



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:40 AM UTC

PDB ID : 3J3U / pdb_00003j3u
EMDB ID : EMD-5609
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 : 10.00 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:

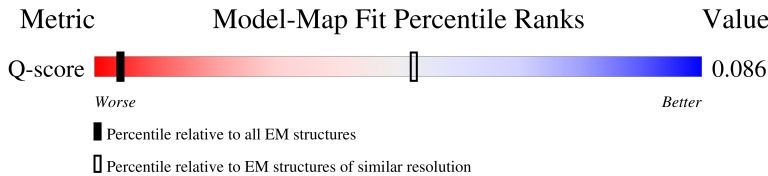
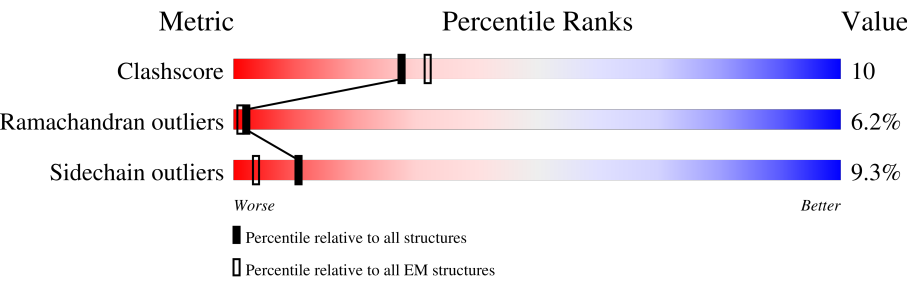
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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	147 (9.50 - 10.50)

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	28%11%57%
1	2	218	26%13%57%
1	3	218	24%13%5%57%
1	4	218	28%13%57%

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Mol	Chain	Length	Quality of chain
1	5	218	28%12%57%
1	6	218	29%11%57%
2	A	810	8%61%28%8%
2	B	810	7%62%29%6%
2	C	810	7%61%30%6%
2	D	810	7%61%30%7%
2	E	810	7%63%28%7%
2	F	810	8%60%30%7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41838 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
			6196	3848	1120	1213	15		
2	B	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		
2	C	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		
2	D	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		
2	E	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		
2	F	798	Total	C	N	O	S	0	0
			6196	3848	1120	1213	15		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	ALA	GLU	engineered mutation	UNP P37571
A	618	ALA	GLU	engineered mutation	UNP P37571

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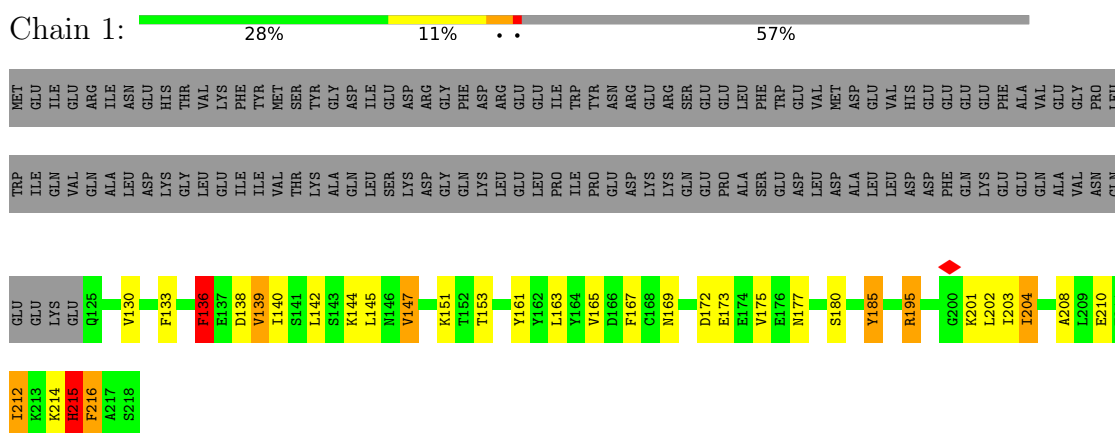
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Chain	Residue	Modelled	Actual	Comment	Reference
B	280	ALA	GLU	engineered mutation	UNP P37571
B	618	ALA	GLU	engineered mutation	UNP P37571
C	280	ALA	GLU	engineered mutation	UNP P37571
C	618	ALA	GLU	engineered mutation	UNP P37571
D	280	ALA	GLU	engineered mutation	UNP P37571
D	618	ALA	GLU	engineered mutation	UNP P37571
E	280	ALA	GLU	engineered mutation	UNP P37571
E	618	ALA	GLU	engineered mutation	UNP P37571
F	280	ALA	GLU	engineered mutation	UNP P37571
F	618	ALA	GLU	engineered mutation	UNP P37571

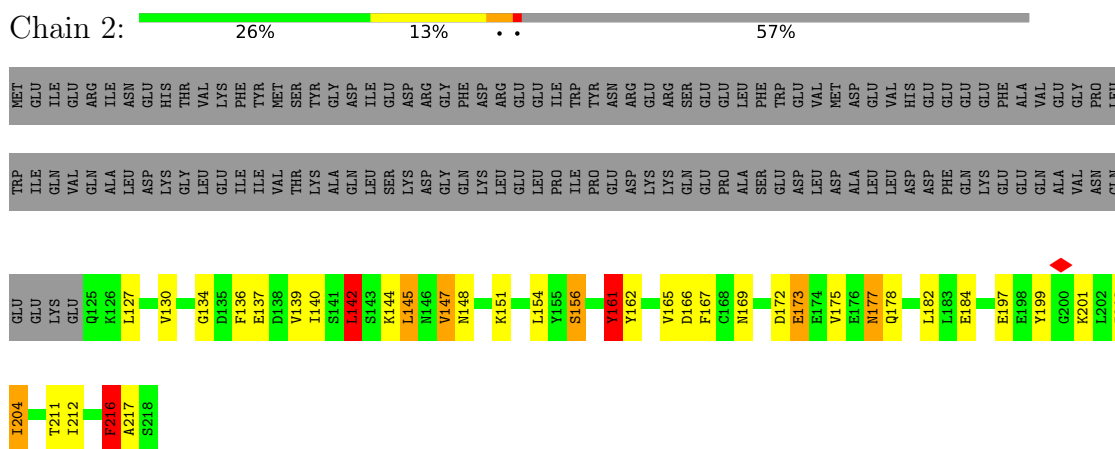
3 Residue-property plots

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.

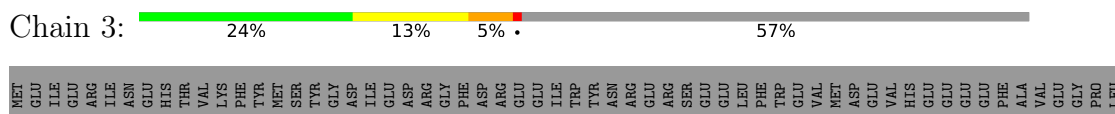
• Molecule 1: Adapter protein MecA 1

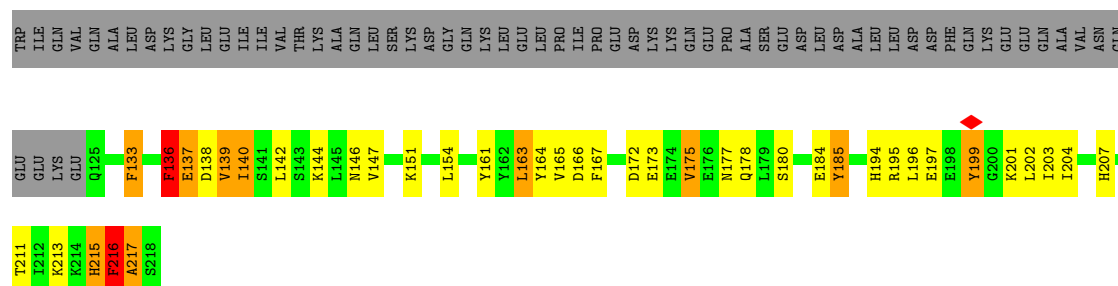


• Molecule 1: Adapter protein MecA 1



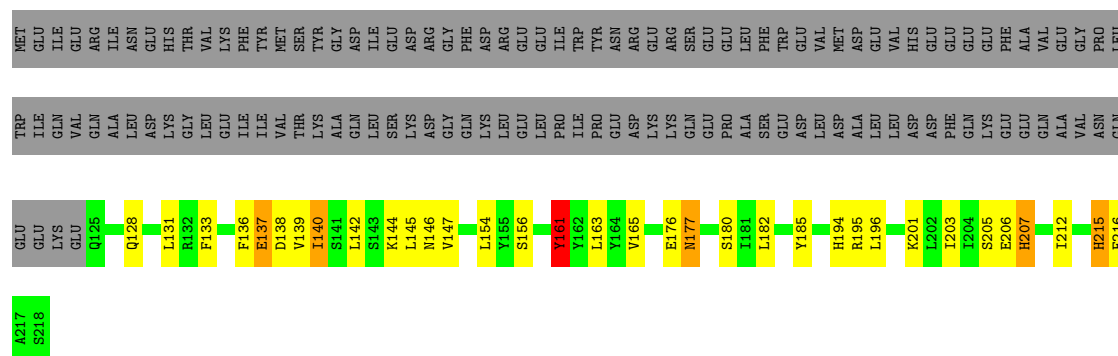
• Molecule 1: Adapter protein MecA 1





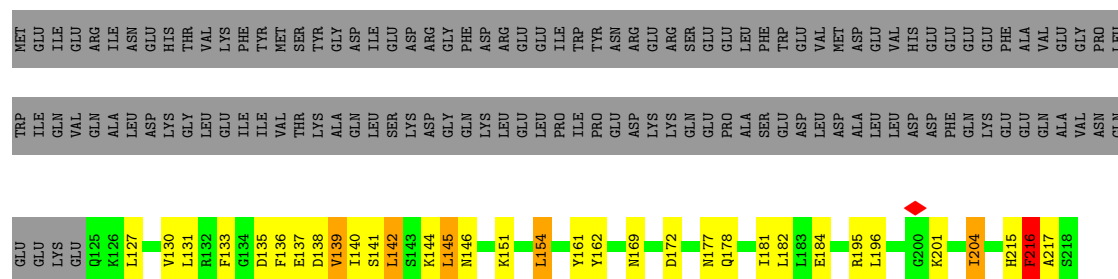
• Molecule 1: Adapter protein MecA 1

Chain 4: 28% 13% . 57%



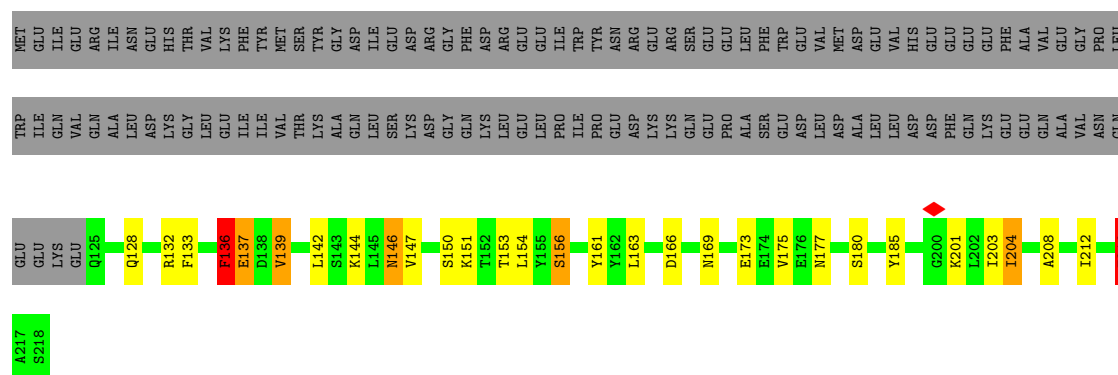
• Molecule 1: Adapter protein MecA 1

Chain 5: 28% 12% . 57%

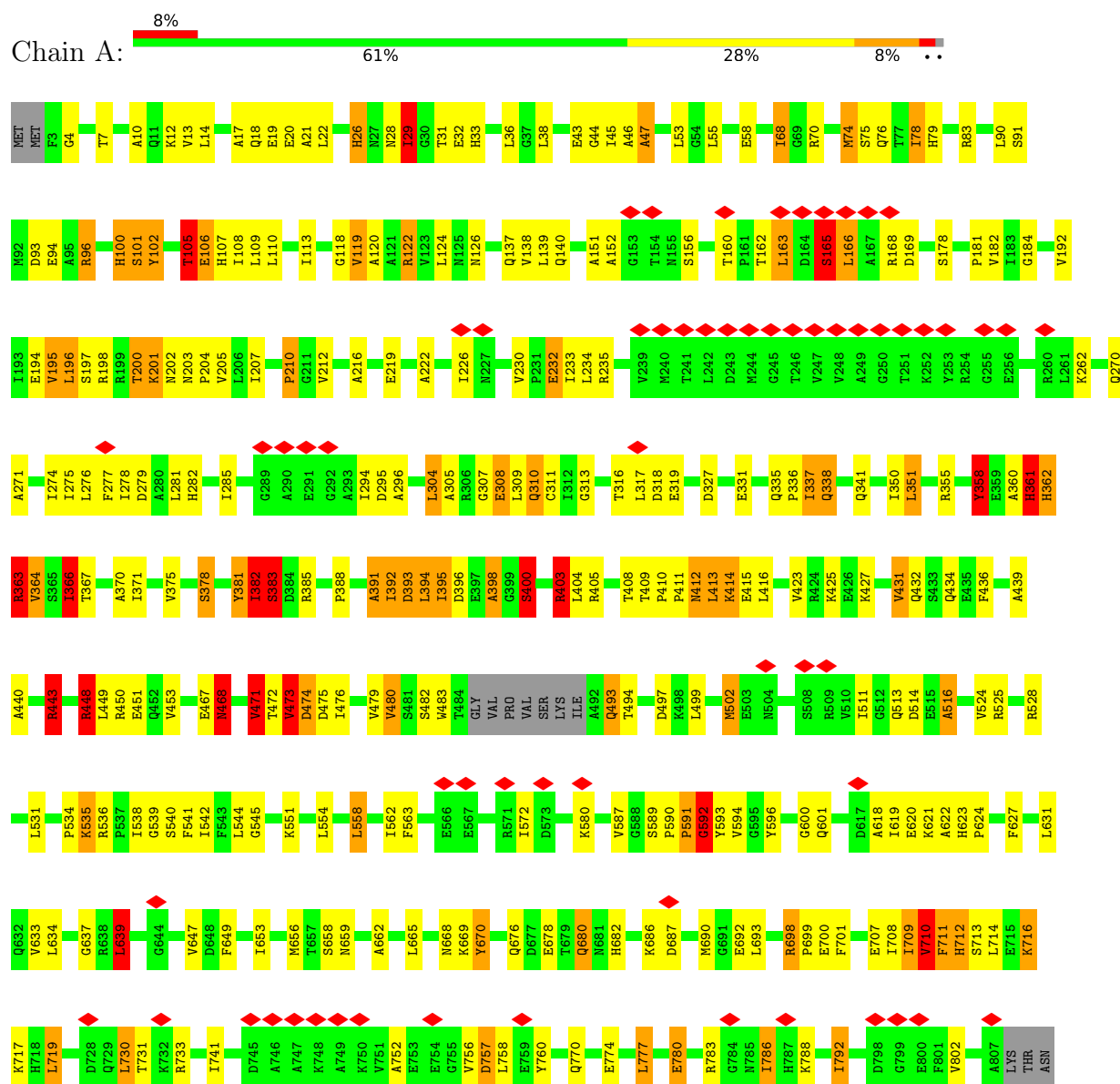


• Molecule 1: Adapter protein MecA 1

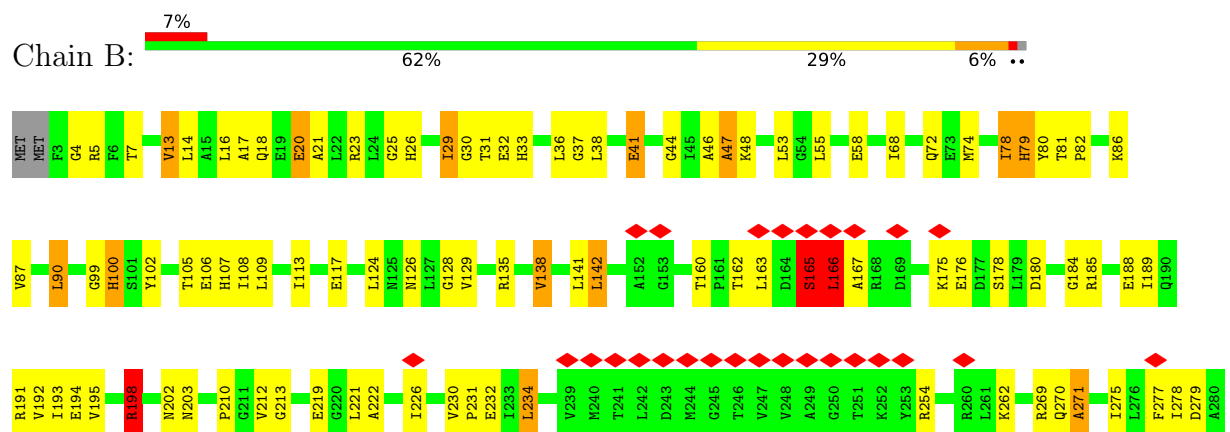
Chain 6: 29% 11% . . 57%

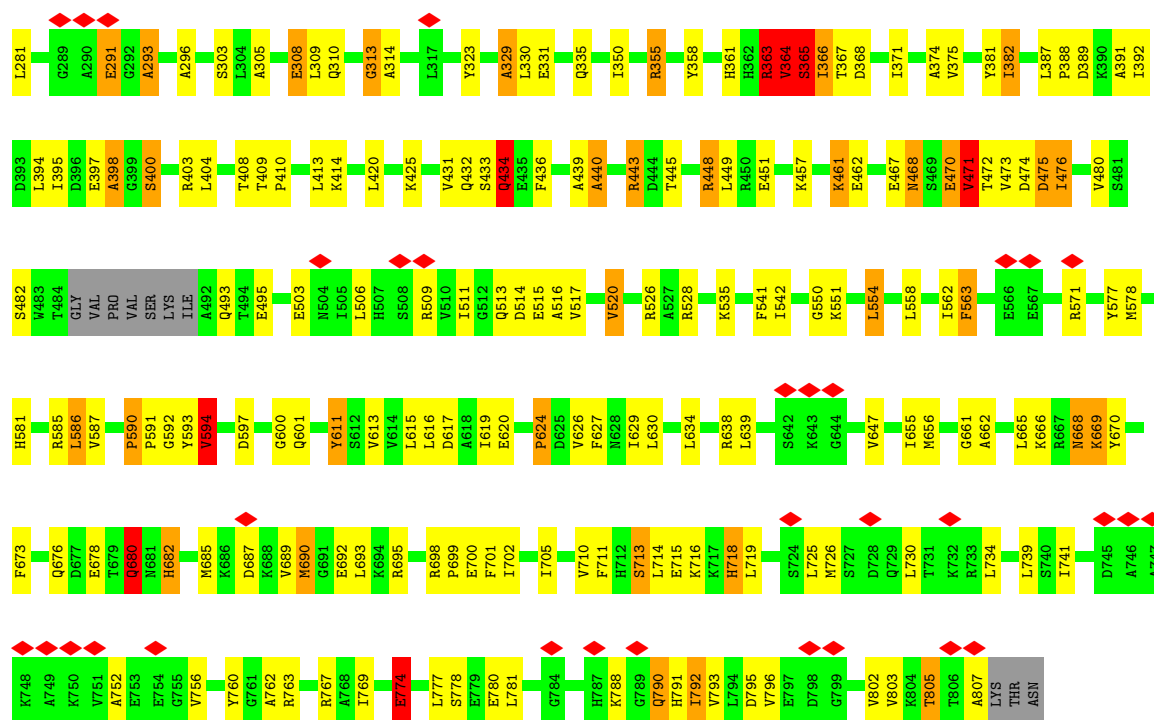


• Molecule 2: Negative regulator of genetic competence ClpC/MecB

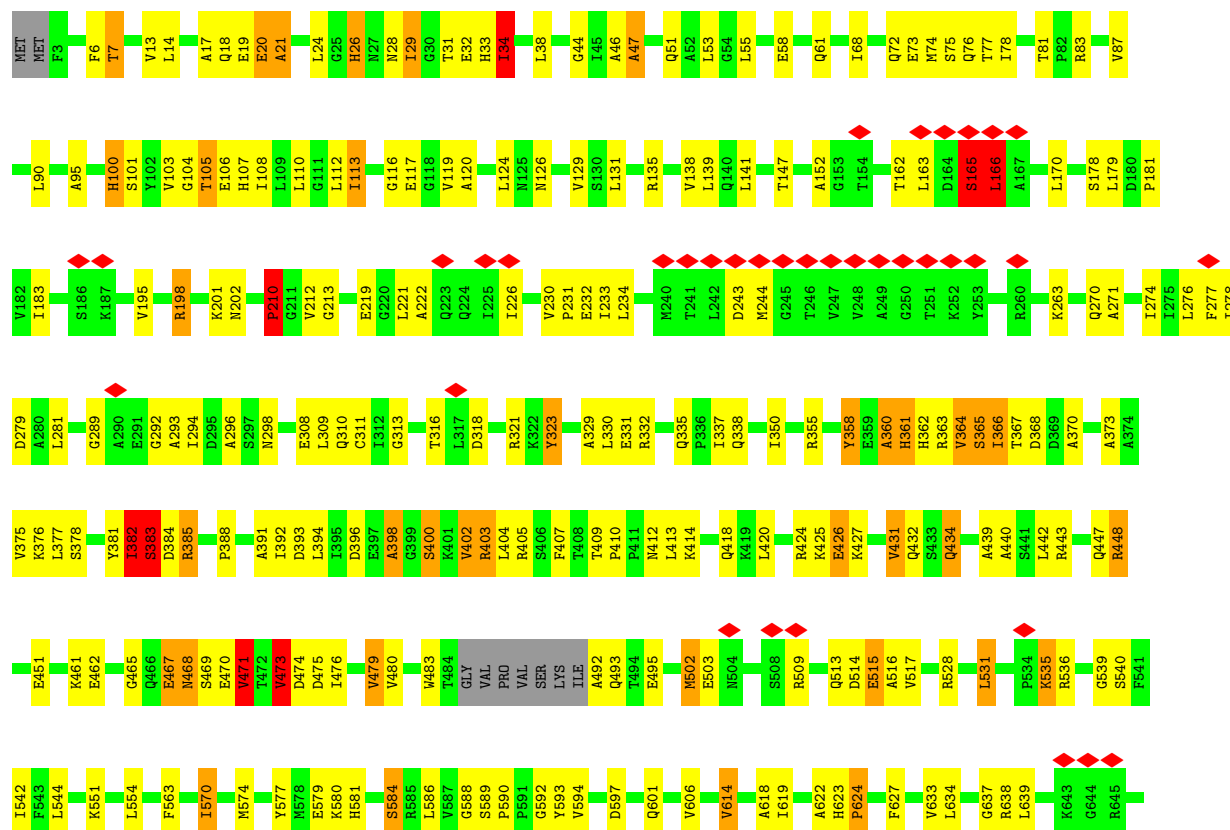


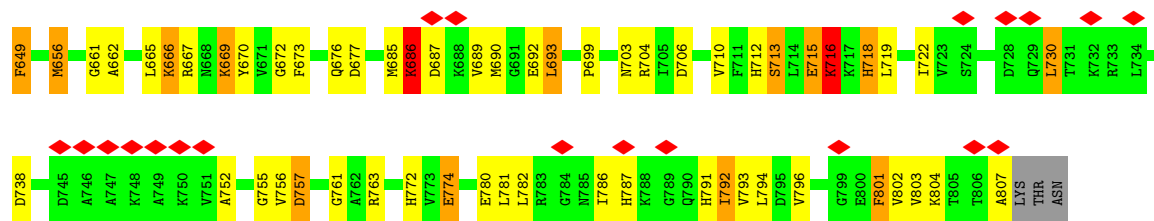
• Molecule 2: Negative regulator of genetic competence ClpC/MecB



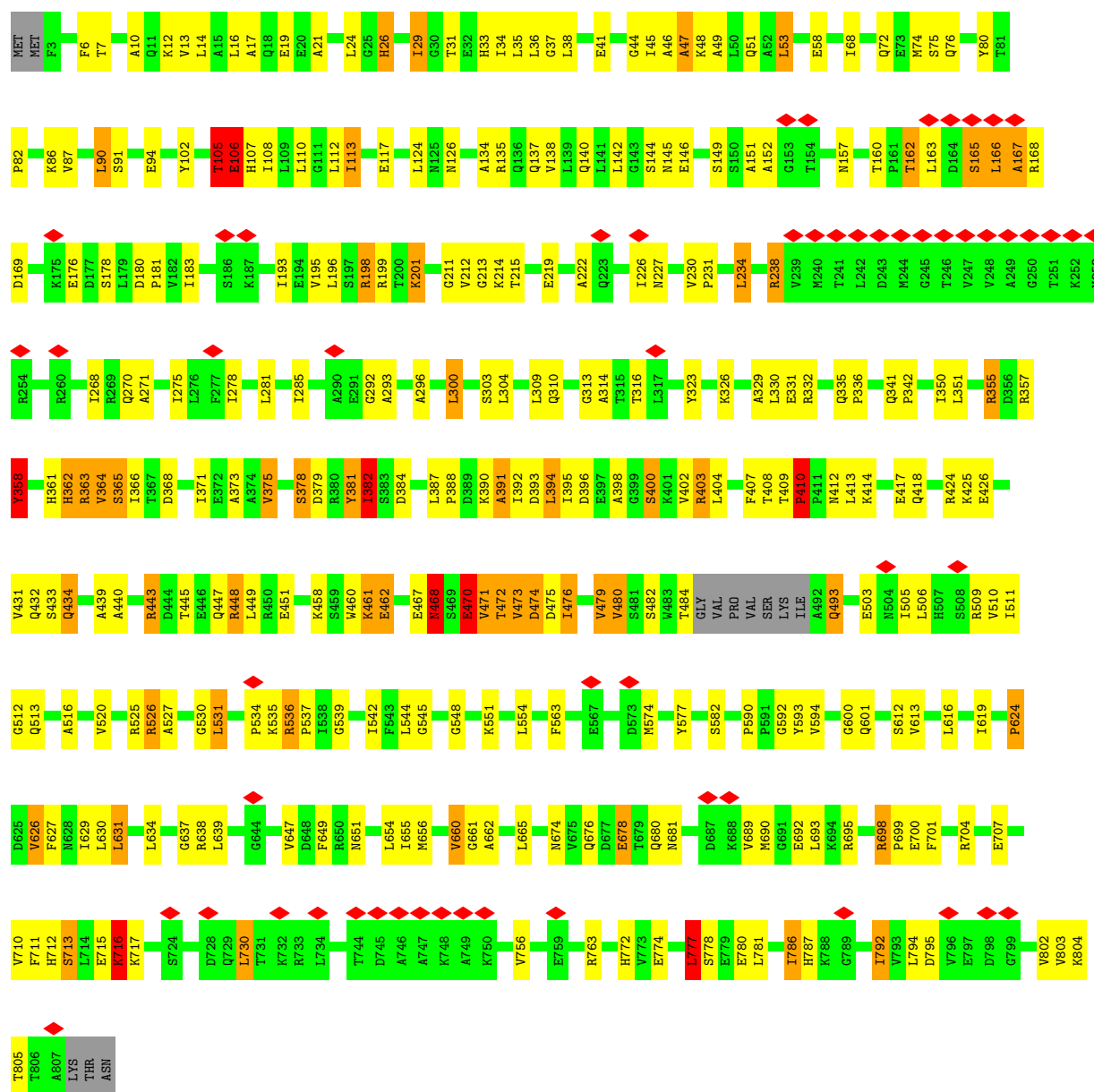


• Molecule 2: Negative regulator of genetic competence ClpC/MecB



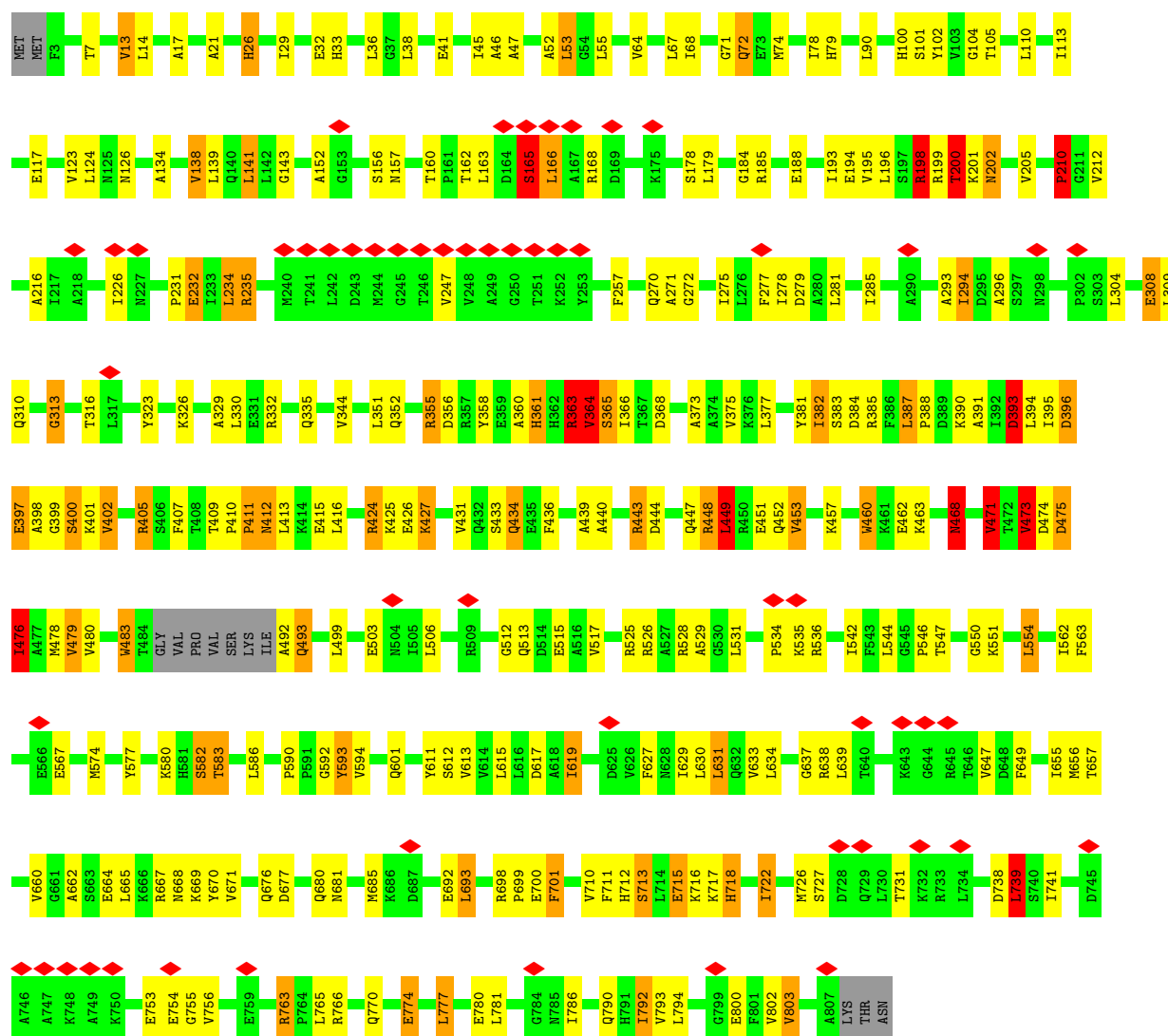


• Molecule 2: Negative regulator of genetic competence ClpC/MecB



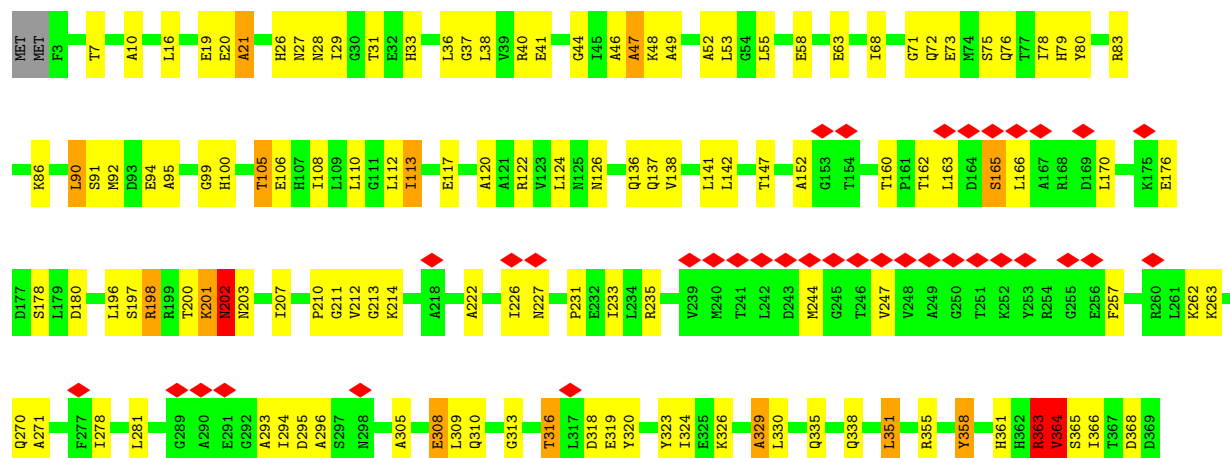
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

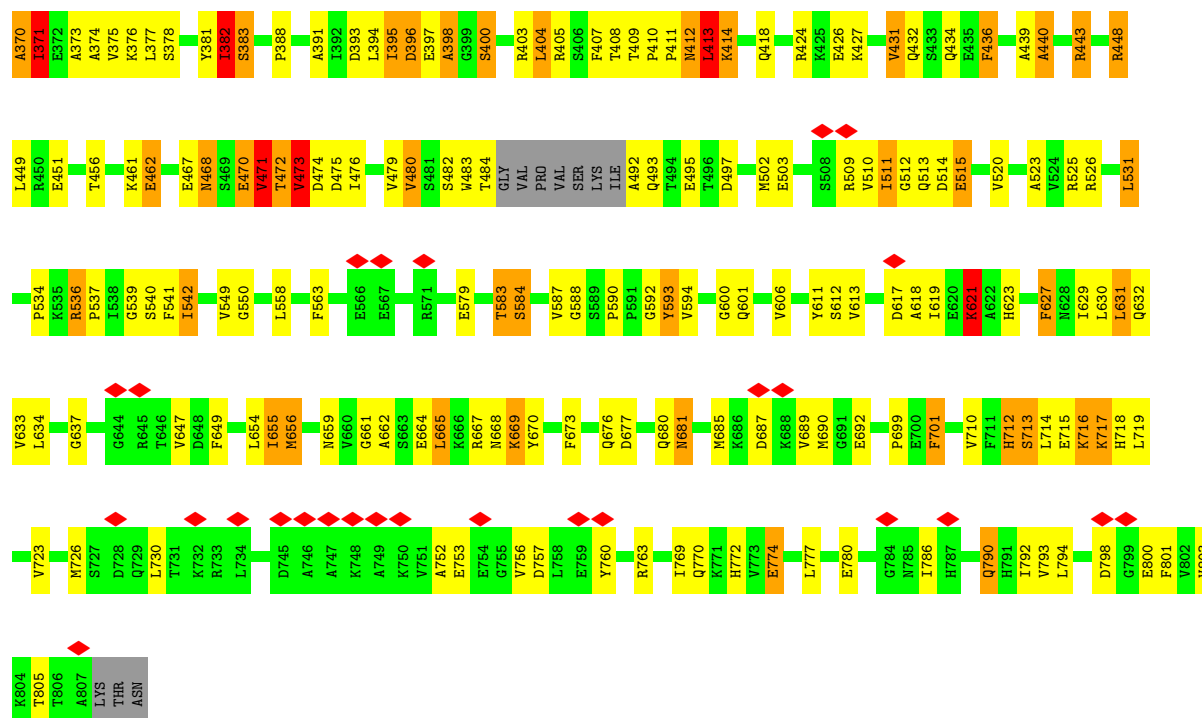




• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain F: 8% 60% 30% 7% ..





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36688	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)	1700	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	7.710	Depositor
Minimum map value	-4.936	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.999	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	1.35	0/791	1.77	20/1064 (1.9%)
1	2	1.36	0/791	1.79	20/1064 (1.9%)
1	3	1.36	1/791 (0.1%)	1.92	28/1064 (2.6%)
1	4	1.30	0/791	1.82	18/1064 (1.7%)
1	5	1.34	0/791	1.81	18/1064 (1.7%)
1	6	1.34	1/791 (0.1%)	1.74	15/1064 (1.4%)
2	A	1.37	8/6265 (0.1%)	1.89	195/8436 (2.3%)
2	B	1.35	3/6265 (0.0%)	1.86	164/8436 (1.9%)
2	C	1.37	5/6265 (0.1%)	1.86	181/8436 (2.1%)
2	D	1.37	4/6265 (0.1%)	1.87	188/8436 (2.2%)
2	E	1.38	2/6265 (0.0%)	1.90	172/8436 (2.0%)
2	F	1.36	6/6265 (0.1%)	1.86	166/8436 (2.0%)
All	All	1.36	30/42336 (0.1%)	1.86	1185/57000 (2.1%)

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	3
1	2	0	3
1	3	0	6
1	4	0	2
1	5	0	1
1	6	0	3
2	A	0	18
2	B	0	18
2	C	0	13
2	D	0	13
2	E	0	14
2	F	0	12
All	All	0	106

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	443	ARG	CA-C	-6.90	1.44	1.52
2	B	668	ASN	CA-C	-6.84	1.48	1.52
2	C	21	ALA	CA-C	-6.63	1.44	1.52
2	C	29	ILE	CA-C	-6.20	1.46	1.53
2	C	313	GLY	CA-C	-6.16	1.47	1.52
1	3	140	ILE	CA-C	-6.00	1.45	1.52
2	F	313	GLY	CA-C	-6.00	1.48	1.52
2	D	313	GLY	CA-C	-5.75	1.48	1.52
2	D	792	ILE	CA-C	-5.74	1.45	1.52
2	D	362	HIS	CA-C	-5.72	1.47	1.53
2	A	29	ILE	CA-C	-5.69	1.46	1.53
2	E	443	ARG	CA-C	-5.67	1.45	1.52
2	A	541	PHE	CA-C	-5.66	1.45	1.52
2	D	157	ASN	CA-C	-5.62	1.48	1.52
2	A	792	ILE	CA-C	-5.58	1.45	1.52
2	F	443	ARG	CA-C	-5.57	1.46	1.52
2	F	541	PHE	CA-C	-5.56	1.45	1.52
2	A	714	LEU	CA-C	-5.48	1.46	1.52
2	C	311	CYS	CA-C	-5.46	1.45	1.52
2	F	21	ALA	CA-C	-5.41	1.46	1.52
2	A	711	PHE	CA-C	-5.39	1.46	1.53
2	E	313	GLY	CA-C	-5.34	1.48	1.52
2	C	792	ILE	CA-C	-5.24	1.45	1.52
2	A	400	SER	N-CA	-5.17	1.39	1.46
2	A	313	GLY	CA-C	-5.14	1.48	1.52
2	B	313	GLY	CA-C	-5.13	1.48	1.52
2	B	541	PHE	CA-C	-5.13	1.46	1.52
1	6	166	ASP	CA-C	-5.08	1.47	1.53
2	F	713	SER	CA-C	-5.08	1.46	1.52
2	F	665	LEU	CA-C	-5.03	1.46	1.52

All (1185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	215	HIS	CA-CB-CG	10.82	124.62	113.80
2	E	536	ARG	N-CA-C	-10.72	98.53	108.07
2	E	79	HIS	N-CA-C	-10.38	94.45	109.18
2	E	780	GLU	N-CA-C	-10.34	101.21	114.04
1	4	140	ILE	N-CA-CB	10.30	121.94	110.51
1	3	215	HIS	CA-CB-CG	10.27	124.07	113.80
2	F	364	VAL	CA-C-N	10.14	139.96	121.70
2	F	364	VAL	C-N-CA	10.14	139.96	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	165	SER	CA-C-N	10.12	139.91	121.70
2	C	165	SER	C-N-CA	10.12	139.91	121.70
2	A	361	HIS	CA-CB-CG	-9.96	103.84	113.80
2	B	79	HIS	N-CA-C	-9.95	95.06	109.18
2	B	593	TYR	N-CA-C	9.79	123.17	111.33
2	E	439	ALA	N-CA-C	-9.78	99.92	112.93
2	B	165	SER	CA-C-N	9.77	139.28	121.70
2	B	165	SER	C-N-CA	9.77	139.28	121.70
2	E	396	ASP	N-CA-C	9.67	121.90	111.36
1	1	215	HIS	CA-CB-CG	9.62	123.42	113.80
2	F	780	GLU	N-CA-C	-9.61	102.13	114.04
2	E	165	SER	CA-C-N	9.57	138.93	121.70
2	E	165	SER	C-N-CA	9.57	138.93	121.70
2	F	510	VAL	CA-C-N	9.53	139.13	121.97
2	F	510	VAL	C-N-CA	9.53	139.13	121.97
2	A	165	SER	CA-C-N	9.44	138.70	121.70
2	A	165	SER	C-N-CA	9.44	138.70	121.70
2	E	711	PHE	CA-CB-CG	-9.31	104.49	113.80
2	D	212	VAL	N-CA-C	-9.20	103.96	112.43
2	E	364	VAL	CA-C-N	9.17	138.20	121.70
2	E	364	VAL	C-N-CA	9.17	138.20	121.70
2	E	739	LEU	CA-C-N	9.15	134.94	122.77
2	E	739	LEU	C-N-CA	9.15	134.94	122.77
2	B	364	VAL	CA-C-N	9.10	138.08	121.70
2	B	364	VAL	C-N-CA	9.10	138.08	121.70
2	F	165	SER	CA-C-N	8.98	137.87	121.70
2	F	165	SER	C-N-CA	8.98	137.87	121.70
1	4	215	HIS	CA-CB-CG	8.93	122.73	113.80
2	D	802	VAL	N-CA-C	-8.92	96.57	108.35
1	6	136	PHE	CA-CB-CG	-8.89	104.91	113.80
2	C	47	ALA	CA-C-N	8.84	131.93	120.44
2	C	47	ALA	C-N-CA	8.84	131.93	120.44
2	C	439	ALA	N-CA-C	-8.80	101.23	112.93
2	A	443	ARG	N-CA-CB	8.77	122.72	109.91
2	B	780	GLU	N-CA-C	-8.73	103.22	114.04
2	D	166	LEU	CA-C-N	8.69	137.34	121.70
2	D	166	LEU	C-N-CA	8.69	137.34	121.70
2	E	793	VAL	N-CA-C	-8.69	96.01	108.17
1	3	203	ILE	N-CA-C	-8.62	104.81	111.62
2	B	219	GLU	CA-C-N	8.60	129.71	119.99
2	B	219	GLU	C-N-CA	8.60	129.71	119.99
2	A	47	ALA	CA-C-N	8.60	131.62	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	47	ALA	C-N-CA	8.60	131.62	120.44
2	C	669	LYS	N-CA-C	-8.44	92.82	110.80
2	D	364	VAL	CA-C-N	8.41	136.84	121.70
2	D	364	VAL	C-N-CA	8.41	136.84	121.70
2	E	669	LYS	CA-C-N	8.40	137.59	121.54
2	E	669	LYS	C-N-CA	8.40	137.59	121.54
2	D	439	ALA	N-CA-C	-8.35	101.82	112.93
2	B	47	ALA	CA-C-N	8.34	131.29	120.44
2	B	47	ALA	C-N-CA	8.34	131.29	120.44
2	B	718	HIS	CA-C-N	8.33	132.37	120.79
2	B	718	HIS	C-N-CA	8.33	132.37	120.79
2	E	590	PRO	N-CA-C	8.27	120.79	110.70
2	A	439	ALA	N-CA-C	-8.24	101.97	112.93
2	F	141	LEU	N-CA-C	-8.22	100.57	110.44
2	B	448	ARG	CA-C-N	8.20	131.60	120.54
2	B	448	ARG	C-N-CA	8.20	131.60	120.54
2	A	212	VAL	N-CA-C	-8.15	105.38	113.20
2	C	593	TYR	N-CA-C	8.13	121.17	111.33
2	C	666	LYS	N-CA-C	-8.10	103.60	113.97
2	D	47	ALA	CA-C-N	8.08	130.95	120.44
2	D	47	ALA	C-N-CA	8.08	130.95	120.44
2	E	802	VAL	N-CA-C	-8.08	97.68	108.35
2	F	257	PHE	CA-CB-CG	8.06	121.86	113.80
2	B	439	ALA	N-CA-C	-8.00	102.29	112.93
2	A	802	VAL	N-CA-C	-7.96	97.84	108.35
2	E	393	ASP	CA-CB-CG	7.94	120.54	112.60
2	B	802	VAL	N-CA-C	-7.93	97.41	108.27
2	C	364	VAL	CA-C-N	7.84	135.81	121.70
2	C	364	VAL	C-N-CA	7.84	135.81	121.70
2	C	382	ILE	CA-C-N	7.83	135.80	121.70
2	C	382	ILE	C-N-CA	7.83	135.80	121.70
2	B	711	PHE	CA-CB-CG	-7.79	106.01	113.80
2	D	234	LEU	N-CA-C	-7.75	103.39	112.92
2	E	105	THR	CA-C-N	7.75	130.51	120.44
2	E	105	THR	C-N-CA	7.75	130.51	120.44
2	F	396	ASP	CA-CB-CG	-7.74	104.86	112.60
2	B	203	ASN	CB-CA-C	-7.73	101.26	110.15
2	C	594	VAL	CA-C-N	7.72	129.80	120.14
2	C	594	VAL	C-N-CA	7.72	129.80	120.14
2	E	660	VAL	N-CA-C	-7.72	104.39	113.42
1	5	142	LEU	N-CA-C	7.72	120.67	111.33
2	A	296	ALA	CA-C-N	7.71	131.64	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	296	ALA	C-N-CA	7.71	131.64	120.38
2	D	448	ARG	CA-C-N	7.70	131.50	120.79
2	D	448	ARG	C-N-CA	7.70	131.50	120.79
2	D	310	GLN	N-CA-C	-7.67	96.79	108.67
2	E	601	GLN	N-CA-C	7.66	119.31	110.97
2	C	780	GLU	N-CA-C	-7.64	104.56	114.04
2	D	165	SER	CA-C-N	7.64	135.46	121.70
2	D	165	SER	C-N-CA	7.64	135.46	121.70
2	C	310	GLN	N-CA-C	-7.64	96.07	108.52
2	C	368	ASP	CA-C-N	7.63	131.53	120.38
2	C	368	ASP	C-N-CA	7.63	131.53	120.38
2	B	270	GLN	CA-C-N	7.62	136.09	121.54
2	B	270	GLN	C-N-CA	7.62	136.09	121.54
2	B	382	ILE	CA-C-N	7.60	135.38	121.70
2	B	382	ILE	C-N-CA	7.60	135.38	121.70
2	F	395	ILE	CB-CA-C	-7.56	102.02	111.70
2	A	710	VAL	N-CA-C	-7.54	97.62	108.17
2	F	296	ALA	CA-C-N	7.54	131.38	120.38
2	F	296	ALA	C-N-CA	7.54	131.38	120.38
2	E	397	GLU	N-CA-CB	7.52	121.15	109.94
2	F	47	ALA	CA-C-N	7.47	130.16	120.44
2	F	47	ALA	C-N-CA	7.47	130.16	120.44
2	E	594	VAL	CA-C-N	7.46	128.26	119.98
2	E	594	VAL	C-N-CA	7.46	128.26	119.98
2	A	780	GLU	N-CA-C	-7.45	104.80	114.04
2	C	407	PHE	CA-CB-CG	-7.45	106.35	113.80
2	C	673	PHE	N-CA-C	-7.44	103.28	113.18
2	A	219	GLU	CA-C-N	7.43	128.39	119.99
2	A	219	GLU	C-N-CA	7.43	128.39	119.99
2	C	222	ALA	CA-C-N	7.42	130.22	120.28
2	C	222	ALA	C-N-CA	7.42	130.22	120.28
2	B	102	TYR	CA-C-N	7.41	130.65	120.35
2	B	102	TYR	C-N-CA	7.41	130.65	120.35
2	B	364	VAL	N-CA-C	-7.37	97.96	108.65
2	A	331	GLU	N-CA-C	-7.36	106.23	114.62
2	D	780	GLU	N-CA-C	-7.36	104.91	114.04
1	2	201	LYS	CA-C-N	7.34	131.83	120.75
1	2	201	LYS	C-N-CA	7.34	131.83	120.75
2	D	480	VAL	N-CA-C	-7.34	103.31	110.72
2	B	105	THR	CA-C-N	7.33	130.33	120.65
2	B	105	THR	C-N-CA	7.33	130.33	120.65
2	E	400	SER	CA-C-N	7.32	131.81	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	400	SER	C-N-CA	7.32	131.81	120.82
2	A	28	ASN	N-CA-C	-7.31	96.99	108.90
2	F	364	VAL	N-CA-C	-7.31	94.14	109.34
2	C	350	ILE	CA-C-N	7.29	130.93	120.79
2	C	350	ILE	C-N-CA	7.29	130.93	120.79
2	C	21	ALA	CB-CA-C	-7.28	99.35	110.92
2	E	396	ASP	CA-CB-CG	-7.28	105.33	112.60
2	D	110	LEU	CA-C-N	7.27	128.05	119.98
2	D	110	LEU	C-N-CA	7.27	128.05	119.98
2	B	331	GLU	N-CA-C	-7.22	105.65	114.75
2	E	718	HIS	CA-CB-CG	7.21	121.01	113.80
2	B	414	LYS	CA-C-N	7.20	130.52	120.29
2	B	414	LYS	C-N-CA	7.20	130.52	120.29
2	A	105	THR	CA-C-N	7.20	129.80	120.44
2	A	105	THR	C-N-CA	7.20	129.80	120.44
2	F	656	MET	N-CA-C	-7.20	97.48	109.07
2	D	408	THR	N-CA-C	-7.18	102.86	111.69
2	F	509	ARG	N-CA-C	-7.18	105.45	114.56
2	D	384	ASP	N-CA-C	-7.17	103.54	114.16
1	3	216	PHE	CA-CB-CG	7.15	120.95	113.80
2	F	439	ALA	N-CA-C	-7.15	103.42	112.93
2	F	584	SER	N-CA-C	-7.14	104.20	114.12
2	E	332	ARG	N-CA-C	-7.11	101.78	110.88
2	B	474	ASP	CA-C-N	7.08	129.65	120.44
2	B	474	ASP	C-N-CA	7.08	129.65	120.44
2	D	378	SER	CA-C-N	7.07	129.75	120.28
2	D	378	SER	C-N-CA	7.07	129.75	120.28
2	A	310	GLN	N-CA-C	-7.06	98.53	109.76
2	C	219	GLU	CA-C-N	7.06	127.96	119.99
2	C	219	GLU	C-N-CA	7.06	127.96	119.99
2	D	219	GLU	CA-C-N	7.05	127.95	119.99
2	D	219	GLU	C-N-CA	7.05	127.95	119.99
2	C	677	ASP	N-CA-C	-7.04	104.49	113.23
2	B	578	MET	N-CA-C	-7.03	103.89	113.30
2	D	462	GLU	N-CA-C	-7.01	103.39	112.23
2	A	542	ILE	N-CA-C	-7.01	98.39	108.48
2	A	270	GLN	CA-C-N	6.98	134.88	121.54
2	A	270	GLN	C-N-CA	6.98	134.88	121.54
2	F	212	VAL	N-CA-C	-6.98	104.63	113.22
2	B	296	ALA	CA-C-N	6.97	130.56	120.38
2	B	296	ALA	C-N-CA	6.97	130.56	120.38
2	C	670	TYR	N-CA-C	6.97	120.84	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	593	TYR	N-CA-C	6.97	119.76	111.33
2	A	204	PRO	N-CA-C	-6.96	100.05	111.68
2	C	448	ARG	CA-C-N	6.96	129.94	120.54
2	C	448	ARG	C-N-CA	6.96	129.94	120.54
2	C	141	LEU	N-CA-C	-6.95	100.02	109.54
2	A	711	PHE	CA-CB-CG	-6.95	106.85	113.80
2	F	178	SER	N-CA-C	-6.95	104.42	113.17
2	E	453	VAL	N-CA-CB	6.93	117.90	110.62
2	C	178	SER	N-CA-C	-6.93	104.44	113.17
2	A	110	LEU	CA-C-N	6.92	128.79	120.14
2	A	110	LEU	C-N-CA	6.92	128.79	120.14
2	D	292	GLY	O-C-N	6.92	125.73	121.85
2	A	448	ARG	CA-C-N	6.92	130.41	120.79
2	A	448	ARG	C-N-CA	6.92	130.41	120.79
2	F	434	GLN	CA-C-N	6.92	134.15	121.70
2	F	434	GLN	C-N-CA	6.92	134.15	121.70
2	A	535	LYS	N-CA-C	-6.91	102.97	111.40
2	A	44	GLY	N-CA-C	-6.87	103.74	112.54
2	F	448	ARG	CA-C-N	6.87	129.82	120.54
2	F	448	ARG	C-N-CA	6.87	129.82	120.54
2	E	451	GLU	CA-C-N	6.87	129.48	120.28
2	E	451	GLU	C-N-CA	6.87	129.48	120.28
2	F	113	ILE	CA-C-N	6.86	129.80	120.54
2	F	113	ILE	C-N-CA	6.86	129.80	120.54
2	E	235	ARG	N-CA-C	-6.86	99.18	109.94
2	D	113	ILE	CA-C-N	6.85	129.79	120.54
2	D	113	ILE	C-N-CA	6.85	129.79	120.54
2	D	222	ALA	CA-C-N	6.85	129.46	120.28
2	D	222	ALA	C-N-CA	6.85	129.46	120.28
2	E	792	ILE	N-CA-C	-6.85	97.75	107.75
2	C	44	GLY	N-CA-C	-6.85	103.78	112.54
2	A	393	ASP	CA-CB-CG	6.82	119.42	112.60
1	6	201	LYS	CA-C-N	6.81	131.03	120.75
1	6	201	LYS	C-N-CA	6.81	131.03	120.75
2	F	451	GLU	CA-C-N	6.80	129.28	120.44
2	F	451	GLU	C-N-CA	6.80	129.28	120.44
2	B	212	VAL	N-CA-C	-6.80	106.68	113.20
2	E	405	ARG	CA-C-N	6.79	129.27	120.44
2	E	405	ARG	C-N-CA	6.79	129.27	120.44
2	C	383	SER	N-CA-CB	6.79	122.04	110.50
2	C	365	SER	CA-C-N	6.78	134.18	121.97
2	C	365	SER	C-N-CA	6.78	134.18	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	234	LEU	N-CA-C	-6.76	105.03	113.28
2	A	222	ALA	CA-C-N	6.75	129.32	120.28
2	A	222	ALA	C-N-CA	6.75	129.32	120.28
2	E	590	PRO	CA-C-O	-6.74	110.78	120.56
2	C	803	VAL	N-CA-C	-6.74	98.74	108.17
2	C	590	PRO	CA-C-O	-6.71	110.83	120.56
2	E	270	GLN	CA-C-N	6.71	134.35	121.54
2	E	270	GLN	C-N-CA	6.71	134.35	121.54
2	E	355	ARG	CA-C-N	6.69	131.41	120.63
2	E	355	ARG	C-N-CA	6.69	131.41	120.63
2	E	296	ALA	CA-C-N	6.69	130.14	120.38
2	E	296	ALA	C-N-CA	6.69	130.14	120.38
2	F	376	LYS	N-CA-C	6.68	119.12	111.11
1	3	138	ASP	CA-CB-CG	-6.67	105.92	112.60
2	A	395	ILE	N-CA-CB	6.67	117.63	110.62
2	D	296	ALA	CA-C-N	6.66	130.11	120.38
2	D	296	ALA	C-N-CA	6.66	130.11	120.38
2	B	78	ILE	N-CA-CB	6.66	118.59	111.46
2	A	594	VAL	CA-C-N	6.66	128.46	120.14
2	A	594	VAL	C-N-CA	6.66	128.46	120.14
2	F	774	GLU	CA-C-N	6.66	129.50	120.38
2	F	774	GLU	C-N-CA	6.66	129.50	120.38
2	F	443	ARG	N-CA-CB	6.66	119.63	109.91
1	3	201	LYS	CA-C-N	6.65	130.78	120.75
1	3	201	LYS	C-N-CA	6.65	130.78	120.75
2	C	330	LEU	N-CA-C	-6.64	103.77	112.41
2	C	802	VAL	N-CA-C	-6.64	99.17	108.27
2	D	362	HIS	CA-CB-CG	-6.64	107.16	113.80
2	D	526	ARG	CA-C-N	6.63	129.16	120.28
2	D	526	ARG	C-N-CA	6.63	129.16	120.28
2	C	364	VAL	N-CA-C	-6.63	98.94	108.42
2	F	536	ARG	N-CA-C	-6.62	101.73	110.40
2	D	711	PHE	N-CA-C	-6.61	98.47	109.24
2	E	669	LYS	N-CA-C	-6.60	96.74	110.80
2	C	656	MET	N-CA-C	-6.60	98.45	109.07
2	D	542	ILE	N-CA-C	-6.59	98.98	108.48
2	A	443	ARG	CB-CA-C	-6.59	100.82	110.96
2	D	214	LYS	CA-C-N	6.58	131.23	120.63
2	D	214	LYS	C-N-CA	6.58	131.23	120.63
2	B	178	SER	N-CA-C	-6.58	104.88	113.17
2	C	804	LYS	N-CA-C	-6.58	99.45	109.85
2	C	542	ILE	N-CA-C	-6.56	99.03	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	93	ASP	CA-CB-CG	-6.55	106.05	112.60
2	D	527	ALA	N-CA-C	6.55	118.42	111.28
2	D	674	ASN	N-CA-C	-6.55	99.11	109.07
2	C	774	GLU	CA-C-N	6.54	129.34	120.38
2	C	774	GLU	C-N-CA	6.54	129.34	120.38
2	E	448	ARG	CA-C-N	6.54	129.88	120.79
2	E	448	ARG	C-N-CA	6.54	129.88	120.79
2	E	101	SER	N-CA-C	-6.53	105.13	113.23
2	F	270	GLN	CA-C-N	6.53	134.01	121.54
2	F	270	GLN	C-N-CA	6.53	134.01	121.54
2	A	539	GLY	N-CA-C	-6.53	97.72	113.18
2	F	482	SER	N-CA-C	6.52	118.05	111.07
2	D	404	LEU	N-CA-C	-6.52	102.66	112.04
2	D	536	ARG	N-CA-C	-6.52	95.41	109.81
2	F	594	VAL	CA-C-N	6.52	127.22	119.98
2	F	594	VAL	C-N-CA	6.52	127.22	119.98
2	A	601	GLN	N-CA-C	6.52	118.07	110.97
2	A	201	LYS	N-CA-C	-6.51	100.84	110.48
2	B	581	HIS	N-CA-C	-6.51	102.47	110.61
2	E	7	THR	CA-C-N	6.50	129.82	120.79
2	E	7	THR	C-N-CA	6.50	129.82	120.79
2	E	462	GLU	N-CA-C	-6.50	103.70	111.69
2	C	479	VAL	N-CA-CB	6.49	119.37	110.54
2	B	29	ILE	CA-C-N	6.49	127.51	120.44
2	B	29	ILE	C-N-CA	6.49	127.51	120.44
2	C	639	LEU	N-CA-C	-6.49	99.25	109.50
2	F	471	VAL	CA-C-N	6.48	133.92	121.54
2	F	471	VAL	C-N-CA	6.48	133.92	121.54
2	F	413	LEU	CA-C-N	6.47	129.60	120.28
2	F	413	LEU	C-N-CA	6.47	129.60	120.28
1	4	140	ILE	CB-CA-C	-6.47	103.60	111.88
2	B	398	ALA	CA-C-N	6.47	134.08	121.41
2	B	398	ALA	C-N-CA	6.47	134.08	121.41
2	B	31	THR	CA-C-N	6.46	129.59	120.28
2	B	31	THR	C-N-CA	6.46	129.59	120.28
2	E	676	GLN	N-CA-C	-6.45	104.55	112.88
2	E	476	ILE	CA-C-N	6.45	128.92	120.28
2	E	476	ILE	C-N-CA	6.45	128.92	120.28
2	B	551	LYS	CA-C-N	6.44	129.23	120.54
2	B	551	LYS	C-N-CA	6.44	129.23	120.54
2	A	405	ARG	CA-C-N	6.43	128.80	120.44
2	A	405	ARG	C-N-CA	6.43	128.80	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	330	LEU	N-CA-C	-6.43	105.01	112.92
2	A	540	SER	N-CA-C	-6.42	99.73	109.95
2	C	467	GLU	CA-C-N	6.42	133.80	121.54
2	C	467	GLU	C-N-CA	6.42	133.80	121.54
2	A	382	ILE	CA-C-N	6.41	133.24	121.70
2	A	382	ILE	C-N-CA	6.41	133.24	121.70
2	D	355	ARG	CA-C-N	6.41	130.95	120.63
2	D	355	ARG	C-N-CA	6.41	130.95	120.63
2	E	412	ASN	CA-C-N	6.41	133.78	121.54
2	E	412	ASN	C-N-CA	6.41	133.78	121.54
2	B	803	VAL	N-CA-C	-6.41	98.51	107.80
2	F	542	ILE	N-CA-C	-6.40	99.26	108.48
2	B	682	HIS	CA-CB-CG	-6.40	107.40	113.80
2	D	468	ASN	CA-CB-CG	-6.40	106.20	112.60
2	D	358	TYR	N-CA-CB	6.40	120.31	110.46
2	A	637	GLY	N-CA-C	-6.39	105.87	115.32
2	C	296	ALA	CA-C-N	6.39	129.71	120.38
2	C	296	ALA	C-N-CA	6.39	129.71	120.38
2	C	796	VAL	N-CA-C	-6.37	99.29	108.53
2	D	637	GLY	N-CA-C	-6.37	106.45	115.43
2	E	593	TYR	N-CA-C	6.37	118.22	111.28
2	A	235	ARG	N-CA-C	-6.37	102.74	112.99
2	E	692	GLU	CA-C-N	6.37	129.29	120.63
2	E	692	GLU	C-N-CA	6.37	129.29	120.63
2	B	310	GLN	N-CA-C	-6.37	97.28	108.23
1	5	138	ASP	CA-CB-CG	-6.36	106.24	112.60
2	C	104	GLY	CA-C-N	6.36	129.09	120.38
2	C	104	GLY	C-N-CA	6.36	129.09	120.38
2	B	594	VAL	CA-C-N	6.34	127.02	119.98
2	B	594	VAL	C-N-CA	6.34	127.02	119.98
1	5	139	VAL	CB-CA-C	-6.33	103.49	112.22
2	A	210	PRO	CA-C-N	6.33	133.09	121.70
2	A	210	PRO	C-N-CA	6.33	133.09	121.70
2	F	540	SER	N-CA-C	-6.32	99.90	109.95
2	E	110	LEU	CA-C-N	6.32	128.04	120.14
2	E	110	LEU	C-N-CA	6.32	128.04	120.14
2	A	126	ASN	N-CA-C	-6.31	105.23	113.12
2	B	680	GLN	N-CA-C	-6.31	105.35	114.12
1	3	180	SER	CA-C-N	6.30	128.73	120.60
1	3	180	SER	C-N-CA	6.30	128.73	120.60
1	5	172	ASP	N-CA-C	6.29	117.80	111.07
2	C	667	ARG	N-CA-C	-6.29	100.26	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	332	ARG	N-CA-C	-6.28	103.80	112.03
2	C	509	ARG	N-CA-C	-6.28	106.25	114.04
2	F	351	LEU	CA-C-N	6.27	128.97	120.38
2	F	351	LEU	C-N-CA	6.27	128.97	120.38
2	E	426	GLU	CA-C-N	6.27	129.50	120.79
2	E	426	GLU	C-N-CA	6.27	129.50	120.79
1	4	138	ASP	CA-CB-CG	-6.27	106.33	112.60
2	A	395	ILE	CB-CA-C	-6.26	103.69	111.70
2	C	563	PHE	N-CA-C	-6.25	106.25	114.31
2	B	476	ILE	CB-CA-C	-6.25	103.84	112.02
2	B	796	VAL	N-CA-C	-6.25	99.47	108.53
1	6	139	VAL	CA-C-N	6.24	128.65	120.60
1	6	139	VAL	C-N-CA	6.24	128.65	120.60
2	B	198	ARG	CD-NE-CZ	-6.24	115.67	124.40
2	C	722	ILE	N-CA-CB	6.24	119.50	110.52
2	F	431	VAL	CB-CA-C	-6.24	102.49	112.16
2	C	26	HIS	CA-C-N	6.23	128.95	120.54
2	C	26	HIS	C-N-CA	6.23	128.95	120.54
2	B	166	LEU	N-CA-CB	6.23	121.09	110.50
2	D	693	LEU	CA-C-N	6.23	129.47	120.38
2	D	693	LEU	C-N-CA	6.23	129.47	120.38
2	B	364	VAL	O-C-N	-6.22	116.04	122.95
2	B	176	GLU	N-CA-C	-6.22	106.01	113.97
2	F	692	GLU	N-CA-C	-6.22	105.52	113.23
2	B	793	VAL	N-CA-C	-6.20	99.48	108.17
2	A	364	VAL	N-CA-C	-6.20	96.44	109.34
2	A	692	GLU	CA-C-N	6.20	129.06	120.63
2	A	692	GLU	C-N-CA	6.20	129.06	120.63
2	A	232	GLU	N-CA-C	6.20	117.70	111.07
2	A	371	ILE	CB-CA-C	-6.19	103.77	111.70
2	A	336	PRO	N-CA-C	-6.19	99.72	112.47
2	F	793	VAL	N-CA-C	-6.19	99.50	108.17
2	F	405	ARG	CA-C-N	6.19	128.49	120.44
2	F	405	ARG	C-N-CA	6.19	128.49	120.44
2	C	404	LEU	N-CA-C	-6.18	103.13	112.04
2	D	563	PHE	N-CA-C	-6.18	106.33	114.31
2	B	234	LEU	N-CA-C	-6.17	105.06	112.59
2	D	364	VAL	N-CA-C	-6.17	99.59	108.42
1	1	136	PHE	CA-CB-CG	-6.17	107.63	113.80
2	A	28	ASN	CA-CB-CG	-6.17	106.43	112.60
1	3	139	VAL	CA-C-N	6.17	128.56	120.60
1	3	139	VAL	C-N-CA	6.17	128.56	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	393	ASP	CB-CA-C	-6.17	100.37	110.85
2	E	411	PRO	CA-C-N	6.17	133.32	121.54
2	E	411	PRO	C-N-CA	6.17	133.32	121.54
2	A	659	ASN	N-CA-C	-6.16	103.18	111.87
2	D	593	TYR	N-CA-C	6.16	117.99	111.28
2	E	700	GLU	CA-C-N	6.15	129.00	120.63
2	E	700	GLU	C-N-CA	6.15	129.00	120.63
2	F	563	PHE	N-CA-C	-6.15	106.38	114.31
1	1	139	VAL	CB-CA-C	-6.15	103.97	112.02
2	C	451	GLU	CA-C-N	6.15	128.43	120.44
2	C	451	GLU	C-N-CA	6.15	128.43	120.44
2	A	107	HIS	CA-CB-CG	-6.14	107.66	113.80
2	F	222	ALA	CA-C-N	6.14	128.51	120.28
2	F	222	ALA	C-N-CA	6.14	128.51	120.28
2	F	398	ALA	CA-C-N	6.14	133.45	121.41
2	F	398	ALA	C-N-CA	6.14	133.45	121.41
2	D	82	PRO	CA-C-N	6.14	128.75	120.65
2	D	82	PRO	C-N-CA	6.14	128.75	120.65
1	1	201	LYS	CA-C-N	6.13	129.41	120.71
1	1	201	LYS	C-N-CA	6.13	129.41	120.71
2	A	408	THR	N-CA-C	-6.13	105.75	113.72
2	D	393	ASP	CB-CA-C	-6.13	100.43	110.85
2	B	113	ILE	CA-C-N	6.13	128.81	120.54
2	B	113	ILE	C-N-CA	6.13	128.81	120.54
2	F	407	PHE	CA-CB-CG	-6.13	107.67	113.80
2	F	443	ARG	CB-CA-C	-6.12	101.53	110.96
2	A	479	VAL	N-CA-CB	6.11	118.85	110.54
2	C	323	TYR	CB-CA-C	-6.11	98.26	110.42
2	A	26	HIS	CA-C-N	6.10	128.46	120.28
2	A	26	HIS	C-N-CA	6.10	128.46	120.28
2	E	309	LEU	N-CA-C	-6.10	102.97	110.65
2	B	792	ILE	CB-CA-C	-6.09	102.12	110.77
2	E	739	LEU	N-CA-C	6.09	123.78	110.80
2	C	126	ASN	N-CA-C	-6.09	105.51	113.12
1	2	156	SER	N-CA-C	-6.07	99.00	108.90
2	B	718	HIS	N-CA-C	-6.07	104.02	112.45
2	C	539	GLY	N-CA-C	-6.07	98.80	113.18
2	F	110	LEU	CA-C-N	6.06	127.72	120.14
2	F	110	LEU	C-N-CA	6.06	127.72	120.14
2	B	7	THR	CA-C-N	6.05	129.20	120.79
2	B	7	THR	C-N-CA	6.05	129.20	120.79
2	D	332	ARG	N-CA-C	-6.05	104.55	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	414	LYS	CA-C-N	6.05	128.88	120.29
2	A	414	LYS	C-N-CA	6.05	128.88	120.29
2	E	551	LYS	CA-C-N	6.04	128.69	120.54
2	E	551	LYS	C-N-CA	6.04	128.69	120.54
2	E	382	ILE	CA-C-N	6.04	132.57	121.70
2	E	382	ILE	C-N-CA	6.04	132.57	121.70
2	A	101	SER	N-CA-C	-6.04	105.57	113.17
2	E	47	ALA	CA-C-N	6.04	128.29	120.44
2	E	47	ALA	C-N-CA	6.04	128.29	120.44
2	E	360	ALA	N-CA-C	-6.04	104.78	111.36
2	C	540	SER	N-CA-C	-6.03	100.36	109.95
2	D	590	PRO	N-CA-C	6.03	118.05	110.70
2	B	692	GLU	CA-C-N	6.02	128.82	120.63
2	B	692	GLU	C-N-CA	6.02	128.82	120.63
2	B	364	VAL	CB-CA-C	6.01	119.96	110.52
2	D	75	SER	CA-C-N	6.01	133.03	121.54
2	D	75	SER	C-N-CA	6.01	133.03	121.54
2	D	36	LEU	CA-C-N	6.01	126.65	119.98
2	D	36	LEU	C-N-CA	6.01	126.65	119.98
2	F	214	LYS	CA-C-N	6.00	130.30	120.63
2	F	214	LYS	C-N-CA	6.00	130.30	120.63
2	B	520	VAL	CB-CA-C	-6.00	104.28	111.97
2	D	368	ASP	CA-C-N	6.00	129.14	120.38
2	D	368	ASP	C-N-CA	6.00	129.14	120.38
2	C	718	HIS	CA-CB-CG	6.00	119.80	113.80
2	D	460	TRP	CB-CA-C	6.00	119.48	111.14
2	B	461	LYS	N-CA-C	-5.99	105.97	113.28
2	D	167	ALA	N-CA-CB	5.99	119.39	110.40
2	D	270	GLN	CA-C-N	5.99	132.98	121.54
2	D	270	GLN	C-N-CA	5.99	132.98	121.54
2	D	660	VAL	N-CA-C	-5.99	106.90	113.43
2	F	699	PRO	CA-C-N	5.98	128.30	120.28
2	F	699	PRO	C-N-CA	5.98	128.30	120.28
2	B	482	SER	N-CA-C	5.98	117.47	111.07
2	E	774	GLU	CA-C-N	5.97	128.56	120.38
2	E	774	GLU	C-N-CA	5.97	128.56	120.38
1	6	175	VAL	N-CA-C	-5.96	105.04	110.82
2	C	316	THR	CA-C-N	5.96	129.76	120.82
2	C	316	THR	C-N-CA	5.96	129.76	120.82
2	C	687	ASP	CA-C-N	5.95	130.11	120.60
2	C	687	ASP	C-N-CA	5.95	130.11	120.60
2	F	473	VAL	CA-C-N	5.95	128.53	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	473	VAL	C-N-CA	5.95	128.53	120.38
2	B	471	VAL	CA-C-N	5.94	132.89	121.54
2	B	471	VAL	C-N-CA	5.94	132.89	121.54
2	E	384	ASP	CA-CB-CG	5.94	118.54	112.60
2	C	7	THR	CA-C-N	5.94	129.05	120.79
2	C	7	THR	C-N-CA	5.94	129.05	120.79
2	E	310	GLN	N-CA-C	-5.94	99.47	108.67
2	C	292	GLY	N-CA-C	-5.93	106.40	115.66
2	E	639	LEU	N-CA-C	-5.93	100.04	109.23
2	D	341	GLN	CA-C-N	5.93	127.25	119.84
2	D	341	GLN	C-N-CA	5.93	127.25	119.84
2	A	200	THR	N-CA-CB	5.92	119.37	110.19
2	A	680	GLN	N-CA-C	-5.92	105.89	114.12
1	5	216	PHE	N-CA-CB	5.92	120.49	110.49
2	A	96	ARG	CA-C-N	5.91	128.69	120.29
2	A	96	ARG	C-N-CA	5.91	128.69	120.29
2	E	619	ILE	CA-C-N	5.91	128.12	120.44
2	E	619	ILE	C-N-CA	5.91	128.12	120.44
1	5	216	PHE	CA-CB-CG	5.90	119.70	113.80
2	A	79	HIS	N-CA-C	-5.90	100.80	109.18
2	D	601	GLN	N-CA-C	5.90	117.40	110.97
2	B	308	GLU	N-CA-C	-5.89	104.22	111.40
2	C	361	HIS	N-CA-C	-5.89	106.64	113.88
2	E	471	VAL	N-CA-C	-5.88	97.10	109.34
2	F	28	ASN	N-CA-C	-5.88	99.31	108.90
2	B	126	ASN	N-CA-C	-5.88	105.77	113.12
2	F	330	LEU	N-CA-C	-5.88	105.29	112.88
2	E	141	LEU	N-CA-C	-5.88	105.70	114.64
2	C	270	GLN	CA-C-N	5.88	132.77	121.54
2	C	270	GLN	C-N-CA	5.88	132.77	121.54
2	E	72	GLN	N-CA-CB	5.88	120.42	110.49
2	B	542	ILE	N-CA-C	-5.87	100.03	108.48
1	4	196	LEU	CA-C-N	5.86	128.41	120.38
1	4	196	LEU	C-N-CA	5.86	128.41	120.38
2	E	637	GLY	N-CA-C	-5.86	107.16	115.43
2	F	404	LEU	N-CA-C	-5.86	103.60	112.04
1	4	161	TYR	CA-CB-CG	-5.86	103.35	113.90
2	A	197	SER	N-CA-C	-5.86	104.52	112.26
2	E	71	GLY	CA-C-N	5.85	132.72	121.54
2	E	71	GLY	C-N-CA	5.85	132.72	121.54
2	C	34	ILE	CA-C-N	5.85	128.05	120.44
2	C	34	ILE	C-N-CA	5.85	128.05	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	44	GLY	N-CA-C	-5.85	105.05	112.54
2	F	318	ASP	N-CA-C	-5.85	105.81	113.12
2	C	244	MET	CA-C-N	5.84	126.46	119.98
2	C	244	MET	C-N-CA	5.84	126.46	119.98
1	1	172	ASP	N-CA-C	5.83	117.31	111.07
2	F	137	GLN	N-CA-C	5.83	118.11	111.11
2	C	551	LYS	CA-C-N	5.83	128.41	120.54
2	C	551	LYS	C-N-CA	5.83	128.41	120.54
2	F	701	PHE	CA-C-N	5.83	130.60	120.86
2	F	701	PHE	C-N-CA	5.83	130.60	120.86
1	2	142	LEU	N-CA-C	5.83	118.38	111.33
2	B	434	GLN	CA-C-N	5.82	132.17	121.70
2	B	434	GLN	C-N-CA	5.82	132.17	121.70
1	4	201	LYS	CA-C-N	5.81	128.97	120.71
1	4	201	LYS	C-N-CA	5.81	128.97	120.71
1	5	139	VAL	N-CA-CB	5.81	119.30	110.58
2	B	5	ARG	N-CA-C	-5.81	97.70	107.99
2	A	74	MET	CA-C-N	5.81	130.60	122.36
2	A	74	MET	C-N-CA	5.81	130.60	122.36
2	C	323	TYR	N-CA-CB	5.81	120.30	110.49
2	F	479	VAL	N-CA-CB	5.80	118.43	110.54
2	A	551	LYS	CA-C-N	5.80	128.37	120.54
2	A	551	LYS	C-N-CA	5.80	128.37	120.54
1	2	178	GLN	CA-C-N	5.79	128.62	120.28
1	2	178	GLN	C-N-CA	5.79	128.62	120.28
2	C	434	GLN	CA-C-N	5.79	132.13	121.70
2	C	434	GLN	C-N-CA	5.79	132.13	121.70
2	C	106	GLU	CA-C-N	5.79	128.84	120.38
2	C	106	GLU	C-N-CA	5.79	128.84	120.38
2	B	90	LEU	CA-C-N	5.79	128.31	120.38
2	B	90	LEU	C-N-CA	5.79	128.31	120.38
2	C	376	LYS	N-CA-C	5.79	118.06	111.11
2	D	447	GLN	N-CA-C	5.79	118.36	111.71
2	E	680	GLN	N-CA-C	-5.78	106.08	114.12
2	F	120	ALA	CB-CA-C	-5.78	101.72	110.92
2	D	358	TYR	CA-CB-CG	5.78	124.31	113.90
2	D	471	VAL	CA-C-N	5.78	132.58	121.54
2	D	471	VAL	C-N-CA	5.78	132.58	121.54
2	F	316	THR	CA-C-N	5.77	129.48	120.82
2	F	316	THR	C-N-CA	5.77	129.48	120.82
2	F	370	ALA	CA-C-N	5.77	128.33	120.77
2	F	370	ALA	C-N-CA	5.77	128.33	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	175	VAL	N-CA-C	-5.77	105.22	110.82
2	A	451	GLU	CA-C-N	5.77	127.94	120.44
2	A	451	GLU	C-N-CA	5.77	127.94	120.44
2	D	351	LEU	CA-C-N	5.76	128.27	120.38
2	D	351	LEU	C-N-CA	5.76	128.27	120.38
2	E	629	ILE	N-CA-C	-5.76	105.23	110.82
2	D	805	THR	N-CA-C	-5.76	100.40	109.50
2	C	637	GLY	N-CA-C	-5.75	106.81	115.32
2	A	337	ILE	CA-C-N	5.75	130.06	122.30
2	A	337	ILE	C-N-CA	5.75	130.06	122.30
2	A	113	ILE	CA-C-N	5.75	128.30	120.54
2	A	113	ILE	C-N-CA	5.75	128.30	120.54
1	3	136	PHE	CA-CB-CG	-5.74	108.06	113.80
2	A	181	PRO	CA-C-N	5.74	132.03	121.70
2	A	181	PRO	C-N-CA	5.74	132.03	121.70
2	C	649	PHE	N-CA-C	-5.74	104.95	112.41
2	A	708	ILE	CA-C-N	5.74	129.77	122.37
2	A	708	ILE	C-N-CA	5.74	129.77	122.37
2	B	408	THR	N-CA-C	-5.74	106.32	113.38
2	E	563	PHE	N-CA-C	-5.74	106.91	114.31
2	F	712	HIS	N-CA-CB	5.74	118.54	109.71
2	F	667	ARG	N-CA-C	5.73	118.38	110.35
1	1	214	LYS	CA-C-N	5.73	133.77	122.31
1	1	214	LYS	C-N-CA	5.73	133.77	122.31
2	A	166	LEU	N-CA-CB	5.73	120.24	110.50
2	A	434	GLN	CA-C-N	5.73	132.01	121.70
2	A	434	GLN	C-N-CA	5.73	132.01	121.70
2	D	178	SER	N-CA-C	-5.73	104.65	111.69
2	D	368	ASP	CA-CB-CG	-5.72	106.88	112.60
2	F	470	GLU	N-CA-CB	5.72	120.29	111.24
2	A	216	ALA	CA-C-N	5.72	128.30	120.46
2	A	216	ALA	C-N-CA	5.72	128.30	120.46
2	D	112	LEU	CA-C-N	5.72	127.98	120.60
2	D	112	LEU	C-N-CA	5.72	127.98	120.60
2	E	178	SER	N-CA-C	-5.72	98.61	110.80
2	F	426	GLU	CA-C-N	5.72	128.75	120.79
2	F	426	GLU	C-N-CA	5.72	128.75	120.79
2	B	350	ILE	CA-C-N	5.72	128.74	120.79
2	B	350	ILE	C-N-CA	5.72	128.74	120.79
2	B	368	ASP	CA-C-N	5.71	128.72	120.38
2	B	368	ASP	C-N-CA	5.71	128.72	120.38
2	D	29	ILE	CB-CA-C	-5.71	105.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	207	HIS	N-CA-C	-5.71	99.06	109.56
2	A	308	GLU	N-CA-C	-5.70	104.44	111.40
2	C	201	LYS	N-CA-C	-5.70	100.99	109.83
2	D	26	HIS	CA-C-N	5.70	128.98	120.31
2	D	26	HIS	C-N-CA	5.70	128.98	120.31
2	D	105	THR	CA-C-N	5.70	127.85	120.44
2	D	105	THR	C-N-CA	5.70	127.85	120.44
2	D	661	GLY	CA-C-N	5.70	132.43	121.54
2	D	661	GLY	C-N-CA	5.70	132.43	121.54
1	2	173	GLU	CA-C-N	5.70	128.97	120.31
1	2	173	GLU	C-N-CA	5.70	128.97	120.31
2	F	310	GLN	N-CA-C	-5.70	99.84	108.67
2	C	110	LEU	CA-C-N	5.69	127.25	120.14
2	C	110	LEU	C-N-CA	5.69	127.25	120.14
2	E	517	VAL	N-CA-C	5.69	116.34	110.36
2	F	803	VAL	N-CA-C	-5.69	100.21	108.17
2	F	408	THR	N-CA-C	-5.69	104.70	111.69
2	A	75	SER	CA-C-N	5.68	132.39	121.54
2	A	75	SER	C-N-CA	5.68	132.39	121.54
2	A	102	TYR	CA-C-N	5.68	128.71	120.98
2	A	102	TYR	C-N-CA	5.68	128.71	120.98
1	2	172	ASP	N-CA-C	5.68	117.14	111.07
2	D	300	LEU	N-CA-C	5.68	117.55	111.36
2	D	445	THR	N-CA-CB	5.67	118.46	110.12
2	C	337	ILE	CA-C-N	5.67	129.95	121.72
2	C	337	ILE	C-N-CA	5.67	129.95	121.72
2	C	676	GLN	N-CA-C	-5.67	105.94	112.92
1	5	201	LYS	CA-C-N	5.67	129.31	120.75
1	5	201	LYS	C-N-CA	5.67	129.31	120.75
1	2	177	ASN	CA-C-N	5.67	129.32	120.82
1	2	177	ASN	C-N-CA	5.67	129.32	120.82
2	D	512	GLY	N-CA-C	-5.67	105.62	112.48
2	E	449	LEU	CA-C-N	5.67	128.67	120.79
2	E	449	LEU	C-N-CA	5.67	128.67	120.79
2	A	700	GLU	CA-C-N	5.67	128.34	120.63
2	A	700	GLU	C-N-CA	5.67	128.34	120.63
1	3	202	LEU	N-CA-C	5.66	118.05	110.35
2	D	316	THR	N-CA-C	-5.66	100.88	108.86
2	D	539	GLY	N-CA-C	-5.65	99.78	113.18
2	E	308	GLU	N-CA-C	-5.65	104.74	111.69
2	E	483	TRP	CB-CG-CD2	-5.65	118.89	126.80
2	E	701	PHE	CA-C-N	5.65	130.29	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	PHE	C-N-CA	5.65	130.29	120.86
2	A	234	LEU	CA-C-N	5.65	129.66	120.23
2	A	234	LEU	C-N-CA	5.65	129.66	120.23
2	A	480	VAL	N-CA-CB	5.64	119.05	110.58
2	E	313	GLY	N-CA-C	-5.64	100.66	110.71
1	6	150	SER	N-CA-C	-5.64	98.15	108.02
2	D	160	THR	CA-C-N	5.64	125.11	119.24
2	D	160	THR	C-N-CA	5.64	125.11	119.24
2	B	676	GLN	N-CA-C	-5.64	105.75	113.30
2	E	444	ASP	CA-CB-CG	-5.64	106.96	112.60
2	E	166	LEU	N-CA-CB	5.64	120.08	110.50
2	F	395	ILE	N-CA-CB	5.63	116.53	110.62
2	D	358	TYR	CB-CA-C	-5.63	99.95	110.36
2	D	238	ARG	N-CA-C	-5.63	99.84	109.24
2	B	629	ILE	N-CA-C	-5.62	105.37	110.82
2	D	309	LEU	N-CA-C	-5.62	101.14	109.11
2	A	398	ALA	CA-C-N	5.61	132.41	121.41
2	A	398	ALA	C-N-CA	5.61	132.41	121.41
2	C	28	ASN	N-CA-C	-5.61	99.75	108.90
2	E	210	PRO	CA-C-N	5.61	131.80	121.70
2	E	210	PRO	C-N-CA	5.61	131.80	121.70
2	A	383	SER	N-CA-CB	5.61	120.04	110.50
2	D	410	PRO	N-CA-CB	-5.61	97.64	103.08
2	F	308	GLU	N-CA-C	-5.61	104.79	111.69
2	A	468	ASN	N-CA-C	5.61	122.74	110.80
1	3	137	GLU	CA-C-N	5.60	128.34	120.28
1	3	137	GLU	C-N-CA	5.60	128.34	120.28
2	D	364	VAL	O-C-N	-5.60	116.84	123.00
2	C	101	SER	N-CA-C	-5.60	106.12	113.17
2	E	803	VAL	N-CA-C	-5.60	99.68	107.80
2	A	719	LEU	N-CA-CB	5.59	118.33	109.82
2	B	590	PRO	CA-C-O	-5.59	112.45	120.56
2	E	434	GLN	CA-C-N	5.59	131.77	121.70
2	E	434	GLN	C-N-CA	5.59	131.77	121.70
2	D	468	ASN	N-CA-C	5.59	122.71	110.80
2	A	351	LEU	CA-C-N	5.59	128.04	120.38
2	A	351	LEU	C-N-CA	5.59	128.04	120.38
2	A	431	VAL	CB-CA-C	-5.59	103.50	112.16
2	C	113	ILE	CA-C-N	5.59	128.08	120.54
2	C	113	ILE	C-N-CA	5.59	128.08	120.54
2	F	497	ASP	N-CA-C	-5.59	105.19	112.23
2	F	382	ILE	CA-C-N	5.58	131.75	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	382	ILE	C-N-CA	5.58	131.75	121.70
1	3	139	VAL	CB-CA-C	-5.58	104.52	112.22
2	C	589	SER	N-CA-C	-5.58	96.54	108.93
2	C	692	GLU	CA-C-N	5.58	128.22	120.63
2	C	692	GLU	C-N-CA	5.58	128.22	120.63
2	D	433	SER	CA-C-N	5.58	132.20	121.54
2	D	433	SER	C-N-CA	5.58	132.20	121.54
2	C	692	GLU	N-CA-C	-5.58	106.31	113.23
2	D	474	ASP	CA-C-N	5.58	127.69	120.44
2	D	474	ASP	C-N-CA	5.58	127.69	120.44
2	B	509	ARG	N-CA-C	-5.57	106.17	114.64
2	D	350	ILE	CA-C-N	5.57	128.54	120.79
2	D	350	ILE	C-N-CA	5.57	128.54	120.79
2	C	274	ILE	CA-C-N	5.57	130.43	123.14
2	C	274	ILE	C-N-CA	5.57	130.43	123.14
2	D	804	LYS	N-CA-C	-5.57	101.06	109.85
1	2	139	VAL	CB-CA-C	-5.57	104.75	112.04
1	4	180	SER	CA-C-N	5.56	128.06	120.77
1	4	180	SER	C-N-CA	5.56	128.06	120.77
2	D	449	LEU	CA-C-N	5.56	128.52	120.79
2	D	449	LEU	C-N-CA	5.56	128.52	120.79
2	D	536	ARG	CB-CA-C	-5.56	99.22	110.17
2	D	676	GLN	N-CA-C	-5.56	104.04	112.99
2	F	617	ASP	CA-C-N	5.56	132.16	121.54
2	F	617	ASP	C-N-CA	5.56	132.16	121.54
1	3	216	PHE	N-CA-CB	5.56	119.88	110.49
2	D	461	LYS	N-CA-C	-5.55	106.51	113.28
2	B	451	GLU	CA-C-N	5.55	127.66	120.44
2	B	451	GLU	C-N-CA	5.55	127.66	120.44
2	E	535	LYS	CA-C-N	5.55	130.11	122.06
2	E	535	LYS	C-N-CA	5.55	130.11	122.06
2	B	563	PHE	N-CA-C	-5.55	107.15	114.31
2	F	502	MET	CG-SD-CE	-5.55	88.69	100.90
2	D	407	PHE	CA-CB-CG	-5.55	108.25	113.80
2	B	291	GLU	N-CA-C	-5.54	108.30	114.62
2	D	292	GLY	N-CA-C	-5.54	105.17	110.21
2	A	362	HIS	CA-CB-CG	-5.54	108.26	113.80
2	A	670	TYR	N-CA-C	5.54	118.48	110.28
2	A	412	ASN	CA-CB-CG	-5.54	107.06	112.60
2	A	497	ASP	N-CA-C	-5.54	105.26	112.23
2	A	358	TYR	CA-CB-CG	5.53	123.86	113.90
2	C	601	GLN	N-CA-C	5.53	117.00	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	184	GLY	CA-C-N	5.53	131.66	121.70
2	E	184	GLY	C-N-CA	5.53	131.66	121.70
2	D	426	GLU	CA-C-N	5.53	128.48	120.79
2	D	426	GLU	C-N-CA	5.53	128.48	120.79
2	A	473	VAL	CA-C-N	5.53	127.95	120.38
2	A	473	VAL	C-N-CA	5.53	127.95	120.38
2	E	677	ASP	N-CA-C	-5.52	106.38	113.23
2	B	180	ASP	CA-CB-CG	-5.52	107.08	112.60
2	C	461	LYS	N-CA-C	-5.52	106.54	113.28
2	C	793	VAL	N-CA-C	-5.52	100.44	108.17
2	A	480	VAL	N-CA-C	-5.52	105.14	110.72
2	B	222	ALA	CA-C-N	5.52	127.67	120.28
2	B	222	ALA	C-N-CA	5.52	127.67	120.28
1	4	207	HIS	CA-C-N	5.52	127.67	120.28
1	4	207	HIS	C-N-CA	5.52	127.67	120.28
2	F	203	ASN	CB-CA-C	-5.52	101.97	109.42
1	2	167	PHE	CA-CB-CG	-5.51	108.28	113.80
2	F	36	LEU	CA-C-N	5.51	126.10	119.98
2	F	36	LEU	C-N-CA	5.51	126.10	119.98
2	F	483	TRP	N-CA-CB	5.51	118.18	110.07
1	1	210	GLU	CA-C-N	5.51	128.11	120.29
1	1	210	GLU	C-N-CA	5.51	128.11	120.29
2	A	480	VAL	CB-CA-C	-5.51	104.62	112.22
2	E	304	LEU	CB-CA-C	-5.51	101.65	110.79
2	E	194	GLU	N-CA-C	-5.50	104.97	110.97
1	1	138	ASP	CA-CB-CG	-5.50	107.10	112.60
2	C	517	VAL	N-CA-C	5.50	116.14	110.36
2	D	34	ILE	CA-C-N	5.50	127.59	120.44
2	D	34	ILE	C-N-CA	5.50	127.59	120.44
2	F	106	GLU	CA-C-N	5.50	128.41	120.38
2	F	106	GLU	C-N-CA	5.50	128.41	120.38
2	C	581	HIS	N-CA-C	-5.50	105.37	113.61
2	B	213	GLY	CA-C-N	5.49	127.91	120.38
2	B	213	GLY	C-N-CA	5.49	127.91	120.38
2	D	700	GLU	CA-C-N	5.49	128.10	120.63
2	D	700	GLU	C-N-CA	5.49	128.10	120.63
2	D	681	ASN	CA-CB-CG	-5.49	107.11	112.60
1	6	146	ASN	CA-C-N	5.48	131.84	121.97
1	6	146	ASN	C-N-CA	5.48	131.84	121.97
2	A	274	ILE	CA-C-N	5.48	130.32	123.14
2	A	274	ILE	C-N-CA	5.48	130.32	123.14
2	A	699	PRO	CA-C-N	5.48	127.89	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	699	PRO	C-N-CA	5.48	127.89	120.38
2	C	462	GLU	N-CA-C	-5.47	104.96	111.69
2	F	677	ASP	N-CA-C	-5.47	106.44	113.23
2	B	194	GLU	N-CA-CB	5.47	117.90	109.91
2	F	371	ILE	CB-CA-C	5.47	118.70	111.70
2	C	699	PRO	CA-C-N	5.47	127.61	120.28
2	C	699	PRO	C-N-CA	5.47	127.61	120.28
2	C	112	LEU	CA-C-N	5.47	127.65	120.60
2	C	112	LEU	C-N-CA	5.47	127.65	120.60
2	F	539	GLY	N-CA-C	-5.46	100.23	113.18
2	B	597	ASP	N-CA-C	5.46	117.04	111.14
1	3	199	TYR	N-CA-C	5.45	119.48	113.21
2	A	467	GLU	CA-C-N	5.45	131.96	121.54
2	A	467	GLU	C-N-CA	5.45	131.96	121.54
2	E	593	TYR	CA-CB-CG	-5.45	104.08	113.90
2	F	176	GLU	N-CA-C	-5.45	106.63	113.72
2	D	777	LEU	N-CA-CB	5.45	118.23	110.16
2	D	382	ILE	CA-C-N	5.45	131.51	121.70
2	D	382	ILE	C-N-CA	5.45	131.51	121.70
2	E	104	GLY	CA-C-N	5.45	127.84	120.38
2	E	104	GLY	C-N-CA	5.45	127.84	120.38
2	F	244	MET	CA-C-N	5.45	126.03	119.98
2	F	244	MET	C-N-CA	5.45	126.03	119.98
2	A	70	ARG	N-CA-C	-5.45	100.44	108.99
2	B	445	THR	N-CA-CB	5.45	118.12	110.12
2	C	418	GLN	CA-C-N	5.45	127.84	120.65
2	C	418	GLN	C-N-CA	5.45	127.84	120.65
1	3	217	ALA	N-CA-C	-5.44	99.21	110.80
2	C	75	SER	CA-C-N	5.44	131.93	121.54
2	C	75	SER	C-N-CA	5.44	131.93	121.54
2	C	116	GLY	CA-C-N	5.44	131.93	121.54
2	C	116	GLY	C-N-CA	5.44	131.93	121.54
2	D	106	GLU	N-CA-CB	5.44	117.90	110.01
2	F	126	ASN	N-CA-C	-5.44	106.32	113.12
1	1	180	SER	CA-C-N	5.44	127.89	120.77
1	1	180	SER	C-N-CA	5.44	127.89	120.77
2	E	205	VAL	N-CA-C	-5.44	98.03	109.34
2	E	722	ILE	N-CA-CB	5.44	118.35	110.52
2	F	227	ASN	CA-C-N	5.43	131.48	121.70
2	F	227	ASN	C-N-CA	5.43	131.48	121.70
2	F	201	LYS	CA-C-N	5.43	131.92	121.54
2	F	201	LYS	C-N-CA	5.43	131.92	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	MET	N-CA-C	5.43	117.63	111.11
2	E	493	GLN	N-CA-C	5.43	122.36	110.80
2	D	126	ASN	N-CA-C	-5.43	106.34	113.12
2	D	181	PRO	CA-C-N	5.43	131.47	121.70
2	D	181	PRO	C-N-CA	5.43	131.47	121.70
2	B	184	GLY	CA-C-N	5.42	131.46	121.70
2	B	184	GLY	C-N-CA	5.42	131.46	121.70
2	D	381	TYR	CA-C-N	5.42	131.74	121.97
2	D	381	TYR	C-N-CA	5.42	131.74	121.97
2	F	383	SER	N-CA-CB	5.42	119.72	110.50
2	B	774	GLU	CA-C-N	5.42	127.81	120.38
2	B	774	GLU	C-N-CA	5.42	127.81	120.38
2	A	106	GLU	CA-C-N	5.42	128.29	120.38
2	A	106	GLU	C-N-CA	5.42	128.29	120.38
2	A	525	ARG	CA-C-N	5.42	127.80	120.65
2	A	525	ARG	C-N-CA	5.42	127.80	120.65
2	F	462	GLU	N-CA-C	-5.41	105.03	111.69
2	E	294	ILE	N-CA-CB	5.41	120.16	111.23
2	F	601	GLN	N-CA-C	5.40	116.86	110.97
2	C	447	GLN	N-CA-C	5.40	117.92	111.71
2	C	514	ASP	CA-C-N	5.40	128.30	120.79
2	C	514	ASP	C-N-CA	5.40	128.30	120.79
2	F	44	GLY	N-CA-C	-5.40	104.16	112.85
2	A	687	ASP	CA-C-N	5.39	129.73	120.72
2	A	687	ASP	C-N-CA	5.39	129.73	120.72
2	D	24	LEU	N-CA-C	-5.39	106.63	114.12
1	5	141	SER	CA-C-N	5.39	127.76	120.38
1	5	141	SER	C-N-CA	5.39	127.76	120.38
2	E	475	ASP	CA-C-N	5.39	127.46	120.56
2	E	475	ASP	C-N-CA	5.39	127.46	120.56
1	5	135	ASP	N-CA-C	-5.39	100.73	108.60
2	F	106	GLU	N-CA-CB	5.39	117.82	110.01
2	F	414	LYS	CA-C-N	5.38	127.93	120.29
2	F	414	LYS	C-N-CA	5.38	127.93	120.29
2	D	213	GLY	CA-C-N	5.38	127.75	120.38
2	D	213	GLY	C-N-CA	5.38	127.75	120.38
1	2	166	ASP	N-CA-C	-5.38	97.06	107.44
1	2	216	PHE	N-CA-CB	5.38	119.58	110.49
2	C	801	PHE	CA-CB-CG	-5.38	108.42	113.80
2	B	13	VAL	N-CA-CB	5.38	117.85	110.54
2	E	330	LEU	N-CA-C	-5.38	105.01	113.02
2	F	95	ALA	N-CA-C	-5.37	106.66	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	676	GLN	N-CA-C	-5.37	106.40	113.17
2	A	160	THR	CA-C-N	5.37	124.82	119.24
2	A	160	THR	C-N-CA	5.37	124.82	119.24
1	1	139	VAL	CA-C-N	5.37	127.52	120.60
1	1	139	VAL	C-N-CA	5.37	127.52	120.60
2	A	304	LEU	CB-CA-C	-5.36	101.74	110.85
2	A	757	ASP	N-CA-CB	5.36	119.54	110.49
2	B	128	GLY	CA-C-N	5.36	131.62	121.97
2	B	128	GLY	C-N-CA	5.36	131.62	121.97
2	B	389	ASP	CA-CB-CG	5.35	117.95	112.60
2	F	198	ARG	N-CA-C	-5.35	101.62	109.81
1	3	173	GLU	CA-C-N	5.35	128.44	120.31
1	3	173	GLU	C-N-CA	5.35	128.44	120.31
2	D	157	ASN	CA-CB-CG	-5.35	107.25	112.60
2	C	95	ALA	N-CA-C	-5.34	106.70	113.43
2	D	479	VAL	N-CA-CB	5.33	117.80	110.54
2	E	356	ASP	N-CA-C	5.33	119.27	112.34
2	E	433	SER	CA-C-N	5.33	131.72	121.54
2	E	433	SER	C-N-CA	5.33	131.72	121.54
2	A	305	ALA	N-CA-C	5.33	117.17	111.36
2	E	29	ILE	CB-CA-C	-5.33	105.48	111.23
2	B	86	LYS	N-CA-CB	5.32	117.93	110.12
2	D	551	LYS	CA-C-N	5.32	127.72	120.54
2	D	551	LYS	C-N-CA	5.32	127.72	120.54
2	E	126	ASN	N-CA-C	-5.32	106.47	113.12
2	B	138	VAL	CB-CA-C	-5.31	105.17	111.97
1	2	161	TYR	CA-CB-CG	-5.31	104.34	113.90
1	5	196	LEU	CA-C-N	5.31	127.66	120.38
1	5	196	LEU	C-N-CA	5.31	127.66	120.38
2	E	52	ALA	N-CA-C	-5.31	104.92	111.40
2	E	755	GLY	N-CA-C	-5.31	108.37	115.32
2	A	195	VAL	N-CA-C	5.31	120.38	109.34
2	E	447	GLN	N-CA-C	5.30	117.81	111.71
2	D	692	GLU	N-CA-C	-5.30	106.66	113.23
2	C	213	GLY	CA-C-N	5.29	127.63	120.38
2	C	213	GLY	C-N-CA	5.29	127.63	120.38
2	C	462	GLU	CB-CA-C	-5.29	101.02	110.70
1	2	175	VAL	N-CA-C	-5.29	105.69	110.82
2	C	179	LEU	N-CA-C	-5.29	102.23	110.42
2	A	563	PHE	N-CA-C	-5.28	107.50	114.31
1	6	180	SER	CA-C-N	5.28	127.68	120.77
1	6	180	SER	C-N-CA	5.28	127.68	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	404	LEU	N-CA-C	-5.28	104.44	112.04
2	E	563	PHE	CA-CB-CG	-5.28	108.53	113.80
2	B	433	SER	CA-C-N	5.27	131.61	121.54
2	B	433	SER	C-N-CA	5.27	131.61	121.54
2	A	316	THR	CA-C-N	5.27	128.73	120.82
2	A	316	THR	C-N-CA	5.27	128.73	120.82
2	A	194	GLU	N-CA-C	-5.27	105.22	110.97
2	B	535	LYS	N-CA-C	-5.27	105.61	111.36
2	D	535	LYS	N-CA-C	-5.27	99.86	109.56
2	E	582	SER	CA-C-N	5.27	131.61	121.54
2	E	582	SER	C-N-CA	5.27	131.61	121.54
2	D	180	ASP	CA-CB-CG	-5.27	107.33	112.60
2	E	754	GLU	N-CA-C	-5.27	106.87	113.72
2	E	763	ARG	CA-C-N	5.26	124.98	119.82
2	E	763	ARG	C-N-CA	5.26	124.98	119.82
2	A	362	HIS	CA-C-N	5.26	131.59	121.54
2	A	362	HIS	C-N-CA	5.26	131.59	121.54
2	C	378	SER	CA-C-N	5.26	127.33	120.28
2	C	378	SER	C-N-CA	5.26	127.33	120.28
2	B	141	LEU	N-CA-C	-5.26	106.64	114.64
2	D	417	GLU	CA-C-N	5.26	127.64	120.54
2	D	417	GLU	C-N-CA	5.26	127.64	120.54
2	E	344	VAL	N-CA-C	5.26	116.62	110.62
2	C	713	SER	N-CA-CB	5.26	117.59	110.38
2	F	180	ASP	CA-CB-CG	-5.26	107.34	112.60
2	D	7	THR	N-CA-C	-5.25	102.28	110.42
2	F	40	ARG	N-CA-C	-5.25	106.92	113.38
2	E	542	ILE	N-CA-C	-5.25	100.92	108.48
1	4	147	VAL	N-CA-C	-5.25	98.42	109.34
2	A	364	VAL	CA-C-N	5.25	131.15	121.70
2	A	364	VAL	C-N-CA	5.25	131.15	121.70
2	C	757	ASP	CA-CB-CG	5.25	117.85	112.60
2	D	531	LEU	CB-CA-C	-5.25	102.39	109.16
2	D	701	PHE	CA-C-N	5.25	129.62	120.86
2	D	701	PHE	C-N-CA	5.25	129.62	120.86
1	1	130	VAL	N-CA-C	-5.25	100.09	107.75
2	E	457	LYS	N-CA-C	-5.25	106.38	112.89
2	F	368	ASP	CA-C-N	5.25	128.04	120.38
2	F	368	ASP	C-N-CA	5.25	128.04	120.38
2	F	680	GLN	N-CA-C	-5.25	106.83	114.12
2	A	639	LEU	N-CA-C	-5.24	101.10	109.23
2	B	687	ASP	CA-C-N	5.24	128.98	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	687	ASP	C-N-CA	5.24	128.98	120.60
2	D	227	ASN	CA-C-N	5.24	131.13	121.70
2	D	227	ASN	C-N-CA	5.24	131.13	121.70
2	F	440	ALA	CA-C-N	5.24	128.27	120.31
2	F	440	ALA	C-N-CA	5.24	128.27	120.31
2	C	166	LEU	N-CA-CB	5.24	119.40	110.50
2	D	176	GLU	N-CA-C	-5.24	106.84	114.12
2	F	681	ASN	CA-CB-CG	-5.24	107.36	112.60
2	B	781	LEU	N-CA-C	-5.23	105.66	111.36
2	F	117	GLU	N-CA-C	-5.23	106.58	113.17
2	E	692	GLU	N-CA-C	-5.23	106.74	113.23
2	A	318	ASP	N-CA-C	-5.22	105.74	112.68
2	D	451	GLU	CA-C-N	5.22	127.22	120.44
2	D	451	GLU	C-N-CA	5.22	127.22	120.44
2	E	216	ALA	CA-C-N	5.22	127.61	120.46
2	E	216	ALA	C-N-CA	5.22	127.61	120.46
2	E	257	PHE	CA-CB-CG	5.22	119.02	113.80
2	F	637	GLY	N-CA-C	-5.22	107.60	115.32
2	C	21	ALA	N-CA-CB	5.21	117.74	109.82
1	1	147	VAL	CA-C-N	5.21	129.54	122.19
1	1	147	VAL	C-N-CA	5.21	129.54	122.19
2	E	468	ASN	N-CA-C	5.21	121.90	110.80
2	A	350	ILE	CA-C-N	5.21	128.03	120.79
2	A	350	ILE	C-N-CA	5.21	128.03	120.79
2	B	669	LYS	CA-C-N	5.21	131.49	121.54
2	B	669	LYS	C-N-CA	5.21	131.49	121.54
2	A	163	LEU	N-CA-C	5.21	119.11	112.34
1	2	139	VAL	CA-C-N	5.21	127.31	120.60
1	2	139	VAL	C-N-CA	5.21	127.31	120.60
2	A	295	ASP	CA-CB-CG	-5.21	107.39	112.60
2	C	331	GLU	N-CA-C	-5.20	104.61	112.99
2	C	243	ASP	CA-C-N	5.20	127.67	120.29
2	C	243	ASP	C-N-CA	5.20	127.67	120.29
2	B	142	LEU	N-CA-C	-5.20	106.53	112.92
1	6	156	SER	N-CA-C	-5.20	100.43	108.90
2	A	90	LEU	CA-C-N	5.19	127.49	120.38
2	A	90	LEU	C-N-CA	5.19	127.49	120.38
2	E	473	VAL	CA-C-N	5.19	127.49	120.38
2	E	473	VAL	C-N-CA	5.19	127.49	120.38
2	B	495	GLU	N-CA-C	-5.19	107.61	114.04
2	C	77	THR	CA-C-N	5.19	131.31	121.97
2	C	77	THR	C-N-CA	5.19	131.31	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	405	ARG	CA-C-N	5.19	127.19	120.44
2	C	405	ARG	C-N-CA	5.19	127.19	120.44
2	E	478	MET	N-CA-CB	5.19	117.75	110.12
2	E	479	VAL	CB-CA-C	-5.19	105.13	112.14
2	C	210	PRO	CA-C-N	5.19	131.04	121.70
2	C	210	PRO	C-N-CA	5.19	131.04	121.70
2	D	330	LEU	N-CA-C	-5.19	105.67	112.41
2	F	99	GLY	CA-C-N	5.18	131.44	121.54
2	F	99	GLY	C-N-CA	5.18	131.44	121.54
2	A	516	ALA	CA-C-N	5.18	127.28	120.60
2	A	516	ALA	C-N-CA	5.18	127.28	120.60
2	B	99	GLY	CA-C-N	5.18	131.44	121.54
2	B	99	GLY	C-N-CA	5.18	131.44	121.54
2	D	536	ARG	N-CA-CB	5.18	119.59	110.37
2	B	805	THR	N-CA-C	-5.18	101.32	109.50
2	F	295	ASP	CA-C-N	5.18	130.20	121.14
2	F	295	ASP	C-N-CA	5.18	130.20	121.14
2	F	467	GLU	CA-C-N	5.18	131.43	121.54
2	F	467	GLU	C-N-CA	5.18	131.43	121.54
2	F	621	LYS	N-CA-C	-5.18	99.77	110.80
2	F	627	PHE	CA-C-N	5.18	127.74	120.28
2	F	627	PHE	C-N-CA	5.18	127.74	120.28
2	C	181	PRO	CA-C-N	5.17	131.01	121.70
2	C	181	PRO	C-N-CA	5.17	131.01	121.70
2	E	200	THR	N-CA-C	-5.17	99.78	110.80
2	A	592	GLY	CA-C-N	5.17	127.47	120.38
2	A	592	GLY	C-N-CA	5.17	127.47	120.38
2	B	462	GLU	CB-CA-C	-5.17	101.25	110.70
2	F	378	SER	CA-C-N	5.16	127.20	120.28
2	F	378	SER	C-N-CA	5.16	127.20	120.28
2	F	659	ASN	N-CA-C	-5.16	105.28	112.03
2	B	106	GLU	CA-C-N	5.16	127.91	120.38
2	B	106	GLU	C-N-CA	5.16	127.91	120.38
2	C	230	VAL	CA-C-N	5.15	126.28	119.84
2	C	230	VAL	C-N-CA	5.15	126.28	119.84
2	B	673	PHE	N-CA-C	-5.15	103.19	111.02
2	D	516	ALA	CA-C-N	5.15	127.25	120.60
2	D	516	ALA	C-N-CA	5.15	127.25	120.60
2	D	713	SER	N-CA-C	-5.15	103.88	110.53
2	E	478	MET	N-CA-C	-5.15	105.66	111.28
1	5	127	LEU	N-CA-C	-5.15	104.76	112.54
2	A	449	LEU	CA-C-N	5.15	127.95	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	449	LEU	C-N-CA	5.15	127.95	120.79
2	D	482	SER	CA-C-N	5.15	127.64	120.63
2	D	482	SER	C-N-CA	5.15	127.64	120.63
2	E	272	GLY	N-CA-C	-5.15	108.17	115.43
2	B	699	PRO	CA-C-N	5.15	127.18	120.28
2	B	699	PRO	C-N-CA	5.15	127.18	120.28
2	D	145	ASN	CA-CB-CG	-5.15	107.45	112.60
2	B	4	GLY	N-CA-C	-5.14	108.23	114.92
2	A	341	GLN	CA-C-N	5.14	125.14	119.90
2	A	341	GLN	C-N-CA	5.14	125.14	119.90
2	D	358	TYR	N-CA-C	-5.14	107.03	113.15
2	B	666	LYS	N-CA-C	-5.14	106.79	113.16
2	D	716	LYS	N-CA-CB	5.14	119.17	110.49
2	D	480	VAL	CB-CA-C	-5.14	105.13	112.22
2	D	493	GLN	N-CA-C	5.14	121.74	110.80
2	D	780	GLU	CA-C-N	5.14	127.58	120.29
2	D	780	GLU	C-N-CA	5.14	127.58	120.29
2	A	692	GLU	N-CA-C	-5.13	106.87	113.23
1	4	206	GLU	CA-C-N	5.13	131.34	121.54
1	4	206	GLU	C-N-CA	5.13	131.34	121.54
2	A	404	LEU	N-CA-C	-5.13	104.66	112.04
2	B	763	ARG	CA-C-N	5.13	124.85	119.82
2	B	763	ARG	C-N-CA	5.13	124.85	119.82
2	D	772	HIS	CA-CB-CG	-5.13	108.67	113.80
2	E	715	GLU	N-CA-C	-5.13	99.93	108.34
2	F	160	THR	CA-C-N	5.13	124.57	119.24
2	F	160	THR	C-N-CA	5.13	124.57	119.24
2	F	629	ILE	N-CA-C	-5.13	105.85	110.82
2	F	757	ASP	N-CA-C	-5.13	99.88	110.80
2	C	355	ARG	CA-C-N	5.12	131.32	121.54
2	C	355	ARG	C-N-CA	5.12	131.32	121.54
2	C	715	GLU	CA-C-N	5.12	131.32	121.54
2	C	715	GLU	C-N-CA	5.12	131.32	121.54
2	E	452	GLN	CA-C-N	5.12	127.48	120.77
2	E	452	GLN	C-N-CA	5.12	127.48	120.77
2	D	467	GLU	CA-C-N	5.12	131.31	121.54
2	D	467	GLU	C-N-CA	5.12	131.31	121.54
2	D	639	LEU	N-CA-C	-5.12	101.41	109.50
2	E	117	GLU	N-CA-C	-5.12	107.08	113.38
2	A	307	GLY	N-CA-C	-5.12	107.75	115.32
2	C	473	VAL	CA-C-N	5.12	127.39	120.38
2	C	473	VAL	C-N-CA	5.12	127.39	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	176	GLU	CA-C-N	5.11	131.30	121.54
1	4	176	GLU	C-N-CA	5.11	131.30	121.54
1	6	139	VAL	CB-CA-C	-5.11	105.33	112.02
2	B	117	GLU	N-CA-C	-5.11	107.10	113.38
2	B	400	SER	CA-C-N	5.11	128.48	120.82
2	B	400	SER	C-N-CA	5.11	128.48	120.82
2	C	393	ASP	CA-C-N	5.11	127.08	120.44
2	C	393	ASP	C-N-CA	5.11	127.08	120.44
1	3	196	LEU	CA-C-N	5.10	127.37	120.38
1	3	196	LEU	C-N-CA	5.10	127.37	120.38
2	E	316	THR	CA-C-N	5.10	128.48	120.82
2	E	316	THR	C-N-CA	5.10	128.48	120.82
1	5	178	GLN	CA-C-N	5.10	127.63	120.28
1	5	178	GLN	C-N-CA	5.10	127.63	120.28
2	A	68	ILE	N-CA-C	-5.10	98.73	109.34
2	C	706	ASP	CA-CB-CG	-5.10	107.50	112.60
2	D	41	GLU	N-CA-C	-5.10	106.84	113.16
2	E	407	PHE	N-CA-C	-5.10	99.94	110.80
2	E	699	PRO	CA-C-N	5.10	127.11	120.28
2	E	699	PRO	C-N-CA	5.10	127.11	120.28
2	F	461	LYS	N-CA-C	-5.10	107.06	113.28
1	3	166	ASP	N-CA-C	-5.10	97.60	107.44
1	3	185	TYR	CA-CB-CG	-5.10	104.73	113.90
2	C	503	GLU	CB-CA-C	-5.10	102.88	110.88
1	6	137	GLU	CA-C-N	5.10	127.62	120.28
1	6	137	GLU	C-N-CA	5.10	127.62	120.28
2	B	520	VAL	N-CA-CB	5.09	116.51	110.55
1	2	127	LEU	N-CA-C	-5.09	104.53	111.56
2	B	36	LEU	CA-C-N	5.09	125.63	119.98
2	B	36	LEU	C-N-CA	5.09	125.63	119.98
2	C	414	LYS	CA-C-N	5.09	127.52	120.29
2	C	414	LYS	C-N-CA	5.09	127.52	120.29
2	D	213	GLY	N-CA-C	-5.09	101.12	113.18
2	D	434	GLN	CA-C-N	5.09	130.86	121.70
2	D	434	GLN	C-N-CA	5.09	130.86	121.70
2	F	687	ASP	CA-C-N	5.09	129.22	120.72
2	F	687	ASP	C-N-CA	5.09	129.22	120.72
2	C	465	GLY	CA-C-N	5.09	129.21	120.71
2	C	465	GLY	C-N-CA	5.09	129.21	120.71
2	D	548	GLY	N-CA-C	-5.09	105.25	114.46
2	C	360	ALA	N-CA-C	-5.08	99.97	110.80
2	E	200	THR	N-CA-CB	5.08	119.08	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	293	ALA	CA-C-N	5.08	131.12	121.97
2	E	293	ALA	C-N-CA	5.08	131.12	121.97
2	E	232	GLU	N-CA-C	5.08	116.63	111.14
2	A	474	ASP	CA-C-N	5.08	127.04	120.44
2	A	474	ASP	C-N-CA	5.08	127.04	120.44
2	A	366	ILE	CA-C-N	5.08	130.84	121.70
2	A	366	ILE	C-N-CA	5.08	130.84	121.70
2	D	649	PHE	N-CA-C	-5.08	106.40	112.59
2	B	180	ASP	N-CA-C	-5.07	102.48	110.14
2	A	572	ILE	N-CA-C	-5.07	101.18	108.48
1	3	213	LYS	CB-CA-C	-5.07	102.37	110.79
2	A	36	LEU	CA-C-N	5.07	125.60	119.98
2	A	36	LEU	C-N-CA	5.07	125.60	119.98
2	A	482	SER	CA-C-N	5.07	127.52	120.63
2	A	482	SER	C-N-CA	5.07	127.52	120.63
2	C	398	ALA	CA-C-N	5.06	131.32	121.41
2	C	398	ALA	C-N-CA	5.06	131.32	121.41
2	F	122	ARG	CA-C-N	5.06	127.66	120.53
2	F	122	ARG	C-N-CA	5.06	127.66	120.53
2	A	792	ILE	N-CA-C	-5.06	100.37	107.75
2	D	629	ILE	N-CA-C	-5.06	105.91	110.82
2	A	7	THR	CA-C-N	5.05	127.81	120.79
2	A	7	THR	C-N-CA	5.05	127.81	120.79
2	D	44	GLY	N-CA-C	-5.05	104.78	112.51
2	B	193	ILE	N-CA-C	-5.05	105.48	112.50
2	B	541	PHE	CA-CB-CG	-5.05	108.75	113.80
2	A	777	LEU	N-CA-CB	5.05	117.64	110.16
2	B	725	LEU	N-CA-C	-5.05	105.43	112.45
2	D	699	PRO	CA-C-N	5.05	127.30	120.38
2	D	699	PRO	C-N-CA	5.05	127.30	120.38
2	D	520	VAL	CB-CA-C	-5.05	105.41	112.02
2	A	413	LEU	CA-C-N	5.05	127.55	120.28
2	A	413	LEU	C-N-CA	5.05	127.55	120.28
2	F	324	ILE	CA-C-N	5.04	127.54	120.28
2	F	324	ILE	C-N-CA	5.04	127.54	120.28
2	B	82	PRO	CA-C-N	5.04	127.30	120.65
2	B	82	PRO	C-N-CA	5.04	127.30	120.65
2	F	480	VAL	N-CA-C	-5.04	105.63	110.72
1	3	172	ASP	N-CA-C	5.04	116.46	111.07
2	B	160	THR	CA-C-N	5.04	124.48	119.24
2	B	160	THR	C-N-CA	5.04	124.48	119.24
2	E	198	ARG	N-CA-C	-5.04	102.03	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	184	GLY	CA-C-N	5.03	130.76	121.70
2	A	184	GLY	C-N-CA	5.03	130.76	121.70
2	F	7	THR	CA-C-N	5.03	127.78	120.79
2	F	7	THR	C-N-CA	5.03	127.78	120.79
2	B	175	LYS	N-CA-C	-5.03	106.56	113.30
2	B	365	SER	CA-C-N	5.03	131.02	121.97
2	B	365	SER	C-N-CA	5.03	131.02	121.97
2	A	122	ARG	CA-C-N	5.03	127.62	120.53
2	A	122	ARG	C-N-CA	5.03	127.62	120.53
2	C	318	ASP	N-CA-C	-5.02	106.00	112.68
2	B	601	GLN	N-CA-C	5.02	116.44	110.97
2	A	169	ASP	CA-C-N	5.02	127.26	120.38
2	A	169	ASP	C-N-CA	5.02	127.26	120.38
2	C	426	GLU	CA-C-N	5.02	127.77	120.79
2	C	426	GLU	C-N-CA	5.02	127.77	120.79
2	C	471	VAL	N-CA-C	-5.02	98.90	109.34
2	F	41	GLU	N-CA-C	-5.02	106.94	113.16
2	F	655	ILE	N-CA-C	-5.02	100.30	107.78
2	E	365	SER	CA-C-N	5.02	131.00	121.97
2	E	365	SER	C-N-CA	5.02	131.00	121.97
2	F	63	GLU	CA-C-N	5.02	126.88	120.56
2	F	63	GLU	C-N-CA	5.02	126.88	120.56
2	D	7	THR	CA-C-N	5.02	127.76	120.79
2	D	7	THR	C-N-CA	5.02	127.76	120.79
2	A	295	ASP	CA-C-N	5.01	129.91	121.14
2	A	295	ASP	C-N-CA	5.01	129.91	121.14
2	B	792	ILE	N-CA-CB	5.01	118.16	111.64
2	C	614	VAL	N-CA-CB	5.01	116.57	110.95
1	1	173	GLU	CA-C-N	5.01	127.93	120.31
1	1	173	GLU	C-N-CA	5.01	127.93	120.31
2	A	205	VAL	N-CA-C	-5.01	98.92	109.34
2	A	471	VAL	CA-C-N	5.01	131.11	121.54
2	A	471	VAL	C-N-CA	5.01	131.11	121.54
2	D	162	THR	CA-C-N	5.01	131.11	121.54
2	D	162	THR	C-N-CA	5.01	131.11	121.54
2	E	26	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
2	C	794	LEU	N-CA-C	-5.01	100.56	108.73
2	E	67	LEU	N-CA-C	-5.01	107.12	113.43
2	F	632	GLN	N-CA-C	-5.01	105.92	112.23
2	B	87	VAL	CB-CA-C	-5.00	104.75	112.05
2	B	700	GLU	CA-C-N	5.00	127.44	120.63
2	B	700	GLU	C-N-CA	5.00	127.44	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	52	ALA	N-CA-C	-5.00	105.30	111.40

There are no chirality outliers.

All (106) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	136	PHE	Sidechain
1	1	161	TYR	Sidechain
1	1	185	TYR	Sidechain
1	2	161	TYR	Sidechain
1	2	162	TYR	Sidechain
1	2	199	TYR	Sidechain
1	3	133	PHE	Sidechain
1	3	164	TYR	Sidechain
1	3	185	TYR	Sidechain
1	3	199	TYR	Sidechain
1	3	215	HIS	Sidechain
1	3	216	PHE	Sidechain
1	4	161	TYR	Sidechain
1	4	185	TYR	Sidechain
1	5	162	TYR	Sidechain
1	6	136	PHE	Sidechain
1	6	161	TYR	Sidechain
1	6	185	TYR	Sidechain
2	A	102	TYR	Sidechain
2	A	122	ARG	Sidechain
2	A	210	PRO	Peptide
2	A	361	HIS	Peptide
2	A	363	ARG	Sidechain
2	A	381	TYR	Sidechain
2	A	403	ARG	Sidechain
2	A	409	THR	Peptide
2	A	448	ARG	Sidechain
2	A	450	ARG	Sidechain
2	A	468	ASN	Peptide
2	A	592	GLY	Peptide
2	A	596	TYR	Sidechain
2	A	670	TYR	Sidechain
2	A	698	ARG	Sidechain
2	A	713	SER	Peptide
2	A	716	LYS	Peptide
2	A	756	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	B	135	ARG	Sidechain
2	B	185	ARG	Sidechain
2	B	191	ARG	Sidechain
2	B	198	ARG	Sidechain
2	B	210	PRO	Peptide
2	B	355	ARG	Sidechain
2	B	358	TYR	Sidechain
2	B	381	TYR	Sidechain
2	B	409	THR	Peptide
2	B	468	ASN	Peptide
2	B	577	TYR	Sidechain
2	B	585	ARG	Sidechain
2	B	592	GLY	Peptide
2	B	611	TYR	Sidechain
2	B	713	SER	Peptide
2	B	716	LYS	Peptide
2	B	756	VAL	Peptide
2	B	80	TYR	Sidechain
2	C	135	ARG	Sidechain
2	C	198	ARG	Sidechain
2	C	210	PRO	Peptide
2	C	323	TYR	Sidechain
2	C	358	TYR	Sidechain
2	C	403	ARG	Sidechain
2	C	409	THR	Peptide
2	C	468	ASN	Peptide
2	C	592	GLY	Peptide
2	C	713	SER	Peptide
2	C	716	LYS	Peptide
2	C	756	VAL	Peptide
2	C	83	ARG	Sidechain
2	D	102	TYR	Sidechain
2	D	198	ARG	Sidechain
2	D	358	TYR	Sidechain
2	D	409	THR	Peptide
2	D	468	ASN	Peptide
2	D	577	TYR	Sidechain
2	D	592	GLY	Peptide
2	D	6	PHE	Sidechain
2	D	651	ASN	Peptide
2	D	698	ARG	Sidechain
2	D	713	SER	Peptide

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Mol	Chain	Res	Type	Group
2	D	716	LYS	Peptide
2	D	756	VAL	Peptide
2	E	102	TYR	Sidechain
2	E	198	ARG	Sidechain
2	E	210	PRO	Peptide
2	E	363	ARG	Sidechain
2	E	385	ARG	Sidechain
2	E	409	THR	Peptide
2	E	424	ARG	Sidechain
2	E	460	TRP	Peptide
2	E	468	ASN	Peptide
2	E	592	GLY	Peptide
2	E	593	TYR	Sidechain
2	E	713	SER	Peptide
2	E	716	LYS	Peptide
2	E	756	VAL	Peptide
2	F	235	ARG	Sidechain
2	F	320	TYR	Sidechain
2	F	323	TYR	Sidechain
2	F	358	TYR	Sidechain
2	F	409	THR	Peptide
2	F	468	ASN	Peptide
2	F	592	GLY	Peptide
2	F	593	TYR	Sidechain
2	F	611	TYR	Sidechain
2	F	716	LYS	Peptide
2	F	756	VAL	Peptide
2	F	763	ARG	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	19	0
1	2	777	0	758	12	0
1	3	777	0	758	20	0
1	4	777	0	758	20	0
1	5	777	0	758	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6	777	0	758	16	0
2	A	6196	0	6289	136	0
2	B	6196	0	6289	122	0
2	C	6196	0	6289	132	0
2	D	6196	0	6289	120	0
2	E	6196	0	6289	145	0
2	F	6196	0	6289	135	0
All	All	41838	0	42282	810	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 (810) 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:E:281:LEU:CD1	2:E:313:GLY:HA3	1.25	1.60
2:E:281:LEU:HD11	2:E:313:GLY:CA	1.17	1.57
2:C:278:ILE:HB	2:C:281:LEU:CD2	1.34	1.52
2:F:278:ILE:CG2	2:F:281:LEU:HD23	1.37	1.50
2:A:278:ILE:HB	2:A:281:LEU:CD2	1.41	1.50
2:B:277:PHE:CE2	2:B:279:ASP:OD1	1.74	1.38
2:C:277:PHE:CE2	2:C:279:ASP:OD1	1.78	1.35
2:F:278:ILE:HB	2:F:281:LEU:CD2	1.60	1.30
2:B:571:ARG:HD3	2:B:617:ASP:OD2	1.29	1.30
2:C:278:ILE:CB	2:C:281:LEU:CD2	2.10	1.29
2:F:278:ILE:CG2	2:F:281:LEU:CD2	2.08	1.29
2:A:277:PHE:CE2	2:A:279:ASP:OD1	1.85	1.28
2:F:278:ILE:CB	2:F:281:LEU:HD21	1.63	1.26
2:B:619:ILE:HG23	2:B:627:PHE:CE1	1.72	1.25
2:C:277:PHE:HE2	2:C:279:ASP:OD1	0.94	1.25
2:F:278:ILE:CB	2:F:281:LEU:CD2	2.17	1.22
2:C:278:ILE:CG2	2:C:281:LEU:HD23	1.67	1.22
2:A:278:ILE:CG2	2:A:281:LEU:HD23	1.71	1.21
2:E:281:LEU:CD1	2:E:313:GLY:CA	1.92	1.20
2:B:619:ILE:HD12	2:B:656:MET:HB3	1.24	1.20
2:A:278:ILE:CB	2:A:281:LEU:CD2	2.21	1.18
2:B:277:PHE:CZ	2:B:279:ASP:OD1	1.96	1.16
2:E:278:ILE:HB	2:E:281:LEU:HD21	1.27	1.13
2:A:278:ILE:CB	2:A:281:LEU:HD21	1.81	1.10
2:C:619:ILE:HD12	2:C:656:MET:HB3	1.22	1.10
2:E:281:LEU:HD11	2:E:313:GLY:HA2	1.25	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:281:LEU:HD12	2:E:313:GLY:HA3	1.30	1.08
2:E:619:ILE:HD12	2:E:656:MET:HB3	1.11	1.07
2:D:619:ILE:HD12	2:D:656:MET:HB3	1.37	1.07
2:C:278:ILE:CB	2:C:281:LEU:HD21	1.74	1.07
2:C:278:ILE:HG22	2:C:281:LEU:HD23	1.32	1.05
2:B:278:ILE:HB	2:B:281:LEU:HD21	1.36	1.04
2:F:278:ILE:HG22	2:F:281:LEU:HD23	1.03	1.02
2:E:278:ILE:HB	2:E:281:LEU:CD2	1.92	0.99
2:F:278:ILE:HG21	2:F:281:LEU:HD23	1.43	0.98
2:E:619:ILE:HD12	2:E:656:MET:CB	1.92	0.98
2:C:619:ILE:CG2	2:C:627:PHE:CE1	2.47	0.97
2:D:278:ILE:HB	2:D:281:LEU:CD2	1.94	0.97
2:E:278:ILE:CG2	2:E:281:LEU:HD23	1.95	0.97
2:E:619:ILE:HG23	2:E:627:PHE:CE1	1.99	0.96
2:B:278:ILE:HB	2:B:281:LEU:CD2	1.93	0.96
2:C:619:ILE:CG2	2:C:627:PHE:CZ	2.48	0.95
2:B:619:ILE:CD1	2:B:656:MET:HB3	1.97	0.95
2:D:619:ILE:HD13	2:D:630:LEU:CD1	1.97	0.94
2:C:278:ILE:HB	2:C:281:LEU:HD21	0.94	0.94
2:E:615:LEU:HD22	2:E:617:ASP:OD1	1.68	0.94
2:B:277:PHE:HE2	2:B:279:ASP:OD1	1.46	0.94
2:C:619:ILE:HG21	2:C:627:PHE:CE1	2.04	0.93
2:A:278:ILE:HG22	2:A:281:LEU:HD23	1.48	0.93
2:D:619:ILE:HD13	2:D:630:LEU:HD11	1.51	0.92
2:D:278:ILE:HB	2:D:281:LEU:HD21	1.52	0.91
2:A:277:PHE:HE2	2:A:279:ASP:OD1	1.40	0.91
2:C:278:ILE:HB	2:C:281:LEU:HD22	1.53	0.90
2:A:277:PHE:CZ	2:A:279:ASP:OD1	2.24	0.90
2:C:278:ILE:CG2	2:C:281:LEU:CD2	2.42	0.89
2:B:619:ILE:HD12	2:B:656:MET:CB	2.03	0.88
2:C:619:ILE:HG21	2:C:627:PHE:HE1	1.38	0.88
2:B:619:ILE:HG23	2:B:627:PHE:HE1	1.24	0.88
2:C:619:ILE:HD12	2:C:656:MET:CB	2.04	0.88
2:A:278:ILE:HB	2:A:281:LEU:HD21	0.90	0.88
2:A:277:PHE:HE2	2:A:279:ASP:CG	1.86	0.84
2:F:278:ILE:HB	2:F:281:LEU:HD21	0.86	0.84
2:B:277:PHE:HE2	2:B:279:ASP:CG	1.84	0.84
2:B:277:PHE:CE2	2:B:279:ASP:CG	2.55	0.84
2:F:278:ILE:HG22	2:F:281:LEU:CD2	1.91	0.84
2:F:278:ILE:HG21	2:F:281:LEU:CD2	2.03	0.84
2:C:619:ILE:CD1	2:C:656:MET:HB3	2.05	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:281:LEU:CG	2:E:313:GLY:HA2	2.09	0.83
2:E:619:ILE:CD1	2:E:656:MET:HB3	2.05	0.82
2:A:278:ILE:CB	2:A:281:LEU:HD23	1.96	0.82
2:E:21:ALA:HA	2:E:33:HIS:CE1	2.16	0.81
2:C:781:LEU:HD13	2:D:531:LEU:HD21	1.63	0.81
2:B:619:ILE:CG2	2:B:627:PHE:CE1	2.60	0.80
2:E:619:ILE:HD11	2:E:656:MET:HG2	1.64	0.79
2:D:619:ILE:HG22	2:D:627:PHE:CE1	2.18	0.79
2:E:619:ILE:HG23	2:E:627:PHE:HE1	1.45	0.79
2:E:281:LEU:CD1	2:E:313:GLY:HA2	1.87	0.78
2:B:571:ARG:CD	2:B:617:ASP:OD2	2.22	0.77
2:C:619:ILE:HG23	2:C:627:PHE:CE1	2.21	0.76
2:B:615:LEU:HD22	2:B:617:ASP:OD1	1.86	0.75
2:C:394:LEU:HD22	2:C:480:VAL:HA	1.68	0.75
2:C:394:LEU:HD13	2:C:480:VAL:HG22	1.68	0.75
2:E:278:ILE:HG22	2:E:281:LEU:HD23	1.67	0.75
2:E:278:ILE:CB	2:E:281:LEU:CD2	2.64	0.75
2:E:781:LEU:HD13	2:F:531:LEU:HD11	1.69	0.75
2:E:619:ILE:HG21	2:E:701:PHE:CE2	2.22	0.74
2:C:619:ILE:HG23	2:C:627:PHE:CZ	2.22	0.74
1:3:194:HIS:CE1	2:D:45:ILE:HD12	2.21	0.74
2:C:619:ILE:CG2	2:C:627:PHE:HE1	1.94	0.74
2:C:619:ILE:CG2	2:C:627:PHE:HZ	1.97	0.73
2:F:394:LEU:HD13	2:F:480:VAL:HG22	1.68	0.73
2:B:777:LEU:HD22	2:B:792:ILE:HG21	1.70	0.73
2:F:619:ILE:HG22	2:F:619:ILE:O	1.86	0.73
2:E:394:LEU:HD13	2:E:480:VAL:HG22	1.69	0.73
2:C:619:ILE:HG22	2:C:619:ILE:O	1.88	0.72
2:E:619:ILE:HG22	2:E:619:ILE:O	1.90	0.72
2:E:619:ILE:CG2	2:E:627:PHE:CE1	2.72	0.72
2:F:619:ILE:HD13	2:F:630:LEU:CD1	2.19	0.72
2:A:619:ILE:HD12	2:A:656:MET:HB3	1.70	0.72
2:A:278:ILE:CG2	2:A:281:LEU:CD2	2.52	0.71
2:C:619:ILE:HG23	2:C:622:ALA:HB3	1.73	0.71
2:A:277:PHE:CE2	2:A:279:ASP:CG	2.66	0.70
2:B:278:ILE:CG2	2:B:281:LEU:HD23	2.20	0.70
2:A:619:ILE:HG22	2:A:619:ILE:O	1.90	0.70
2:E:619:ILE:CD1	2:E:656:MET:HG2	2.21	0.69
2:A:17:ALA:HB1	2:A:29:ILE:HD11	1.74	0.69
2:A:395:ILE:HA	2:A:476:ILE:HD12	1.73	0.69
2:E:278:ILE:CG2	2:E:281:LEU:CD2	2.69	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:619:ILE:CD1	2:C:656:MET:CG	2.71	0.68
2:E:281:LEU:HD11	2:E:313:GLY:HA3	0.79	0.68
2:D:619:ILE:HD13	2:D:630:LEU:HD13	1.74	0.67
2:C:278:ILE:O	2:C:281:LEU:CD2	2.42	0.67
2:D:21:ALA:HA	2:D:33:HIS:CE1	2.30	0.67
2:B:619:ILE:HG21	2:B:701:PHE:HE2	1.60	0.67
2:C:619:ILE:HG22	2:C:627:PHE:HZ	1.59	0.67
2:D:476:ILE:O	2:D:480:VAL:HG23	1.95	0.67
2:A:26:HIS:CG	2:A:33:HIS:CE1	2.82	0.67
2:E:619:ILE:CD1	2:E:656:MET:CG	2.73	0.67
2:F:511:ILE:HG22	2:F:512:GLY:H	1.60	0.66
2:B:513:GLN:HE21	2:B:714:LEU:HD11	1.59	0.66
2:D:10:ALA:HB1	2:D:108:ILE:HD11	1.76	0.66
2:E:619:ILE:HD13	2:E:630:LEU:HD12	1.77	0.66
2:E:619:ILE:CD1	2:E:630:LEU:CD1	2.73	0.66
2:F:394:LEU:HD22	2:F:480:VAL:HA	1.76	0.65
2:A:394:LEU:HD13	2:A:480:VAL:HG22	1.79	0.65
1:4:136:PHE:CZ	2:D:431:VAL:HG11	2.32	0.65
2:B:571:ARG:HD3	2:B:617:ASP:CG	2.19	0.65
2:E:281:LEU:CG	2:E:313:GLY:CA	2.69	0.65
1:6:216:PHE:CD1	2:F:440:ALA:HA	2.32	0.65
2:C:277:PHE:HE2	2:C:279:ASP:CG	1.95	0.65
2:A:29:ILE:HD13	2:A:29:ILE:O	1.98	0.64
2:E:26:HIS:CE1	2:E:68:ILE:HB	2.33	0.64
2:F:197:SER:O	2:F:233:ILE:HG21	1.97	0.64
2:D:619:ILE:HD12	2:D:656:MET:CB	2.22	0.64
2:D:631:LEU:HD13	2:D:698:ARG:HH22	1.63	0.63
2:B:278:ILE:CB	2:B:281:LEU:CD2	2.74	0.63
2:D:394:LEU:HD13	2:D:480:VAL:HG22	1.80	0.63
2:E:619:ILE:HD13	2:E:630:LEU:CD1	2.29	0.63
2:E:38:LEU:HD22	2:E:46:ALA:CB	2.29	0.62
2:F:38:LEU:HD11	2:F:112:LEU:HD12	1.81	0.62
2:C:619:ILE:HD11	2:C:656:MET:CG	2.29	0.62
2:B:619:ILE:HD11	2:B:656:MET:HG2	1.81	0.62
2:F:476:ILE:O	2:F:480:VAL:HG23	1.99	0.62
2:E:45:ILE:HG23	2:E:141:LEU:HB2	1.81	0.62
2:A:10:ALA:HB1	2:A:108:ILE:HD11	1.81	0.62
2:D:619:ILE:HG23	2:D:626:VAL:CG1	2.29	0.62
1:4:142:LEU:HD12	1:4:146:ASN:HD22	1.64	0.61
2:E:544:LEU:HD11	2:E:693:LEU:HD13	1.80	0.61
2:D:90:LEU:HG	2:E:156:SER:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:619:ILE:HG21	2:E:701:PHE:HE2	1.63	0.61
2:E:792:ILE:HG23	2:E:803:VAL:CG1	2.31	0.61
2:F:370:ALA:O	2:F:373:ALA:HB3	2.01	0.61
2:C:570:ILE:HD12	2:C:614:VAL:HG22	1.83	0.61
2:F:665:LEU:HD21	2:F:710:VAL:HB	1.82	0.61
1:3:216:PHE:CD1	2:C:440:ALA:HA	2.36	0.61
2:D:619:ILE:HG21	2:D:630:LEU:CD1	2.30	0.61
2:B:21:ALA:HA	2:B:33:HIS:CE1	2.35	0.61
2:B:619:ILE:CD1	2:B:656:MET:HG2	2.31	0.61
2:B:619:ILE:HG21	2:B:701:PHE:CE2	2.35	0.60
2:E:398:ALA:HB1	2:E:475:ASP:CG	2.26	0.60
2:F:26:HIS:CE1	2:F:68:ILE:HB	2.37	0.60
2:F:619:ILE:HD13	2:F:630:LEU:HD12	1.82	0.60
2:C:619:ILE:CD1	2:C:656:MET:HG2	2.31	0.60
2:E:361:HIS:O	2:F:233:ILE:HG23	2.02	0.60
2:D:38:LEU:O	2:D:47:ALA:HB2	2.01	0.60
2:D:278:ILE:CG2	2:D:281:LEU:HD23	2.32	0.60
2:C:278:ILE:O	2:C:281:LEU:HD21	2.02	0.60
2:E:277:PHE:HE2	2:E:279:ASP:OD2	1.84	0.59
2:F:10:ALA:HB1	2:F:108:ILE:HD11	1.84	0.59
2:F:38:LEU:O	2:F:47:ALA:HB2	2.03	0.59
2:A:524:VAL:HG13	2:A:538:ILE:HD12	1.84	0.59
2:F:777:LEU:HD11	2:F:794:LEU:HD11	1.85	0.59
2:C:619:ILE:CG2	2:C:619:ILE:O	2.50	0.59
2:D:665:LEU:HD21	2:D:689:VAL:HG11	1.85	0.59
2:C:21:ALA:HB2	2:C:29:ILE:CG1	2.32	0.59
2:F:473:VAL:HG23	2:F:474:ASP:H	1.67	0.59
2:C:619:ILE:CD1	2:C:656:MET:CB	2.75	0.59
2:E:786:ILE:HG21	2:E:803:VAL:HG12	1.84	0.59
2:A:427:LYS:O	2:A:431:VAL:HG23	2.03	0.58
2:D:26:HIS:CE1	2:D:68:ILE:HB	2.38	0.58
2:A:398:ALA:HB1	2:A:475:ASP:CG	2.27	0.58
2:F:619:ILE:CG2	2:F:627:PHE:CD2	2.87	0.58
2:B:714:LEU:HD13	2:B:762:ALA:HB2	1.86	0.58
2:B:374:ALA:HA	2:B:394:LEU:HD12	1.85	0.58
2:F:395:ILE:HA	2:F:476:ILE:HD11	1.84	0.58
2:C:38:LEU:O	2:C:47:ALA:HB2	2.04	0.58
2:D:38:LEU:HD22	2:D:46:ALA:CB	2.34	0.58
2:E:619:ILE:HG23	2:E:627:PHE:CD1	2.38	0.58
2:F:305:ALA:HB2	2:F:329:ALA:HB1	1.84	0.58
2:D:619:ILE:HG22	2:D:627:PHE:HE1	1.64	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:ALA:HA	2:F:33:HIS:CE1	2.39	0.58
2:B:109:LEU:HD23	2:B:138:VAL:HG22	1.86	0.57
2:C:278:ILE:O	2:C:281:LEU:HG	2.04	0.57
2:B:619:ILE:CD1	2:B:656:MET:CB	2.70	0.57
2:C:278:ILE:CA	2:C:281:LEU:HD21	2.33	0.57
2:D:278:ILE:CB	2:D:281:LEU:CD2	2.76	0.57
2:A:278:ILE:HG21	2:A:281:LEU:HD23	1.78	0.57
2:C:38:LEU:HD22	2:C:46:ALA:CB	2.34	0.57
2:F:665:LEU:HD23	2:F:685:MET:HB3	1.85	0.57
2:B:619:ILE:HD13	2:B:701:PHE:HZ	1.69	0.57
2:F:351:LEU:HB3	2:F:395:ILE:HD11	1.87	0.57
2:B:777:LEU:CD2	2:B:792:ILE:HG21	2.35	0.57
2:D:373:ALA:HB3	2:D:476:ILE:HG21	1.86	0.57
2:C:476:ILE:O	2:C:480:VAL:HG23	2.04	0.57
2:D:619:ILE:HG23	2:D:626:VAL:HG11	1.86	0.57
2:C:21:ALA:HB2	2:C:29:ILE:HG12	1.85	0.57
2:A:46:ALA:H	2:A:105:THR:HB	1.70	0.57
2:D:730:LEU:HD21	2:D:774:GLU:HB3	1.86	0.57
2:F:358:TYR:HB3	2:F:361:HIS:CE1	2.40	0.56
2:F:198:ARG:HH12	2:F:335:GLN:HG3	1.70	0.56
2:A:361:HIS:CE1	2:B:234:LEU:HD11	2.41	0.56
1:6:154:LEU:HB3	1:6:204:ILE:HD12	1.85	0.56
2:A:633:VAL:HG23	2:A:639:LEU:HD23	1.86	0.56
2:B:30:GLY:H	2:B:33:HIS:CE1	2.24	0.56
2:D:382:ILE:HB	2:D:484:THR:HG23	1.88	0.56
2:A:619:ILE:O	2:A:619:ILE:CG2	2.53	0.56
2:D:278:ILE:HG22	2:D:281:LEU:HD23	1.87	0.56
2:A:619:ILE:CD1	2:A:656:MET:HG2	2.36	0.56
2:C:606:VAL:HG21	2:C:649:PHE:CE1	2.40	0.56
2:A:203:ASN:HD21	2:A:304:LEU:HD22	1.71	0.56
2:B:739:LEU:HD11	2:B:792:ILE:HD11	1.87	0.55
2:C:623:HIS:CD2	2:C:624:PRO:HD2	2.41	0.55
2:C:730:LEU:HD11	2:C:774:GLU:HG2	1.88	0.55
2:D:357:ARG:HH21	2:E:200:THR:HA	1.70	0.55
2:D:616:LEU:HB2	2:D:619:ILE:HD11	1.88	0.55
2:C:26:HIS:CG	2:C:33:HIS:CE1	2.94	0.55
2:F:619:ILE:CD1	2:F:630:LEU:CD1	2.83	0.55
2:A:631:LEU:HD22	2:A:698:ARG:HH22	1.70	0.55
2:D:364:VAL:HG12	2:D:365:SER:HA	1.87	0.55
2:E:731:THR:HG22	2:E:741:ILE:HB	1.88	0.55
1:5:216:PHE:CD1	2:E:440:ALA:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LEU:HD22	2:B:46:ALA:CB	2.37	0.55
2:B:619:ILE:HD11	2:B:656:MET:CG	2.36	0.55
2:E:506:LEU:HD13	2:E:554:LEU:HD11	1.88	0.55
2:A:18:GLN:OE1	2:A:29:ILE:HD12	2.07	0.55
2:E:278:ILE:HG21	2:E:281:LEU:HD23	1.84	0.55
2:F:681:ASN:HB3	2:F:685:MET:HE3	1.88	0.55
2:B:682:HIS:CE1	2:B:718:HIS:CE1	2.95	0.55
1:4:154:LEU:HD22	1:4:212:ILE:HD11	1.88	0.54
2:C:772:HIS:CE1	2:C:801:PHE:CE2	2.95	0.54
2:D:362:HIS:CD2	2:E:232:GLU:HB2	2.42	0.54
2:E:26:HIS:CG	2:E:33:HIS:CE1	2.94	0.54
2:E:513:GLN:HE22	2:E:550:GLY:HA3	1.72	0.54
2:C:31:THR:HB	2:C:120:ALA:H	1.72	0.54
2:E:739:LEU:CD2	2:F:531:LEU:HD12	2.37	0.54
2:E:667:ARG:HB2	2:E:681:ASN:HD21	1.72	0.54
2:C:276:LEU:HD23	2:C:309:LEU:HA	1.89	0.54
1:3:140:ILE:HG12	1:3:216:PHE:HB3	1.89	0.54
2:D:281:LEU:HG	2:D:314:ALA:H	1.73	0.54
1:2:216:PHE:CD1	2:B:440:ALA:HA	2.43	0.54
2:B:303:SER:HB3	2:B:309:LEU:HB2	1.90	0.54
2:D:198:ARG:HH12	2:D:335:GLN:HG3	1.72	0.54
2:F:373:ALA:HB2	2:F:492:ALA:N	2.23	0.54
1:6:133:PHE:CE2	1:6:163:LEU:HB2	2.42	0.54
2:D:526:ARG:O	2:D:531:LEU:HD23	2.08	0.53
2:B:26:HIS:CE1	2:B:68:ILE:HB	2.44	0.53
2:E:38:LEU:HD22	2:E:46:ALA:HB1	1.90	0.53
2:F:377:LEU:HD13	2:F:495:GLU:HB2	1.90	0.53
2:B:790:GLN:HE21	2:B:805:THR:HG23	1.72	0.53
2:F:16:LEU:HB3	2:F:37:GLY:HA2	1.91	0.53
2:A:544:LEU:HB2	2:A:710:VAL:HG22	1.90	0.53
2:B:713:SER:HA	2:B:714:LEU:HD12	1.90	0.53
2:C:373:ALA:HB2	2:C:492:ALA:N	2.24	0.53
2:E:198:ARG:HH12	2:E:335:GLN:HG3	1.72	0.53
2:A:587:VAL:HA	2:B:594:VAL:H	1.74	0.53
2:D:398:ALA:HB1	2:D:475:ASP:CG	2.33	0.53
2:F:27:ASN:HA	2:F:75:SER:HA	1.89	0.53
2:A:278:ILE:O	2:A:281:LEU:HG	2.09	0.53
2:D:91:SER:CB	2:D:108:ILE:HD13	2.39	0.53
2:F:503:GLU:H	2:F:525:ARG:HH21	1.56	0.53
2:A:55:LEU:HD13	2:A:124:LEU:HD22	1.90	0.53
2:B:613:VAL:CG1	2:B:655:ILE:HD12	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:665:LEU:HD21	2:C:710:VAL:CG1	2.39	0.53
2:E:198:ARG:HH11	2:E:201:LYS:HB2	1.74	0.53
2:E:416:LEU:HB3	2:E:453:VAL:HG22	1.90	0.53
2:A:13:VAL:HB	2:A:38:LEU:HD23	1.91	0.53
2:C:396:ASP:HB3	2:D:198:ARG:HD3	1.90	0.53
2:F:665:LEU:HD11	2:F:689:VAL:HG11	1.91	0.53
1:1:136:PHE:CE2	1:1:216:PHE:CD2	2.97	0.53
1:2:156:SER:HB2	1:2:203:ILE:HD11	1.91	0.53
1:3:204:ILE:HG21	1:3:211:THR:CB	2.39	0.53
2:E:402:VAL:HG13	2:E:405:ARG:HE	1.73	0.53
2:E:619:ILE:CD1	2:E:656:MET:CB	2.74	0.53
2:A:619:ILE:HG23	2:A:627:PHE:CE1	2.44	0.52
2:F:31:THR:H	2:F:83:ARG:HH21	1.57	0.52
1:3:133:PHE:CD2	1:3:139:VAL:HG22	2.43	0.52
1:3:136:PHE:CE1	2:C:431:VAL:HG11	2.45	0.52
2:D:473:VAL:HG23	2:D:474:ASP:H	1.73	0.52
2:E:64:VAL:HG22	2:E:123:VAL:HG21	1.92	0.52
1:4:136:PHE:CZ	1:4:161:TYR:CE1	2.97	0.52
1:6:216:PHE:CZ	2:F:431:VAL:HG22	2.45	0.52
2:D:168:ARG:HE	2:D:169:ASP:H	1.57	0.52
2:E:619:ILE:O	2:E:619:ILE:CG2	2.56	0.52
2:D:678:GLU:CD	2:D:678:GLU:H	2.17	0.52
2:E:281:LEU:HG	2:E:313:GLY:HA2	1.90	0.52
2:F:91:SER:CB	2:F:108:ILE:HD13	2.40	0.52
2:E:17:ALA:HA	2:E:33:HIS:HB3	1.91	0.52
2:F:723:VAL:HA	2:F:769:ILE:HD11	1.92	0.52
2:A:558:LEU:HD13	2:A:653:ILE:HG21	1.90	0.52
2:B:55:LEU:HD13	2:B:124:LEU:HD22	1.92	0.52
2:C:398:ALA:HB1	2:C:475:ASP:CG	2.34	0.52
2:E:14:LEU:O	2:E:17:ALA:HB3	2.10	0.52
2:E:547:THR:H	2:E:763:ARG:HE	1.56	0.52
2:E:665:LEU:HD22	2:E:712:HIS:HA	1.92	0.52
1:6:203:ILE:HG22	2:F:436:PHE:CZ	2.45	0.52
2:A:26:HIS:CD2	2:A:33:HIS:CE1	2.98	0.52
2:B:665:LEU:HD21	2:B:710:VAL:HB	1.90	0.52
2:D:278:ILE:O	2:D:281:LEU:HD21	2.10	0.52
2:E:377:LEU:HD12	2:E:480:VAL:HG21	1.92	0.52
2:E:387:LEU:HD22	2:E:387:LEU:H	1.74	0.52
1:1:216:PHE:CD1	2:A:440:ALA:HA	2.45	0.52
2:A:38:LEU:O	2:A:47:ALA:HB2	2.10	0.52
2:A:156:SER:H	2:F:90:LEU:HG	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:THR:HG23	2:D:87:VAL:HG21	1.90	0.52
2:B:616:LEU:HD13	2:B:630:LEU:HD22	1.92	0.51
2:D:363:ARG:HD2	2:D:403:ARG:H	1.75	0.51
2:B:26:HIS:CG	2:B:33:HIS:CE1	2.98	0.51
2:B:619:ILE:CD1	2:B:656:MET:CG	2.88	0.51
2:D:786:ILE:HD13	2:D:792:ILE:HG23	1.91	0.51
1:1:216:PHE:CZ	2:A:431:VAL:HG22	2.45	0.51
2:D:619:ILE:CG2	2:D:626:VAL:HG13	2.41	0.51
2:E:168:ARG:HH22	2:E:179:LEU:HD13	1.75	0.51
2:E:615:LEU:CD2	2:E:617:ASP:OD1	2.51	0.51
2:C:619:ILE:HG22	2:C:627:PHE:CZ	2.35	0.51
2:D:14:LEU:O	2:D:17:ALA:HB3	2.11	0.51
2:E:722:ILE:HG23	2:E:765:LEU:HD22	1.91	0.51
2:F:26:HIS:CG	2:F:33:HIS:CE1	2.98	0.51
2:F:790:GLN:HE21	2:F:805:THR:HG23	1.75	0.51
2:B:361:HIS:CD2	2:B:363:ARG:HB2	2.46	0.51
2:C:46:ALA:HB2	2:C:105:THR:O	2.10	0.51
2:A:17:ALA:CB	2:A:29:ILE:HD11	2.40	0.51
2:B:192:VAL:CG1	2:B:221:LEU:HD21	2.40	0.51
2:D:278:ILE:O	2:D:281:LEU:CD2	2.58	0.51
1:5:216:PHE:HA	2:E:440:ALA:HA	1.93	0.51
2:F:665:LEU:HA	2:F:685:MET:HG2	1.93	0.51
2:A:619:ILE:HG21	2:A:701:PHE:CE2	2.45	0.50
2:D:505:ILE:HG22	2:D:509:ARG:HH22	1.75	0.50
2:F:664:GLU:O	2:F:685:MET:HE2	2.11	0.50
2:C:17:ALA:HB1	2:C:29:ILE:CG2	2.41	0.50
2:A:476:ILE:O	2:A:480:VAL:HG23	2.11	0.50
2:C:513:GLN:H	2:C:718:HIS:CD2	2.29	0.50
2:D:660:VAL:HG21	2:D:695:ARG:HH22	1.76	0.50
2:F:211:GLY:H	2:F:213:GLY:H	1.59	0.50
2:F:363:ARG:HH22	2:F:470:GLU:CD	2.19	0.50
2:F:427:LYS:HG3	2:F:443:ARG:HA	1.92	0.50
2:A:528:ARG:HE	2:A:562:ILE:HG23	1.77	0.50
2:F:382:ILE:HB	2:F:484:THR:HG23	1.93	0.50
1:1:133:PHE:CE2	1:1:163:LEU:HB2	2.46	0.50
2:A:96:ARG:HE	2:A:101:SER:HA	1.76	0.50
2:B:46:ALA:HB1	2:B:109:LEU:HB2	1.93	0.50
2:B:100:HIS:CD2	2:B:107:HIS:CE1	2.99	0.50
2:D:613:VAL:CG1	2:D:655:ILE:HD12	2.42	0.50
2:F:619:ILE:O	2:F:619:ILE:CG2	2.59	0.50
2:A:31:THR:HB	2:A:120:ALA:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:378:SER:OG	2:A:394:LEU:HD11	2.12	0.50
2:B:506:LEU:HD13	2:B:554:LEU:HD11	1.93	0.50
2:D:31:THR:CG2	2:D:87:VAL:HG21	2.42	0.50
2:C:730:LEU:HD11	2:C:774:GLU:CG	2.42	0.50
2:D:545:GLY:HA2	2:D:665:LEU:HD22	1.94	0.50
2:F:786:ILE:HD13	2:F:792:ILE:HD11	1.94	0.50
2:B:277:PHE:HE2	2:B:279:ASP:OD2	1.95	0.49
2:D:619:ILE:HG22	2:D:619:ILE:O	2.12	0.49
2:A:786:ILE:HD13	2:A:792:ILE:HG23	1.93	0.49
2:C:278:ILE:O	2:C:281:LEU:CG	2.61	0.49
2:C:198:ARG:HH12	2:C:335:GLN:HG3	1.78	0.49
2:E:281:LEU:HD11	2:E:313:GLY:N	2.09	0.49
2:E:619:ILE:HG21	2:E:701:PHE:CZ	2.47	0.49
2:A:536:ARG:HH22	2:F:770:GLN:HG3	1.77	0.49
2:A:619:ILE:HD12	2:A:656:MET:CB	2.41	0.49
2:B:619:ILE:HD13	2:B:701:PHE:CZ	2.47	0.49
2:C:100:HIS:CD2	2:C:107:HIS:CE1	3.01	0.49
2:D:619:ILE:CG2	2:D:626:VAL:CG1	2.90	0.49
1:5:136:PHE:CD1	1:5:161:TYR:CE1	3.00	0.49
2:E:361:HIS:CD2	2:F:233:ILE:HG22	2.48	0.49
2:E:397:GLU:HA	2:F:198:ARG:HE	1.78	0.49
1:4:137:GLU:CD	2:D:443:ARG:HE	2.21	0.49
2:A:46:ALA:HB2	2:A:105:THR:O	2.13	0.49
2:C:278:ILE:CB	2:C:281:LEU:HD23	1.94	0.49
1:5:133:PHE:CG	1:5:139:VAL:HG22	2.48	0.49
2:B:278:ILE:HG22	2:B:281:LEU:HD23	1.94	0.49
2:C:370:ALA:O	2:C:373:ALA:HB3	2.12	0.49
2:B:398:ALA:HB1	2:B:475:ASP:HB3	1.95	0.49
2:C:786:ILE:HD12	2:C:792:ILE:HD13	1.95	0.49
1:3:140:ILE:CB	2:C:443:ARG:HE	2.26	0.48
2:A:394:LEU:HD22	2:A:480:VAL:HA	1.93	0.48
2:B:20:GLU:HB3	2:B:33:HIS:CG	2.47	0.48
2:C:716:LYS:H	2:C:719:LEU:HD12	1.78	0.48
2:F:371:ILE:O	2:F:374:ALA:HB3	2.12	0.48
2:D:371:ILE:HD12	2:D:395:ILE:HD13	1.95	0.48
2:D:387:LEU:H	2:D:387:LEU:HD22	1.78	0.48
2:B:281:LEU:HG	2:B:314:ALA:H	1.78	0.48
2:B:714:LEU:HD23	2:B:718:HIS:CG	2.48	0.48
2:C:685:MET:HG3	2:C:712:HIS:CD2	2.47	0.48
2:B:29:ILE:HG23	2:B:33:HIS:HD1	1.78	0.48
2:C:46:ALA:H	2:C:105:THR:HB	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:26:HIS:CG	2:E:33:HIS:HE1	2.30	0.48
2:F:46:ALA:HB2	2:F:105:THR:O	2.13	0.48
2:F:363:ARG:CG	2:F:403:ARG:HE	2.26	0.48
1:5:136:PHE:CZ	1:5:154:LEU:HD22	2.49	0.48
2:C:289:GLY:H	2:C:321:ARG:HH12	1.60	0.48
2:C:619:ILE:HD11	2:C:656:MET:HG3	1.95	0.48
2:E:394:LEU:HD22	2:E:480:VAL:HA	1.96	0.48
1:6:216:PHE:CE1	2:F:440:ALA:HA	2.47	0.48
2:C:370:ALA:HB1	2:C:476:ILE:HD12	1.96	0.48
2:C:394:LEU:HD21	2:C:483:TRP:CE3	2.48	0.48
2:C:535:LYS:HZ3	2:C:536:ARG:HG3	1.78	0.48
2:F:631:LEU:HD23	2:F:701:PHE:HA	1.96	0.48
1:1:140:ILE:HD13	1:1:216:PHE:O	2.12	0.48
2:A:355:ARG:HA	2:A:358:TYR:CE1	2.49	0.48
2:B:364:VAL:HG23	2:B:365:SER:HA	1.95	0.48
2:D:355:ARG:HD3	2:D:371:ILE:HD11	1.95	0.48
2:D:396:ASP:HB3	2:E:198:ARG:HD3	1.94	0.48
2:E:619:ILE:HD12	2:E:656:MET:CG	2.37	0.48
1:4:215:HIS:O	1:4:216:PHE:CD1	2.67	0.48
2:C:18:GLN:O	2:C:21:ALA:HB3	2.14	0.48
2:C:584:SER:HB3	2:D:582:SER:H	1.79	0.48
2:E:352:GLN:HE22	2:E:368:ASP:HA	1.79	0.48
1:3:136:PHE:CE1	1:3:161:TYR:CE1	3.01	0.47
2:B:278:ILE:CB	2:B:281:LEU:HD23	2.44	0.47
2:B:394:LEU:HD22	2:B:480:VAL:HG22	1.96	0.47
2:D:619:ILE:HG23	2:D:626:VAL:HG13	1.96	0.47
2:E:13:VAL:HG11	2:E:38:LEU:HD23	1.96	0.47
2:E:427:LYS:HG3	2:E:443:ARG:HA	1.95	0.47
2:A:730:LEU:HA	2:A:733:ARG:HE	1.79	0.47
2:C:730:LEU:HD21	2:C:774:GLU:HG3	1.95	0.47
2:D:689:VAL:HG11	2:D:710:VAL:HG13	1.96	0.47
2:E:476:ILE:O	2:E:480:VAL:HG23	2.15	0.47
2:F:398:ALA:HB1	2:F:475:ASP:CG	2.39	0.47
2:C:719:LEU:HD21	2:C:755:GLY:HA3	1.96	0.47
2:F:665:LEU:CD1	2:F:689:VAL:HG11	2.44	0.47
2:B:32:GLU:HG3	2:B:33:HIS:CD2	2.50	0.47
2:D:16:LEU:HB3	2:D:37:GLY:HA2	1.96	0.47
2:F:719:LEU:HD22	2:F:752:ALA:O	2.14	0.47
2:A:382:ILE:HA	2:A:383:SER:HB3	1.96	0.47
2:B:665:LEU:HD23	2:B:685:MET:HB3	1.97	0.47
2:E:619:ILE:HD13	2:E:701:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:196:LEU:HD12	2:A:275:ILE:HD12	1.96	0.47
2:A:619:ILE:HG21	2:A:701:PHE:HE2	1.80	0.47
2:C:26:HIS:CE1	2:C:68:ILE:HB	2.50	0.47
2:C:473:VAL:HG23	2:C:474:ASP:H	1.80	0.47
2:C:791:HIS:H	2:C:807:ALA:HB2	1.80	0.47
2:D:46:ALA:H	2:D:105:THR:HB	1.79	0.47
2:E:399:GLY:CA	2:E:471:VAL:HG13	2.45	0.47
2:E:739:LEU:HD13	2:E:741:ILE:HD11	1.97	0.47
2:E:741:ILE:HD12	2:E:777:LEU:HG	1.97	0.47
1:1:140:ILE:HD12	2:A:443:ARG:CZ	2.44	0.47
1:3:184:GLU:HA	2:C:81:THR:HG22	1.96	0.47
2:F:363:ARG:CG	2:F:403:ARG:HB2	2.45	0.47
1:3:146:ASN:HB2	1:3:178:GLN:HE22	1.80	0.47
2:A:589:SER:H	2:B:591:PRO:HA	1.80	0.47
2:B:739:LEU:HD13	2:B:788:LYS:HA	1.97	0.47
2:E:46:ALA:HA	2:E:138:VAL:HG13	1.96	0.47
2:E:398:ALA:HA	2:E:401:LYS:HB3	1.97	0.47
2:A:18:GLN:O	2:A:21:ALA:HB3	2.15	0.47
2:D:168:ARG:NE	2:D:169:ASP:H	2.13	0.47
2:E:685:MET:O	2:E:710:VAL:HG11	2.15	0.47
2:F:777:LEU:HD22	2:F:792:ILE:HG21	1.96	0.47
2:E:278:ILE:CB	2:E:281:LEU:HD23	2.39	0.46
2:F:38:LEU:HD13	2:F:46:ALA:HB1	1.96	0.46
2:F:716:LYS:H	2:F:717:LYS:HB3	1.79	0.46
2:A:26:HIS:CE1	2:A:68:ILE:HB	2.50	0.46
2:C:6:PHE:HA	2:C:103:VAL:H	1.81	0.46
2:F:515:GLU:CD	2:F:515:GLU:H	2.23	0.46
2:B:668:ASN:HB3	2:B:715:GLU:HB2	1.97	0.46
2:E:777:LEU:HG	2:E:792:ILE:HG21	1.96	0.46
2:F:613:VAL:CG1	2:F:655:ILE:HD12	2.46	0.46
2:F:665:LEU:HG	2:F:689:VAL:HG21	1.97	0.46
2:F:726:MET:HB2	2:F:769:ILE:HD13	1.97	0.46
2:D:786:ILE:HD13	2:D:803:VAL:HG11	1.97	0.46
2:F:772:HIS:CE1	2:F:801:PHE:CD1	3.03	0.46
2:B:305:ALA:HB2	2:B:329:ALA:CB	2.45	0.46
2:F:370:ALA:HB1	2:F:476:ILE:HD12	1.97	0.46
2:F:619:ILE:HG23	2:F:627:PHE:CD2	2.50	0.46
1:1:153:THR:HG23	1:1:202:LEU:HD21	1.98	0.46
1:2:140:ILE:HB	2:B:443:ARG:HH11	1.81	0.46
2:A:232:GLU:H	2:F:403:ARG:HD2	1.80	0.46
2:C:20:GLU:HB3	2:C:33:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:727:SER:O	2:E:731:THR:HG23	2.16	0.46
2:A:398:ALA:C	2:A:400:SER:H	2.24	0.46
2:C:14:LEU:O	2:C:17:ALA:HB3	2.15	0.46
2:D:506:LEU:HD13	2:D:554:LEU:HD11	1.97	0.46
2:F:713:SER:HA	2:F:718:HIS:CG	2.50	0.46
2:E:515:GLU:CD	2:E:712:HIS:CD2	2.93	0.46
1:1:216:PHE:CE1	2:A:443:ARG:HB2	2.50	0.46
2:A:165:SER:HB2	2:A:166:LEU:HB2	1.98	0.46
2:A:385:ARG:HH22	2:B:335:GLN:HA	1.81	0.46
2:A:780:GLU:HG2	2:A:783:ARG:HH21	1.81	0.46
2:B:734:LEU:HB2	2:B:741:ILE:HD11	1.98	0.46
2:E:36:LEU:HD11	2:E:64:VAL:HG11	1.98	0.46
2:E:411:PRO:HA	2:E:460:TRP:CE2	2.51	0.46
2:F:395:ILE:HA	2:F:476:ILE:CD1	2.46	0.46
2:A:91:SER:CB	2:A:108:ILE:HD13	2.46	0.46
2:E:383:SER:H	2:E:390:LYS:HD3	1.82	0.46
2:E:613:VAL:CG1	2:E:655:ILE:HD12	2.46	0.46
2:E:739:LEU:HD22	2:E:741:ILE:HD11	1.97	0.46
1:1:202:LEU:HD23	1:1:203:ILE:N	2.31	0.45
2:A:83:ARG:HH21	2:A:119:VAL:HG22	1.81	0.45
2:E:619:ILE:CG2	2:E:701:PHE:HE2	2.26	0.45
2:A:198:ARG:CD	2:A:201:LYS:HB2	2.46	0.45
2:A:416:LEU:HB3	2:A:453:VAL:HG22	1.96	0.45
2:C:13:VAL:HB	2:C:38:LEU:HD23	1.99	0.45
2:C:361:HIS:CD2	2:D:234:LEU:HD12	2.51	0.45
2:C:703:ASN:HB2	2:C:704:ARG:HH11	1.80	0.45
1:1:142:LEU:HA	1:1:185:TYR:CD2	2.51	0.45
2:B:41:GLU:HG2	2:B:47:ALA:HB2	1.98	0.45
2:B:730:LEU:CD2	2:B:774:GLU:HG3	2.47	0.45
2:D:17:ALA:HA	2:D:33:HIS:HB3	1.99	0.45
2:E:45:ILE:HG22	2:E:138:VAL:HG12	1.99	0.45
2:F:523:ALA:HA	2:F:526:ARG:HE	1.80	0.45
2:B:615:LEU:CD2	2:B:617:ASP:OD1	2.59	0.45
2:C:20:GLU:HB3	2:C:33:HIS:CG	2.51	0.45
2:C:26:HIS:HB2	2:C:33:HIS:CE1	2.51	0.45
2:E:358:TYR:CE2	2:F:200:THR:HA	2.51	0.45
1:4:142:LEU:HD11	1:4:182:LEU:HD22	1.99	0.45
1:6:216:PHE:CE2	2:F:431:VAL:HG22	2.52	0.45
2:A:355:ARG:HE	2:A:395:ILE:HG21	1.82	0.45
2:B:558:LEU:CD1	2:B:655:ILE:HD11	2.47	0.45
2:B:624:PRO:HA	2:B:627:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:212:ILE:HD12	1:4:216:PHE:CD2	2.52	0.45
2:B:26:HIS:CD2	2:B:33:HIS:NE2	2.85	0.45
2:D:777:LEU:HD21	2:D:794:LEU:HB2	1.99	0.45
2:E:373:ALA:HB2	2:E:492:ALA:HA	1.98	0.45
2:E:499:LEU:HD11	2:E:529:ALA:HB2	1.99	0.45
2:F:55:LEU:HD13	2:F:124:LEU:HD22	1.99	0.45
1:2:203:ILE:HG21	2:B:434:GLN:HE21	1.82	0.45
1:4:194:HIS:CE1	2:E:141:LEU:O	2.70	0.45
2:D:394:LEU:H	2:D:394:LEU:HG	1.60	0.45
2:B:476:ILE:O	2:B:480:VAL:HG23	2.16	0.45
2:B:528:ARG:CZ	2:B:562:ILE:HA	2.47	0.45
2:B:558:LEU:HD12	2:B:655:ILE:HD11	1.99	0.45
2:B:689:VAL:HG11	2:B:710:VAL:HG12	1.98	0.45
2:D:361:HIS:CE1	2:E:234:LEU:HD12	2.52	0.45
2:E:460:TRP:CG	2:E:463:LYS:HB2	2.52	0.45
2:A:198:ARG:HH12	2:A:335:GLN:HG3	1.81	0.45
2:A:366:ILE:HB	2:A:367:THR:HA	1.99	0.45
2:B:38:LEU:O	2:B:47:ALA:HB2	2.17	0.45
2:B:702:ILE:HA	2:B:705:ILE:HD12	1.97	0.45
2:C:382:ILE:HA	2:C:383:SER:CB	2.47	0.45
2:C:515:GLU:OE2	2:C:712:HIS:CD2	2.70	0.45
2:E:770:GLN:HA	2:E:774:GLU:CD	2.42	0.45
2:F:520:VAL:HG11	2:F:558:LEU:HD11	1.98	0.45
1:2:136:PHE:HA	1:2:161:TYR:CD2	2.52	0.45
2:A:317:LEU:HD12	2:A:317:LEU:H	1.82	0.45
2:C:367:THR:O	2:C:370:ALA:HB3	2.17	0.45
2:F:661:GLY:HA3	2:F:689:VAL:HG13	1.99	0.45
2:F:713:SER:HA	2:F:718:HIS:CD2	2.52	0.45
2:A:20:GLU:HB3	2:A:33:HIS:CD2	2.52	0.44
2:B:730:LEU:HD23	2:B:774:GLU:HG3	1.99	0.44
2:D:574:MET:SD	2:D:619:ILE:HG12	2.57	0.44
2:E:411:PRO:HA	2:E:460:TRP:CD2	2.52	0.44
2:C:55:LEU:HD13	2:C:124:LEU:HD22	1.99	0.44
2:D:137:GLN:HA	2:D:140:GLN:HG2	1.99	0.44
2:F:27:ASN:HB2	2:F:76:GLN:H	1.83	0.44
1:1:133:PHE:CD2	1:1:139:VAL:HG22	2.51	0.44
1:5:204:ILE:HD13	1:5:204:ILE:N	2.32	0.44
2:A:278:ILE:O	2:A:281:LEU:CD2	2.65	0.44
2:C:21:ALA:HA	2:C:33:HIS:CE1	2.53	0.44
2:D:503:GLU:H	2:D:525:ARG:HH21	1.65	0.44
2:D:619:ILE:HG21	2:D:630:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:277:PHE:CE2	2:E:279:ASP:OD2	2.59	0.44
2:E:394:LEU:HA	2:E:479:VAL:HG11	2.00	0.44
2:E:449:LEU:O	2:E:453:VAL:HG23	2.17	0.44
2:F:583:THR:HG23	2:F:584:SER:H	1.82	0.44
1:2:184:GLU:HA	2:B:81:THR:HG22	2.00	0.44
2:A:14:LEU:O	2:A:17:ALA:HB3	2.18	0.44
2:D:113:ILE:HG21	2:D:135:ARG:HB2	1.99	0.44
2:E:631:LEU:HD13	2:E:698:ARG:HH22	1.82	0.44
1:5:139:VAL:HG21	1:5:154:LEU:HD11	1.98	0.44
2:F:278:ILE:HD11	2:F:309:LEU:HD11	1.99	0.44
2:B:25:GLY:O	2:B:26:HIS:CD2	2.71	0.44
2:D:35:LEU:HD11	2:D:124:LEU:HD21	1.99	0.44
2:D:458:LYS:HA	2:D:461:LYS:HG2	2.00	0.44
2:D:624:PRO:HA	2:D:627:PHE:CD2	2.53	0.44
1:3:194:HIS:HE1	2:D:45:ILE:HD12	1.79	0.44
1:4:133:PHE:CD2	1:4:139:VAL:HG22	2.53	0.44
1:4:133:PHE:CE2	1:4:163:LEU:HB2	2.53	0.44
1:4:136:PHE:CE2	2:D:431:VAL:HG11	2.52	0.44
2:A:21:ALA:HB2	2:A:29:ILE:CG2	2.48	0.44
2:B:395:ILE:HA	2:B:476:ILE:CD1	2.48	0.44
2:B:503:GLU:CD	2:B:503:GLU:H	2.26	0.44
2:C:686:LYS:HA	2:C:710:VAL:HG11	2.00	0.44
2:E:55:LEU:HD13	2:E:124:LEU:HD22	2.00	0.44
1:3:140:ILE:HD12	1:3:140:ILE:H	1.82	0.44
2:A:198:ARG:CZ	2:F:397:GLU:HA	2.48	0.44
2:A:351:LEU:HD22	2:A:392:ILE:HG12	1.99	0.44
2:B:397:GLU:HA	2:C:198:ARG:CZ	2.48	0.44
2:C:17:ALA:HB2	2:C:34:ILE:HA	2.00	0.44
2:C:781:LEU:HD12	2:C:787:HIS:HA	1.99	0.44
2:E:196:LEU:HD11	2:E:275:ILE:HD12	2.00	0.44
2:F:370:ALA:HB2	2:F:472:THR:C	2.43	0.44
2:F:715:GLU:H	2:F:718:HIS:HB3	1.83	0.44
2:B:619:ILE:O	2:B:619:ILE:HG22	2.18	0.44
2:B:719:LEU:HD13	2:B:752:ALA:O	2.18	0.44
2:C:198:ARG:HH22	2:C:335:GLN:NE2	2.16	0.44
2:E:281:LEU:HD12	2:E:313:GLY:CA	2.10	0.44
2:F:394:LEU:CD2	2:F:480:VAL:HA	2.46	0.44
1:3:204:ILE:HG21	1:3:211:THR:HB	2.00	0.43
2:A:394:LEU:H	2:A:394:LEU:HG	1.57	0.43
2:A:394:LEU:HD21	2:A:483:TRP:CE3	2.53	0.43
2:B:517:VAL:HG22	2:B:554:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:198:ARG:HB2	2:C:202:ASN:HA	2.00	0.43
2:F:730:LEU:HD23	2:F:774:GLU:HG2	1.99	0.43
1:4:215:HIS:C	2:D:440:ALA:HB2	2.43	0.43
2:A:282:HIS:CG	2:A:319:GLU:HB3	2.53	0.43
1:2:142:LEU:HD21	1:2:182:LEU:HA	2.00	0.43
1:2:204:ILE:HD11	1:2:212:ILE:CD1	2.48	0.43
1:3:133:PHE:CE2	1:3:163:LEU:HB2	2.52	0.43
1:3:195:ARG:HH11	2:D:146:GLU:H	1.65	0.43
2:A:391:ALA:HA	2:A:394:LEU:HD12	2.00	0.43
2:A:624:PRO:HA	2:A:627:PHE:CD2	2.53	0.43
2:A:633:VAL:HG13	2:A:649:PHE:CG	2.53	0.43
2:C:358:TYR:CZ	2:C:364:VAL:HG21	2.53	0.43
2:E:633:VAL:HG13	2:E:649:PHE:CD1	2.53	0.43
2:F:26:HIS:H	2:F:26:HIS:CD2	2.37	0.43
1:2:140:ILE:HG12	1:2:216:PHE:HB3	1.99	0.43
1:6:137:GLU:CB	2:F:443:ARG:HD3	2.49	0.43
2:A:545:GLY:H	2:A:665:LEU:HD13	1.84	0.43
2:B:366:ILE:HB	2:B:367:THR:HA	1.99	0.43
2:C:633:VAL:HG13	2:C:649:PHE:CG	2.53	0.43
2:D:29:ILE:HB	2:D:80:TYR:HA	2.00	0.43
2:D:398:ALA:C	2:D:400:SER:H	2.26	0.43
1:3:140:ILE:CG1	1:3:216:PHE:HB3	2.49	0.43
1:6:137:GLU:HB2	2:F:443:ARG:HH11	1.84	0.43
2:B:17:ALA:HA	2:B:33:HIS:HB3	2.00	0.43
2:F:316:THR:H	2:F:319:GLU:HB2	1.82	0.43
1:2:161:TYR:CE1	2:B:431:VAL:HG11	2.54	0.43
1:4:156:SER:HB2	1:4:203:ILE:HD11	1.98	0.43
1:5:140:ILE:HG12	1:5:216:PHE:CB	2.49	0.43
2:D:106:GLU:CD	2:D:106:GLU:H	2.26	0.43
2:F:413:LEU:HD13	2:F:456:THR:HB	2.01	0.43
1:4:136:PHE:CE2	1:4:161:TYR:CD1	3.07	0.43
1:5:146:ASN:HD21	1:5:181:ILE:HG22	1.84	0.43
2:A:362:HIS:CE1	2:B:232:GLU:HB3	2.53	0.43
2:D:777:LEU:O	2:D:781:LEU:HG	2.19	0.43
2:E:397:GLU:HB2	2:F:198:ARG:HH21	1.84	0.43
2:F:363:ARG:HG2	2:F:403:ARG:HB2	2.00	0.43
2:F:412:ASN:C	2:F:414:LYS:H	2.27	0.43
1:1:195:ARG:HE	1:1:195:ARG:HA	1.84	0.43
2:A:276:LEU:HD23	2:A:309:LEU:HA	2.01	0.43
2:A:536:ARG:HH12	2:F:770:GLN:HB2	1.84	0.43
2:A:678:GLU:C	2:A:680:GLN:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:PHE:CD1	2:B:611:TYR:HB2	2.53	0.43
2:C:577:TYR:CD1	2:C:597:ASP:HB2	2.54	0.43
2:D:530:GLY:C	2:D:531:LEU:HD22	2.44	0.43
2:E:739:LEU:HD21	2:F:531:LEU:HD12	2.00	0.43
2:F:49:ALA:O	2:F:53:LEU:HD22	2.18	0.43
1:3:136:PHE:HB2	2:C:427:LYS:HZ3	1.84	0.43
1:6:139:VAL:HG13	1:6:154:LEU:HD13	2.01	0.43
2:A:516:ALA:HB2	2:A:710:VAL:O	2.19	0.43
2:C:361:HIS:CE1	2:D:198:ARG:O	2.72	0.43
2:D:778:SER:HA	2:D:781:LEU:HD12	2.01	0.43
2:E:363:ARG:HG2	2:E:364:VAL:HG23	2.00	0.43
2:A:619:ILE:HG23	2:A:627:PHE:HE1	1.83	0.43
2:A:731:THR:HG22	2:A:741:ILE:HB	2.01	0.43
2:B:678:GLU:C	2:B:680:GLN:H	2.26	0.43
2:C:358:TYR:CE2	2:C:364:VAL:HG21	2.54	0.43
2:C:377:LEU:HD13	2:C:495:GLU:HB2	2.01	0.43
2:C:570:ILE:HD12	2:C:606:VAL:HG22	2.00	0.43
2:C:665:LEU:HD23	2:C:685:MET:HB2	2.00	0.43
2:D:278:ILE:CB	2:D:281:LEU:HD23	2.47	0.43
2:D:704:ARG:HG3	2:D:704:ARG:HH11	1.84	0.43
1:6:136:PHE:CD1	2:F:431:VAL:HG21	2.54	0.42
1:2:147:VAL:HG13	1:2:148:ASN:H	1.83	0.42
2:C:113:ILE:HG23	2:C:131:LEU:HB3	2.01	0.42
2:D:26:HIS:HB2	2:D:33:HIS:HE1	1.83	0.42
2:D:513:GLN:HG3	2:D:712:HIS:H	1.84	0.42
2:F:633:VAL:HG13	2:F:649:PHE:CG	2.54	0.42
1:4:136:PHE:CD2	1:4:216:PHE:CE2	3.07	0.42
2:B:281:LEU:HD21	2:B:313:GLY:HA2	1.89	0.42
2:E:53:LEU:HD21	2:E:134:ALA:HA	2.00	0.42
2:A:233:ILE:H	2:F:403:ARG:NH1	2.17	0.42
2:B:739:LEU:HD11	2:B:792:ILE:CD1	2.49	0.42
2:C:385:ARG:HH21	2:D:331:GLU:HA	1.85	0.42
2:E:363:ARG:HH21	2:E:468:ASN:HA	1.84	0.42
1:1:204:ILE:HD11	1:1:212:ILE:HD11	2.02	0.42
2:A:17:ALA:HA	2:A:33:HIS:HB3	2.00	0.42
2:B:661:GLY:CA	2:B:689:VAL:HG13	2.50	0.42
2:C:363:ARG:HD3	2:C:400:SER:HA	2.01	0.42
2:D:510:VAL:HG21	2:D:554:LEU:HA	2.02	0.42
1:6:212:ILE:HG23	1:6:216:PHE:HB3	2.02	0.42
2:A:686:LYS:HB2	2:A:712:HIS:CE1	2.55	0.42
2:D:53:LEU:HD21	2:D:134:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:503:GLU:H	2:E:525:ARG:NH2	2.17	0.42
2:F:382:ILE:HA	2:F:383:SER:HB2	2.00	0.42
2:A:21:ALA:HA	2:A:33:HIS:CE1	2.54	0.42
2:A:192:VAL:O	2:A:196:LEU:HD22	2.19	0.42
2:B:516:ALA:HB2	2:B:710:VAL:O	2.20	0.42
2:C:476:ILE:HA	2:C:479:VAL:HG22	2.01	0.42
1:1:216:PHE:CE2	2:A:431:VAL:HG22	2.55	0.42
2:A:370:ALA:CB	2:A:471:VAL:HG13	2.50	0.42
2:B:16:LEU:HB3	2:B:37:GLY:HA2	2.02	0.42
2:C:278:ILE:C	2:C:281:LEU:HD21	2.44	0.42
2:C:544:LEU:HD21	2:C:693:LEU:HD12	2.02	0.42
2:E:528:ARG:HD2	2:E:562:ILE:HD12	2.01	0.42
2:F:53:LEU:HD22	2:F:53:LEU:H	1.85	0.42
1:6:132:ARG:HH22	2:A:151:ALA:H	1.68	0.42
2:B:14:LEU:O	2:B:17:ALA:HB3	2.19	0.42
2:B:371:ILE:O	2:B:374:ALA:HB3	2.19	0.42
2:B:791:HIS:H	2:B:807:ALA:HB3	1.85	0.42
2:F:20:GLU:HB2	2:F:33:HIS:CG	2.55	0.42
2:F:21:ALA:CB	2:F:29:ILE:HG12	2.50	0.42
1:1:202:LEU:HD23	1:1:203:ILE:H	1.84	0.42
1:3:136:PHE:CZ	1:3:154:LEU:CD2	3.03	0.42
2:A:427:LYS:HE2	2:A:443:ARG:HA	2.02	0.42
2:A:719:LEU:HD13	2:A:752:ALA:O	2.20	0.42
2:A:770:GLN:HA	2:A:774:GLU:HG2	2.02	0.42
2:D:387:LEU:HA	2:D:390:LYS:HE2	2.02	0.42
1:4:136:PHE:HB3	2:D:443:ARG:HG3	2.02	0.41
2:A:619:ILE:HD12	2:A:656:MET:CG	2.50	0.41
2:C:366:ILE:O	2:C:471:VAL:HG13	2.20	0.41
2:C:483:TRP:HE1	2:D:336:PRO:HD2	1.85	0.41
2:D:26:HIS:CG	2:D:33:HIS:CE1	3.08	0.41
2:F:361:HIS:HD2	2:F:403:ARG:HH21	1.68	0.41
1:1:133:PHE:CZ	1:1:142:LEU:HD13	2.55	0.41
1:1:153:THR:HA	1:1:208:ALA:HB2	2.01	0.41
2:C:363:ARG:HG2	2:C:403:ARG:HH21	1.84	0.41
2:F:772:HIS:HE1	2:F:801:PHE:CD1	2.37	0.41
2:A:38:LEU:HD22	2:A:46:ALA:CB	2.50	0.41
2:B:269:ARG:C	2:B:271:ALA:H	2.28	0.41
2:D:777:LEU:HD11	2:D:794:LEU:HB2	2.02	0.41
2:E:503:GLU:H	2:E:525:ARG:HH21	1.68	0.41
2:E:512:GLY:HA3	2:E:718:HIS:CD2	2.55	0.41
2:E:792:ILE:HG23	2:E:803:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:46:ALA:HB1	2:A:109:LEU:HB2	2.03	0.41
2:A:203:ASN:HA	2:A:311:CYS:O	2.20	0.41
2:A:499:LEU:O	2:A:502:MET:HB2	2.21	0.41
2:B:165:SER:HB2	2:B:166:LEU:HB2	2.02	0.41
2:B:189:ILE:HG23	2:B:221:LEU:HD23	2.02	0.41
2:C:719:LEU:HD13	2:C:752:ALA:O	2.20	0.41
1:6:156:SER:HB2	1:6:203:ILE:HD11	2.01	0.41
2:B:778:SER:HA	2:C:531:LEU:HD23	2.03	0.41
2:F:427:LYS:O	2:F:431:VAL:HG23	2.20	0.41
2:F:542:ILE:HD13	2:F:656:MET:HB2	2.02	0.41
1:4:131:LEU:HD11	1:4:182:LEU:HD13	2.01	0.41
2:A:351:LEU:HD11	2:A:391:ALA:HB1	2.02	0.41
2:A:396:ASP:HB3	2:B:198:ARG:HD3	2.03	0.41
2:A:544:LEU:HD21	2:A:693:LEU:CD1	2.50	0.41
2:C:502:MET:HE2	2:C:528:ARG:HH11	1.86	0.41
2:C:515:GLU:HG3	2:C:516:ALA:H	1.85	0.41
2:C:588:GLY:H	2:D:594:VAL:HG13	1.84	0.41
1:5:216:PHE:CD1	2:E:443:ARG:HB2	2.56	0.41
2:A:360:ALA:HA	2:A:362:HIS:CE1	2.55	0.41
2:A:524:VAL:CG1	2:A:538:ILE:HD12	2.49	0.41
2:B:714:LEU:HD23	2:B:718:HIS:CD2	2.56	0.41
2:D:49:ALA:O	2:D:53:LEU:HD22	2.21	0.41
2:D:787:HIS:CE1	2:E:531:LEU:HD11	2.56	0.41
2:E:26:HIS:CD2	2:E:33:HIS:NE2	2.89	0.41
2:F:606:VAL:HG11	2:F:649:PHE:CD1	2.54	0.41
2:E:619:ILE:HD11	2:E:630:LEU:HD13	2.03	0.41
2:F:196:LEU:C	2:F:198:ARG:H	2.29	0.41
2:F:198:ARG:HB2	2:F:202:ASN:HA	2.02	0.41
2:F:355:ARG:NH1	2:F:371:ILE:HD13	2.36	0.41
1:3:165:VAL:HG11	1:3:167:PHE:CZ	2.56	0.41
1:4:195:ARG:HE	2:E:143:GLY:N	2.19	0.41
1:5:131:LEU:HD11	1:5:182:LEU:HD13	2.03	0.41
1:5:136:PHE:CZ	1:5:154:LEU:CD2	3.04	0.41
1:6:136:PHE:CD2	1:6:216:PHE:CE1	3.09	0.41
2:A:137:GLN:HA	2:A:140:GLN:HG2	2.02	0.41
2:A:202:ASN:HA	2:A:310:GLN:HE21	1.86	0.41
2:A:709:ILE:HG21	2:A:711:PHE:CE2	2.55	0.41
2:C:426:GLU:HB3	2:C:442:LEU:HD13	2.03	0.41
2:D:470:GLU:HG2	2:D:472:THR:HG23	2.03	0.41
2:E:615:LEU:HD21	2:E:657:THR:HG23	2.01	0.41
2:E:619:ILE:CD1	2:E:630:LEU:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:664:GLU:HG3	2:E:685:MET:HA	2.02	0.41
1:4:136:PHE:CD2	1:4:216:PHE:CZ	3.08	0.41
1:6:153:THR:HA	1:6:208:ALA:HB2	2.03	0.41
2:A:45:ILE:HB	2:A:106:GLU:HB3	2.03	0.41
2:A:730:LEU:HD11	2:A:774:GLU:HB3	2.03	0.41
2:D:375:VAL:HG12	2:D:379:ASP:OD1	2.21	0.41
2:D:394:LEU:O	2:D:479:VAL:HG21	2.21	0.41
2:D:403:ARG:HH21	2:E:231:PRO:HA	1.85	0.41
2:D:619:ILE:CG2	2:D:619:ILE:O	2.69	0.41
2:E:281:LEU:CD2	2:E:313:GLY:HA2	2.51	0.41
2:F:198:ARG:HH11	2:F:201:LYS:HB3	1.86	0.41
2:A:366:ILE:O	2:A:471:VAL:HG12	2.21	0.40
2:A:474:ASP:HA	2:A:494:THR:H	1.85	0.40
2:B:363:ARG:HG2	2:B:403:ARG:HB2	2.03	0.40
2:E:393:ASP:HB2	2:F:335:GLN:HG3	2.02	0.40
2:F:630:LEU:O	2:F:634:LEU:HD13	2.21	0.40
1:2:154:LEU:CD2	1:2:212:ILE:HD11	2.50	0.40
2:A:363:ARG:HB2	2:A:403:ARG:HB3	2.02	0.40
2:B:627:PHE:HB2	2:B:698:ARG:HE	1.86	0.40
2:D:94:GLU:O	2:D:107:HIS:CD2	2.74	0.40
2:E:199:ARG:HA	2:E:202:ASN:HB3	2.03	0.40
2:F:29:ILE:HB	2:F:80:TYR:HA	2.02	0.40
2:B:291:GLU:HG2	2:B:293:ALA:H	1.86	0.40
2:C:24:LEU:HD11	2:C:61:GLN:HE22	1.86	0.40
2:C:402:VAL:HG21	2:C:470:GLU:HB3	2.03	0.40
2:D:358:TYR:CE2	2:D:364:VAL:HG21	2.57	0.40
2:D:375:VAL:HA	2:D:391:ALA:HB2	2.04	0.40
2:E:667:ARG:CB	2:E:681:ASN:HD21	2.32	0.40
1:1:167:PHE:CD1	1:1:175:VAL:HG22	2.56	0.40
1:1:215:HIS:C	2:A:440:ALA:HB2	2.46	0.40
2:A:232:GLU:N	2:F:403:ARG:HH11	2.20	0.40
2:A:351:LEU:N	2:A:351:LEU:HD23	2.36	0.40
2:A:633:VAL:HG22	2:A:649:PHE:CE2	2.56	0.40
2:B:364:VAL:HA	2:B:365:SER:O	2.22	0.40
2:C:427:LYS:HG3	2:C:443:ARG:HA	2.04	0.40
2:C:661:GLY:HA3	2:C:689:VAL:HG13	2.03	0.40
2:E:165:SER:HB2	2:E:166:LEU:HB2	2.02	0.40
2:E:473:VAL:HG23	2:E:474:ASP:H	1.87	0.40
2:F:363:ARG:HD2	2:F:403:ARG:H	1.85	0.40
2:F:685:MET:HB2	2:F:712:HIS:CE1	2.57	0.40
1:3:194:HIS:NE2	2:D:45:ILE:HD12	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:338:GLN:CD	2:A:338:GLN:H	2.27	0.40
2:A:361:HIS:HE1	2:B:234:LEU:HD11	1.83	0.40
2:A:473:VAL:HB	2:A:493:GLN:H	1.86	0.40
2:C:165:SER:HB2	2:C:166:LEU:HB2	2.04	0.40
2:D:13:VAL:HG21	2:D:38:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	92/218 (42%)	77 (84%)	10 (11%)	5 (5%)	1	15
1	2	92/218 (42%)	76 (83%)	8 (9%)	8 (9%)	0	9
1	3	92/218 (42%)	79 (86%)	9 (10%)	4 (4%)	2	17
1	4	92/218 (42%)	77 (84%)	10 (11%)	5 (5%)	1	15
1	5	92/218 (42%)	76 (83%)	10 (11%)	6 (6%)	1	12
1	6	92/218 (42%)	76 (83%)	11 (12%)	5 (5%)	1	15
2	A	794/810 (98%)	632 (80%)	113 (14%)	49 (6%)	1	13
2	B	794/810 (98%)	634 (80%)	118 (15%)	42 (5%)	1	15
2	C	794/810 (98%)	630 (79%)	110 (14%)	54 (7%)	1	11
2	D	794/810 (98%)	624 (79%)	121 (15%)	49 (6%)	1	13
2	E	794/810 (98%)	628 (79%)	120 (15%)	46 (6%)	1	14
2	F	794/810 (98%)	629 (79%)	106 (13%)	59 (7%)	1	10
All	All	5316/6168 (86%)	4238 (80%)	746 (14%)	332 (6%)	2	13

All (332) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	147	VAL
1	3	147	VAL
1	4	207	HIS
1	6	147	VAL
2	A	76	GLN
2	A	78	ILE
2	A	271	ALA
2	A	294	ILE
2	A	363	ARG
2	A	366	ILE
2	A	382	ILE
2	A	468	ASN
2	A	472	THR
2	A	473	VAL
2	A	591	PRO
2	A	669	LYS
2	A	712	HIS
2	A	757	ASP
2	B	100	HIS
2	B	129	VAL
2	B	230	VAL
2	B	271	ALA
2	B	365	SER
2	B	366	ILE
2	B	382	ILE
2	B	468	ASN
2	B	472	THR
2	B	473	VAL
2	C	76	GLN
2	C	78	ILE
2	C	100	HIS
2	C	117	GLU
2	C	183	ILE
2	C	294	ILE
2	C	383	SER
2	C	468	ASN
2	C	471	VAL
2	C	473	VAL
2	C	669	LYS
2	C	757	ASP
2	D	76	GLN
2	D	167	ALA
2	D	183	ILE

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Mol	Chain	Res	Type
2	D	293	ALA
2	D	382	ILE
2	D	468	ASN
2	D	472	THR
2	D	473	VAL
2	D	493	GLN
2	D	716	LYS
2	D	717	LYS
2	E	72	GLN
2	E	271	ALA
2	E	294	ILE
2	E	363	ARG
2	E	365	SER
2	E	410	PRO
2	E	412	ASN
2	E	468	ASN
2	E	473	VAL
2	E	670	TYR
2	E	739	LEU
2	F	100	HIS
2	F	202	ASN
2	F	294	ILE
2	F	364	VAL
2	F	365	SER
2	F	366	ILE
2	F	382	ILE
2	F	468	ASN
2	F	472	THR
2	F	473	VAL
2	F	511	ILE
2	F	579	GLU
2	F	583	THR
2	F	587	VAL
2	F	618	ALA
2	F	621	LYS
2	F	668	ASN
2	F	760	TYR
1	3	217	ALA
1	4	145	LEU
1	4	205	SER
1	5	217	ALA
2	A	100	HIS

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Mol	Chain	Res	Type
2	A	118	GLY
2	A	165	SER
2	A	327	ASP
2	A	493	GLN
2	A	590	PRO
2	A	592	GLY
2	A	662	ALA
2	A	668	ASN
2	A	716	LYS
2	B	72	GLN
2	B	165	SER
2	B	202	ASN
2	B	363	ARG
2	B	470	GLU
2	B	471	VAL
2	B	493	GLN
2	C	73	GLU
2	C	129	VAL
2	C	165	SER
2	C	212	VAL
2	C	360	ALA
2	C	366	ILE
2	C	375	VAL
2	C	412	ASN
2	C	493	GLN
2	C	580	LYS
2	C	618	ALA
2	D	151	ALA
2	D	163	LEU
2	D	165	SER
2	D	201	LYS
2	D	365	SER
2	D	366	ILE
2	D	412	ASN
2	D	470	GLU
2	D	662	ALA
2	E	100	HIS
2	E	165	SER
2	E	200	THR
2	E	202	ASN
2	E	366	ILE
2	E	413	LEU

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Mol	Chain	Res	Type
2	E	471	VAL
2	E	493	GLN
2	E	662	ALA
2	E	738	ASP
2	F	78	ILE
2	F	165	SER
2	F	271	ALA
2	F	375	VAL
2	F	471	VAL
2	F	493	GLN
2	F	534	PRO
2	F	669	LYS
2	F	714	LEU
2	F	717	LYS
1	1	144	LYS
1	1	145	LEU
1	1	169	ASN
1	1	177	ASN
1	1	216	PHE
1	2	144	LYS
1	2	145	LEU
1	2	169	ASN
1	2	177	ASN
1	2	217	ALA
1	3	144	LYS
1	3	177	ASN
1	4	144	LYS
1	4	177	ASN
1	5	144	LYS
1	5	169	ASN
1	5	177	ASN
1	5	216	PHE
1	6	144	LYS
1	6	177	ASN
1	6	216	PHE
2	A	4	GLY
2	A	152	ALA
2	A	162	THR
2	A	375	VAL
2	A	391	ALA
2	A	413	LEU
2	A	580	LYS

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Mol	Chain	Res	Type
2	A	600	GLY
2	A	618	ALA
2	A	690	MET
2	B	162	THR
2	B	329	ALA
2	B	391	ALA
2	B	413	LEU
2	B	434	GLN
2	B	550	GLY
2	B	586	LEU
2	B	662	ALA
2	B	669	LYS
2	B	690	MET
2	C	152	ALA
2	C	163	LEU
2	C	271	ALA
2	C	365	SER
2	C	384	ASP
2	C	391	ALA
2	C	413	LEU
2	C	662	ALA
2	C	672	GLY
2	C	716	LYS
2	C	761	GLY
2	D	149	SER
2	D	166	LEU
2	D	211	GLY
2	D	231	PRO
2	D	271	ALA
2	D	326	LYS
2	D	375	VAL
2	D	388	PRO
2	D	391	ALA
2	D	410	PRO
2	D	413	LEU
2	D	434	GLN
2	D	600	GLY
2	D	612	SER
2	E	152	ALA
2	E	162	THR
2	E	212	VAL
2	E	364	VAL

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Mol	Chain	Res	Type
2	E	375	VAL
2	E	391	ALA
2	E	434	GLN
2	E	580	LYS
2	E	582	SER
2	E	583	THR
2	E	612	SER
2	E	668	ASN
2	F	71	GLY
2	F	73	GLU
2	F	142	LEU
2	F	147	THR
2	F	152	ALA
2	F	162	THR
2	F	163	LEU
2	F	210	PRO
2	F	391	ALA
2	F	550	GLY
2	F	588	GLY
2	F	590	PRO
2	F	662	ALA
1	2	216	PHE
1	5	145	LEU
2	A	388	PRO
2	A	400	SER
2	A	412	ASN
2	A	534	PRO
2	A	622	ALA
2	A	717	LYS
2	B	163	LEU
2	B	375	VAL
2	B	388	PRO
2	B	400	SER
2	B	410	PRO
2	B	760	TYR
2	C	162	THR
2	C	232	GLU
2	C	293	ALA
2	C	329	ALA
2	C	362	HIS
2	C	382	ILE
2	C	388	PRO

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Mol	Chain	Res	Type
2	C	400	SER
2	C	410	PRO
2	C	579	GLU
2	C	586	LEU
2	C	686	LYS
2	C	690	MET
2	D	117	GLU
2	D	152	ALA
2	D	162	THR
2	D	199	ARG
2	D	329	ALA
2	D	342	PRO
2	D	400	SER
2	D	690	MET
2	E	163	LEU
2	E	329	ALA
2	E	388	PRO
2	E	400	SER
2	F	166	LEU
2	F	293	ALA
2	F	329	ALA
2	F	363	ARG
2	F	388	PRO
2	F	400	SER
2	F	412	ASN
2	F	413	LEU
2	F	600	GLY
2	F	612	SER
2	F	623	HIS
2	F	673	PHE
2	F	690	MET
1	6	169	ASN
2	A	163	LEU
2	A	178	SER
2	A	226	ILE
2	A	410	PRO
2	A	623	HIS
2	A	707	GLU
2	B	590	PRO
2	C	166	LEU
2	C	226	ILE
2	C	434	GLN

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Mol	Chain	Res	Type
2	C	584	SER
2	C	738	ASP
2	D	215	THR
2	D	226	ILE
2	D	534	PRO
2	E	226	ILE
2	E	326	LYS
2	F	226	ILE
2	F	326	LYS
2	F	798	ASP
2	A	383	SER
2	A	471	VAL
2	B	166	LEU
2	B	167	ALA
2	B	226	ILE
2	B	293	ALA
2	B	323	TYR
2	B	440	ALA
2	B	670	TYR
2	C	147	THR
2	D	144	SER
2	D	323	TYR
2	E	323	TYR
2	E	717	LYS
2	D	536	ARG
2	E	534	PRO
2	F	537	PRO
2	B	600	GLY
2	E	210	PRO
2	A	423	VAL
2	C	210	PRO
2	E	160	THR
2	E	671	VAL
2	F	410	PRO
1	2	134	GLY
2	D	537	PRO
2	E	546	PRO

5.3.2 Protein sidechains [i](#)

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%)	78 (89%)	10 (11%)	5	18
1	3	88/201 (44%)	81 (92%)	7 (8%)	11	31
1	4	88/201 (44%)	83 (94%)	5 (6%)	18	40
1	5	88/201 (44%)	79 (90%)	9 (10%)	7	23
1	6	88/201 (44%)	81 (92%)	7 (8%)	11	31
2	A	666/685 (97%)	594 (89%)	72 (11%)	6	21
2	B	666/685 (97%)	601 (90%)	65 (10%)	7	24
2	C	666/685 (97%)	611 (92%)	55 (8%)	10	30
2	D	666/685 (97%)	602 (90%)	64 (10%)	8	25
2	E	666/685 (97%)	601 (90%)	65 (10%)	7	24
2	F	666/685 (97%)	611 (92%)	55 (8%)	10	30
All	All	4524/5316 (85%)	4103 (91%)	421 (9%)	11	26

All (421) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	147	VAL
1	1	151	LYS
1	1	165	VAL
1	1	195	ARG
1	1	204	ILE
1	1	212	ILE
1	1	215	HIS
1	2	130	VAL
1	2	137	GLU
1	2	142	LEU
1	2	145	LEU
1	2	151	LYS
1	2	165	VAL
1	2	173	GLU
1	2	197	GLU
1	2	204	ILE
1	2	211	THR
1	3	136	PHE

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Mol	Chain	Res	Type
1	3	137	GLU
1	3	142	LEU
1	3	151	LYS
1	3	163	LEU
1	3	175	VAL
1	3	197	GLU
1	4	128	GLN
1	4	137	GLU
1	4	140	ILE
1	4	165	VAL
1	4	177	ASN
1	5	130	VAL
1	5	137	GLU
1	5	142	LEU
1	5	145	LEU
1	5	151	LYS
1	5	154	LEU
1	5	184	GLU
1	5	195	ARG
1	5	204	ILE
1	6	128	GLN
1	6	142	LEU
1	6	146	ASN
1	6	151	LYS
1	6	173	GLU
1	6	204	ILE
1	6	216	PHE
2	A	12	LYS
2	A	19	GLU
2	A	22	LEU
2	A	29	ILE
2	A	32	GLU
2	A	43	GLU
2	A	53	LEU
2	A	58	GLU
2	A	74	MET
2	A	78	ILE
2	A	94	GLU
2	A	100	HIS
2	A	105	THR
2	A	119	VAL
2	A	138	VAL

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Mol	Chain	Res	Type
2	A	139	LEU
2	A	168	ARG
2	A	182	VAL
2	A	195	VAL
2	A	196	LEU
2	A	200	THR
2	A	207	ILE
2	A	230	VAL
2	A	262	LYS
2	A	285	ILE
2	A	308	GLU
2	A	337	ILE
2	A	338	GLN
2	A	358	TYR
2	A	363	ARG
2	A	364	VAL
2	A	366	ILE
2	A	378	SER
2	A	381	TYR
2	A	392	ILE
2	A	393	ASP
2	A	394	LEU
2	A	403	ARG
2	A	411	PRO
2	A	414	LYS
2	A	415	GLU
2	A	425	LYS
2	A	432	GLN
2	A	436	PHE
2	A	443	ARG
2	A	448	ARG
2	A	473	VAL
2	A	502	MET
2	A	511	ILE
2	A	513	GLN
2	A	514	ASP
2	A	531	LEU
2	A	535	LYS
2	A	554	LEU
2	A	558	LEU
2	A	591	PRO
2	A	593	TYR

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Mol	Chain	Res	Type
2	A	620	GLU
2	A	621	LYS
2	A	634	LEU
2	A	639	LEU
2	A	647	VAL
2	A	658	SER
2	A	682	HIS
2	A	709	ILE
2	A	710	VAL
2	A	730	LEU
2	A	758	LEU
2	A	760	TYR
2	A	777	LEU
2	A	786	ILE
2	A	788	LYS
2	B	13	VAL
2	B	18	GLN
2	B	20	GLU
2	B	23	ARG
2	B	41	GLU
2	B	48	LYS
2	B	53	LEU
2	B	58	GLU
2	B	74	MET
2	B	78	ILE
2	B	79	HIS
2	B	90	LEU
2	B	108	ILE
2	B	142	LEU
2	B	188	GLU
2	B	195	VAL
2	B	231	PRO
2	B	254	ARG
2	B	262	LYS
2	B	275	ILE
2	B	308	GLU
2	B	355	ARG
2	B	363	ARG
2	B	364	VAL
2	B	387	LEU
2	B	392	ILE
2	B	420	LEU

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Mol	Chain	Res	Type
2	B	425	LYS
2	B	432	GLN
2	B	436	PHE
2	B	443	ARG
2	B	448	ARG
2	B	449	LEU
2	B	457	LYS
2	B	461	LYS
2	B	467	GLU
2	B	470	GLU
2	B	471	VAL
2	B	475	ASP
2	B	511	ILE
2	B	514	ASP
2	B	515	GLU
2	B	520	VAL
2	B	526	ARG
2	B	554	LEU
2	B	586	LEU
2	B	587	VAL
2	B	594	VAL
2	B	620	GLU
2	B	624	PRO
2	B	626	VAL
2	B	634	LEU
2	B	638	ARG
2	B	639	LEU
2	B	647	VAL
2	B	680	GLN
2	B	690	MET
2	B	693	LEU
2	B	695	ARG
2	B	726	MET
2	B	767	ARG
2	B	769	ILE
2	B	774	GLU
2	B	790	GLN
2	B	795	ASP
2	C	7	THR
2	C	19	GLU
2	C	20	GLU
2	C	32	GLU

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Mol	Chain	Res	Type
2	C	34	ILE
2	C	51	GLN
2	C	53	LEU
2	C	58	GLU
2	C	72	GLN
2	C	74	MET
2	C	87	VAL
2	C	90	LEU
2	C	105	THR
2	C	108	ILE
2	C	119	VAL
2	C	138	VAL
2	C	139	LEU
2	C	170	LEU
2	C	195	VAL
2	C	221	LEU
2	C	231	PRO
2	C	233	ILE
2	C	263	LYS
2	C	298	ASN
2	C	308	GLU
2	C	338	GLN
2	C	381	TYR
2	C	385	ARG
2	C	392	ILE
2	C	402	VAL
2	C	420	LEU
2	C	424	ARG
2	C	425	LYS
2	C	431	VAL
2	C	432	GLN
2	C	448	ARG
2	C	467	GLU
2	C	469	SER
2	C	473	VAL
2	C	515	GLU
2	C	531	LEU
2	C	535	LYS
2	C	554	LEU
2	C	570	ILE
2	C	574	MET
2	C	624	PRO

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Mol	Chain	Res	Type
2	C	634	LEU
2	C	638	ARG
2	C	666	LYS
2	C	686	LYS
2	C	693	LEU
2	C	715	GLU
2	C	730	LEU
2	C	763	ARG
2	C	782	LEU
2	D	12	LYS
2	D	19	GLU
2	D	48	LYS
2	D	51	GLN
2	D	53	LEU
2	D	58	GLU
2	D	72	GLN
2	D	74	MET
2	D	86	LYS
2	D	90	LEU
2	D	105	THR
2	D	106	GLU
2	D	138	VAL
2	D	142	LEU
2	D	193	ILE
2	D	195	VAL
2	D	196	LEU
2	D	201	LYS
2	D	230	VAL
2	D	238	ARG
2	D	268	ILE
2	D	275	ILE
2	D	285	ILE
2	D	300	LEU
2	D	303	SER
2	D	304	LEU
2	D	358	TYR
2	D	363	ARG
2	D	378	SER
2	D	381	TYR
2	D	392	ILE
2	D	394	LEU
2	D	402	VAL

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Mol	Chain	Res	Type
2	D	403	ARG
2	D	410	PRO
2	D	414	LYS
2	D	418	GLN
2	D	424	ARG
2	D	425	LYS
2	D	432	GLN
2	D	443	ARG
2	D	448	ARG
2	D	462	GLU
2	D	470	GLU
2	D	471	VAL
2	D	476	ILE
2	D	511	ILE
2	D	544	LEU
2	D	624	PRO
2	D	626	VAL
2	D	631	LEU
2	D	634	LEU
2	D	638	ARG
2	D	647	VAL
2	D	654	LEU
2	D	678	GLU
2	D	680	GLN
2	D	707	GLU
2	D	715	GLU
2	D	730	LEU
2	D	763	ARG
2	D	777	LEU
2	D	786	ILE
2	D	795	ASP
2	E	13	VAL
2	E	32	GLU
2	E	41	GLU
2	E	53	LEU
2	E	74	MET
2	E	78	ILE
2	E	90	LEU
2	E	113	ILE
2	E	138	VAL
2	E	139	LEU
2	E	157	ASN

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Mol	Chain	Res	Type
2	E	185	ARG
2	E	188	GLU
2	E	193	ILE
2	E	195	VAL
2	E	234	LEU
2	E	235	ARG
2	E	247	VAL
2	E	285	ILE
2	E	308	GLU
2	E	351	LEU
2	E	355	ARG
2	E	361	HIS
2	E	381	TYR
2	E	382	ILE
2	E	387	LEU
2	E	393	ASP
2	E	395	ILE
2	E	396	ASP
2	E	402	VAL
2	E	415	GLU
2	E	424	ARG
2	E	425	LYS
2	E	427	LYS
2	E	431	VAL
2	E	436	PHE
2	E	448	ARG
2	E	449	LEU
2	E	471	VAL
2	E	473	VAL
2	E	476	ILE
2	E	483	TRP
2	E	526	ARG
2	E	554	LEU
2	E	567	GLU
2	E	574	MET
2	E	577	TYR
2	E	583	THR
2	E	586	LEU
2	E	611	TYR
2	E	631	LEU
2	E	634	LEU
2	E	638	ARG

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Mol	Chain	Res	Type
2	E	647	VAL
2	E	693	LEU
2	E	713	SER
2	E	715	GLU
2	E	726	MET
2	E	739	LEU
2	E	753	GLU
2	E	766	ARG
2	E	777	LEU
2	E	790	GLN
2	E	794	LEU
2	E	800	GLU
2	F	19	GLU
2	F	48	LYS
2	F	58	GLU
2	F	72	GLN
2	F	79	HIS
2	F	86	LYS
2	F	90	LEU
2	F	92	MET
2	F	94	GLU
2	F	105	THR
2	F	113	ILE
2	F	136	GLN
2	F	138	VAL
2	F	170	LEU
2	F	202	ASN
2	F	207	ILE
2	F	231	PRO
2	F	247	VAL
2	F	262	LYS
2	F	263	LYS
2	F	308	GLU
2	F	338	GLN
2	F	363	ARG
2	F	364	VAL
2	F	371	ILE
2	F	381	TYR
2	F	393	ASP
2	F	396	ASP
2	F	400	SER
2	F	404	LEU

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Mol	Chain	Res	Type
2	F	411	PRO
2	F	418	GLN
2	F	424	ARG
2	F	432	GLN
2	F	436	PHE
2	F	448	ARG
2	F	449	LEU
2	F	462	GLU
2	F	471	VAL
2	F	513	GLN
2	F	514	ASP
2	F	515	GLU
2	F	531	LEU
2	F	536	ARG
2	F	549	VAL
2	F	621	LYS
2	F	631	LEU
2	F	647	VAL
2	F	654	LEU
2	F	669	LYS
2	F	670	TYR
2	F	676	GLN
2	F	753	GLU
2	F	790	GLN
2	F	800	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	207	HIS
1	3	178	GLN
1	3	207	HIS
1	4	146	ASN
1	4	159	ASN
1	4	178	GLN
1	4	194	HIS
1	5	128	GLN
1	5	178	GLN
1	5	207	HIS
1	6	128	GLN
1	6	148	ASN
1	6	194	HIS

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Mol	Chain	Res	Type
2	A	11	GLN
2	A	79	HIS
2	A	107	HIS
2	A	126	ASN
2	A	270	GLN
2	A	310	GLN
2	A	338	GLN
2	A	341	GLN
2	A	468	ASN
2	A	507	HIS
2	A	581	HIS
2	A	681	ASN
2	A	703	ASN
2	A	791	HIS
2	B	79	HIS
2	B	100	HIS
2	B	132	ASN
2	B	137	GLN
2	B	338	GLN
2	B	341	GLN
2	B	432	GLN
2	B	464	GLN
2	B	493	GLN
2	B	504	ASN
2	B	581	HIS
2	B	601	GLN
2	B	623	HIS
2	B	682	HIS
2	B	703	ASN
2	B	718	HIS
2	B	729	GLN
2	B	737	GLN
2	B	787	HIS
2	C	11	GLN
2	C	33	HIS
2	C	100	HIS
2	C	126	ASN
2	C	273	ASN
2	C	341	GLN
2	C	361	HIS
2	C	447	GLN
2	C	581	HIS

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Mol	Chain	Res	Type
2	C	601	GLN
2	C	651	ASN
2	C	703	ASN
2	C	718	HIS
2	C	772	HIS
2	D	11	GLN
2	D	26	HIS
2	D	79	HIS
2	D	125	ASN
2	D	136	GLN
2	D	228	ASN
2	D	270	GLN
2	D	338	GLN
2	D	341	GLN
2	D	352	GLN
2	D	361	HIS
2	D	447	GLN
2	D	623	HIS
2	D	632	GLN
2	D	659	ASN
2	D	674	ASN
2	D	682	HIS
2	D	791	HIS
2	E	11	GLN
2	E	26	HIS
2	E	76	GLN
2	E	79	HIS
2	E	100	HIS
2	E	126	ASN
2	E	140	GLN
2	E	273	ASN
2	E	282	HIS
2	E	352	GLN
2	E	434	GLN
2	E	466	GLN
2	E	504	ASN
2	E	674	ASN
2	E	681	ASN
2	E	712	HIS
2	E	729	GLN
2	F	11	GLN
2	F	33	HIS

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Mol	Chain	Res	Type
2	F	76	GLN
2	F	79	HIS
2	F	100	HIS
2	F	126	ASN
2	F	140	GLN
2	F	228	ASN
2	F	270	GLN
2	F	338	GLN
2	F	341	GLN
2	F	352	GLN
2	F	362	HIS
2	F	507	HIS
2	F	601	GLN
2	F	676	GLN
2	F	680	GLN
2	F	703	ASN
2	F	718	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 ⓘ

There are no chain breaks in this entry.

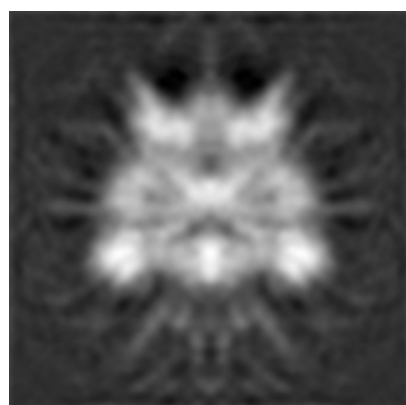
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5609. These allow visual inspection of the internal detail of the map and identification of artifacts.

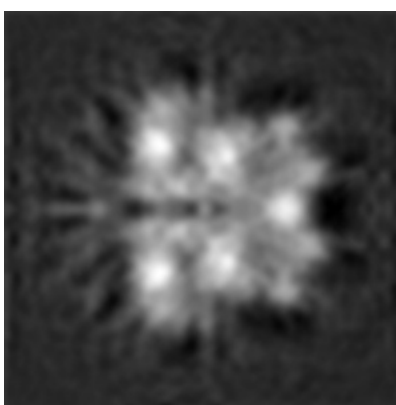
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

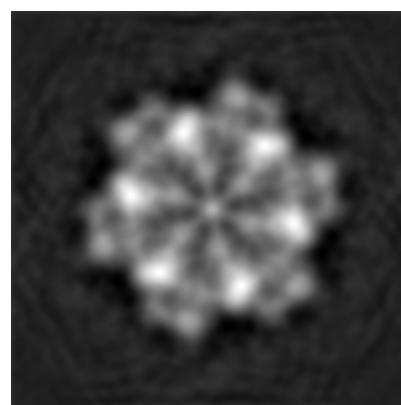
6.1.1 Primary map



X



Y

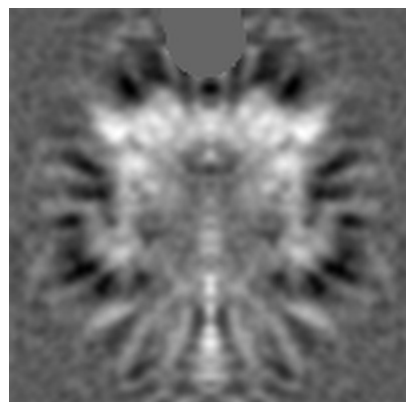


Z

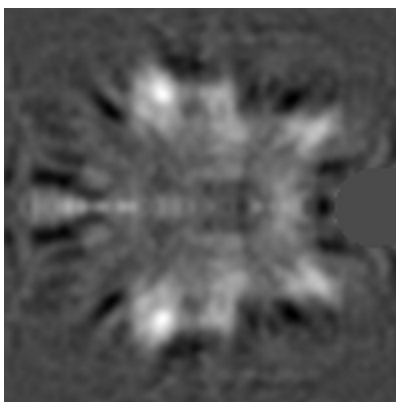
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

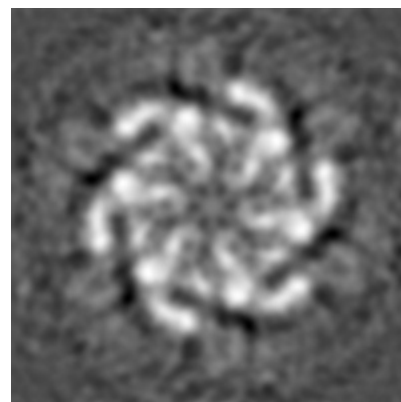
6.2.1 Primary map



X Index: 75



Y Index: 75

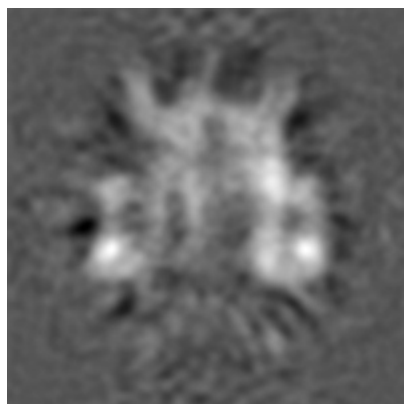


Z Index: 75

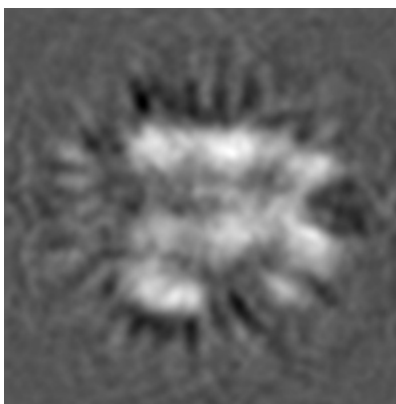
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

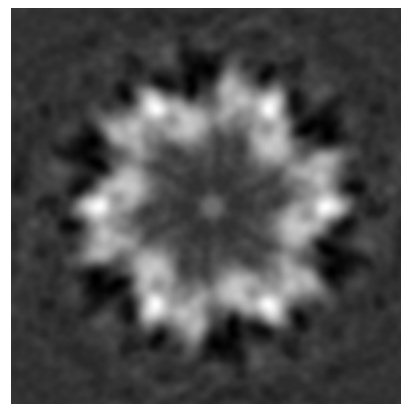
6.3.1 Primary map



X Index: 96



Y Index: 100

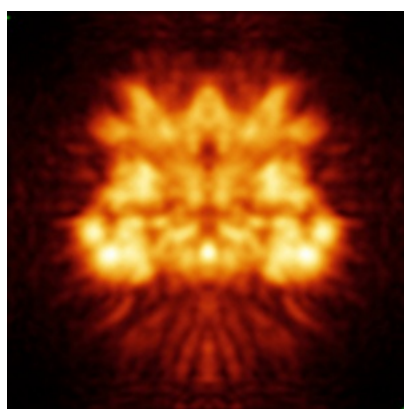


Z Index: 58

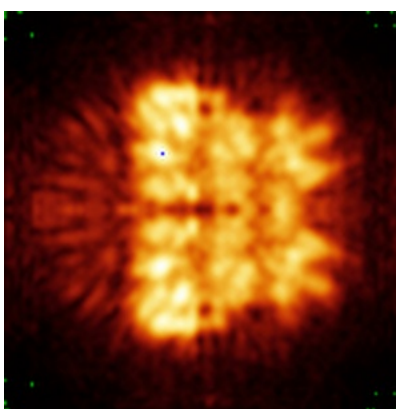
The images above show the largest variance slices of the map in three orthogonal directions.

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

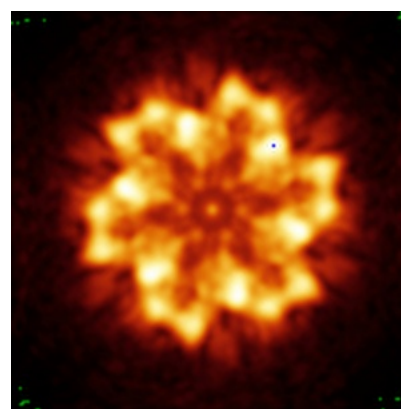
6.4.1 Primary map



X



Y

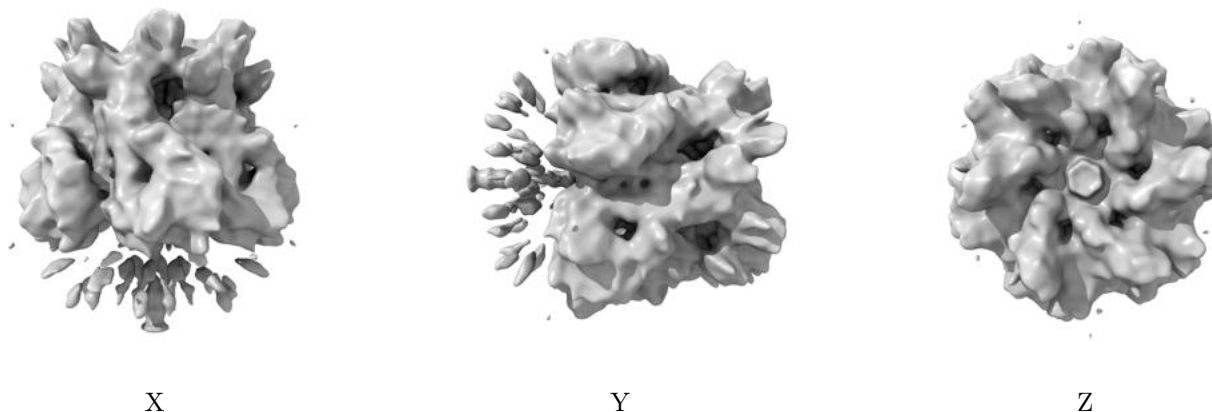


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

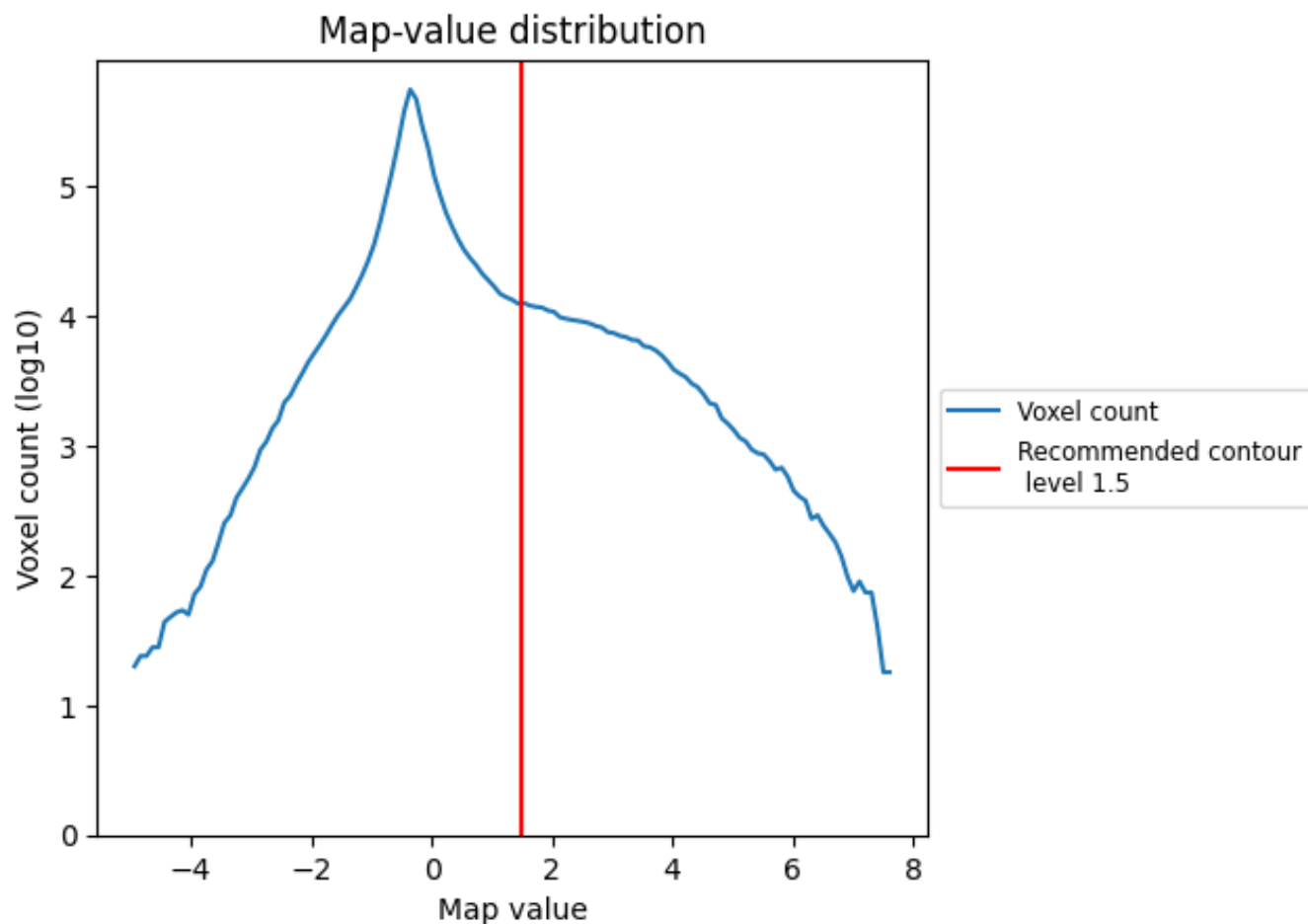
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

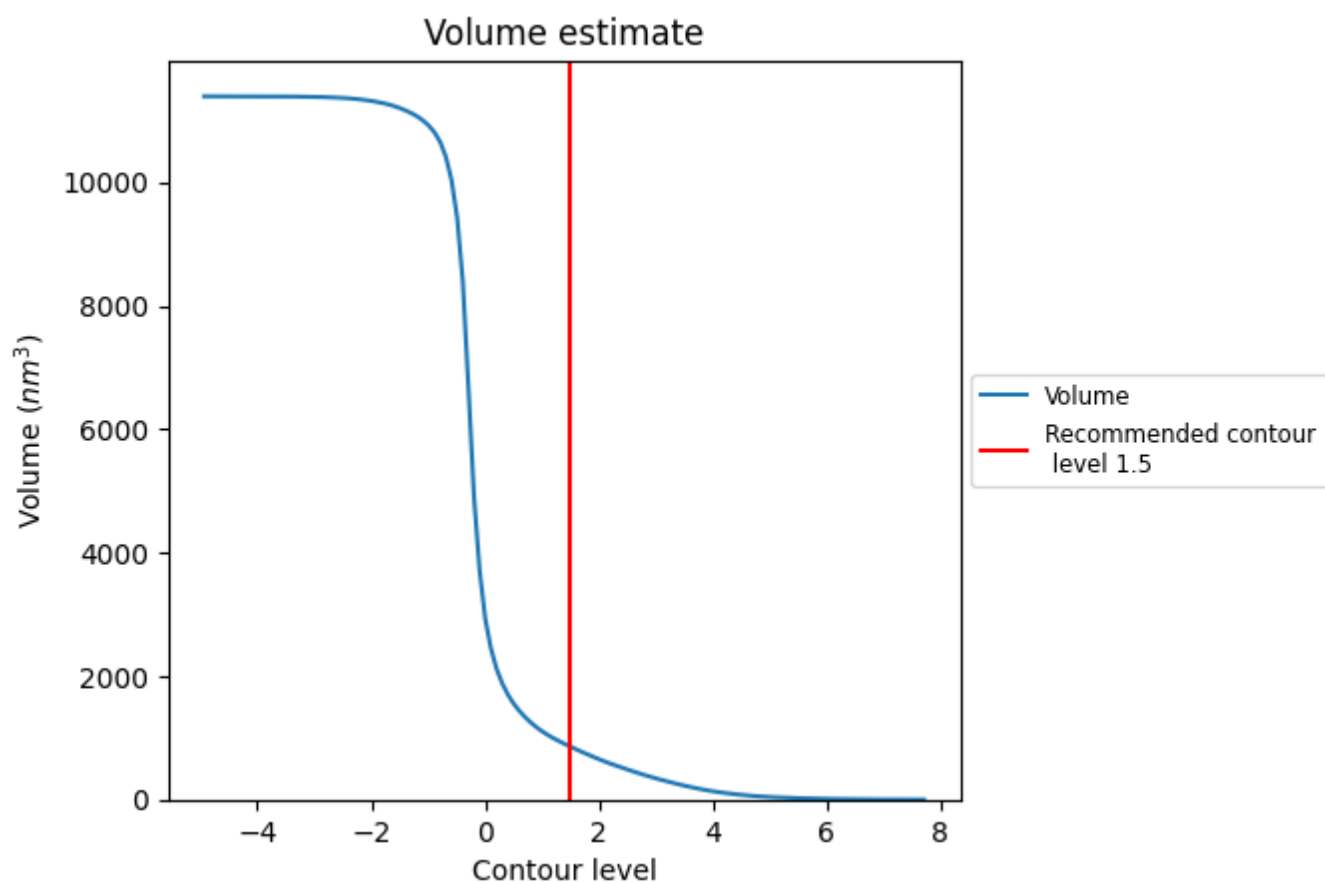
This section contains the results of statistical analysis of the map.

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.

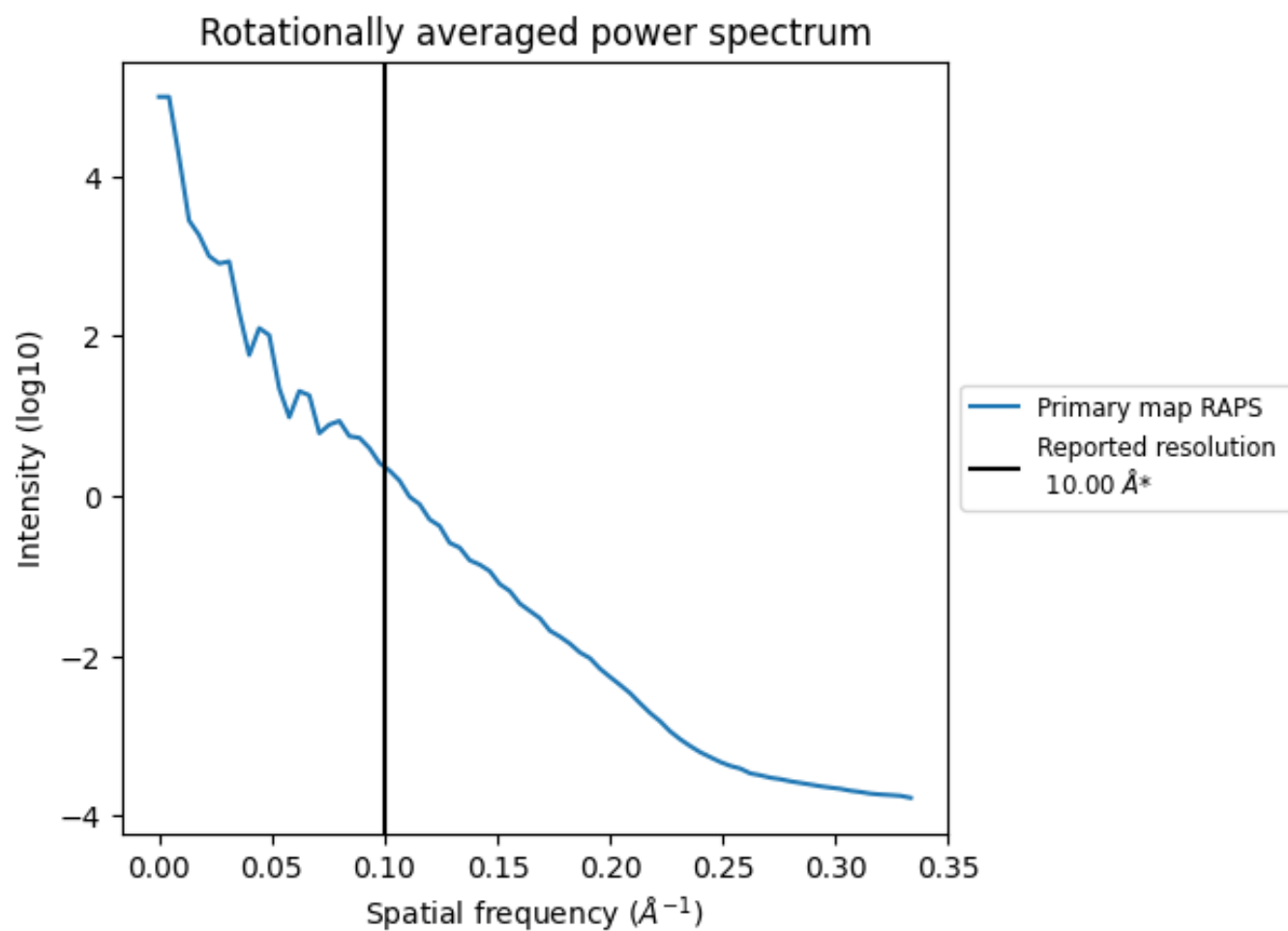
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 856 nm³; this corresponds to an approximate mass of 773 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 0.100 Å⁻¹

8 Fourier-Shell correlation

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

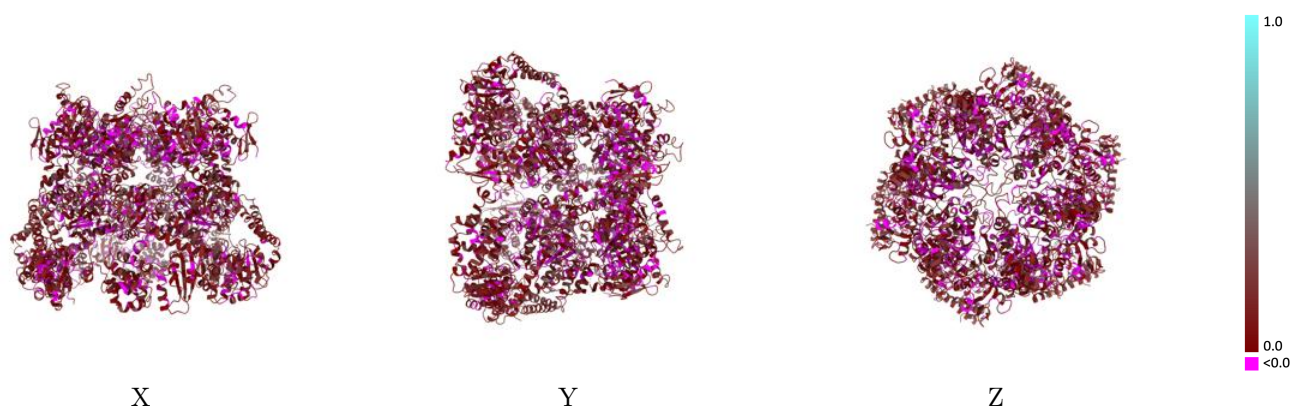
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5609 and PDB model 3J3U. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

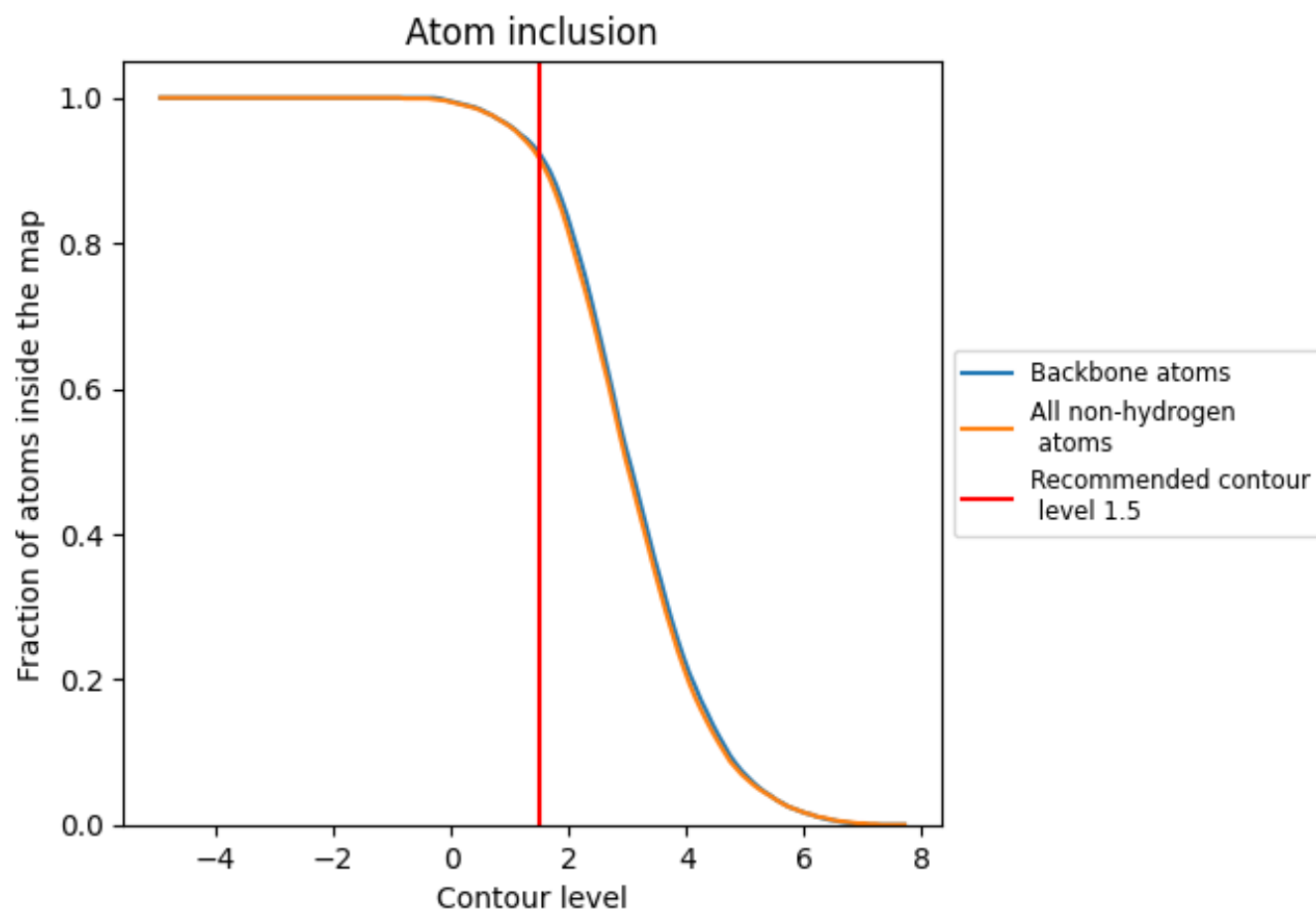


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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	0.9170	0.0860
1	0.9740	0.0870
2	0.9770	0.0920
3	0.9820	0.0860
4	0.9820	0.0770
5	0.9880	0.0780
6	0.9800	0.0860
A	0.9040	0.0890
B	0.9030	0.0870
C	0.9110	0.0860
D	0.9100	0.0850
E	0.9150	0.0820
F	0.9070	0.0890

1.0

0.0

<0.0