/791 (0.1%)	1.90	20/1064 (1.9%)
2	A	1.40	10/6269 (0.2%)	1.92	190/8441 (2.3%)
2	B	1.40	5/6269 (0.1%)	1.95	210/8441 (2.5%)
2	C	1.38	3/6269 (0.0%)	1.93	200/8441 (2.4%)
2	D	1.39	10/6269 (0.2%)	1.95	227/8441 (2.7%)
2	E	1.38	10/6269 (0.2%)	1.94	225/8441 (2.7%)
2	F	1.40	7/6269 (0.1%)	1.92	206/8441 (2.4%)
All	All	1.39	51/42360 (0.1%)	1.93	1392/57030 (2.4%)

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	1	0	1
1	2	0	1
1	3	0	4
1	4	0	1
1	5	0	1
1	6	0	2
2	A	0	19
2	B	0	20
2	C	0	12
2	D	0	17
2	E	0	15
2	F	0	14
All	All	0	107

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	697	PHE	CA-C	-9.01	1.48	1.53
2	A	196	LEU	CA-C	-7.93	1.47	1.52
2	B	469	SER	CA-C	-7.09	1.49	1.53
2	D	196	LEU	CA-C	-7.05	1.45	1.53
2	E	793	VAL	CA-C	-6.46	1.45	1.52
2	B	689	VAL	CA-C	-6.34	1.45	1.52
2	A	792	ILE	CA-C	-6.28	1.44	1.52
2	E	792	ILE	CA-C	-6.23	1.44	1.52
2	F	21	ALA	CA-C	-6.20	1.45	1.52
2	F	689	VAL	CA-C	-6.06	1.45	1.52
2	D	685	MET	CA-C	-5.82	1.45	1.52
2	E	136	GLN	CA-C	-5.74	1.45	1.52
2	A	793	VAL	CA-C	-5.64	1.46	1.52
2	D	689	VAL	CA-C	-5.63	1.46	1.52
2	E	439	ALA	CA-C	-5.58	1.47	1.52
2	D	439	ALA	CA-C	-5.58	1.47	1.52
2	E	397	GLU	CA-C	-5.57	1.45	1.52
2	C	21	ALA	CA-C	-5.47	1.45	1.52
2	F	792	ILE	CA-C	-5.45	1.45	1.52
2	A	689	VAL	CA-C	-5.45	1.45	1.52
1	4	166	ASP	CA-C	-5.42	1.47	1.53
2	F	98	LEU	CA-C	-5.40	1.46	1.52
2	A	136	GLN	CA-C	-5.38	1.46	1.52
2	A	311	CYS	CA-C	-5.37	1.45	1.52
1	4	216	PHE	CA-C	-5.37	1.46	1.52
2	D	793	VAL	CA-C	-5.36	1.46	1.52
2	A	313	GLY	CA-C	-5.35	1.48	1.52
2	A	794	LEU	CA-C	-5.34	1.46	1.52
2	B	794	LEU	CA-C	-5.32	1.46	1.52
2	D	311	CYS	CA-C	-5.29	1.46	1.52
2	C	67	LEU	CA-C	-5.28	1.49	1.52
2	E	689	VAL	CA-C	-5.28	1.46	1.52
2	B	439	ALA	CA-C	-5.23	1.47	1.52
2	B	78	ILE	CA-C	-5.21	1.48	1.53
1	2	166	ASP	CA-C	-5.20	1.47	1.53
2	D	471	VAL	CA-C	-5.20	1.46	1.52
2	E	21	ALA	CA-C	-5.18	1.46	1.52
2	E	794	LEU	CA-C	-5.16	1.46	1.52
1	2	153	THR	CA-C	-5.16	1.46	1.52
2	A	28	ASN	N-CA	-5.15	1.39	1.46
2	F	471	VAL	CA-C	-5.14	1.46	1.52
2	E	471	VAL	CA-C	-5.11	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	439	ALA	CA-C	-5.11	1.47	1.52
1	5	207	HIS	N-CA	-5.11	1.42	1.47
2	C	106	GLU	CA-C	-5.09	1.46	1.52
2	D	29	ILE	CA-C	-5.09	1.47	1.53
2	D	24	LEU	CA-C	-5.04	1.45	1.52
2	E	681	ASN	CA-C	-5.03	1.46	1.52
1	6	216	PHE	N-CA	-5.03	1.41	1.46
2	F	612	SER	CA-C	-5.01	1.46	1.52
2	D	402	VAL	CA-CB	-5.01	1.47	1.54

All (1392) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	215	HIS	CA-CB-CG	11.28	125.08	113.80
1	2	203	ILE	N-CA-C	-11.20	102.77	111.62
2	C	285	ILE	N-CA-C	11.02	121.85	110.72
2	E	627	PHE	CA-CB-CG	-10.60	103.20	113.80
2	A	165	SER	CA-C-N	10.40	140.43	121.70
2	A	165	SER	C-N-CA	10.40	140.43	121.70
2	F	590	PRO	N-CA-C	9.95	122.83	110.70
2	B	165	SER	CA-C-N	9.83	139.40	121.70
2	B	165	SER	C-N-CA	9.83	139.40	121.70
2	F	165	SER	CA-C-N	9.81	139.35	121.70
2	F	165	SER	C-N-CA	9.81	139.35	121.70
2	B	410	PRO	N-CA-C	-9.77	98.78	110.70
2	F	79	HIS	N-CA-C	-9.77	95.31	109.18
2	E	590	PRO	N-CA-C	9.75	122.60	110.70
2	D	165	SER	CA-C-N	9.70	139.17	121.70
2	D	165	SER	C-N-CA	9.70	139.17	121.70
1	6	130	VAL	N-CA-C	-9.62	93.70	107.75
2	F	627	PHE	CA-CB-CG	-9.56	104.24	113.80
2	B	79	HIS	N-CA-C	-9.54	95.64	109.18
2	E	364	VAL	CA-C-N	9.53	138.86	121.70
2	E	364	VAL	C-N-CA	9.53	138.86	121.70
2	F	439	ALA	N-CA-C	-9.53	100.26	112.93
2	D	802	VAL	N-CA-C	-9.44	95.34	108.27
2	E	79	HIS	N-CA-C	-9.40	95.83	109.18
1	6	216	PHE	CA-CB-CG	-9.39	104.41	113.80
2	C	79	HIS	N-CA-C	-9.32	95.95	109.18
2	C	165	SER	CA-C-N	9.29	138.42	121.70
2	C	165	SER	C-N-CA	9.29	138.42	121.70
2	C	689	VAL	N-CA-C	-9.29	102.29	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	689	VAL	N-CA-C	-9.29	102.29	110.74
2	D	364	VAL	CA-C-N	9.28	138.41	121.70
2	D	364	VAL	C-N-CA	9.28	138.41	121.70
2	B	511	ILE	N-CA-C	-9.27	103.90	112.43
2	B	802	VAL	N-CA-C	-9.23	95.63	108.27
2	B	364	VAL	CA-C-N	9.21	138.28	121.70
2	B	364	VAL	C-N-CA	9.21	138.28	121.70
2	E	689	VAL	N-CA-C	-9.08	102.47	110.74
2	A	79	HIS	N-CA-C	-8.96	96.45	109.18
2	E	421	ASP	CA-CB-CG	8.87	121.47	112.60
2	E	165	SER	CA-C-N	8.77	137.49	121.70
2	E	165	SER	C-N-CA	8.77	137.49	121.70
2	C	544	LEU	N-CA-C	-8.77	96.83	110.42
2	A	802	VAL	N-CA-C	-8.75	96.80	108.35
2	B	183	ILE	CA-C-N	8.73	128.39	120.10
2	B	183	ILE	C-N-CA	8.73	128.39	120.10
2	B	110	LEU	CA-C-N	8.72	129.66	119.98
2	B	110	LEU	C-N-CA	8.72	129.66	119.98
2	C	588	GLY	N-CA-C	-8.70	92.55	113.18
2	D	805	THR	N-CA-C	-8.66	95.81	109.50
1	6	129	PHE	CA-CB-CG	-8.63	105.17	113.80
2	F	593	TYR	N-CA-C	8.63	121.77	111.33
2	A	366	ILE	CA-C-N	8.61	137.20	121.70
2	A	366	ILE	C-N-CA	8.61	137.20	121.70
2	E	101	SER	N-CA-C	-8.61	102.55	113.23
2	A	47	ALA	CA-C-N	8.57	131.58	120.44
2	A	47	ALA	C-N-CA	8.57	131.58	120.44
2	B	439	ALA	N-CA-C	-8.53	101.58	112.93
2	F	511	ILE	N-CA-C	-8.51	104.16	113.43
2	A	382	ILE	CA-C-N	8.47	136.95	121.70
2	A	382	ILE	C-N-CA	8.47	136.95	121.70
2	F	711	PHE	N-CA-C	-8.46	96.18	109.72
2	E	366	ILE	CA-C-N	8.40	136.82	121.70
2	E	366	ILE	C-N-CA	8.40	136.82	121.70
2	B	361	HIS	CA-CB-CG	8.34	122.14	113.80
2	C	105	THR	N-CA-C	8.32	121.40	111.33
1	3	130	VAL	N-CA-C	-8.28	95.66	107.75
2	C	364	VAL	CA-C-N	8.22	136.50	121.70
2	C	364	VAL	C-N-CA	8.22	136.50	121.70
2	A	689	VAL	N-CA-C	-8.21	102.86	110.82
2	C	360	ALA	N-CA-C	-8.20	100.93	113.89
1	5	129	PHE	CA-CB-CG	-8.18	105.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	47	ALA	CA-C-N	8.15	131.04	120.44
2	D	47	ALA	C-N-CA	8.15	131.04	120.44
2	C	439	ALA	N-CA-C	-8.14	102.10	112.93
2	E	233	ILE	N-CA-C	-8.14	104.77	112.83
2	A	107	HIS	CA-CB-CG	-8.09	105.71	113.80
2	C	752	ALA	N-CA-C	8.07	121.00	111.71
2	D	470	GLU	N-CA-C	-8.06	97.49	108.38
2	B	47	ALA	CA-C-N	8.06	130.91	120.44
2	B	47	ALA	C-N-CA	8.06	130.91	120.44
2	E	439	ALA	N-CA-C	-8.04	102.23	112.93
2	C	743	LEU	N-CA-C	-8.04	96.13	109.24
2	A	426	GLU	CA-C-N	8.04	131.96	120.79
2	A	426	GLU	C-N-CA	8.04	131.96	120.79
2	E	802	VAL	N-CA-C	-8.01	97.29	108.27
2	C	106	GLU	N-CA-CB	8.01	121.62	110.01
2	F	669	LYS	N-CA-C	-7.96	103.58	112.57
1	3	149	GLY	N-CA-C	-7.93	104.81	115.36
2	E	805	THR	N-CA-C	-7.93	96.97	109.50
2	E	176	GLU	N-CA-C	-7.92	101.65	112.03
1	1	156	SER	N-CA-C	-7.89	96.03	108.90
1	3	129	PHE	CA-CB-CG	-7.87	105.93	113.80
2	D	350	ILE	CB-CA-C	-7.86	101.92	111.97
2	F	802	VAL	N-CA-C	-7.83	98.02	108.35
2	A	110	LEU	CA-C-N	7.82	128.66	119.98
2	A	110	LEU	C-N-CA	7.82	128.66	119.98
2	C	431	VAL	CB-CA-C	-7.81	100.05	112.16
1	2	217	ALA	N-CA-C	-7.81	98.32	110.42
2	A	534	PRO	N-CA-C	-7.81	105.63	114.92
2	E	166	LEU	CA-C-N	7.80	135.74	121.70
2	E	166	LEU	C-N-CA	7.80	135.74	121.70
2	D	331	GLU	N-CA-C	-7.77	105.76	114.62
2	F	697	PHE	N-CA-C	-7.76	101.30	108.75
2	B	232	GLU	N-CA-C	7.74	120.70	111.33
2	F	95	ALA	N-CA-C	-7.74	104.45	114.04
2	B	201	LYS	N-CA-C	-7.72	97.37	109.72
2	C	593	TYR	N-CA-C	7.71	120.66	111.33
1	2	156	SER	N-CA-C	-7.70	96.35	108.90
2	A	593	TYR	N-CA-C	7.69	120.63	111.33
2	A	669	LYS	N-CA-C	-7.68	94.44	110.80
1	2	136	PHE	CA-CB-CG	-7.66	106.14	113.80
2	A	594	VAL	CA-C-N	7.66	128.49	119.98
2	A	594	VAL	C-N-CA	7.66	128.49	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	433	SER	CA-C-N	7.64	136.14	121.54
2	F	433	SER	C-N-CA	7.64	136.14	121.54
2	E	780	GLU	N-CA-C	-7.63	104.58	114.04
2	A	359	GLU	N-CA-C	-7.61	103.73	113.16
2	E	428	ASP	CA-CB-CG	-7.60	105.00	112.60
1	3	149	GLY	CA-C-N	7.59	133.64	122.86
1	3	149	GLY	C-N-CA	7.59	133.64	122.86
2	B	382	ILE	CA-C-N	7.57	135.33	121.70
2	B	382	ILE	C-N-CA	7.57	135.33	121.70
2	E	167	ALA	N-CA-CB	7.56	121.74	110.40
2	B	360	ALA	N-CA-C	-7.55	103.63	112.92
2	A	677	ASP	N-CA-C	-7.55	103.87	113.23
2	E	711	PHE	N-CA-C	-7.55	97.94	109.41
1	5	217	ALA	N-CA-C	-7.51	98.08	110.17
2	E	688	LYS	CA-C-N	7.51	130.04	120.88
2	E	688	LYS	C-N-CA	7.51	130.04	120.88
2	A	439	ALA	N-CA-C	-7.50	102.96	112.93
2	B	426	GLU	CA-C-N	7.49	131.21	120.79
2	B	426	GLU	C-N-CA	7.49	131.21	120.79
2	B	639	LEU	N-CA-C	-7.49	97.67	109.50
2	D	361	HIS	N-CA-C	-7.48	101.31	110.88
2	E	639	LEU	N-CA-C	-7.48	97.68	109.50
2	C	410	PRO	N-CA-CB	-7.47	95.83	103.08
2	D	408	THR	N-CA-C	-7.44	104.05	113.43
2	C	119	VAL	N-CA-C	-7.43	103.21	110.72
2	E	57	SER	CA-C-N	7.42	130.44	120.65
2	E	57	SER	C-N-CA	7.42	130.44	120.65
2	A	623	HIS	CA-CB-CG	7.41	121.21	113.80
2	F	376	LYS	N-CA-C	7.41	120.00	111.11
2	A	659	ASN	N-CA-C	-7.39	101.37	110.61
2	A	511	ILE	N-CA-C	-7.38	104.05	111.88
2	C	805	THR	N-CA-C	-7.38	97.84	109.50
1	1	201	LYS	CA-C-N	7.36	131.87	120.75
1	1	201	LYS	C-N-CA	7.36	131.87	120.75
2	B	410	PRO	CA-C-O	-7.36	109.88	120.56
2	C	793	VAL	N-CA-C	-7.36	97.87	108.17
2	C	511	ILE	N-CA-C	-7.36	95.31	106.42
2	C	47	ALA	CA-C-N	7.33	129.96	120.44
2	C	47	ALA	C-N-CA	7.33	129.96	120.44
2	C	368	ASP	CA-C-N	7.33	131.08	120.38
2	C	368	ASP	C-N-CA	7.33	131.08	120.38
2	C	697	PHE	CA-CB-CG	-7.31	106.49	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	439	ALA	N-CA-C	-7.30	103.22	112.93
1	4	156	SER	N-CA-C	-7.30	97.00	108.90
2	E	382	ILE	CA-C-N	7.29	134.83	121.70
2	E	382	ILE	C-N-CA	7.29	134.83	121.70
2	D	180	ASP	N-CA-C	-7.29	97.73	109.40
2	D	688	LYS	CA-C-N	7.29	129.78	120.88
2	D	688	LYS	C-N-CA	7.29	129.78	120.88
2	A	180	ASP	N-CA-C	-7.28	99.98	110.40
2	B	28	ASN	CA-CB-CG	-7.28	105.33	112.60
2	C	791	HIS	CA-CB-CG	-7.27	106.53	113.80
2	C	350	ILE	CA-C-N	7.24	130.85	120.79
2	C	350	ILE	C-N-CA	7.24	130.85	120.79
2	C	646	THR	N-CA-C	-7.22	96.75	108.52
2	A	176	GLU	N-CA-C	-7.22	104.50	113.38
2	B	104	GLY	CA-C-N	7.21	130.26	120.38
2	B	104	GLY	C-N-CA	7.21	130.26	120.38
2	D	359	GLU	N-CA-C	-7.20	104.53	113.38
2	A	568	SER	N-CA-C	-7.19	95.48	110.80
2	E	331	GLU	N-CA-C	-7.17	104.57	113.38
2	B	677	ASP	N-CA-C	-7.16	104.35	113.23
2	D	310	GLN	N-CA-C	-7.16	95.39	107.99
2	F	428	ASP	CA-CB-CG	-7.12	105.48	112.60
2	A	718	HIS	CA-C-N	7.11	130.68	120.79
2	A	718	HIS	C-N-CA	7.11	130.68	120.79
2	F	361	HIS	N-CA-C	-7.11	104.86	113.97
2	A	29	ILE	N-CA-C	-7.10	96.66	107.73
2	C	176	GLU	N-CA-C	-7.08	96.53	109.56
2	D	639	LEU	N-CA-C	-7.08	98.32	109.50
2	D	105	THR	N-CA-C	7.06	119.87	111.33
2	E	26	HIS	CA-C-N	7.04	129.72	120.28
2	E	26	HIS	C-N-CA	7.04	129.72	120.28
2	C	350	ILE	CB-CA-C	-7.04	102.96	111.97
2	D	682	HIS	CA-CB-CG	7.04	120.84	113.80
2	A	629	ILE	N-CA-C	-7.02	104.01	110.82
2	E	19	GLU	N-CA-CB	7.01	120.58	110.06
1	5	156	SER	N-CA-C	-6.99	97.51	108.90
2	E	743	LEU	N-CA-C	-6.98	97.86	109.24
2	C	232	GLU	CA-C-N	6.98	129.35	120.56
2	C	232	GLU	C-N-CA	6.98	129.35	120.56
2	D	692	GLU	CA-C-N	6.97	130.12	120.63
2	D	692	GLU	C-N-CA	6.97	130.12	120.63
2	F	141	LEU	N-CA-C	-6.97	103.79	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	729	GLN	N-CA-C	-6.96	103.46	112.23
2	B	366	ILE	CA-C-N	6.96	134.22	121.70
2	B	366	ILE	C-N-CA	6.96	134.22	121.70
2	B	410	PRO	CB-CA-C	6.96	119.41	110.92
1	4	175	VAL	N-CA-C	-6.95	104.08	110.82
2	D	667	ARG	N-CA-C	-6.95	102.07	111.87
2	B	57	SER	CA-C-N	6.95	129.82	120.65
2	B	57	SER	C-N-CA	6.95	129.82	120.65
2	F	296	ALA	CA-C-N	6.94	130.51	120.38
2	F	296	ALA	C-N-CA	6.94	130.51	120.38
2	F	409	THR	N-CA-C	-6.93	98.30	109.40
2	E	646	THR	N-CA-C	-6.93	97.23	108.52
2	D	677	ASP	N-CA-C	-6.92	104.65	113.23
2	E	593	TYR	N-CA-C	6.92	119.70	111.33
2	F	426	GLU	CA-C-N	6.91	130.40	120.79
2	F	426	GLU	C-N-CA	6.91	130.40	120.79
2	E	110	LEU	CA-C-N	6.91	128.78	120.14
2	E	110	LEU	C-N-CA	6.91	128.78	120.14
2	F	105	THR	N-CA-C	6.90	119.68	111.33
2	F	28	ASN	CA-CB-CG	-6.89	105.71	112.60
2	F	106	GLU	N-CA-CB	6.89	120.01	110.01
2	A	763	ARG	CA-C-N	6.88	126.56	119.82
2	A	763	ARG	C-N-CA	6.88	126.56	119.82
2	F	405	ARG	CA-C-N	6.88	129.38	120.44
2	F	405	ARG	C-N-CA	6.88	129.38	120.44
2	A	544	LEU	N-CA-C	-6.88	99.76	110.42
2	B	646	THR	N-CA-C	-6.87	97.32	108.52
2	A	681	ASN	N-CA-C	-6.87	103.58	112.23
2	C	696	ALA	CA-C-N	6.86	131.11	120.75
2	C	696	ALA	C-N-CA	6.86	131.11	120.75
2	F	590	PRO	CA-C-O	-6.86	110.62	120.56
2	E	47	ALA	CA-C-N	6.84	129.34	120.44
2	E	47	ALA	C-N-CA	6.84	129.34	120.44
2	F	568	SER	N-CA-C	-6.84	96.23	110.80
2	B	296	ALA	CA-C-N	6.84	130.36	120.38
2	B	296	ALA	C-N-CA	6.84	130.36	120.38
2	B	689	VAL	N-CA-CB	6.83	118.84	110.64
2	E	28	ASN	CA-CB-CG	-6.82	105.78	112.60
2	C	28	ASN	CA-CB-CG	-6.82	105.78	112.60
2	A	590	PRO	N-CA-C	6.81	119.01	110.70
2	F	331	GLU	N-CA-C	-6.81	104.86	113.43
2	F	692	GLU	CA-C-N	6.79	129.87	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	692	GLU	C-N-CA	6.79	129.87	120.63
2	B	36	LEU	CA-C-N	6.78	127.50	119.98
2	B	36	LEU	C-N-CA	6.78	127.50	119.98
2	D	333	ARG	N-CA-C	-6.77	96.39	110.80
2	F	175	LYS	N-CA-C	-6.76	105.56	113.88
2	E	581	HIS	CA-C-N	6.76	129.34	120.28
2	E	581	HIS	C-N-CA	6.76	129.34	120.28
2	E	752	ALA	N-CA-C	6.74	119.46	111.71
1	4	139	VAL	CA-C-N	6.74	129.29	120.60
1	4	139	VAL	C-N-CA	6.74	129.29	120.60
2	A	471	VAL	CA-C-N	6.74	134.41	121.54
2	A	471	VAL	C-N-CA	6.74	134.41	121.54
2	C	222	ALA	CA-C-N	6.73	129.30	120.28
2	C	222	ALA	C-N-CA	6.73	129.30	120.28
2	F	659	ASN	CA-CB-CG	-6.73	105.87	112.60
2	D	448	ARG	CA-C-N	6.73	130.14	120.79
2	D	448	ARG	C-N-CA	6.73	130.14	120.79
2	A	646	THR	N-CA-C	-6.72	97.56	108.52
2	C	118	GLY	CA-C-N	6.72	129.97	120.42
2	C	118	GLY	C-N-CA	6.72	129.97	120.42
1	5	167	PHE	N-CA-C	-6.72	98.97	109.25
2	D	548	GLY	CA-C-N	6.72	129.67	120.46
2	D	548	GLY	C-N-CA	6.72	129.67	120.46
2	E	792	ILE	N-CA-C	-6.72	97.94	107.75
2	D	511	ILE	N-CA-C	-6.71	104.76	111.88
1	5	145	LEU	CA-C-N	6.71	130.24	120.71
1	5	145	LEU	C-N-CA	6.71	130.24	120.71
2	A	393	ASP	CA-C-N	6.70	129.15	120.44
2	A	393	ASP	C-N-CA	6.70	129.15	120.44
2	E	685	MET	N-CA-CB	6.70	120.18	110.20
2	F	360	ALA	N-CA-C	-6.70	104.73	113.17
2	E	234	LEU	N-CA-C	-6.69	100.49	110.06
2	A	270	GLN	CA-C-N	6.68	134.29	121.54
2	A	270	GLN	C-N-CA	6.68	134.29	121.54
2	E	222	ALA	CA-C-N	6.68	129.23	120.28
2	E	222	ALA	C-N-CA	6.68	129.23	120.28
2	A	448	ARG	CA-C-N	6.68	130.07	120.79
2	A	448	ARG	C-N-CA	6.68	130.07	120.79
2	C	28	ASN	N-CA-C	-6.67	98.03	108.90
2	C	333	ARG	N-CA-C	-6.66	96.61	110.80
2	B	316	THR	CA-C-N	6.66	130.80	120.82
2	B	316	THR	C-N-CA	6.66	130.80	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	108	ILE	N-CA-C	6.65	116.78	110.53
2	B	176	GLU	N-CA-C	-6.65	104.39	113.30
2	C	794	LEU	N-CA-C	-6.65	97.69	108.52
1	3	175	VAL	N-CA-C	-6.64	104.38	110.82
1	2	130	VAL	N-CA-C	-6.64	98.06	107.75
2	C	363	ARG	N-CA-C	-6.63	96.67	110.80
2	F	201	LYS	CB-CA-C	-6.62	102.96	111.50
2	E	677	ASP	N-CA-C	-6.61	105.04	113.23
2	D	669	LYS	N-CA-C	-6.61	96.73	110.80
2	A	72	GLN	CA-C-N	6.60	129.13	120.28
2	A	72	GLN	C-N-CA	6.60	129.13	120.28
2	B	178	SER	N-CA-C	-6.60	105.14	113.72
2	D	666	LYS	N-CA-C	-6.58	105.13	112.57
1	2	207	HIS	N-CA-C	-6.56	103.44	112.03
2	E	594	VAL	CA-C-N	6.55	127.25	119.98
2	E	594	VAL	C-N-CA	6.55	127.25	119.98
2	B	692	GLU	CA-C-N	6.55	129.53	120.63
2	B	692	GLU	C-N-CA	6.55	129.53	120.63
2	F	351	LEU	CA-C-N	6.54	129.34	120.38
2	F	351	LEU	C-N-CA	6.54	129.34	120.38
2	A	639	LEU	N-CA-C	-6.53	99.18	109.50
2	A	404	LEU	N-CA-C	-6.52	102.65	112.04
2	A	364	VAL	CA-C-N	6.52	133.43	121.70
2	A	364	VAL	C-N-CA	6.52	133.43	121.70
2	B	548	GLY	CA-C-N	6.52	129.39	120.46
2	B	548	GLY	C-N-CA	6.52	129.39	120.46
2	F	7	THR	CA-C-N	6.52	129.85	120.79
2	F	7	THR	C-N-CA	6.52	129.85	120.79
2	F	471	VAL	CA-C-N	6.52	133.99	121.54
2	F	471	VAL	C-N-CA	6.52	133.99	121.54
2	D	213	GLY	N-CA-C	-6.51	97.75	113.18
2	D	632	GLN	CB-CA-C	-6.51	98.78	110.70
2	E	679	THR	N-CA-C	6.51	120.90	113.15
2	A	428	ASP	CA-CB-CG	-6.51	106.09	112.60
2	E	93	ASP	CA-CB-CG	-6.51	106.09	112.60
2	D	659	ASN	N-CA-C	-6.49	103.01	111.71
2	E	581	HIS	N-CA-C	-6.49	105.24	112.57
2	E	44	GLY	N-CA-C	-6.48	97.81	113.18
2	B	413	LEU	CA-C-N	6.48	130.97	120.60
2	B	413	LEU	C-N-CA	6.48	130.97	120.60
2	C	80	TYR	CA-CB-CG	-6.48	102.24	113.90
2	F	180	ASP	N-CA-C	-6.47	100.36	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	LYS	N-CA-C	-6.47	100.11	110.14
2	D	674	ASN	CA-C-N	6.47	129.32	120.46
2	D	674	ASN	C-N-CA	6.47	129.32	120.46
2	E	135	ARG	CA-C-N	6.47	129.19	120.65
2	E	135	ARG	C-N-CA	6.47	129.19	120.65
2	B	699	PRO	CA-C-N	6.47	129.59	120.28
2	B	699	PRO	C-N-CA	6.47	129.59	120.28
2	C	110	LEU	CA-C-N	6.47	128.22	120.14
2	C	110	LEU	C-N-CA	6.47	128.22	120.14
2	C	461	LYS	N-CA-C	-6.46	105.39	113.28
2	E	448	ARG	CA-C-N	6.46	129.18	120.65
2	E	448	ARG	C-N-CA	6.46	129.18	120.65
2	D	718	HIS	N-CA-C	-6.46	103.47	112.45
2	D	693	LEU	N-CA-C	-6.45	103.87	111.03
2	F	176	GLU	N-CA-C	-6.44	104.90	112.89
1	6	175	VAL	N-CA-C	-6.44	104.58	110.82
2	C	363	ARG	N-CA-CB	6.44	121.37	110.49
1	2	201	LYS	CA-C-N	6.42	130.45	120.75
1	2	201	LYS	C-N-CA	6.42	130.45	120.75
2	D	405	ARG	CA-C-N	6.42	128.79	120.44
2	D	405	ARG	C-N-CA	6.42	128.79	120.44
2	F	382	ILE	CA-C-N	6.42	133.26	121.70
2	F	382	ILE	C-N-CA	6.42	133.26	121.70
2	C	678	GLU	CB-CA-C	-6.41	100.02	110.79
2	F	793	VAL	N-CA-C	-6.41	99.20	108.17
2	D	624	PRO	CA-C-N	6.40	129.38	120.29
2	D	624	PRO	C-N-CA	6.40	129.38	120.29
2	D	308	GLU	N-CA-C	-6.39	104.39	111.36
2	C	780	GLU	N-CA-C	-6.38	106.12	114.04
2	A	693	LEU	N-CA-C	-6.38	103.95	111.03
2	C	382	ILE	CA-C-N	6.38	133.18	121.70
2	C	382	ILE	C-N-CA	6.38	133.18	121.70
2	B	469	SER	N-CA-C	-6.38	103.55	108.78
2	D	183	ILE	CA-C-N	6.37	126.39	120.34
2	D	183	ILE	C-N-CA	6.37	126.39	120.34
2	B	359	GLU	N-CA-C	-6.37	104.66	112.88
2	A	764	PRO	CA-C-N	6.36	129.32	120.29
2	A	764	PRO	C-N-CA	6.36	129.32	120.29
2	E	95	ALA	N-CA-C	-6.36	106.15	114.04
2	A	186	SER	N-CA-C	6.35	121.19	112.04
2	A	765	LEU	N-CA-C	-6.35	104.44	111.36
2	B	7	THR	CA-C-N	6.35	129.61	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	THR	C-N-CA	6.35	129.61	120.79
2	E	377	LEU	CA-C-N	6.34	129.30	120.29
2	E	377	LEU	C-N-CA	6.34	129.30	120.29
2	A	692	GLU	CA-C-N	6.34	129.25	120.63
2	A	692	GLU	C-N-CA	6.34	129.25	120.63
2	E	729	GLN	N-CA-C	-6.34	103.90	111.69
2	B	95	ALA	N-CA-C	-6.33	106.19	114.04
2	D	421	ASP	CA-CB-CG	6.33	118.93	112.60
1	5	201	LYS	CA-C-N	6.33	130.31	120.75
1	5	201	LYS	C-N-CA	6.33	130.31	120.75
2	D	509	ARG	N-CA-C	-6.32	106.53	114.56
2	B	629	ILE	N-CA-C	-6.32	104.69	110.82
2	F	369	ASP	CA-CB-CG	-6.32	106.28	112.60
1	1	139	VAL	CA-C-N	6.31	128.74	120.60
1	1	139	VAL	C-N-CA	6.31	128.74	120.60
2	F	113	ILE	CA-C-N	6.30	129.05	120.54
2	F	113	ILE	C-N-CA	6.30	129.05	120.54
2	A	804	LYS	N-CA-C	-6.30	99.90	109.85
2	E	198	ARG	N-CA-C	-6.30	100.59	110.36
2	B	529	ALA	N-CA-C	-6.28	105.55	113.72
2	E	676	GLN	N-CA-C	-6.28	105.62	113.28
2	F	632	GLN	N-CA-C	-6.28	103.96	111.69
1	3	167	PHE	N-CA-C	-6.28	99.64	109.25
2	B	667	ARG	N-CA-C	-6.28	97.43	110.80
2	D	384	ASP	CA-CB-CG	6.28	118.88	112.60
2	E	59	LYS	CA-C-N	6.28	128.38	120.72
2	E	59	LYS	C-N-CA	6.28	128.38	120.72
2	C	433	SER	CA-C-N	6.28	133.53	121.54
2	C	433	SER	C-N-CA	6.28	133.53	121.54
2	E	637	GLY	N-CA-C	-6.28	104.09	114.76
2	F	696	ALA	N-CA-C	-6.27	105.94	113.97
2	B	398	ALA	CA-C-N	6.27	133.70	121.41
2	B	398	ALA	C-N-CA	6.27	133.70	121.41
2	C	104	GLY	CA-C-N	6.27	128.97	120.38
2	C	104	GLY	C-N-CA	6.27	128.97	120.38
2	F	509	ARG	N-CA-C	-6.27	106.60	114.56
2	C	688	LYS	CA-C-N	6.27	128.53	120.88
2	C	688	LYS	C-N-CA	6.27	128.53	120.88
2	D	449	LEU	CA-C-N	6.26	129.50	120.79
2	D	449	LEU	C-N-CA	6.26	129.50	120.79
1	6	139	VAL	CA-C-N	6.25	128.67	120.60
1	6	139	VAL	C-N-CA	6.25	128.67	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	448	ARG	CA-C-N	6.25	129.47	120.79
2	C	448	ARG	C-N-CA	6.25	129.47	120.79
1	2	180	SER	CA-C-N	6.24	128.66	120.60
1	2	180	SER	C-N-CA	6.24	128.66	120.60
2	E	28	ASN	N-CA-C	-6.24	98.73	108.90
2	D	350	ILE	CA-C-N	6.24	129.46	120.79
2	D	350	ILE	C-N-CA	6.24	129.46	120.79
2	E	705	ILE	N-CA-CB	6.24	117.33	110.53
2	C	270	GLN	CA-C-N	6.23	133.43	121.54
2	C	270	GLN	C-N-CA	6.23	133.43	121.54
2	C	345	ASP	CA-C-N	6.22	128.62	120.28
2	C	345	ASP	C-N-CA	6.22	128.62	120.28
2	D	113	ILE	CA-C-N	6.22	128.93	120.54
2	D	113	ILE	C-N-CA	6.22	128.93	120.54
2	A	434	GLN	CA-C-N	6.21	132.88	121.70
2	A	434	GLN	C-N-CA	6.21	132.88	121.70
1	3	178	GLN	CA-C-N	6.21	129.23	120.28
1	3	178	GLN	C-N-CA	6.21	129.23	120.28
2	A	217	ILE	CB-CA-C	-6.21	103.75	112.14
2	F	28	ASN	N-CA-C	-6.21	98.78	108.90
2	A	296	ALA	CA-C-N	6.21	129.44	120.38
2	A	296	ALA	C-N-CA	6.21	129.44	120.38
2	E	426	GLU	CA-C-N	6.20	129.41	120.79
2	E	426	GLU	C-N-CA	6.20	129.41	120.79
2	D	464	GLN	N-CA-C	-6.20	103.12	112.04
2	F	47	ALA	CA-C-N	6.20	128.50	120.44
2	F	47	ALA	C-N-CA	6.20	128.50	120.44
1	5	130	VAL	N-CA-C	-6.19	98.71	107.75
2	D	669	LYS	N-CA-CB	6.19	120.95	110.49
2	B	244	MET	CA-C-N	6.19	126.85	119.98
2	B	244	MET	C-N-CA	6.19	126.85	119.98
2	E	678	GLU	CB-CA-C	-6.19	100.65	110.86
2	D	361	HIS	CA-C-N	6.18	133.35	121.54
2	D	361	HIS	C-N-CA	6.18	133.35	121.54
2	D	519	ALA	CA-C-N	6.18	128.35	120.56
2	D	519	ALA	C-N-CA	6.18	128.35	120.56
2	D	184	GLY	CA-C-N	6.18	132.82	121.70
2	D	184	GLY	C-N-CA	6.18	132.82	121.70
2	B	397	GLU	N-CA-CB	6.18	119.14	109.94
2	B	552	THR	CA-C-N	6.18	129.18	120.28
2	B	552	THR	C-N-CA	6.18	129.18	120.28
2	D	583	THR	CA-C-N	6.17	130.07	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	583	THR	C-N-CA	6.17	130.07	120.75
2	F	201	LYS	N-CA-CB	6.17	119.51	110.25
2	D	95	ALA	N-CA-C	-6.17	105.66	113.43
2	B	763	ARG	CA-C-N	6.17	125.86	119.82
2	B	763	ARG	C-N-CA	6.17	125.86	119.82
2	B	332	ARG	N-CA-C	-6.16	103.07	112.99
2	A	794	LEU	N-CA-C	-6.16	98.69	108.73
2	E	629	ILE	N-CA-C	-6.15	104.85	110.82
2	E	650	ARG	N-CA-C	-6.15	105.53	113.16
2	C	253	TYR	CA-C-N	6.15	129.02	120.29
2	C	253	TYR	C-N-CA	6.15	129.02	120.29
2	F	372	GLU	CA-C-N	6.15	128.80	120.44
2	F	372	GLU	C-N-CA	6.15	128.80	120.44
2	A	350	ILE	CA-C-N	6.14	129.33	120.79
2	A	350	ILE	C-N-CA	6.14	129.33	120.79
2	F	743	LEU	N-CA-C	-6.14	99.23	109.24
2	A	563	PHE	N-CA-C	-6.14	106.39	114.31
2	D	376	LYS	N-CA-C	6.14	118.48	111.11
2	C	764	PRO	CA-C-N	6.14	129.01	120.29
2	C	764	PRO	C-N-CA	6.14	129.01	120.29
2	E	774	GLU	CA-C-N	6.14	128.79	120.38
2	E	774	GLU	C-N-CA	6.14	128.79	120.38
2	B	729	GLN	N-CA-C	-6.13	104.50	112.23
2	F	757	ASP	N-CA-CB	6.13	120.86	110.49
2	A	63	GLU	CA-C-N	6.12	128.27	120.56
2	A	63	GLU	C-N-CA	6.12	128.27	120.56
2	C	180	ASP	N-CA-C	-6.12	100.90	110.14
2	F	409	THR	CA-C-N	6.12	126.68	120.38
2	F	409	THR	C-N-CA	6.12	126.68	120.38
2	D	210	PRO	CA-C-N	6.10	132.68	121.70
2	D	210	PRO	C-N-CA	6.10	132.68	121.70
2	D	729	GLN	N-CA-C	-6.10	104.18	111.69
2	A	752	ALA	N-CA-C	6.10	118.73	111.71
2	D	360	ALA	N-CA-C	-6.10	105.49	113.17
2	E	360	ALA	N-CA-C	-6.10	105.33	112.89
2	A	711	PHE	N-CA-C	-6.10	100.69	110.14
2	B	763	ARG	CA-C-O	-6.10	112.94	118.79
1	5	139	VAL	CA-C-N	6.09	128.46	120.60
1	5	139	VAL	C-N-CA	6.09	128.46	120.60
2	C	468	ASN	CA-CB-CG	6.09	118.69	112.60
2	C	509	ARG	N-CA-C	-6.08	106.50	114.04
2	A	294	ILE	N-CA-CB	6.07	121.24	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ASN	CA-CB-CG	-6.07	106.53	112.60
2	F	677	ASP	N-CA-C	-6.06	105.72	113.23
2	C	388	PRO	CA-C-N	6.05	128.31	120.44
2	C	388	PRO	C-N-CA	6.05	128.31	120.44
1	6	208	ALA	N-CA-C	6.05	117.54	111.07
2	F	699	PRO	CA-C-N	6.05	128.99	120.28
2	F	699	PRO	C-N-CA	6.05	128.99	120.28
2	C	753	GLU	N-CA-C	6.05	120.20	112.34
2	A	104	GLY	CA-C-N	6.05	128.66	120.38
2	A	104	GLY	C-N-CA	6.05	128.66	120.38
2	F	728	ASP	CA-CB-CG	-6.05	106.55	112.60
2	B	331	GLU	N-CA-C	-6.04	104.56	112.41
2	B	107	HIS	CA-CB-CG	-6.04	107.76	113.80
2	C	329	ALA	N-CA-C	-6.04	105.74	112.57
2	D	369	ASP	CA-CB-CG	-6.04	106.56	112.60
2	E	24	LEU	N-CA-C	-6.04	105.72	114.12
2	C	95	ALA	N-CA-C	-6.04	106.55	114.04
2	B	650	ARG	N-CA-C	-6.04	105.68	113.16
2	A	197	SER	N-CA-C	-6.03	100.72	109.59
2	C	244	MET	CA-C-N	6.03	126.67	119.98
2	C	244	MET	C-N-CA	6.03	126.67	119.98
2	D	382	ILE	CA-C-N	6.03	132.55	121.70
2	D	382	ILE	C-N-CA	6.03	132.55	121.70
2	B	471	VAL	CA-C-N	6.02	133.03	121.54
2	B	471	VAL	C-N-CA	6.02	133.03	121.54
1	6	156	SER	N-CA-C	-6.02	99.09	108.90
2	A	689	VAL	N-CA-CB	6.01	119.18	110.52
2	C	186	SER	N-CA-C	6.01	120.69	112.04
2	D	492	ALA	CA-C-N	6.01	133.02	121.54
2	D	492	ALA	C-N-CA	6.01	133.02	121.54
2	E	396	ASP	N-CA-C	6.01	117.91	111.36
2	F	59	LYS	CA-C-N	6.01	128.05	120.72
2	F	59	LYS	C-N-CA	6.01	128.05	120.72
2	A	244	MET	CA-C-N	6.01	126.65	119.98
2	A	244	MET	C-N-CA	6.01	126.65	119.98
2	E	501	ASN	CA-CB-CG	-6.01	106.59	112.60
2	F	263	LYS	CA-C-N	6.00	128.69	120.46
2	F	263	LYS	C-N-CA	6.00	128.69	120.46
2	E	641	ASP	CA-C-N	6.00	133.00	121.54
2	E	641	ASP	C-N-CA	6.00	133.00	121.54
1	6	178	GLN	CA-C-N	6.00	128.92	120.28
1	6	178	GLN	C-N-CA	6.00	128.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	157	PHE	N-CA-C	-6.00	98.48	108.32
2	D	404	LEU	N-CA-C	-6.00	103.40	112.04
2	B	697	PHE	CA-CB-CG	-5.99	107.81	113.80
2	C	393	ASP	CB-CA-C	-5.99	100.68	110.85
2	B	59	LYS	CA-C-N	5.98	128.02	120.72
2	B	59	LYS	C-N-CA	5.98	128.02	120.72
2	F	178	SER	N-CA-C	-5.97	104.52	112.94
2	A	676	GLN	N-CA-C	-5.97	106.98	114.56
2	F	639	LEU	N-CA-C	-5.96	100.08	109.50
2	B	641	ASP	CA-C-N	5.96	132.93	121.54
2	B	641	ASP	C-N-CA	5.96	132.93	121.54
2	C	592	GLY	CA-C-N	5.96	128.55	120.38
2	C	592	GLY	C-N-CA	5.96	128.55	120.38
2	B	568	SER	N-CA-C	-5.96	98.11	110.80
2	D	346	GLU	CA-C-N	5.96	129.07	120.79
2	D	346	GLU	C-N-CA	5.96	129.07	120.79
2	E	398	ALA	N-CA-C	-5.95	105.28	112.54
2	B	452	GLN	CA-C-N	5.95	128.14	120.70
2	B	452	GLN	C-N-CA	5.95	128.14	120.70
1	6	147	VAL	CA-C-N	5.95	132.90	121.54
1	6	147	VAL	C-N-CA	5.95	132.90	121.54
2	A	7	THR	CA-C-N	5.95	129.06	120.79
2	A	7	THR	C-N-CA	5.95	129.06	120.79
2	A	175	LYS	N-CA-C	-5.95	105.99	113.72
2	F	364	VAL	CA-C-N	5.94	132.39	121.70
2	F	364	VAL	C-N-CA	5.94	132.39	121.70
2	E	272	GLY	N-CA-C	-5.94	107.06	115.43
2	E	397	GLU	N-CA-CB	5.94	118.79	109.94
2	D	743	LEU	N-CA-C	-5.93	99.57	109.24
2	E	58	GLU	CA-C-N	5.93	128.23	120.28
2	E	58	GLU	C-N-CA	5.93	128.23	120.28
2	A	36	LEU	CA-C-N	5.93	126.56	119.98
2	A	36	LEU	C-N-CA	5.93	126.56	119.98
2	C	641	ASP	CA-C-N	5.92	132.86	121.54
2	C	641	ASP	C-N-CA	5.92	132.86	121.54
1	6	141	SER	CA-C-N	5.92	128.49	120.38
1	6	141	SER	C-N-CA	5.92	128.49	120.38
2	D	28	ASN	N-CA-C	-5.92	99.75	109.40
2	B	448	ARG	CA-C-N	5.91	129.01	120.79
2	B	448	ARG	C-N-CA	5.91	129.01	120.79
2	B	480	VAL	N-CA-CB	5.91	119.45	110.58
2	D	355	ARG	CA-C-N	5.91	130.15	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	355	ARG	C-N-CA	5.91	130.15	120.63
2	B	404	LEU	N-CA-C	-5.90	103.54	112.04
2	F	693	LEU	N-CA-C	-5.90	104.48	111.03
2	A	678	GLU	N-CA-C	-5.90	104.20	111.40
2	E	433	SER	CA-C-N	5.90	132.80	121.54
2	E	433	SER	C-N-CA	5.90	132.80	121.54
2	A	166	LEU	N-CA-CB	5.89	120.52	110.50
2	D	502	MET	N-CA-C	5.89	118.18	111.11
2	D	681	ASN	N-CA-C	-5.89	104.81	112.23
2	B	637	GLY	N-CA-C	-5.89	104.71	114.48
2	F	404	LEU	N-CA-C	-5.89	103.56	112.04
2	A	667	ARG	N-CA-C	-5.89	103.51	112.99
2	C	426	GLU	CA-C-N	5.89	128.97	120.79
2	C	426	GLU	C-N-CA	5.89	128.97	120.79
2	F	104	GLY	CA-C-N	5.89	128.44	120.38
2	F	104	GLY	C-N-CA	5.89	128.44	120.38
2	A	95	ALA	N-CA-C	-5.88	106.75	114.04
2	A	105	THR	N-CA-C	5.88	118.44	111.33
2	E	632	GLN	N-CA-C	-5.87	104.47	111.69
2	E	350	ILE	CB-CA-C	-5.87	104.46	111.97
2	F	58	GLU	CA-C-N	5.87	128.14	120.28
2	F	58	GLU	C-N-CA	5.87	128.14	120.28
2	C	629	ILE	N-CA-C	-5.86	105.13	110.82
2	F	669	LYS	CA-C-N	5.86	132.74	121.54
2	F	669	LYS	C-N-CA	5.86	132.74	121.54
2	E	175	LYS	N-CA-C	-5.86	105.33	112.88
2	D	434	GLN	CA-C-N	5.85	132.24	121.70
2	D	434	GLN	C-N-CA	5.85	132.24	121.70
2	B	180	ASP	N-CA-C	-5.85	100.04	109.40
2	D	763	ARG	CA-C-N	5.85	127.15	119.84
2	D	763	ARG	C-N-CA	5.85	127.15	119.84
1	1	175	VAL	CA-C-N	5.85	128.39	120.38
1	1	175	VAL	C-N-CA	5.85	128.39	120.38
2	D	433	SER	N-CA-C	-5.84	105.82	113.12
2	F	210	PRO	CA-C-N	5.84	132.22	121.70
2	F	210	PRO	C-N-CA	5.84	132.22	121.70
2	D	62	LYS	CA-C-N	5.84	128.03	120.44
2	D	62	LYS	C-N-CA	5.84	128.03	120.44
2	D	58	GLU	CA-C-N	5.83	128.09	120.28
2	D	58	GLU	C-N-CA	5.83	128.09	120.28
2	C	673	PHE	N-CA-C	-5.83	98.39	110.80
2	D	132	ASN	CA-CB-CG	-5.83	106.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	250	GLY	N-CA-C	-5.83	107.06	115.27
2	D	389	ASP	CA-C-N	5.83	130.45	121.19
2	D	389	ASP	C-N-CA	5.83	130.45	121.19
2	C	501	ASN	CA-CB-CG	-5.82	106.78	112.60
2	B	330	LEU	N-CA-C	-5.82	105.80	114.64
2	B	666	LYS	CA-C-N	5.82	132.65	121.54
2	B	666	LYS	C-N-CA	5.82	132.65	121.54
2	E	96	ARG	CA-C-N	5.82	128.55	120.29
2	E	96	ARG	C-N-CA	5.82	128.55	120.29
2	F	705	ILE	N-CA-C	-5.82	101.21	108.89
2	F	270	GLN	CA-C-N	5.81	132.64	121.54
2	F	270	GLN	C-N-CA	5.81	132.64	121.54
2	A	160	THR	CA-C-N	5.81	125.28	119.24
2	A	160	THR	C-N-CA	5.81	125.28	119.24
2	C	519	ALA	CA-C-N	5.81	127.88	120.56
2	C	519	ALA	C-N-CA	5.81	127.88	120.56
2	C	677	ASP	N-CA-C	-5.81	106.03	113.23
2	D	212	VAL	N-CA-C	-5.81	104.67	111.00
2	E	667	ARG	N-CA-C	-5.80	101.42	110.42
2	A	402	VAL	CB-CA-C	5.80	120.02	112.24
2	F	467	GLU	CA-C-N	5.80	132.62	121.54
2	F	467	GLU	C-N-CA	5.80	132.62	121.54
2	E	356	ASP	CA-CB-CG	-5.80	106.80	112.60
2	A	729	GLN	CA-C-N	5.80	128.30	120.65
2	A	729	GLN	C-N-CA	5.80	128.30	120.65
2	E	80	TYR	CA-CB-CG	-5.79	103.47	113.90
2	B	434	GLN	CA-C-N	5.79	132.12	121.70
2	B	434	GLN	C-N-CA	5.79	132.12	121.70
2	C	351	LEU	CA-C-N	5.79	128.31	120.38
2	C	351	LEU	C-N-CA	5.79	128.31	120.38
2	B	13	VAL	N-CA-CB	5.79	118.41	110.54
2	B	764	PRO	CA-C-N	5.79	128.51	120.29
2	B	764	PRO	C-N-CA	5.79	128.51	120.29
2	C	293	ALA	CA-C-N	5.79	132.38	121.97
2	C	293	ALA	C-N-CA	5.79	132.38	121.97
2	D	296	ALA	CA-C-N	5.79	128.83	120.38
2	D	296	ALA	C-N-CA	5.79	128.83	120.38
2	E	461	LYS	N-CA-C	-5.79	106.22	113.28
2	E	106	GLU	CA-C-N	5.78	128.82	120.38
2	E	106	GLU	C-N-CA	5.78	128.82	120.38
2	B	270	GLN	CA-C-N	5.77	132.56	121.54
2	B	270	GLN	C-N-CA	5.77	132.56	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	467	GLU	N-CA-C	5.77	120.61	112.93
2	D	423	VAL	CA-CB-CG1	-5.77	100.59	110.40
2	E	316	THR	CA-C-N	5.77	129.47	120.82
2	E	316	THR	C-N-CA	5.77	129.47	120.82
2	B	176	GLU	CA-C-N	5.77	132.55	121.54
2	B	176	GLU	C-N-CA	5.77	132.55	121.54
2	C	58	GLU	CA-C-N	5.77	128.01	120.28
2	C	58	GLU	C-N-CA	5.77	128.01	120.28
2	F	57	SER	CA-C-N	5.77	128.26	120.65
2	F	57	SER	C-N-CA	5.77	128.26	120.65
2	A	729	GLN	N-CA-C	-5.76	104.60	111.69
2	F	792	ILE	N-CA-C	-5.76	99.33	107.75
2	B	346	GLU	CA-C-N	5.76	128.80	120.79
2	B	346	GLU	C-N-CA	5.76	128.80	120.79
2	C	802	VAL	N-CA-C	-5.76	100.75	108.35
2	E	346	GLU	CA-C-N	5.76	128.79	120.79
2	E	346	GLU	C-N-CA	5.76	128.79	120.79
2	D	351	LEU	CA-C-N	5.75	128.26	120.38
2	D	351	LEU	C-N-CA	5.75	128.26	120.38
2	B	101	SER	N-CA-C	-5.75	105.10	111.36
2	C	296	ALA	CA-C-N	5.75	128.77	120.38
2	C	296	ALA	C-N-CA	5.75	128.77	120.38
2	E	457	LYS	N-CA-C	-5.75	105.76	112.89
1	5	196	LEU	CA-C-N	5.74	128.24	120.38
1	5	196	LEU	C-N-CA	5.74	128.24	120.38
2	C	160	THR	CA-C-N	5.74	125.21	119.24
2	C	160	THR	C-N-CA	5.74	125.21	119.24
2	F	6	PHE	CA-C-N	5.74	132.50	121.54
2	F	6	PHE	C-N-CA	5.74	132.50	121.54
2	D	365	SER	CA-C-N	5.73	132.29	121.97
2	D	365	SER	C-N-CA	5.73	132.29	121.97
2	C	361	HIS	N-CA-C	-5.73	103.89	112.54
2	F	294	ILE	N-CA-CB	5.72	120.67	111.23
2	A	421	ASP	CA-CB-CG	5.71	118.31	112.60
2	B	138	VAL	CA-C-N	5.71	128.26	120.54
2	B	138	VAL	C-N-CA	5.71	128.26	120.54
2	B	97	LYS	CB-CA-C	-5.71	101.88	110.90
2	B	436	PHE	CA-CB-CG	-5.71	108.09	113.80
2	C	667	ARG	N-CA-C	-5.71	100.73	109.41
2	D	87	VAL	CB-CA-C	-5.71	104.44	112.14
2	D	668	ASN	CA-C-N	5.71	132.44	121.54
2	D	668	ASN	C-N-CA	5.71	132.44	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	389	ASP	CA-C-N	5.71	130.26	121.19
2	F	389	ASP	C-N-CA	5.71	130.26	121.19
2	E	244	MET	CA-C-N	5.70	126.31	119.98
2	E	244	MET	C-N-CA	5.70	126.31	119.98
1	2	216	PHE	N-CA-C	-5.70	108.12	114.62
2	B	480	VAL	CB-CA-C	-5.70	104.35	112.22
2	F	448	ARG	CA-C-N	5.70	128.71	120.79
2	F	448	ARG	C-N-CA	5.70	128.71	120.79
1	5	180	SER	CA-C-N	5.69	128.23	120.77
1	5	180	SER	C-N-CA	5.69	128.23	120.77
2	B	472	THR	N-CA-CB	5.69	120.11	110.49
2	C	792	ILE	N-CA-C	-5.69	99.44	107.75
2	F	184	GLY	CA-C-N	5.69	131.94	121.70
2	F	184	GLY	C-N-CA	5.69	131.94	121.70
1	2	216	PHE	CA-CB-CG	-5.69	108.11	113.80
2	A	641	ASP	CA-C-N	5.69	132.40	121.54
2	A	641	ASP	C-N-CA	5.69	132.40	121.54
2	D	441	SER	CA-C-N	5.69	128.36	120.29
2	D	441	SER	C-N-CA	5.69	128.36	120.29
1	6	164	TYR	N-CA-CB	5.68	119.91	110.47
2	E	423	VAL	CA-CB-CG1	-5.68	100.74	110.40
2	B	60	ILE	N-CA-C	-5.68	105.08	110.42
2	D	501	ASN	CA-CB-CG	-5.68	106.92	112.60
1	5	190	SER	CA-C-N	5.67	128.10	120.50
1	5	190	SER	C-N-CA	5.67	128.10	120.50
2	B	427	LYS	CA-C-N	5.67	132.37	121.54
2	B	427	LYS	C-N-CA	5.67	132.37	121.54
1	2	164	TYR	N-CA-C	-5.67	97.96	107.99
2	D	368	ASP	CA-C-N	5.67	128.65	120.38
2	D	368	ASP	C-N-CA	5.67	128.65	120.38
2	B	364	VAL	N-CA-C	-5.66	97.56	109.34
2	B	19	GLU	N-CA-CB	5.66	118.55	110.06
2	D	629	ILE	N-CA-C	-5.66	105.33	110.82
2	B	647	VAL	N-CA-C	-5.66	99.60	107.80
2	E	158	ALA	CA-C-N	5.66	129.74	120.63
2	E	158	ALA	C-N-CA	5.66	129.74	120.63
2	A	62	LYS	CA-C-N	5.66	127.79	120.44
2	A	62	LYS	C-N-CA	5.66	127.79	120.44
1	5	173	GLU	CA-C-N	5.65	128.90	120.31
1	5	173	GLU	C-N-CA	5.65	128.90	120.31
2	D	236	ASP	CA-C-N	5.65	128.73	120.71
2	D	236	ASP	C-N-CA	5.65	128.73	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	316	THR	CA-C-N	5.65	129.29	120.82
2	F	316	THR	C-N-CA	5.65	129.29	120.82
2	F	517	VAL	N-CA-C	5.65	116.29	110.36
2	C	462	GLU	N-CA-C	-5.65	105.12	112.23
2	D	274	ILE	CA-C-N	5.64	130.53	123.14
2	D	274	ILE	C-N-CA	5.64	130.53	123.14
2	D	316	THR	CA-C-N	5.64	129.28	120.82
2	D	316	THR	C-N-CA	5.64	129.28	120.82
2	F	253	TYR	CA-C-N	5.64	128.30	120.29
2	F	253	TYR	C-N-CA	5.64	128.30	120.29
2	B	464	GLN	N-CA-C	-5.63	103.92	112.04
2	D	160	THR	CA-C-N	5.63	125.10	119.24
2	D	160	THR	C-N-CA	5.63	125.10	119.24
2	A	184	GLY	CA-C-N	5.63	131.84	121.70
2	A	184	GLY	C-N-CA	5.63	131.84	121.70
2	B	743	LEU	N-CA-C	-5.63	100.06	109.24
2	A	268	ILE	CA-C-N	5.63	132.29	121.54
2	A	268	ILE	C-N-CA	5.63	132.29	121.54
2	E	442	LEU	CA-C-N	5.63	128.08	120.65
2	E	442	LEU	C-N-CA	5.63	128.08	120.65
2	C	719	LEU	N-CA-C	5.62	117.88	111.02
2	F	60	ILE	N-CA-C	-5.62	105.14	110.42
2	B	268	ILE	CA-C-N	5.62	132.27	121.54
2	B	268	ILE	C-N-CA	5.62	132.27	121.54
2	B	666	LYS	N-CA-C	-5.62	102.03	110.06
2	C	59	LYS	CA-C-N	5.62	127.58	120.72
2	C	59	LYS	C-N-CA	5.62	127.58	120.72
2	E	764	PRO	CA-C-N	5.62	128.27	120.29
2	E	764	PRO	C-N-CA	5.62	128.27	120.29
2	A	451	GLU	CA-C-N	5.62	127.74	120.44
2	A	451	GLU	C-N-CA	5.62	127.74	120.44
2	C	514	ASP	CA-CB-CG	-5.60	107.00	112.60
2	F	365	SER	CA-C-N	5.60	132.05	121.97
2	F	365	SER	C-N-CA	5.60	132.05	121.97
2	C	692	GLU	CA-C-N	5.60	128.24	120.63
2	C	692	GLU	C-N-CA	5.60	128.24	120.63
2	A	753	GLU	N-CA-C	5.59	119.61	112.34
2	C	441	SER	CA-C-N	5.59	128.23	120.29
2	C	441	SER	C-N-CA	5.59	128.23	120.29
2	E	699	PRO	CA-C-N	5.59	127.78	120.28
2	E	699	PRO	C-N-CA	5.59	127.78	120.28
2	D	363	ARG	N-CA-CB	5.59	119.94	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	442	LEU	CA-C-N	5.59	128.03	120.65
2	D	442	LEU	C-N-CA	5.59	128.03	120.65
2	F	126	ASN	N-CA-C	-5.59	106.13	113.12
2	F	464	GLN	N-CA-C	-5.59	103.99	112.04
2	F	101	SER	N-CA-C	-5.59	105.27	111.36
1	2	127	LEU	N-CA-C	-5.58	105.68	112.88
2	F	373	ALA	CA-C-N	5.58	130.07	121.19
2	F	373	ALA	C-N-CA	5.58	130.07	121.19
2	D	593	TYR	N-CA-C	5.58	118.08	111.33
2	E	585	ARG	CA-C-N	5.58	132.20	121.54
2	E	585	ARG	C-N-CA	5.58	132.20	121.54
2	D	106	GLU	N-CA-CB	5.58	118.10	110.01
2	E	270	GLN	CA-C-N	5.58	132.20	121.54
2	E	270	GLN	C-N-CA	5.58	132.20	121.54
2	C	404	LEU	N-CA-C	-5.58	104.01	112.04
2	B	405	ARG	CA-C-N	5.57	127.75	120.28
2	B	405	ARG	C-N-CA	5.57	127.75	120.28
2	C	716	LYS	N-CA-C	-5.57	106.47	113.72
2	E	790	GLN	N-CA-CB	5.57	118.19	110.17
1	4	207	HIS	CA-C-N	5.57	127.74	120.28
1	4	207	HIS	C-N-CA	5.57	127.74	120.28
2	D	21	ALA	CB-CA-C	-5.57	102.07	110.92
2	D	203	ASN	CB-CA-C	-5.57	101.90	109.42
2	F	502	MET	N-CA-C	5.57	117.79	111.11
2	E	471	VAL	CA-C-N	5.57	132.17	121.54
2	E	471	VAL	C-N-CA	5.57	132.17	121.54
2	B	406	SER	CB-CA-C	-5.56	101.56	110.79
2	B	501	ASN	CA-CB-CG	-5.56	107.04	112.60
2	C	543	PHE	N-CA-C	-5.56	98.14	107.99
2	E	441	SER	CA-C-N	5.56	128.19	120.29
2	E	441	SER	C-N-CA	5.56	128.19	120.29
1	5	216	PHE	CA-CB-CG	-5.56	108.24	113.80
2	B	355	ARG	CB-CA-C	5.56	119.52	110.96
1	5	204	ILE	N-CA-C	-5.56	100.66	108.27
2	C	474	ASP	N-CA-C	5.56	118.05	111.33
2	D	313	GLY	N-CA-C	-5.55	100.83	110.71
2	B	210	PRO	CA-C-N	5.55	131.69	121.70
2	B	210	PRO	C-N-CA	5.55	131.69	121.70
2	B	235	ARG	CA-C-N	5.55	132.14	121.54
2	B	235	ARG	C-N-CA	5.55	132.14	121.54
2	B	467	GLU	CA-C-O	-5.55	112.37	120.13
2	B	365	SER	CA-C-N	5.54	131.95	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	365	SER	C-N-CA	5.54	131.95	121.97
2	A	637	GLY	N-CA-C	-5.54	105.34	114.76
2	A	351	LEU	CA-C-N	5.54	128.02	120.54
2	A	351	LEU	C-N-CA	5.54	128.02	120.54
2	A	513	GLN	CA-C-N	5.54	128.25	120.28
2	A	513	GLN	C-N-CA	5.54	128.25	120.28
2	E	338	GLN	N-CA-C	5.53	117.75	108.96
2	D	409	THR	CA-C-N	5.52	126.07	120.38
2	D	409	THR	C-N-CA	5.52	126.07	120.38
2	E	182	VAL	CA-C-N	5.52	131.91	121.97
2	E	182	VAL	C-N-CA	5.52	131.91	121.97
2	F	63	GLU	CA-C-N	5.52	127.51	120.56
2	F	63	GLU	C-N-CA	5.52	127.51	120.56
2	B	475	ASP	CA-C-N	5.52	128.25	120.42
2	B	475	ASP	C-N-CA	5.52	128.25	120.42
2	B	184	GLY	CA-C-N	5.51	131.62	121.70
2	B	184	GLY	C-N-CA	5.51	131.62	121.70
2	E	105	THR	CA-C-N	5.51	127.61	120.44
2	E	105	THR	C-N-CA	5.51	127.61	120.44
2	E	711	PHE	N-CA-CB	5.51	120.19	111.43
2	B	451	GLU	CA-C-N	5.51	127.60	120.44
2	B	451	GLU	C-N-CA	5.51	127.60	120.44
2	D	126	ASN	N-CA-C	-5.51	106.24	113.12
2	D	203	ASN	N-CA-C	5.50	118.20	109.40
2	D	272	GLY	N-CA-C	-5.50	108.04	115.36
2	E	593	TYR	CB-CA-C	-5.50	101.33	110.68
2	F	431	VAL	N-CA-CB	5.50	120.06	110.65
2	B	792	ILE	N-CA-C	-5.50	99.72	107.75
1	3	157	PHE	N-CA-C	-5.50	99.31	108.32
2	C	272	GLY	N-CA-C	-5.50	107.66	115.30
2	E	350	ILE	CA-C-N	5.50	128.43	120.79
2	E	350	ILE	C-N-CA	5.50	128.43	120.79
2	C	639	LEU	N-CA-C	-5.49	100.71	109.23
2	F	166	LEU	N-CA-CB	5.49	119.84	110.50
2	F	629	ILE	N-CA-C	-5.49	105.49	110.82
2	A	138	VAL	CB-CA-C	-5.49	104.94	111.97
2	B	793	VAL	N-CA-C	-5.49	100.48	108.17
1	3	137	GLU	CA-C-N	5.49	128.18	120.28
1	3	137	GLU	C-N-CA	5.49	128.18	120.28
2	B	722	ILE	N-CA-C	-5.49	105.50	110.82
2	C	143	GLY	N-CA-C	-5.48	100.19	113.18
2	E	318	ASP	N-CA-C	-5.48	106.27	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	102	TYR	N-CA-C	-5.48	100.25	108.96
2	D	268	ILE	CB-CA-C	5.48	120.28	111.29
2	D	698	ARG	N-CA-C	-5.48	102.56	110.40
1	3	204	ILE	N-CA-C	-5.48	100.77	108.27
2	B	669	LYS	N-CA-CB	5.48	118.10	109.83
2	A	27	ASN	CA-C-N	5.47	131.15	122.94
2	A	27	ASN	C-N-CA	5.47	131.15	122.94
2	C	93	ASP	CA-CB-CG	-5.47	107.12	112.60
2	F	272	GLY	N-CA-C	-5.47	108.08	115.36
2	C	637	GLY	N-CA-C	-5.47	107.70	115.30
2	F	378	SER	CA-C-N	5.47	127.61	120.28
2	F	378	SER	C-N-CA	5.47	127.61	120.28
2	D	416	LEU	CA-C-N	5.47	127.92	120.54
2	D	416	LEU	C-N-CA	5.47	127.92	120.54
2	E	449	LEU	CA-C-N	5.47	128.39	120.79
2	E	449	LEU	C-N-CA	5.47	128.39	120.79
1	1	213	LYS	CB-CA-C	-5.46	101.72	110.79
2	D	338	GLN	N-CA-C	5.46	117.64	108.96
2	E	462	GLU	N-CA-C	-5.46	105.35	112.23
2	D	647	VAL	N-CA-C	-5.46	99.88	107.80
1	3	180	SER	CA-C-N	5.46	127.92	120.77
1	3	180	SER	C-N-CA	5.46	127.92	120.77
2	B	659	ASN	N-CA-CB	5.46	119.71	110.49
2	B	719	LEU	N-CA-C	5.46	122.42	110.80
2	D	345	ASP	CA-C-N	5.45	127.59	120.28
2	D	345	ASP	C-N-CA	5.45	127.59	120.28
2	F	680	GLN	N-CA-C	-5.45	106.54	114.12
2	F	201	LYS	N-CA-C	-5.45	103.96	111.81
1	4	207	HIS	N-CA-C	-5.45	99.19	110.80
2	A	82	PRO	CA-C-N	5.45	127.84	120.65
2	A	82	PRO	C-N-CA	5.45	127.84	120.65
2	A	96	ARG	CA-C-N	5.45	127.85	120.44
2	A	96	ARG	C-N-CA	5.45	127.85	120.44
2	D	697	PHE	CA-CB-CG	-5.45	108.35	113.80
2	F	18	GLN	CB-CA-C	-5.45	101.75	110.79
2	D	552	THR	CA-C-N	5.44	128.12	120.28
2	D	552	THR	C-N-CA	5.44	128.12	120.28
1	6	190	SER	N-CA-C	-5.44	104.33	112.54
2	D	220	GLY	CA-C-N	5.44	127.83	120.65
2	D	220	GLY	C-N-CA	5.44	127.83	120.65
2	A	102	TYR	N-CA-C	-5.44	99.87	108.73
2	D	632	GLN	N-CA-C	-5.43	105.00	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	787	HIS	CA-C-N	5.43	128.81	121.05
2	A	787	HIS	C-N-CA	5.43	128.81	121.05
2	E	794	LEU	N-CA-C	-5.43	99.67	108.52
1	5	207	HIS	N-CA-C	-5.42	105.62	113.21
2	C	63	GLU	CA-C-N	5.42	127.39	120.56
2	C	63	GLU	C-N-CA	5.42	127.39	120.56
2	B	461	LYS	N-CA-C	-5.42	106.67	113.28
2	A	461	LYS	N-CA-C	-5.42	106.67	113.28
2	B	805	THR	N-CA-C	-5.42	100.94	109.50
2	D	270	GLN	CA-C-N	5.42	131.89	121.54
2	D	270	GLN	C-N-CA	5.42	131.89	121.54
2	C	346	GLU	CA-C-N	5.42	128.32	120.79
2	C	346	GLU	C-N-CA	5.42	128.32	120.79
2	F	434	GLN	CA-C-N	5.42	131.45	121.70
2	F	434	GLN	C-N-CA	5.42	131.45	121.70
2	F	430	ALA	CA-C-O	-5.42	115.13	120.82
2	B	661	GLY	CA-C-N	5.41	131.88	121.54
2	B	661	GLY	C-N-CA	5.41	131.88	121.54
2	C	503	GLU	CA-C-N	5.41	127.79	120.38
2	C	503	GLU	C-N-CA	5.41	127.79	120.38
2	E	63	GLU	CA-C-N	5.41	127.38	120.56
2	E	63	GLU	C-N-CA	5.41	127.38	120.56
2	E	220	GLY	CA-C-N	5.41	127.78	120.65
2	E	220	GLY	C-N-CA	5.41	127.78	120.65
2	E	450	ARG	CA-C-N	5.41	127.78	120.38
2	E	450	ARG	C-N-CA	5.41	127.78	120.38
2	E	160	THR	CA-C-N	5.40	125.48	119.32
2	E	160	THR	C-N-CA	5.40	125.48	119.32
2	F	293	ALA	CA-C-N	5.40	131.69	121.97
2	F	293	ALA	C-N-CA	5.40	131.69	121.97
2	E	365	SER	CA-C-N	5.40	131.69	121.97
2	E	365	SER	C-N-CA	5.40	131.69	121.97
2	F	33	HIS	CA-CB-CG	-5.40	108.40	113.80
1	1	180	SER	CA-C-N	5.40	127.84	120.77
1	1	180	SER	C-N-CA	5.40	127.84	120.77
1	2	152	THR	N-CA-C	-5.40	99.52	108.75
2	B	423	VAL	CA-CB-CG1	-5.40	101.22	110.40
2	D	398	ALA	CA-C-N	5.40	131.99	121.41
2	D	398	ALA	C-N-CA	5.40	131.99	121.41
2	F	244	MET	CA-C-N	5.39	125.97	119.98
2	F	244	MET	C-N-CA	5.39	125.97	119.98
2	A	565	ASP	N-CA-C	-5.39	99.89	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	657	THR	N-CA-C	-5.39	102.21	110.14
2	F	145	ASN	N-CA-C	-5.39	99.53	108.75
2	F	346	GLU	CA-C-N	5.39	128.28	120.79
2	F	346	GLU	C-N-CA	5.39	128.28	120.79
2	A	106	GLU	CA-C-N	5.39	128.25	120.38
2	A	106	GLU	C-N-CA	5.39	128.25	120.38
1	5	175	VAL	N-CA-C	-5.39	105.59	110.82
2	D	793	VAL	N-CA-C	-5.39	100.63	108.17
1	4	166	ASP	N-CA-C	-5.39	97.05	107.44
2	D	582	SER	CA-C-N	5.38	128.88	120.75
2	D	582	SER	C-N-CA	5.38	128.88	120.75
2	F	497	ASP	CA-C-N	5.38	127.50	120.28
2	F	497	ASP	C-N-CA	5.38	127.50	120.28
2	C	451	GLU	CA-C-N	5.38	127.44	120.44
2	C	451	GLU	C-N-CA	5.38	127.44	120.44
2	F	646	THR	N-CA-C	-5.38	99.75	108.52
1	2	158	GLU	CA-C-N	5.38	131.81	121.54
1	2	158	GLU	C-N-CA	5.38	131.81	121.54
2	B	254	ARG	CA-C-N	5.38	125.95	119.98
2	B	254	ARG	C-N-CA	5.38	125.95	119.98
2	C	361	HIS	CA-CB-CG	5.38	119.18	113.80
2	D	300	LEU	CA-C-N	5.38	127.47	120.26
2	D	300	LEU	C-N-CA	5.38	127.47	120.26
2	F	692	GLU	N-CA-C	-5.38	106.56	113.23
2	C	693	LEU	N-CA-C	-5.38	105.06	111.03
2	D	467	GLU	CA-C-N	5.37	131.80	121.54
2	D	467	GLU	C-N-CA	5.37	131.80	121.54
2	C	704	ARG	N-CA-C	-5.37	107.10	113.97
2	D	181	PRO	CA-C-N	5.37	131.36	121.70
2	D	181	PRO	C-N-CA	5.37	131.36	121.70
2	D	792	ILE	N-CA-C	-5.37	99.91	107.75
2	B	342	PRO	N-CA-C	-5.37	101.41	112.47
2	B	80	TYR	CA-CB-CG	-5.37	104.24	113.90
2	F	350	ILE	CA-C-N	5.37	128.25	120.79
2	F	350	ILE	C-N-CA	5.37	128.25	120.79
2	A	105	THR	CB-CA-C	-5.36	101.56	110.68
2	F	368	ASP	CA-C-N	5.35	128.20	120.38
2	F	368	ASP	C-N-CA	5.35	128.20	120.38
2	D	57	SER	CA-C-N	5.35	127.71	120.65
2	D	57	SER	C-N-CA	5.35	127.71	120.65
2	D	545	GLY	CA-C-N	5.34	126.52	119.84
2	D	545	GLY	C-N-CA	5.34	126.52	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	364	VAL	O-C-N	-5.34	118.33	122.97
2	E	763	ARG	CA-C-N	5.34	125.05	119.82
2	E	763	ARG	C-N-CA	5.34	125.05	119.82
2	E	474	ASP	N-CA-C	5.34	117.79	111.33
2	D	237	LYS	CA-C-N	5.33	130.94	122.62
2	D	237	LYS	C-N-CA	5.33	130.94	122.62
2	E	404	LEU	N-CA-C	-5.33	105.59	112.68
2	C	546	PRO	CA-C-N	5.33	131.72	121.54
2	C	546	PRO	C-N-CA	5.33	131.72	121.54
2	B	181	PRO	CA-C-N	5.33	131.29	121.70
2	B	181	PRO	C-N-CA	5.33	131.29	121.70
2	C	502	MET	N-CA-C	5.33	117.50	111.11
2	F	685	MET	N-CA-C	-5.33	105.52	112.23
2	B	804	LYS	N-CA-C	-5.32	101.44	109.85
2	F	501	ASN	CA-CB-CG	-5.32	107.28	112.60
2	D	27	ASN	CA-C-N	5.32	130.92	122.94
2	D	27	ASN	C-N-CA	5.32	130.92	122.94
2	D	268	ILE	CA-C-N	5.32	131.70	121.54
2	D	268	ILE	C-N-CA	5.32	131.70	121.54
2	E	428	ASP	CA-C-N	5.32	127.66	120.38
2	E	428	ASP	C-N-CA	5.32	127.66	120.38
2	C	434	GLN	CA-C-N	5.31	131.26	121.70
2	C	434	GLN	C-N-CA	5.31	131.26	121.70
2	F	381	TYR	CA-C-N	5.31	131.53	121.97
2	F	381	TYR	C-N-CA	5.31	131.53	121.97
2	F	667	ARG	N-CA-C	-5.31	99.49	110.80
2	A	447	GLN	CA-C-N	5.31	128.17	120.79
2	A	447	GLN	C-N-CA	5.31	128.17	120.79
2	D	678	GLU	N-CA-C	-5.31	104.92	111.40
2	F	36	LEU	CA-C-N	5.31	125.87	119.98
2	F	36	LEU	C-N-CA	5.31	125.87	119.98
2	F	345	ASP	CA-C-N	5.31	127.39	120.28
2	F	345	ASP	C-N-CA	5.31	127.39	120.28
2	E	475	ASP	CA-C-N	5.30	127.95	120.42
2	E	475	ASP	C-N-CA	5.30	127.95	120.42
2	E	601	GLN	N-CA-C	5.30	116.75	110.97
2	C	362	HIS	CA-C-N	5.30	131.66	121.54
2	C	362	HIS	C-N-CA	5.30	131.66	121.54
1	3	173	GLU	CA-C-N	5.30	128.36	120.31
1	3	173	GLU	C-N-CA	5.30	128.36	120.31
2	C	113	ILE	CA-C-N	5.30	127.69	120.54
2	C	113	ILE	C-N-CA	5.30	127.69	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	60	ILE	N-CA-C	-5.29	105.44	110.42
2	B	175	LYS	N-CA-C	-5.29	106.84	113.72
2	C	423	VAL	CA-CB-CG1	-5.29	101.41	110.40
2	A	23	ARG	N-CA-C	5.29	119.22	112.34
1	2	190	SER	CA-C-N	5.29	131.49	121.97
1	2	190	SER	C-N-CA	5.29	131.49	121.97
1	5	157	PHE	N-CA-C	-5.29	99.65	108.32
2	B	673	PHE	N-CA-C	-5.29	105.54	112.41
2	E	319	GLU	CA-C-N	5.29	127.36	120.28
2	E	319	GLU	C-N-CA	5.29	127.36	120.28
2	C	158	ALA	CA-C-N	5.29	129.14	120.63
2	C	158	ALA	C-N-CA	5.29	129.14	120.63
2	A	632	GLN	N-CA-C	-5.28	105.57	112.23
2	E	793	VAL	N-CA-C	-5.28	100.77	108.17
2	A	316	THR	CA-C-N	5.28	128.74	120.82
2	A	316	THR	C-N-CA	5.28	128.74	120.82
2	A	590	PRO	CA-C-O	-5.28	112.90	120.56
2	C	428	ASP	CA-CB-CG	-5.28	107.32	112.60
2	E	126	ASN	N-CA-C	-5.28	106.52	113.12
2	A	220	GLY	CA-C-N	5.28	127.62	120.65
2	A	220	GLY	C-N-CA	5.28	127.62	120.65
2	E	268	ILE	CA-C-N	5.28	131.62	121.54
2	E	268	ILE	C-N-CA	5.28	131.62	121.54
1	6	133	PHE	N-CA-C	-5.27	101.10	109.59
2	D	169	ASP	CA-C-N	5.27	127.60	120.38
2	D	169	ASP	C-N-CA	5.27	127.60	120.38
1	3	181	ILE	CA-C-N	5.27	127.66	120.54
1	3	181	ILE	C-N-CA	5.27	127.66	120.54
2	B	693	LEU	N-CA-C	-5.27	105.18	111.03
2	C	464	GLN	N-CA-CB	5.27	118.36	110.19
2	A	473	VAL	CA-C-N	5.26	127.59	120.38
2	A	473	VAL	C-N-CA	5.26	127.59	120.38
2	A	743	LEU	N-CA-C	-5.26	100.66	109.24
2	E	502	MET	N-CA-C	5.26	117.43	111.11
2	B	467	GLU	N-CA-C	5.26	119.68	112.68
2	B	63	GLU	CA-C-N	5.26	127.19	120.56
2	B	63	GLU	C-N-CA	5.26	127.19	120.56
2	B	222	ALA	CA-C-N	5.26	127.33	120.28
2	B	222	ALA	C-N-CA	5.26	127.33	120.28
2	B	544	LEU	N-CA-C	-5.26	102.27	110.42
2	D	564	GLY	N-CA-C	-5.26	107.99	115.30
2	B	594	VAL	CA-C-N	5.26	125.82	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	594	VAL	C-N-CA	5.26	125.82	119.98
2	B	806	THR	N-CA-C	-5.26	100.74	108.99
2	D	232	GLU	CA-C-N	5.26	127.38	120.60
2	D	232	GLU	C-N-CA	5.26	127.38	120.60
2	D	474	ASP	CA-C-N	5.26	127.27	120.44
2	D	474	ASP	C-N-CA	5.26	127.27	120.44
2	F	420	LEU	CB-CA-C	-5.25	101.75	110.68
2	A	757	ASP	CA-C-N	5.25	127.32	120.28
2	A	757	ASP	C-N-CA	5.25	127.32	120.28
2	A	183	ILE	CA-C-N	5.25	125.32	120.34
2	A	183	ILE	C-N-CA	5.25	125.32	120.34
2	D	407	PHE	CA-CB-CG	-5.25	108.55	113.80
2	C	365	SER	CA-C-N	5.24	131.41	121.97
2	C	365	SER	C-N-CA	5.24	131.41	121.97
2	D	273	ASN	N-CA-C	-5.24	106.40	114.16
2	E	804	LYS	N-CA-C	-5.24	101.57	109.85
2	B	502	MET	N-CA-C	5.24	117.40	111.11
2	E	397	GLU	CB-CA-C	-5.24	102.42	110.81
2	F	519	ALA	CA-C-N	5.24	127.16	120.56
2	F	519	ALA	C-N-CA	5.24	127.16	120.56
2	C	711	PHE	N-CA-C	-5.24	101.17	109.76
2	D	635	GLU	N-CA-C	5.24	119.57	111.56
2	F	402	VAL	CB-CA-C	5.24	119.26	112.24
2	B	160	THR	CA-C-N	5.24	125.29	119.32
2	B	160	THR	C-N-CA	5.24	125.29	119.32
2	D	363	ARG	N-CA-C	-5.24	99.65	110.80
1	6	157	PHE	N-CA-C	-5.23	99.74	108.32
2	D	767	ARG	CB-CA-C	-5.23	101.78	110.68
1	2	213	LYS	CB-CA-C	-5.23	102.10	110.79
2	B	393	ASP	CB-CA-C	-5.23	101.95	110.85
2	E	642	SER	CA-C-N	5.23	129.55	122.07
2	E	642	SER	C-N-CA	5.23	129.55	122.07
1	3	127	LEU	N-CA-C	-5.23	105.89	113.21
1	4	180	SER	CA-C-N	5.23	127.62	120.77
1	4	180	SER	C-N-CA	5.23	127.62	120.77
2	E	540	SER	N-CA-C	-5.23	101.63	109.95
2	A	331	GLU	N-CA-C	-5.23	105.77	113.61
2	B	519	ALA	CA-C-N	5.23	127.15	120.56
2	B	519	ALA	C-N-CA	5.23	127.15	120.56
2	F	268	ILE	CA-C-N	5.23	131.53	121.54
2	F	268	ILE	C-N-CA	5.23	131.53	121.54
2	E	543	PHE	N-CA-CB	5.23	118.76	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	ILE	N-CA-CB	5.23	116.31	110.51
2	B	126	ASN	N-CA-C	-5.22	106.59	113.12
2	C	416	LEU	CA-C-N	5.22	127.59	120.54
2	C	416	LEU	C-N-CA	5.22	127.59	120.54
2	F	110	LEU	CA-C-N	5.22	126.67	120.14
2	F	110	LEU	C-N-CA	5.22	126.67	120.14
2	A	234	LEU	N-CA-C	-5.22	99.77	108.34
1	1	141	SER	CA-C-N	5.22	127.53	120.38
1	1	141	SER	C-N-CA	5.22	127.53	120.38
2	B	28	ASN	N-CA-C	-5.22	100.89	109.40
2	D	678	GLU	CB-CA-C	-5.22	102.02	110.79
2	F	87	VAL	CB-CA-C	-5.22	105.09	112.14
2	F	370	ALA	CB-CA-C	-5.21	102.66	110.90
2	F	641	ASP	CA-C-N	5.21	131.50	121.54
2	F	641	ASP	C-N-CA	5.21	131.50	121.54
2	D	660	VAL	N-CA-C	-5.21	106.06	111.58
2	F	41	GLU	N-CA-C	-5.21	106.70	113.16
2	A	210	PRO	CA-C-N	5.21	131.07	121.70
2	A	210	PRO	C-N-CA	5.21	131.07	121.70
2	D	681	ASN	CA-C-N	5.21	131.49	121.54
2	D	681	ASN	C-N-CA	5.21	131.49	121.54
2	E	263	LYS	CA-C-N	5.21	127.12	120.56
2	E	263	LYS	C-N-CA	5.21	127.12	120.56
1	2	157	PHE	N-CA-C	-5.20	99.79	108.32
1	5	166	ASP	N-CA-C	-5.20	97.39	107.44
2	B	323	TYR	N-CA-CB	5.20	119.28	110.49
2	B	497	ASP	CA-C-N	5.20	127.25	120.28
2	B	497	ASP	C-N-CA	5.20	127.25	120.28
2	B	611	TYR	N-CA-C	-5.20	100.69	109.07
2	E	674	ASN	N-CA-CB	5.20	119.28	110.49
2	E	87	VAL	CB-CA-C	-5.20	105.12	112.14
2	E	433	SER	N-CA-C	-5.20	106.62	113.12
2	E	742	GLU	N-CA-CB	5.20	120.43	111.13
2	A	694	LYS	N-CA-C	5.19	118.40	111.75
1	4	158	GLU	CA-C-N	5.19	131.45	121.54
1	4	158	GLU	C-N-CA	5.19	131.45	121.54
2	A	126	ASN	N-CA-C	-5.19	106.64	113.12
2	F	366	ILE	N-CA-CB	5.19	119.79	111.23
2	B	318	ASP	N-CA-C	-5.18	106.64	113.12
2	B	358	TYR	CA-CB-CG	5.18	123.23	113.90
2	E	712	HIS	N-CA-C	-5.18	101.03	108.60
2	E	364	VAL	N-CA-C	-5.18	100.95	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	565	ASP	N-CA-C	-5.18	100.46	108.90
2	F	329	ALA	N-CA-C	-5.18	105.42	112.26
2	C	106	GLU	CA-C-N	5.18	127.47	120.38
2	C	106	GLU	C-N-CA	5.18	127.47	120.38
2	C	692	GLU	N-CA-C	-5.18	106.81	113.23
2	E	138	VAL	CB-CA-C	-5.18	105.34	111.97
2	F	503	GLU	CA-C-N	5.18	127.47	120.38
2	F	503	GLU	C-N-CA	5.18	127.47	120.38
2	A	647	VAL	N-CA-C	-5.17	100.30	107.80
2	E	378	SER	CA-C-N	5.17	127.21	120.28
2	E	378	SER	C-N-CA	5.17	127.21	120.28
2	A	167	ALA	CA-C-N	5.17	128.55	120.75
2	A	167	ALA	C-N-CA	5.17	128.55	120.75
2	D	451	GLU	CA-C-N	5.17	127.16	120.44
2	D	451	GLU	C-N-CA	5.17	127.16	120.44
2	E	693	LEU	CA-C-N	5.17	127.92	120.38
2	E	693	LEU	C-N-CA	5.17	127.92	120.38
2	C	493	GLN	N-CA-C	5.16	121.79	110.80
2	E	563	PHE	N-CA-C	-5.16	107.65	114.31
2	A	198	ARG	N-CA-C	-5.16	99.81	110.80
2	A	697	PHE	CA-CB-CG	-5.16	108.64	113.80
2	F	45	ILE	CB-CA-C	-5.16	105.17	112.14
2	C	360	ALA	CA-C-N	5.16	130.69	121.15
2	C	360	ALA	C-N-CA	5.16	130.69	121.15
2	D	548	GLY	N-CA-C	-5.16	108.50	115.36
2	F	552	THR	CA-C-N	5.16	127.71	120.28
2	F	552	THR	C-N-CA	5.16	127.71	120.28
2	B	268	ILE	CB-CA-C	5.16	119.75	111.29
2	C	29	ILE	N-CA-CB	-5.15	105.41	111.39
2	E	351	LEU	CA-C-N	5.15	127.44	120.38
2	E	351	LEU	C-N-CA	5.15	127.44	120.38
2	A	346	GLU	CA-C-N	5.15	127.95	120.79
2	A	346	GLU	C-N-CA	5.15	127.95	120.79
2	B	150	SER	CA-C-N	5.15	131.38	121.54
2	B	150	SER	C-N-CA	5.15	131.38	121.54
2	F	93	ASP	CA-CB-CG	-5.15	107.45	112.60
2	C	542	ILE	N-CA-C	-5.14	101.07	108.48
2	D	718	HIS	CA-C-N	5.14	127.94	120.79
2	D	718	HIS	C-N-CA	5.14	127.94	120.79
2	B	547	THR	N-CA-CB	5.14	119.18	110.49
2	E	652	THR	N-CA-CB	5.14	119.18	110.49
2	B	689	VAL	N-CA-C	-5.14	106.06	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	753	GLU	N-CA-C	5.14	118.65	112.38
2	C	449	LEU	CA-C-N	5.14	127.93	120.79
2	C	449	LEU	C-N-CA	5.14	127.93	120.79
2	B	180	ASP	CA-C-N	5.13	124.58	119.24
2	B	180	ASP	C-N-CA	5.13	124.58	119.24
2	D	60	ILE	CA-C-N	5.13	127.67	120.28
2	D	60	ILE	C-N-CA	5.13	127.67	120.28
1	4	216	PHE	N-CA-CB	5.13	120.31	111.13
2	D	471	VAL	CA-C-N	5.13	131.34	121.54
2	D	471	VAL	C-N-CA	5.13	131.34	121.54
1	3	133	PHE	N-CA-C	-5.13	101.33	109.59
2	A	712	HIS	N-CA-C	-5.13	101.28	109.23
2	E	102	TYR	CA-C-N	5.13	131.20	121.97
2	E	102	TYR	C-N-CA	5.13	131.20	121.97
2	E	416	LEU	CA-C-N	5.13	127.46	120.54
2	E	416	LEU	C-N-CA	5.13	127.46	120.54
2	B	105	THR	CB-CA-C	-5.13	101.97	110.68
2	C	198	ARG	N-CA-C	-5.13	100.94	108.79
2	C	469	SER	N-CA-C	-5.13	99.88	110.80
2	F	13	VAL	N-CA-CB	5.12	117.51	110.54
2	D	404	LEU	CA-C-N	5.12	128.88	120.63
2	D	404	LEU	C-N-CA	5.12	128.88	120.63
2	E	104	GLY	CA-C-N	5.12	127.40	120.38
2	E	104	GLY	C-N-CA	5.12	127.40	120.38
2	F	711	PHE	N-CA-CB	5.12	119.84	111.08
2	F	404	LEU	CA-C-N	5.12	128.87	120.63
2	F	404	LEU	C-N-CA	5.12	128.87	120.63
2	C	590	PRO	CA-C-O	-5.12	113.14	120.56
2	B	220	GLY	CA-C-N	5.12	127.40	120.65
2	B	220	GLY	C-N-CA	5.12	127.40	120.65
2	C	655	ILE	N-CA-C	-5.12	100.16	107.78
2	A	293	ALA	CA-C-N	5.11	131.17	121.97
2	A	293	ALA	C-N-CA	5.11	131.17	121.97
2	A	356	ASP	CA-CB-CG	-5.11	107.49	112.60
2	E	705	ILE	N-CA-C	-5.11	102.14	108.89
1	3	154	LEU	CA-C-N	5.11	131.91	122.92
1	3	154	LEU	C-N-CA	5.11	131.91	122.92
2	D	537	PRO	CA-C-N	5.11	127.46	120.46
2	D	537	PRO	C-N-CA	5.11	127.46	120.46
2	A	436	PHE	CA-CB-CG	-5.11	108.69	113.80
2	C	431	VAL	N-CA-CB	5.11	119.39	110.65
1	4	173	GLU	CA-C-N	5.11	128.07	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	173	GLU	C-N-CA	5.11	128.07	120.31
2	C	481	SER	CA-C-N	5.11	127.12	120.28
2	C	481	SER	C-N-CA	5.11	127.12	120.28
2	D	400	SER	CA-C-N	5.11	128.48	120.82
2	D	400	SER	C-N-CA	5.11	128.48	120.82
2	F	222	ALA	CA-C-N	5.11	127.12	120.28
2	F	222	ALA	C-N-CA	5.11	127.12	120.28
2	F	787	HIS	CA-C-N	5.11	128.35	121.05
2	F	787	HIS	C-N-CA	5.11	128.35	121.05
2	E	235	ARG	CA-C-N	5.10	129.61	122.36
2	E	235	ARG	C-N-CA	5.10	129.61	122.36
2	A	243	ASP	CA-C-N	5.10	128.07	120.31
2	A	243	ASP	C-N-CA	5.10	128.07	120.31
2	A	402	VAL	CA-CB-CG2	-5.10	101.72	110.40
2	C	126	ASN	N-CA-C	-5.10	106.74	113.12
2	C	660	VAL	N-CA-C	-5.10	104.72	111.09
2	F	410	PRO	O-C-N	-5.10	115.44	121.46
2	A	462	GLU	N-CA-C	-5.10	105.81	112.23
2	A	135	ARG	CA-C-N	5.09	127.38	120.65
2	A	135	ARG	C-N-CA	5.09	127.38	120.65
2	A	503	GLU	CA-C-N	5.09	127.36	120.38
2	A	503	GLU	C-N-CA	5.09	127.36	120.38
2	E	407	PHE	CA-CB-CG	-5.09	108.70	113.80
2	E	497	ASP	CA-C-N	5.09	127.11	120.28
2	E	497	ASP	C-N-CA	5.09	127.11	120.28
2	F	160	THR	CA-C-N	5.09	125.13	119.32
2	F	160	THR	C-N-CA	5.09	125.13	119.32
1	3	139	VAL	CA-C-N	5.09	127.17	120.60
1	3	139	VAL	C-N-CA	5.09	127.17	120.60
2	D	428	ASP	CA-CB-CG	-5.09	107.51	112.60
2	B	186	SER	N-CA-C	5.09	119.52	112.45
2	D	503	GLU	CA-C-N	5.09	127.35	120.38
2	D	503	GLU	C-N-CA	5.09	127.35	120.38
2	E	552	THR	CA-C-N	5.09	127.60	120.28
2	E	552	THR	C-N-CA	5.09	127.60	120.28
1	1	130	VAL	N-CA-C	-5.08	100.33	107.75
2	C	467	GLU	CA-C-N	5.08	131.25	121.54
2	C	467	GLU	C-N-CA	5.08	131.25	121.54
2	C	184	GLY	CA-C-N	5.08	130.85	121.70
2	C	184	GLY	C-N-CA	5.08	130.85	121.70
2	E	757	ASP	N-CA-CB	5.08	119.08	110.49
1	6	167	PHE	N-CA-C	-5.08	101.48	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	692	GLU	N-CA-C	-5.08	106.93	113.23
2	C	505	ILE	N-CA-C	-5.08	105.47	111.00
2	B	243	ASP	CA-C-N	5.08	127.50	120.29
2	B	243	ASP	C-N-CA	5.08	127.50	120.29
2	F	475	ASP	CA-C-N	5.08	127.63	120.42
2	F	475	ASP	C-N-CA	5.08	127.63	120.42
2	E	434	GLN	CA-C-N	5.07	130.83	121.70
2	E	434	GLN	C-N-CA	5.07	130.83	121.70
2	F	370	ALA	CA-C-N	5.07	127.41	120.77
2	F	370	ALA	C-N-CA	5.07	127.41	120.77
2	A	3	PHE	CA-CB-CG	5.07	118.87	113.80
2	C	20	GLU	CA-C-N	5.07	127.38	120.54
2	C	20	GLU	C-N-CA	5.07	127.38	120.54
2	D	166	LEU	N-CA-CB	5.07	119.12	110.50
2	E	544	LEU	N-CA-C	-5.07	102.56	110.42
2	E	728	ASP	CA-CB-CG	-5.07	107.53	112.60
1	1	164	TYR	N-CA-C	-5.07	99.02	107.99
2	B	350	ILE	CA-C-N	5.07	127.83	120.79
2	B	350	ILE	C-N-CA	5.07	127.83	120.79
2	A	692	GLU	N-CA-C	-5.06	106.95	113.23
2	B	559	ALA	CA-C-N	5.06	127.37	120.54
2	B	559	ALA	C-N-CA	5.06	127.37	120.54
2	E	725	LEU	CA-C-N	5.06	127.06	120.28
2	E	725	LEU	C-N-CA	5.06	127.06	120.28
2	F	107	HIS	CB-CA-C	-5.06	102.08	110.68
1	1	157	PHE	N-CA-C	-5.05	100.03	108.32
2	C	85	LYS	CA-C-N	5.05	127.05	120.28
2	C	85	LYS	C-N-CA	5.05	127.05	120.28
2	E	410	PRO	N-CA-CB	-5.05	98.18	103.08
2	F	408	THR	N-CA-C	-5.05	104.76	112.04
2	A	57	SER	CA-C-N	5.05	127.32	120.65
2	A	57	SER	C-N-CA	5.05	127.32	120.65
2	C	376	LYS	N-CA-C	5.05	117.44	111.33
2	E	393	ASP	CA-CB-CG	5.05	117.65	112.60
1	1	216	PHE	CA-CB-CG	-5.05	108.75	113.80
1	5	145	LEU	N-CA-C	-5.05	100.05	110.80
2	D	577	TYR	CA-C-N	5.05	131.19	121.54
2	D	577	TYR	C-N-CA	5.05	131.19	121.54
2	E	412	ASN	N-CA-CB	5.05	119.03	110.49
2	A	493	GLN	N-CA-C	5.05	121.55	110.80
1	2	139	VAL	CA-C-N	5.05	127.11	120.60
1	2	139	VAL	C-N-CA	5.05	127.11	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	TYR	N-CA-C	-5.05	99.57	108.20
2	B	431	VAL	CB-CA-C	-5.05	104.34	112.16
2	F	446	GLU	CA-C-N	5.05	127.55	120.28
2	F	446	GLU	C-N-CA	5.05	127.55	120.28
2	A	725	LEU	N-CA-C	-5.04	105.44	112.45
2	F	217	ILE	CB-CA-C	-5.04	105.33	112.14
2	E	41	GLU	N-CA-C	-5.04	106.91	113.16
1	3	166	ASP	N-CA-C	-5.04	97.71	107.44
2	B	187	LYS	N-CA-C	5.04	118.69	112.54
2	C	433	SER	N-CA-C	-5.04	106.82	113.12
2	D	26	HIS	CE1-NE2-CD2	-5.04	103.96	109.00
2	E	253	TYR	CA-C-N	5.04	127.44	120.29
2	E	253	TYR	C-N-CA	5.04	127.44	120.29
2	F	447	GLN	CA-C-N	5.04	127.79	120.79
2	F	447	GLN	C-N-CA	5.04	127.79	120.79
2	F	475	ASP	CA-CB-CG	-5.04	107.56	112.60
2	B	678	GLU	CB-CA-C	-5.04	102.55	110.86
2	E	366	ILE	CB-CA-C	5.04	119.55	111.29
2	A	19	GLU	CA-CB-CG	5.03	124.17	114.10
2	D	217	ILE	CB-CA-C	-5.03	105.35	112.14
2	A	542	ILE	N-CA-C	-5.03	101.24	108.48
2	F	461	LYS	N-CA-C	-5.03	107.14	113.28
2	F	805	THR	N-CA-C	-5.03	101.55	109.50
1	1	158	GLU	CA-C-N	5.03	131.14	121.54
1	1	158	GLU	C-N-CA	5.03	131.14	121.54
2	A	222	ALA	CA-C-N	5.03	127.02	120.28
2	A	222	ALA	C-N-CA	5.03	127.02	120.28
2	B	632	GLN	N-CA-C	-5.03	105.89	112.23
1	4	127	LEU	N-CA-C	-5.03	104.78	111.87
2	C	384	ASP	CA-CB-CG	5.03	117.62	112.60
2	D	542	ILE	N-CA-C	-5.03	101.24	108.48
2	A	536	ARG	CA-C-N	5.02	125.74	120.11
2	A	536	ARG	C-N-CA	5.02	125.74	120.11
2	C	791	HIS	CB-CG-CD2	-5.02	124.67	131.20
2	D	329	ALA	N-CA-C	-5.02	105.88	112.41
2	E	184	GLY	CA-C-N	5.02	130.74	121.70
2	E	184	GLY	C-N-CA	5.02	130.74	121.70
2	C	542	ILE	N-CA-CB	5.02	120.13	111.39
2	C	268	ILE	CA-C-N	5.02	131.13	121.54
2	C	268	ILE	C-N-CA	5.02	131.13	121.54
2	C	135	ARG	CA-C-N	5.02	127.27	120.65
2	C	135	ARG	C-N-CA	5.02	127.27	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	396	ASP	CA-C-N	5.02	127.31	120.54
2	E	396	ASP	C-N-CA	5.02	127.31	120.54
2	A	699	PRO	CA-C-N	5.01	127.00	120.28
2	A	699	PRO	C-N-CA	5.01	127.00	120.28
2	C	765	LEU	CA-C-N	5.01	127.76	120.79
2	C	765	LEU	C-N-CA	5.01	127.76	120.79
2	D	82	PRO	CA-C-N	5.01	127.26	120.65
2	D	82	PRO	C-N-CA	5.01	127.26	120.65
2	D	296	ALA	N-CA-C	-5.01	106.68	112.89
2	D	667	ARG	CA-C-N	5.01	131.11	121.54
2	D	667	ARG	C-N-CA	5.01	131.11	121.54
2	B	514	ASP	CA-CB-CG	-5.01	107.59	112.60
2	F	23	ARG	N-CA-C	5.01	118.85	112.34
2	C	369	ASP	CA-CB-CG	-5.01	107.59	112.60
1	3	201	LYS	CA-C-N	5.00	127.82	120.71
1	3	201	LYS	C-N-CA	5.00	127.82	120.71
1	4	190	SER	CA-C-N	5.00	127.28	120.63
1	4	190	SER	C-N-CA	5.00	127.28	120.63
2	C	257	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (107) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	161	TYR	Sidechain
1	2	199	TYR	Sidechain
1	3	164	TYR	Sidechain
1	3	185	TYR	Sidechain
1	3	194	HIS	Sidechain
1	3	216	PHE	Sidechain
1	4	161	TYR	Sidechain
1	5	185	TYR	Sidechain
1	6	164	TYR	Sidechain
1	6	215	HIS	Sidechain
2	A	185	ARG	Sidechain
2	A	210	PRO	Peptide
2	A	355	ARG	Sidechain
2	A	363	ARG	Sidechain
2	A	409	THR	Peptide
2	A	424	ARG	Sidechain
2	A	468	ASN	Peptide
2	A	592	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	A	596	TYR	Sidechain
2	A	627	PHE	Sidechain
2	A	667	ARG	Sidechain
2	A	697	PHE	Sidechain
2	A	716	LYS	Peptide,Mainchain
2	A	756	VAL	Peptide
2	A	760	TYR	Sidechain
2	A	767	ARG	Sidechain
2	A	776	ARG	Sidechain
2	A	80	TYR	Sidechain
2	B	107	HIS	Sidechain
2	B	199	ARG	Sidechain
2	B	210	PRO	Peptide
2	B	23	ARG	Sidechain
2	B	355	ARG	Sidechain
2	B	358	TYR	Sidechain
2	B	363	ARG	Sidechain
2	B	403	ARG	Sidechain
2	B	409	THR	Peptide
2	B	468	ASN	Peptide
2	B	536	ARG	Sidechain
2	B	592	GLY	Peptide
2	B	627	PHE	Sidechain
2	B	667	ARG	Sidechain
2	B	697	PHE	Sidechain
2	B	716	LYS	Peptide,Mainchain
2	B	756	VAL	Peptide
2	B	760	TYR	Sidechain
2	B	80	TYR	Sidechain
2	C	210	PRO	Peptide
2	C	28	ASN	Mainchain
2	C	358	TYR	Sidechain
2	C	409	THR	Peptide
2	C	468	ASN	Peptide
2	C	541	PHE	Peptide
2	C	592	GLY	Peptide
2	C	697	PHE	Sidechain
2	C	716	LYS	Peptide
2	C	756	VAL	Peptide
2	C	791	HIS	Sidechain
2	C	80	TYR	Sidechain
2	D	210	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	D	355	ARG	Sidechain
2	D	363	ARG	Sidechain
2	D	381	TYR	Sidechain
2	D	405	ARG	Sidechain
2	D	409	THR	Peptide
2	D	468	ASN	Peptide
2	D	556	ARG	Sidechain
2	D	592	GLY	Peptide
2	D	593	TYR	Sidechain
2	D	611	TYR	Sidechain
2	D	667	ARG	Sidechain
2	D	697	PHE	Sidechain
2	D	716	LYS	Peptide,Mainchain
2	D	756	VAL	Peptide
2	D	760	TYR	Sidechain
2	E	198	ARG	Sidechain
2	E	210	PRO	Peptide
2	E	381	TYR	Sidechain
2	E	409	THR	Peptide
2	E	468	ASN	Peptide
2	E	5	ARG	Sidechain
2	E	592	GLY	Peptide
2	E	593	TYR	Sidechain
2	E	627	PHE	Sidechain
2	E	667	ARG	Sidechain
2	E	716	LYS	Peptide,Mainchain
2	E	756	VAL	Peptide
2	E	80	TYR	Sidechain
2	E	96	ARG	Sidechain
2	F	102	TYR	Sidechain
2	F	114	ARG	Sidechain
2	F	210	PRO	Peptide
2	F	381	TYR	Sidechain
2	F	409	THR	Peptide
2	F	424	ARG	Sidechain
2	F	468	ASN	Peptide
2	F	592	GLY	Peptide
2	F	667	ARG	Sidechain
2	F	697	PHE	Sidechain
2	F	716	LYS	Peptide,Mainchain
2	F	756	VAL	Peptide
2	F	80	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	1	777	0	758	17	0
1	2	777	0	758	15	0
1	3	777	0	758	21	0
1	4	777	0	758	13	0
1	5	777	0	758	14	0
1	6	777	0	758	12	0
2	A	6200	0	6290	119	0
2	B	6200	0	6290	136	0
2	C	6200	0	6290	114	0
2	D	6200	0	6290	143	0
2	E	6200	0	6290	119	0
2	F	6200	0	6290	120	0
All	All	41862	0	42288	791	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 10.

All (791) 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)
2:A:619:ILE:CD1	2:A:656:MET:HB3	1.24	1.66
2:A:619:ILE:CD1	2:A:656:MET:CB	2.18	1.21
2:F:619:ILE:HD12	2:F:656:MET:HB3	1.23	1.21
2:E:619:ILE:CD1	2:E:656:MET:HB3	1.69	1.20
2:F:619:ILE:CG2	2:F:627:PHE:CZ	2.27	1.18
2:C:615:LEU:HD22	2:C:617:ASP:OD1	1.47	1.13
2:E:619:ILE:HG23	2:E:627:PHE:CZ	1.84	1.12
2:D:619:ILE:HD12	2:D:656:MET:HB3	1.15	1.11
2:F:619:ILE:HG21	2:F:627:PHE:CE1	1.85	1.11
2:A:619:ILE:HD11	2:A:656:MET:HB3	1.20	1.10
2:E:619:ILE:CG2	2:E:627:PHE:CZ	2.34	1.09
2:F:619:ILE:CG2	2:F:627:PHE:HZ	1.64	1.09
2:C:616:LEU:HB3	2:C:619:ILE:HD11	1.36	1.08
2:A:619:ILE:HD12	2:A:656:MET:CB	1.81	1.04
2:E:619:ILE:HD12	2:E:656:MET:HB3	1.10	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ILE:CD1	2:B:656:MET:HB3	1.87	1.03
2:E:619:ILE:HG23	2:E:627:PHE:HZ	1.14	1.03
2:B:619:ILE:HD12	2:B:656:MET:HB3	1.01	1.01
2:E:619:ILE:HG21	2:E:627:PHE:CE1	1.99	0.98
2:F:619:ILE:HG22	2:F:627:PHE:HZ	1.31	0.96
2:F:619:ILE:HG21	2:F:627:PHE:HE1	1.24	0.94
2:D:619:ILE:CG2	2:D:627:PHE:HE1	1.81	0.94
2:A:619:ILE:HD12	2:A:656:MET:HB3	0.94	0.93
2:B:619:ILE:HD12	2:B:656:MET:CB	1.97	0.93
2:A:619:ILE:HD11	2:A:656:MET:CB	1.90	0.93
2:E:619:ILE:CG2	2:E:627:PHE:CE1	2.51	0.93
2:F:619:ILE:CG2	2:F:627:PHE:CE1	2.49	0.93
2:B:616:LEU:HB2	2:B:619:ILE:HD11	1.53	0.90
2:D:619:ILE:CG2	2:D:627:PHE:CE1	2.54	0.89
2:D:619:ILE:HG23	2:D:627:PHE:HE1	1.37	0.89
2:F:619:ILE:HG22	2:F:627:PHE:CZ	2.07	0.88
2:A:394:LEU:HD13	2:A:480:VAL:HG22	1.54	0.86
2:B:619:ILE:CG2	2:B:627:PHE:HE1	1.89	0.86
2:C:616:LEU:CB	2:C:619:ILE:HD11	2.05	0.85
2:C:619:ILE:HG22	2:C:619:ILE:O	1.76	0.85
2:D:619:ILE:CD1	2:D:656:MET:HB3	2.05	0.84
2:B:619:ILE:CG2	2:B:627:PHE:CE1	2.62	0.83
2:C:615:LEU:CD2	2:C:617:ASP:OD1	2.26	0.82
2:C:619:ILE:CG2	2:C:627:PHE:HE1	1.92	0.82
2:F:619:ILE:HG23	2:F:627:PHE:CZ	2.18	0.79
2:C:394:LEU:HD13	2:C:480:VAL:HG22	1.64	0.79
2:F:571:ARG:CZ	2:F:617:ASP:OD2	2.31	0.78
2:B:619:ILE:HG22	2:B:627:PHE:CE1	2.18	0.77
2:E:619:ILE:HD12	2:E:656:MET:CB	2.05	0.76
2:C:26:HIS:CD2	2:C:33:HIS:CE1	2.75	0.75
2:E:619:ILE:HG21	2:E:627:PHE:HE1	1.52	0.72
2:F:619:ILE:CD1	2:F:656:MET:HB3	2.13	0.72
2:F:513:GLN:H	2:F:718:HIS:CD2	2.08	0.72
2:D:619:ILE:HG22	2:D:627:PHE:CE1	2.25	0.72
2:E:619:ILE:HG22	2:E:619:ILE:O	1.91	0.71
2:F:26:HIS:CD2	2:F:33:HIS:CE1	2.79	0.71
2:B:21:ALA:HA	2:B:33:HIS:CE1	2.25	0.71
2:D:619:ILE:HG22	2:D:697:PHE:HE1	1.55	0.71
2:F:619:ILE:HD12	2:F:656:MET:CB	2.14	0.71
2:E:107:HIS:HA	2:E:110:LEU:HD12	1.73	0.70
2:F:619:ILE:HG22	2:F:619:ILE:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:LEU:HD13	2:D:124:LEU:HD22	1.74	0.69
2:C:574:MET:HG3	2:C:619:ILE:HG12	1.74	0.69
2:B:619:ILE:HG23	2:B:627:PHE:HE1	1.57	0.68
2:C:693:LEU:HD12	2:C:697:PHE:CD2	2.28	0.68
2:B:363:ARG:HH11	2:B:399:GLY:HA2	1.59	0.68
2:C:26:HIS:CG	2:C:33:HIS:CE1	2.81	0.68
2:D:363:ARG:HH11	2:D:399:GLY:HA2	1.60	0.67
2:D:363:ARG:HH12	2:D:471:VAL:HA	1.60	0.67
2:A:544:LEU:HD21	2:A:693:LEU:HD13	1.77	0.66
2:A:682:HIS:CD2	2:A:712:HIS:CE1	2.84	0.66
2:D:53:LEU:HD21	2:D:134:ALA:HA	1.77	0.66
2:D:197:SER:HA	2:D:234:LEU:HD23	1.77	0.66
2:D:544:LEU:HD11	2:D:693:LEU:HD13	1.77	0.66
2:C:619:ILE:O	2:C:619:ILE:CG2	2.43	0.66
2:E:507:HIS:CD2	2:E:517:VAL:HG11	2.32	0.65
2:F:26:HIS:CG	2:F:33:HIS:CE1	2.84	0.65
1:4:142:LEU:HD23	1:4:185:TYR:CD2	2.30	0.65
2:F:619:ILE:HG23	2:F:627:PHE:HZ	1.56	0.65
2:C:55:LEU:HD13	2:C:124:LEU:HD22	1.79	0.65
2:A:21:ALA:HA	2:A:33:HIS:CE1	2.33	0.64
2:F:751:VAL:HG22	2:F:772:HIS:CB	2.27	0.64
2:A:394:LEU:HD21	2:A:483:TRP:CE2	2.32	0.64
2:F:741:ILE:HG22	2:F:792:ILE:HD12	1.80	0.64
2:B:669:LYS:H	2:B:685:MET:HE1	1.63	0.64
2:C:619:ILE:HG23	2:C:622:ALA:HB3	1.80	0.64
2:E:619:ILE:HD11	2:E:656:MET:HB3	1.77	0.64
2:C:24:LEU:HD11	2:C:61:GLN:HE22	1.62	0.63
2:C:619:ILE:CG2	2:C:627:PHE:CE1	2.78	0.63
1:1:163:LEU:HD11	1:1:209:LEU:HD21	1.79	0.63
2:B:106:GLU:CD	2:B:142:LEU:HD11	2.24	0.63
2:F:351:LEU:HD13	2:F:391:ALA:HB1	1.79	0.63
1:5:154:LEU:HB3	1:5:204:ILE:HD12	1.81	0.63
2:A:619:ILE:CG2	2:A:627:PHE:CE1	2.82	0.63
2:A:727:SER:O	2:A:731:THR:HG23	1.99	0.62
2:B:26:HIS:CD2	2:B:33:HIS:HE2	2.16	0.62
2:D:619:ILE:HD12	2:D:656:MET:CB	2.10	0.62
2:C:619:ILE:HG22	2:C:697:PHE:HE1	1.64	0.62
2:D:665:LEU:HD23	2:D:685:MET:HG3	1.82	0.62
2:D:682:HIS:CG	2:D:712:HIS:CE1	2.88	0.62
2:F:427:LYS:HG3	2:F:443:ARG:HA	1.81	0.62
2:C:544:LEU:HD11	2:C:693:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:544:LEU:HD23	2:A:658:SER:HB2	1.82	0.61
2:D:21:ALA:HB2	2:D:29:ILE:CG1	2.30	0.61
2:D:26:HIS:CE1	2:D:68:ILE:HB	2.35	0.61
2:F:21:ALA:HA	2:F:33:HIS:CE1	2.34	0.61
2:B:20:GLU:HB2	2:B:33:HIS:CD2	2.35	0.61
2:E:55:LEU:HD13	2:E:124:LEU:HD22	1.83	0.61
2:F:363:ARG:HH11	2:F:399:GLY:HA2	1.65	0.61
2:C:693:LEU:HD12	2:C:697:PHE:HD2	1.64	0.61
2:B:507:HIS:CD2	2:B:517:VAL:HG11	2.36	0.60
2:D:46:ALA:HB1	2:D:109:LEU:HB2	1.83	0.60
2:A:476:ILE:O	2:A:480:VAL:HG23	2.01	0.60
2:C:198:ARG:N	2:C:233:ILE:HG21	2.17	0.60
2:D:786:ILE:HG21	2:D:792:ILE:HG23	1.83	0.60
2:F:233:ILE:H	2:F:233:ILE:HD12	1.66	0.60
2:B:633:VAL:HG23	2:B:639:LEU:HD23	1.83	0.60
2:E:507:HIS:CG	2:E:517:VAL:HG11	2.37	0.60
2:A:363:ARG:HH12	2:A:471:VAL:HA	1.67	0.60
2:A:383:SER:H	2:A:390:LYS:HD2	1.67	0.59
2:E:24:LEU:HB2	2:E:33:HIS:HE2	1.66	0.59
2:C:364:VAL:H	2:C:470:GLU:H	1.50	0.59
2:D:685:MET:O	2:D:689:VAL:HG23	2.02	0.59
2:B:723:VAL:HG21	2:B:752:ALA:HA	1.83	0.59
2:D:363:ARG:HH21	2:D:402:VAL:HG11	1.66	0.59
2:A:395:ILE:HA	2:A:476:ILE:HD12	1.85	0.59
2:D:507:HIS:CD2	2:D:517:VAL:HG11	2.38	0.59
2:A:786:ILE:HG21	2:A:792:ILE:HG23	1.85	0.59
2:D:387:LEU:H	2:D:387:LEU:HD22	1.67	0.59
2:F:715:GLU:HB2	2:F:718:HIS:CD2	2.38	0.59
1:2:142:LEU:HD13	1:2:209:LEU:HD21	1.85	0.58
2:A:619:ILE:HG22	2:A:697:PHE:HE1	1.68	0.58
2:E:25:GLY:HA3	2:E:73:GLU:HA	1.85	0.58
2:A:402:VAL:CG2	2:A:478:MET:HE1	2.33	0.58
2:B:633:VAL:HG13	2:B:649:PHE:HB3	1.85	0.58
2:D:547:THR:H	2:D:763:ARG:HH21	1.51	0.58
2:F:351:LEU:CD1	2:F:391:ALA:HB1	2.33	0.58
1:5:164:TYR:CG	1:5:193:ILE:HD13	2.39	0.58
2:E:574:MET:HG2	2:E:619:ILE:HG12	1.85	0.58
2:E:633:VAL:HG13	2:E:649:PHE:HB3	1.85	0.58
2:B:665:LEU:HD11	2:B:689:VAL:HG11	1.86	0.58
2:D:437:GLU:HA	2:D:440:ALA:HB3	1.84	0.58
2:C:21:ALA:HB2	2:C:29:ILE:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:619:ILE:CD1	2:E:656:MET:CB	2.64	0.58
2:F:719:LEU:HD12	2:F:720:THR:H	1.68	0.58
2:F:747:ALA:O	2:F:751:VAL:HG23	2.03	0.58
2:A:624:PRO:HA	2:A:627:PHE:CD2	2.39	0.58
2:F:522:LYS:HA	2:F:525:ARG:HE	1.69	0.58
2:F:289:GLY:H	2:F:321:ARG:HH12	1.49	0.57
2:B:627:PHE:HB2	2:B:698:ARG:HE	1.70	0.57
2:D:619:ILE:HG22	2:D:697:PHE:CE1	2.39	0.57
2:A:723:VAL:HG21	2:A:752:ALA:HA	1.86	0.57
2:E:21:ALA:HA	2:E:33:HIS:CE1	2.39	0.57
2:A:28:ASN:HB2	2:A:81:THR:HG23	1.86	0.57
2:A:233:ILE:HA	2:F:361:HIS:HA	1.87	0.57
2:D:548:GLY:O	2:D:762:ALA:HB3	2.04	0.57
2:A:402:VAL:HG13	2:A:405:ARG:HE	1.69	0.57
2:E:427:LYS:HG3	2:E:443:ARG:HA	1.86	0.57
2:B:616:LEU:CB	2:B:619:ILE:HD11	2.31	0.57
2:B:624:PRO:HA	2:B:627:PHE:CD2	2.40	0.57
1:3:136:PHE:CD1	2:C:431:VAL:HG11	2.40	0.57
2:A:427:LYS:HG3	2:A:443:ARG:HA	1.87	0.57
1:3:216:PHE:CZ	2:C:439:ALA:HB3	2.40	0.56
1:4:142:LEU:HD21	1:4:182:LEU:HA	1.86	0.56
1:2:194:HIS:CE1	2:C:141:LEU:HD22	2.40	0.56
1:3:142:LEU:HD23	1:3:142:LEU:O	2.05	0.56
2:B:276:LEU:HD23	2:B:309:LEU:HA	1.88	0.56
2:D:399:GLY:O	2:E:233:ILE:HD13	2.05	0.56
2:F:544:LEU:HD13	2:F:690:MET:HE2	1.87	0.56
1:2:133:PHE:CZ	1:2:142:LEU:HD12	2.40	0.56
2:D:398:ALA:HB1	2:D:475:ASP:HB3	1.87	0.56
1:1:140:ILE:HD13	1:1:216:PHE:CE1	2.41	0.56
2:C:403:ARG:HH21	2:D:232:GLU:H	1.54	0.56
2:D:351:LEU:HD13	2:D:391:ALA:HB1	1.87	0.56
2:E:685:MET:HG3	2:E:712:HIS:CG	2.41	0.56
2:F:627:PHE:CD2	2:F:697:PHE:HA	2.40	0.56
2:C:507:HIS:CD2	2:C:517:VAL:HG11	2.41	0.55
2:F:26:HIS:CE1	2:F:68:ILE:HB	2.41	0.55
1:1:140:ILE:HD13	1:1:216:PHE:CD1	2.42	0.55
2:A:619:ILE:CD1	2:A:656:MET:CG	2.83	0.55
2:B:545:GLY:H	2:B:665:LEU:HD13	1.70	0.55
2:E:619:ILE:CG2	2:E:619:ILE:O	2.54	0.55
2:E:685:MET:HG3	2:E:712:HIS:CD2	2.42	0.55
1:3:130:VAL:HG22	1:3:164:TYR:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:484:THR:HG23	2:A:611:TYR:CE1	2.42	0.55
2:B:49:ALA:HB1	2:B:137:GLN:HB3	1.88	0.55
2:E:685:MET:HE3	2:E:712:HIS:HB3	1.86	0.55
2:E:363:ARG:HB3	2:E:399:GLY:HA2	1.89	0.55
1:2:208:ALA:O	1:2:212:ILE:HD13	2.07	0.55
1:3:142:LEU:HD21	1:3:182:LEU:HD22	1.87	0.55
2:B:512:GLY:HA2	2:B:722:ILE:HD11	1.88	0.55
2:E:751:VAL:HG22	2:E:772:HIS:CG	2.42	0.55
2:F:21:ALA:HB2	2:F:29:ILE:HG12	1.89	0.55
2:F:633:VAL:HG11	2:F:654:LEU:HD11	1.88	0.55
2:A:542:ILE:HG13	2:A:705:ILE:HD13	1.89	0.55
2:F:776:ARG:HE	2:F:801:PHE:HB3	1.72	0.54
2:C:394:LEU:HD23	2:C:479:VAL:HG22	1.90	0.54
2:F:661:GLY:H	2:F:689:VAL:HG13	1.73	0.54
1:5:216:PHE:HA	2:E:440:ALA:HB2	1.89	0.54
2:D:17:ALA:HB1	2:D:29:ILE:HG21	1.88	0.54
2:D:21:ALA:HB2	2:D:29:ILE:HG13	1.89	0.54
2:D:394:LEU:HD13	2:D:480:VAL:HG22	1.89	0.54
2:A:401:LYS:HD3	2:A:478:MET:HE3	1.90	0.54
2:A:26:HIS:CD2	2:A:33:HIS:CE1	2.95	0.54
2:B:741:ILE:HG21	2:B:777:LEU:HD13	1.89	0.54
2:E:351:LEU:CD1	2:E:391:ALA:HB1	2.38	0.54
1:5:142:LEU:HD13	1:5:209:LEU:HD21	1.89	0.54
2:B:90:LEU:HA	2:C:156:SER:H	1.73	0.54
2:A:387:LEU:HD12	2:A:387:LEU:H	1.72	0.54
1:1:137:GLU:HA	1:1:140:ILE:HD12	1.89	0.53
2:A:437:GLU:HA	2:A:440:ALA:HB3	1.90	0.53
2:E:53:LEU:HD21	2:E:134:ALA:HA	1.90	0.53
2:F:616:LEU:HB2	2:F:619:ILE:HD11	1.88	0.53
1:5:140:ILE:HD11	1:5:216:PHE:CD1	2.42	0.53
2:A:556:ARG:HE	2:A:571:ARG:HH22	1.56	0.53
2:B:9:ARG:HB3	2:B:105:THR:H	1.72	0.53
2:B:682:HIS:CE1	2:B:712:HIS:CE1	2.96	0.53
2:C:624:PRO:HA	2:C:627:PHE:CD2	2.43	0.53
2:D:26:HIS:CG	2:D:33:HIS:CE1	2.97	0.53
2:D:106:GLU:HG2	2:D:107:HIS:CD2	2.43	0.53
2:D:374:ALA:HA	2:D:394:LEU:HD12	1.90	0.53
2:F:199:ARG:HH21	2:F:310:GLN:HE22	1.55	0.53
2:E:26:HIS:HB2	2:E:33:HIS:CE1	2.43	0.53
2:B:630:LEU:O	2:B:634:LEU:HD13	2.08	0.53
2:C:361:HIS:CG	2:C:361:HIS:O	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:ILE:HG23	2:D:141:LEU:HB2	1.91	0.53
2:E:351:LEU:HD13	2:E:391:ALA:HB1	1.91	0.53
2:D:355:ARG:HE	2:D:364:VAL:HG12	1.73	0.53
2:E:371:ILE:HD12	2:E:395:ILE:HD13	1.91	0.53
2:E:667:ARG:H	2:E:667:ARG:HH11	1.57	0.53
1:6:142:LEU:HD21	1:6:182:LEU:HD22	1.90	0.53
2:A:619:ILE:HG22	2:A:627:PHE:CE1	2.44	0.53
2:C:100:HIS:CG	2:C:102:TYR:O	2.61	0.53
2:E:195:VAL:HG13	2:E:198:ARG:HH11	1.73	0.53
2:C:542:ILE:HG13	2:C:705:ILE:HD13	1.91	0.53
2:C:545:GLY:H	2:C:661:GLY:HA3	1.73	0.53
2:D:476:ILE:O	2:D:480:VAL:HG23	2.09	0.53
2:D:542:ILE:HG13	2:D:705:ILE:HD13	1.91	0.53
2:F:619:ILE:CG2	2:F:619:ILE:O	2.55	0.53
1:3:216:PHE:HA	2:C:440:ALA:HB2	1.91	0.53
2:C:95:ALA:HA	2:C:107:HIS:CD2	2.44	0.53
2:F:571:ARG:NH2	2:F:617:ASP:OD2	2.41	0.53
2:B:361:HIS:CG	2:C:233:ILE:HG12	2.44	0.53
2:F:387:LEU:H	2:F:387:LEU:HD22	1.73	0.53
1:5:133:PHE:CZ	1:5:142:LEU:HD12	2.45	0.52
2:B:53:LEU:HD21	2:B:134:ALA:HA	1.90	0.52
2:E:46:ALA:HB1	2:E:109:LEU:HB2	1.91	0.52
2:E:747:ALA:HB1	2:E:801:PHE:CZ	2.45	0.52
1:1:216:PHE:CE1	2:A:440:ALA:HA	2.44	0.52
2:C:506:LEU:HD21	2:C:558:LEU:HD23	1.91	0.52
2:D:26:HIS:HB2	2:D:33:HIS:CE1	2.44	0.52
2:B:619:ILE:HG22	2:B:697:PHE:HE1	1.74	0.52
2:F:362:HIS:HB2	2:F:403:ARG:HH21	1.74	0.52
2:A:374:ALA:HA	2:A:476:ILE:HG21	1.90	0.52
2:D:26:HIS:CD2	2:D:33:HIS:NE2	2.77	0.52
2:E:361:HIS:HA	2:F:233:ILE:HA	1.90	0.52
2:B:394:LEU:HD13	2:B:480:VAL:HG22	1.92	0.52
2:F:630:LEU:O	2:F:634:LEU:HD13	2.09	0.52
2:C:21:ALA:HA	2:C:33:HIS:CE1	2.45	0.52
2:F:423:VAL:HG11	2:F:445:THR:HB	1.92	0.52
2:F:639:LEU:HD13	2:F:640:THR:H	1.74	0.52
1:6:203:ILE:HA	2:F:434:GLN:HE22	1.74	0.52
2:E:342:PRO:HG2	2:E:350:ILE:HD11	1.92	0.52
2:B:355:ARG:HD3	2:B:366:ILE:H	1.75	0.51
2:B:669:LYS:HD3	2:B:712:HIS:CD2	2.44	0.51
2:D:394:LEU:HD23	2:D:479:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:702:ILE:HA	2:D:705:ILE:HD12	1.91	0.51
2:F:786:ILE:HD12	2:F:792:ILE:HD13	1.91	0.51
1:2:216:PHE:HA	2:B:440:ALA:HB2	1.92	0.51
2:A:619:ILE:HG22	2:A:619:ILE:O	2.09	0.51
2:B:26:HIS:CG	2:B:33:HIS:CE1	2.98	0.51
2:D:21:ALA:HA	2:D:33:HIS:CE1	2.45	0.51
2:D:540:SER:HB2	2:D:706:ASP:H	1.74	0.51
2:F:111:GLY:HA2	2:F:114:ARG:HH11	1.75	0.51
2:A:26:HIS:CG	2:A:33:HIS:CE1	2.98	0.51
2:B:427:LYS:O	2:B:431:VAL:HG23	2.09	0.51
2:B:741:ILE:HG22	2:B:792:ILE:HB	1.92	0.51
2:D:701:PHE:CE2	2:D:705:ILE:HD11	2.46	0.51
1:1:154:LEU:HD11	1:1:161:TYR:HB3	1.92	0.51
2:A:423:VAL:HG11	2:A:445:THR:HB	1.92	0.51
2:C:363:ARG:HH21	2:C:470:GLU:CD	2.18	0.51
2:D:46:ALA:HB2	2:D:105:THR:O	2.09	0.51
2:D:235:ARG:HH22	2:D:238:ARG:HH22	1.58	0.51
2:F:26:HIS:CD2	2:F:33:HIS:HE1	2.26	0.51
2:C:46:ALA:H	2:C:105:THR:HB	1.75	0.51
2:C:403:ARG:HE	2:D:231:PRO:HB2	1.76	0.51
2:A:26:HIS:CE1	2:A:68:ILE:HB	2.46	0.51
2:A:363:ARG:HD2	2:A:403:ARG:HB2	1.93	0.51
2:A:777:LEU:HD22	2:A:792:ILE:HG21	1.93	0.51
2:C:303:SER:HB3	2:C:309:LEU:HB2	1.92	0.51
2:D:619:ILE:HG23	2:D:627:PHE:CE1	2.26	0.51
2:C:254:ARG:HD3	2:C:254:ARG:H	1.76	0.51
2:D:109:LEU:HD23	2:D:138:VAL:HG22	1.92	0.51
2:D:715:GLU:HB3	2:D:717:LYS:HZ3	1.76	0.51
2:E:363:ARG:CZ	2:E:471:VAL:HA	2.41	0.51
2:A:731:THR:HG22	2:A:741:ILE:O	2.10	0.51
2:F:507:HIS:CD2	2:F:517:VAL:HG11	2.46	0.51
2:F:355:ARG:HB3	2:F:365:SER:HA	1.92	0.50
1:3:142:LEU:HD22	1:3:209:LEU:HD13	1.93	0.50
2:F:398:ALA:HB1	2:F:475:ASP:HB3	1.93	0.50
1:4:140:ILE:HG21	2:D:443:ARG:HE	1.76	0.50
2:C:742:GLU:HB3	2:C:791:HIS:CE1	2.46	0.50
2:A:192:VAL:HG13	2:A:204:PRO:HG2	1.93	0.50
2:B:423:VAL:HG11	2:B:445:THR:HB	1.94	0.50
2:B:743:LEU:HD21	2:B:773:VAL:HG22	1.93	0.50
2:C:743:LEU:HG	2:C:794:LEU:HD23	1.93	0.50
2:E:394:LEU:HD13	2:E:480:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:164:TYR:CG	1:4:193:ILE:HD13	2.46	0.50
2:B:93:ASP:HB3	2:C:158:ALA:H	1.77	0.50
2:C:26:HIS:CE1	2:C:68:ILE:HB	2.46	0.50
2:C:619:ILE:HG23	2:C:622:ALA:CB	2.41	0.50
2:E:543:PHE:HB2	2:E:657:THR:HA	1.92	0.50
2:B:38:LEU:O	2:B:47:ALA:HB2	2.12	0.50
2:E:685:MET:O	2:E:689:VAL:HG23	2.11	0.50
2:F:195:VAL:HA	2:F:198:ARG:HE	1.76	0.50
2:F:498:LYS:HB2	2:F:528:ARG:HH12	1.76	0.50
1:3:136:PHE:CG	2:C:431:VAL:HG11	2.47	0.50
2:A:544:LEU:HD22	2:A:660:VAL:HG12	1.93	0.50
2:A:348:ILE:HG22	2:A:352:GLN:HE21	1.77	0.50
2:B:424:ARG:HE	2:B:427:LYS:HD3	1.77	0.50
2:B:727:SER:HB3	2:B:743:LEU:HD13	1.94	0.50
2:D:45:ILE:HG22	2:D:138:VAL:HG12	1.94	0.50
2:E:371:ILE:O	2:E:374:ALA:HB3	2.12	0.50
2:F:18:GLN:O	2:F:21:ALA:HB3	2.12	0.50
2:F:36:LEU:HB3	2:F:40:ARG:HE	1.77	0.50
2:D:627:PHE:HB2	2:D:698:ARG:HE	1.77	0.49
2:A:46:ALA:HB2	2:A:105:THR:O	2.12	0.49
2:C:370:ALA:HB1	2:C:471:VAL:HG13	1.94	0.49
2:E:98:LEU:CD1	2:E:110:LEU:HD13	2.42	0.49
2:F:394:LEU:HD23	2:F:479:VAL:HG22	1.94	0.49
1:5:142:LEU:HD11	1:5:182:LEU:HD22	1.94	0.49
2:F:184:GLY:HA2	2:F:185:ARG:HB2	1.94	0.49
1:2:203:ILE:HG23	2:B:434:GLN:HE21	1.78	0.49
2:A:20:GLU:HB3	2:A:33:HIS:CD2	2.47	0.49
2:B:39:VAL:HG11	2:B:60:ILE:HD12	1.93	0.49
2:B:571:ARG:NE	2:B:617:ASP:OD2	2.46	0.49
2:C:36:LEU:HB3	2:C:40:ARG:HE	1.78	0.49
2:D:371:ILE:O	2:D:374:ALA:HB3	2.13	0.49
2:E:18:GLN:O	2:E:21:ALA:HB3	2.12	0.49
1:2:136:PHE:CE2	1:2:216:PHE:CD2	3.00	0.49
2:A:777:LEU:CD2	2:A:792:ILE:HG21	2.43	0.49
2:B:506:LEU:HB2	2:B:517:VAL:HG13	1.95	0.49
2:E:49:ALA:O	2:E:53:LEU:HD22	2.13	0.49
2:B:303:SER:HB3	2:B:309:LEU:HB2	1.95	0.49
1:5:216:PHE:CE1	2:E:440:ALA:HA	2.48	0.49
2:B:355:ARG:CD	2:B:366:ILE:H	2.25	0.49
2:B:355:ARG:CG	2:B:366:ILE:H	2.26	0.49
2:C:355:ARG:HB2	2:C:364:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:417:GLU:H	2:F:417:GLU:CD	2.21	0.49
1:4:195:ARG:HA	1:4:195:ARG:HH21	1.78	0.49
2:A:631:LEU:HD13	2:A:698:ARG:HH12	1.78	0.49
2:B:36:LEU:HD11	2:B:64:VAL:HG11	1.95	0.49
2:D:398:ALA:HB1	2:D:475:ASP:CB	2.42	0.49
1:3:152:THR:OG1	1:3:163:LEU:HD21	2.13	0.48
2:C:285:ILE:HD11	2:C:323:TYR:CE1	2.47	0.48
2:E:98:LEU:HD12	2:E:110:LEU:HD13	1.94	0.48
2:E:544:LEU:HD23	2:E:689:VAL:HG11	1.95	0.48
2:F:26:HIS:CG	2:F:33:HIS:HE1	2.30	0.48
2:A:743:LEU:HD11	2:A:773:VAL:CG2	2.43	0.48
2:B:46:ALA:HB2	2:B:105:THR:O	2.13	0.48
2:B:198:ARG:HB2	2:B:202:ASN:HA	1.95	0.48
2:D:522:LYS:HA	2:D:525:ARG:HE	1.78	0.48
2:D:741:ILE:HD13	2:D:777:LEU:CD1	2.43	0.48
2:E:498:LYS:O	2:E:502:MET:HE2	2.13	0.48
1:1:142:LEU:HD23	1:1:185:TYR:CE2	2.48	0.48
1:4:136:PHE:CE2	1:4:216:PHE:CE2	3.02	0.48
2:A:398:ALA:C	2:A:400:SER:H	2.22	0.48
2:C:364:VAL:HG22	2:C:471:VAL:CG2	2.43	0.48
2:C:387:LEU:HD12	2:C:387:LEU:H	1.78	0.48
1:6:139:VAL:HG11	1:6:154:LEU:HD13	1.96	0.48
2:A:77:THR:HG21	2:A:450:ARG:HH22	1.79	0.48
2:A:619:ILE:HG22	2:A:697:PHE:CE1	2.47	0.48
2:D:639:LEU:HD13	2:D:640:THR:H	1.79	0.48
2:B:619:ILE:CD1	2:B:656:MET:CB	2.75	0.48
2:E:21:ALA:HB2	2:E:29:ILE:HG12	1.94	0.48
2:E:46:ALA:HB2	2:E:105:THR:O	2.13	0.48
2:F:667:ARG:HH22	2:F:684:ASP:HB2	1.78	0.48
1:3:164:TYR:CD1	1:3:193:ILE:HD13	2.48	0.48
2:D:627:PHE:HB3	2:D:701:PHE:CG	2.48	0.48
1:5:203:ILE:HG23	2:E:434:GLN:OE1	2.14	0.48
2:A:53:LEU:HD21	2:A:134:ALA:HA	1.95	0.48
2:B:361:HIS:HA	2:C:233:ILE:HA	1.96	0.48
2:C:398:ALA:C	2:C:400:SER:H	2.21	0.48
2:D:377:LEU:HD21	2:D:492:ALA:HA	1.95	0.48
2:D:751:VAL:HG22	2:D:772:HIS:CD2	2.49	0.48
2:D:762:ALA:HB1	2:D:765:LEU:CD1	2.43	0.48
2:C:457:LYS:HZ1	2:C:460:TRP:CD1	2.31	0.48
2:D:483:TRP:HE1	2:E:198:ARG:HH22	1.62	0.48
2:E:188:GLU:HG3	2:E:339:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:136:PHE:CE2	1:3:216:PHE:CD2	3.02	0.47
1:3:153:THR:O	1:3:163:LEU:HD22	2.14	0.47
2:A:49:ALA:O	2:A:53:LEU:HD22	2.14	0.47
2:A:402:VAL:HG21	2:A:475:ASP:CG	2.38	0.47
2:F:38:LEU:O	2:F:47:ALA:HB2	2.14	0.47
2:F:705:ILE:HG21	2:F:708:ILE:HD13	1.95	0.47
1:1:142:LEU:HD23	1:1:185:TYR:CD2	2.49	0.47
2:C:38:LEU:O	2:C:47:ALA:HB2	2.13	0.47
2:C:619:ILE:HD12	2:C:656:MET:HB3	1.95	0.47
2:E:100:HIS:HB2	2:E:107:HIS:CE1	2.48	0.47
2:E:506:LEU:HB2	2:E:517:VAL:HG13	1.96	0.47
2:F:751:VAL:HG22	2:F:772:HIS:HB3	1.95	0.47
2:F:563:PHE:CE1	2:F:611:TYR:CD1	3.02	0.47
2:A:507:HIS:CD2	2:A:517:VAL:HG11	2.50	0.47
2:C:98:LEU:HD11	2:C:139:LEU:HD22	1.96	0.47
2:F:27:ASN:HA	2:F:75:SER:HA	1.97	0.47
2:A:394:LEU:HD11	2:A:483:TRP:CZ3	2.49	0.47
2:B:370:ALA:HB1	2:B:476:ILE:HD12	1.96	0.47
2:C:484:THR:HG23	2:C:611:TYR:CE2	2.48	0.47
2:F:543:PHE:HB2	2:F:657:THR:HG22	1.95	0.47
1:1:140:ILE:HG21	2:A:443:ARG:HD2	1.97	0.47
1:1:180:SER:HB3	2:A:68:ILE:HD11	1.96	0.47
2:B:27:ASN:HA	2:B:75:SER:HA	1.97	0.47
2:F:431:VAL:HG22	2:F:439:ALA:HB1	1.97	0.47
1:3:154:LEU:HD22	1:3:212:ILE:HD11	1.96	0.47
1:3:195:ARG:HH21	2:D:144:SER:H	1.62	0.47
1:3:204:ILE:HD11	1:3:212:ILE:HD11	1.96	0.47
2:A:363:ARG:HE	2:A:467:GLU:HB3	1.79	0.47
2:A:364:VAL:HG11	2:A:471:VAL:HG21	1.96	0.47
2:A:743:LEU:HD12	2:A:794:LEU:HD13	1.96	0.47
2:D:623:HIS:CD2	2:D:624:PRO:HD2	2.49	0.47
2:E:271:ALA:HB2	2:E:308:GLU:HA	1.96	0.47
2:A:747:ALA:HB1	2:A:801:PHE:CZ	2.50	0.47
2:B:403:ARG:HG2	2:B:403:ARG:HH11	1.80	0.47
2:E:670:TYR:CE1	2:E:756:VAL:HG13	2.50	0.47
2:C:18:GLN:O	2:C:21:ALA:HB3	2.14	0.47
2:C:403:ARG:HE	2:D:231:PRO:CB	2.27	0.47
2:E:623:HIS:CD2	2:E:624:PRO:HD2	2.50	0.47
2:E:743:LEU:HD11	2:E:773:VAL:HG22	1.97	0.47
2:F:786:ILE:HG21	2:F:792:ILE:HG23	1.97	0.47
2:A:381:TYR:HB2	2:A:484:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ALA:HB2	2:B:107:HIS:CG	2.50	0.46
2:B:100:HIS:HB2	2:B:107:HIS:CE1	2.50	0.46
2:D:362:HIS:O	2:E:233:ILE:HD11	2.15	0.46
2:B:60:ILE:HG23	2:B:123:VAL:HG11	1.97	0.46
2:B:751:VAL:HG22	2:B:772:HIS:HB2	1.97	0.46
2:E:109:LEU:HD23	2:E:138:VAL:CG2	2.45	0.46
2:A:413:LEU:HB2	2:A:460:TRP:HE1	1.81	0.46
2:A:563:PHE:CD2	2:A:611:TYR:CD1	3.04	0.46
2:D:427:LYS:HA	2:D:442:LEU:HB2	1.98	0.46
2:A:276:LEU:HD23	2:A:309:LEU:HA	1.97	0.46
2:B:402:VAL:HG23	2:B:475:ASP:OD1	2.16	0.46
2:A:420:LEU:O	2:A:420:LEU:HD23	2.16	0.46
2:C:423:VAL:HG11	2:C:445:THR:HB	1.97	0.46
2:D:427:LYS:HD3	2:D:427:LYS:C	2.41	0.46
2:F:31:THR:HB	2:F:120:ALA:HB2	1.96	0.46
1:2:142:LEU:HD21	1:2:182:LEU:HG	1.98	0.46
2:B:139:LEU:O	2:B:142:LEU:HD13	2.16	0.46
2:C:660:VAL:HG21	2:C:697:PHE:CE2	2.51	0.46
2:E:787:HIS:H	2:E:790:GLN:HG2	1.80	0.46
1:6:210:GLU:CD	1:6:210:GLU:H	2.23	0.46
2:A:559:ALA:HA	2:A:563:PHE:CD1	2.51	0.46
2:C:417:GLU:CD	2:C:417:GLU:H	2.24	0.46
2:C:498:LYS:O	2:C:502:MET:HE2	2.16	0.46
2:C:619:ILE:HG21	2:C:627:PHE:HE1	1.78	0.46
2:D:17:ALA:HB1	2:D:29:ILE:CG2	2.46	0.46
2:E:727:SER:O	2:E:731:THR:HG23	2.16	0.46
1:2:142:LEU:HD22	1:2:146:ASN:HB2	1.98	0.46
1:4:154:LEU:HD22	1:4:212:ILE:HD11	1.98	0.46
2:A:109:LEU:HD23	2:A:138:VAL:HG22	1.97	0.46
2:B:623:HIS:CD2	2:B:624:PRO:HD2	2.51	0.46
2:B:747:ALA:HB1	2:B:801:PHE:CE1	2.51	0.46
2:D:363:ARG:NH1	2:D:399:GLY:HA2	2.30	0.46
2:F:665:LEU:HG	2:F:689:VAL:HG21	1.98	0.46
1:2:136:PHE:CD1	2:B:431:VAL:HG11	2.51	0.46
2:A:374:ALA:CA	2:A:476:ILE:HG21	2.45	0.46
2:A:396:ASP:HB3	2:B:198:ARG:HB3	1.96	0.46
2:A:619:ILE:CG2	2:A:619:ILE:O	2.63	0.46
2:B:87:VAL:HG13	2:B:112:LEU:HA	1.97	0.46
2:B:20:GLU:HB3	2:B:23:ARG:HH21	1.80	0.45
2:B:26:HIS:CE1	2:B:68:ILE:HB	2.50	0.45
2:D:34:ILE:HD11	2:D:84:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:571:ARG:NE	2:D:617:ASP:OD2	2.49	0.45
2:D:777:LEU:HD21	2:D:794:LEU:HD11	1.97	0.45
2:E:574:MET:SD	2:E:626:VAL:HG11	2.56	0.45
2:E:739:LEU:HD11	2:E:792:ILE:HD11	1.98	0.45
2:F:201:LYS:C	2:F:203:ASN:H	2.24	0.45
2:B:406:SER:HB3	2:B:407:PHE:CD1	2.51	0.45
2:B:727:SER:O	2:B:731:THR:HG23	2.16	0.45
2:C:542:ILE:CG1	2:C:705:ILE:HD13	2.46	0.45
2:D:21:ALA:HB2	2:D:29:ILE:HD11	1.98	0.45
2:D:370:ALA:HB1	2:D:471:VAL:HG13	1.99	0.45
2:D:723:VAL:HG21	2:D:752:ALA:HA	1.97	0.45
2:E:352:GLN:HG3	2:E:371:ILE:HG21	1.98	0.45
2:F:751:VAL:HA	2:F:772:HIS:CD2	2.52	0.45
1:2:164:TYR:CD1	1:2:193:ILE:HD13	2.50	0.45
2:A:199:ARG:H	2:F:396:ASP:HB3	1.80	0.45
2:B:26:HIS:HE1	2:B:68:ILE:HB	1.81	0.45
2:C:685:MET:HE3	2:C:712:HIS:ND1	2.31	0.45
2:E:32:GLU:HB2	2:E:64:VAL:HG13	1.97	0.45
1:4:137:GLU:HA	1:4:140:ILE:HD12	1.99	0.45
1:4:203:ILE:CG2	2:D:434:GLN:HE21	2.29	0.45
1:5:136:PHE:CE2	1:5:203:ILE:HG21	2.51	0.45
2:A:355:ARG:HD3	2:A:366:ILE:H	1.82	0.45
2:C:357:ARG:C	2:C:359:GLU:H	2.24	0.45
2:C:410:PRO:HG2	2:C:412:ASN:H	1.82	0.45
2:E:106:GLU:HG3	2:E:107:HIS:CD2	2.52	0.45
2:F:100:HIS:CD2	2:F:107:HIS:CE1	3.04	0.45
2:F:751:VAL:HG22	2:F:772:HIS:HB2	1.99	0.45
2:A:38:LEU:O	2:A:47:ALA:HB2	2.17	0.45
2:B:348:ILE:HG22	2:B:352:GLN:HE21	1.82	0.45
2:B:394:LEU:HD23	2:B:479:VAL:HG22	1.97	0.45
2:A:685:MET:HA	2:A:689:VAL:HG23	1.99	0.45
2:C:661:GLY:HA2	2:C:689:VAL:HG22	1.99	0.45
2:A:363:ARG:HA	2:A:468:ASN:HA	1.99	0.45
2:B:743:LEU:HB3	2:B:747:ALA:HB3	1.98	0.45
2:E:483:TRP:HE1	2:F:198:ARG:HH12	1.63	0.45
2:E:674:ASN:HB3	2:E:676:GLN:H	1.82	0.45
2:F:100:HIS:HB3	2:F:107:HIS:CE1	2.51	0.45
2:F:587:VAL:HG22	2:F:589:SER:H	1.82	0.45
2:F:616:LEU:CB	2:F:619:ILE:HD11	2.46	0.45
2:C:26:HIS:CE1	2:C:32:GLU:CD	2.95	0.45
2:C:363:ARG:HG3	2:C:403:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:476:ILE:O	2:E:480:VAL:HG23	2.17	0.45
1:6:142:LEU:HD23	1:6:182:LEU:HA	1.97	0.45
2:C:403:ARG:HG3	2:D:231:PRO:HB3	1.99	0.45
2:C:574:MET:CG	2:C:619:ILE:HG12	2.46	0.45
2:E:394:LEU:HD23	2:E:479:VAL:HG22	1.99	0.45
2:D:53:LEU:HB3	2:D:129:VAL:HG21	1.99	0.45
2:D:278:ILE:HD11	2:D:309:LEU:HD23	1.99	0.45
1:1:133:PHE:CE2	1:1:163:LEU:HD12	2.52	0.44
2:A:32:GLU:HG2	2:A:33:HIS:CD2	2.52	0.44
2:A:371:ILE:O	2:A:374:ALA:HB3	2.17	0.44
2:A:619:ILE:HG23	2:A:627:PHE:HE1	1.81	0.44
2:B:363:ARG:HH12	2:B:471:VAL:HA	1.82	0.44
2:D:731:THR:HG22	2:D:741:ILE:HD12	1.99	0.44
2:D:777:LEU:CD2	2:D:792:ILE:HG21	2.47	0.44
2:E:26:HIS:CE1	2:E:68:ILE:HB	2.52	0.44
2:F:398:ALA:C	2:F:400:SER:H	2.24	0.44
2:F:623:HIS:CD2	2:F:624:PRO:HD2	2.52	0.44
1:6:204:ILE:HG21	1:6:211:THR:HB	2.00	0.44
2:A:113:ILE:HG21	2:A:135:ARG:HB2	2.00	0.44
2:A:510:VAL:HG21	2:A:554:LEU:HA	1.99	0.44
2:E:355:ARG:HG3	2:E:371:ILE:HD11	1.99	0.44
1:4:181:ILE:H	1:4:181:ILE:HD12	1.81	0.44
2:A:665:LEU:HD21	2:A:689:VAL:HG21	1.99	0.44
2:C:714:LEU:HD22	2:C:718:HIS:CD2	2.51	0.44
2:D:77:THR:HB	2:D:79:HIS:CD2	2.53	0.44
2:D:624:PRO:HA	2:D:627:PHE:CD2	2.52	0.44
2:E:394:LEU:HD21	2:E:483:TRP:CZ2	2.53	0.44
2:F:100:HIS:CD2	2:F:107:HIS:HE1	2.35	0.44
2:F:669:LYS:HG2	2:F:712:HIS:CE1	2.52	0.44
2:A:665:LEU:CD2	2:A:689:VAL:HG21	2.48	0.44
2:B:420:LEU:HD13	2:B:453:VAL:HG21	1.99	0.44
2:B:693:LEU:O	2:B:697:PHE:CD2	2.70	0.44
2:D:394:LEU:CD1	2:D:480:VAL:HG22	2.47	0.44
2:F:420:LEU:O	2:F:420:LEU:HD23	2.18	0.44
1:3:139:VAL:CG1	1:3:212:ILE:HD13	2.47	0.44
2:D:26:HIS:HB2	2:D:33:HIS:HE1	1.83	0.44
2:E:55:LEU:HD11	2:E:129:VAL:HG11	2.00	0.44
1:1:203:ILE:HG22	1:1:204:ILE:HD13	1.99	0.44
1:5:204:ILE:HD11	1:5:212:ILE:HD11	1.99	0.44
2:A:431:VAL:HG13	2:A:439:ALA:HB1	1.99	0.44
2:B:45:ILE:HG22	2:B:138:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:HIS:CE1	2:B:283:THR:HG23	2.52	0.44
2:C:6:PHE:HA	2:C:102:TYR:HA	2.00	0.44
2:C:371:ILE:O	2:C:374:ALA:HB3	2.17	0.44
2:E:10:ALA:HB1	2:E:108:ILE:HD11	1.99	0.44
2:E:579:GLU:HA	2:E:593:TYR:CD2	2.53	0.44
2:A:363:ARG:HH11	2:A:399:GLY:HA2	1.82	0.44
2:A:631:LEU:HA	2:A:634:LEU:HD22	2.00	0.44
2:D:660:VAL:HG21	2:D:696:ALA:HB2	1.99	0.44
2:E:382:ILE:HG12	2:E:651:ASN:HD21	1.82	0.44
2:F:468:ASN:HD22	2:F:468:ASN:H	1.65	0.44
2:F:739:LEU:HD11	2:F:792:ILE:HD11	1.98	0.44
2:A:20:GLU:HB2	2:A:33:HIS:CG	2.52	0.44
2:A:53:LEU:HD11	2:A:137:GLN:HB2	2.00	0.44
2:B:59:LYS:HG2	2:B:127:LEU:HD22	1.99	0.44
2:C:32:GLU:HB2	2:C:64:VAL:HG13	1.99	0.44
2:C:476:ILE:O	2:C:480:VAL:HG23	2.18	0.44
2:E:20:GLU:HB3	2:E:33:HIS:CD2	2.52	0.44
2:B:619:ILE:HG22	2:B:619:ILE:O	2.18	0.44
2:C:55:LEU:HD11	2:C:129:VAL:HG11	1.99	0.44
2:E:398:ALA:HB1	2:E:475:ASP:HB3	2.00	0.44
2:A:351:LEU:HD22	2:A:392:ILE:HG12	1.99	0.43
2:B:32:GLU:HB2	2:B:64:VAL:HG13	2.00	0.43
2:B:402:VAL:HG22	2:B:405:ARG:CZ	2.48	0.43
2:C:24:LEU:HD13	2:C:69:GLY:HA2	2.00	0.43
2:C:384:ASP:HB3	2:C:385:ARG:HE	1.82	0.43
2:D:417:GLU:H	2:D:417:GLU:CD	2.25	0.43
2:A:510:VAL:HG12	2:A:512:GLY:H	1.84	0.43
2:A:639:LEU:HD23	2:A:640:THR:H	1.83	0.43
2:A:702:ILE:HA	2:A:705:ILE:HD12	2.01	0.43
2:D:394:LEU:HD21	2:D:483:TRP:CH2	2.53	0.43
2:D:619:ILE:HG22	2:D:619:ILE:O	2.17	0.43
2:A:231:PRO:HB2	2:F:403:ARG:HD3	2.00	0.43
2:B:371:ILE:O	2:B:374:ALA:HB3	2.18	0.43
2:B:399:GLY:O	2:C:233:ILE:HD11	2.17	0.43
2:C:198:ARG:HD2	2:C:202:ASN:HA	1.99	0.43
2:D:402:VAL:HG21	2:D:475:ASP:CG	2.44	0.43
2:E:59:LYS:HG2	2:E:127:LEU:HD22	1.99	0.43
2:F:21:ALA:HA	2:F:33:HIS:ND1	2.33	0.43
1:6:133:PHE:CZ	1:6:186:ALA:HB2	2.52	0.43
1:6:153:THR:O	1:6:163:LEU:HD22	2.18	0.43
2:D:193:ILE:HD13	2:D:225:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:701:PHE:CZ	2:D:705:ILE:HD11	2.54	0.43
2:E:623:HIS:CG	2:E:624:PRO:HD2	2.53	0.43
2:F:59:LYS:HG2	2:F:127:LEU:HD22	1.99	0.43
1:3:133:PHE:CD2	1:3:139:VAL:HG22	2.53	0.43
2:B:301:LYS:HB2	2:B:302:PRO:HD3	2.00	0.43
2:C:348:ILE:HG21	2:C:372:GLU:HG2	2.01	0.43
2:C:627:PHE:HB2	2:C:698:ARG:HE	1.83	0.43
2:D:712:HIS:H	2:D:712:HIS:CD2	2.35	0.43
2:E:6:PHE:HA	2:E:102:TYR:HA	2.00	0.43
2:E:520:VAL:HG11	2:E:558:LEU:HD11	2.01	0.43
2:E:627:PHE:HB3	2:E:701:PHE:CG	2.53	0.43
2:A:588:GLY:HA3	2:B:594:VAL:H	1.84	0.43
2:B:374:ALA:HA	2:B:394:LEU:HD12	2.01	0.43
2:C:381:TYR:HB2	2:C:611:TYR:CE2	2.54	0.43
2:E:21:ALA:CB	2:E:29:ILE:HG12	2.49	0.43
2:E:110:LEU:HD23	2:E:135:ARG:HG2	2.00	0.43
1:3:140:ILE:HD11	1:3:216:PHE:CD1	2.54	0.43
1:6:137:GLU:HA	1:6:140:ILE:HD12	2.00	0.43
2:C:730:LEU:HD11	2:C:774:GLU:HG2	2.00	0.43
2:D:580:LYS:HD3	2:D:581:HIS:CE1	2.54	0.43
2:D:665:LEU:HD22	2:D:712:HIS:HA	2.00	0.43
1:5:143:SER:C	1:5:145:LEU:H	2.26	0.43
2:B:394:LEU:HD21	2:B:483:TRP:CH2	2.54	0.43
2:B:406:SER:HB2	2:B:463:LYS:HE2	2.01	0.43
2:F:31:THR:HG23	2:F:83:ARG:HG3	2.01	0.43
2:F:402:VAL:HG12	2:F:467:GLU:HB3	2.00	0.43
2:F:664:GLU:HA	2:F:667:ARG:HE	1.84	0.43
2:B:742:GLU:OE1	2:B:793:VAL:HG13	2.19	0.43
2:C:363:ARG:HH12	2:C:475:ASP:HB3	1.84	0.43
2:D:22:LEU:HD12	2:D:22:LEU:H	1.82	0.43
2:D:483:TRP:NE1	2:E:198:ARG:HH22	2.17	0.43
2:D:510:VAL:HG12	2:D:512:GLY:H	1.84	0.43
2:C:410:PRO:HB2	2:C:411:PRO:HD2	2.00	0.43
2:E:367:THR:O	2:E:370:ALA:HB3	2.19	0.43
2:E:394:LEU:HD21	2:E:483:TRP:CE2	2.54	0.43
2:F:53:LEU:HD21	2:F:134:ALA:HA	2.00	0.43
2:A:363:ARG:HD2	2:A:403:ARG:H	1.83	0.42
2:A:619:ILE:HD11	2:A:656:MET:CG	2.44	0.42
2:B:407:PHE:CD1	2:C:229:GLU:HB3	2.53	0.42
2:D:747:ALA:O	2:D:751:VAL:HG23	2.19	0.42
1:3:143:SER:C	1:3:145:LEU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:20:GLU:CB	2:A:33:HIS:CD2	3.02	0.42
2:D:6:PHE:CD2	2:D:103:VAL:HG23	2.54	0.42
2:D:370:ALA:HB2	2:D:472:THR:HA	2.01	0.42
2:D:515:GLU:CD	2:D:669:LYS:HZ3	2.27	0.42
2:E:359:GLU:HA	2:E:362:HIS:CD2	2.54	0.42
2:E:397:GLU:CB	2:E:479:VAL:HG21	2.50	0.42
2:F:192:VAL:HG13	2:F:204:PRO:HG2	2.01	0.42
2:B:53:LEU:HD12	2:B:129:VAL:HG13	2.01	0.42
2:B:546:PRO:HD2	2:B:549:VAL:HG21	1.99	0.42
2:C:46:ALA:HB2	2:C:105:THR:O	2.19	0.42
2:D:26:HIS:CD2	2:D:33:HIS:CE1	3.07	0.42
2:E:410:PRO:HG2	2:E:413:LEU:H	1.85	0.42
2:E:513:GLN:HA	2:E:718:HIS:CE1	2.54	0.42
2:F:98:LEU:HD12	2:F:110:LEU:HD13	2.00	0.42
1:5:175:VAL:HA	1:5:178:GLN:HE21	1.84	0.42
2:A:46:ALA:HB1	2:A:109:LEU:HB2	2.00	0.42
2:D:351:LEU:CD1	2:D:391:ALA:HB1	2.49	0.42
2:D:742:GLU:HB3	2:D:791:HIS:CE1	2.54	0.42
2:E:166:LEU:HA	2:E:167:ALA:CB	2.49	0.42
1:1:216:PHE:HA	2:A:440:ALA:HB2	2.00	0.42
2:A:22:LEU:HD22	2:A:22:LEU:H	1.85	0.42
2:A:743:LEU:HB3	2:A:747:ALA:HB3	2.02	0.42
2:F:371:ILE:O	2:F:374:ALA:HB3	2.20	0.42
1:6:142:LEU:HB2	1:6:185:TYR:CD2	2.55	0.42
2:B:571:ARG:NH2	2:B:617:ASP:OD2	2.52	0.42
2:D:6:PHE:HA	2:D:102:TYR:HA	2.01	0.42
2:D:271:ALA:HA	2:D:274:ILE:HG22	2.02	0.42
2:D:392:ILE:HA	2:D:395:ILE:HD12	2.01	0.42
2:D:549:VAL:HG13	2:D:714:LEU:CD2	2.49	0.42
2:E:581:HIS:CE1	2:E:585:ARG:CZ	3.02	0.42
2:F:100:HIS:CE1	2:F:102:TYR:HB2	2.55	0.42
2:F:374:ALA:HB1	2:F:391:ALA:HA	2.01	0.42
1:2:154:LEU:HB2	1:2:208:ALA:HB1	2.01	0.42
1:2:215:HIS:HB2	2:B:436:PHE:HB3	2.00	0.42
1:5:216:PHE:CE2	2:E:439:ALA:HB3	2.55	0.42
2:B:113:ILE:HG21	2:B:135:ARG:HB2	2.01	0.42
2:C:281:LEU:HG	2:C:285:ILE:HD13	2.01	0.42
2:E:483:TRP:CD1	2:F:335:GLN:HG3	2.55	0.42
2:F:46:ALA:H	2:F:105:THR:HB	1.84	0.42
2:A:403:ARG:HA	2:A:467:GLU:HG3	2.01	0.42
2:A:664:GLU:O	2:A:685:MET:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:HIS:CD2	2:B:33:HIS:NE2	2.86	0.42
2:B:743:LEU:HA	2:B:794:LEU:HB2	2.02	0.42
2:B:777:LEU:HD11	2:B:794:LEU:HD11	2.02	0.42
2:D:361:HIS:CG	2:E:233:ILE:HG23	2.55	0.42
2:D:682:HIS:CD2	2:D:712:HIS:CE1	3.07	0.42
2:E:370:ALA:HB2	2:E:472:THR:HA	2.00	0.42
2:F:374:ALA:HB2	2:F:476:ILE:HG12	2.02	0.42
2:A:786:ILE:HD12	2:A:792:ILE:HD13	2.00	0.42
2:B:398:ALA:HB1	2:B:475:ASP:HB3	2.01	0.42
2:B:427:LYS:HD2	2:B:443:ARG:HA	2.02	0.42
2:D:627:PHE:HB3	2:D:701:PHE:CD2	2.55	0.42
1:1:128:GLN:HG3	1:1:166:ASP:HA	2.02	0.42
1:1:133:PHE:CZ	1:1:163:LEU:HD12	2.55	0.42
2:A:739:LEU:HD21	2:A:792:ILE:HD11	2.02	0.42
2:B:355:ARG:HA	2:B:358:TYR:CZ	2.55	0.42
2:B:412:ASN:C	2:B:414:LYS:H	2.27	0.42
2:C:373:ALA:HB2	2:C:473:VAL:HG13	2.02	0.42
2:E:201:LYS:C	2:E:203:ASN:H	2.27	0.42
2:E:634:LEU:HD22	2:E:701:PHE:CE1	2.54	0.42
2:F:502:MET:HA	2:F:505:ILE:HG12	2.02	0.42
2:A:142:LEU:HG	2:A:144:SER:H	1.85	0.41
2:A:383:SER:H	2:A:390:LYS:CD	2.31	0.41
2:B:507:HIS:CD2	2:B:517:VAL:CG1	3.02	0.41
2:C:413:LEU:HB2	2:C:460:TRP:CZ2	2.55	0.41
2:D:117:GLU:CD	2:D:118:GLY:H	2.27	0.41
2:D:631:LEU:HA	2:D:634:LEU:HD22	2.02	0.41
2:E:743:LEU:HD21	2:E:773:VAL:HG22	2.02	0.41
2:F:382:ILE:H	2:F:383:SER:HB2	1.84	0.41
2:F:392:ILE:HA	2:F:395:ILE:HD12	2.02	0.41
2:B:183:ILE:HD12	2:B:350:ILE:HA	2.01	0.41
2:C:361:HIS:CE1	2:C:396:ASP:HA	2.55	0.41
2:D:20:GLU:HB2	2:D:33:HIS:CG	2.55	0.41
2:D:25:GLY:C	2:D:26:HIS:CD2	2.98	0.41
2:E:366:ILE:HB	2:E:367:THR:HA	2.02	0.41
2:F:395:ILE:HA	2:F:476:ILE:HD11	2.02	0.41
2:A:165:SER:HB2	2:A:166:LEU:HB2	2.02	0.41
2:D:714:LEU:HD12	2:D:762:ALA:HB2	2.02	0.41
2:F:427:LYS:HG3	2:F:443:ARG:CA	2.48	0.41
2:F:507:HIS:CE1	2:F:518:VAL:HG22	2.56	0.41
2:B:106:GLU:CG	2:B:142:LEU:HD11	2.50	0.41
2:B:476:ILE:O	2:B:479:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:507:HIS:CE1	2:D:518:VAL:HG22	2.56	0.41
2:D:747:ALA:HB1	2:D:801:PHE:CZ	2.56	0.41
2:E:9:ARG:HB2	2:E:105:THR:HB	2.03	0.41
2:E:303:SER:HB3	2:E:309:LEU:HB2	2.02	0.41
2:F:53:LEU:HD12	2:F:129:VAL:HG13	2.02	0.41
2:F:484:THR:HG22	2:F:563:PHE:HA	2.02	0.41
1:1:140:ILE:HG23	1:1:216:PHE:HB3	2.03	0.41
2:B:364:VAL:HG11	2:B:471:VAL:HG13	2.03	0.41
2:E:445:THR:O	2:E:449:LEU:HD23	2.20	0.41
2:F:474:ASP:HA	2:F:493:GLN:H	1.85	0.41
2:C:304:LEU:HD22	2:C:311:CYS:SG	2.60	0.41
2:D:21:ALA:HB2	2:D:29:ILE:CD1	2.51	0.41
2:D:70:ARG:H	2:D:70:ARG:HD2	1.85	0.41
2:D:400:SER:HA	2:E:233:ILE:HD12	2.02	0.41
2:F:579:GLU:HA	2:F:593:TYR:CD1	2.55	0.41
1:4:203:ILE:HG21	2:D:434:GLN:HE21	1.85	0.41
1:6:127:LEU:CB	1:6:175:VAL:HG21	2.50	0.41
2:B:26:HIS:CB	2:B:33:HIS:HE1	2.33	0.41
2:B:627:PHE:CE2	2:B:697:PHE:HA	2.55	0.41
2:B:632:GLN:HB2	2:B:639:LEU:HD22	2.03	0.41
2:C:437:GLU:HA	2:C:440:ALA:HB3	2.01	0.41
1:1:194:HIS:CD2	2:B:141:LEU:HD22	2.55	0.41
1:2:216:PHE:CZ	2:B:439:ALA:HB3	2.55	0.41
1:3:171:THR:O	1:3:175:VAL:HG23	2.21	0.41
1:4:128:GLN:HG3	1:4:166:ASP:HA	2.02	0.41
2:A:324:ILE:HD13	2:F:385:ARG:HH12	1.86	0.41
2:A:362:HIS:CE1	2:B:232:GLU:OE2	2.74	0.41
2:B:656:MET:HE1	2:B:705:ILE:HG12	2.02	0.41
2:C:5:ARG:HH22	2:C:357:ARG:HH21	1.69	0.41
2:C:615:LEU:HD21	2:C:657:THR:HG23	2.03	0.41
1:4:147:VAL:HG13	1:4:148:ASN:H	1.85	0.41
2:B:109:LEU:HD23	2:B:138:VAL:HG22	2.02	0.41
2:B:589:SER:H	2:C:584:SER:HA	1.86	0.41
2:B:739:LEU:HD13	2:B:741:ILE:HG23	2.03	0.41
2:C:545:GLY:N	2:C:661:GLY:HA3	2.36	0.41
2:C:741:ILE:HA	2:C:792:ILE:HB	2.01	0.41
2:D:59:LYS:HG2	2:D:127:LEU:HD22	2.02	0.41
2:D:110:LEU:HD21	2:D:138:VAL:HB	2.03	0.41
2:F:100:HIS:HD2	2:F:107:HIS:CE1	2.39	0.41
2:F:746:ALA:HB1	2:F:796:VAL:HB	2.03	0.41
2:B:188:GLU:HG3	2:B:339:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:HIS:HB2	2:C:233:ILE:HG23	2.03	0.41
2:B:395:ILE:HA	2:B:471:VAL:HG11	2.03	0.41
2:B:719:LEU:HD12	2:B:752:ALA:HB1	2.02	0.41
2:C:480:VAL:HG13	2:C:483:TRP:CZ3	2.56	0.41
2:D:394:LEU:CD2	2:D:479:VAL:HG22	2.51	0.41
2:D:665:LEU:HD11	2:D:710:VAL:HG13	2.02	0.41
2:B:624:PRO:HA	2:B:627:PHE:CE2	2.56	0.40
2:D:20:GLU:HB3	2:D:33:HIS:CD2	2.56	0.40
2:D:98:LEU:HD12	2:D:110:LEU:HD13	2.02	0.40
2:E:741:ILE:HG22	2:E:792:ILE:HD12	2.04	0.40
1:6:127:LEU:HA	1:6:175:VAL:HG21	2.03	0.40
2:B:387:LEU:H	2:B:387:LEU:HD22	1.86	0.40
2:C:427:LYS:HG3	2:C:443:ARG:HA	2.03	0.40
2:C:685:MET:HB2	2:C:712:HIS:CE1	2.56	0.40
2:D:620:GLU:O	2:D:696:ALA:HB1	2.21	0.40
2:E:686:LYS:HB2	2:E:712:HIS:HE1	1.86	0.40
2:F:94:GLU:O	2:F:107:HIS:CD2	2.74	0.40
2:F:271:ALA:HB2	2:F:308:GLU:HA	2.03	0.40
1:2:133:PHE:CD1	1:2:186:ALA:HB2	2.57	0.40
1:3:139:VAL:HG11	1:3:212:ILE:HD13	2.03	0.40
2:B:235:ARG:NE	2:B:236:ASP:H	2.19	0.40
2:B:420:LEU:HD23	2:B:420:LEU:C	2.46	0.40
2:B:570:ILE:HG13	2:B:606:VAL:HG22	2.03	0.40
2:B:742:GLU:O	2:B:794:LEU:HD12	2.22	0.40
2:D:55:LEU:HD11	2:D:129:VAL:HG11	2.04	0.40
2:E:710:VAL:CG1	2:E:712:HIS:CE1	3.04	0.40
2:A:87:VAL:HG13	2:A:112:LEU:HA	2.02	0.40
2:A:110:LEU:HD11	2:A:142:LEU:HD13	2.04	0.40
2:A:370:ALA:CB	2:A:471:VAL:HG13	2.51	0.40
2:C:363:ARG:HD3	2:C:399:GLY:HA2	2.02	0.40
2:D:14:LEU:O	2:D:17:ALA:HB3	2.22	0.40
2:D:506:LEU:HD21	2:D:558:LEU:HD23	2.04	0.40
2:D:714:LEU:HD22	2:D:718:HIS:CD2	2.56	0.40
2:D:727:SER:O	2:D:731:THR:HG23	2.22	0.40
2:E:484:THR:HG23	2:E:611:TYR:CD2	2.57	0.40
2:C:627:PHE:CD2	2:C:697:PHE:HA	2.57	0.40
2:D:91:SER:HB2	2:D:108:ILE:HD13	2.03	0.40
2:E:484:THR:HG23	2:E:611:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	92/218 (42%)	78 (85%)	8 (9%)	6 (6%)	1	12
1	2	92/218 (42%)	78 (85%)	9 (10%)	5 (5%)	1	15
1	3	92/218 (42%)	74 (80%)	12 (13%)	6 (6%)	1	12
1	4	92/218 (42%)	79 (86%)	8 (9%)	5 (5%)	1	15
1	5	92/218 (42%)	76 (83%)	12 (13%)	4 (4%)	2	17
1	6	92/218 (42%)	76 (83%)	13 (14%)	3 (3%)	3	21
2	A	794/810 (98%)	627 (79%)	109 (14%)	58 (7%)	1	10
2	B	794/810 (98%)	625 (79%)	117 (15%)	52 (6%)	1	12
2	C	794/810 (98%)	623 (78%)	118 (15%)	53 (7%)	1	12
2	D	794/810 (98%)	614 (77%)	125 (16%)	55 (7%)	1	11
2	E	794/810 (98%)	629 (79%)	107 (14%)	58 (7%)	1	10
2	F	794/810 (98%)	628 (79%)	112 (14%)	54 (7%)	1	11
All	All	5316/6168 (86%)	4207 (79%)	750 (14%)	359 (7%)	2	11

All (359) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	207	HIS
1	2	145	LEU
1	2	147	VAL
1	3	145	LEU
1	3	146	ASN
1	5	148	ASN
2	A	100	HIS
2	A	271	ALA
2	A	294	ILE
2	A	366	ILE
2	A	412	ASN
2	A	468	ASN

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Mol	Chain	Res	Type
2	A	472	THR
2	A	493	GLN
2	A	579	GLU
2	A	650	ARG
2	A	669	LYS
2	B	100	HIS
2	B	150	SER
2	B	151	ALA
2	B	343	SER
2	B	365	SER
2	B	366	ILE
2	B	410	PRO
2	B	468	ASN
2	B	470	GLU
2	B	493	GLN
2	B	531	LEU
2	B	652	THR
2	B	667	ARG
2	C	78	ILE
2	C	271	ALA
2	C	294	ILE
2	C	363	ARG
2	C	365	SER
2	C	366	ILE
2	C	434	GLN
2	C	468	ASN
2	C	472	THR
2	C	493	GLN
2	C	547	THR
2	C	589	SER
2	C	590	PRO
2	C	642	SER
2	C	713	SER
2	D	293	ALA
2	D	333	ARG
2	D	339	VAL
2	D	365	SER
2	D	410	PRO
2	D	412	ASN
2	D	468	ASN
2	D	471	VAL
2	D	473	VAL

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Mol	Chain	Res	Type
2	D	535	LYS
2	D	591	PRO
2	D	669	LYS
2	D	762	ALA
2	E	150	SER
2	E	167	ALA
2	E	183	ILE
2	E	293	ALA
2	E	363	ARG
2	E	366	ILE
2	E	412	ASN
2	E	468	ASN
2	E	473	VAL
2	E	493	GLN
2	E	585	ARG
2	E	674	ASN
2	F	7	THR
2	F	78	ILE
2	F	117	GLU
2	F	183	ILE
2	F	294	ILE
2	F	410	PRO
2	F	412	ASN
2	F	434	GLN
2	F	468	ASN
2	F	472	THR
2	F	493	GLN
2	F	547	THR
2	F	668	ASN
2	F	670	TYR
1	1	147	VAL
1	4	145	LEU
1	4	147	VAL
1	5	147	VAL
1	6	145	LEU
2	A	68	ILE
2	A	144	SER
2	A	157	ASN
2	A	165	SER
2	A	183	ILE
2	A	391	ALA
2	A	471	VAL

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Mol	Chain	Res	Type
2	A	473	VAL
2	A	652	THR
2	A	662	ALA
2	A	675	VAL
2	B	99	GLY
2	B	163	LEU
2	B	165	SER
2	B	177	ASP
2	B	212	VAL
2	B	271	ALA
2	B	291	GLU
2	B	294	ILE
2	B	383	SER
2	B	547	THR
2	B	579	GLU
2	B	642	SER
2	B	659	ASN
2	B	662	ALA
2	B	674	ASN
2	B	716	LYS
2	B	757	ASP
2	C	99	GLY
2	C	150	SER
2	C	165	SER
2	C	212	VAL
2	C	293	ALA
2	C	362	HIS
2	C	412	ASN
2	C	568	SER
2	C	662	ALA
2	D	72	GLN
2	D	99	GLY
2	D	100	HIS
2	D	165	SER
2	D	166	LEU
2	D	178	SER
2	D	183	ILE
2	D	362	HIS
2	D	363	ARG
2	D	366	ILE
2	D	413	LEU
2	D	493	GLN

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Mol	Chain	Res	Type
2	D	578	MET
2	D	662	ALA
2	D	738	ASP
2	E	100	HIS
2	E	152	ALA
2	E	165	SER
2	E	177	ASP
2	E	271	ALA
2	E	365	SER
2	E	383	SER
2	E	384	ASP
2	E	410	PRO
2	E	434	GLN
2	E	618	ALA
2	E	642	SER
2	E	662	ALA
2	E	738	ASP
2	E	759	GLU
2	F	100	HIS
2	F	118	GLY
2	F	150	SER
2	F	165	SER
2	F	168	ARG
2	F	271	ALA
2	F	343	SER
2	F	366	ILE
2	F	662	ALA
2	F	673	PHE
2	F	717	LYS
2	F	757	ASP
1	1	144	LYS
1	1	177	ASN
1	2	144	LYS
1	2	177	ASN
1	3	144	LYS
1	3	177	ASN
1	4	144	LYS
1	4	177	ASN
1	5	177	ASN
1	6	177	ASN
2	A	99	GLY
2	A	151	ALA

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Mol	Chain	Res	Type
2	A	162	THR
2	A	163	LEU
2	A	167	ALA
2	A	330	LEU
2	A	375	VAL
2	A	388	PRO
2	A	410	PRO
2	A	413	LEU
2	A	585	ARG
2	A	707	GLU
2	A	738	ASP
2	A	760	TYR
2	B	364	VAL
2	B	384	ASP
2	B	391	ALA
2	B	591	PRO
2	B	738	ASP
2	C	148	GLY
2	C	162	THR
2	C	163	LEU
2	C	364	VAL
2	C	375	VAL
2	C	391	ALA
2	C	410	PRO
2	C	413	LEU
2	C	550	GLY
2	C	580	LYS
2	C	757	ASP
2	C	761	GLY
2	C	788	LYS
2	D	143	GLY
2	D	150	SER
2	D	163	LEU
2	D	291	GLU
2	D	326	LYS
2	D	375	VAL
2	D	388	PRO
2	D	391	ALA
2	D	400	SER
2	D	472	THR
2	D	592	GLY
2	E	72	GLN

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Mol	Chain	Res	Type
2	E	73	GLU
2	E	162	THR
2	E	163	LEU
2	E	210	PRO
2	E	391	ALA
2	E	413	LEU
2	E	472	THR
2	E	580	LYS
2	F	152	ALA
2	F	162	THR
2	F	163	LEU
2	F	177	ASP
2	F	185	ARG
2	F	384	ASP
2	F	388	PRO
2	F	391	ALA
2	F	413	LEU
2	F	568	SER
2	F	738	ASP
1	1	145	LEU
1	4	217	ALA
1	6	144	LYS
2	A	150	SER
2	A	152	ALA
2	A	210	PRO
2	A	293	ALA
2	A	343	SER
2	A	550	GLY
2	A	690	MET
2	B	152	ALA
2	B	162	THR
2	B	226	ILE
2	B	388	PRO
2	B	400	SER
2	B	413	LEU
2	B	550	GLY
2	C	226	ILE
2	C	384	ASP
2	C	388	PRO
2	C	471	VAL
2	C	661	GLY
2	C	686	LYS

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Mol	Chain	Res	Type
2	D	145	ASN
2	D	162	THR
2	D	197	SER
2	D	364	VAL
2	D	550	GLY
2	D	686	LYS
2	E	143	GLY
2	E	231	PRO
2	E	375	VAL
2	E	388	PRO
2	E	400	SER
2	E	550	GLY
2	E	586	LEU
2	E	686	LYS
2	F	166	LEU
2	F	293	ALA
2	F	375	VAL
2	F	531	LEU
2	F	550	GLY
2	F	642	SER
2	F	671	VAL
1	1	191	ILE
1	5	144	LYS
2	A	70	ARG
2	A	198	ARG
2	A	202	ASN
2	A	226	ILE
2	A	228	ASN
2	A	400	SER
2	A	469	SER
2	A	642	SER
2	B	375	VAL
2	B	434	GLN
2	B	472	THR
2	B	717	LYS
2	C	147	THR
2	C	400	SER
2	C	579	GLU
2	D	167	ALA
2	D	226	ILE
2	D	674	ASN
2	E	209	GLU

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Mol	Chain	Res	Type
2	E	226	ILE
2	E	469	SER
2	E	534	PRO
2	E	690	MET
2	E	698	ARG
2	E	713	SER
2	F	226	ILE
2	F	400	SER
1	3	216	PHE
2	A	434	GLN
2	A	600	GLY
2	B	166	LEU
2	C	118	GLY
2	C	152	ALA
2	C	323	TYR
2	D	228	ASN
2	D	251	THR
2	D	343	SER
2	D	531	LEU
2	D	760	TYR
2	E	5	ARG
2	E	103	VAL
2	E	323	TYR
2	E	600	GLY
2	E	757	ASP
2	F	99	GLY
2	F	686	LYS
2	F	758	LEU
1	3	191	ILE
2	C	210	PRO
2	C	512	GLY
2	E	661	GLY
2	F	212	VAL
2	F	382	ILE
2	F	610	PRO
2	A	212	VAL
2	A	382	ILE
2	B	600	GLY
2	C	588	GLY
2	D	68	ILE
2	E	212	VAL
2	F	471	VAL

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Mol	Chain	Res	Type
1	2	191	ILE
2	A	761	GLY
2	B	182	VAL
2	B	660	VAL
2	D	382	ILE
2	F	210	PRO
2	A	364	VAL
2	B	382	ILE
2	B	534	PRO
2	C	392	ILE
2	A	160	THR

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	1	88/201 (44%)	81 (92%)	7 (8%)	11	31
1	2	88/201 (44%)	77 (88%)	11 (12%)	4	16
1	3	88/201 (44%)	79 (90%)	9 (10%)	7	23
1	4	88/201 (44%)	78 (89%)	10 (11%)	5	18
1	5	88/201 (44%)	77 (88%)	11 (12%)	4	16
1	6	88/201 (44%)	80 (91%)	8 (9%)	9	27
2	A	667/686 (97%)	584 (88%)	83 (12%)	4	17
2	B	667/686 (97%)	586 (88%)	81 (12%)	5	17
2	C	667/686 (97%)	586 (88%)	81 (12%)	5	17
2	D	667/686 (97%)	589 (88%)	78 (12%)	5	18
2	E	667/686 (97%)	599 (90%)	68 (10%)	7	23
2	F	667/686 (97%)	587 (88%)	80 (12%)	5	17
All	All	4530/5322 (85%)	4003 (88%)	527 (12%)	7	18

All (527) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	130	VAL
1	1	137	GLU
1	1	147	VAL
1	1	151	LYS
1	1	175	VAL
1	1	204	ILE
1	1	216	PHE
1	2	130	VAL
1	2	140	ILE
1	2	142	LEU
1	2	145	LEU
1	2	147	VAL
1	2	151	LYS
1	2	170	MET
1	2	175	VAL
1	2	214	LYS
1	2	215	HIS
1	2	216	PHE
1	3	130	VAL
1	3	145	LEU
1	3	151	LYS
1	3	152	THR
1	3	165	VAL
1	3	195	ARG
1	3	204	ILE
1	3	214	LYS
1	3	216	PHE
1	4	136	PHE
1	4	137	GLU
1	4	145	LEU
1	4	147	VAL
1	4	151	LYS
1	4	163	LEU
1	4	175	VAL
1	4	195	ARG
1	4	203	ILE
1	4	204	ILE
1	5	130	VAL
1	5	137	GLU
1	5	142	LEU
1	5	144	LYS
1	5	146	ASN
1	5	151	LYS

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Mol	Chain	Res	Type
1	5	170	MET
1	5	176	GLU
1	5	202	LEU
1	5	204	ILE
1	5	216	PHE
1	6	130	VAL
1	6	142	LEU
1	6	145	LEU
1	6	151	LYS
1	6	170	MET
1	6	175	VAL
1	6	204	ILE
1	6	215	HIS
2	A	3	PHE
2	A	8	GLU
2	A	19	GLU
2	A	22	LEU
2	A	41	GLU
2	A	43	GLU
2	A	53	LEU
2	A	74	MET
2	A	76	GLN
2	A	78	ILE
2	A	94	GLU
2	A	105	THR
2	A	119	VAL
2	A	132	ASN
2	A	138	VAL
2	A	139	LEU
2	A	142	LEU
2	A	155	ASN
2	A	170	LEU
2	A	185	ARG
2	A	187	LYS
2	A	194	GLU
2	A	209	GLU
2	A	224	GLN
2	A	238	ARG
2	A	247	VAL
2	A	262	LYS
2	A	268	ILE
2	A	294	ILE

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Mol	Chain	Res	Type
2	A	303	SER
2	A	315	THR
2	A	324	ILE
2	A	335	GLN
2	A	337	ILE
2	A	341	GLN
2	A	354	LEU
2	A	355	ARG
2	A	364	VAL
2	A	379	ASP
2	A	380	ARG
2	A	392	ILE
2	A	415	GLU
2	A	423	VAL
2	A	424	ARG
2	A	427	LYS
2	A	443	ARG
2	A	449	LEU
2	A	452	GLN
2	A	457	LYS
2	A	461	LYS
2	A	462	GLU
2	A	463	LYS
2	A	470	GLU
2	A	471	VAL
2	A	475	ASP
2	A	497	ASP
2	A	503	GLU
2	A	511	ILE
2	A	563	PHE
2	A	578	MET
2	A	597	ASP
2	A	624	PRO
2	A	626	VAL
2	A	632	GLN
2	A	634	LEU
2	A	641	ASP
2	A	647	VAL
2	A	671	VAL
2	A	673	PHE
2	A	674	ASN
2	A	675	VAL

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Mol	Chain	Res	Type
2	A	676	GLN
2	A	678	GLU
2	A	687	ASP
2	A	694	LYS
2	A	700	GLU
2	A	713	SER
2	A	717	LYS
2	A	729	GLN
2	A	730	LEU
2	A	741	ILE
2	A	763	ARG
2	A	795	ASP
2	B	18	GLN
2	B	20	GLU
2	B	27	ASN
2	B	41	GLU
2	B	45	ILE
2	B	72	GLN
2	B	74	MET
2	B	78	ILE
2	B	97	LYS
2	B	100	HIS
2	B	105	THR
2	B	117	GLU
2	B	119	VAL
2	B	137	GLN
2	B	138	VAL
2	B	139	LEU
2	B	166	LEU
2	B	168	ARG
2	B	170	LEU
2	B	185	ARG
2	B	194	GLU
2	B	214	LYS
2	B	230	VAL
2	B	232	GLU
2	B	235	ARG
2	B	262	LYS
2	B	268	ILE
2	B	269	ARG
2	B	308	GLU
2	B	309	LEU

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Mol	Chain	Res	Type
2	B	321	ARG
2	B	348	ILE
2	B	355	ARG
2	B	358	TYR
2	B	361	HIS
2	B	363	ARG
2	B	364	VAL
2	B	385	ARG
2	B	387	LEU
2	B	392	ILE
2	B	415	GLU
2	B	423	VAL
2	B	424	ARG
2	B	425	LYS
2	B	449	LEU
2	B	451	GLU
2	B	452	GLN
2	B	457	LYS
2	B	471	VAL
2	B	472	THR
2	B	476	ILE
2	B	478	MET
2	B	479	VAL
2	B	480	VAL
2	B	483	TRP
2	B	503	GLU
2	B	511	ILE
2	B	531	LEU
2	B	567	GLU
2	B	578	MET
2	B	586	LEU
2	B	597	ASP
2	B	609	LYS
2	B	620	GLU
2	B	624	PRO
2	B	639	LEU
2	B	641	ASP
2	B	643	LYS
2	B	647	VAL
2	B	682	HIS
2	B	693	LEU
2	B	695	ARG

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Mol	Chain	Res	Type
2	B	716	LYS
2	B	719	LEU
2	B	721	GLU
2	B	730	LEU
2	B	739	LEU
2	B	742	GLU
2	B	769	ILE
2	B	790	GLN
2	B	795	ASP
2	C	18	GLN
2	C	19	GLU
2	C	20	GLU
2	C	27	ASN
2	C	31	THR
2	C	32	GLU
2	C	45	ILE
2	C	53	LEU
2	C	72	GLN
2	C	74	MET
2	C	83	ARG
2	C	105	THR
2	C	108	ILE
2	C	135	ARG
2	C	138	VAL
2	C	139	LEU
2	C	166	LEU
2	C	188	GLU
2	C	193	ILE
2	C	194	GLU
2	C	195	VAL
2	C	202	ASN
2	C	247	VAL
2	C	269	ARG
2	C	285	ILE
2	C	308	GLU
2	C	323	TYR
2	C	342	PRO
2	C	346	GLU
2	C	363	ARG
2	C	364	VAL
2	C	379	ASP
2	C	380	ARG

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Mol	Chain	Res	Type
2	C	392	ILE
2	C	397	GLU
2	C	401	LYS
2	C	410	PRO
2	C	415	GLU
2	C	420	LEU
2	C	423	VAL
2	C	424	ARG
2	C	427	LYS
2	C	431	VAL
2	C	434	GLN
2	C	443	ARG
2	C	447	GLN
2	C	449	LEU
2	C	452	GLN
2	C	460	TRP
2	C	463	LYS
2	C	478	MET
2	C	479	VAL
2	C	480	VAL
2	C	495	GLU
2	C	503	GLU
2	C	549	VAL
2	C	576	GLU
2	C	586	LEU
2	C	603	THR
2	C	609	LYS
2	C	621	LYS
2	C	624	PRO
2	C	634	LEU
2	C	639	LEU
2	C	647	VAL
2	C	653	ILE
2	C	665	LEU
2	C	669	LYS
2	C	679	THR
2	C	680	GLN
2	C	683	LYS
2	C	688	LYS
2	C	713	SER
2	C	716	LYS
2	C	729	GLN

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Mol	Chain	Res	Type
2	C	730	LEU
2	C	741	ILE
2	C	742	GLU
2	C	767	ARG
2	C	790	GLN
2	C	795	ASP
2	D	19	GLU
2	D	22	LEU
2	D	31	THR
2	D	32	GLU
2	D	41	GLU
2	D	53	LEU
2	D	62	LYS
2	D	74	MET
2	D	85	LYS
2	D	90	LEU
2	D	94	GLU
2	D	105	THR
2	D	106	GLU
2	D	117	GLU
2	D	136	GLN
2	D	138	VAL
2	D	139	LEU
2	D	185	ARG
2	D	194	GLU
2	D	224	GLN
2	D	234	LEU
2	D	237	LYS
2	D	262	LYS
2	D	269	ARG
2	D	308	GLU
2	D	337	ILE
2	D	342	PRO
2	D	361	HIS
2	D	364	VAL
2	D	366	ILE
2	D	380	ARG
2	D	381	TYR
2	D	387	LEU
2	D	392	ILE
2	D	397	GLU
2	D	401	LYS

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Mol	Chain	Res	Type
2	D	403	ARG
2	D	412	ASN
2	D	414	LYS
2	D	419	LYS
2	D	420	LEU
2	D	423	VAL
2	D	424	ARG
2	D	428	ASP
2	D	431	VAL
2	D	432	GLN
2	D	452	GLN
2	D	457	LYS
2	D	462	GLU
2	D	471	VAL
2	D	479	VAL
2	D	480	VAL
2	D	503	GLU
2	D	511	ILE
2	D	531	LEU
2	D	546	PRO
2	D	563	PHE
2	D	567	GLU
2	D	570	ILE
2	D	574	MET
2	D	578	MET
2	D	593	TYR
2	D	606	VAL
2	D	609	LYS
2	D	623	HIS
2	D	634	LEU
2	D	636	ASP
2	D	639	LEU
2	D	647	VAL
2	D	683	LYS
2	D	686	LYS
2	D	695	ARG
2	D	729	GLN
2	D	730	LEU
2	D	742	GLU
2	D	758	LEU
2	D	790	GLN
2	D	804	LYS

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Mol	Chain	Res	Type
2	E	18	GLN
2	E	45	ILE
2	E	53	LEU
2	E	62	LYS
2	E	78	ILE
2	E	100	HIS
2	E	108	ILE
2	E	119	VAL
2	E	139	LEU
2	E	262	LYS
2	E	263	LYS
2	E	265	MET
2	E	269	ARG
2	E	270	GLN
2	E	299	ILE
2	E	316	THR
2	E	337	ILE
2	E	342	PRO
2	E	355	ARG
2	E	359	GLU
2	E	363	ARG
2	E	364	VAL
2	E	366	ILE
2	E	378	SER
2	E	380	ARG
2	E	382	ILE
2	E	384	ASP
2	E	392	ILE
2	E	393	ASP
2	E	397	GLU
2	E	400	SER
2	E	401	LYS
2	E	410	PRO
2	E	415	GLU
2	E	421	ASP
2	E	423	VAL
2	E	424	ARG
2	E	427	LYS
2	E	435	GLU
2	E	452	GLN
2	E	457	LYS
2	E	461	LYS

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Mol	Chain	Res	Type
2	E	462	GLU
2	E	479	VAL
2	E	480	VAL
2	E	503	GLU
2	E	511	ILE
2	E	542	ILE
2	E	544	LEU
2	E	597	ASP
2	E	624	PRO
2	E	626	VAL
2	E	639	LEU
2	E	647	VAL
2	E	665	LEU
2	E	667	ARG
2	E	671	VAL
2	E	685	MET
2	E	689	VAL
2	E	697	PHE
2	E	711	PHE
2	E	719	LEU
2	E	730	LEU
2	E	741	ILE
2	E	759	GLU
2	E	790	GLN
2	E	791	HIS
2	E	795	ASP
2	F	19	GLU
2	F	20	GLU
2	F	35	LEU
2	F	45	ILE
2	F	62	LYS
2	F	72	GLN
2	F	74	MET
2	F	83	ARG
2	F	94	GLU
2	F	105	THR
2	F	108	ILE
2	F	110	LEU
2	F	119	VAL
2	F	137	GLN
2	F	138	VAL
2	F	170	LEU

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Mol	Chain	Res	Type
2	F	185	ARG
2	F	209	GLU
2	F	262	LYS
2	F	269	ARG
2	F	304	LEU
2	F	337	ILE
2	F	341	GLN
2	F	351	LEU
2	F	361	HIS
2	F	364	VAL
2	F	379	ASP
2	F	380	ARG
2	F	381	TYR
2	F	385	ARG
2	F	387	LEU
2	F	392	ILE
2	F	397	GLU
2	F	412	ASN
2	F	414	LYS
2	F	415	GLU
2	F	423	VAL
2	F	424	ARG
2	F	427	LYS
2	F	431	VAL
2	F	443	ARG
2	F	449	LEU
2	F	452	GLN
2	F	468	ASN
2	F	471	VAL
2	F	473	VAL
2	F	475	ASP
2	F	476	ILE
2	F	478	MET
2	F	479	VAL
2	F	503	GLU
2	F	513	GLN
2	F	570	ILE
2	F	579	GLU
2	F	586	LEU
2	F	589	SER
2	F	593	TYR
2	F	624	PRO

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Mol	Chain	Res	Type
2	F	636	ASP
2	F	639	LEU
2	F	641	ASP
2	F	647	VAL
2	F	653	ILE
2	F	658	SER
2	F	664	GLU
2	F	669	LYS
2	F	676	GLN
2	F	692	GLU
2	F	697	PHE
2	F	704	ARG
2	F	710	VAL
2	F	714	LEU
2	F	719	LEU
2	F	729	GLN
2	F	730	LEU
2	F	741	ILE
2	F	742	GLU
2	F	769	ILE
2	F	790	GLN
2	F	793	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	194	HIS
1	1	207	HIS
1	2	207	HIS
1	3	148	ASN
1	3	159	ASN
1	3	207	HIS
1	4	159	ASN
1	4	207	HIS
1	5	146	ASN
1	5	207	HIS
1	6	194	HIS
2	A	26	HIS
2	A	33	HIS
2	A	137	GLN
2	A	155	ASN
2	A	190	GLN

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Mol	Chain	Res	Type
2	A	282	HIS
2	A	341	GLN
2	A	352	GLN
2	A	418	GLN
2	A	507	HIS
2	A	581	HIS
2	A	676	GLN
2	A	682	HIS
2	A	791	HIS
2	B	27	ASN
2	B	28	ASN
2	B	79	HIS
2	B	107	HIS
2	B	224	GLN
2	B	270	GLN
2	B	273	ASN
2	B	282	HIS
2	B	298	ASN
2	B	338	GLN
2	B	341	GLN
2	B	352	GLN
2	B	361	HIS
2	B	412	ASN
2	B	434	GLN
2	B	468	ASN
2	B	507	HIS
2	B	581	HIS
2	B	674	ASN
2	B	680	GLN
2	B	682	HIS
2	B	718	HIS
2	B	787	HIS
2	C	26	HIS
2	C	33	HIS
2	C	100	HIS
2	C	107	HIS
2	C	125	ASN
2	C	352	GLN
2	C	418	GLN
2	C	466	GLN
2	C	507	HIS
2	C	601	GLN

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Mol	Chain	Res	Type
2	C	623	HIS
2	C	628	ASN
2	C	737	GLN
2	C	787	HIS
2	C	791	HIS
2	D	26	HIS
2	D	28	ASN
2	D	33	HIS
2	D	79	HIS
2	D	100	HIS
2	D	107	HIS
2	D	136	GLN
2	D	137	GLN
2	D	190	GLN
2	D	224	GLN
2	D	270	GLN
2	D	352	GLN
2	D	447	GLN
2	D	507	HIS
2	D	581	HIS
2	D	628	ASN
2	D	682	HIS
2	D	703	ASN
2	D	712	HIS
2	D	718	HIS
2	D	770	GLN
2	D	772	HIS
2	D	785	ASN
2	E	125	ASN
2	E	136	GLN
2	E	155	ASN
2	E	190	GLN
2	E	270	GLN
2	E	362	HIS
2	E	418	GLN
2	E	464	GLN
2	E	468	ASN
2	E	507	HIS
2	E	581	HIS
2	E	682	HIS
2	E	772	HIS
2	F	26	HIS

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Mol	Chain	Res	Type
2	F	33	HIS
2	F	100	HIS
2	F	107	HIS
2	F	155	ASN
2	F	190	GLN
2	F	273	ASN
2	F	310	GLN
2	F	361	HIS
2	F	466	GLN
2	F	468	ASN
2	F	507	HIS
2	F	581	HIS
2	F	623	HIS
2	F	628	ASN
2	F	676	GLN
2	F	681	ASN
2	F	682	HIS
2	F	718	HIS
2	F	729	GLN
2	F	770	GLN
2	F	772	HIS
2	F	787	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

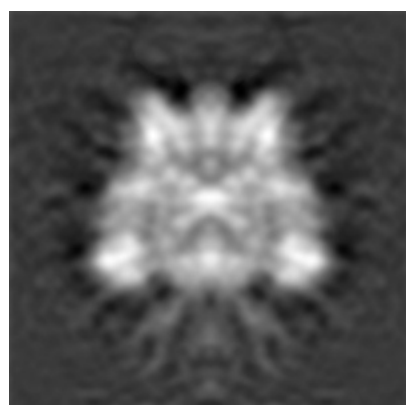
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5608. These allow visual inspection of the internal detail of the map and identification of artifacts.

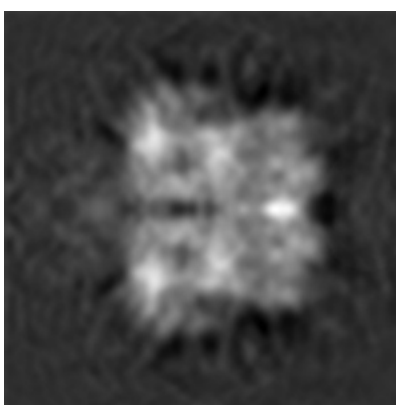
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

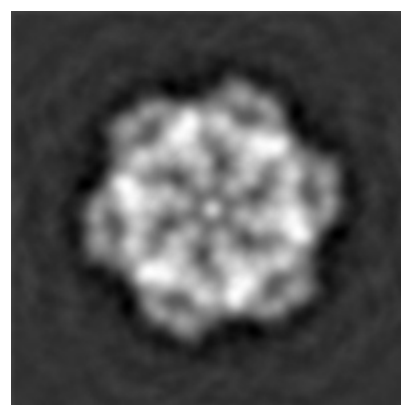
6.1.1 Primary map



X



Y

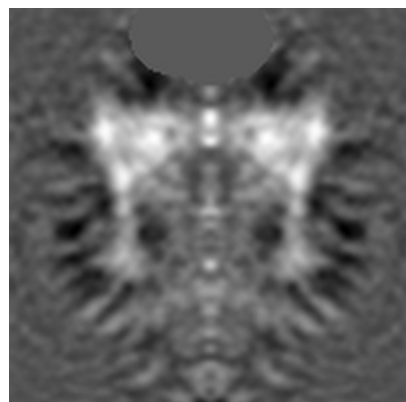


Z

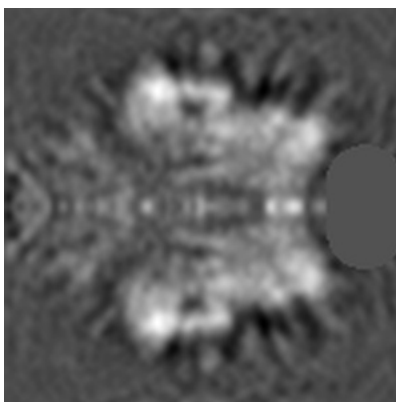
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

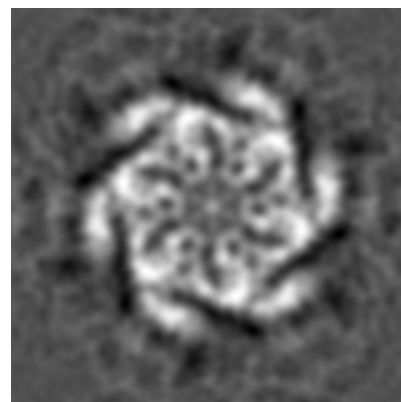
6.2.1 Primary map



X Index: 75



Y Index: 75

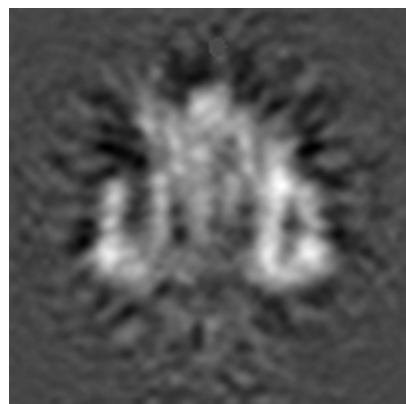


Z Index: 75

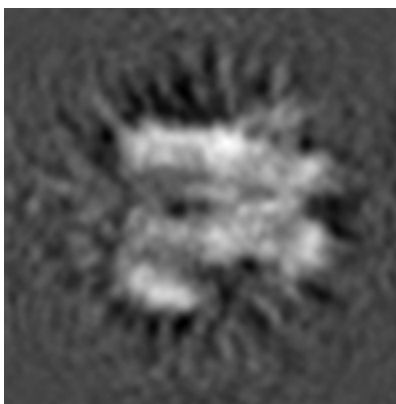
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

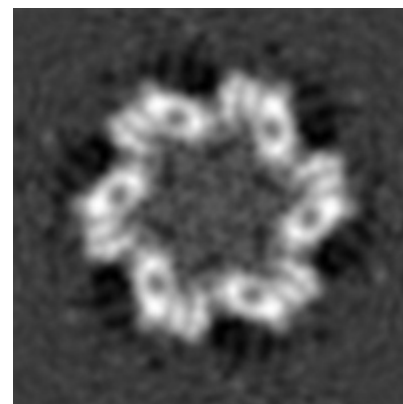
6.3.1 Primary map



X Index: 98



Y Index: 100

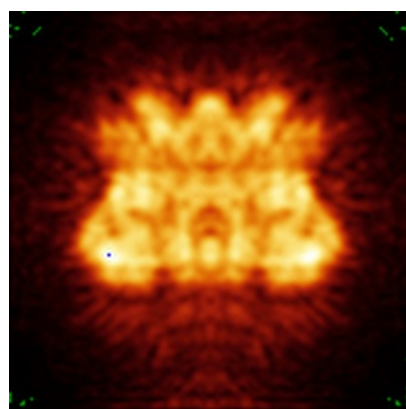


Z Index: 57

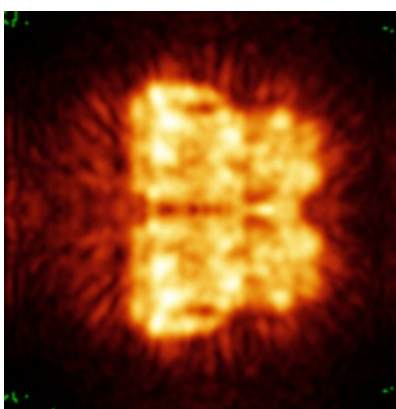
The images above show the largest variance slices of the map in three orthogonal directions.

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

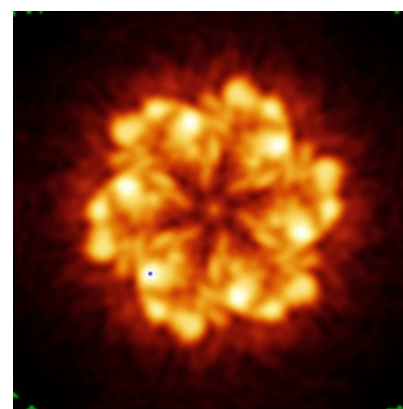
6.4.1 Primary map



X



Y

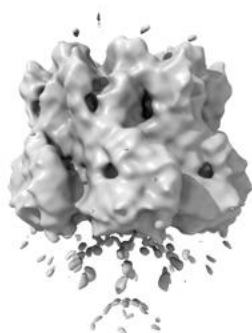


Z

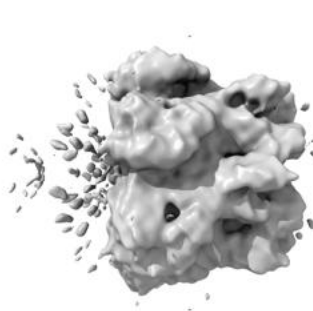
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

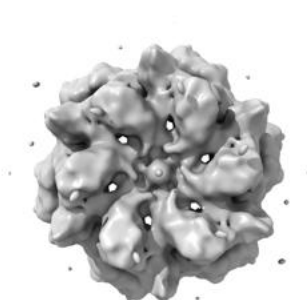
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

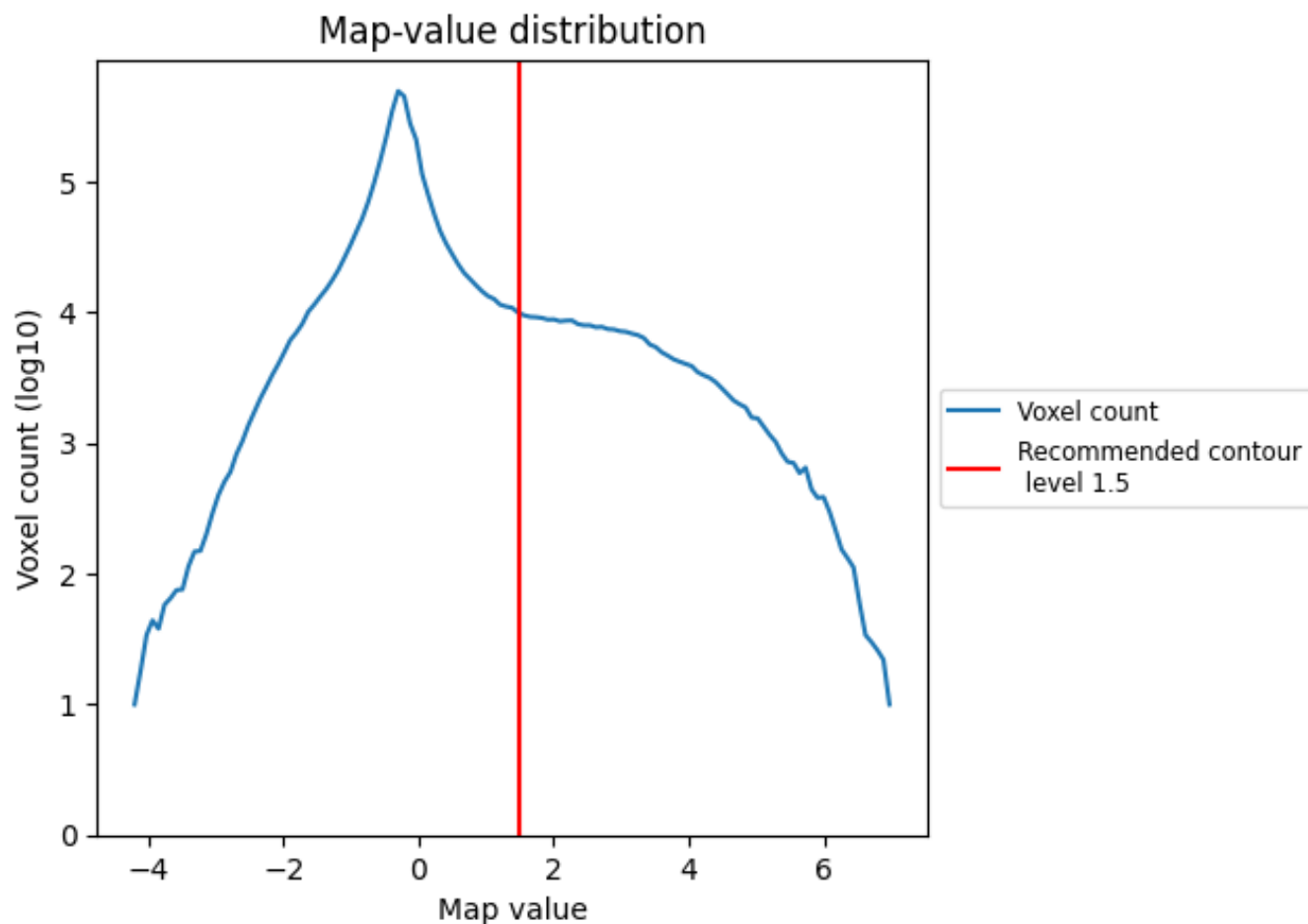
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

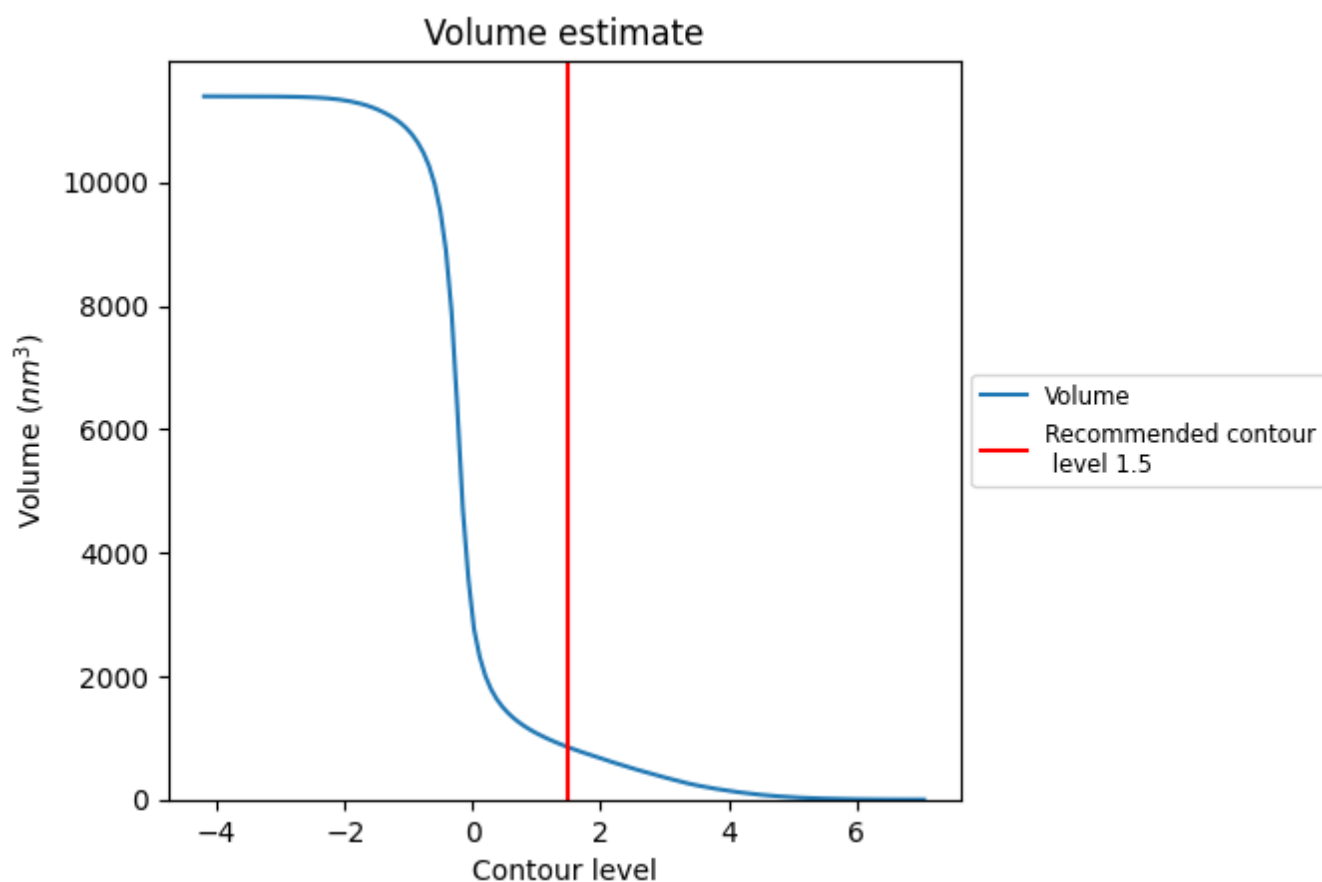
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

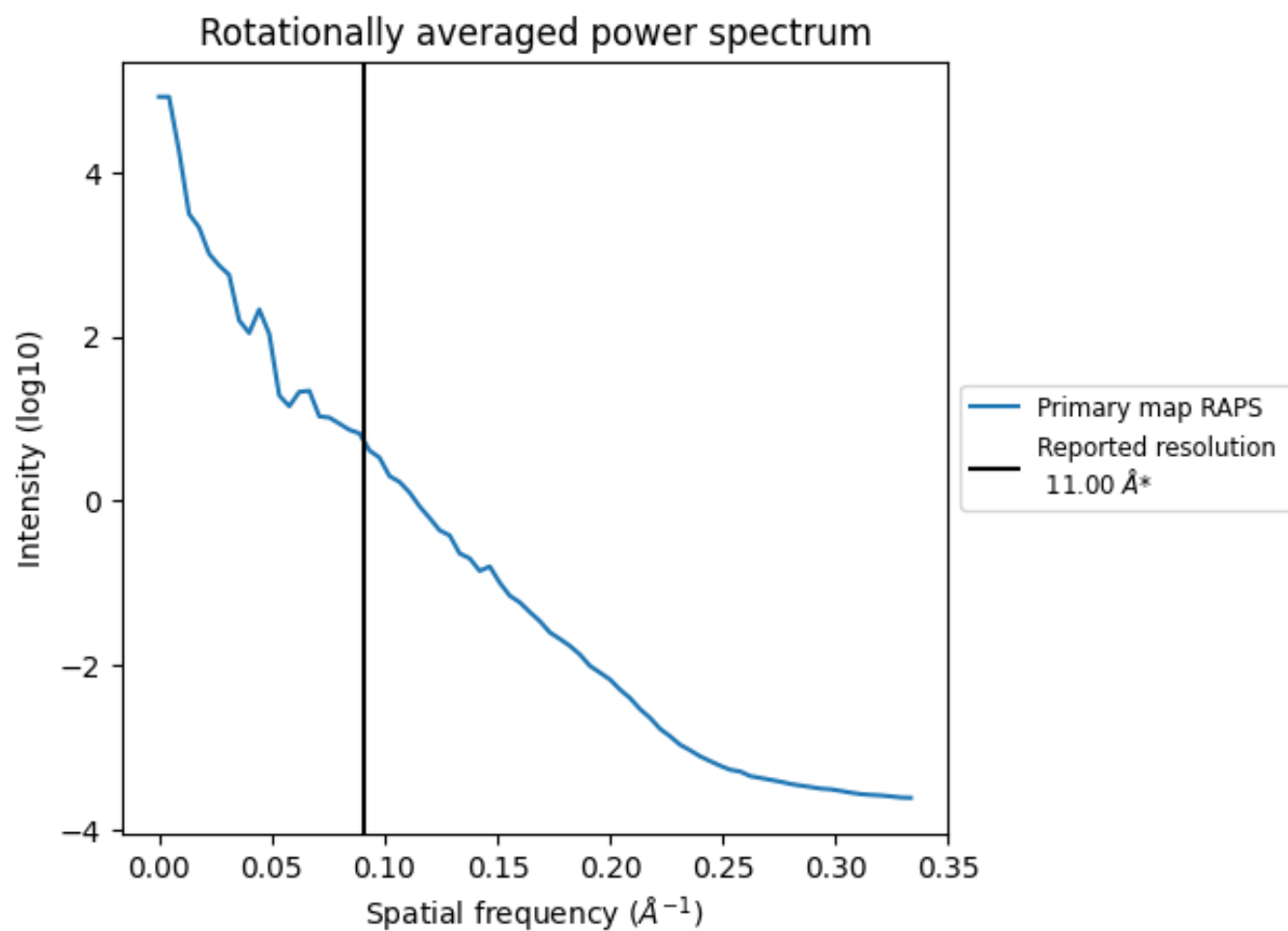
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 846 nm^3 ; this corresponds to an approximate mass of 764 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 0.091 Å⁻¹

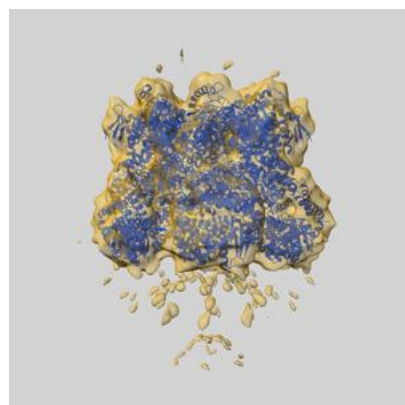
8 Fourier-Shell correlation

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

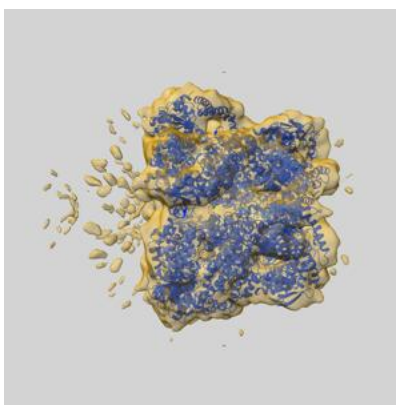
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5608 and PDB model 3J3S. Per-residue inclusion information can be found in section 3 on page 6.

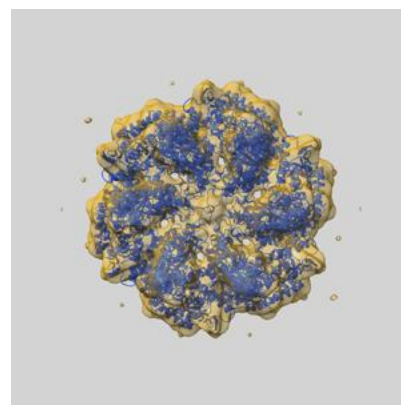
9.1 Map-model overlay [i](#)



X



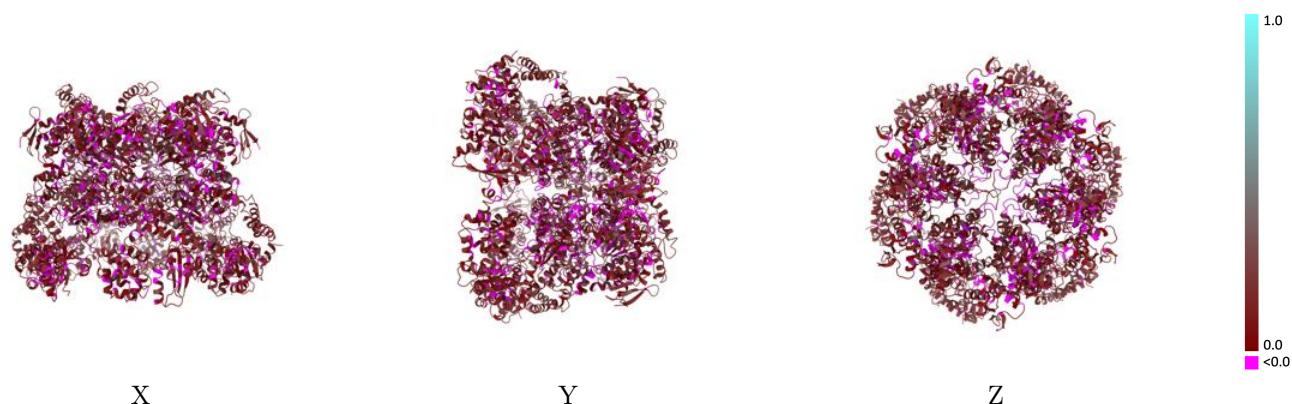
Y



Z

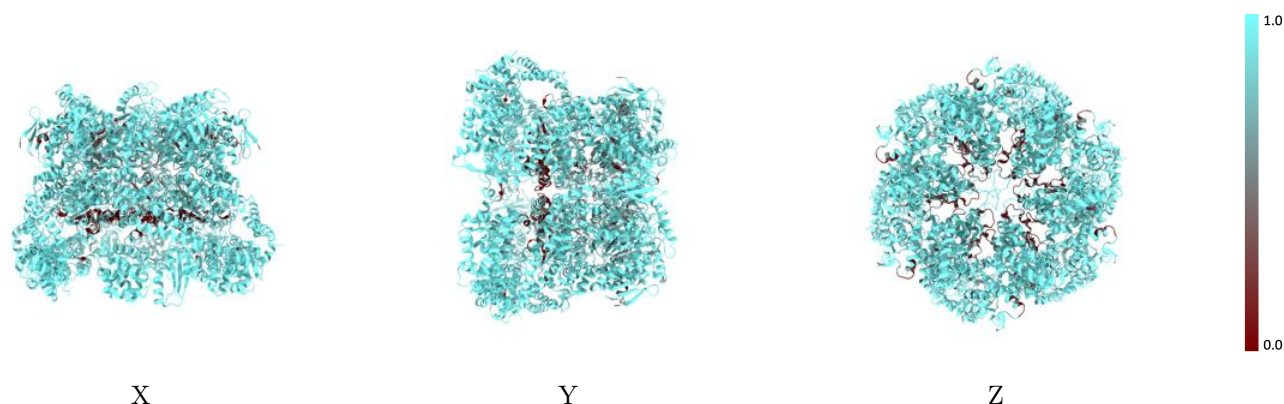
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



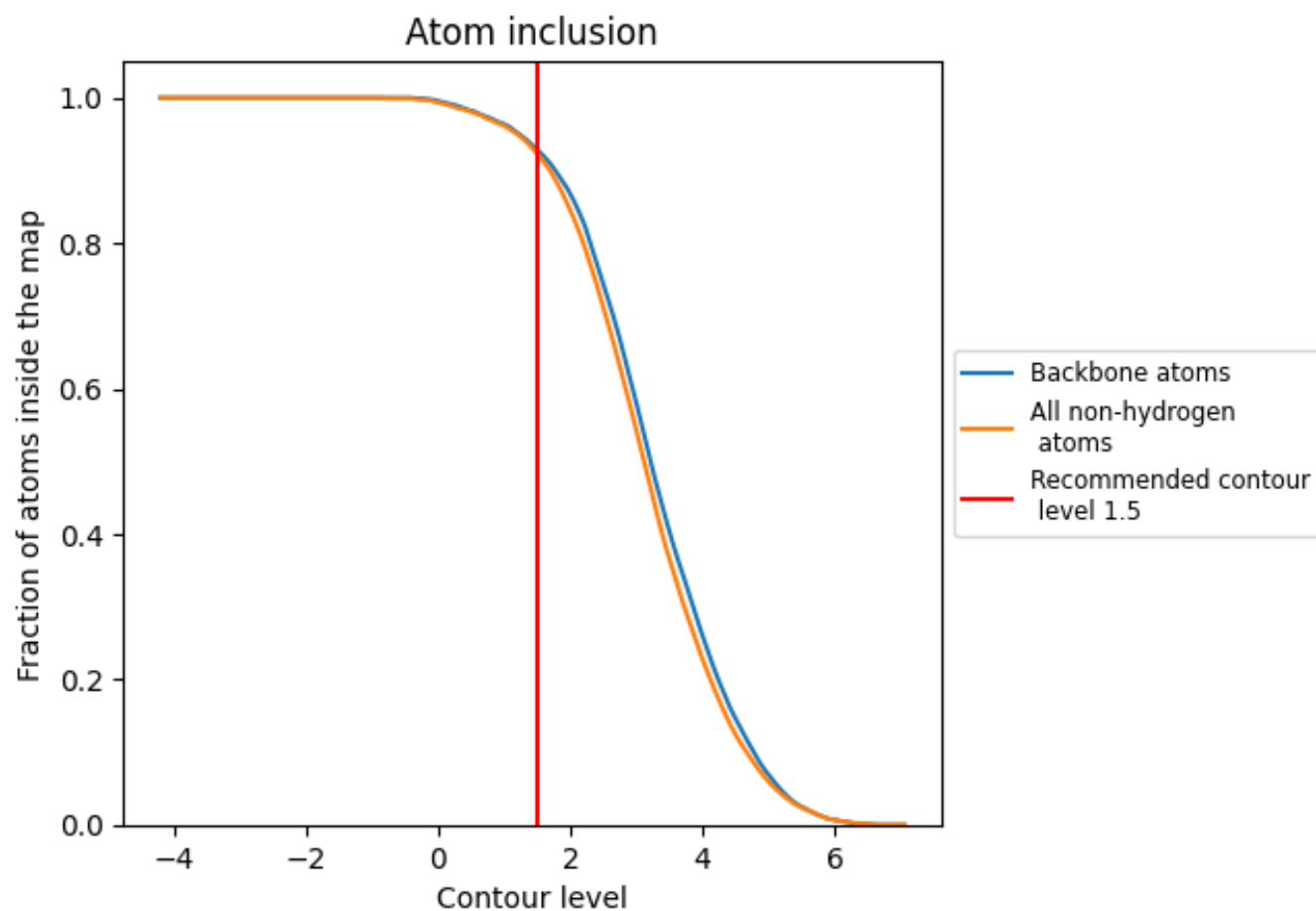
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9230	0.1040
1	0.9570	0.0990
2	0.9620	0.0980
3	0.9650	0.1010
4	0.9770	0.0890
5	0.9740	0.0890
6	0.9620	0.1000
A	0.9140	0.1050
B	0.9140	0.1060
C	0.9200	0.1050
D	0.9210	0.1010
E	0.9190	0.1030
F	0.9170	0.1060

