



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:58 AM UTC

PDB ID : 5MG3 / pdb_00005mg3
EMDB ID : EMD-3506
Title : EM fitted model of bacterial holo-translocon
Authors : Schaffitzel, C.; Botte, M.
Deposited on : 2016-11-20
Resolution : 14.00 Å(reported)

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:

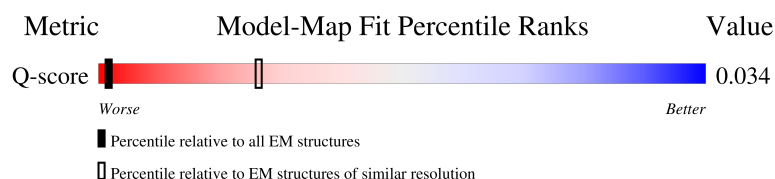
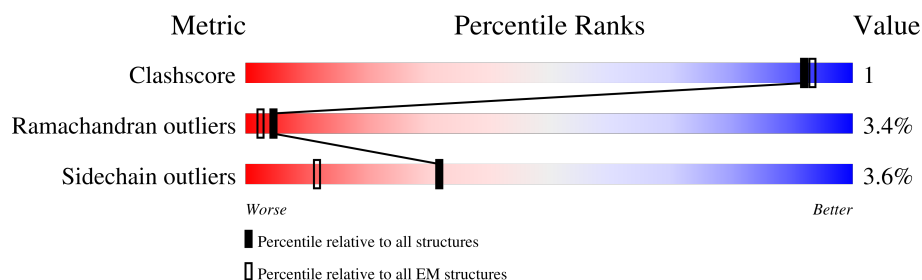
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 14.00 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	61 (13.50 - 14.50)

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	Y	458	
2	E	140	
3	G	136	
4	D	622	

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Mol	Chain	Length	Quality of chain
5	F	323	41%43%6%11%
6	C	559	35%41%5%19%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26650 atoms, of which 13553 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 Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	Y	443	7004	2259	3581	566	580	18	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-14	VAL	-	expression tag	UNP P0AGA2
Y	-13	TRP	-	expression tag	UNP P0AGA2
Y	-12	ASN	-	expression tag	UNP P0AGA2
Y	-11	CYS	-	expression tag	UNP P0AGA2
Y	-10	GLU	-	expression tag	UNP P0AGA2
Y	-9	ARG	-	expression tag	UNP P0AGA2
Y	-8	ILE	-	expression tag	UNP P0AGA2
Y	-7	THR	-	expression tag	UNP P0AGA2
Y	-6	ILE	-	expression tag	UNP P0AGA2
Y	-5	SER	-	expression tag	UNP P0AGA2
Y	-4	HIS	-	expression tag	UNP P0AGA2
Y	-3	ARG	-	expression tag	UNP P0AGA2
Y	-2	LYS	-	expression tag	UNP P0AGA2
Y	-1	GLN	-	expression tag	UNP P0AGA2
Y	0	THR	-	expression tag	UNP P0AGA2

- Molecule 2 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	E	65	1062	332	552	91	86	1	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	369	MET	-	initiating methionine	UNP P0AG96
E	370	HIS	-	expression tag	UNP P0AG96

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Chain	Residue	Modelled	Actual	Comment	Reference
E	371	HIS	-	expression tag	UNP P0AG96
E	372	HIS	-	expression tag	UNP P0AG96
E	373	HIS	-	expression tag	UNP P0AG96
E	374	HIS	-	expression tag	UNP P0AG96
E	375	HIS	-	expression tag	UNP P0AG96
E	376	ASP	-	expression tag	UNP P0AG96
E	377	ASP	-	expression tag	UNP P0AG96
E	378	ASP	-	expression tag	UNP P0AG96
E	379	ASP	-	expression tag	UNP P0AG96
E	380	LYS	-	expression tag	UNP P0AG96
E	381	ALA	-	expression tag	UNP P0AG96
E	382	MET	-	expression tag	UNP P0AG96
E	383	GLY	-	expression tag	UNP P0AG96

- Molecule 3 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	32	Total	C	H	N	O	S	0	0
			480	151	244	39	44	2		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	439	VAL	-	expression tag	UNP P0AG99
G	440	GLY	-	expression tag	UNP P0AG99
G	441	THR	-	expression tag	UNP P0AG99
G	442	GLY	-	expression tag	UNP P0AG99
G	443	TRP	-	expression tag	UNP P0AG99
G	444	TYR	-	expression tag	UNP P0AG99
G	445	SER	-	expression tag	UNP P0AG99
G	446	GLY	-	expression tag	UNP P0AG99
G	447	SER	-	expression tag	UNP P0AG99
G	448	PRO	-	expression tag	UNP P0AG99
G	449	GLY	-	expression tag	UNP P0AG99
G	450	ILE	-	expression tag	UNP P0AG99
G	451	LEU	-	expression tag	UNP P0AG99
G	452	TYR	-	expression tag	UNP P0AG99
G	453	HIS	-	expression tag	UNP P0AG99
G	454	TRP	-	expression tag	UNP P0AG99
G	455	PRO	-	expression tag	UNP P0AG99
G	456	GLU	-	expression tag	UNP P0AG99
G	457	VAL	-	expression tag	UNP P0AG99

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Chain	Residue	Modelled	Actual	Comment	Reference
G	458	LEU	-	expression tag	UNP P0AG99
G	459	ARG	-	expression tag	UNP P0AG99
G	460	ILE	-	expression tag	UNP P0AG99
G	461	GLN	-	expression tag	UNP P0AG99
G	462	GLU	-	expression tag	UNP P0AG99
G	463	LEU	-	expression tag	UNP P0AG99
G	464	ILE	-	expression tag	UNP P0AG99

- Molecule 4 is a protein called Protein translocase subunit SecD.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	414	Total	C	H	N	O	S	0	0
			6419	1991	3291	545	582	10		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP P0AG90
D	-5	HIS	-	expression tag	UNP P0AG90
D	-4	HIS	-	expression tag	UNP P0AG90
D	-3	HIS	-	expression tag	UNP P0AG90
D	-2	HIS	-	expression tag	UNP P0AG90
D	-1	HIS	-	expression tag	UNP P0AG90
D	0	HIS	-	expression tag	UNP P0AG90
D	1	MET	-	expression tag	UNP P0AG90
D	142	VAL	ALA	conflict	UNP P0AG90

- Molecule 5 is a protein called Protein translocase subunit SecF.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	289	Total	C	H	N	O	S	0	0
			4502	1434	2291	366	398	13		

- Molecule 6 is a protein called Membrane protein insertase YidC.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	C	455	Total	C	H	N	O	S	0	0
			7183	2336	3594	582	650	21		

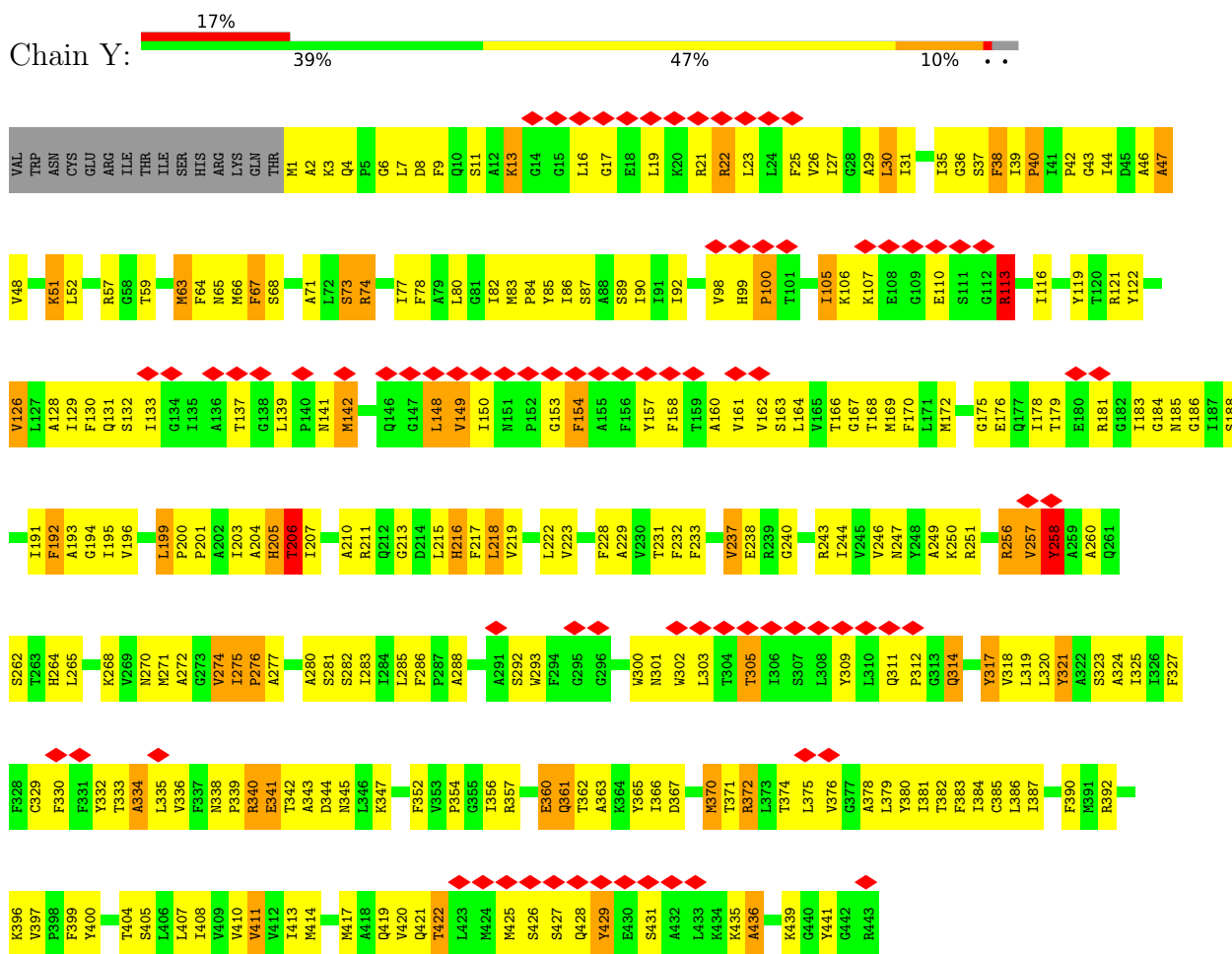
There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	MET	-	initiating methionine	UNP P25714
C	-3	ASP	-	expression tag	UNP P25714
C	-2	PRO	-	expression tag	UNP P25714
C	-1	SER	-	expression tag	UNP P25714
C	0	SER	-	expression tag	UNP P25714
C	1	ARG	-	expression tag	UNP P25714
C	228	ALA	GLU	conflict	UNP P25714
C	229	ALA	LYS	conflict	UNP P25714
C	231	ALA	GLU	conflict	UNP P25714
C	232	ALA	LYS	conflict	UNP P25714
C	234	ALA	LYS	conflict	UNP P25714
C	549	HIS	-	expression tag	UNP P25714
C	550	HIS	-	expression tag	UNP P25714
C	551	HIS	-	expression tag	UNP P25714
C	552	HIS	-	expression tag	UNP P25714
C	553	HIS	-	expression tag	UNP P25714
C	554	HIS	-	expression tag	UNP P25714

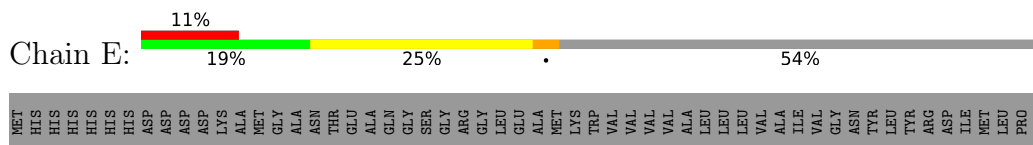
3 Residue-property plots

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: Protein translocase subunit SecY

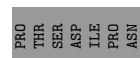


• Molecule 2: Protein translocase subunit SecE

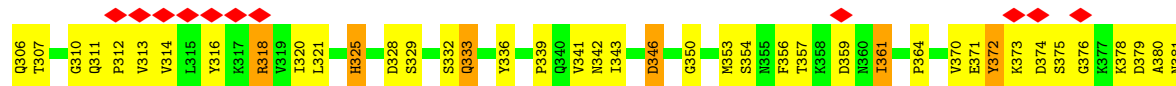


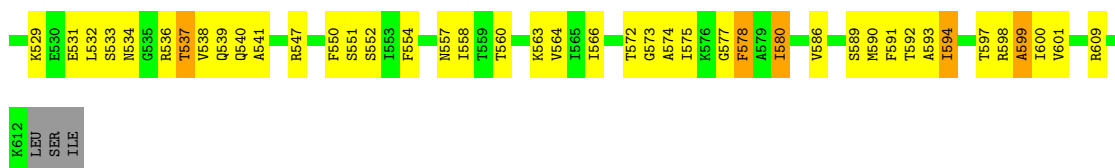


Chain G: 12% 10% 76%

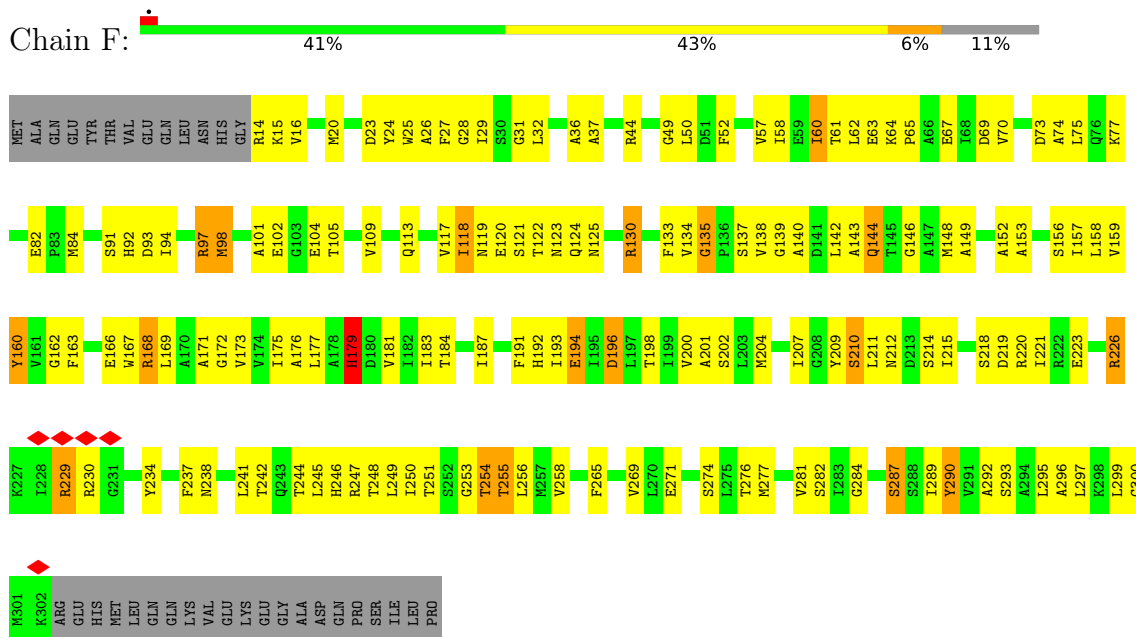


Chain D: 29% 33% 5% 33%

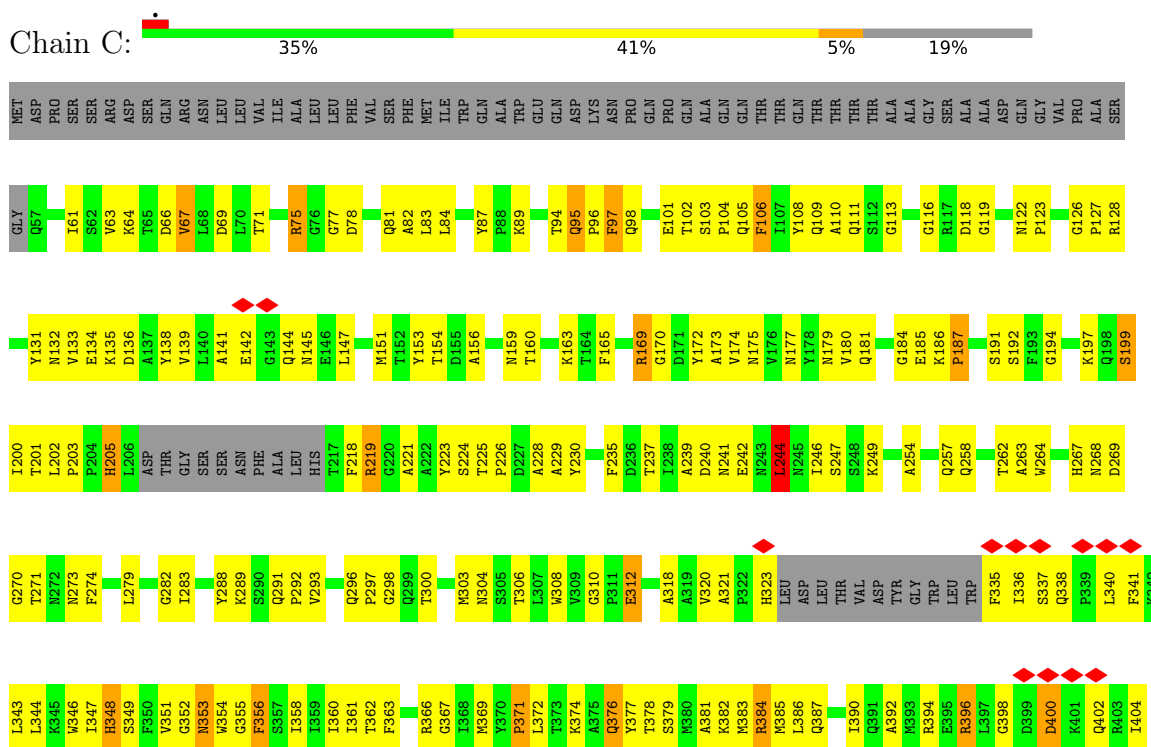


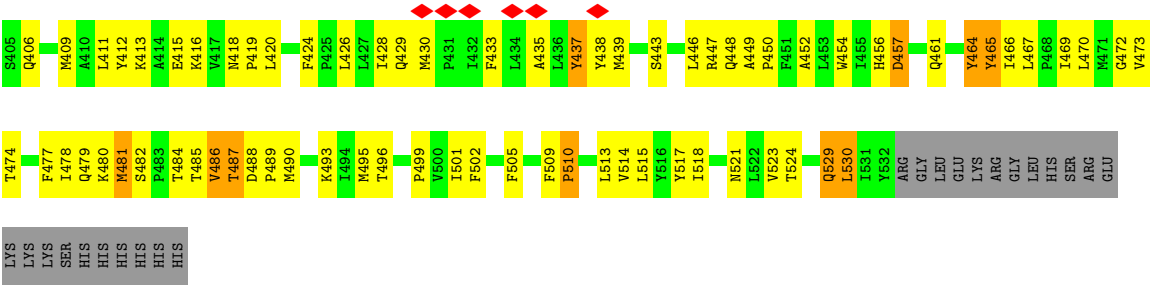


• Molecule 5: Protein translocase subunit SecF



• Molecule 6: Membrane protein insertase YidC





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53648	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	153.928	Depositor
Minimum map value	-63.993	Depositor
Average map value	1.728	Depositor
Map value standard deviation	15.464	Depositor
Recommended contour level	8.5	Depositor
Map size ($\text{\AA}$)	190.40001, 190.40001, 190.40001	wwPDB
Map dimensions	140, 140, 140	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	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	Y	2.32	118/3501 (3.4%)	2.59	300/4744 (6.3%)
2	E	2.33	19/518 (3.7%)	2.60	43/702 (6.1%)
3	G	2.20	6/238 (2.5%)	2.53	16/320 (5.0%)
4	D	2.23	114/3163 (3.6%)	2.51	231/4288 (5.4%)
5	F	2.14	55/2250 (2.4%)	2.58	183/3049 (6.0%)
6	C	2.16	116/3683 (3.1%)	2.45	257/5013 (5.1%)
All	All	2.22	428/13353 (3.2%)	2.53	1030/18116 (5.7%)

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	Y	0	11
2	E	0	3
4	D	0	9
5	F	0	13
6	C	0	21
All	All	0	57

All (428) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	317	TYR	CG-CD2	22.02	1.85	1.39
1	Y	317	TYR	CG-CD1	21.22	1.83	1.39
1	Y	317	TYR	CE2-CZ	18.32	1.82	1.38
1	Y	317	TYR	CE1-CZ	18.09	1.81	1.38
1	Y	317	TYR	CD1-CE1	11.81	1.74	1.38
1	Y	317	TYR	CD2-CE2	11.38	1.72	1.38
1	Y	199	LEU	CA-C	10.45	1.66	1.52
4	D	234	LEU	CA-C	9.37	1.65	1.52
1	Y	219	VAL	CA-CB	9.35	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	497	LEU	CA-CB	9.09	1.63	1.53
2	E	505	GLY	CA-C	-9.09	1.42	1.52
1	Y	387	ILE	CA-CB	8.98	1.60	1.53
4	D	598	ARG	N-CA	8.89	1.57	1.46
1	Y	149	VAL	CA-CB	8.27	1.65	1.54
4	D	434	GLN	C-N	8.23	1.43	1.33
5	F	64	LYS	N-CA	-8.10	1.39	1.46
6	C	264	TRP	C-N	8.02	1.42	1.33
1	Y	142	MET	CA-C	8.02	1.62	1.52
1	Y	286	PHE	N-CA	7.97	1.53	1.46
6	C	165	PHE	CA-C	-7.96	1.43	1.52
4	D	254	ASP	CA-C	7.95	1.63	1.52
6	C	154	THR	CA-C	-7.92	1.43	1.52
6	C	226	PRO	CA-C	-7.90	1.42	1.52
6	C	67	VAL	CA-CB	7.88	1.63	1.54
1	Y	68	SER	CA-CB	7.86	1.65	1.53
6	C	323	HIS	CB-CG	7.85	1.61	1.50
5	F	179	HIS	C-N	7.84	1.44	1.34
4	D	601	VAL	CA-C	7.76	1.62	1.52
4	D	297	ARG	C-N	7.63	1.42	1.33
1	Y	275	ILE	CA-CB	-7.63	1.50	1.54
6	C	78	ASP	CA-C	7.61	1.61	1.52
1	Y	427	SER	CA-CB	7.59	1.65	1.53
1	Y	126	VAL	N-CA	7.54	1.53	1.46
4	D	313	VAL	C-N	7.52	1.43	1.33
1	Y	385	CYS	N-CA	-7.47	1.36	1.46
1	Y	131	GLN	N-CA	-7.43	1.37	1.46
4	D	470	ILE	CA-C	7.42	1.62	1.52
6	C	153	TYR	CA-C	7.41	1.61	1.52
6	C	133	VAL	N-CA	7.40	1.54	1.46
3	G	509	SER	C-N	7.39	1.43	1.33
6	C	363	PHE	N-CA	7.33	1.55	1.46
5	F	149	ALA	CA-C	-7.32	1.43	1.52
6	C	320	VAL	CA-C	7.30	1.61	1.52
1	Y	413	ILE	CA-CB	-7.29	1.46	1.54
4	D	13	LEU	N-CA	-7.29	1.37	1.46
2	E	456	ALA	CA-C	-7.28	1.43	1.52
6	C	349	SER	CA-C	-7.27	1.43	1.52
6	C	433	PHE	CA-C	7.26	1.62	1.52
4	D	376	GLY	N-CA	7.25	1.54	1.45
4	D	580	ILE	CA-CB	7.25	1.62	1.54
6	C	156	ALA	CA-C	7.24	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	413	ASN	CA-CB	-7.24	1.43	1.53
6	C	66	ASP	CA-C	7.22	1.61	1.52
3	G	522	LEU	N-CA	7.21	1.55	1.46
2	E	501	SER	CA-CB	7.21	1.65	1.53
4	D	254	ASP	CA-CB	7.18	1.63	1.53
1	Y	205	HIS	CA-CB	7.16	1.65	1.53
4	D	336	TYR	C-N	7.13	1.43	1.33
1	Y	148	LEU	CB-CG	7.13	1.67	1.53
1	Y	223	VAL	N-CA	7.13	1.55	1.46
5	F	249	LEU	CA-C	7.12	1.61	1.52
5	F	52	PHE	C-N	7.10	1.43	1.33
6	C	443	SER	CA-C	-7.09	1.44	1.52
5	F	67	GLU	C-N	7.05	1.42	1.33
6	C	381	ALA	CA-C	-7.04	1.44	1.52
5	F	179	HIS	ND1-CE1	7.03	1.39	1.32
6	C	518	ILE	CA-C	7.03	1.61	1.52
1	Y	397	VAL	CA-C	7.01	1.60	1.52
4	D	541	ALA	N-CA	-6.99	1.38	1.46
6	C	435	ALA	C-N	6.98	1.43	1.33
4	D	238	VAL	N-CA	-6.98	1.37	1.46
2	E	484	VAL	CA-CB	-6.96	1.46	1.54
6	C	145	ASN	CA-C	6.95	1.62	1.52
6	C	78	ASP	N-CA	-6.94	1.37	1.45
4	D	343	ILE	CA-CB	-6.89	1.45	1.54
4	D	6	PRO	CA-C	6.89	1.60	1.52
1	Y	396	LYS	CA-CB	6.88	1.65	1.53
6	C	247	SER	CA-C	6.87	1.61	1.52
5	F	109	VAL	CA-CB	-6.87	1.47	1.54
4	D	310	GLY	C-N	6.85	1.41	1.33
5	F	57	VAL	CA-C	6.83	1.61	1.52
1	Y	365	TYR	C-N	6.83	1.41	1.33
1	Y	330	PHE	CA-C	6.81	1.60	1.52
1	Y	150	ILE	CA-CB	6.79	1.61	1.54
1	Y	405	SER	N-CA	-6.79	1.37	1.46
4	D	11	VAL	CA-C	-6.79	1.44	1.52
1	Y	141	ASN	CA-C	-6.76	1.41	1.52
6	C	244	LEU	CA-C	6.75	1.61	1.52
6	C	360	ILE	CA-CB	6.74	1.62	1.54
5	F	97	ARG	CA-CB	6.72	1.65	1.53
5	F	117	VAL	C-N	6.71	1.41	1.33
6	C	127	PRO	CA-CB	-6.69	1.44	1.53
1	Y	191	ILE	CA-CB	-6.69	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	122	THR	C-N	6.68	1.43	1.33
4	D	16	VAL	C-N	6.65	1.42	1.33
1	Y	23	LEU	CA-C	6.65	1.62	1.52
4	D	510	ILE	CA-C	6.63	1.61	1.52
2	E	472	LEU	C-N	6.62	1.43	1.34
6	C	225	THR	N-CA	6.61	1.51	1.45
5	F	60	ILE	CA-C	6.56	1.60	1.52
4	D	415	ASN	CA-C	6.54	1.61	1.52
2	E	468	ARG	C-N	6.53	1.42	1.33
6	C	87	TYR	CA-CB	6.53	1.61	1.53
1	Y	87	SER	CA-CB	6.51	1.63	1.53
5	F	167	TRP	CA-C	6.48	1.61	1.52
4	D	598	ARG	CD-NE	6.48	1.55	1.46
5	F	271	GLU	N-CA	6.48	1.54	1.46
4	D	441	ILE	N-CA	-6.48	1.37	1.46
1	Y	59	THR	CA-C	6.46	1.60	1.52
6	C	341	PHE	CA-C	6.45	1.61	1.52
4	D	243	VAL	CA-CB	6.44	1.60	1.53
4	D	356	PHE	C-N	6.43	1.42	1.33
5	F	138	VAL	CA-C	6.41	1.60	1.52
4	D	235	ARG	N-CA	-6.40	1.38	1.46
2	E	482	THR	CA-C	6.40	1.60	1.52
6	C	173	ALA	CA-CB	6.39	1.62	1.53
6	C	505	PHE	CA-C	6.38	1.61	1.52
4	D	291	ALA	N-CA	-6.38	1.38	1.46
6	C	362	THR	C-N	6.38	1.42	1.33
4	D	373	LYS	CA-C	-6.37	1.44	1.52
6	C	160	THR	CA-CB	-6.37	1.44	1.53
6	C	258	GLN	C-O	-6.36	1.16	1.23
4	D	383	ARG	CD-NE	6.36	1.55	1.46
6	C	467	LEU	CA-C	6.36	1.60	1.52
1	Y	201	PRO	CA-C	6.35	1.58	1.52
1	Y	382	THR	C-N	6.33	1.42	1.34
4	D	586	VAL	CA-C	-6.32	1.42	1.52
1	Y	260	ALA	N-CA	-6.31	1.38	1.46
1	Y	417	MET	CA-CB	-6.30	1.43	1.53
6	C	416	LYS	CA-C	-6.29	1.45	1.53
4	D	17	ILE	N-CA	-6.29	1.38	1.46
4	D	533	SER	CA-CB	6.26	1.63	1.53
4	D	293	ALA	CA-CB	6.26	1.63	1.53
5	F	50	LEU	CA-C	6.25	1.58	1.52
4	D	342	ASN	N-CA	-6.24	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	497	LEU	CA-C	6.24	1.60	1.52
6	C	499	PRO	CA-CB	6.24	1.62	1.53
1	Y	164	LEU	C-O	-6.24	1.17	1.24
5	F	92	HIS	CD2-NE2	6.23	1.44	1.37
4	D	252	GLY	CA-C	-6.23	1.44	1.51
5	F	244	THR	N-CA	6.22	1.53	1.46
2	E	449	THR	C-N	-6.21	1.27	1.33
4	D	557	ASN	CA-C	6.17	1.60	1.52
4	D	447	MET	CA-CB	6.17	1.63	1.53
2	E	461	ARG	CD-NE	6.15	1.54	1.46
4	D	297	ARG	CA-C	6.14	1.61	1.52
4	D	232	ASN	N-CA	6.14	1.53	1.46
1	Y	130	PHE	CA-C	6.14	1.61	1.52
6	C	269	ASP	CA-CB	6.13	1.63	1.53
1	Y	30	LEU	C-O	6.12	1.31	1.24
5	F	172	GLY	N-CA	6.09	1.53	1.45
4	D	572	THR	CA-C	-6.09	1.45	1.52
1	Y	320	LEU	C-N	6.07	1.41	1.33
4	D	531	GLU	CA-CB	6.07	1.62	1.53
6	C	102	THR	CA-C	-6.04	1.44	1.52
5	F	179	HIS	CA-CB	6.04	1.62	1.53
1	Y	200	PRO	C-N	6.04	1.38	1.33
4	D	7	LEU	N-CA	-6.04	1.39	1.46
6	C	225	THR	CA-C	-6.02	1.46	1.52
1	Y	164	LEU	C-N	6.02	1.41	1.33
6	C	237	THR	CA-CB	-6.02	1.45	1.53
6	C	387	GLN	C-N	6.01	1.41	1.34
6	C	474	THR	N-CA	6.00	1.53	1.46
4	D	389	GLN	N-CA	5.99	1.53	1.46
2	E	491	GLY	N-CA	5.98	1.53	1.45
6	C	111	GLN	N-CA	-5.97	1.39	1.46
1	Y	329	CYS	CA-CB	5.96	1.64	1.53
1	Y	113	ARG	CA-CB	5.95	1.63	1.53
6	C	291	GLN	CA-C	5.95	1.60	1.53
5	F	120	GLU	C-N	5.94	1.40	1.33
5	F	183	ILE	CA-CB	5.93	1.61	1.54
6	C	321	ALA	CA-C	-5.93	1.47	1.53
6	C	267	HIS	ND1-CE1	5.92	1.38	1.32
4	D	456	ALA	CA-C	5.92	1.60	1.52
1	Y	205	HIS	ND1-CE1	5.91	1.38	1.32
1	Y	428	GLN	N-CA	-5.91	1.39	1.46
1	Y	86	ILE	N-CA	-5.91	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	181	ARG	CD-NE	5.91	1.54	1.46
3	G	539	SER	CA-CB	5.89	1.62	1.53
1	Y	363	ALA	CA-C	-5.88	1.45	1.52
6	C	353	ASN	N-CA	-5.88	1.39	1.46
6	C	318	ALA	CA-C	5.88	1.60	1.52
1	Y	68	SER	N-CA	5.87	1.53	1.46
3	G	529	ILE	N-CA	5.87	1.53	1.46
2	E	501	SER	C-N	5.86	1.41	1.33
1	Y	13	LYS	N-CA	5.85	1.53	1.46
6	C	293	VAL	CA-CB	-5.85	1.47	1.54
1	Y	357	ARG	CD-NE	5.84	1.54	1.46
4	D	441	ILE	CA-C	-5.83	1.47	1.53
6	C	180	VAL	CA-CB	-5.83	1.47	1.54
6	C	273	ASN	CA-C	-5.82	1.45	1.52
1	Y	380	TYR	N-CA	-5.82	1.39	1.46
6	C	187	PRO	CA-CB	-5.82	1.45	1.53
4	D	503	SER	C-N	5.81	1.40	1.33
4	D	228	GLN	C-N	5.80	1.41	1.33
4	D	318	ARG	CD-NE	5.80	1.54	1.46
4	D	408	ILE	CA-CB	-5.80	1.47	1.54
6	C	224	SER	N-CA	-5.79	1.38	1.45
1	Y	64	PHE	CA-CB	5.79	1.62	1.53
6	C	69	ASP	C-N	5.79	1.41	1.33
1	Y	420	VAL	CA-C	-5.78	1.44	1.52
5	F	175	ILE	C-N	5.78	1.41	1.33
6	C	298	GLY	C-N	5.78	1.41	1.33
1	Y	217	PHE	CA-CB	5.77	1.63	1.53
6	C	429	GLN	C-N	5.77	1.40	1.33
1	Y	240	GLY	C-O	-5.77	1.17	1.24
5	F	57	VAL	CA-CB	-5.77	1.47	1.54
6	C	194	GLY	C-O	-5.76	1.16	1.23
1	Y	9	PHE	N-CA	-5.76	1.38	1.46
1	Y	441	TYR	CA-CB	5.76	1.64	1.53
1	Y	330	PHE	CA-CB	5.75	1.62	1.53
4	D	421	SER	CA-C	5.75	1.60	1.52
1	Y	345	ASN	CA-C	-5.75	1.45	1.52
1	Y	185	ASN	CA-CB	5.74	1.61	1.53
1	Y	347	LYS	CA-CB	5.74	1.60	1.53
1	Y	404	THR	C-O	-5.74	1.16	1.24
1	Y	334	ALA	CA-C	-5.73	1.45	1.52
4	D	269	ALA	C-N	5.73	1.40	1.33
6	C	352	GLY	C-N	5.71	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	296	ALA	C-N	5.71	1.41	1.33
4	D	361	ILE	C-N	5.70	1.42	1.33
5	F	258	VAL	N-CA	-5.69	1.40	1.46
4	D	524	ILE	CA-C	5.69	1.61	1.52
6	C	413	LYS	CA-CB	5.69	1.60	1.53
1	Y	383	PHE	CG-CD2	5.68	1.50	1.38
6	C	493	LYS	C-N	5.68	1.41	1.33
5	F	171	ALA	CA-C	-5.68	1.45	1.52
6	C	83	LEU	CB-CG	5.68	1.64	1.53
1	Y	52	LEU	C-N	5.67	1.41	1.33
1	Y	256	ARG	N-CA	-5.66	1.39	1.46
4	D	243	VAL	N-CA	-5.66	1.39	1.46
1	Y	161	VAL	CA-CB	-5.65	1.48	1.54
5	F	281	VAL	N-CA	-5.65	1.39	1.46
1	Y	153	GLY	C-N	5.64	1.42	1.33
4	D	536	ARG	C-N	5.64	1.41	1.33
6	C	186	LYS	CA-C	-5.63	1.45	1.52
6	C	257	GLN	CA-CB	5.63	1.62	1.53
1	Y	66	MET	CA-CB	5.63	1.62	1.53
6	C	424	PHE	CA-C	5.62	1.59	1.52
4	D	412	ASN	CA-CB	5.62	1.62	1.53
6	C	387	GLN	N-CA	-5.61	1.41	1.46
5	F	246	HIS	CA-CB	5.61	1.62	1.53
1	Y	332	TYR	CA-C	5.61	1.60	1.52
5	F	162	GLY	CA-C	5.61	1.58	1.52
6	C	184	GLY	C-N	5.61	1.40	1.33
5	F	251	THR	C-O	-5.61	1.17	1.23
1	Y	268	LYS	CA-C	5.60	1.60	1.52
3	G	512	SER	CA-CB	5.58	1.61	1.53
6	C	478	ILE	CA-CB	-5.58	1.48	1.54
6	C	419	PRO	CA-C	-5.57	1.47	1.53
4	D	241	LEU	CA-C	-5.57	1.45	1.52
4	D	375	SER	C-N	5.56	1.40	1.33
1	Y	219	VAL	CA-C	5.56	1.59	1.52
5	F	247	ARG	CA-C	-5.55	1.45	1.52
6	C	229	ALA	N-CA	5.55	1.52	1.46
1	Y	74	ARG	CD-NE	5.55	1.54	1.46
1	Y	35	ILE	C-O	-5.55	1.17	1.24
5	F	183	ILE	C-N	5.54	1.41	1.33
5	F	297	LEU	CA-CB	-5.54	1.44	1.53
5	F	98	MET	CA-CB	5.54	1.61	1.53
4	D	404	ASN	N-CA	5.54	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	422	THR	CA-CB	-5.54	1.45	1.53
1	Y	268	LYS	C-N	5.53	1.40	1.33
4	D	374	ASP	CA-CB	5.53	1.62	1.53
6	C	354	TRP	C-N	5.52	1.42	1.33
4	D	422	LEU	CA-CB	5.51	1.61	1.53
6	C	139	VAL	CA-C	-5.51	1.46	1.52
4	D	560	THR	N-CA	5.51	1.52	1.46
1	Y	106	LYS	CA-CB	5.51	1.62	1.53
6	C	110	ALA	N-CA	-5.51	1.39	1.45
2	E	479	ALA	N-CA	-5.50	1.39	1.46
1	Y	232	PHE	C-N	5.50	1.41	1.33
1	Y	408	ILE	CA-CB	-5.50	1.48	1.54
4	D	594	ILE	C-N	5.50	1.38	1.33
1	Y	42	PRO	N-CA	-5.48	1.40	1.47
1	Y	204	ALA	CA-C	5.47	1.60	1.52
1	Y	305	THR	CA-C	5.46	1.60	1.52
4	D	455	GLU	CA-CB	5.46	1.62	1.53
4	D	418	ARG	NE-CZ	-5.46	1.27	1.33
6	C	398	GLY	N-CA	5.46	1.53	1.45
2	E	448	ALA	C-N	5.46	1.41	1.33
4	D	332	SER	CA-C	5.45	1.59	1.52
1	Y	132	SER	N-CA	5.45	1.52	1.46
6	C	219	ARG	N-CA	5.45	1.53	1.46
6	C	489	PRO	CA-CB	5.43	1.62	1.53
5	F	123	ASN	CA-CB	5.43	1.62	1.53
1	Y	21	ARG	N-CA	5.42	1.52	1.46
5	F	74	ALA	CA-C	5.42	1.59	1.52
5	F	130	ARG	CA-C	-5.42	1.46	1.52
6	C	479	GLN	CA-CB	5.41	1.62	1.53
4	D	255	ARG	CD-NE	5.41	1.53	1.46
4	D	284	VAL	CA-C	-5.41	1.48	1.52
5	F	293	SER	CA-CB	5.41	1.61	1.53
1	Y	203	ILE	C-O	-5.41	1.17	1.24
5	F	143	ALA	C-N	5.39	1.41	1.33
1	Y	265	LEU	CA-CB	5.39	1.60	1.53
1	Y	272	ALA	N-CA	-5.39	1.39	1.46
1	Y	390	PHE	CA-CB	5.38	1.61	1.53
6	C	297	PRO	C-O	-5.38	1.16	1.23
4	D	290	GLN	C-N	5.37	1.41	1.33
1	Y	42	PRO	N-CD	-5.37	1.40	1.47
4	D	264	GLN	CA-CB	5.37	1.62	1.53
5	F	94	ILE	CA-C	-5.37	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	395	ILE	N-CA	-5.36	1.39	1.46
2	E	459	GLU	N-CA	-5.36	1.40	1.46
1	Y	400	TYR	CA-C	5.36	1.60	1.52
1	Y	36	GLY	C-O	-5.35	1.16	1.23
6	C	205	HIS	CD2-NE2	5.35	1.43	1.37
4	D	371	GLU	CA-C	5.34	1.58	1.52
1	Y	233	PHE	CA-C	-5.34	1.46	1.52
4	D	444	THR	CA-C	-5.33	1.45	1.52
6	C	113	GLY	CA-C	5.33	1.57	1.52
6	C	218	PHE	N-CA	-5.33	1.40	1.46
6	C	283	ILE	CA-CB	5.33	1.60	1.54
4	D	534	ASN	CA-CB	5.32	1.62	1.53
6	C	530	LEU	C-O	-5.32	1.17	1.23
6	C	465	TYR	CA-CB	5.31	1.63	1.53
5	F	244	THR	C-N	5.30	1.40	1.33
6	C	61	ILE	N-CA	5.30	1.52	1.46
4	D	272	ILE	C-N	-5.30	1.26	1.34
6	C	141	ALA	CA-CB	5.29	1.60	1.53
6	C	289	LYS	C-N	5.29	1.40	1.33
4	D	401	ARG	C-N	5.28	1.40	1.33
1	Y	65	ASN	CA-C	5.28	1.60	1.52
6	C	282	GLY	C-N	5.28	1.40	1.33
4	D	353	MET	CA-CB	5.26	1.61	1.53
2	E	486	SER	C-O	-5.26	1.18	1.24
4	D	257	VAL	CA-CB	5.25	1.61	1.54
2	E	490	TRP	NE1-CE2	-5.25	1.31	1.37
4	D	503	SER	CA-CB	5.24	1.62	1.53
4	D	609	ARG	CD-NE	5.24	1.53	1.46
6	C	201	THR	N-CA	-5.24	1.39	1.46
1	Y	257	VAL	CA-C	5.24	1.58	1.52
1	Y	119	TYR	CA-C	-5.24	1.46	1.52
1	Y	341	GLU	CA-CB	5.24	1.62	1.53
4	D	469	ILE	CA-C	5.24	1.59	1.52
1	Y	370	MET	N-CA	-5.23	1.40	1.46
4	D	425	ARG	CA-CB	5.23	1.61	1.53
1	Y	168	THR	N-CA	5.22	1.52	1.46
2	E	473	HIS	C-N	5.22	1.41	1.34
4	D	592	THR	CA-CB	5.21	1.61	1.53
4	D	354	SER	CA-C	5.21	1.59	1.52
6	C	181	GLN	C-N	-5.21	1.27	1.33
5	F	282	SER	CA-C	5.20	1.59	1.52
1	Y	352	PHE	CA-C	-5.20	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	78	ASP	C-N	5.18	1.39	1.33
4	D	236	ASN	C-N	5.18	1.41	1.33
6	C	447	ARG	CD-NE	5.17	1.53	1.46
6	C	378	THR	CA-C	-5.17	1.45	1.52
6	C	151	MET	C-N	5.17	1.40	1.33
6	C	293	VAL	CA-C	-5.17	1.46	1.52
6	C	228	ALA	N-CA	5.16	1.52	1.45
5	F	15	LYS	C-N	5.16	1.40	1.33
4	D	278	THR	C-N	5.16	1.41	1.33
4	D	494	MET	N-CA	5.16	1.52	1.46
6	C	523	VAL	CA-CB	-5.16	1.48	1.54
1	Y	188	SER	C-N	5.15	1.40	1.33
5	F	229	ARG	CD-NE	5.15	1.53	1.46
6	C	529	GLN	C-N	5.15	1.40	1.33
4	D	287	ASN	CA-C	-5.15	1.46	1.52
4	D	467	PHE	CA-C	-5.15	1.46	1.52
4	D	372	TYR	C-N	5.15	1.40	1.33
4	D	262	GLY	N-CA	-5.14	1.38	1.45
4	D	325	HIS	CA-CB	5.14	1.62	1.53
6	C	235	PHE	C-N	5.14	1.41	1.33
1	Y	40	PRO	N-CD	5.14	1.54	1.47
4	D	438	GLU	C-N	5.14	1.40	1.33
4	D	439	ARG	C-N	5.14	1.40	1.33
6	C	291	GLN	CA-CB	5.14	1.61	1.53
4	D	462	LEU	CA-CB	-5.14	1.45	1.53
4	D	558	ILE	N-CA	-5.14	1.40	1.46
6	C	383	MET	CA-C	5.13	1.59	1.52
4	D	575	ILE	C-O	-5.13	1.18	1.24
6	C	279	LEU	CA-C	-5.13	1.45	1.52
5	F	299	LEU	C-N	5.13	1.40	1.33
4	D	261	PRO	N-CA	-5.13	1.41	1.47
4	D	563	LYS	N-CA	5.12	1.52	1.46
5	F	166	GLU	N-CA	-5.12	1.40	1.46
4	D	539	GLN	C-O	-5.12	1.18	1.24
1	Y	335	LEU	C-N	5.12	1.40	1.33
4	D	240	GLN	C-O	-5.12	1.17	1.24
1	Y	384	ILE	C-N	5.12	1.41	1.33
6	C	241	ASN	CA-CB	5.12	1.62	1.53
1	Y	250	LYS	CA-C	5.11	1.59	1.52
4	D	513	THR	CA-C	5.11	1.59	1.52
1	Y	237	VAL	CA-C	5.11	1.59	1.52
1	Y	211	ARG	CA-CB	5.11	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	457	ARG	NE-CZ	5.11	1.38	1.33
6	C	404	ILE	CA-C	5.11	1.59	1.52
4	D	23	TYR	CA-C	5.10	1.59	1.52
6	C	71	THR	CA-CB	5.10	1.61	1.53
1	Y	26	VAL	C-N	5.10	1.39	1.33
1	Y	354	PRO	N-CA	-5.10	1.41	1.47
4	D	333	GLN	C-O	-5.10	1.18	1.24
6	C	268	ASN	C-N	5.10	1.40	1.33
2	E	490	TRP	CZ2-CH2	5.09	1.47	1.37
4	D	314	VAL	N-CA	5.09	1.53	1.46
5	F	65	PRO	N-CD	-5.09	1.40	1.47
6	C	430	MET	CA-CB	5.09	1.60	1.53
6	C	450	PRO	N-CA	-5.09	1.41	1.47
5	F	221	ILE	CA-CB	5.09	1.60	1.54
6	C	304	ASN	CA-C	-5.08	1.46	1.52
1	Y	167	GLY	N-CA	5.08	1.52	1.45
1	Y	129	ILE	CB-CG1	5.08	1.63	1.53
4	D	538	VAL	CA-C	-5.08	1.47	1.52
4	D	392	VAL	CA-CB	-5.08	1.47	1.54
6	C	254	ALA	CA-C	5.08	1.58	1.52
1	Y	21	ARG	CD-NE	5.07	1.53	1.46
5	F	152	ALA	CA-CB	5.06	1.61	1.53
6	C	134	GLU	N-CA	-5.06	1.40	1.46
3	G	536	ASN	CA-C	-5.05	1.46	1.52
5	F	177	LEU	CA-C	5.05	1.59	1.52
6	C	356	PHE	CA-CB	5.05	1.61	1.53
6	C	416	LYS	CA-CB	5.05	1.58	1.53
1	Y	222	LEU	N-CA	-5.04	1.40	1.46
1	Y	354	PRO	CA-CB	5.04	1.60	1.53
1	Y	303	LEU	CA-C	5.04	1.59	1.52
6	C	77	GLY	C-N	5.04	1.40	1.33
5	F	15	LYS	CA-C	-5.04	1.46	1.53
6	C	390	ILE	CA-CB	5.03	1.61	1.54
6	C	81	GLN	C-N	5.03	1.39	1.33
5	F	219	ASP	C-N	5.03	1.40	1.33
4	D	534	ASN	CA-C	5.03	1.59	1.52
5	F	25	TRP	N-CA	-5.03	1.40	1.46
4	D	437	GLU	CA-C	5.02	1.59	1.52
6	C	361	ILE	CA-C	5.02	1.60	1.52
1	Y	184	GLY	CA-C	5.02	1.57	1.51
4	D	305	LYS	C-N	5.01	1.40	1.33

All (1030) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	226	ARG	NE-CZ-NH1	13.30	134.80	121.50
6	C	321	ALA	N-CA-C	11.42	124.14	109.64
1	Y	210	ALA	N-CA-C	10.90	123.16	111.28
4	D	235	ARG	N-CA-C	10.87	124.22	111.71
1	Y	126	VAL	N-CA-C	-10.66	103.20	111.62
1	Y	323	SER	N-CA-C	10.61	122.60	111.14
5	F	140	ALA	N-CA-C	10.22	122.42	111.28
5	F	212	ASN	CA-C-N	10.16	133.65	120.44
5	F	212	ASN	C-N-CA	10.16	133.65	120.44
4	D	297	ARG	NE-CZ-NH1	10.11	131.61	121.50
6	C	310	GLY	CA-C-N	10.04	130.67	119.93
6	C	310	GLY	C-N-CA	10.04	130.67	119.93
4	D	431	ALA	N-CA-C	-9.82	97.54	110.40
6	C	199	SER	CA-C-O	9.75	131.88	121.15
6	C	452	ALA	N-CA-C	9.61	124.06	111.75
6	C	349	SER	N-CA-C	9.57	121.71	111.28
6	C	109	GLN	O-C-N	-9.51	113.25	123.42
4	D	452	GLN	CA-C-N	9.48	130.43	120.00
4	D	452	GLN	C-N-CA	9.48	130.43	120.00
1	Y	408	ILE	N-CA-C	9.44	120.28	110.36
4	D	413	ASN	CA-C-O	-9.41	111.80	119.71
6	C	132	ASN	CA-CB-CG	-9.36	103.24	112.60
1	Y	367	ASP	CA-CB-CG	9.23	121.83	112.60
4	D	379	ASP	CA-CB-CG	9.23	121.83	112.60
3	G	523	LEU	N-CA-C	9.22	122.48	111.33
1	Y	283	ILE	N-CA-C	9.09	122.42	111.05
5	F	94	ILE	O-C-N	-9.09	113.87	123.14
5	F	250	ILE	N-CA-C	9.07	119.12	110.42
2	E	459	GLU	N-CA-C	9.01	120.71	111.07
5	F	226	ARG	CA-C-O	-9.01	110.87	120.42
1	Y	166	THR	CA-C-N	8.85	129.81	119.98
1	Y	166	THR	C-N-CA	8.85	129.81	119.98
1	Y	216	HIS	CB-CG-CD2	-8.85	119.70	131.20
4	D	396	ALA	CA-C-O	-8.75	111.86	121.23
1	Y	9	PHE	CA-CB-CG	8.73	122.53	113.80
4	D	598	ARG	N-CA-C	8.71	121.93	111.82
1	Y	68	SER	N-CA-C	8.70	120.76	111.28
5	F	74	ALA	N-CA-C	8.69	120.75	111.28
2	E	493	ASP	CA-CB-CG	8.61	121.21	112.60
5	F	292	ALA	N-CA-C	8.57	121.40	111.11
6	C	122	ASN	O-C-N	-8.56	114.36	121.38
6	C	175	ASN	OD1-CG-ND2	-8.48	114.12	122.60
4	D	275	ALA	N-CA-C	8.46	122.50	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	226	ARG	NH1-CZ-NH2	-8.44	108.32	119.30
2	E	452	PHE	CA-CB-CG	-8.42	105.38	113.80
6	C	456	HIS	CA-CB-CG	-8.42	105.38	113.80
4	D	350	GLY	CA-C-N	8.42	131.56	120.28
4	D	350	GLY	C-N-CA	8.42	131.56	120.28
1	Y	154	PHE	CA-CB-CG	-8.36	105.44	113.80
1	Y	338	ASN	CA-C-O	-8.33	112.37	119.36
6	C	136	ASP	CA-CB-CG	8.32	120.92	112.60
1	Y	276	PRO	CA-C-N	8.31	131.41	120.28
1	Y	276	PRO	C-N-CA	8.31	131.41	120.28
6	C	400	ASP	CA-CB-CG	8.30	120.90	112.60
4	D	547	ARG	O-C-N	-8.26	112.74	122.15
6	C	142	GLU	N-CA-C	8.17	120.86	110.24
4	D	359	ASP	CA-CB-CG	8.15	120.75	112.60
1	Y	160	ALA	CA-C-N	8.12	131.08	120.60
1	Y	160	ALA	C-N-CA	8.12	131.08	120.60
4	D	268	ARG	NE-CZ-NH2	-8.10	111.91	119.20
6	C	240	ASP	CA-CB-CG	8.07	120.67	112.60
5	F	247	ARG	CD-NE-CZ	-8.06	113.12	124.40
5	F	168	ARG	NE-CZ-NH2	-8.05	111.96	119.20
5	F	254	THR	N-CA-C	8.02	119.65	111.07
3	G	513	GLY	N-CA-C	7.99	124.18	111.64
6	C	273	ASN	OD1-CG-ND2	-7.95	114.65	122.60
1	Y	275	ILE	CA-C-O	-7.95	112.67	118.71
1	Y	381	ILE	N-CA-C	7.94	118.70	110.36
1	Y	26	VAL	O-C-N	7.94	130.16	121.90
4	D	438	GLU	CA-C-N	7.94	135.06	122.83
4	D	438	GLU	C-N-CA	7.94	135.06	122.83
1	Y	199	LEU	CA-C-N	7.92	128.54	120.38
1	Y	199	LEU	C-N-CA	7.92	128.54	120.38
1	Y	370	MET	N-CA-C	7.92	119.92	111.28
6	C	218	PHE	CA-CB-CG	-7.92	105.88	113.80
1	Y	195	ILE	N-CA-C	-7.92	104.65	112.17
4	D	591	PHE	CA-CB-CG	-7.91	105.89	113.80
6	C	510	PRO	N-CA-C	7.90	123.59	111.34
6	C	113	GLY	N-CA-C	7.87	121.88	110.63
5	F	271	GLU	O-C-N	-7.86	113.91	122.09
2	E	456	ALA	CA-C-N	7.86	130.65	120.44
2	E	456	ALA	C-N-CA	7.86	130.65	120.44
4	D	353	MET	CA-C-N	7.86	130.65	120.44
4	D	353	MET	C-N-CA	7.86	130.65	120.44
6	C	177	ASN	CA-CB-CG	-7.84	104.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	122	ASN	OD1-CG-ND2	-7.83	114.77	122.60
1	Y	392	ARG	NE-CZ-NH1	7.82	129.32	121.50
6	C	291	GLN	O-C-N	-7.82	115.37	121.47
5	F	31	GLY	N-CA-C	7.81	122.36	112.83
5	F	214	SER	CA-C-O	7.80	129.05	120.63
1	Y	199	LEU	O-C-N	-7.80	112.35	121.32
1	Y	270	ASN	CA-C-N	7.77	131.02	120.38
1	Y	270	ASN	C-N-CA	7.77	131.02	120.38
1	Y	200	PRO	N-CA-C	7.75	120.15	110.70
5	F	156	SER	N-CA-C	7.75	119.72	111.28
4	D	525	ASN	CA-C-O	7.73	128.61	120.42
5	F	196	ASP	CA-CB-CG	-7.73	104.87	112.60
5	F	64	LYS	N-CA-C	7.72	123.28	113.25
6	C	239	ALA	CA-C-N	7.71	135.89	122.32
6	C	239	ALA	C-N-CA	7.71	135.89	122.32
1	Y	186	GLY	O-C-N	-7.70	114.59	122.60
6	C	267	HIS	CE1-NE2-CD2	-7.68	101.32	109.00
1	Y	387	ILE	O-C-N	-7.65	114.64	120.07
5	F	27	PHE	CA-C-N	7.64	128.42	119.94
5	F	27	PHE	C-N-CA	7.64	128.42	119.94
6	C	402	GLN	N-CA-C	7.62	122.02	112.87
5	F	26	ALA	CA-C-N	7.61	130.80	120.38
5	F	26	ALA	C-N-CA	7.61	130.80	120.38
1	Y	338	ASN	CA-C-N	7.60	129.34	119.84
1	Y	338	ASN	C-N-CA	7.60	129.34	119.84
1	Y	376	VAL	N-CA-C	7.59	119.24	109.30
5	F	97	ARG	CD-NE-CZ	7.57	135.00	124.40
4	D	3	ASN	OD1-CG-ND2	-7.57	115.03	122.60
6	C	437	TYR	O-C-N	-7.52	114.32	122.07
5	F	144	GLN	CB-CG-CD	7.49	125.34	112.60
1	Y	246	VAL	CA-C-O	-7.49	113.48	121.19
5	F	276	THR	CA-C-N	7.49	130.65	120.54
5	F	276	THR	C-N-CA	7.49	130.65	120.54
4	D	297	ARG	NE-CZ-NH2	-7.44	112.50	119.20
4	D	532	LEU	CA-C-N	7.44	130.11	120.44
4	D	532	LEU	C-N-CA	7.44	130.11	120.44
1	Y	133	ILE	CA-C-O	-7.43	113.22	120.95
4	D	268	ARG	NE-CZ-NH1	7.43	128.93	121.50
5	F	143	ALA	N-CA-C	7.41	119.00	111.07
1	Y	200	PRO	N-CA-CB	7.41	110.27	103.08
5	F	142	LEU	N-CA-C	7.41	119.00	111.07
6	C	262	THR	CA-C-O	-7.40	112.75	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	332	SER	N-CA-C	-7.39	97.38	108.99
6	C	486	VAL	O-C-N	-7.38	113.34	122.57
1	Y	319	LEU	O-C-N	-7.38	114.30	122.12
5	F	247	ARG	NE-CZ-NH2	-7.38	112.56	119.20
5	F	168	ARG	NE-CZ-NH1	7.37	128.87	121.50
5	F	176	ALA	CA-C-O	-7.37	113.09	120.82
1	Y	244	ILE	N-CA-C	7.36	117.98	108.12
1	Y	126	VAL	CB-CA-C	7.34	117.58	111.05
5	F	277	MET	CA-C-N	7.34	129.98	120.44
5	F	277	MET	C-N-CA	7.34	129.98	120.44
5	F	49	GLY	O-C-N	-7.32	116.92	123.88
5	F	187	ILE	CA-C-N	7.32	130.09	120.28
5	F	187	ILE	C-N-CA	7.32	130.09	120.28
1	Y	386	LEU	CA-C-N	7.32	124.85	120.24
1	Y	386	LEU	C-N-CA	7.32	124.85	120.24
4	D	510	ILE	CA-C-N	7.31	129.77	120.56
4	D	510	ILE	C-N-CA	7.31	129.77	120.56
4	D	531	GLU	CA-C-N	7.31	129.94	120.44
4	D	531	GLU	C-N-CA	7.31	129.94	120.44
4	D	413	ASN	N-CA-C	7.31	118.56	109.57
1	Y	175	GLY	O-C-N	-7.30	114.32	122.28
4	D	380	ALA	N-CA-CB	-7.29	100.27	111.56
2	E	499	LEU	N-CA-C	7.26	119.28	111.36
4	D	9	LYS	CA-C-O	7.25	128.24	120.55
6	C	372	LEU	CA-C-N	7.25	129.87	120.44
6	C	372	LEU	C-N-CA	7.25	129.87	120.44
1	Y	113	ARG	NH1-CZ-NH2	7.23	128.70	119.30
6	C	159	ASN	CA-CB-CG	-7.22	105.38	112.60
5	F	253	GLY	CA-C-N	7.20	129.80	120.44
5	F	253	GLY	C-N-CA	7.20	129.80	120.44
1	Y	200	PRO	CA-C-N	7.19	128.17	120.83
1	Y	200	PRO	C-N-CA	7.19	128.17	120.83
1	Y	300	TRP	CB-CG-CD2	-7.19	116.73	126.80
2	E	485	MET	CG-SD-CE	-7.19	85.08	100.90
1	Y	8	ASP	CA-C-N	7.19	131.38	120.82
1	Y	8	ASP	C-N-CA	7.19	131.38	120.82
6	C	338	GLN	O-C-N	-7.17	113.08	121.32
1	Y	228	PHE	N-CA-C	7.16	119.09	111.28
1	Y	186	GLY	CA-C-N	7.15	129.57	120.56
1	Y	186	GLY	C-N-CA	7.15	129.57	120.56
6	C	267	HIS	CG-CD2-NE2	7.15	114.35	107.20
6	C	338	GLN	OE1-CD-NE2	-7.15	115.45	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	143	ALA	O-C-N	-7.13	114.73	122.07
4	D	385	VAL	N-CA-C	7.13	119.89	109.63
6	C	474	THR	N-CA-C	7.13	119.05	111.28
6	C	473	VAL	N-CA-C	7.11	117.24	110.42
1	Y	257	VAL	CA-C-O	-7.11	112.35	120.74
1	Y	413	ILE	N-CA-C	7.10	117.82	110.36
1	Y	262	SER	CA-C-N	7.10	131.53	121.02
1	Y	262	SER	C-N-CA	7.10	131.53	121.02
6	C	249	LYS	N-CA-CB	7.10	120.51	110.36
5	F	246	HIS	CA-C-N	7.09	130.12	120.54
5	F	246	HIS	C-N-CA	7.09	130.12	120.54
2	E	477	ILE	N-CA-C	7.09	117.85	110.62
1	Y	319	LEU	CA-C-O	7.08	128.06	120.55
1	Y	324	ALA	CA-C-O	7.08	128.11	119.97
4	D	393	ILE	N-CA-C	7.08	117.87	110.72
4	D	529	LYS	N-CA-C	7.04	118.61	111.07
1	Y	312	PRO	CA-C-N	7.04	129.00	120.13
1	Y	312	PRO	C-N-CA	7.04	129.00	120.13
1	Y	342	THR	O-C-N	-7.03	114.78	122.09
4	D	9	LYS	N-CA-C	7.03	118.94	111.28
1	Y	333	THR	CA-C-N	7.02	134.96	121.54
1	Y	333	THR	C-N-CA	7.02	134.96	121.54
6	C	418	ASN	CA-CB-CG	-7.02	105.58	112.60
5	F	58	ILE	CA-C-O	7.01	127.75	120.39
6	C	480	LYS	N-CA-C	7.01	119.57	110.53
6	C	470	LEU	N-CA-C	6.99	118.90	111.28
6	C	384	ARG	NE-CZ-NH2	-6.98	112.92	119.20
4	D	359	ASP	N-CA-CB	-6.97	99.90	110.01
1	Y	247	ASN	N-CA-C	6.97	120.73	109.02
1	Y	80	LEU	CA-C-N	6.96	131.34	120.00
1	Y	80	LEU	C-N-CA	6.96	131.34	120.00
6	C	274	PHE	CA-CB-CG	-6.94	106.86	113.80
6	C	385	MET	CG-SD-CE	-6.94	85.63	100.90
1	Y	344	ASP	O-C-N	-6.92	114.12	122.22
5	F	105	THR	CA-CB-CG2	6.91	122.24	110.50
5	F	255	THR	CA-CB-CG2	-6.89	98.78	110.50
1	Y	199	LEU	N-CA-CB	6.89	122.64	110.37
5	F	162	GLY	N-CA-C	6.88	120.49	112.50
4	D	239	ASN	OD1-CG-ND2	-6.88	115.72	122.60
2	E	455	GLU	CA-C-N	6.87	129.49	120.28
2	E	455	GLU	C-N-CA	6.87	129.49	120.28
1	Y	286	PHE	CA-CB-CG	6.87	120.67	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	336	ILE	CA-C-N	6.86	134.65	121.54
6	C	336	ILE	C-N-CA	6.86	134.65	121.54
1	Y	175	GLY	CA-C-O	6.85	127.84	120.30
4	D	406	PHE	CB-CA-C	6.84	121.89	109.37
4	D	282	ARG	NE-CZ-NH1	6.84	128.34	121.50
6	C	409	MET	N-CA-C	6.83	119.56	111.71
1	Y	107	LYS	N-CA-CB	6.82	120.06	109.48
1	Y	371	THR	O-C-N	-6.82	114.89	122.12
1	Y	205	HIS	CE1-NE2-CD2	-6.82	102.18	109.00
1	Y	264	HIS	CE1-NE2-CD2	-6.82	102.18	109.00
1	Y	113	ARG	NE-CZ-NH2	-6.81	113.07	119.20
4	D	397	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	Y	237	VAL	O-C-N	6.79	128.56	121.91
1	Y	274	VAL	CA-C-N	6.79	126.95	120.43
1	Y	274	VAL	C-N-CA	6.79	126.95	120.43
6	C	502	PHE	N-CA-C	6.79	118.33	111.07
2	E	450	VAL	O-C-N	-6.78	115.81	122.12
4	D	237	ARG	CA-C-O	-6.77	111.80	119.79
2	E	485	MET	N-CA-CB	6.77	120.07	110.12
1	Y	408	ILE	N-CA-CB	6.75	118.01	110.51
5	F	214	SER	N-CA-C	6.75	119.50	111.33
1	Y	250	LYS	CA-C-O	-6.75	114.15	121.44
4	D	284	VAL	O-C-N	-6.74	115.60	122.75
6	C	379	SER	CA-C-O	6.74	127.24	119.35
4	D	574	ALA	N-CA-C	6.74	118.62	111.28
6	C	371	PRO	CA-C-N	6.74	129.63	120.54
6	C	371	PRO	C-N-CA	6.74	129.63	120.54
5	F	276	THR	O-C-N	-6.73	115.14	122.07
6	C	437	TYR	CA-C-O	6.73	127.89	120.82
6	C	481	MET	N-CA-CB	6.73	121.86	110.49
6	C	369	MET	CA-C-N	6.73	128.50	120.09
6	C	369	MET	C-N-CA	6.73	128.50	120.09
1	Y	258	TYR	N-CA-CB	6.71	121.84	110.49
6	C	181	GLN	CA-C-N	6.71	131.97	122.05
6	C	181	GLN	C-N-CA	6.71	131.97	122.05
4	D	328	ASP	N-CA-CB	6.70	121.78	111.46
1	Y	426	SER	CA-C-O	6.70	127.52	120.42
1	Y	325	ILE	CA-C-N	6.70	129.63	120.46
1	Y	325	ILE	C-N-CA	6.70	129.63	120.46
3	G	522	LEU	CA-C-O	-6.70	113.80	120.70
4	D	435	ILE	O-C-N	-6.69	115.73	122.62
1	Y	414	MET	CA-C-N	6.69	129.54	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	414	MET	C-N-CA	6.69	129.54	120.44
1	Y	311	GLN	N-CA-CB	-6.68	100.35	110.30
4	D	353	MET	CG-SD-CE	-6.66	86.24	100.90
2	E	444	THR	CA-CB-OG1	6.66	119.59	109.60
2	E	473	HIS	CA-CB-CG	6.66	120.46	113.80
6	C	323	HIS	CE1-NE2-CD2	-6.65	102.35	109.00
6	C	398	GLY	CA-C-N	6.65	129.49	120.38
6	C	398	GLY	C-N-CA	6.65	129.49	120.38
6	C	469	ILE	CA-C-O	6.65	127.89	120.85
4	D	504	MET	CA-C-N	6.64	126.42	119.05
4	D	504	MET	C-N-CA	6.64	126.42	119.05
4	D	550	PHE	CA-C-O	6.64	126.35	119.05
1	Y	264	HIS	CA-CB-CG	6.63	120.43	113.80
1	Y	314	GLN	N-CA-C	6.63	124.47	109.81
4	D	385	VAL	O-C-N	-6.63	115.61	122.63
6	C	386	LEU	CA-C-N	6.63	129.14	120.26
6	C	386	LEU	C-N-CA	6.63	129.14	120.26
6	C	267	HIS	CA-C-O	6.62	127.29	119.28
1	Y	372	ARG	N-CA-C	-6.61	104.96	113.16
5	F	274	SER	CA-C-N	6.61	129.14	120.28
5	F	274	SER	C-N-CA	6.61	129.14	120.28
4	D	472	TYR	CA-C-N	6.61	130.80	121.02
4	D	472	TYR	C-N-CA	6.61	130.80	121.02
5	F	215	ILE	CA-C-O	6.61	128.38	121.05
1	Y	99	HIS	CB-CG-ND1	6.61	132.61	122.70
4	D	287	ASN	OD1-CG-ND2	-6.60	116.00	122.60
4	D	573	GLY	O-C-N	-6.60	114.12	122.70
6	C	437	TYR	CA-C-N	6.60	129.02	120.44
6	C	437	TYR	C-N-CA	6.60	129.02	120.44
5	F	113	GLN	CA-C-N	6.59	129.78	120.42
5	F	113	GLN	C-N-CA	6.59	129.78	120.42
5	F	218	SER	N-CA-C	6.59	118.54	111.36
3	G	522	LEU	O-C-N	6.58	129.20	122.09
6	C	184	GLY	N-CA-C	-6.58	104.36	115.62
4	D	513	THR	N-CA-CB	6.58	120.44	110.30
1	Y	210	ALA	N-CA-CB	-6.58	100.45	110.12
1	Y	4	GLN	O-C-N	-6.57	113.76	121.32
4	D	541	ALA	N-CA-C	6.57	118.99	111.11
6	C	192	SER	CA-C-O	6.57	128.52	121.16
4	D	254	ASP	CA-C-O	6.57	127.90	119.95
5	F	215	ILE	O-C-N	-6.57	115.07	121.90
1	Y	311	GLN	O-C-N	-6.57	114.64	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	457	ARG	CA-C-N	6.57	129.08	120.28
2	E	457	ARG	C-N-CA	6.57	129.08	120.28
6	C	346	TRP	CD2-CE2-CZ2	-6.56	115.84	122.40
5	F	287	SER	N-CA-C	6.56	118.08	111.07
5	F	290	TYR	CA-C-N	6.55	128.95	120.56
5	F	290	TYR	C-N-CA	6.55	128.95	120.56
6	C	406	GLN	CA-C-N	6.54	129.04	120.28
6	C	406	GLN	C-N-CA	6.54	129.04	120.28
3	G	518	ARG	N-CA-C	6.54	120.47	112.23
5	F	20	MET	N-CA-C	6.53	118.95	111.11
5	F	204	MET	CA-C-N	6.53	129.27	120.65
5	F	204	MET	C-N-CA	6.53	129.27	120.65
2	E	483	ALA	N-CA-C	6.53	118.39	111.28
5	F	134	VAL	O-C-N	-6.52	116.12	123.10
4	D	490	ILE	N-CA-CB	6.51	118.17	110.55
5	F	184	THR	N-CA-C	6.51	118.38	111.28
1	Y	27	ILE	N-CA-C	-6.51	106.33	113.43
5	F	207	ILE	CA-C-O	6.51	128.76	120.76
2	E	506	LEU	N-CA-C	6.50	118.37	111.28
6	C	320	VAL	N-CA-C	6.50	116.66	110.42
6	C	348	HIS	CA-CB-CG	-6.49	107.31	113.80
6	C	75	ARG	NE-CZ-NH1	6.49	127.99	121.50
5	F	265	PHE	CA-CB-CG	-6.49	107.31	113.80
1	Y	207	ILE	CA-C-N	6.48	133.92	121.54
1	Y	207	ILE	C-N-CA	6.48	133.92	121.54
5	F	289	ILE	N-CA-C	6.48	119.15	111.05
4	D	566	ILE	CB-CA-C	-6.46	103.41	112.14
6	C	443	SER	N-CA-C	6.46	119.35	110.24
1	Y	422	THR	CA-C-N	6.45	129.44	120.29
1	Y	422	THR	C-N-CA	6.45	129.44	120.29
3	G	535	GLY	CA-C-N	6.44	129.74	120.79
3	G	535	GLY	C-N-CA	6.44	129.74	120.79
6	C	392	ALA	CA-C-N	6.44	131.96	122.82
6	C	392	ALA	C-N-CA	6.44	131.96	122.82
1	Y	407	LEU	N-CA-C	-6.44	102.88	111.96
2	E	467	THR	CA-C-N	6.44	129.85	120.71
2	E	467	THR	C-N-CA	6.44	129.85	120.71
1	Y	13	LYS	N-CA-C	6.43	116.94	107.88
6	C	449	ALA	CA-C-O	-6.42	114.57	119.32
1	Y	11	SER	N-CA-CB	6.42	119.41	110.17
1	Y	99	HIS	CA-C-N	6.41	127.85	119.84
1	Y	99	HIS	C-N-CA	6.41	127.85	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	558	ILE	CA-C-N	6.39	128.85	120.28
4	D	558	ILE	C-N-CA	6.39	128.85	120.28
6	C	122	ASN	CA-C-O	6.39	125.08	119.71
1	Y	133	ILE	CB-CA-C	-6.39	103.51	112.14
6	C	282	GLY	O-C-N	-6.39	116.15	122.41
4	D	590	MET	N-CA-C	6.39	118.77	111.11
1	Y	340	ARG	CA-C-N	6.38	133.73	121.54
1	Y	340	ARG	C-N-CA	6.38	133.73	121.54
1	Y	40	PRO	O-C-N	-6.38	114.03	122.64
5	F	290	TYR	N-CA-C	6.37	118.30	111.36
4	D	310	GLY	CA-C-O	-6.37	115.96	122.26
4	D	250	ARG	NH1-CZ-NH2	-6.37	111.02	119.30
4	D	459	ALA	CA-C-N	6.37	127.01	119.94
4	D	459	ALA	C-N-CA	6.37	127.01	119.94
5	F	277	MET	CG-SD-CE	-6.36	86.92	100.90
6	C	465	TYR	CA-C-N	6.36	128.57	120.56
6	C	465	TYR	C-N-CA	6.36	128.57	120.56
1	Y	160	ALA	N-CA-C	6.35	117.87	111.07
4	D	287	ASN	CA-CB-CG	-6.35	106.25	112.60
5	F	148	MET	CA-C-N	6.35	128.79	120.28
5	F	148	MET	C-N-CA	6.35	128.79	120.28
6	C	412	TYR	O-C-N	-6.35	115.12	122.93
1	Y	311	GLN	N-CA-C	6.34	121.37	112.75
4	D	269	ALA	CA-C-O	6.34	126.03	119.05
1	Y	436	ALA	O-C-N	-6.33	114.17	122.59
6	C	169	ARG	N-CA-C	6.33	118.90	109.59
4	D	226	ALA	CA-C-N	6.33	129.46	120.53
4	D	226	ALA	C-N-CA	6.33	129.46	120.53
4	D	230	ASN	N-CA-C	-6.33	104.72	112.88
4	D	407	ARG	NE-CZ-NH1	6.33	127.83	121.50
5	F	271	GLU	N-CA-C	6.32	118.70	111.11
4	D	236	ASN	CA-CB-CG	-6.32	106.28	112.60
1	Y	26	VAL	N-CA-CB	6.30	118.64	110.57
1	Y	116	ILE	CA-C-N	6.30	130.27	120.82
1	Y	116	ILE	C-N-CA	6.30	130.27	120.82
6	C	358	ILE	CA-C-O	6.30	127.84	121.17
5	F	98	MET	O-C-N	-6.29	117.06	121.65
4	D	261	PRO	N-CA-C	6.29	120.71	111.03
1	Y	119	TYR	N-CA-C	6.28	117.92	111.14
4	D	534	ASN	CA-CB-CG	-6.28	106.33	112.60
6	C	197	LYS	N-CA-CB	6.27	121.35	110.81
1	Y	100	PRO	CA-C-N	6.26	128.68	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	100	PRO	C-N-CA	6.26	128.68	120.28
4	D	500	ALA	CA-C-N	6.26	133.28	121.69
4	D	500	ALA	C-N-CA	6.26	133.28	121.69
1	Y	217	PHE	CA-C-N	6.26	131.82	123.00
1	Y	217	PHE	C-N-CA	6.26	131.82	123.00
4	D	19	ILE	N-CA-C	6.25	118.86	111.05
5	F	258	VAL	CA-C-N	6.25	130.54	120.30
5	F	258	VAL	C-N-CA	6.25	130.54	120.30
1	Y	64	PHE	CA-C-O	6.24	127.55	121.00
4	D	512	LEU	O-C-N	-6.23	115.65	122.07
1	Y	352	PHE	CA-CB-CG	-6.23	107.57	113.80
1	Y	286	PHE	N-CA-C	6.23	121.22	112.75
4	D	318	ARG	N-CA-CB	6.23	121.02	110.49
6	C	128	ARG	CA-C-O	-6.23	113.65	120.69
1	Y	435	LYS	N-CA-C	6.22	119.37	110.10
4	D	552	SER	CA-C-N	6.22	128.40	120.56
4	D	552	SER	C-N-CA	6.22	128.40	120.56
1	Y	318	VAL	CA-C-N	6.22	128.62	120.28
1	Y	318	VAL	C-N-CA	6.22	128.62	120.28
4	D	239	ASN	CA-CB-CG	-6.22	106.38	112.60
4	D	597	THR	N-CA-CB	6.22	119.48	110.47
4	D	289	ASP	N-CA-C	6.21	117.72	111.07
4	D	422	LEU	CB-CA-C	6.21	120.64	110.88
5	F	84	MET	CA-C-N	6.21	131.35	121.66
5	F	84	MET	C-N-CA	6.21	131.35	121.66
4	D	321	LEU	CA-C-O	-6.21	113.52	120.66
2	E	502	PHE	CA-CB-CG	6.20	120.00	113.80
4	D	267	ALA	CA-C-O	6.20	127.01	119.38
2	E	484	VAL	O-C-N	-6.20	115.45	121.90
6	C	521	ASN	CA-C-N	6.20	129.20	120.28
6	C	521	ASN	C-N-CA	6.20	129.20	120.28
5	F	238	ASN	N-CA-CB	6.20	118.99	110.01
6	C	454	TRP	CA-CB-CG	6.19	125.37	113.60
1	Y	170	PHE	CA-C-N	6.19	128.58	120.28
1	Y	170	PHE	C-N-CA	6.19	128.58	120.28
5	F	92	HIS	CE1-NE2-CD2	-6.19	102.81	109.00
6	C	530	LEU	O-C-N	-6.19	115.34	122.89
5	F	73	ASP	CB-CA-C	6.18	120.66	110.90
1	Y	425	MET	O-C-N	-6.17	115.12	122.15
6	C	466	ILE	N-CA-C	6.17	116.34	110.42
4	D	245	GLU	N-CA-CB	-6.16	103.45	111.09
4	D	508	ALA	O-C-N	-6.16	115.59	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	270	GLY	CA-C-N	6.16	129.51	120.82
6	C	270	GLY	C-N-CA	6.16	129.51	120.82
6	C	488	ASP	CA-C-N	6.16	125.38	118.97
6	C	488	ASP	C-N-CA	6.16	125.38	118.97
4	D	463	VAL	O-C-N	-6.16	114.84	121.80
6	C	219	ARG	N-CA-C	6.16	123.92	110.80
6	C	430	MET	CA-C-N	6.16	125.72	119.19
6	C	430	MET	C-N-CA	6.16	125.72	119.19
1	Y	163	SER	N-CA-CB	6.15	119.17	110.12
2	E	486	SER	CA-C-N	6.15	128.52	120.28
2	E	486	SER	C-N-CA	6.15	128.52	120.28
6	C	200	ILE	N-CA-C	6.15	118.74	111.05
1	Y	216	HIS	CB-CG-ND1	6.15	131.92	122.70
4	D	381	ASN	N-CA-C	6.15	119.38	110.28
5	F	254	THR	O-C-N	6.15	128.40	122.07
1	Y	238	GLU	CA-C-N	6.14	128.80	120.38
1	Y	238	GLU	C-N-CA	6.14	128.80	120.38
6	C	185	GLU	N-CA-C	6.14	119.83	111.17
6	C	435	ALA	CA-C-N	6.14	128.51	120.28
6	C	435	ALA	C-N-CA	6.14	128.51	120.28
1	Y	285	LEU	CA-C-N	6.14	128.49	120.26
1	Y	285	LEU	C-N-CA	6.14	128.49	120.26
5	F	201	ALA	N-CA-C	6.14	117.97	111.28
4	D	306	GLN	N-CA-C	6.13	117.96	111.28
5	F	200	VAL	N-CA-C	6.13	116.30	110.42
6	C	242	GLU	CB-CG-CD	6.12	123.01	112.60
1	Y	282	SER	CA-C-O	-6.12	113.93	120.42
1	Y	137	THR	CA-C-N	6.11	128.32	122.27
1	Y	137	THR	C-N-CA	6.11	128.32	122.27
1	Y	262	SER	O-C-N	-6.11	116.03	123.30
4	D	311	GLN	O-C-N	-6.11	117.19	121.65
6	C	450	PRO	CA-C-N	6.11	128.71	120.65
6	C	450	PRO	C-N-CA	6.11	128.71	120.65
5	F	274	SER	O-C-N	-6.10	115.65	122.12
4	D	547	ARG	NH1-CZ-NH2	-6.10	111.37	119.30
4	D	288	VAL	CA-C-N	6.10	128.37	120.44
4	D	288	VAL	C-N-CA	6.10	128.37	120.44
1	Y	250	LYS	N-CA-C	6.09	118.16	110.24
6	C	101	GLU	CA-C-O	6.08	127.80	120.99
5	F	104	GLU	N-CA-CB	6.08	119.49	110.49
5	F	158	LEU	CA-C-O	6.08	127.40	120.90
1	Y	411	VAL	CA-C-O	-6.08	113.91	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	158	PHE	CA-C-N	6.08	128.42	120.28
1	Y	158	PHE	C-N-CA	6.08	128.42	120.28
1	Y	223	VAL	O-C-N	-6.07	115.39	122.07
4	D	474	LYS	N-CA-CB	6.07	119.04	110.36
6	C	338	GLN	N-CA-C	6.06	123.21	109.81
4	D	357	THR	N-CA-C	6.06	117.56	111.07
1	Y	215	LEU	CA-C-O	-6.06	114.53	121.19
1	Y	302	TRP	N-CA-C	6.06	118.99	109.96
4	D	541	ALA	N-CA-CB	-6.06	100.91	109.94
5	F	255	THR	N-CA-C	6.05	117.96	111.36
6	C	396	ARG	CA-C-O	6.05	126.82	119.38
6	C	348	HIS	ND1-CE1-NE2	6.05	114.45	108.40
1	Y	339	PRO	O-C-N	-6.04	114.48	122.64
1	Y	47	ALA	CA-C-N	6.04	132.85	121.97
1	Y	47	ALA	C-N-CA	6.04	132.85	121.97
1	Y	425	MET	CA-C-N	6.03	128.85	120.29
1	Y	425	MET	C-N-CA	6.03	128.85	120.29
4	D	511	VAL	N-CA-C	6.03	116.21	110.42
1	Y	126	VAL	N-CA-CB	6.02	116.58	111.64
1	Y	218	LEU	O-C-N	-6.02	116.29	123.27
4	D	594	ILE	CA-CB-CG1	6.01	120.62	110.40
6	C	428	ILE	CA-C-N	6.01	128.82	120.29
6	C	428	ILE	C-N-CA	6.01	128.82	120.29
5	F	169	LEU	CB-CA-C	-6.00	99.14	110.67
4	D	574	ALA	CA-C-N	6.00	128.34	120.60
4	D	574	ALA	C-N-CA	6.00	128.34	120.60
6	C	271	THR	N-CA-CB	6.00	118.87	109.69
6	C	348	HIS	CE1-NE2-CD2	-6.00	103.00	109.00
6	C	452	ALA	CA-C-O	-6.00	113.48	120.20
2	E	471	THR	O-C-N	-5.99	114.63	122.59
4	D	467	PHE	N-CA-C	5.99	117.48	111.07
1	Y	314	GLN	CA-C-N	5.99	125.37	118.85
1	Y	314	GLN	C-N-CA	5.99	125.37	118.85
6	C	98	GLN	CA-C-O	-5.99	114.04	120.92
5	F	173	VAL	O-C-N	-5.98	115.78	121.94
6	C	482	SER	O-C-N	-5.98	114.44	121.32
5	F	284	GLY	O-C-N	-5.98	115.90	122.24
6	C	366	ARG	NH1-CZ-NH2	-5.97	111.54	119.30
1	Y	8	ASP	CA-CB-CG	-5.96	106.64	112.60
4	D	547	ARG	NE-CZ-NH2	5.96	124.56	119.20
4	D	488	ILE	N-CA-C	5.95	116.61	110.36
5	F	130	ARG	CA-C-N	5.95	131.38	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	130	ARG	C-N-CA	5.95	131.38	122.75
6	C	177	ASN	CA-C-N	5.95	130.93	122.72
6	C	177	ASN	C-N-CA	5.95	130.93	122.72
1	Y	158	PHE	O-C-N	5.94	128.41	122.12
4	D	295	SER	CA-C-O	5.94	126.83	120.24
6	C	323	HIS	CG-CD2-NE2	5.94	113.14	107.20
1	Y	39	ILE	N-CA-CB	5.93	115.60	110.08
1	Y	345	ASN	CA-C-N	5.93	130.72	120.58
1	Y	345	ASN	C-N-CA	5.93	130.72	120.58
3	G	526	LEU	CA-C-O	5.93	126.83	119.78
5	F	49	GLY	N-CA-C	5.92	118.86	110.74
6	C	135	LYS	CB-CA-C	5.92	121.15	109.66
1	Y	421	GLN	N-CA-C	5.92	117.73	111.28
1	Y	157	TYR	CA-C-N	5.92	128.21	120.28
1	Y	157	TYR	C-N-CA	5.92	128.21	120.28
5	F	192	HIS	N-CA-C	5.91	119.55	111.39
6	C	151	MET	O-C-N	-5.91	116.48	123.22
6	C	103	SER	O-C-N	-5.91	114.53	121.32
6	C	340	LEU	N-CA-C	-5.90	104.43	111.69
5	F	74	ALA	CA-C-N	5.90	128.67	120.29
5	F	74	ALA	C-N-CA	5.90	128.67	120.29
5	F	94	ILE	CA-C-O	5.90	127.45	120.72
4	D	480	THR	CA-C-O	5.90	125.88	119.15
5	F	184	THR	N-CA-CB	5.90	118.79	110.12
6	C	513	LEU	N-CA-C	5.89	117.38	111.07
4	D	477	LEU	CA-C-N	5.89	128.20	120.60
4	D	477	LEU	C-N-CA	5.89	128.20	120.60
4	D	593	ALA	CA-C-N	5.89	128.53	120.46
4	D	593	ALA	C-N-CA	5.89	128.53	120.46
1	Y	213	GLY	CA-C-N	5.88	133.02	122.38
1	Y	213	GLY	C-N-CA	5.88	133.02	122.38
6	C	296	GLN	N-CA-C	5.88	118.82	110.24
4	D	578	PHE	O-C-N	-5.88	115.92	122.03
6	C	355	GLY	CA-C-N	5.88	128.08	120.44
6	C	355	GLY	C-N-CA	5.88	128.08	120.44
1	Y	110	GLU	N-CA-C	5.87	118.34	110.35
5	F	242	THR	CA-C-N	5.87	128.63	120.29
5	F	242	THR	C-N-CA	5.87	128.63	120.29
6	C	199	SER	O-C-N	-5.87	115.81	122.97
4	D	577	GLY	CA-C-N	5.87	128.40	120.65
4	D	577	GLY	C-N-CA	5.87	128.40	120.65
4	D	404	ASN	OD1-CG-ND2	-5.87	116.73	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	408	ILE	CB-CA-C	-5.86	101.88	110.62
6	C	163	LYS	N-CA-CB	-5.86	101.52	110.65
1	Y	68	SER	N-CA-CB	5.85	118.72	110.12
4	D	399	GLN	O-C-N	-5.85	114.81	122.59
6	C	177	ASN	N-CA-C	-5.85	98.88	108.41
1	Y	130	PHE	CA-CB-CG	-5.84	107.96	113.80
4	D	293	ALA	N-CA-C	5.84	117.64	111.28
4	D	564	VAL	O-C-N	5.84	127.84	121.83
6	C	344	LEU	CA-C-N	5.84	128.58	120.29
6	C	344	LEU	C-N-CA	5.84	128.58	120.29
4	D	307	THR	CA-C-O	5.83	126.60	120.42
6	C	416	LYS	CA-C-N	5.83	128.45	120.35
6	C	416	LYS	C-N-CA	5.83	128.45	120.35
5	F	242	THR	CA-CB-OG1	5.82	118.34	109.60
1	Y	85	TYR	CA-C-N	5.82	128.43	120.46
1	Y	85	TYR	C-N-CA	5.82	128.43	120.46
6	C	308	TRP	CE3-CZ3-CH2	-5.82	113.54	121.10
2	E	492	LEU	O-C-N	-5.81	115.42	122.22
4	D	295	SER	CA-C-N	5.81	127.41	120.14
4	D	295	SER	C-N-CA	5.81	127.41	120.14
4	D	534	ASN	N-CA-C	5.81	120.23	113.20
5	F	57	VAL	CA-C-N	-5.81	115.53	123.14
5	F	57	VAL	C-N-CA	-5.81	115.53	123.14
5	F	93	ASP	CA-C-O	5.80	126.96	120.70
5	F	219	ASP	CB-CA-C	5.80	119.98	110.88
6	C	122	ASN	CB-CG-OD1	5.80	132.39	120.80
4	D	255	ARG	NH1-CZ-NH2	-5.79	111.77	119.30
5	F	146	GLY	CA-C-N	5.79	128.04	120.28
5	F	146	GLY	C-N-CA	5.79	128.04	120.28
5	F	23	ASP	N-CA-CB	-5.79	101.62	110.01
5	F	77	LYS	CA-C-O	-5.79	114.42	120.55
1	Y	374	THR	O-C-N	-5.78	114.90	122.59
4	D	409	THR	O-C-N	-5.78	116.64	123.11
4	D	354	SER	N-CA-C	-5.78	104.89	111.07
5	F	289	ILE	O-C-N	5.78	127.70	121.87
5	F	210	SER	N-CA-CB	5.77	120.25	110.49
6	C	524	THR	CA-C-N	5.77	127.83	120.56
6	C	524	THR	C-N-CA	5.77	127.83	120.56
1	Y	233	PHE	CA-CB-CG	-5.77	108.03	113.80
1	Y	374	THR	CA-CB-OG1	5.76	118.24	109.60
4	D	361	ILE	O-C-N	-5.76	115.37	122.57
5	F	250	ILE	CA-C-O	5.76	127.27	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	439	MET	CA-C-N	5.76	128.57	120.28
6	C	439	MET	C-N-CA	5.76	128.57	120.28
6	C	304	ASN	O-C-N	-5.75	116.34	123.36
6	C	464	TYR	N-CA-CB	5.75	120.22	110.49
4	D	384	ALA	CA-C-N	5.75	128.20	120.50
4	D	384	ALA	C-N-CA	5.75	128.20	120.50
2	E	450	VAL	CA-C-N	5.74	132.03	121.70
2	E	450	VAL	C-N-CA	5.74	132.03	121.70
4	D	597	THR	O-C-N	-5.74	114.99	122.39
5	F	135	GLY	O-C-N	-5.74	116.03	121.77
1	Y	17	GLY	N-CA-C	-5.73	102.04	110.87
4	D	378	LYS	CA-C-N	5.73	132.18	122.26
4	D	378	LYS	C-N-CA	5.73	132.18	122.26
1	Y	275	ILE	O-C-N	5.73	124.09	120.42
6	C	84	LEU	O-C-N	-5.73	114.54	121.02
1	Y	78	PHE	O-C-N	-5.73	115.30	122.35
1	Y	194	GLY	N-CA-C	5.72	122.44	113.86
6	C	353	ASN	O-C-N	-5.72	115.00	122.20
1	Y	98	VAL	O-C-N	-5.71	115.43	122.57
6	C	97	PHE	CB-CA-C	5.71	119.20	109.72
3	G	518	ARG	CD-NE-CZ	5.71	132.39	124.40
6	C	472	GLY	CA-C-N	5.70	127.74	120.56
6	C	472	GLY	C-N-CA	5.70	127.74	120.56
1	Y	129	ILE	N-CA-C	5.70	115.78	110.42
1	Y	77	ILE	N-CA-C	5.70	118.17	111.05
5	F	281	VAL	N-CA-C	-5.69	106.25	112.80
4	D	450	ILE	N-CA-C	5.69	115.88	110.42
4	D	554	PHE	N-CA-C	5.69	117.17	110.97
5	F	36	ALA	O-C-N	-5.69	116.21	122.07
6	C	502	PHE	CA-C-N	5.68	127.83	120.44
6	C	502	PHE	C-N-CA	5.68	127.83	120.44
6	C	419	PRO	N-CA-CB	-5.68	98.58	102.73
4	D	341	VAL	N-CA-CB	-5.68	104.18	110.99
6	C	126	GLY	CA-C-N	5.68	126.94	119.84
6	C	126	GLY	C-N-CA	5.68	126.94	119.84
6	C	306	THR	N-CA-C	-5.67	100.16	109.40
5	F	158	LEU	CA-C-N	5.67	128.23	120.46
5	F	158	LEU	C-N-CA	5.67	128.23	120.46
1	Y	31	ILE	N-CA-C	5.66	116.39	110.62
6	C	523	VAL	O-C-N	-5.66	116.38	121.87
3	G	537	ILE	N-CA-C	-5.66	107.30	112.96
2	E	456	ALA	O-C-N	-5.65	116.13	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	202	LEU	CA-C-N	5.65	126.20	120.38
6	C	202	LEU	C-N-CA	5.65	126.20	120.38
1	Y	162	VAL	CA-C-N	5.65	127.85	120.28
1	Y	162	VAL	C-N-CA	5.65	127.85	120.28
4	D	483	LEU	N-CA-C	5.64	117.10	111.07
4	D	312	PRO	O-C-N	-5.63	115.73	122.89
6	C	529	GLN	O-C-N	-5.63	117.34	123.26
4	D	343	ILE	CA-C-O	5.63	127.26	120.67
6	C	484	THR	CB-CA-C	5.63	121.61	110.42
6	C	82	ALA	N-CA-C	-5.62	100.16	108.99
1	Y	38	PHE	CA-C-O	5.62	125.59	119.24
5	F	105	THR	N-CA-CB	5.62	117.53	110.45
6	C	514	VAL	N-CA-C	5.62	115.81	110.42
4	D	243	VAL	N-CA-CB	5.62	118.06	111.66
5	F	24	TYR	CA-C-N	5.62	127.81	120.28
5	F	24	TYR	C-N-CA	5.62	127.81	120.28
5	F	276	THR	CA-CB-CG2	-5.62	100.95	110.50
1	Y	205	HIS	CG-CD2-NE2	5.61	112.81	107.20
1	Y	309	TYR	O-C-N	-5.61	115.15	122.39
1	Y	378	ALA	N-CA-CB	-5.61	103.80	111.65
2	E	458	THR	N-CA-CB	5.60	118.36	110.12
1	Y	99	HIS	CG-CD2-NE2	5.60	112.80	107.20
1	Y	283	ILE	O-C-N	-5.60	116.21	121.87
1	Y	193	ALA	N-CA-C	5.60	117.38	111.28
1	Y	301	ASN	O-C-N	-5.60	115.14	122.59
6	C	306	THR	CA-C-N	5.60	131.06	123.11
6	C	306	THR	C-N-CA	5.60	131.06	123.11
6	C	323	HIS	CA-CB-CG	-5.59	108.21	113.80
6	C	469	ILE	CB-CG1-CD1	5.59	125.53	113.80
2	E	468	ARG	CD-NE-CZ	5.58	132.22	124.40
4	D	578	PHE	CA-CB-CG	5.58	119.38	113.80
4	D	600	ILE	N-CA-C	5.58	116.98	110.62
4	D	589	SER	O-C-N	-5.57	116.21	122.12
5	F	124	GLN	CA-C-N	5.57	132.19	121.54
5	F	124	GLN	C-N-CA	5.57	132.19	121.54
6	C	466	ILE	N-CA-CB	5.57	117.07	110.55
4	D	230	ASN	O-C-N	-5.57	115.62	122.25
6	C	95	GLN	CB-CG-CD	5.57	122.07	112.60
2	E	502	PHE	CB-CG-CD2	5.57	130.16	120.70
3	G	516	MET	CA-C-N	5.57	128.61	120.71
3	G	516	MET	C-N-CA	5.57	128.61	120.71
4	D	455	GLU	CA-C-N	5.56	127.73	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	455	GLU	C-N-CA	5.56	127.73	120.28
6	C	452	ALA	CB-CA-C	-5.56	99.67	110.46
5	F	160	TYR	N-CA-CB	5.56	118.13	110.07
6	C	341	PHE	CA-C-O	-5.56	114.96	121.07
4	D	436	VAL	N-CA-CB	-5.55	103.17	112.06
6	C	203	PRO	CB-CA-C	5.55	117.69	110.92
4	D	346	ASP	CA-CB-CG	5.55	118.15	112.60
4	D	552	SER	CA-C-O	5.55	126.35	119.97
1	Y	78	PHE	CA-C-O	5.55	126.38	119.78
1	Y	84	PRO	N-CA-CB	5.54	109.40	103.52
5	F	234	TYR	CA-C-N	5.54	127.71	120.28
5	F	234	TYR	C-N-CA	5.54	127.71	120.28
5	F	163	PHE	CA-C-N	5.54	127.65	120.44
5	F	163	PHE	C-N-CA	5.54	127.65	120.44
1	Y	169	MET	CA-C-O	5.54	126.64	120.82
1	Y	367	ASP	N-CA-C	5.54	117.00	111.07
4	D	407	ARG	CG-CD-NE	-5.54	99.81	112.00
1	Y	39	ILE	N-CA-C	5.54	114.38	108.95
4	D	408	ILE	N-CA-CB	5.54	121.02	111.39
1	Y	376	VAL	N-CA-CB	5.54	117.36	110.05
1	Y	382	THR	N-CA-CB	5.53	118.82	110.30
4	D	551	SER	CA-C-O	-5.53	114.68	120.55
1	Y	188	SER	O-C-N	5.53	127.98	122.12
4	D	586	VAL	N-CA-C	5.53	118.85	111.44
4	D	443	PRO	N-CA-C	5.51	119.89	111.34
4	D	550	PHE	CA-CB-CG	-5.51	108.28	113.80
6	C	490	MET	N-CA-C	5.51	118.18	109.96
1	Y	2	ALA	N-CA-C	5.51	118.68	110.52
6	C	461	GLN	CA-C-N	5.51	129.03	120.60
6	C	461	GLN	C-N-CA	5.51	129.03	120.60
6	C	308	TRP	CA-CB-CG	5.50	124.06	113.60
6	C	264	TRP	CE2-CD2-CE3	5.50	124.30	118.80
4	D	265	ASP	N-CA-C	5.50	122.52	110.80
5	F	179	HIS	CG-CD2-NE2	5.50	112.70	107.20
4	D	599	ALA	N-CA-C	5.50	118.03	111.71
6	C	95	GLN	O-C-N	-5.49	116.07	121.18
5	F	138	VAL	CA-C-O	5.49	126.66	120.95
1	Y	44	ILE	N-CA-C	-5.49	104.99	113.16
4	D	475	PHE	CA-CB-CG	5.49	119.28	113.80
4	D	22	LEU	CA-C-O	5.48	125.70	119.18
1	Y	422	THR	OG1-CB-CG2	-5.48	98.34	109.30
2	E	457	ARG	NE-CZ-NH2	-5.47	114.28	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	364	PRO	N-CA-CB	-5.47	98.54	103.36
6	C	170	GLY	O-C-N	5.47	128.74	122.34
6	C	446	LEU	N-CA-C	-5.47	105.91	112.59
4	D	460	GLY	CA-C-N	5.46	127.91	120.54
4	D	460	GLY	C-N-CA	5.46	127.91	120.54
6	C	144	GLN	O-C-N	-5.46	116.92	123.31
1	Y	256	ARG	CG-CD-NE	-5.46	100.00	112.00
4	D	318	ARG	NE-CZ-NH2	5.46	124.11	119.20
5	F	256	LEU	O-C-N	-5.46	116.34	122.12
6	C	84	LEU	CA-C-N	5.46	124.97	119.19
6	C	84	LEU	C-N-CA	5.46	124.97	119.19
1	Y	205	HIS	CA-CB-CG	-5.45	108.35	113.80
6	C	374	LYS	N-CA-C	5.45	117.31	111.36
4	D	418	ARG	NE-CZ-NH1	5.45	126.95	121.50
1	Y	82	ILE	N-CA-C	-5.45	107.44	112.83
1	Y	9	PHE	CA-C-N	5.45	128.97	120.75
1	Y	9	PHE	C-N-CA	5.45	128.97	120.75
5	F	62	LEU	N-CA-C	-5.44	99.81	109.06
1	Y	281	SER	N-CA-C	-5.44	104.77	111.40
1	Y	59	THR	CA-CB-OG1	5.44	117.76	109.60
6	C	64	LYS	N-CA-C	5.43	118.26	109.40
6	C	61	ILE	O-C-N	-5.43	117.33	122.98
1	Y	37	SER	CA-C-O	-5.42	112.97	119.15
5	F	282	SER	N-CA-C	-5.42	106.67	113.72
6	C	262	THR	CB-CA-C	5.42	120.02	109.33
2	E	498	ARG	CA-CB-CG	-5.42	103.25	114.10
5	F	237	PHE	CA-C-N	5.42	127.49	120.44
5	F	237	PHE	C-N-CA	5.42	127.49	120.44
4	D	246	PRO	N-CA-CB	-5.42	97.56	103.25
1	Y	184	GLY	CA-C-O	5.42	126.95	122.24
6	C	312	GLU	O-C-N	-5.42	115.38	122.59
2	E	507	ARG	N-CA-C	5.42	119.87	112.88
6	C	174	VAL	N-CA-C	-5.42	99.35	107.37
4	D	370	VAL	N-CA-C	5.41	120.60	109.34
6	C	415	GLU	CA-C-N	5.41	129.84	121.83
6	C	415	GLU	C-N-CA	5.41	129.84	121.83
5	F	52	PHE	O-C-N	-5.41	115.40	122.43
4	D	409	THR	N-CA-C	5.41	118.31	110.42
6	C	119	GLY	CA-C-N	5.40	124.92	119.19
6	C	119	GLY	C-N-CA	5.40	124.92	119.19
4	D	276	THR	CA-CB-OG1	5.40	117.70	109.60
4	D	525	ASN	CA-CB-CG	-5.39	107.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	478	VAL	N-CA-CB	5.39	118.66	110.58
1	Y	13	LYS	CA-C-O	-5.38	115.38	121.25
1	Y	160	ALA	CA-C-O	-5.38	115.17	120.82
5	F	77	LYS	N-CA-C	5.38	117.14	111.28
1	Y	324	ALA	O-C-N	-5.38	115.65	122.27
4	D	286	THR	CA-C-O	5.38	126.33	120.58
6	C	116	GLY	N-CA-C	-5.37	104.48	111.52
5	F	137	SER	N-CA-CB	5.37	118.57	110.30
6	C	501	ILE	CA-CB-CG1	5.37	119.53	110.40
1	Y	25	PHE	CB-CG-CD1	-5.37	111.57	120.70
5	F	248	THR	CA-CB-CG2	5.37	119.63	110.50
1	Y	321	TYR	CA-CB-CG	5.37	123.56	113.90
1	Y	26	VAL	N-CA-C	5.37	115.57	110.53
1	Y	121	ARG	NE-CZ-NH1	5.37	126.87	121.50
5	F	284	GLY	CA-C-O	5.37	126.19	120.40
6	C	225	THR	CA-C-N	-5.37	114.73	120.47
6	C	225	THR	C-N-CA	-5.37	114.73	120.47
1	Y	271	MET	CA-C-N	5.36	127.46	120.28
1	Y	271	MET	C-N-CA	5.36	127.46	120.28
5	F	28	GLY	O-C-N	-5.36	117.04	122.18
6	C	64	LYS	CA-C-O	5.36	126.48	120.70
4	D	589	SER	N-CA-CB	5.35	117.99	110.12
1	Y	372	ARG	NE-CZ-NH1	5.35	126.85	121.50
2	E	502	PHE	N-CA-C	5.35	117.11	111.28
1	Y	73	SER	N-CA-CB	5.35	119.53	110.49
4	D	407	ARG	CB-CA-C	-5.35	100.47	109.72
5	F	24	TYR	N-CA-C	5.35	118.02	111.82
1	Y	329	CYS	CA-C-N	5.35	130.30	122.39
1	Y	329	CYS	C-N-CA	5.35	130.30	122.39
4	D	580	ILE	O-C-N	-5.35	116.59	121.94
6	C	376	GLN	CA-C-N	5.35	127.39	120.44
6	C	376	GLN	C-N-CA	5.35	127.39	120.44
1	Y	9	PHE	N-CA-C	5.34	117.19	110.24
1	Y	231	THR	N-CA-CB	5.34	118.53	110.30
1	Y	19	LEU	CA-C-O	-5.34	113.10	119.35
1	Y	360	GLU	CA-C-N	5.34	127.96	120.28
1	Y	360	GLU	C-N-CA	5.34	127.96	120.28
4	D	407	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
6	C	515	LEU	N-CA-C	5.33	117.09	111.28
4	D	320	ILE	N-CA-CB	5.33	118.20	110.68
1	Y	39	ILE	CA-CB-CG2	5.33	119.56	110.50
4	D	518	VAL	N-CA-C	5.33	116.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	63	MET	N-CA-C	5.33	117.08	111.28
5	F	159	VAL	O-C-N	-5.33	116.70	121.87
1	Y	139	LEU	O-C-N	-5.32	115.20	121.32
6	C	177	ASN	N-CA-CB	5.32	118.95	110.65
1	Y	250	LYS	O-C-N	5.32	129.63	122.82
4	D	280	GLU	CA-C-O	-5.32	114.63	120.69
1	Y	106	LYS	CA-C-O	5.32	127.72	121.87
6	C	147	LEU	O-C-N	-5.32	117.02	123.29
5	F	121	SER	N-CA-C	5.31	117.15	109.07
6	C	479	GLN	OE1-CD-NE2	-5.31	117.29	122.60
6	C	95	GLN	CB-CA-C	5.31	118.59	109.82
6	C	335	PHE	CB-CG-CD1	5.31	129.73	120.70
1	Y	128	ALA	O-C-N	-5.31	116.57	122.09
2	E	467	THR	O-C-N	-5.31	117.33	123.33
6	C	384	ARG	NH1-CZ-NH2	5.31	126.20	119.30
6	C	194	GLY	O-C-N	5.30	129.59	122.70
4	D	473	LYS	N-CA-CB	5.30	117.89	109.51
1	Y	375	LEU	N-CA-C	5.30	117.97	110.50
5	F	226	ARG	O-C-N	5.30	128.19	122.15
6	C	477	PHE	CA-CB-CG	5.30	119.10	113.80
1	Y	378	ALA	CA-C-N	5.30	127.64	120.44
1	Y	378	ALA	C-N-CA	5.30	127.64	120.44
6	C	296	GLN	CA-C-O	-5.30	115.18	120.64
1	Y	249	ALA	N-CA-CB	5.29	118.61	110.61
1	Y	264	HIS	ND1-CE1-NE2	5.29	113.69	108.40
6	C	191	SER	CA-C-N	5.29	128.39	120.87
6	C	191	SER	C-N-CA	5.29	128.39	120.87
1	Y	321	TYR	N-CA-CB	5.29	117.68	110.01
4	D	456	ALA	CB-CA-C	-5.29	102.01	110.79
5	F	300	GLY	N-CA-C	5.29	119.08	112.73
6	C	63	VAL	CB-CA-C	-5.29	104.44	110.73
5	F	210	SER	CA-C-N	5.29	131.64	121.54
5	F	210	SER	C-N-CA	5.29	131.64	121.54
1	Y	1	MET	CG-SD-CE	-5.29	89.27	100.90
4	D	423	LEU	N-CA-C	5.27	118.50	111.75
2	E	465	TRP	CB-CG-CD1	-5.27	119.00	126.90
1	Y	67	PHE	CA-C-N	5.27	127.34	120.28
1	Y	67	PHE	C-N-CA	5.27	127.34	120.28
1	Y	330	PHE	CA-CB-CG	-5.26	108.54	113.80
5	F	221	ILE	CA-C-N	5.26	127.59	120.65
5	F	221	ILE	C-N-CA	5.26	127.59	120.65
6	C	360	ILE	N-CA-C	5.26	115.47	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	230	ARG	NE-CZ-NH2	-5.26	114.47	119.20
5	F	181	VAL	CB-CA-C	5.25	118.69	111.97
4	D	311	GLN	CA-C-N	5.25	125.26	119.90
4	D	311	GLN	C-N-CA	5.25	125.26	119.90
6	C	122	ASN	CB-CA-C	5.25	117.54	109.50
1	Y	280	ALA	N-CA-C	5.25	117.00	111.28
1	Y	431	SER	N-CA-CB	5.25	118.79	110.55
5	F	82	GLU	O-C-N	-5.25	115.28	121.32
4	D	281	PHE	O-C-N	-5.24	117.14	123.27
4	D	538	VAL	O-C-N	5.24	127.32	121.97
1	Y	37	SER	N-CA-CB	5.24	118.34	110.53
4	D	482	ALA	CA-C-N	5.24	127.25	120.44
4	D	482	ALA	C-N-CA	5.24	127.25	120.44
6	C	192	SER	O-C-N	-5.24	116.50	122.89
1	Y	64	PHE	CA-C-N	5.23	129.51	121.19
1	Y	64	PHE	C-N-CA	5.23	129.51	121.19
5	F	159	VAL	CA-C-N	5.23	127.55	120.44
5	F	159	VAL	C-N-CA	5.23	127.55	120.44
1	Y	191	ILE	N-CA-CB	-5.23	104.43	110.55
1	Y	309	TYR	CA-C-O	5.23	125.75	119.43
1	Y	379	LEU	N-CA-C	5.23	116.79	111.14
1	Y	130	PHE	CA-C-N	5.23	127.23	120.44
1	Y	130	PHE	C-N-CA	5.23	127.23	120.44
4	D	388	LYS	N-CA-C	5.23	119.22	113.21
6	C	343	LEU	O-C-N	-5.23	116.66	122.09
1	Y	25	PHE	CB-CG-CD2	5.22	129.58	120.70
6	C	221	ALA	N-CA-CB	-5.22	102.74	111.20
6	C	413	LYS	CA-C-N	5.22	127.23	120.44
6	C	413	LYS	C-N-CA	5.22	127.23	120.44
4	D	264	GLN	CA-C-O	-5.22	115.80	121.44
1	Y	362	THR	N-CA-C	5.22	121.92	110.80
4	D	269	ALA	CA-C-N	5.22	128.05	120.79
4	D	269	ALA	C-N-CA	5.22	128.05	120.79
2	E	503	ILE	N-CA-C	5.22	115.94	110.62
1	Y	3	LYS	N-CA-C	-5.21	101.15	109.07
6	C	353	ASN	N-CA-C	-5.21	105.25	113.02
6	C	367	GLY	O-C-N	-5.21	116.79	122.68
1	Y	42	PRO	CB-CA-C	5.21	118.25	111.64
1	Y	89	SER	N-CA-CB	5.21	117.77	110.12
1	Y	293	TRP	N-CA-C	5.21	117.03	111.36
5	F	168	ARG	CD-NE-CZ	-5.21	117.11	124.40
5	F	75	LEU	CA-C-N	5.20	127.56	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	75	LEU	C-N-CA	5.20	127.56	120.54
4	D	239	ASN	CA-C-N	5.20	131.47	121.54
4	D	239	ASN	C-N-CA	5.20	131.47	121.54
5	F	192	HIS	CA-CB-CG	-5.20	108.60	113.80
1	Y	439	LYS	O-C-N	-5.20	116.73	122.91
5	F	153	ALA	CA-C-O	-5.20	115.04	120.55
1	Y	419	GLN	OE1-CD-NE2	-5.19	117.41	122.60
5	F	176	ALA	CA-C-N	5.19	127.66	120.29
5	F	176	ALA	C-N-CA	5.19	127.66	120.29
6	C	185	GLU	O-C-N	-5.19	116.64	122.86
4	D	329	SER	CA-C-O	5.18	126.54	120.43
1	Y	139	LEU	N-CA-CB	5.18	119.58	110.37
4	D	373	LYS	O-C-N	-5.17	117.52	123.42
6	C	369	MET	O-C-N	-5.17	115.71	122.59
4	D	468	MET	CA-C-N	5.17	127.07	120.56
4	D	468	MET	C-N-CA	5.17	127.07	120.56
4	D	513	THR	CA-C-N	5.17	127.21	120.28
4	D	513	THR	C-N-CA	5.17	127.21	120.28
5	F	153	ALA	CA-C-N	5.17	127.16	120.44
5	F	153	ALA	C-N-CA	5.17	127.16	120.44
2	E	477	ILE	N-CA-CB	-5.17	103.51	110.54
4	D	390	GLU	CB-CA-C	-5.17	101.76	110.44
5	F	256	LEU	CA-C-O	5.17	126.03	120.55
1	Y	206	THR	CA-CB-OG1	5.16	117.34	109.60
1	Y	327	PHE	CA-CB-CG	-5.16	108.64	113.80
1	Y	405	SER	N-CA-C	5.16	118.36	111.75
6	C	160	THR	CA-CB-OG1	5.16	117.34	109.60
6	C	509	PHE	CA-CB-CG	-5.16	108.64	113.80
2	E	502	PHE	CB-CG-CD1	-5.16	111.94	120.70
1	Y	166	THR	CA-CB-CG2	-5.15	101.74	110.50
1	Y	229	ALA	N-CA-C	5.15	116.97	111.36
6	C	409	MET	CA-C-N	5.15	127.18	120.28
6	C	409	MET	C-N-CA	5.15	127.18	120.28
6	C	75	ARG	NE-CZ-NH2	-5.15	114.57	119.20
4	D	580	ILE	N-CA-C	5.15	115.77	110.36
4	D	432	PRO	N-CA-C	5.14	119.28	111.15
6	C	486	VAL	CA-C-O	5.14	127.21	120.78
1	Y	218	LEU	CA-C-N	5.14	127.51	120.46
1	Y	218	LEU	C-N-CA	5.14	127.51	120.46
1	Y	380	TYR	N-CA-C	5.14	116.57	111.07
1	Y	408	ILE	O-C-N	5.14	127.08	121.94
4	D	566	ILE	N-CA-C	5.13	115.86	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	228	ALA	CA-C-N	5.13	128.00	120.71
6	C	228	ALA	C-N-CA	5.13	128.00	120.71
4	D	399	GLN	CA-C-N	5.13	128.15	120.87
4	D	399	GLN	C-N-CA	5.13	128.15	120.87
5	F	70	VAL	CA-C-N	5.13	127.16	120.28
5	F	70	VAL	C-N-CA	5.13	127.16	120.28
1	Y	100	PRO	CB-CA-C	5.13	120.02	111.56
6	C	437	TYR	N-CA-CB	5.12	117.44	110.01
6	C	282	GLY	CA-C-O	5.12	126.00	119.80
3	G	517	THR	O-C-N	-5.12	116.58	122.87
4	D	424	LEU	O-C-N	-5.12	116.56	122.09
6	C	81	GLN	CA-C-O	5.12	126.83	120.54
1	Y	43	GLY	CA-C-N	5.12	128.74	121.02
1	Y	43	GLY	C-N-CA	5.12	128.74	121.02
4	D	402	LEU	CA-C-O	5.12	125.77	120.30
6	C	308	TRP	CD2-CE2-CZ2	-5.11	117.29	122.40
5	F	139	GLY	O-C-N	-5.11	117.28	122.19
6	C	300	THR	N-CA-CB	5.11	118.59	110.57
1	Y	381	ILE	O-C-N	-5.11	116.83	121.94
4	D	430	ILE	N-CA-C	5.11	116.27	109.37
5	F	101	ALA	N-CA-C	5.11	117.75	110.24
5	F	255	THR	CB-CA-C	-5.11	102.17	110.85
2	E	472	LEU	N-CA-C	5.11	117.24	111.11
4	D	250	ARG	NE-CZ-NH2	5.11	123.79	119.20
5	F	241	LEU	CA-C-O	5.11	125.96	120.70
5	F	293	SER	N-CA-C	5.11	116.84	111.28
4	D	343	ILE	O-C-N	-5.10	117.67	123.18
6	C	89	LYS	CA-C-O	5.10	125.45	119.28
6	C	292	PRO	N-CA-CB	-5.10	97.89	103.25
3	G	515	PHE	CA-C-N	-5.10	116.21	122.84
3	G	515	PHE	C-N-CA	-5.10	116.21	122.84
6	C	269	ASP	CA-C-O	5.10	127.83	121.81
4	D	497	LEU	CA-C-O	-5.10	115.24	121.15
4	D	552	SER	O-C-N	-5.10	116.00	122.27
1	Y	192	PHE	CA-C-O	-5.10	115.15	120.55
6	C	109	GLN	CA-C-O	5.10	126.68	121.23
5	F	223	GLU	N-CA-C	5.09	116.83	111.28
6	C	263	ALA	N-CA-CB	-5.09	103.16	111.66
4	D	342	ASN	OD1-CG-ND2	5.09	127.69	122.60
6	C	474	THR	CA-CB-OG1	5.09	117.24	109.60
1	Y	183	ILE	CA-CB-CG1	5.09	119.05	110.40
5	F	69	ASP	CA-C-N	5.09	127.43	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	69	ASP	C-N-CA	5.09	127.43	120.46
1	Y	318	VAL	O-C-N	-5.08	116.94	121.87
4	D	429	LEU	O-C-N	5.08	129.08	122.42
6	C	457	ASP	N-CA-CB	5.08	119.08	110.49
1	Y	300	TRP	CA-C-N	5.07	131.23	121.54
1	Y	300	TRP	C-N-CA	5.07	131.23	121.54
1	Y	429	TYR	O-C-N	-5.07	117.39	123.27
5	F	26	ALA	N-CA-CB	5.07	117.57	110.12
1	Y	150	ILE	CA-CB-CG2	-5.06	101.89	110.50
1	Y	272	ALA	N-CA-C	5.06	116.80	111.28
4	D	240	GLN	CA-C-N	5.06	130.50	122.60
4	D	240	GLN	C-N-CA	5.06	130.50	122.60
6	C	141	ALA	N-CA-C	5.06	114.92	108.24
4	D	237	ARG	CD-NE-CZ	-5.06	117.32	124.40
4	D	508	ALA	CA-C-N	5.06	125.60	119.98
4	D	508	ALA	C-N-CA	5.06	125.60	119.98
6	C	94	THR	N-CA-C	-5.06	107.14	113.72
6	C	179	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	Y	277	ALA	N-CA-C	5.05	116.79	111.28
4	D	592	THR	CA-C-O	5.05	125.91	120.55
6	C	110	ALA	O-C-N	-5.05	117.29	123.10
6	C	415	GLU	CB-CG-CD	5.05	121.18	112.60
4	D	433	ILE	N-CA-C	-5.05	101.04	108.11
1	Y	16	LEU	CA-C-O	5.04	128.17	122.37
1	Y	92	ILE	N-CA-C	-5.04	107.84	112.83
4	D	498	PRO	N-CA-CB	-5.04	97.96	103.25
1	Y	428	GLN	N-CA-C	5.04	116.46	111.07
4	D	237	ARG	NE-CZ-NH1	5.04	126.53	121.50
4	D	261	PRO	O-C-N	-5.04	117.22	123.01
6	C	438	TYR	CB-CA-C	5.04	118.79	110.88
6	C	448	GLN	OE1-CD-NE2	-5.04	117.56	122.60
6	C	495	MET	N-CA-C	5.03	116.45	111.07
5	F	118	ILE	O-C-N	-5.03	117.44	122.62
4	D	285	ASN	OD1-CG-ND2	-5.03	117.57	122.60
5	F	61	THR	O-C-N	-5.03	117.36	123.29
6	C	361	ILE	CA-C-O	5.03	125.90	120.47
5	F	202	SER	N-CA-C	5.03	116.45	111.07
5	F	295	LEU	O-C-N	-5.02	116.42	122.15
1	Y	4	GLN	CB-CG-CD	5.02	121.14	112.60
1	Y	37	SER	N-CA-C	-5.02	107.21	113.38
1	Y	99	HIS	ND1-CG-CD2	-5.02	101.08	106.10
5	F	102	GLU	N-CA-C	5.02	117.17	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	382	LYS	CA-C-O	-5.02	115.92	122.14
1	Y	29	ALA	CA-C-N	5.02	127.26	120.44
1	Y	29	ALA	C-N-CA	5.02	127.26	120.44
1	Y	292	SER	N-CA-C	5.01	116.44	111.07
5	F	37	ALA	N-CA-CB	-5.01	102.50	110.22
6	C	118	ASP	CA-C-N	5.01	129.74	121.87
6	C	118	ASP	C-N-CA	5.01	129.74	121.87
1	Y	410	VAL	N-CA-C	5.01	115.73	110.62
1	Y	216	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
1	Y	90	ILE	CA-CB-CG2	5.01	119.02	110.50
1	Y	243	ARG	NE-CZ-NH2	-5.01	114.69	119.20
3	G	515	PHE	CA-C-O	-5.01	114.94	120.30
4	D	272	ILE	CA-C-N	5.01	127.92	120.31
4	D	272	ILE	C-N-CA	5.01	127.92	120.31
6	C	69	ASP	O-C-N	-5.01	115.38	122.99
1	Y	51	LYS	N-CA-C	5.01	121.46	110.80
4	D	598	ARG	N-CA-CB	-5.00	102.52	110.28
5	F	158	LEU	N-CA-C	5.00	117.11	111.11
5	F	159	VAL	N-CA-C	5.00	115.72	110.62
6	C	180	VAL	CB-CA-C	-5.00	103.37	110.83
1	Y	216	HIS	ND1-CE1-NE2	5.00	113.40	108.40

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	108	TYR	Sidechain
6	C	131	TYR	Sidechain
6	C	138	TYR	Sidechain
6	C	169	ARG	Sidechain
6	C	172	TYR	Sidechain
6	C	205	HIS	Mainchain
6	C	219	ARG	Sidechain
6	C	223	TYR	Sidechain
6	C	230	TYR	Sidechain
6	C	288	TYR	Sidechain
6	C	356	PHE	Sidechain
6	C	377	TYR	Sidechain
6	C	384	ARG	Sidechain
6	C	396	ARG	Sidechain
6	C	437	TYR	Sidechain
6	C	464	TYR	Sidechain

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Mol	Chain	Res	Type	Group
6	C	465	TYR	Sidechain
6	C	496	THR	Mainchain
6	C	517	TYR	Sidechain
6	C	75	ARG	Sidechain
6	C	97	PHE	Sidechain
4	D	10	TYR	Sidechain
4	D	250	ARG	Sidechain
4	D	268	ARG	Sidechain
4	D	282	ARG	Sidechain
4	D	316	TYR	Sidechain
4	D	372	TYR	Sidechain
4	D	387	VAL	Peptide
4	D	418	ARG	Sidechain
4	D	578	PHE	Sidechain
2	E	454	ARG	Sidechain
2	E	468	ARG	Sidechain
2	E	498	ARG	Sidechain
5	F	130	ARG	Sidechain
5	F	133	PHE	Sidechain
5	F	135	GLY	Peptide
5	F	160	TYR	Sidechain
5	F	168	ARG	Sidechain
5	F	179	HIS	Sidechain
5	F	209	TYR	Sidechain,Peptide
5	F	226	ARG	Sidechain
5	F	229	ARG	Sidechain
5	F	287	SER	Peptide
5	F	290	TYR	Sidechain
5	F	44	ARG	Sidechain
1	Y	113	ARG	Sidechain
1	Y	122	TYR	Sidechain
1	Y	154	PHE	Sidechain
1	Y	206	THR	Peptide
1	Y	22	ARG	Sidechain
1	Y	256	ARG	Sidechain
1	Y	372	ARG	Sidechain
1	Y	38	PHE	Sidechain
1	Y	399	PHE	Sidechain
1	Y	429	TYR	Sidechain
1	Y	7	LEU	Peptide

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	Y	3423	3581	3583	17	0
2	E	510	552	551	0	0
3	G	236	244	243	1	0
4	D	3128	3291	3292	10	0
5	F	2211	2291	2290	6	0
6	C	3589	3594	3591	8	0
All	All	13097	13553	13550	39	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 1.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:317:TYR:CE1	1:Y:317:TYR:CZ	1.81	1.62
1:Y:317:TYR:CG	1:Y:317:TYR:CD1	1.83	1.61
1:Y:317:TYR:CG	1:Y:317:TYR:CD2	1.85	1.61
1:Y:317:TYR:CZ	1:Y:317:TYR:CE2	1.82	1.59
6:C:486:VAL:HG22	6:C:487:THR:H	1.62	0.64
1:Y:176:GLU:CD	6:C:394:ARG:HH21	2.14	0.56
1:Y:361:GLN:H	1:Y:361:GLN:CD	2.16	0.52
1:Y:274:VAL:HG21	1:Y:411:VAL:HG21	1.91	0.52
6:C:351:VAL:HG12	6:C:353:ASN:HD22	1.74	0.51
1:Y:63:MET:HE2	1:Y:288:ALA:HB1	1.92	0.50
4:D:239:ASN:HD21	4:D:246:PRO:HB3	1.78	0.48
4:D:445:LEU:HD11	5:F:269:VAL:HG11	1.95	0.48
3:G:529:ILE:H	3:G:529:ILE:HD12	1.78	0.47
4:D:275:ALA:HB3	4:D:386:LEU:HD12	1.97	0.47
1:Y:67:PHE:HB3	1:Y:83:MET:HB2	1.98	0.46
1:Y:47:ALA:HA	1:Y:74:ARG:HA	1.97	0.46
6:C:244:LEU:HD11	6:C:246:ILE:HD12	1.99	0.45
4:D:231:ILE:HG21	4:D:256:ILE:HD12	1.99	0.45
6:C:95:GLN:HA	6:C:96:PRO:HD2	1.89	0.45
1:Y:257:VAL:HG12	1:Y:258:TYR:CD1	2.52	0.44
1:Y:30:LEU:HD21	1:Y:192:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:29:ILE:HD12	5:F:29:ILE:HA	1.92	0.44
5:F:118:ILE:O	5:F:119:ASN:HB2	2.18	0.43
5:F:194:GLU:CD	5:F:194:GLU:H	2.26	0.43
1:Y:275:ILE:HB	1:Y:276:PRO:HD3	2.01	0.43
6:C:486:VAL:HG22	6:C:487:THR:N	2.31	0.43
1:Y:105:ILE:HG22	1:Y:336:VAL:HG13	2.00	0.43
1:Y:148:LEU:HD12	1:Y:149:VAL:H	1.84	0.42
4:D:537:THR:HG21	4:D:540:GLN:HB2	2.01	0.42
5:F:32:LEU:HD21	6:C:530:LEU:HA	2.02	0.42
5:F:191:PHE:CD2	5:F:193:ILE:HD11	2.55	0.42
4:D:416:GLU:H	4:D:416:GLU:CD	2.27	0.42
1:Y:196:VAL:HG22	1:Y:196:VAL:O	2.20	0.41
4:D:507:ILE:HA	4:D:510:ILE:HD12	2.01	0.41
1:Y:172:MET:HE2	1:Y:172:MET:HA	2.03	0.41
4:D:240:GLN:H	4:D:303:GLU:CD	2.29	0.41
4:D:259:GLU:HG3	4:D:435:ILE:HD12	2.03	0.41
6:C:106:PHE:CD1	6:C:199:SER:HB2	2.56	0.40
4:D:4:ARG:HG2	4:D:599:ALA:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	441/458 (96%)	367 (83%)	50 (11%)	24 (5%)	1	15
2	E	63/140 (45%)	57 (90%)	5 (8%)	1 (2%)	7	38
3	G	30/136 (22%)	29 (97%)	1 (3%)	0	100	100
4	D	410/622 (66%)	373 (91%)	25 (6%)	12 (3%)	3	23
5	F	287/323 (89%)	257 (90%)	24 (8%)	6 (2%)	5	30
6	C	449/559 (80%)	395 (88%)	40 (9%)	14 (3%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1680/2238 (75%)	1478 (88%)	145 (9%)	57 (3%)	4	21

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	48	VAL
1	Y	71	ALA
1	Y	113	ARG
1	Y	199	LEU
1	Y	305	THR
1	Y	341	GLU
4	D	318	ARG
4	D	389	GLN
4	D	537	THR
5	F	196	ASP
5	F	210	SER
6	C	337	SER
1	Y	57	ARG
1	Y	73	SER
1	Y	258	TYR
2	E	449	THR
4	D	240	GLN
4	D	258	VAL
4	D	265	ASP
4	D	399	GLN
4	D	475	PHE
5	F	125	ASN
5	F	211	LEU
6	C	312	GLU
6	C	348	HIS
6	C	411	LEU
6	C	426	LEU
1	Y	22	ARG
1	Y	105	ILE
1	Y	205	HIS
1	Y	206	THR
1	Y	334	ALA
1	Y	343	ALA
1	Y	360	GLU
4	D	325	HIS
4	D	346	ASP
6	C	244	LEU

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Mol	Chain	Res	Type
6	C	347	ILE
6	C	457	ASP
1	Y	46	ALA
1	Y	314	GLN
1	Y	436	ALA
4	D	417	ALA
5	F	16	VAL
5	F	91	SER
6	C	106	PHE
6	C	481	MET
1	Y	142	MET
1	Y	251	ARG
6	C	485	THR
6	C	105	GLN
6	C	420	LEU
4	D	288	VAL
1	Y	100	PRO
1	Y	356	ILE
6	C	371	PRO
1	Y	6	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	359/374 (96%)	344 (96%)	15 (4%)	26	48
2	E	54/110 (49%)	52 (96%)	2 (4%)	30	51
3	G	27/106 (26%)	27 (100%)	0	100	100
4	D	337/509 (66%)	327 (97%)	10 (3%)	36	57
5	F	237/267 (89%)	223 (94%)	14 (6%)	18	39
6	C	387/475 (82%)	377 (97%)	10 (3%)	40	62
All	All	1401/1841 (76%)	1350 (96%)	51 (4%)	32	52

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	13	LYS
1	Y	40	PRO
1	Y	51	LYS
1	Y	126	VAL
1	Y	178	ILE
1	Y	179	THR
1	Y	216	HIS
1	Y	218	LEU
1	Y	237	VAL
1	Y	321	TYR
1	Y	340	ARG
1	Y	361	GLN
1	Y	366	ILE
1	Y	370	MET
1	Y	422	THR
2	E	458	THR
2	E	475	THR
4	D	297	ARG
4	D	333	GLN
4	D	339	PRO
4	D	361	ILE
4	D	432	PRO
4	D	440	THR
4	D	474	LYS
4	D	498	PRO
4	D	580	ILE
4	D	594	ILE
5	F	14	ARG
5	F	60	ILE
5	F	63	GLU
5	F	97	ARG
5	F	98	MET
5	F	144	GLN
5	F	157	ILE
5	F	179	HIS
5	F	194	GLU
5	F	198	THR
5	F	220	ARG
5	F	245	LEU
5	F	254	THR
5	F	255	THR
6	C	67	VAL
6	C	104	PRO

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Mol	Chain	Res	Type
6	C	123	PRO
6	C	187	PRO
6	C	303	MET
6	C	376	GLN
6	C	400	ASP
6	C	487	THR
6	C	510	PRO
6	C	529	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	212	GLN
3	G	514	ASN
4	D	27	ASN
4	D	239	ASN
4	D	240	GLN
4	D	249	GLN
4	D	360	ASN
4	D	394	ASN
4	D	397	ASN
5	F	47	ASN
6	C	73	ASN
6	C	304	ASN
6	C	348	HIS
6	C	353	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

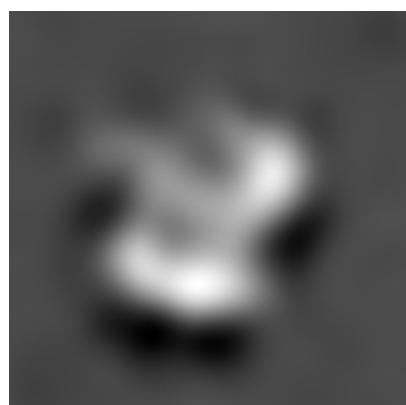
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3506. 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](#)

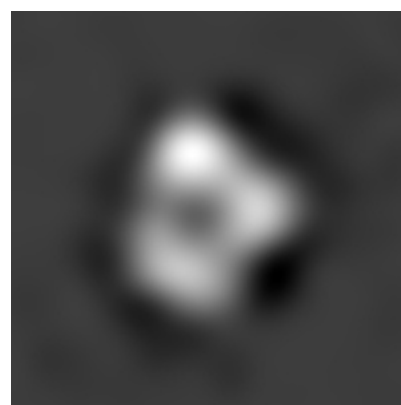
6.1.1 Primary map



X



Y

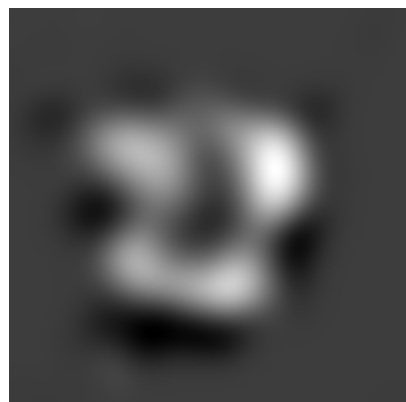


Z

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

6.2 Central slices [i](#)

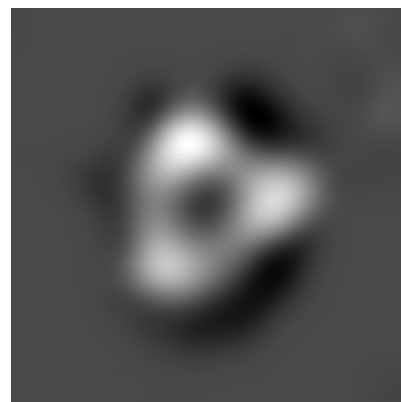
6.2.1 Primary map



X Index: 70



Y Index: 70



Z Index: 70

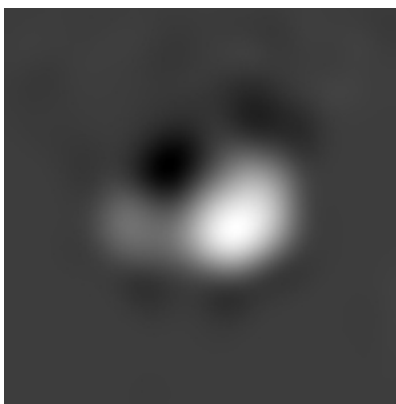
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 61



Y Index: 91

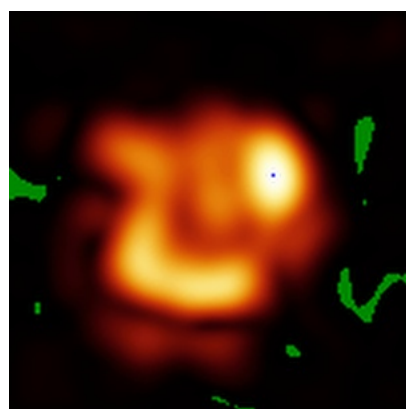


Z Index: 45

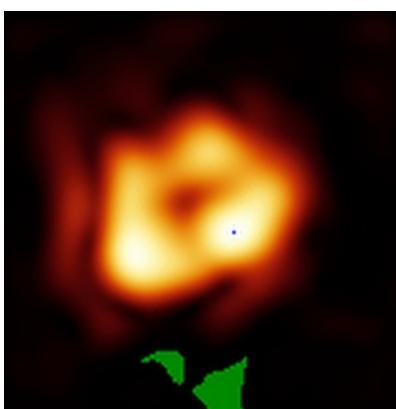
The images above show the largest variance slices of the map in three orthogonal directions.

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

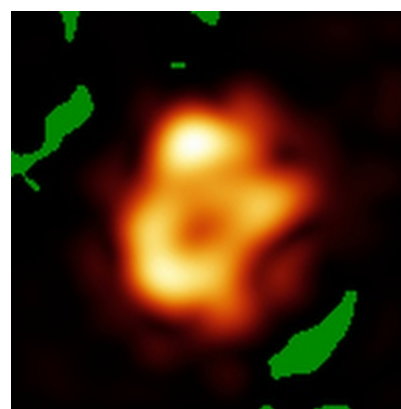
6.4.1 Primary map



X



Y

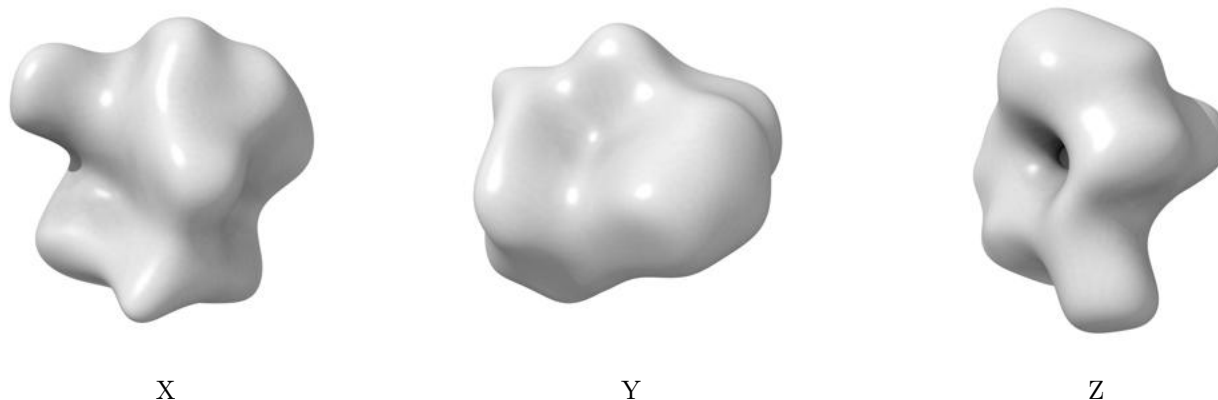


Z

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 8.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

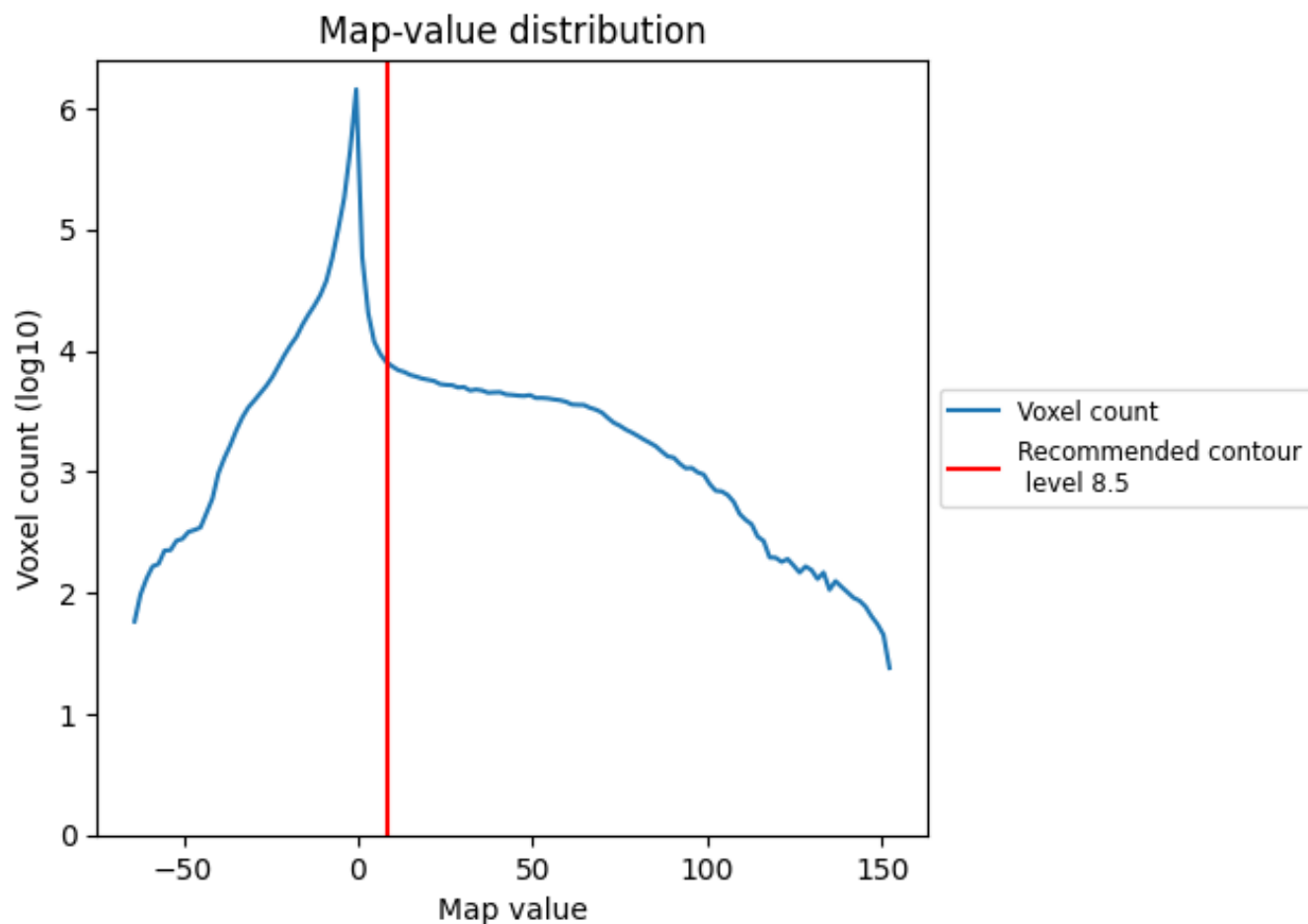
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

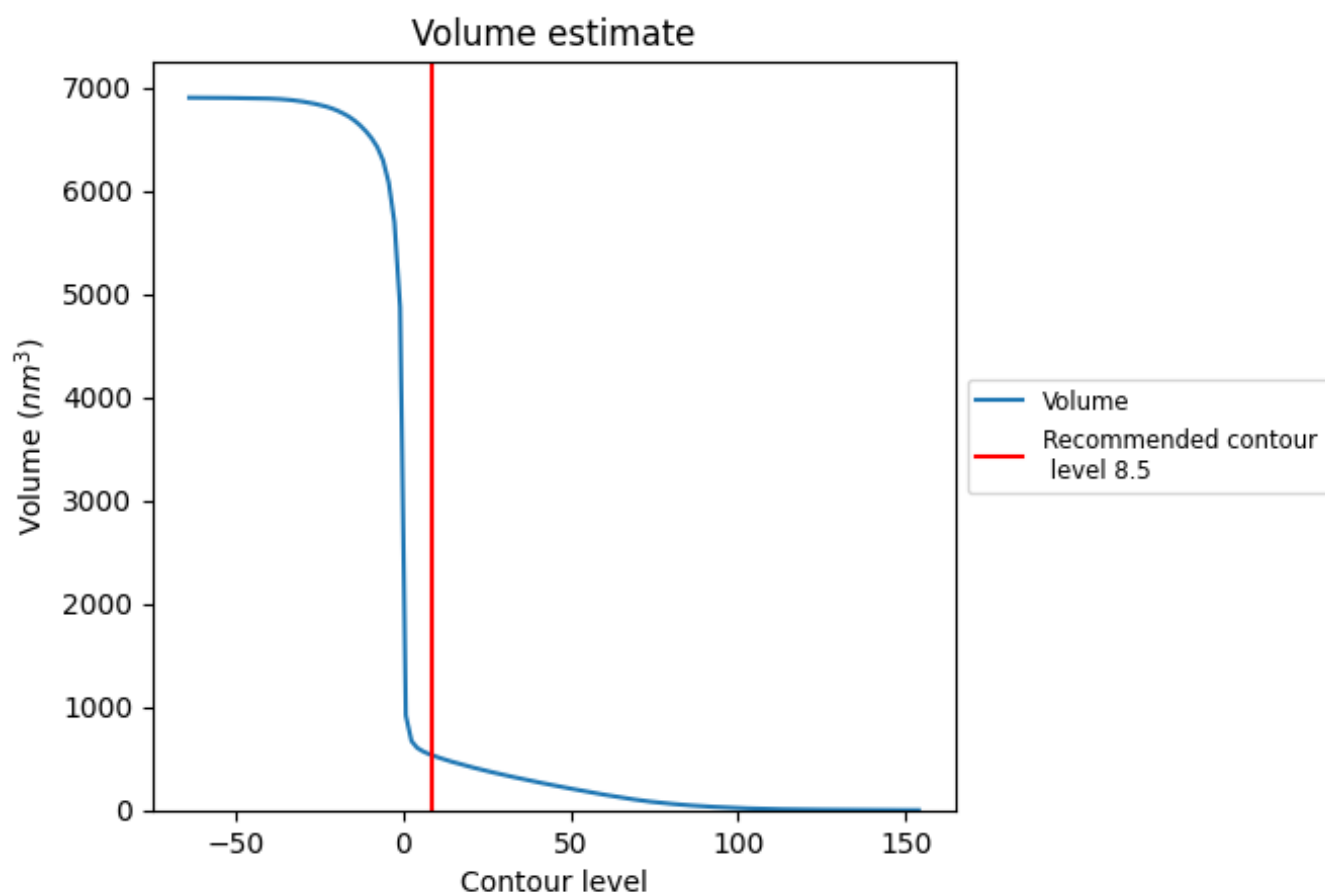
This section contains the results of statistical analysis of the map.

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.

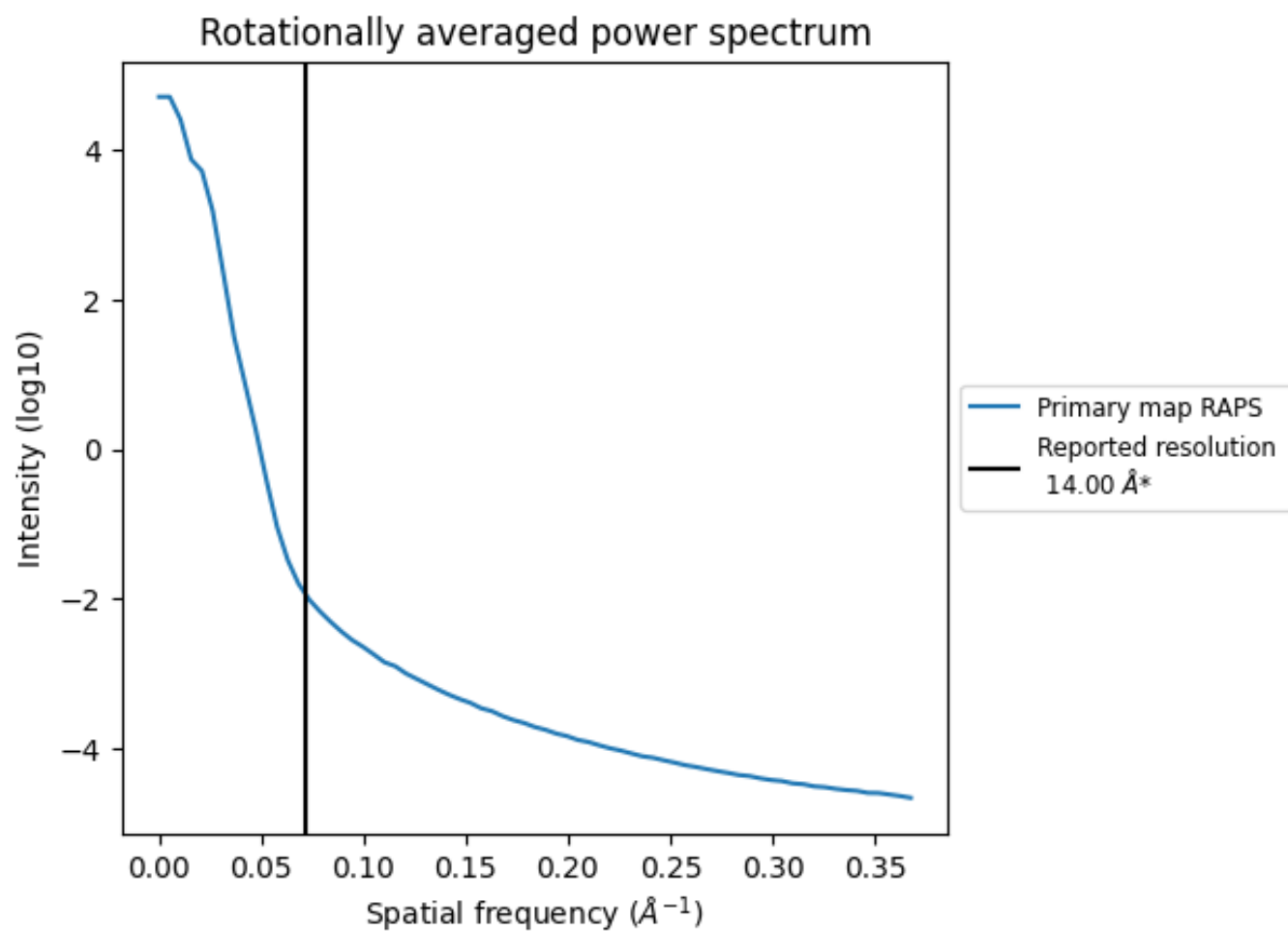
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 533 nm^3 ; this corresponds to an approximate mass of 481 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 ⓘ

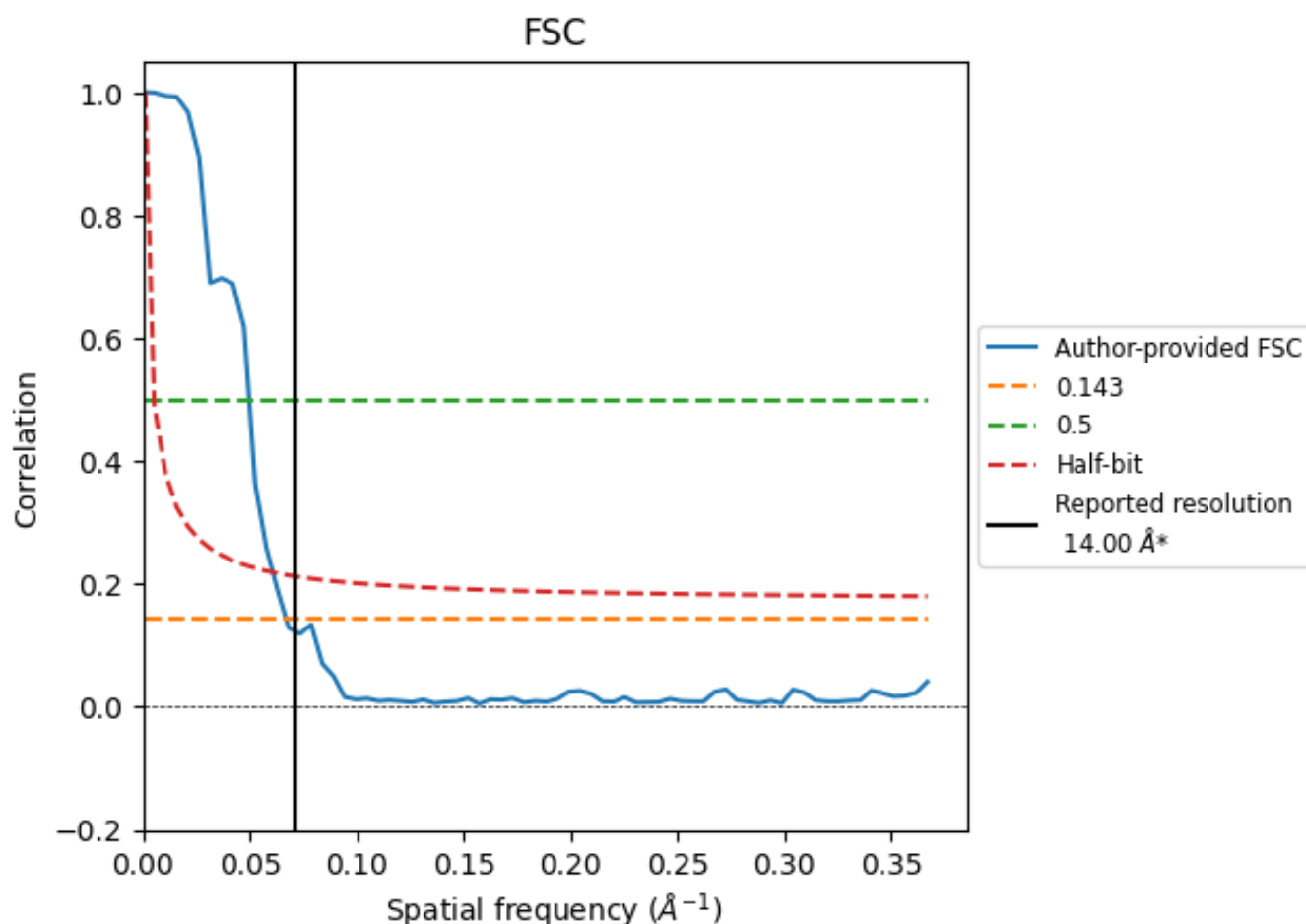


*Reported resolution corresponds to spatial frequency of 0.071 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.071 Å⁻¹

8.2 Resolution estimates [i](#)

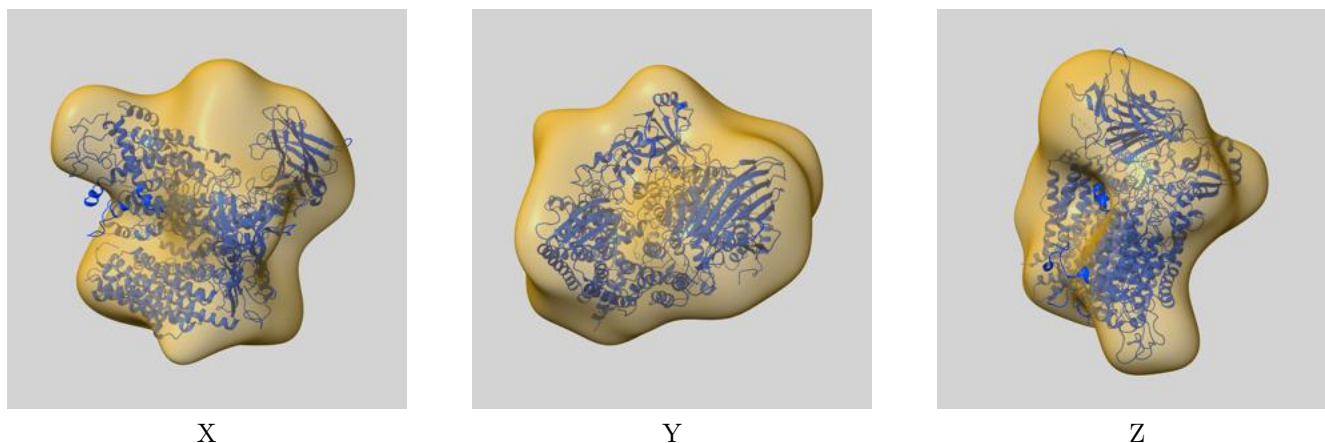
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	14.00	-	-
Author-provided FSC curve	14.95	20.16	16.47
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

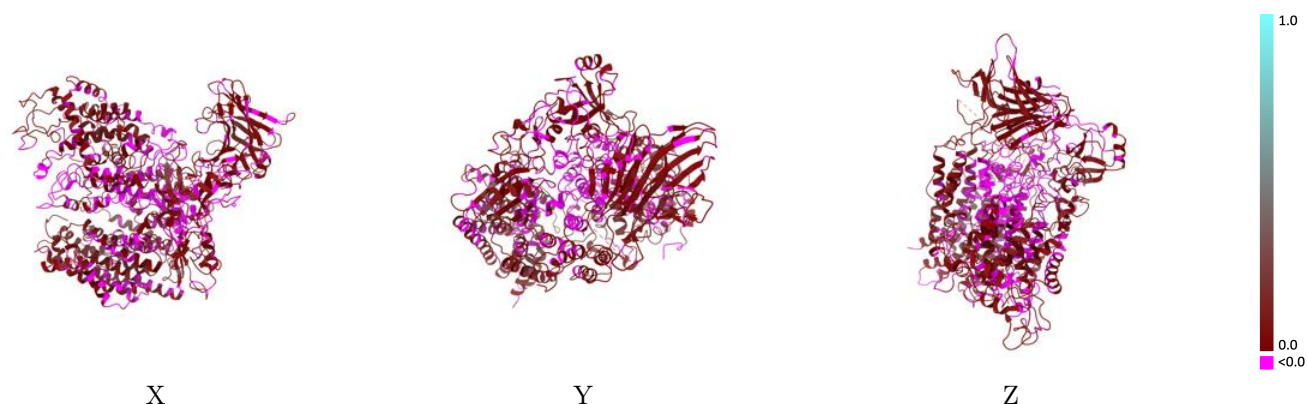
This section contains information regarding the fit between EMDB map EMD-3506 and PDB model 5MG3. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



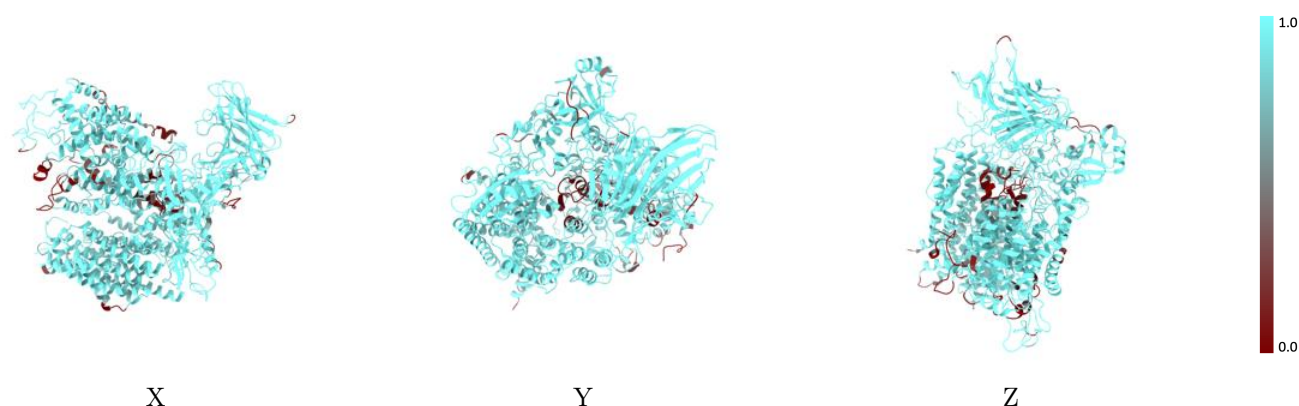
The images above show the 3D surface view of the map at the recommended contour level 8.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



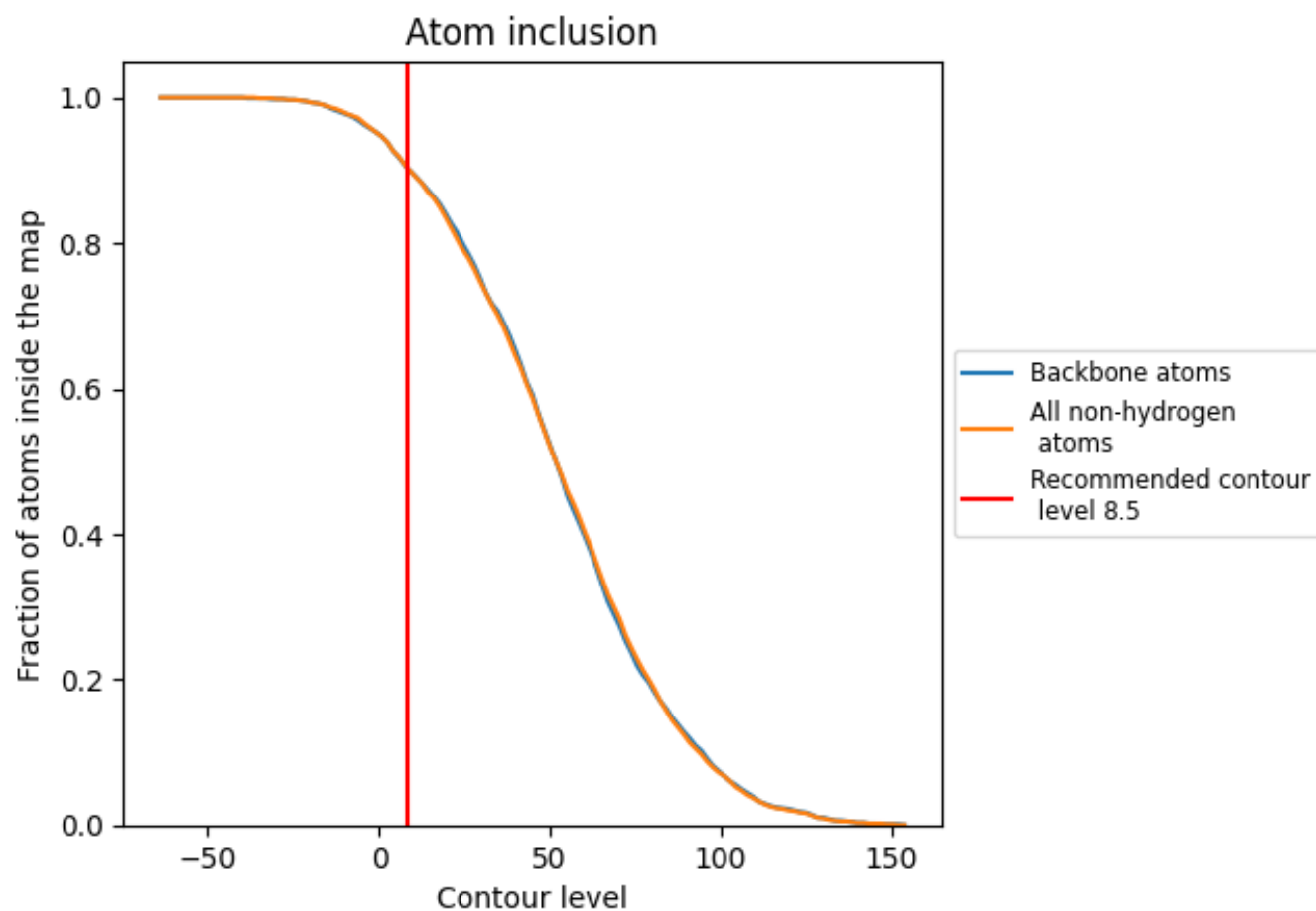
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (8.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (8.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9020	0.0340
C	0.9490	0.0350
D	0.9390	0.0380
E	0.7700	0.0180
F	0.9760	0.0580
G	0.9920	-0.0030
Y	0.8100	0.0180

