



Full wwPDB EM Validation Report ⓘ

May 1, 2025 – 01:44 pm BST

PDB ID : 9Q96 / pdb_00009q96
EMDB ID : EMD-52919
Title : Cryo-EM Structure of Bacterial RNA polymerase-sigma54 transcription open complex with wild type sigma54, from RPi(-10-1)
Authors : Gao, F.; Zhang, X.
Deposited on : 2025-02-26
Resolution : 4.60 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

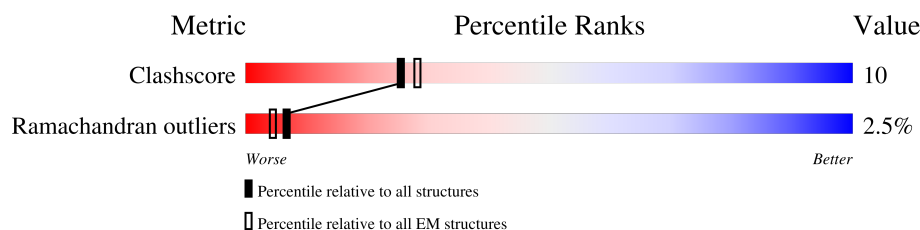
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

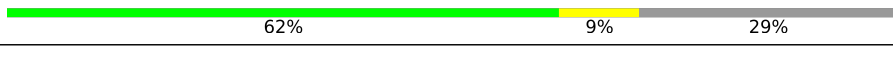

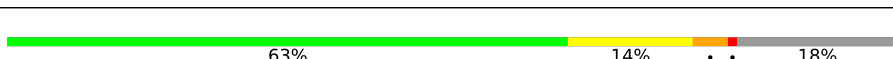


The reported resolution of this entry is 4.60 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	 64% 27% 6%
1	B	329	 62% 9% 29%
2	C	1342	 60% 36% 4%
3	D	1407	 59% 31% 10%
4	E	91	 63% 14% 18%
5	M	497	 49% 12% 36%
6	N	46	 24% 74% 2%
7	T	46	 24% 50% 15% 11%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19633 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	309	Total	C	N	O	0	0
			1526	908	309	309		
1	B	235	Total	C	N	O	0	0
			1160	690	235	235		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	1341	Total	C	N	O	0	0
			6599	3917	1341	1341		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	1345	Total	C	N	O	0	0
			6619	3929	1345	1345		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	75	Total	C	N	O	0	0
			371	221	75	75		

- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	316	Total	C	N	O	0	0
			1570	938	316	316		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	initiating methionine	UNP A0A377VEN9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-18	GLY	-	expression tag	UNP A0A377VEN9
M	-17	SER	-	expression tag	UNP A0A377VEN9
M	-16	SER	-	expression tag	UNP A0A377VEN9
M	-15	HIS	-	expression tag	UNP A0A377VEN9
M	-14	HIS	-	expression tag	UNP A0A377VEN9
M	-13	HIS	-	expression tag	UNP A0A377VEN9
M	-12	HIS	-	expression tag	UNP A0A377VEN9
M	-11	HIS	-	expression tag	UNP A0A377VEN9
M	-10	HIS	-	expression tag	UNP A0A377VEN9
M	-9	SER	-	expression tag	UNP A0A377VEN9
M	-8	SER	-	expression tag	UNP A0A377VEN9
M	-7	GLY	-	expression tag	UNP A0A377VEN9
M	-6	LEU	-	expression tag	UNP A0A377VEN9
M	-5	VAL	-	expression tag	UNP A0A377VEN9
M	-4	PRO	-	expression tag	UNP A0A377VEN9
M	-3	ARG	-	expression tag	UNP A0A377VEN9
M	-2	GLY	-	expression tag	UNP A0A377VEN9
M	-1	SER	-	expression tag	UNP A0A377VEN9
M	0	HIS	-	expression tag	UNP A0A377VEN9
M	1	MET	-	expression tag	UNP A0A377VEN9
M	2	LYS	-	expression tag	UNP A0A377VEN9
M	3	GLN	-	expression tag	UNP A0A377VEN9
M	4	GLY	-	expression tag	UNP A0A377VEN9
M	5	LEU	-	expression tag	UNP A0A377VEN9
M	6	GLN	-	expression tag	UNP A0A377VEN9
M	7	LEU	-	expression tag	UNP A0A377VEN9
M	8	ARG	-	expression tag	UNP A0A377VEN9
M	9	LEU	-	expression tag	UNP A0A377VEN9
M	10	SER	-	expression tag	UNP A0A377VEN9
M	11	GLN	-	expression tag	UNP A0A377VEN9
M	12	GLN	-	expression tag	UNP A0A377VEN9
M	13	LEU	-	expression tag	UNP A0A377VEN9
M	14	ALA	-	expression tag	UNP A0A377VEN9
M	15	MET	-	expression tag	UNP A0A377VEN9
M	16	THR	-	expression tag	UNP A0A377VEN9
M	17	PRO	-	expression tag	UNP A0A377VEN9
M	18	GLN	-	expression tag	UNP A0A377VEN9
M	19	LEU	-	expression tag	UNP A0A377VEN9
M	20	GLN	-	expression tag	UNP A0A377VEN9
M	21	GLN	-	expression tag	UNP A0A377VEN9
M	22	ALA	-	expression tag	UNP A0A377VEN9
M	23	ILE	-	expression tag	UNP A0A377VEN9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	24	ARG	-	expression tag	UNP A0A377VEN9
M	25	LEU	-	expression tag	UNP A0A377VEN9

- Molecule 6 is a DNA chain called NIFH PROMOTER NON-TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	46	Total	C	N	O	P	0	0
			946	448	173	279	46		

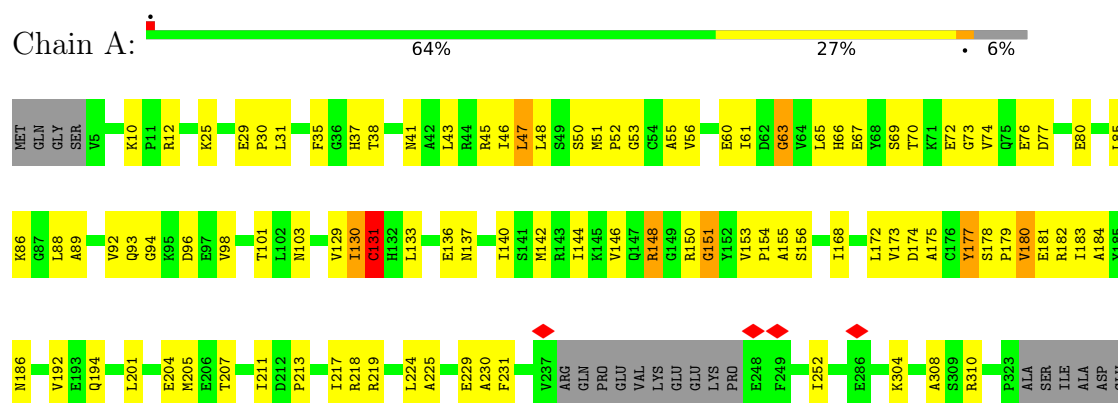
- Molecule 7 is a DNA chain called NIFH PROMOTER TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	41	Total	C	N	O	P	0	0
			842	396	165	240	41		

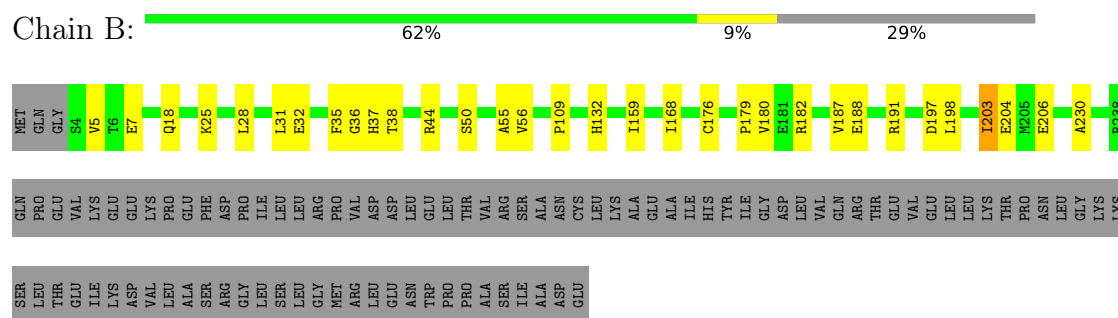
3 Residue-property plots

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.

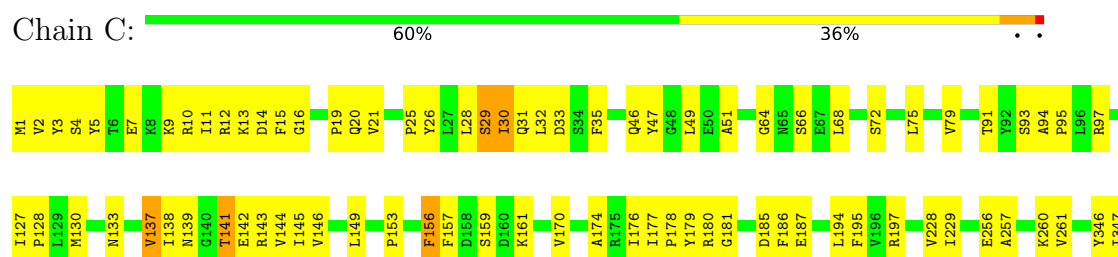
• Molecule 1: DNA-directed RNA polymerase subunit alpha

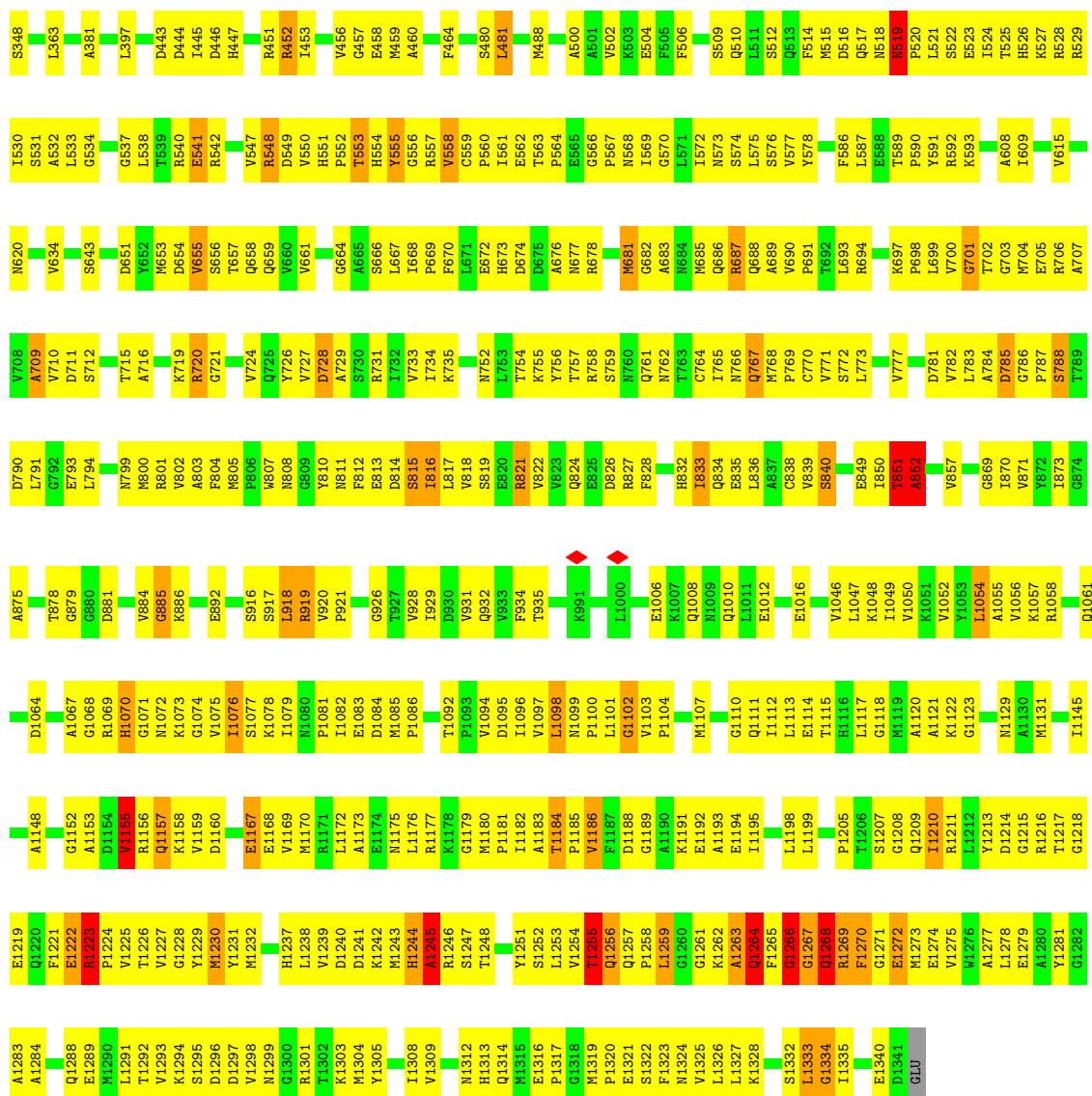


• Molecule 1: DNA-directed RNA polymerase subunit alpha



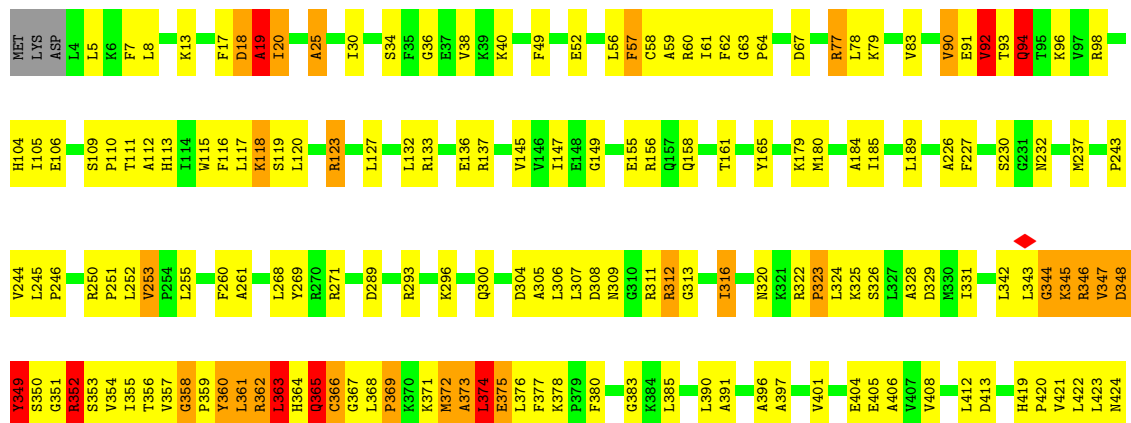
• Molecule 2: DNA-directed RNA polymerase subunit beta



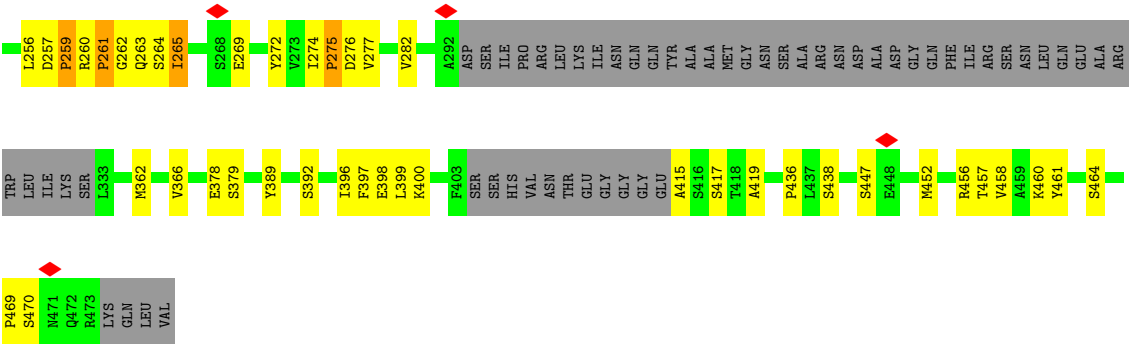


• Molecule 3: DNA-directed RNA polymerase subunit beta'

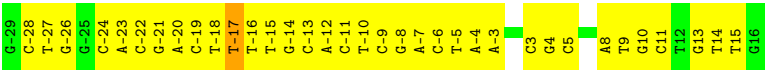
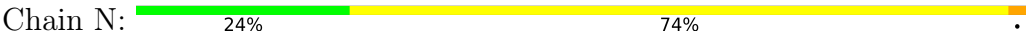
Chain D: 59% 31% 5% • •



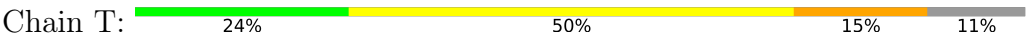




• Molecule 6: NIFH PROMOTER NON-TEMPLATE DNA



• Molecule 7: NIFH PROMOTER TEMPLATE DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	20233, 20233, 79678, 20233	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.228	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	220.0, 220.0, 220.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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	A	2.36	81/1524 (5.3%)	1.86	41/2119 (1.9%)
1	B	1.81	20/1159 (1.7%)	1.51	9/1612 (0.6%)
2	C	2.78	562/6598 (8.5%)	2.22	403/9172 (4.4%)
3	D	2.62	476/6614 (7.2%)	2.18	359/9188 (3.9%)
4	E	1.94	9/370 (2.4%)	1.83	9/514 (1.8%)
5	M	1.45	15/1567 (1.0%)	1.61	29/2183 (1.3%)
6	N	0.37	0/1060	0.72	1/1635 (0.1%)
7	T	0.52	1/945 (0.1%)	1.21	15/1453 (1.0%)
All	All	2.40	1164/19837 (5.9%)	1.99	866/27876 (3.1%)

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	A	0	6
2	C	0	24
3	D	0	24
4	E	0	1
5	M	0	1
All	All	0	56

All (1164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	526	HIS	C-O	-17.65	1.03	1.24
2	C	555	TYR	C-O	17.36	1.44	1.24
2	C	1225	VAL	C-O	17.25	1.41	1.24
2	C	813	GLU	C-O	15.82	1.39	1.24
2	C	827	ARG	N-CA	15.49	1.65	1.46
3	D	597	GLY	C-O	15.48	1.39	1.23
2	C	1243	MET	CA-C	15.39	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	360	TYR	N-CA	15.30	1.66	1.46
3	D	113	HIS	CA-C	-15.13	1.39	1.53
3	D	362	ARG	N-CA	-15.10	1.27	1.46
2	C	149	LEU	C-O	14.86	1.40	1.24
3	D	1323	ALA	C-O	14.84	1.41	1.24
3	D	357	VAL	CA-C	14.80	1.68	1.53
3	D	623	GLN	C-O	14.62	1.41	1.24
2	C	794	LEU	C-O	14.59	1.42	1.24
2	C	1238	LEU	N-CA	14.31	1.63	1.45
2	C	1247	SER	N-CA	13.94	1.61	1.46
2	C	143	ARG	C-O	-13.78	1.06	1.24
2	C	668	ILE	CA-C	13.73	1.63	1.53
3	D	359	PRO	CA-CB	13.54	1.73	1.53
3	D	352	ARG	N-CA	13.53	1.62	1.46
3	D	369	PRO	N-CA	13.51	1.63	1.47
3	D	360	TYR	CA-C	13.36	1.70	1.52
2	C	1298	VAL	C-O	13.28	1.36	1.24
3	D	429	LEU	C-O	13.12	1.41	1.23
2	C	519	ASN	N-CA	13.12	1.64	1.46
3	D	472	LEU	CA-CB	-13.11	1.36	1.53
5	M	190	VAL	C-O	13.03	1.37	1.24
2	C	1246	ARG	CA-C	-12.74	1.37	1.52
3	D	373	ALA	N-CA	12.66	1.62	1.46
2	C	577	VAL	C-O	12.62	1.38	1.24
3	D	492	SER	C-O	-12.56	1.08	1.24
2	C	1299	ASN	CA-C	12.46	1.69	1.52
3	D	462	ASP	N-CA	12.42	1.60	1.46
2	C	590	PRO	CA-C	-12.34	1.40	1.52
3	D	425	ARG	C-O	-12.27	1.10	1.24
2	C	699	LEU	C-O	-12.26	1.07	1.24
2	C	931	VAL	C-O	12.26	1.36	1.24
2	C	518	ASN	N-CA	12.22	1.61	1.46
3	D	462	ASP	CA-C	12.22	1.68	1.52
3	D	451	PRO	C-O	12.17	1.40	1.24
2	C	177	ILE	N-CA	12.15	1.55	1.45
1	A	181	GLU	N-CA	12.13	1.61	1.46
2	C	683	ALA	C-O	12.13	1.38	1.24
2	C	803	ALA	C-O	12.12	1.37	1.24
2	C	1078	LYS	C-O	12.11	1.38	1.23
3	D	894	VAL	C-O	-12.00	1.09	1.24
3	D	1365	TYR	C-O	-11.99	1.08	1.24
3	D	1363	TYR	C-O	11.96	1.37	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1099	ASN	CA-C	-11.93	1.38	1.52
3	D	492	SER	CA-C	-11.91	1.39	1.52
2	C	1246	ARG	N-CA	11.91	1.60	1.45
3	D	345	LYS	CA-CB	11.87	1.71	1.53
2	C	697	LYS	N-CA	11.78	1.61	1.45
3	D	769	VAL	N-CA	11.75	1.60	1.46
1	B	31	LEU	C-O	11.74	1.38	1.23
2	C	757	THR	C-O	-11.72	1.10	1.23
2	C	1177	ARG	C-O	-11.72	1.10	1.24
2	C	804	PHE	N-CA	11.66	1.60	1.46
2	C	1068	GLY	N-CA	11.66	1.56	1.45
1	A	182	ARG	N-CA	11.64	1.59	1.45
2	C	690	VAL	CA-C	-11.57	1.40	1.52
2	C	1111	GLN	C-O	11.54	1.37	1.24
3	D	456	ALA	N-CA	11.50	1.60	1.46
3	D	908	ILE	CA-C	-11.42	1.40	1.52
3	D	1340	LYS	C-O	-11.31	1.09	1.23
2	C	452	ARG	C-O	11.31	1.38	1.23
3	D	833	GLU	C-O	-11.30	1.14	1.25
2	C	562	GLU	CA-CB	11.27	1.67	1.53
3	D	622	ASP	C-O	11.27	1.37	1.24
2	C	879	GLY	C-O	-11.24	1.09	1.24
3	D	421	VAL	C-O	11.19	1.34	1.23
2	C	764	CYS	N-CA	11.12	1.60	1.45
2	C	762	ASN	CA-C	11.11	1.67	1.53
2	C	153	PRO	C-O	11.10	1.36	1.23
2	C	524	ILE	N-CA	-11.09	1.34	1.46
3	D	901	ARG	C-O	11.05	1.36	1.23
3	D	808	VAL	C-O	-11.01	1.10	1.24
2	C	770	CYS	N-CA	11.00	1.59	1.46
1	B	44	ARG	C-O	10.96	1.36	1.24
2	C	9	LYS	C-O	-10.89	1.11	1.24
3	D	545	HIS	C-O	-10.85	1.14	1.24
2	C	515	MET	C-O	10.83	1.37	1.23
3	D	377	PHE	CA-C	10.82	1.68	1.52
3	D	1256	ILE	N-CA	-10.82	1.33	1.46
2	C	834	GLN	C-O	10.82	1.37	1.23
3	D	308	ASP	N-CA	10.78	1.59	1.46
2	C	659	GLN	CA-C	-10.76	1.39	1.52
3	D	488	ASN	CA-C	-10.73	1.39	1.52
2	C	758	ARG	CA-C	10.71	1.66	1.52
2	C	677	ASN	C-O	10.68	1.38	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	678	ARG	CA-C	10.66	1.66	1.52
2	C	818	VAL	CA-CB	10.56	1.69	1.54
3	D	470	VAL	CA-CB	-10.54	1.43	1.53
2	C	1113	LEU	C-O	10.51	1.37	1.24
2	C	133	ASN	N-CA	-10.51	1.32	1.46
1	A	151	GLY	N-CA	10.44	1.60	1.45
2	C	1086	PRO	N-CA	10.41	1.59	1.47
3	D	1359	ALA	CA-C	-10.39	1.39	1.52
3	D	1326	GLN	CA-C	-10.30	1.39	1.52
3	D	632	ALA	CA-C	-10.26	1.39	1.52
3	D	808	VAL	CA-CB	10.24	1.68	1.54
2	C	834	GLN	CA-C	-10.21	1.39	1.52
2	C	1271	GLY	C-O	10.21	1.33	1.23
3	D	889	ASP	CA-CB	10.18	1.69	1.53
2	C	1231	TYR	C-O	10.18	1.35	1.24
5	M	154	LEU	C-O	-10.17	1.11	1.24
3	D	365	GLN	CA-CB	10.07	1.68	1.53
2	C	1211	ARG	N-CA	10.05	1.58	1.46
2	C	514	PHE	C-O	10.04	1.36	1.23
3	D	914	ALA	CA-CB	-10.02	1.40	1.53
2	C	693	LEU	CA-C	-10.00	1.40	1.52
3	D	458	ASN	C-O	-10.00	1.10	1.23
3	D	476	ALA	CA-CB	-9.99	1.37	1.53
3	D	781	LYS	C-O	-9.97	1.12	1.24
3	D	770	LEU	C-O	9.95	1.35	1.24
2	C	667	LEU	C-O	9.89	1.37	1.24
2	C	521	LEU	N-CA	-9.89	1.34	1.46
1	A	129	VAL	C-O	-9.86	1.11	1.24
2	C	1184	THR	N-CA	9.86	1.58	1.46
1	A	178	SER	C-O	-9.85	1.11	1.24
2	C	551	HIS	CA-C	9.81	1.65	1.52
2	C	821	ARG	N-CA	-9.76	1.34	1.46
1	A	41	ASN	C-O	9.72	1.35	1.24
2	C	701	GLY	C-O	9.72	1.33	1.23
3	D	885	VAL	N-CA	9.72	1.58	1.46
3	D	916	GLY	C-O	9.69	1.37	1.23
2	C	1277	ALA	CA-CB	-9.69	1.37	1.53
3	D	366	CYS	CA-C	-9.68	1.39	1.52
2	C	1247	SER	CA-C	-9.67	1.46	1.52
2	C	1096	ILE	N-CA	9.67	1.58	1.46
3	D	784	ALA	C-O	-9.66	1.10	1.24
3	D	506	VAL	C-O	9.66	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	468	VAL	C-O	9.66	1.33	1.24
3	D	440	VAL	C-O	9.62	1.33	1.24
2	C	1334	GLY	C-O	9.61	1.36	1.23
3	D	1323	ALA	CA-C	-9.61	1.40	1.52
3	D	501	VAL	N-CA	-9.59	1.34	1.46
2	C	1111	GLN	N-CA	-9.58	1.34	1.46
2	C	138	ILE	C-O	9.57	1.34	1.24
2	C	520	PRO	C-O	9.57	1.37	1.24
2	C	765	ILE	N-CA	9.57	1.58	1.46
1	A	96	ASP	C-O	-9.55	1.11	1.24
2	C	1264	GLN	C-O	9.53	1.35	1.24
2	C	700	VAL	CA-C	9.51	1.64	1.52
2	C	1268	GLN	CA-CB	9.51	1.69	1.53
2	C	1248	THR	C-O	9.50	1.34	1.23
2	C	811	ASN	CA-C	-9.47	1.41	1.52
3	D	460	ASP	CA-C	-9.47	1.41	1.53
3	D	742	GLY	C-O	-9.47	1.12	1.24
2	C	522	SER	N-CA	-9.45	1.34	1.46
3	D	783	LEU	C-O	9.43	1.35	1.24
3	D	899	TYR	CA-CB	9.40	1.69	1.53
3	D	469	HIS	C-O	9.38	1.35	1.23
3	D	1248	ILE	C-O	9.37	1.33	1.24
2	C	1313	HIS	N-CA	9.34	1.58	1.46
3	D	483	LEU	CA-C	-9.27	1.40	1.52
1	A	51	MET	C-O	9.26	1.36	1.24
2	C	512	SER	C-O	9.26	1.34	1.24
3	D	917	VAL	C-O	9.24	1.36	1.24
2	C	1274	GLU	CA-C	-9.23	1.40	1.52
3	D	372	MET	C-O	-9.23	1.12	1.24
2	C	1101	LEU	C-O	9.23	1.35	1.24
1	A	85	LEU	CA-C	-9.22	1.39	1.52
3	D	888	CYS	C-O	9.21	1.35	1.24
2	C	769	PRO	CA-CB	-9.21	1.41	1.53
3	D	722	ILE	C-O	9.21	1.34	1.24
2	C	765	ILE	CA-C	-9.21	1.40	1.52
3	D	629	PHE	N-CA	-9.21	1.35	1.46
2	C	1322	SER	N-CA	-9.20	1.35	1.46
5	M	186	ASP	CA-C	-9.20	1.42	1.52
2	C	1277	ALA	C-O	9.18	1.35	1.24
3	D	1352	ILE	C-O	-9.17	1.13	1.24
4	E	13	ILE	C-O	9.17	1.33	1.24
2	C	1325	VAL	N-CA	-9.16	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	26	ARG	C-O	-9.16	1.12	1.24
3	D	423	LEU	CA-C	-9.15	1.42	1.52
2	C	828	PHE	N-CA	9.14	1.57	1.46
2	C	525	THR	CA-C	-9.10	1.40	1.52
3	D	351	GLY	C-O	9.10	1.33	1.23
2	C	548	ARG	CA-CB	9.09	1.67	1.53
2	C	777	VAL	C-O	9.08	1.33	1.24
2	C	800	MET	CA-CB	9.08	1.69	1.53
3	D	351	GLY	N-CA	9.08	1.55	1.44
2	C	557	ARG	N-CA	-9.07	1.34	1.46
2	C	1270	PHE	CA-CB	-9.04	1.37	1.53
2	C	526	HIS	N-CA	9.02	1.57	1.46
3	D	539	SER	C-O	-9.01	1.14	1.24
3	D	92	VAL	CA-C	9.00	1.64	1.52
2	C	1232	MET	CA-C	-8.98	1.41	1.52
3	D	582	ILE	CA-C	8.97	1.65	1.52
3	D	514	THR	CA-CB	-8.96	1.41	1.53
2	C	1239	VAL	N-CA	8.93	1.58	1.46
2	C	803	ALA	CA-C	-8.92	1.41	1.52
2	C	808	ASN	CA-C	8.90	1.65	1.53
3	D	104	HIS	CA-C	-8.90	1.41	1.52
3	D	445	LYS	N-CA	-8.89	1.34	1.46
2	C	1192	GLU	N-CA	8.88	1.57	1.46
2	C	705	GLU	C-O	8.85	1.35	1.24
3	D	1336	ALA	CA-C	-8.81	1.41	1.52
1	A	133	LEU	N-CA	-8.79	1.35	1.46
2	C	12	ARG	N-CA	8.78	1.57	1.45
2	C	687	ARG	N-CA	-8.78	1.35	1.46
2	C	839	VAL	C-O	8.76	1.32	1.24
3	D	1277	GLY	N-CA	8.75	1.58	1.45
2	C	1181	PRO	C-O	-8.72	1.06	1.23
2	C	177	ILE	CA-CB	8.71	1.60	1.54
3	D	443	GLU	C-O	8.71	1.34	1.24
2	C	704	MET	CA-C	8.69	1.65	1.52
3	D	599	LYS	C-O	8.69	1.34	1.24
2	C	1323	PHE	N-CA	8.69	1.57	1.46
2	C	815	SER	CA-CB	-8.68	1.40	1.53
2	C	1295	SER	CA-CB	8.63	1.68	1.53
3	D	761	ALA	CA-C	8.63	1.62	1.52
2	C	29	SER	C-O	8.62	1.34	1.24
1	B	38	THR	C-O	8.58	1.33	1.24
3	D	491	LEU	C-O	8.56	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	655	VAL	C-O	8.54	1.34	1.24
2	C	1107	MET	N-CA	8.54	1.58	1.46
3	D	809	VAL	C-O	-8.53	1.14	1.24
1	A	151	GLY	C-O	-8.53	1.12	1.23
2	C	819	SER	CA-C	-8.53	1.41	1.52
3	D	917	VAL	N-CA	-8.53	1.35	1.46
3	D	434	ILE	C-O	-8.52	1.15	1.24
2	C	97	ARG	C-O	-8.51	1.13	1.24
1	A	204	GLU	C-O	8.48	1.34	1.24
5	M	152	GLY	C-O	-8.46	1.12	1.23
3	D	914	ALA	C-N	-8.43	1.22	1.33
2	C	1239	VAL	CA-C	8.41	1.65	1.52
2	C	1275	VAL	C-O	8.40	1.33	1.24
2	C	1047	LEU	C-O	-8.39	1.13	1.24
3	D	64	PRO	CA-C	-8.38	1.43	1.53
1	B	197	ASP	C-O	8.37	1.34	1.24
2	C	1058	ARG	CA-C	8.37	1.62	1.52
3	D	1321	SER	C-O	8.36	1.35	1.23
2	C	1273	MET	CA-CB	-8.35	1.39	1.53
2	C	934	PHE	C-O	-8.35	1.14	1.23
2	C	757	THR	CA-C	-8.35	1.42	1.52
3	D	521	LYS	CA-CB	8.34	1.67	1.53
2	C	916	SER	C-O	-8.34	1.13	1.24
2	C	1240	ASP	N-CA	-8.33	1.35	1.46
5	M	153	TYR	CA-CB	8.33	1.67	1.53
3	D	374	LEU	N-CA	8.32	1.56	1.46
3	D	638	SER	C-O	-8.31	1.13	1.24
2	C	685	MET	C-O	-8.30	1.13	1.24
2	C	1227	VAL	N-CA	8.27	1.56	1.46
3	D	456	ALA	CA-C	-8.27	1.42	1.52
2	C	1229	TYR	CA-CB	8.27	1.63	1.53
2	C	706	ARG	C-O	8.25	1.33	1.24
3	D	841	GLY	N-CA	8.25	1.58	1.45
1	A	225	ALA	C-O	-8.25	1.14	1.24
3	D	444	GLY	N-CA	8.23	1.54	1.45
3	D	902	ASP	C-O	8.23	1.34	1.24
3	D	40	LYS	N-CA	8.22	1.56	1.45
1	A	70	THR	N-CA	8.22	1.55	1.45
2	C	669	PRO	CA-C	-8.22	1.42	1.52
3	D	92	VAL	C-O	-8.20	1.14	1.24
2	C	755	LYS	CA-CB	-8.19	1.41	1.53
2	C	653	MET	C-O	8.19	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	521	LEU	CA-C	8.18	1.63	1.52
3	D	585	LYS	C-O	8.18	1.34	1.24
2	C	1231	TYR	CA-CB	8.17	1.64	1.53
3	D	434	ILE	CA-CB	-8.17	1.44	1.54
3	D	452	LEU	C-O	8.16	1.34	1.24
3	D	484	MET	N-CA	8.16	1.56	1.46
3	D	372	MET	CA-C	-8.15	1.41	1.52
3	D	620	PHE	C-O	8.14	1.33	1.24
3	D	112	ALA	CA-CB	8.14	1.65	1.53
3	D	1330	ARG	C-O	8.13	1.33	1.24
3	D	406	ALA	C-O	-8.13	1.13	1.24
2	C	819	SER	N-CA	8.12	1.55	1.46
3	D	436	ALA	C-O	8.11	1.34	1.23
2	C	590	PRO	N-CA	8.10	1.55	1.46
2	C	1172	LEU	CA-C	-8.10	1.42	1.52
3	D	119	SER	N-CA	8.09	1.56	1.46
2	C	801	ARG	C-O	8.08	1.33	1.24
2	C	818	VAL	C-O	-8.08	1.16	1.24
3	D	360	TYR	CA-CB	-8.08	1.39	1.53
2	C	727	VAL	CA-C	-8.07	1.43	1.52
3	D	519	ASN	C-O	-8.07	1.17	1.24
1	A	211	ILE	CA-CB	8.07	1.64	1.54
3	D	900	GLY	C-O	-8.07	1.12	1.24
1	A	205	MET	C-O	-8.06	1.14	1.23
2	C	1214	ASP	C-O	-8.03	1.13	1.23
2	C	552	PRO	CA-CB	-8.02	1.40	1.53
3	D	488	ASN	C-O	8.02	1.33	1.24
2	C	458	GLU	C-O	8.01	1.33	1.24
2	C	810	TYR	CA-C	-8.01	1.41	1.52
3	D	422	LEU	CA-CB	8.00	1.69	1.53
3	D	455	ALA	CA-C	-7.99	1.43	1.52
3	D	841	GLY	C-O	7.99	1.33	1.24
3	D	549	LYS	C-O	-7.98	1.14	1.24
2	C	850	ILE	CA-C	7.98	1.62	1.52
3	D	361	LEU	C-O	-7.97	1.14	1.24
3	D	545	HIS	N-CA	-7.96	1.36	1.46
3	D	794	GLY	N-CA	-7.96	1.35	1.45
3	D	419	HIS	CA-C	7.95	1.62	1.52
2	C	701	GLY	CA-C	-7.95	1.43	1.51
3	D	501	VAL	C-N	7.95	1.43	1.33
4	E	28	ARG	CA-C	-7.92	1.42	1.52
3	D	787	ALA	C-O	7.91	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	550	VAL	CA-CB	7.91	1.63	1.53
2	C	724	VAL	C-O	-7.91	1.15	1.23
2	C	1283	ALA	N-CA	-7.90	1.35	1.46
2	C	694	ARG	C-O	7.89	1.33	1.24
3	D	366	CYS	N-CA	7.88	1.56	1.46
1	A	56	VAL	CA-CB	-7.87	1.45	1.54
2	C	690	VAL	CA-CB	7.87	1.64	1.54
2	C	1226	THR	C-O	7.86	1.33	1.24
5	M	186	ASP	N-CA	7.86	1.53	1.46
3	D	1256	ILE	CA-C	7.84	1.62	1.52
2	C	672	GLU	CA-CB	-7.84	1.41	1.53
1	A	224	LEU	CA-C	-7.84	1.42	1.52
2	C	1295	SER	C-O	-7.83	1.14	1.24
4	E	40	PRO	C-O	-7.82	1.14	1.23
3	D	423	LEU	N-CA	7.82	1.55	1.45
3	D	912	GLY	CA-C	7.82	1.62	1.51
3	D	325	LYS	CA-C	-7.81	1.42	1.52
3	D	1252	HIS	C-O	7.80	1.33	1.24
2	C	687	ARG	CA-CB	7.79	1.66	1.53
2	C	731	ARG	CA-CB	7.78	1.66	1.53
3	D	909	ILE	CA-CB	-7.77	1.45	1.54
2	C	1316	GLU	N-CA	7.77	1.57	1.46
2	C	689	ALA	CA-C	-7.76	1.42	1.53
2	C	1077	SER	N-CA	-7.76	1.36	1.46
3	D	422	LEU	N-CA	7.76	1.55	1.46
2	C	726	TYR	CA-C	-7.75	1.42	1.52
3	D	419	HIS	CA-CB	-7.72	1.41	1.53
2	C	1268	GLN	N-CA	7.72	1.56	1.46
2	C	591	TYR	CA-C	-7.72	1.43	1.52
3	D	717	VAL	C-O	-7.72	1.16	1.24
2	C	1333	LEU	C-O	-7.71	1.14	1.23
2	C	1115	THR	CA-C	-7.70	1.43	1.52
3	D	105	ILE	CA-CB	7.70	1.66	1.54
3	D	922	SER	CA-C	7.69	1.62	1.52
3	D	430	HIS	CA-C	-7.69	1.42	1.53
2	C	510	GLN	CA-C	7.68	1.62	1.52
2	C	1123	GLY	C-O	7.68	1.33	1.23
2	C	1222	GLU	N-CA	7.67	1.55	1.46
1	A	56	VAL	CA-C	7.67	1.62	1.52
3	D	720	ASN	CA-C	-7.67	1.43	1.52
3	D	482	ALA	C-O	7.66	1.34	1.24
2	C	681	MET	CA-CB	7.65	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1357	ILE	C-O	-7.64	1.14	1.24
2	C	1215	GLY	CA-C	-7.63	1.41	1.51
2	C	1278	LEU	C-O	7.63	1.33	1.24
2	C	1229	TYR	C-O	-7.61	1.15	1.24
2	C	1257	GLN	CA-C	-7.61	1.43	1.52
3	D	363	LEU	N-CA	-7.61	1.36	1.46
3	D	924	GLY	N-CA	-7.60	1.35	1.45
3	D	1315	ALA	CA-C	7.59	1.64	1.52
2	C	668	ILE	CA-CB	-7.59	1.46	1.53
3	D	354	VAL	CA-C	7.59	1.62	1.52
2	C	1267	GLY	C-N	-7.58	1.23	1.33
3	D	483	LEU	N-CA	7.57	1.55	1.46
3	D	514	THR	C-O	-7.57	1.14	1.23
2	C	502	VAL	CA-CB	7.57	1.63	1.54
2	C	1210	ILE	CA-CB	7.56	1.66	1.55
3	D	465	GLN	C-O	7.56	1.33	1.23
3	D	823	THR	C-O	-7.56	1.14	1.24
1	A	229	GLU	N-CA	-7.56	1.36	1.46
2	C	885	GLY	N-CA	7.56	1.52	1.44
2	C	822	VAL	CA-C	7.55	1.62	1.52
3	D	619	ILE	C-O	7.55	1.33	1.24
3	D	766	GLY	N-CA	7.55	1.55	1.45
2	C	1259	LEU	C-O	-7.54	1.13	1.23
2	C	1049	ILE	N-CA	7.53	1.55	1.46
2	C	682	GLY	CA-C	7.53	1.60	1.52
2	C	1222	GLU	CA-C	-7.52	1.43	1.52
3	D	910	ASN	N-CA	7.52	1.54	1.45
2	C	697	LYS	C-O	7.51	1.33	1.23
2	C	827	ARG	C-O	7.51	1.33	1.23
3	D	1141	VAL	C-O	7.51	1.32	1.24
3	D	358	GLY	CA-C	7.50	1.62	1.51
1	A	65	LEU	N-CA	-7.49	1.36	1.46
2	C	1284	ALA	C-O	7.48	1.34	1.24
2	C	137	VAL	C-O	7.48	1.32	1.24
2	C	674	ASP	N-CA	-7.48	1.37	1.45
3	D	442	ILE	CA-C	-7.45	1.43	1.52
1	A	177	TYR	N-CA	7.45	1.55	1.46
2	C	1071	GLY	CA-C	7.45	1.62	1.51
2	C	1179	GLY	C-O	7.45	1.33	1.23
2	C	764	CYS	CA-CB	7.44	1.65	1.53
3	D	519	ASN	CA-C	7.44	1.59	1.52
2	C	1069	ARG	C-O	7.44	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1225	VAL	C-N	7.44	1.44	1.33
3	D	628	GLY	N-CA	7.44	1.56	1.45
2	C	10	ARG	CA-C	-7.43	1.44	1.52
3	D	1356	LEU	N-CA	7.43	1.55	1.45
2	C	1209	GLN	CA-C	7.43	1.61	1.52
2	C	875	ALA	CA-C	-7.42	1.43	1.52
2	C	1199	LEU	C-O	-7.42	1.14	1.24
3	D	588	PRO	N-CA	-7.42	1.37	1.47
2	C	1321	GLU	CA-CB	7.41	1.65	1.53
3	D	907	HIS	C-O	-7.41	1.14	1.23
1	A	50	SER	C-O	-7.41	1.14	1.23
2	C	1158	LYS	N-CA	-7.39	1.36	1.46
2	C	690	VAL	N-CA	7.38	1.55	1.46
2	C	1279	GLU	CA-C	-7.38	1.43	1.52
5	M	262	GLY	N-CA	7.38	1.56	1.45
3	D	437	PHE	CA-CB	7.37	1.67	1.53
3	D	633	ALA	CA-C	-7.35	1.43	1.52
2	C	568	ASN	C-O	-7.34	1.15	1.23
1	A	31	LEU	C-O	-7.34	1.14	1.23
2	C	1114	GLU	C-O	7.34	1.32	1.24
3	D	629	PHE	C-O	7.34	1.32	1.24
2	C	518	ASN	CA-C	-7.33	1.43	1.52
2	C	822	VAL	C-O	7.33	1.32	1.24
2	C	1283	ALA	CA-C	-7.33	1.43	1.53
3	D	883	ARG	CA-C	-7.33	1.43	1.52
3	D	1359	ALA	C-O	-7.33	1.14	1.23
1	A	47	LEU	N-CA	-7.32	1.37	1.46
2	C	808	ASN	N-CA	-7.31	1.35	1.46
2	C	451	ARG	C-O	-7.30	1.15	1.24
3	D	802	ASP	C-O	7.30	1.33	1.24
2	C	832	HIS	C-O	7.30	1.33	1.24
2	C	710	VAL	CA-CB	-7.29	1.43	1.54
2	C	522	SER	CA-C	7.29	1.63	1.52
2	C	1098	LEU	C-O	-7.29	1.14	1.23
3	D	1258	ARG	CA-C	-7.29	1.43	1.52
2	C	815	SER	N-CA	7.28	1.55	1.45
2	C	1215	GLY	N-CA	-7.26	1.34	1.45
2	C	668	ILE	C-O	-7.26	1.15	1.24
3	D	553	THR	C-O	7.26	1.32	1.23
3	D	359	PRO	N-CA	7.24	1.56	1.47
2	C	516	ASP	C-O	-7.24	1.15	1.24
3	D	96	LYS	N-CA	-7.24	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	838	CYS	N-CA	7.23	1.54	1.46
2	C	689	ALA	N-CA	7.22	1.55	1.45
1	B	198	LEU	CA-CB	-7.21	1.44	1.53
2	C	526	HIS	CA-CB	-7.21	1.41	1.53
2	C	928	VAL	CA-C	-7.21	1.44	1.52
3	D	349	TYR	C-O	7.20	1.33	1.24
3	D	777	HIS	N-CA	7.20	1.54	1.46
2	C	1086	PRO	CA-C	-7.19	1.43	1.52
3	D	510	LEU	CA-CB	7.19	1.64	1.53
2	C	551	HIS	C-O	7.18	1.33	1.23
2	C	1244	HIS	CA-C	7.17	1.57	1.52
3	D	494	ALA	N-CA	-7.17	1.36	1.46
3	D	1365	TYR	CA-C	7.17	1.62	1.52
2	C	589	THR	CA-CB	7.17	1.64	1.54
2	C	657	THR	C-O	7.16	1.33	1.24
2	C	157	PHE	N-CA	7.15	1.54	1.45
2	C	1172	LEU	C-O	7.14	1.32	1.24
2	C	791	LEU	C-O	7.14	1.32	1.23
2	C	1054	LEU	CA-C	7.14	1.61	1.52
2	C	1229	TYR	CA-C	7.14	1.62	1.52
3	D	632	ALA	N-CA	7.14	1.55	1.46
2	C	762	ASN	CA-CB	-7.13	1.42	1.53
2	C	1095	ASP	CA-C	-7.12	1.43	1.52
3	D	305	ALA	C-O	-7.12	1.14	1.24
1	A	80	GLU	CA-C	7.12	1.62	1.52
3	D	1363	TYR	CA-C	-7.12	1.43	1.52
2	C	558	VAL	C-O	-7.10	1.15	1.24
3	D	368	LEU	N-CA	7.09	1.58	1.45
2	C	527	LYS	CA-C	7.09	1.62	1.52
3	D	839	VAL	C-O	-7.09	1.16	1.24
2	C	531	SER	N-CA	7.08	1.54	1.46
3	D	365	GLN	CA-C	-7.07	1.43	1.53
2	C	531	SER	C-O	7.07	1.32	1.24
2	C	587	LEU	N-CA	7.07	1.54	1.46
3	D	491	LEU	CA-C	7.07	1.61	1.52
3	D	376	LEU	C-O	7.06	1.32	1.24
3	D	623	GLN	N-CA	-7.06	1.37	1.46
3	D	363	LEU	C-O	7.05	1.32	1.24
3	D	1331	VAL	C-O	7.05	1.32	1.24
3	D	459	ALA	CA-C	7.05	1.60	1.52
3	D	725	MET	CA-CB	-7.04	1.42	1.53
1	A	37	HIS	N-CA	-7.03	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1257	GLN	C-O	7.03	1.31	1.24
2	C	1070	HIS	CA-CB	-7.02	1.42	1.53
2	C	1293	VAL	C-O	-7.02	1.15	1.24
2	C	659	GLN	C-O	7.01	1.32	1.24
2	C	68	LEU	C-O	-7.01	1.15	1.23
3	D	764	ARG	C-O	7.01	1.32	1.24
2	C	666	SER	C-O	7.00	1.33	1.24
3	D	94	GLN	N-CA	7.00	1.55	1.46
3	D	482	ALA	N-CA	-7.00	1.37	1.46
2	C	145	ILE	N-CA	6.99	1.55	1.46
2	C	765	ILE	C-O	6.98	1.31	1.24
2	C	1334	GLY	N-CA	6.97	1.55	1.45
3	D	471	PRO	C-N	6.96	1.40	1.33
1	A	60	GLU	CA-C	-6.96	1.44	1.52
3	D	490	ILE	N-CA	-6.95	1.36	1.46
3	D	1364	ALA	N-CA	6.95	1.54	1.46
2	C	30	ILE	CA-CB	-6.95	1.44	1.54
3	D	111	THR	C-O	-6.95	1.15	1.23
3	D	739	GLN	C-O	-6.95	1.15	1.24
3	D	891	ASP	N-CA	6.95	1.55	1.46
3	D	834	PRO	CA-C	-6.94	1.43	1.52
3	D	17	PHE	N-CA	-6.94	1.36	1.45
2	C	146	VAL	CA-C	-6.93	1.43	1.52
3	D	798	ARG	C-O	-6.93	1.16	1.24
2	C	787	PRO	CA-CB	6.92	1.63	1.54
3	D	351	GLY	CA-C	-6.92	1.43	1.51
2	C	818	VAL	CA-C	-6.90	1.44	1.52
3	D	412	LEU	CA-CB	-6.90	1.42	1.53
2	C	1159	VAL	CA-C	-6.90	1.43	1.52
2	C	176	ILE	CA-C	6.89	1.60	1.52
2	C	576	SER	CA-CB	-6.89	1.42	1.53
2	C	1148	ALA	CA-C	-6.89	1.44	1.52
2	C	1230	MET	CA-C	-6.89	1.44	1.52
3	D	706	VAL	C-O	6.89	1.31	1.24
2	C	1297	ASP	C-O	6.89	1.32	1.24
3	D	794	GLY	CA-C	-6.89	1.43	1.51
3	D	518	VAL	C-O	6.88	1.33	1.24
3	D	577	ALA	CA-C	-6.88	1.44	1.52
2	C	1283	ALA	C-O	6.88	1.31	1.23
2	C	1103	VAL	N-CA	-6.88	1.38	1.46
3	D	513	MET	C-O	6.88	1.32	1.24
3	D	94	GLN	CA-CB	6.87	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	145	ILE	C-O	-6.87	1.16	1.24
3	D	534	GLU	CA-C	-6.85	1.43	1.52
1	A	63	GLY	CA-C	6.84	1.61	1.51
2	C	782	VAL	C-O	-6.84	1.17	1.24
2	C	673	HIS	CA-C	6.83	1.64	1.52
2	C	808	ASN	C-O	6.83	1.33	1.23
3	D	807	LEU	CA-C	6.83	1.61	1.52
3	D	470	VAL	CA-C	-6.83	1.47	1.53
3	D	602	SER	N-CA	6.83	1.54	1.46
3	D	783	LEU	CA-C	-6.83	1.44	1.52
3	D	543	SER	CA-CB	6.82	1.65	1.53
3	D	1180	VAL	C-O	-6.82	1.16	1.24
3	D	271	ARG	C-O	6.81	1.32	1.24
2	C	812	PHE	C-O	6.81	1.32	1.23
2	C	1188	ASP	N-CA	6.81	1.54	1.46
2	C	1218	GLY	N-CA	6.80	1.55	1.45
2	C	656	SER	N-CA	6.80	1.53	1.45
3	D	466	MET	N-CA	6.80	1.54	1.46
3	D	803	VAL	CA-C	-6.79	1.43	1.52
3	D	439	PRO	C-O	6.79	1.31	1.23
3	D	19	ALA	C-N	-6.78	1.24	1.33
3	D	895	CYS	C-O	6.78	1.32	1.23
2	C	458	GLU	N-CA	-6.77	1.38	1.46
3	D	20	ILE	CA-CB	6.77	1.63	1.54
3	D	512	TYR	C-O	-6.77	1.15	1.24
3	D	438	GLU	C-N	6.76	1.41	1.33
2	C	1086	PRO	C-O	6.76	1.31	1.23
2	C	754	THR	CA-C	-6.74	1.44	1.52
3	D	640	GLY	N-CA	6.74	1.51	1.45
2	C	566	GLY	C-O	-6.72	1.14	1.24
1	A	66	HIS	C-O	6.72	1.32	1.24
2	C	781	ASP	C-O	6.72	1.32	1.23
2	C	1094	VAL	CA-CB	-6.71	1.47	1.54
3	D	1214	PRO	CA-C	-6.71	1.44	1.52
1	A	41	ASN	N-CA	-6.71	1.38	1.46
3	D	484	MET	CA-C	6.70	1.62	1.52
3	D	615	LYS	CA-C	6.69	1.60	1.52
2	C	32	LEU	N-CA	6.69	1.54	1.46
2	C	530	ILE	C-O	6.69	1.31	1.24
2	C	537	GLY	C-O	-6.69	1.13	1.23
2	C	12	ARG	C-O	6.68	1.32	1.23
2	C	1288	GLN	CA-C	-6.68	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	90	VAL	C-O	-6.68	1.17	1.23
2	C	840	SER	N-CA	6.67	1.54	1.46
3	D	361	LEU	CA-C	-6.67	1.43	1.52
3	D	328	ALA	CA-C	-6.65	1.44	1.52
1	A	38	THR	C-O	6.65	1.31	1.24
2	C	1081	PRO	C-O	6.65	1.32	1.24
2	C	734	ILE	CA-C	-6.64	1.44	1.52
3	D	577	ALA	N-CA	-6.63	1.38	1.46
2	C	1054	LEU	C-O	6.63	1.32	1.23
3	D	364	HIS	C-O	6.63	1.32	1.24
1	A	74	VAL	CA-CB	-6.63	1.46	1.54
2	C	1298	VAL	CA-C	6.62	1.60	1.52
3	D	476	ALA	N-CA	-6.62	1.38	1.46
3	D	767	LEU	C-O	-6.62	1.15	1.24
2	C	733	VAL	N-CA	6.61	1.54	1.46
1	A	153	VAL	N-CA	-6.61	1.41	1.46
3	D	268	LEU	N-CA	-6.61	1.38	1.46
3	D	405	GLU	N-CA	-6.61	1.37	1.45
2	C	145	ILE	CA-C	6.61	1.60	1.52
2	C	691	PRO	C-O	6.60	1.30	1.23
2	C	1097	VAL	C-O	-6.58	1.17	1.24
2	C	1279	GLU	C-O	6.58	1.31	1.24
2	C	130	MET	C-O	6.58	1.32	1.24
2	C	1219	GLU	C-O	-6.58	1.16	1.23
1	B	204	GLU	CA-C	-6.57	1.44	1.52
2	C	733	VAL	C-O	-6.57	1.16	1.24
2	C	572	ILE	C-O	6.57	1.31	1.24
2	C	1226	THR	N-CA	6.56	1.54	1.46
2	C	1082	ILE	C-O	6.56	1.31	1.24
3	D	693	VAL	C-O	6.56	1.31	1.24
2	C	693	LEU	N-CA	6.56	1.54	1.46
2	C	514	PHE	N-CA	6.55	1.54	1.46
2	C	787	PRO	CA-C	6.55	1.59	1.52
2	C	1328	LYS	CA-C	-6.55	1.43	1.52
3	D	1256	ILE	C-O	6.55	1.31	1.24
3	D	633	ALA	C-O	-6.55	1.16	1.24
3	D	781	LYS	N-CA	6.55	1.54	1.46
2	C	1157	GLN	C-O	6.54	1.32	1.24
3	D	499	ILE	N-CA	6.54	1.54	1.46
3	D	924	GLY	CA-C	-6.54	1.42	1.51
3	D	352	ARG	C-O	-6.52	1.15	1.23
3	D	19	ALA	CA-C	6.52	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	859	PRO	CA-C	-6.51	1.46	1.52
2	C	875	ALA	N-CA	6.50	1.53	1.46
1	B	18	GLN	CA-C	-6.50	1.44	1.52
2	C	1182	ILE	CA-CB	-6.50	1.46	1.54
2	C	510	GLN	N-CA	-6.50	1.38	1.46
3	D	621	ALA	C-O	6.50	1.31	1.24
3	D	598	LYS	CA-CB	-6.49	1.43	1.53
3	D	780	ARG	C-O	6.49	1.31	1.24
2	C	456	VAL	CA-CB	-6.49	1.45	1.54
2	C	567	PRO	C-O	-6.49	1.16	1.24
3	D	488	ASN	N-CA	6.48	1.54	1.46
1	A	61	ILE	C-O	6.48	1.30	1.23
2	C	932	GLN	C-O	6.47	1.31	1.23
3	D	886	VAL	CA-CB	6.46	1.63	1.54
3	D	794	GLY	C-O	6.46	1.31	1.24
2	C	1046	VAL	CA-C	-6.46	1.44	1.52
1	B	180	VAL	CA-C	-6.46	1.44	1.52
2	C	674	ASP	CA-CB	6.46	1.63	1.53
2	C	1183	ALA	N-CA	6.45	1.54	1.46
2	C	794	LEU	CA-C	-6.43	1.44	1.52
3	D	1248	ILE	CA-C	-6.43	1.44	1.52
2	C	1120	ALA	C-O	6.43	1.32	1.24
2	C	1303	LYS	C-O	6.43	1.32	1.24
1	A	168	ILE	C-O	6.42	1.31	1.24
3	D	439	PRO	N-CA	-6.42	1.39	1.46
3	D	369	PRO	C-O	6.41	1.30	1.23
1	A	173	VAL	CA-C	-6.41	1.45	1.52
2	C	801	ARG	CA-C	6.41	1.60	1.52
3	D	250	ARG	C-O	-6.41	1.16	1.24
1	A	153	VAL	C-O	-6.40	1.17	1.24
3	D	431	ARG	CA-CB	-6.40	1.42	1.53
3	D	621	ALA	CA-C	-6.40	1.44	1.52
3	D	772	TYR	CA-C	-6.40	1.44	1.52
3	D	1143	ASP	CA-C	6.40	1.61	1.52
2	C	444	ASP	C-O	-6.39	1.16	1.24
2	C	593	LYS	CA-C	-6.39	1.44	1.52
3	D	859	PRO	C-O	-6.39	1.15	1.23
1	B	187	VAL	CA-CB	6.38	1.62	1.54
2	C	519	ASN	C-N	-6.38	1.25	1.33
3	D	918	ILE	CA-CB	-6.38	1.45	1.54
2	C	49	LEU	C-O	6.38	1.32	1.24
3	D	421	VAL	N-CA	6.37	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	469	HIS	CA-C	-6.37	1.45	1.52
3	D	1333	THR	CA-C	6.37	1.61	1.52
3	D	747	MET	C-O	-6.37	1.16	1.23
2	C	703	GLY	CA-C	-6.36	1.43	1.52
2	C	1176	LEU	C-O	6.36	1.32	1.24
3	D	502	PRO	CA-CB	-6.35	1.45	1.53
3	D	455	ALA	C-O	6.35	1.31	1.24
2	C	1224	PRO	CA-C	-6.35	1.45	1.53
2	C	1258	PRO	C-O	-6.35	1.16	1.23
3	D	922	SER	C-O	-6.35	1.16	1.24
3	D	630	ALA	CA-C	-6.35	1.44	1.52
2	C	1102	GLY	N-CA	6.34	1.53	1.45
3	D	413	ASP	C-O	6.34	1.31	1.24
3	D	914	ALA	C-O	6.33	1.30	1.23
3	D	610	ARG	N-CA	6.33	1.53	1.46
2	C	488	MET	C-O	-6.32	1.18	1.24
2	C	818	VAL	N-CA	6.32	1.53	1.46
2	C	1264	GLN	C-N	6.30	1.41	1.33
3	D	78	LEU	CA-C	6.30	1.61	1.52
1	A	76	GLU	N-CA	-6.30	1.37	1.45
3	D	104	HIS	C-O	-6.29	1.16	1.23
3	D	1353	VAL	C-O	-6.29	1.15	1.24
2	C	1052	VAL	CA-C	6.29	1.60	1.52
2	C	10	ARG	C-O	6.28	1.31	1.23
3	D	371	LYS	C-O	-6.28	1.16	1.24
2	C	1101	LEU	C-N	6.27	1.41	1.33
2	C	731	ARG	C-O	6.27	1.31	1.23
3	D	461	PHE	C-O	6.27	1.32	1.23
3	D	1356	LEU	C-O	6.27	1.32	1.23
2	C	1081	PRO	CA-C	6.27	1.61	1.52
3	D	899	TYR	C-O	6.26	1.31	1.24
1	A	154	PRO	C-O	6.26	1.31	1.23
2	C	4	SER	CA-C	-6.26	1.45	1.52
3	D	1317	GLU	C-O	6.26	1.31	1.24
2	C	1251	TYR	N-CA	6.25	1.54	1.45
2	C	1326	LEU	C-O	6.25	1.31	1.24
3	D	471	PRO	C-O	6.25	1.30	1.23
2	C	506	PHE	C-O	-6.24	1.16	1.24
1	A	45	ARG	CA-C	6.24	1.61	1.52
3	D	1249	ASN	N-CA	6.22	1.53	1.45
3	D	913	GLU	CA-C	-6.22	1.44	1.53
3	D	631	TYR	C-O	6.22	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1347	LEU	C-O	6.22	1.31	1.24
3	D	408	VAL	N-CA	-6.21	1.39	1.46
2	C	1312	ASN	C-O	6.21	1.31	1.24
2	C	677	ASN	C-N	-6.20	1.25	1.33
2	C	1292	THR	N-CA	-6.20	1.38	1.46
2	C	533	LEU	CA-CB	-6.19	1.44	1.53
3	D	1321	SER	C-N	-6.19	1.25	1.33
2	C	686	GLN	CA-C	6.18	1.61	1.52
2	C	95	PRO	C-O	-6.17	1.17	1.23
2	C	1289	GLU	C-O	-6.17	1.16	1.24
3	D	499	ILE	C-O	-6.17	1.16	1.24
3	D	859	PRO	N-CA	-6.17	1.40	1.46
7	T	-3	DG	P-OP2	6.17	1.60	1.48
3	D	1323	ALA	N-CA	6.17	1.53	1.46
2	C	772	SER	C-O	6.16	1.31	1.24
2	C	700	VAL	C-O	6.16	1.30	1.24
2	C	734	ILE	N-CA	-6.16	1.39	1.46
3	D	1262	ARG	CA-C	6.15	1.61	1.53
2	C	1055	ALA	C-O	-6.15	1.17	1.24
3	D	786	THR	CA-C	6.15	1.60	1.52
2	C	1240	ASP	CA-C	6.14	1.61	1.52
2	C	1255	THR	CA-CB	6.14	1.63	1.53
3	D	359	PRO	C-N	6.14	1.42	1.33
2	C	443	ASP	C-O	-6.14	1.16	1.23
2	C	1241	ASP	CA-C	-6.14	1.44	1.52
3	D	514	THR	CA-C	-6.14	1.45	1.53
3	D	840	LEU	CA-C	-6.13	1.45	1.52
2	C	1216	ARG	CA-CB	-6.12	1.44	1.53
2	C	578	TYR	C-O	6.12	1.32	1.23
2	C	840	SER	CA-C	-6.12	1.45	1.52
3	D	485	MET	C-O	6.12	1.31	1.23
2	C	573	ASN	CA-C	-6.11	1.45	1.52
2	C	1170	MET	C-O	6.11	1.31	1.24
3	D	601	ILE	CA-C	-6.11	1.43	1.52
2	C	1083	GLU	CA-C	6.11	1.61	1.52
5	M	123	TYR	CA-CB	-6.11	1.43	1.53
1	A	186	ASN	CA-C	-6.10	1.45	1.52
1	A	52	PRO	N-CA	-6.10	1.41	1.46
3	D	596	LEU	CA-CB	-6.10	1.45	1.53
3	D	17	PHE	CA-C	6.10	1.60	1.52
2	C	569	ILE	CA-CB	6.09	1.62	1.54
2	C	785	ASP	CA-C	6.09	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1097	VAL	N-CA	6.09	1.53	1.46
3	D	609	TYR	CA-C	-6.09	1.45	1.52
3	D	40	LYS	CA-C	-6.09	1.46	1.52
3	D	246	PRO	CA-CB	-6.09	1.48	1.53
3	D	380	PHE	C-O	6.09	1.31	1.24
2	C	1266	GLY	CA-C	-6.08	1.44	1.52
5	M	191	ALA	CA-CB	6.08	1.63	1.53
3	D	746	LEU	C-O	6.08	1.31	1.23
3	D	807	LEU	CA-CB	-6.08	1.43	1.53
3	D	19	ALA	C-O	-6.07	1.16	1.24
3	D	1311	LYS	N-CA	-6.07	1.38	1.46
1	B	36	GLY	C-O	6.07	1.32	1.23
1	A	96	ASP	CA-C	6.06	1.61	1.52
2	C	12	ARG	CA-C	6.06	1.60	1.52
2	C	128	PRO	CA-C	-6.06	1.44	1.52
1	A	219	ARG	CA-C	-6.06	1.45	1.52
2	C	702	THR	C-O	-6.06	1.15	1.24
2	C	881	ASP	N-CA	6.05	1.53	1.46
3	D	1362	GLY	C-N	-6.05	1.26	1.33
2	C	1081	PRO	CA-CB	-6.04	1.45	1.53
2	C	1067	ALA	C-O	6.04	1.30	1.24
2	C	549	ASP	CA-C	-6.04	1.45	1.52
2	C	1231	TYR	C-N	6.04	1.41	1.33
3	D	378	LYS	CA-C	6.03	1.60	1.52
1	A	43	LEU	N-CA	-6.03	1.39	1.46
3	D	472	LEU	N-CA	6.01	1.55	1.45
2	C	827	ARG	C-N	-6.01	1.25	1.33
3	D	20	ILE	C-O	-6.01	1.17	1.24
2	C	197	ARG	C-O	6.01	1.31	1.24
2	C	767	GLN	N-CA	6.01	1.53	1.46
1	A	88	LEU	C-O	6.00	1.31	1.24
2	C	824	GLN	C-O	-6.00	1.17	1.24
2	C	1208	GLY	C-O	-6.00	1.15	1.23
2	C	1237	HIS	CA-CB	5.99	1.60	1.52
3	D	1366	HIS	CA-C	-5.99	1.44	1.52
1	A	56	VAL	N-CA	5.99	1.54	1.46
3	D	1328	THR	CA-C	-5.99	1.44	1.52
1	A	172	LEU	N-CA	-5.98	1.38	1.45
2	C	1335	ILE	CA-C	-5.98	1.45	1.52
3	D	434	ILE	C-N	-5.96	1.25	1.33
2	C	12	ARG	CA-CB	5.96	1.63	1.53
2	C	586	PHE	C-O	5.96	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	482	ALA	CA-C	-5.96	1.44	1.52
3	D	620	PHE	CA-CB	-5.95	1.43	1.53
3	D	363	LEU	CA-C	5.94	1.60	1.52
3	D	1140	ARG	CA-C	5.94	1.60	1.52
2	C	1170	MET	N-CA	-5.94	1.38	1.46
5	M	265	ILE	N-CA	5.93	1.53	1.46
2	C	1227	VAL	C-O	-5.93	1.17	1.24
2	C	20	GLN	CA-C	-5.93	1.45	1.52
3	D	261	ALA	C-O	-5.93	1.16	1.23
3	D	1251	LYS	C-O	5.93	1.31	1.24
1	A	92	VAL	C-O	-5.93	1.16	1.23
1	A	218	ARG	C-O	5.92	1.30	1.24
3	D	106	GLU	N-CA	5.92	1.53	1.46
3	D	1328	THR	C-O	5.92	1.31	1.24
2	C	768	MET	C-O	-5.92	1.16	1.24
2	C	524	ILE	CA-C	5.91	1.59	1.52
3	D	246	PRO	C-O	-5.91	1.20	1.25
3	D	923	ILE	N-CA	-5.91	1.39	1.46
1	A	35	PHE	C-O	5.91	1.31	1.24
1	B	37	HIS	CA-CB	-5.91	1.44	1.53
3	D	1346	GLY	N-CA	5.90	1.49	1.44
3	D	478	LEU	N-CA	-5.90	1.38	1.46
5	M	152	GLY	N-CA	5.89	1.53	1.45
2	C	94	ALA	CA-CB	-5.89	1.45	1.54
2	C	21	VAL	CA-CB	-5.89	1.46	1.54
2	C	721	GLY	C-O	-5.89	1.16	1.23
3	D	90	VAL	CA-CB	-5.88	1.46	1.53
3	D	345	LYS	CA-C	5.88	1.60	1.52
2	C	156	PHE	N-CA	5.88	1.53	1.45
3	D	495	ASN	C-O	5.87	1.31	1.24
3	D	429	LEU	N-CA	-5.86	1.38	1.46
3	D	496	GLY	N-CA	5.86	1.53	1.45
2	C	935	THR	N-CA	5.86	1.53	1.45
2	C	1115	THR	CA-CB	5.86	1.62	1.53
1	A	69	SER	CA-C	-5.85	1.45	1.53
2	C	15	PHE	C-O	-5.85	1.16	1.24
1	B	191	ARG	N-CA	5.85	1.53	1.46
2	C	1261	GLY	N-CA	-5.85	1.39	1.45
2	C	1281	TYR	CA-C	-5.85	1.44	1.52
2	C	694	ARG	N-CA	5.84	1.53	1.46
2	C	1103	VAL	CA-C	5.84	1.59	1.52
2	C	93	SER	CA-CB	5.84	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	252	LEU	C-O	-5.84	1.16	1.24
3	D	1308	GLY	C-O	5.84	1.31	1.23
2	C	143	ARG	C-N	-5.84	1.26	1.33
2	C	1182	ILE	N-CA	5.84	1.53	1.46
3	D	375	GLU	C-O	5.83	1.31	1.24
2	C	547	VAL	N-CA	5.83	1.54	1.46
2	C	563	THR	CA-CB	5.83	1.62	1.54
3	D	1252	HIS	N-CA	-5.82	1.39	1.46
2	C	460	ALA	CA-CB	5.82	1.62	1.53
2	C	19	PRO	C-O	5.82	1.30	1.23
5	M	275	PRO	CA-CB	-5.82	1.45	1.53
2	C	1076	ILE	N-CA	-5.81	1.39	1.46
3	D	493	PRO	CA-CB	-5.81	1.49	1.53
1	A	184	ALA	CA-C	-5.81	1.45	1.52
3	D	536	LEU	N-CA	5.81	1.53	1.46
2	C	1232	MET	C-O	-5.81	1.16	1.23
3	D	516	ASP	C-O	-5.81	1.16	1.23
3	D	1334	GLU	C-O	5.81	1.30	1.24
4	E	26	ARG	CA-C	-5.81	1.45	1.52
3	D	776	THR	C-O	5.80	1.31	1.24
2	C	1123	GLY	N-CA	-5.80	1.38	1.45
3	D	608	CYS	CA-C	-5.80	1.45	1.52
2	C	1152	GLY	N-CA	5.80	1.51	1.45
2	C	573	ASN	N-CA	5.79	1.53	1.45
3	D	1355	ARG	CA-CB	5.79	1.63	1.53
2	C	538	LEU	N-CA	5.79	1.53	1.46
3	D	913	GLU	C-O	-5.79	1.16	1.23
2	C	1110	GLY	CA-C	-5.78	1.45	1.51
1	A	131	CYS	C-N	-5.78	1.26	1.33
3	D	1310	THR	CA-C	5.77	1.60	1.53
1	A	155	ALA	CA-C	5.77	1.60	1.52
2	C	1186	VAL	CA-CB	-5.77	1.46	1.54
2	C	1265	PHE	N-CA	5.76	1.54	1.46
3	D	110	PRO	N-CA	5.76	1.53	1.47
2	C	729	ALA	C-O	5.76	1.30	1.24
2	C	719	LYS	C-O	5.75	1.31	1.23
3	D	585	LYS	CA-C	-5.75	1.45	1.52
2	C	1256	GLN	CA-C	-5.75	1.46	1.53
2	C	878	THR	CA-C	-5.74	1.45	1.52
2	C	1160	ASP	N-CA	-5.74	1.38	1.45
2	C	1117	LEU	CA-C	-5.73	1.45	1.52
2	C	1122	LYS	C-N	-5.73	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	GLU	C-O	5.72	1.31	1.24
2	C	1210	ILE	N-CA	5.72	1.52	1.46
3	D	624	ILE	CA-C	5.72	1.60	1.52
3	D	625	MET	C-O	5.72	1.30	1.24
3	D	1326	GLN	N-CA	-5.71	1.38	1.46
3	D	355	ILE	CA-CB	5.71	1.61	1.54
2	C	25	PRO	CA-CB	-5.71	1.45	1.53
2	C	33	ASP	C-O	5.70	1.31	1.24
3	D	613	GLY	N-CA	5.70	1.54	1.45
3	D	761	ALA	CA-CB	5.70	1.63	1.53
2	C	562	GLU	CA-C	-5.69	1.45	1.52
2	C	1118	GLY	N-CA	5.69	1.52	1.45
3	D	397	ALA	C-O	5.69	1.30	1.24
2	C	793	GLU	CA-C	-5.69	1.45	1.52
3	D	513	MET	CA-C	-5.68	1.45	1.52
3	D	517	CYS	CA-C	5.68	1.59	1.52
1	A	150	ARG	N-CA	-5.67	1.39	1.46
2	C	556	GLY	CA-C	-5.67	1.43	1.51
4	E	52	ARG	CA-C	-5.67	1.45	1.52
2	C	615	VAL	CA-CB	-5.67	1.47	1.54
2	C	523	GLU	C-O	5.66	1.30	1.24
2	C	702	THR	C-N	-5.66	1.25	1.33
2	C	807	TRP	CA-C	5.66	1.59	1.53
3	D	566	LYS	C-O	5.66	1.30	1.24
2	C	1322	SER	CA-C	5.65	1.60	1.52
3	D	25	ALA	N-CA	-5.65	1.39	1.46
3	D	542	ALA	CA-C	-5.65	1.45	1.52
2	C	790	ASP	CA-C	-5.65	1.46	1.52
3	D	550	VAL	C-O	-5.64	1.18	1.24
3	D	474	LEU	CA-C	-5.64	1.45	1.52
2	C	1230	MET	CA-CB	-5.64	1.44	1.53
3	D	510	LEU	N-CA	-5.64	1.39	1.46
2	C	664	GLY	C-O	-5.63	1.17	1.23
3	D	784	ALA	CA-C	5.63	1.60	1.52
1	A	142	MET	CA-C	-5.62	1.45	1.52
3	D	1350	ASN	C-O	5.62	1.31	1.24
2	C	1244	HIS	N-CA	-5.61	1.40	1.46
2	C	827	ARG	CA-CB	-5.61	1.43	1.53
3	D	307	LEU	C-O	-5.61	1.17	1.24
2	C	735	LYS	CA-C	-5.61	1.46	1.52
3	D	353	SER	CA-CB	5.61	1.61	1.53
2	C	658	GLN	N-CA	-5.61	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1327	GLU	C-O	5.60	1.30	1.24
2	C	1278	LEU	CA-CB	-5.60	1.44	1.53
2	C	688	GLN	CA-CB	5.59	1.62	1.53
2	C	1228	GLY	N-CA	5.59	1.53	1.45
2	C	1057	LYS	N-CA	5.59	1.52	1.46
1	B	203	ILE	C-O	5.59	1.30	1.24
2	C	1321	GLU	N-CA	5.58	1.53	1.46
3	D	227	PHE	CA-CB	-5.58	1.44	1.53
2	C	871	VAL	CA-CB	-5.58	1.48	1.54
2	C	804	PHE	C-O	5.57	1.30	1.24
3	D	306	LEU	C-O	-5.57	1.16	1.24
3	D	579	LEU	N-CA	-5.57	1.38	1.46
2	C	759	SER	C-N	-5.57	1.26	1.34
1	B	28	LEU	CA-CB	-5.56	1.45	1.53
2	C	709	ALA	CA-CB	5.56	1.62	1.53
1	A	47	LEU	CA-CB	5.56	1.62	1.53
1	A	174	ASP	C-O	5.56	1.30	1.24
3	D	1229	VAL	C-O	5.56	1.30	1.24
1	A	148	ARG	CA-CB	-5.55	1.44	1.53
2	C	178	PRO	CA-CB	-5.55	1.45	1.53
2	C	1223	ARG	CA-C	-5.55	1.45	1.52
2	C	840	SER	C-O	-5.55	1.17	1.24
3	D	503	SER	C-O	-5.54	1.16	1.23
2	C	1244	HIS	CA-CB	5.54	1.61	1.53
1	A	67	GLU	CA-C	-5.54	1.45	1.52
1	B	188	GLU	CA-C	-5.54	1.46	1.52
3	D	585	LYS	N-CA	5.54	1.53	1.46
2	C	805	MET	C-N	-5.53	1.26	1.33
2	C	1221	PHE	N-CA	5.53	1.52	1.46
1	A	217	ILE	C-O	5.53	1.30	1.24
2	C	1320	PRO	N-CA	5.52	1.53	1.47
3	D	647	PRO	CA-CB	-5.52	1.46	1.53
2	C	826	ASP	CA-C	-5.52	1.45	1.52
3	D	1142	ALA	CA-CB	-5.52	1.44	1.53
3	D	792	ASN	C-O	5.52	1.30	1.24
2	C	527	LYS	C-O	-5.52	1.16	1.24
2	C	731	ARG	CA-C	-5.51	1.45	1.52
3	D	360	TYR	C-N	-5.51	1.25	1.33
3	D	896	ALA	C-O	-5.51	1.17	1.24
3	D	475	GLU	C-O	5.51	1.30	1.24
2	C	1272	GLU	C-N	5.50	1.41	1.34
2	C	47	TYR	N-CA	-5.50	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	137	VAL	CA-C	5.50	1.58	1.52
2	C	1288	GLN	CA-CB	-5.50	1.44	1.53
2	C	1320	PRO	CA-C	-5.50	1.45	1.52
2	C	816	ILE	CA-C	-5.49	1.45	1.52
2	C	884	VAL	N-CA	5.49	1.53	1.46
4	E	22	VAL	C-O	-5.49	1.18	1.24
3	D	807	LEU	C-N	-5.48	1.26	1.33
4	E	5	THR	C-O	-5.48	1.17	1.24
3	D	180	MET	C-O	-5.47	1.17	1.24
2	C	805	MET	N-CA	5.47	1.53	1.46
2	C	548	ARG	CA-C	5.47	1.59	1.52
2	C	1219	GLU	CA-C	-5.47	1.46	1.52
5	M	122	ASP	C-O	5.45	1.30	1.24
3	D	550	VAL	CA-C	5.45	1.59	1.52
4	E	50	ALA	CA-CB	-5.45	1.44	1.53
1	B	179	PRO	CA-C	-5.45	1.46	1.53
2	C	137	VAL	CA-CB	-5.45	1.47	1.54
3	D	791	ALA	N-CA	-5.45	1.40	1.46
2	C	703	GLY	C-O	5.44	1.31	1.24
3	D	766	GLY	C-O	5.44	1.31	1.23
2	C	1056	VAL	CA-CB	-5.44	1.47	1.54
2	C	620	ASN	C-O	5.44	1.30	1.23
3	D	366	CYS	CA-CB	5.44	1.62	1.53
2	C	691	PRO	CA-CB	-5.43	1.46	1.53
3	D	49	PHE	CA-C	5.43	1.60	1.53
2	C	1324	ASN	C-O	5.43	1.30	1.24
2	C	634	VAL	CA-C	-5.43	1.46	1.52
2	C	1193	ALA	C-O	5.43	1.30	1.24
3	D	251	PRO	CA-C	5.42	1.59	1.52
3	D	888	CYS	CA-C	-5.42	1.45	1.52
3	D	915	ILE	C-O	5.42	1.30	1.24
2	C	5	TYR	C-O	-5.41	1.17	1.24
2	C	1223	ARG	N-CA	5.41	1.53	1.46
3	D	424	ASN	CA-C	-5.41	1.45	1.52
2	C	457	GLY	C-O	5.41	1.31	1.23
2	C	1226	THR	C-N	5.41	1.42	1.33
2	C	839	VAL	N-CA	5.41	1.52	1.46
3	D	431	ARG	C-O	5.40	1.30	1.24
2	C	11	ILE	N-CA	5.40	1.52	1.46
3	D	598	LYS	C-O	5.40	1.30	1.24
2	C	670	PHE	C-O	-5.40	1.17	1.24
2	C	1057	LYS	C-O	5.40	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	525	THR	C-O	5.40	1.30	1.24
3	D	57	PHE	C-O	5.40	1.30	1.24
2	C	1084	ASP	N-CA	-5.39	1.39	1.46
3	D	500	ILE	N-CA	5.39	1.53	1.46
2	C	181	GLY	N-CA	5.39	1.51	1.44
2	C	516	ASP	CA-CB	5.39	1.59	1.53
1	A	30	PRO	N-CA	5.38	1.54	1.47
3	D	383	GLY	C-O	5.37	1.30	1.23
3	D	363	LEU	CA-CB	5.37	1.62	1.53
3	D	793	SER	C-O	5.37	1.30	1.24
2	C	849	GLU	C-O	-5.36	1.17	1.23
3	D	1321	SER	CA-C	5.36	1.60	1.53
2	C	452	ARG	CA-CB	5.36	1.66	1.53
2	C	1246	ARG	CA-CB	-5.36	1.43	1.53
5	M	181	ARG	CA-C	5.36	1.59	1.52
3	D	534	GLU	C-N	-5.36	1.26	1.33
3	D	1330	ARG	N-CA	-5.36	1.40	1.46
3	D	30	ILE	CA-CB	-5.35	1.47	1.54
2	C	1332	SER	CA-C	5.35	1.60	1.52
3	D	269	TYR	N-CA	-5.35	1.39	1.46
3	D	919	ALA	C-O	5.35	1.30	1.24
2	C	1078	LYS	CA-CB	5.35	1.62	1.53
2	C	731	ARG	N-CA	5.35	1.52	1.46
3	D	1355	ARG	C-O	5.35	1.30	1.23
1	A	207	THR	CA-C	-5.34	1.46	1.52
2	C	574	SER	N-CA	-5.34	1.39	1.46
2	C	835	GLU	N-CA	5.34	1.52	1.46
3	D	300	GLN	N-CA	5.33	1.52	1.46
1	B	35	PHE	CA-C	-5.33	1.45	1.52
2	C	563	THR	C-O	5.33	1.30	1.24
3	D	743	MET	CA-C	-5.33	1.46	1.53
3	D	1260	MET	CA-C	5.33	1.59	1.52
2	C	754	THR	N-CA	-5.33	1.39	1.46
2	C	1153	ALA	N-CA	5.33	1.52	1.46
1	A	180	VAL	N-CA	-5.33	1.39	1.46
2	C	673	HIS	N-CA	-5.32	1.38	1.46
2	C	674	ASP	C-O	5.32	1.30	1.23
2	C	1173	ALA	CA-CB	-5.32	1.45	1.53
3	D	111	THR	CA-C	-5.32	1.46	1.52
3	D	232	ASN	C-O	-5.32	1.17	1.23
3	D	724	MET	CA-C	-5.32	1.45	1.52
2	C	1102	GLY	CA-C	5.32	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	244	VAL	CA-CB	-5.31	1.47	1.54
3	D	780	ARG	CA-C	-5.31	1.45	1.52
3	D	1343	GLU	CA-CB	5.31	1.60	1.54
2	C	931	VAL	C-N	5.31	1.40	1.33
2	C	810	TYR	C-O	-5.30	1.17	1.24
3	D	428	THR	N-CA	-5.30	1.39	1.46
2	C	523	GLU	N-CA	5.29	1.52	1.46
1	A	156	SER	N-CA	-5.29	1.39	1.46
2	C	833	ILE	N-CA	-5.29	1.40	1.46
2	C	1167	GLU	C-O	-5.29	1.18	1.23
3	D	819	GLY	C-O	5.29	1.29	1.23
3	D	456	ALA	C-O	5.28	1.30	1.24
1	A	25	LYS	C-O	-5.28	1.17	1.23
2	C	137	VAL	N-CA	5.28	1.52	1.46
3	D	120	LEU	C-O	5.28	1.31	1.23
3	D	253	VAL	CA-CB	5.27	1.60	1.54
3	D	469	HIS	C-N	5.27	1.38	1.33
2	C	752	ASN	N-CA	-5.27	1.39	1.46
2	C	812	PHE	CA-C	-5.27	1.46	1.52
3	D	744	ARG	N-CA	5.27	1.52	1.46
2	C	783	LEU	CA-C	5.27	1.59	1.52
3	D	412	LEU	C-O	5.27	1.30	1.24
1	A	46	ILE	C-O	-5.26	1.17	1.24
3	D	546	ALA	N-CA	-5.26	1.39	1.46
2	C	813	GLU	CA-C	5.25	1.58	1.53
3	D	1329	THR	CA-CB	-5.25	1.45	1.53
3	D	431	ARG	CA-C	5.25	1.59	1.52
2	C	926	GLY	C-O	-5.24	1.18	1.24
2	C	1210	ILE	C-O	5.24	1.29	1.23
3	D	787	ALA	CA-C	5.24	1.59	1.52
1	A	47	LEU	C-O	5.24	1.30	1.24
3	D	18	ASP	N-CA	-5.24	1.39	1.45
1	A	89	ALA	N-CA	5.24	1.52	1.46
1	A	12	ARG	C-O	-5.22	1.17	1.23
2	C	673	HIS	C-O	5.22	1.31	1.24
3	D	545	HIS	CA-CB	5.22	1.60	1.53
3	D	630	ALA	CA-CB	-5.22	1.44	1.53
2	C	1326	LEU	N-CA	-5.22	1.40	1.46
3	D	296	LYS	C-O	5.22	1.30	1.24
1	A	218	ARG	N-CA	-5.21	1.40	1.46
2	C	756	TYR	CA-CB	-5.21	1.45	1.53
3	D	504	GLN	CA-CB	5.21	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	ASP	CA-C	5.21	1.59	1.52
3	D	701	LEU	CA-C	-5.21	1.45	1.52
3	D	730	ALA	N-CA	-5.21	1.39	1.46
3	D	535	ARG	CA-C	-5.20	1.46	1.52
2	C	4	SER	C-O	-5.20	1.18	1.23
2	C	1207	SER	C-O	-5.20	1.17	1.24
2	C	771	VAL	C-O	5.20	1.31	1.24
1	A	37	HIS	C-O	5.19	1.30	1.24
3	D	539	SER	CA-C	5.19	1.59	1.53
2	C	180	ARG	N-CA	5.18	1.52	1.46
2	C	852	ALA	N-CA	5.18	1.52	1.46
3	D	19	ALA	CA-CB	5.18	1.62	1.53
3	D	98	ARG	CA-C	5.18	1.59	1.52
2	C	1321	GLU	CA-C	-5.18	1.45	1.52
3	D	375	GLU	CA-C	-5.18	1.47	1.52
3	D	536	LEU	C-O	5.18	1.30	1.24
2	C	1048	LYS	N-CA	5.17	1.52	1.45
3	D	1246	VAL	C-O	5.17	1.30	1.24
2	C	1305	TYR	N-CA	5.17	1.52	1.46
2	C	1317	PRO	CA-CB	-5.17	1.46	1.53
3	D	1247	LYS	CA-CB	5.17	1.60	1.53
3	D	1266	ILE	C-O	-5.17	1.18	1.24
3	D	1310	THR	C-O	-5.17	1.17	1.23
2	C	569	ILE	C-O	-5.17	1.18	1.24
2	C	1056	VAL	N-CA	-5.17	1.40	1.46
2	C	1319	MET	C-O	5.16	1.30	1.24
3	D	542	ALA	C-O	-5.16	1.18	1.24
2	C	142	GLU	CA-CB	-5.16	1.45	1.53
2	C	464	PHE	CA-CB	-5.16	1.44	1.53
2	C	1075	VAL	CA-CB	-5.16	1.45	1.55
3	D	367	GLY	CA-C	-5.16	1.44	1.51
1	A	48	LEU	N-CA	5.15	1.52	1.46
2	C	1224	PRO	N-CA	5.15	1.52	1.47
3	D	1255	VAL	C-N	-5.15	1.27	1.33
1	A	61	ILE	CA-CB	-5.14	1.46	1.55
3	D	420	PRO	CA-CB	5.14	1.60	1.53
2	C	26	TYR	C-O	-5.13	1.17	1.24
2	C	16	GLY	N-CA	5.13	1.52	1.45
3	D	326	SER	CA-C	5.13	1.59	1.52
1	A	77	ASP	CA-C	-5.13	1.45	1.53
2	C	711	ASP	CA-CB	5.12	1.61	1.53
2	C	711	ASP	CA-C	-5.12	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	92	VAL	C-N	-5.12	1.26	1.33
3	D	881	LYS	C-O	-5.12	1.17	1.24
2	C	1092	THR	CA-C	-5.11	1.46	1.52
3	D	892	PHE	CA-C	5.11	1.59	1.52
2	C	1228	GLY	C-O	5.11	1.30	1.23
2	C	1131	MET	C-O	-5.10	1.18	1.24
3	D	1364	ALA	CA-C	5.10	1.59	1.52
2	C	699	LEU	N-CA	5.10	1.52	1.46
2	C	1069	ARG	N-CA	5.10	1.52	1.46
2	C	1077	SER	C-O	5.10	1.30	1.24
3	D	367	GLY	N-CA	5.10	1.52	1.45
2	C	128	PRO	N-CA	5.10	1.53	1.47
2	C	592	ARG	CA-CB	-5.10	1.45	1.53
3	D	486	SER	N-CA	5.10	1.52	1.46
3	D	777	HIS	CA-C	-5.10	1.46	1.52
1	B	206	GLU	CA-C	-5.10	1.46	1.52
3	D	116	PHE	CA-C	-5.09	1.46	1.52
2	C	761	GLN	CA-C	5.09	1.60	1.52
2	C	1296	ASP	N-CA	5.09	1.52	1.45
2	C	802	VAL	CA-CB	-5.09	1.47	1.55
2	C	1231	TYR	N-CA	5.08	1.52	1.46
3	D	600	ALA	CA-C	5.08	1.59	1.52
2	C	1155	VAL	C-O	5.08	1.30	1.24
1	B	50	SER	CA-C	-5.08	1.46	1.52
2	C	870	ILE	CA-C	5.08	1.59	1.52
2	C	11	ILE	CA-CB	-5.08	1.48	1.54
2	C	728	ASP	CA-C	-5.08	1.46	1.52
2	C	1068	GLY	C-O	5.08	1.30	1.23
2	C	1232	MET	N-CA	-5.08	1.40	1.45
2	C	577	VAL	CA-C	-5.07	1.46	1.52
2	C	14	ASP	C-O	-5.07	1.17	1.24
3	D	309	ASN	N-CA	5.07	1.52	1.46
3	D	506	VAL	CA-CB	-5.07	1.48	1.54
2	C	589	THR	CA-C	-5.06	1.46	1.52
3	D	626	TYR	N-CA	-5.06	1.40	1.46
3	D	701	LEU	C-O	-5.06	1.17	1.24
5	M	188	VAL	C-O	-5.06	1.18	1.24
3	D	436	ALA	N-CA	5.06	1.52	1.45
3	D	917	VAL	CA-CB	-5.06	1.47	1.54
2	C	93	SER	CA-C	-5.05	1.46	1.53
2	C	447	HIS	CA-C	5.05	1.59	1.52
3	D	13	LYS	C-O	-5.05	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1264	GLN	CA-CB	5.05	1.62	1.53
2	C	31	GLN	N-CA	5.05	1.52	1.46
2	C	520	PRO	CA-CB	5.04	1.61	1.53
2	C	35	PHE	CA-CB	-5.04	1.45	1.53
2	C	1096	ILE	CA-C	5.04	1.59	1.52
1	A	86	LYS	N-CA	5.04	1.52	1.46
1	A	213	PRO	N-CA	-5.04	1.41	1.47
2	C	541	GLU	N-CA	5.03	1.52	1.46
1	A	201	LEU	CA-C	-5.03	1.46	1.52
3	D	401	VAL	CA-C	5.02	1.59	1.52
3	D	462	ASP	C-N	5.02	1.40	1.33
2	C	1213	TYR	C-O	5.02	1.30	1.24
3	D	545	HIS	CA-C	-5.02	1.46	1.53
3	D	237	MET	N-CA	5.02	1.52	1.46
3	D	919	ALA	N-CA	-5.02	1.40	1.46
3	D	511	TYR	CA-C	-5.02	1.45	1.52
1	A	69	SER	N-CA	5.01	1.52	1.45
1	B	198	LEU	CA-C	-5.01	1.46	1.52
3	D	52	GLU	C-O	-5.01	1.17	1.23
3	D	353	SER	C-O	5.01	1.28	1.24
2	C	459	MET	CA-C	5.00	1.59	1.52
2	C	555	TYR	CA-C	-5.00	1.46	1.52
3	D	450	HIS	CA-C	5.00	1.58	1.53

All (866) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	462	ASP	N-CA-C	-18.12	86.03	113.02
3	D	765	GLU	CA-C-N	-16.15	100.29	120.64
3	D	765	GLU	C-N-CA	-16.15	100.29	120.64
5	M	186	ASP	N-CA-CB	15.84	129.11	110.42
3	D	358	GLY	CA-C-N	-14.10	102.21	119.84
3	D	358	GLY	C-N-CA	-14.10	102.21	119.84
2	C	786	GLY	CA-C-N	-14.06	105.34	120.66
2	C	786	GLY	C-N-CA	-14.06	105.34	120.66
3	D	492	SER	CA-C-O	-13.73	109.16	119.32
2	C	554	HIS	N-CA-CB	-13.32	91.26	110.57
2	C	527	LYS	N-CA-C	-12.32	97.96	113.23
3	D	353	SER	N-CA-CB	12.09	129.83	110.97
2	C	1180	MET	CB-CA-C	-12.03	92.06	109.38
2	C	1267	GLY	CA-C-N	-11.92	98.77	121.54
2	C	1267	GLY	C-N-CA	-11.92	98.77	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1270	PHE	CA-C-N	11.76	132.90	122.43
2	C	1270	PHE	C-N-CA	11.76	132.90	122.43
5	M	272	TYR	N-CA-CB	-11.52	94.63	110.29
2	C	813	GLU	CA-C-N	-11.37	104.86	122.60
2	C	813	GLU	C-N-CA	-11.37	104.86	122.60
2	C	1081	PRO	CB-CA-C	-11.12	93.21	111.56
2	C	787	PRO	N-CA-C	-11.06	93.30	111.77
2	C	1153	ALA	CA-C-O	-10.81	109.26	121.15
3	D	347	VAL	N-CA-C	10.71	124.18	108.65
3	D	346	ARG	N-CA-C	-10.67	96.44	110.53
3	D	345	LYS	CB-CA-C	10.62	127.67	109.51
3	D	543	SER	N-CA-C	-10.55	100.41	113.28
3	D	113	HIS	CB-CA-C	-10.54	93.82	112.27
2	C	577	VAL	CA-C-N	-10.51	105.20	122.54
2	C	577	VAL	C-N-CA	-10.51	105.20	122.54
2	C	1169	VAL	CB-CA-C	-10.40	98.83	111.94
3	D	1323	ALA	O-C-N	10.38	134.73	122.17
2	C	1070	HIS	N-CA-C	10.26	124.42	112.93
7	T	3	DG	C2'-C3'-O3'	-10.12	96.33	111.50
2	C	554	HIS	N-CA-C	-10.08	101.62	113.21
2	C	827	ARG	CB-CA-C	-10.06	91.60	109.62
2	C	704	MET	N-CA-C	10.04	124.63	112.38
3	D	1310	THR	N-CA-C	-9.98	97.67	112.04
3	D	373	ALA	O-C-N	-9.89	109.43	122.59
2	C	1217	THR	N-CA-C	-9.89	101.22	113.28
2	C	1159	VAL	CB-CA-C	-9.77	96.28	111.71
3	D	484	MET	N-CA-C	9.73	124.97	113.20
7	T	0	DC	C2'-C3'-O3'	-9.73	96.90	111.50
3	D	914	ALA	CA-C-O	9.68	131.05	120.89
3	D	456	ALA	N-CA-C	-9.67	100.70	111.14
2	C	1246	ARG	CB-CA-C	-9.62	91.01	109.66
3	D	345	LYS	N-CA-C	-9.58	95.09	110.32
5	M	256	LEU	N-CA-C	9.49	121.70	111.36
7	T	-1	DC	P-O5'-C5'	9.46	134.19	120.00
3	D	369	PRO	CB-CA-C	-9.44	100.03	111.46
2	C	1333	LEU	O-C-N	-9.42	110.52	122.20
2	C	1238	LEU	CA-C-N	-9.41	105.03	120.64
2	C	1238	LEU	C-N-CA	-9.41	105.03	120.64
3	D	506	VAL	N-CA-C	9.34	121.27	110.62
2	C	851	THR	N-CA-C	9.31	121.78	108.00
3	D	617	THR	N-CA-C	9.30	122.61	111.82
7	T	0	DC	N1-C1'-C2'	9.27	127.40	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	530	ILE	CA-C-O	9.19	129.55	120.27
3	D	96	LYS	N-CA-C	-9.15	101.03	113.30
3	D	300	GLN	N-CA-CB	9.14	123.56	110.12
2	C	1294	LYS	N-CA-CB	-9.06	97.43	110.57
2	C	794	LEU	CB-CA-C	-9.06	95.87	110.81
3	D	913	GLU	CA-C-O	-9.04	111.54	121.94
7	T	0	DC	C4'-C3'-O3'	-9.03	96.46	110.00
2	C	1064	ASP	N-CA-C	9.03	121.12	111.28
3	D	504	GLN	CB-CA-C	9.01	128.34	110.42
5	M	156	ILE	CB-CA-C	8.97	126.01	111.29
1	A	155	ALA	N-CA-C	8.96	122.18	111.33
3	D	1262	ARG	N-CA-CB	-8.91	98.18	110.38
3	D	583	VAL	CB-CA-C	-8.87	101.31	110.89
4	E	32	VAL	N-CA-C	-8.84	102.25	110.82
2	C	833	ILE	N-CA-CB	-8.84	99.23	111.25
3	D	928	THR	N-CA-C	-8.82	101.67	111.28
3	D	1320	ILE	N-CA-C	8.82	119.61	110.62
2	C	851	THR	CB-CA-C	-8.81	104.00	116.34
7	T	11	DG	C4'-C3'-O3'	-8.80	96.80	110.00
3	D	377	PHE	N-CA-CB	-8.78	97.74	110.56
3	D	373	ALA	N-CA-C	-8.75	92.16	110.80
2	C	1288	GLN	CB-CA-C	-8.71	93.94	110.67
2	C	765	ILE	N-CA-CB	8.68	123.62	111.82
3	D	252	LEU	N-CA-C	8.67	123.42	113.02
2	C	1232	MET	N-CA-C	8.66	123.85	110.42
3	D	344	GLY	CA-C-N	-8.63	107.30	122.07
3	D	344	GLY	C-N-CA	-8.63	107.30	122.07
2	C	819	SER	N-CA-CB	8.63	122.66	109.97
2	C	678	ARG	CB-CA-C	8.63	124.53	110.90
2	C	1268	GLN	CB-CA-C	8.62	127.57	110.42
3	D	534	GLU	N-CA-CB	8.60	123.81	109.78
2	C	811	ASN	N-CA-C	-8.60	92.97	108.02
5	M	261	PRO	N-CA-CB	8.60	112.28	103.25
3	D	622	ASP	O-C-N	8.59	131.02	122.09
2	C	555	TYR	N-CA-CB	8.58	122.44	109.91
2	C	445	ILE	CB-CA-C	-8.58	100.38	112.22
5	M	185	PHE	CA-C-N	-8.53	109.21	119.78
5	M	185	PHE	C-N-CA	-8.53	109.21	119.78
3	D	313	GLY	N-CA-C	8.52	124.31	111.18
2	C	700	VAL	CB-CA-C	-8.50	97.41	110.50
2	C	528	ARG	CB-CA-C	-8.48	96.97	111.23
2	C	700	VAL	CA-C-O	8.48	130.17	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	681	MET	N-CA-CB	8.48	122.37	110.07
3	D	380	PHE	N-CA-CB	-8.45	97.70	110.12
3	D	769	VAL	CB-CA-C	-8.39	101.05	112.04
3	D	539	SER	CA-C-N	-8.39	109.78	122.28
3	D	539	SER	C-N-CA	-8.39	109.78	122.28
5	M	186	ASP	N-CA-C	8.39	123.59	112.35
3	D	765	GLU	O-C-N	-8.38	113.38	123.19
3	D	808	VAL	N-CA-CB	-8.36	97.43	111.23
3	D	461	PHE	N-CA-CB	-8.36	98.44	111.23
2	C	1077	SER	N-CA-C	-8.32	100.89	112.45
3	D	90	VAL	N-CA-C	8.31	119.25	108.12
2	C	144	VAL	N-CA-C	8.30	120.58	109.37
1	B	179	PRO	CB-CA-C	-8.29	100.19	112.04
2	C	677	ASN	CA-C-O	8.29	129.29	119.60
3	D	885	VAL	N-CA-CB	-8.24	97.63	111.23
2	C	828	PHE	N-CA-C	8.24	128.35	110.80
2	C	1263	ALA	CA-C-O	-8.23	108.73	120.51
2	C	1182	ILE	N-CA-C	8.23	120.48	109.37
2	C	1104	PRO	CB-CA-C	-8.20	100.03	113.06
2	C	452	ARG	CA-C-O	-8.18	111.86	121.11
3	D	807	LEU	O-C-N	-8.17	113.73	122.96
2	C	515	MET	CA-C-O	-8.15	112.09	121.47
2	C	758	ARG	N-CA-C	-8.15	99.26	110.35
3	D	898	CYS	CA-C-N	-8.15	105.97	121.54
3	D	898	CYS	C-N-CA	-8.15	105.97	121.54
3	D	924	GLY	N-CA-C	8.14	124.01	114.16
3	D	1321	SER	N-CA-C	-8.12	100.06	110.53
3	D	1246	VAL	CB-CA-C	-8.10	100.62	111.15
3	D	896	ALA	N-CA-C	8.10	122.59	112.87
2	C	1182	ILE	CB-CA-C	-8.09	98.40	111.59
3	D	502	PRO	CA-C-O	-8.09	112.58	121.23
7	T	2	DG	C2'-C3'-O3'	-8.06	99.41	111.50
2	C	1107	MET	CA-C-O	8.06	131.62	122.27
2	C	669	PRO	CB-CA-C	-8.03	100.76	111.12
3	D	885	VAL	N-CA-C	-8.02	92.65	109.34
1	B	32	GLU	CA-C-O	-8.02	112.37	121.19
3	D	477	GLN	N-CA-C	8.00	121.01	111.33
2	C	764	CYS	N-CA-CB	7.97	122.40	110.29
2	C	1079	ILE	CA-C-O	-7.96	111.50	120.74
3	D	471	PRO	CA-C-O	-7.93	111.80	121.31
2	C	672	GLU	CB-CA-C	-7.92	98.45	110.88
3	D	519	ASN	CB-CA-C	-7.91	106.48	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	146	VAL	CB-CA-C	-7.89	100.40	111.21
3	D	374	LEU	N-CA-CB	7.87	123.79	110.49
2	C	144	VAL	CA-C-N	-7.87	113.02	122.93
2	C	144	VAL	C-N-CA	-7.87	113.02	122.93
2	C	857	VAL	CA-C-N	7.86	129.01	120.44
2	C	857	VAL	C-N-CA	7.86	129.01	120.44
2	C	177	ILE	CA-C-O	7.86	124.03	119.94
2	C	1271	GLY	N-CA-C	-7.86	101.81	112.57
3	D	1355	ARG	N-CA-CB	-7.84	99.29	111.05
2	C	1231	TYR	CA-C-O	-7.83	112.08	120.46
3	D	425	ARG	CA-C-O	-7.81	111.96	120.24
3	D	897	HIS	N-CA-C	-7.79	103.57	113.23
3	D	456	ALA	O-C-N	7.79	130.50	122.09
2	C	802	VAL	N-CA-C	-7.78	96.87	108.85
7	T	2	DG	C4'-C3'-O3'	7.78	121.67	110.00
5	M	186	ASP	CB-CA-C	-7.78	100.36	113.04
3	D	351	GLY	CA-C-N	-7.75	106.75	121.63
3	D	351	GLY	C-N-CA	-7.75	106.75	121.63
2	C	815	SER	N-CA-C	7.74	119.92	110.41
2	C	810	TYR	N-CA-CB	7.73	123.00	110.40
2	C	527	LYS	O-C-N	-7.73	111.87	122.46
2	C	794	LEU	CA-C-N	-7.71	111.49	123.13
2	C	794	LEU	C-N-CA	-7.71	111.49	123.13
1	A	73	GLY	N-CA-C	7.68	131.38	113.18
3	D	451	PRO	N-CA-CB	7.68	111.52	103.15
3	D	586	GLY	N-CA-C	7.67	131.37	113.18
2	C	137	VAL	CB-CA-C	-7.65	99.93	111.33
3	D	893	GLY	CA-C-N	-7.65	108.20	121.97
3	D	893	GLY	C-N-CA	-7.65	108.20	121.97
2	C	1245	ALA	N-CA-C	7.65	127.09	110.80
3	D	812	ASP	N-CA-C	7.64	119.40	111.14
3	D	77	ARG	N-CA-C	7.63	122.20	108.69
3	D	1363	TYR	O-C-N	7.60	129.90	122.07
3	D	739	GLN	CA-C-O	7.60	128.73	119.38
2	C	1097	VAL	CB-CA-C	-7.59	99.40	110.63
7	T	-1	DC	O3'-P-O5'	7.58	115.38	104.00
3	D	470	VAL	N-CA-C	7.55	115.68	107.60
3	D	58	CYS	N-CA-C	7.54	120.48	110.53
3	D	489	ASN	N-CA-C	7.52	122.43	107.62
2	C	530	ILE	N-CA-C	-7.51	96.66	107.77
3	D	348	ASP	N-CA-C	7.50	121.48	109.79
2	C	13	LYS	N-CA-C	7.49	120.72	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	586	PHE	CA-C-O	-7.49	112.70	121.16
2	C	1322	SER	CB-CA-C	7.48	123.57	110.85
3	D	365	GLN	CB-CA-C	-7.48	96.11	111.22
2	C	1081	PRO	CA-C-N	-7.47	109.82	120.42
2	C	1081	PRO	C-N-CA	-7.47	109.82	120.42
3	D	1318	SER	N-CA-C	7.46	119.90	109.15
2	C	1335	ILE	CA-C-O	-7.42	112.60	120.39
3	D	903	LEU	N-CA-C	-7.41	95.01	110.80
2	C	1096	ILE	CB-CA-C	7.41	123.44	111.29
3	D	1329	THR	N-CA-C	-7.41	103.14	111.14
3	D	360	TYR	O-C-N	-7.40	112.75	122.59
3	D	807	LEU	N-CA-C	-7.40	99.53	110.48
2	C	577	VAL	O-C-N	7.38	129.57	121.90
2	C	1244	HIS	CA-C-N	-7.37	107.47	121.54
2	C	1244	HIS	C-N-CA	-7.37	107.47	121.54
2	C	515	MET	O-C-N	7.36	131.28	122.96
2	C	1298	VAL	CA-C-N	-7.36	110.30	120.38
2	C	1298	VAL	C-N-CA	-7.36	110.30	120.38
2	C	1231	TYR	O-C-N	7.36	132.40	123.13
2	C	555	TYR	CA-C-N	-7.35	107.01	121.41
2	C	555	TYR	C-N-CA	-7.35	107.01	121.41
2	C	1094	VAL	N-CA-C	7.32	120.17	109.63
3	D	468	VAL	CB-CA-C	-7.31	99.24	110.50
1	A	182	ARG	N-CA-C	7.31	121.58	109.95
3	D	326	SER	N-CA-CB	-7.31	99.67	111.22
1	A	51	MET	CA-C-N	-7.29	112.98	120.85
1	A	51	MET	C-N-CA	-7.29	112.98	120.85
2	C	1056	VAL	CA-C-N	-7.28	112.68	122.72
2	C	1056	VAL	C-N-CA	-7.28	112.68	122.72
3	D	625	MET	CA-C-O	7.27	128.26	120.55
3	D	1356	LEU	N-CA-C	7.27	119.95	110.43
3	D	361	LEU	N-CA-C	7.26	126.26	110.80
3	D	808	VAL	CB-CA-C	-7.24	99.41	111.29
3	D	592	VAL	N-CA-C	7.24	122.02	112.98
3	D	806	ASP	N-CA-C	-7.23	104.33	113.01
2	C	10	ARG	CB-CA-C	-7.22	99.70	110.24
3	D	1321	SER	CA-C-O	7.22	130.24	121.94
2	C	1209	GLN	N-CA-CB	-7.20	99.76	110.85
4	E	4	VAL	N-CA-C	7.19	117.91	110.36
2	C	1107	MET	O-C-N	-7.19	114.23	122.86
3	D	892	PHE	CA-C-O	7.18	127.72	119.18
1	A	76	GLU	N-CA-C	7.17	119.82	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	677	ASN	CA-C-N	-7.17	110.69	120.44
2	C	677	ASN	C-N-CA	-7.17	110.69	120.44
2	C	697	LYS	CB-CA-C	-7.16	97.72	109.46
2	C	929	ILE	N-CA-C	-7.15	104.00	111.58
2	C	704	MET	CA-C-O	7.15	128.14	119.49
3	D	1214	PRO	CB-CA-C	-7.15	101.58	110.95
2	C	1328	LYS	N-CA-C	7.14	119.93	111.71
3	D	640	GLY	O-C-N	-7.12	117.86	123.27
2	C	133	ASN	N-CA-CB	-7.11	99.96	110.49
2	C	766	ASN	CB-CA-C	7.11	121.88	109.80
3	D	897	HIS	N-CA-CB	7.10	121.52	110.44
2	C	609	ILE	CB-CA-C	-7.08	102.45	112.22
2	C	1238	LEU	CA-C-O	-7.07	113.12	121.11
3	D	17	PHE	N-CA-CB	-7.05	100.22	111.43
2	C	561	ILE	N-CA-C	-7.04	104.99	111.67
3	D	1349	GLU	N-CA-C	-7.02	103.56	111.07
2	C	1323	PHE	CB-CA-C	-7.02	98.74	110.68
4	E	40	PRO	CA-C-O	-7.02	113.72	121.23
2	C	1074	GLY	CA-C-N	-7.00	114.78	122.27
2	C	1074	GLY	C-N-CA	-7.00	114.78	122.27
2	C	26	TYR	N-CA-C	7.00	121.27	112.87
2	C	801	ARG	CA-C-O	6.99	128.05	120.43
3	D	535	ARG	CA-C-O	-6.99	112.48	120.24
2	C	1221	PHE	N-CA-CB	6.98	120.30	110.04
3	D	250	ARG	CA-C-N	-6.97	113.52	120.21
3	D	250	ARG	C-N-CA	-6.97	113.52	120.21
2	C	1101	LEU	N-CA-C	6.97	121.23	112.87
2	C	1159	VAL	O-C-N	6.97	129.55	122.79
1	A	181	GLU	N-CA-CB	6.96	122.25	110.49
2	C	1086	PRO	CB-CA-C	-6.96	101.96	111.21
7	T	-3	DG	C2'-C3'-O3'	6.96	121.94	111.50
1	A	182	ARG	O-C-N	6.95	131.91	123.16
2	C	1237	HIS	CA-C-O	-6.95	113.70	120.92
3	D	368	LEU	CB-CA-C	6.95	117.67	109.47
3	D	574	VAL	CB-CA-C	-6.94	99.91	111.29
2	C	703	GLY	N-CA-C	6.92	124.42	114.67
3	D	1244	GLN	N-CA-CB	6.91	120.71	110.49
3	D	486	SER	N-CA-C	-6.90	104.83	113.18
3	D	488	ASN	CA-C-O	-6.90	113.17	120.55
2	C	1078	LYS	CA-C-N	-6.89	113.90	122.93
2	C	1078	LYS	C-N-CA	-6.89	113.90	122.93
3	D	36	GLY	CA-C-O	-6.89	116.75	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1237	HIS	N-CA-CB	-6.89	100.09	110.35
2	C	517	GLN	N-CA-C	-6.88	104.00	112.88
2	C	929	ILE	N-CA-CB	-6.87	97.69	110.40
3	D	109	SER	CA-C-N	-6.87	112.58	119.99
3	D	109	SER	C-N-CA	-6.87	112.58	119.99
2	C	1296	ASP	CB-CA-C	-6.85	98.07	109.99
1	A	181	GLU	CA-C-N	-6.85	111.84	122.87
1	A	181	GLU	C-N-CA	-6.85	111.84	122.87
3	D	36	GLY	N-CA-C	-6.85	104.59	111.85
2	C	1099	ASN	CA-C-O	-6.84	113.30	119.59
2	C	1239	VAL	CB-CA-C	-6.84	96.24	111.77
3	D	1344	LEU	N-CA-CB	-6.84	101.58	111.70
2	C	808	ASN	N-CA-CB	-6.84	101.91	112.30
3	D	485	MET	CB-CA-C	-6.83	96.98	109.54
2	C	1145	ILE	N-CA-C	-6.82	104.12	110.53
2	C	799	ASN	O-C-N	-6.82	115.26	123.10
2	C	530	ILE	N-CA-CB	-6.81	102.56	111.82
3	D	1324	SER	N-CA-C	6.81	121.44	113.20
2	C	522	SER	N-CA-C	6.81	122.60	111.37
3	D	1348	LYS	N-CA-CB	6.80	120.12	110.12
2	C	808	ASN	CA-C-O	6.80	129.24	120.81
3	D	1255	VAL	N-CA-C	6.80	117.50	110.36
3	D	113	HIS	CA-C-O	-6.79	113.47	122.44
3	D	488	ASN	N-CA-CB	6.79	120.19	110.13
2	C	1078	LYS	CA-C-O	-6.79	113.42	120.89
2	C	534	GLY	CA-C-N	6.79	128.32	119.84
2	C	534	GLY	C-N-CA	6.79	128.32	119.84
3	D	453	VAL	CA-C-O	6.78	128.02	119.48
3	D	366	CYS	N-CA-CB	6.78	121.95	110.49
2	C	1231	TYR	N-CA-C	-6.77	96.01	107.99
2	C	1097	VAL	N-CA-C	6.77	117.58	108.11
1	B	187	VAL	N-CA-CB	6.76	121.99	111.99
2	C	1115	THR	N-CA-C	-6.75	103.85	111.14
2	C	731	ARG	N-CA-CB	6.74	123.18	111.39
2	C	768	MET	CB-CA-C	6.74	120.12	110.02
3	D	1145	PHE	N-CA-C	-6.72	104.55	112.89
2	C	1054	LEU	N-CA-CB	-6.72	99.58	111.08
3	D	344	GLY	O-C-N	-6.72	113.96	122.70
2	C	693	LEU	N-CA-C	-6.70	103.22	111.40
3	D	470	VAL	CB-CA-C	-6.69	103.48	111.18
2	C	1321	GLU	CA-C-N	-6.69	110.79	120.29
2	C	1321	GLU	C-N-CA	-6.69	110.79	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	309	ASN	N-CA-C	-6.67	105.14	113.28
2	C	1277	ALA	CA-C-N	-6.67	110.83	120.29
2	C	1277	ALA	C-N-CA	-6.67	110.83	120.29
3	D	492	SER	O-C-N	6.66	127.48	121.35
2	C	653	MET	CB-CA-C	-6.64	98.60	110.03
3	D	390	LEU	N-CA-C	6.63	120.96	112.34
2	C	550	VAL	CB-CA-C	-6.63	102.45	111.33
2	C	1195	ILE	N-CA-C	-6.63	103.77	111.00
3	D	1347	LEU	CA-C-N	-6.62	111.41	120.28
3	D	1347	LEU	C-N-CA	-6.62	111.41	120.28
2	C	1216	ARG	N-CA-C	-6.62	103.88	112.68
2	C	1317	PRO	CB-CA-C	-6.62	102.41	111.21
2	C	1242	LYS	N-CA-C	6.61	121.47	112.68
3	D	427	PRO	CA-C-N	-6.60	114.00	122.77
3	D	427	PRO	C-N-CA	-6.60	114.00	122.77
3	D	808	VAL	CA-C-O	-6.58	112.56	120.78
3	D	1312	ALA	N-CA-C	-6.58	103.31	112.45
2	C	157	PHE	CA-C-O	-6.57	113.43	121.11
2	C	698	PRO	N-CA-C	-6.57	100.88	111.19
2	C	817	LEU	N-CA-C	6.57	119.94	109.24
2	C	1198	LEU	CA-C-O	6.57	127.52	120.10
2	C	1283	ALA	CA-C-O	-6.56	113.75	120.84
2	C	177	ILE	CB-CA-C	-6.56	103.53	110.16
3	D	380	PHE	CA-C-O	6.56	127.50	120.55
3	D	915	ILE	CB-CA-C	6.56	122.05	111.29
3	D	513	MET	CB-CA-C	-6.53	100.62	110.88
3	D	887	SER	CA-C-N	6.53	134.01	121.54
3	D	887	SER	C-N-CA	6.53	134.01	121.54
2	C	670	PHE	N-CA-C	6.52	124.70	110.80
2	C	681	MET	N-CA-C	-6.52	104.09	111.14
2	C	1279	GLU	O-C-N	6.52	129.03	122.12
3	D	442	ILE	O-C-N	6.52	130.66	123.09
3	D	423	LEU	CB-CA-C	-6.52	97.44	109.37
3	D	533	ALA	N-CA-C	-6.52	104.18	111.28
2	C	11	ILE	O-C-N	-6.50	116.35	123.18
2	C	702	THR	CA-C-N	-6.48	112.36	122.86
2	C	702	THR	C-N-CA	-6.48	112.36	122.86
2	C	1238	LEU	N-CA-C	6.48	120.09	109.72
3	D	452	LEU	CA-C-N	-6.48	112.19	121.52
3	D	452	LEU	C-N-CA	-6.48	112.19	121.52
2	C	668	ILE	N-CA-C	6.46	113.44	107.56
2	C	816	ILE	CB-CA-C	-6.45	100.72	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	505	ASP	CA-C-O	-6.45	112.56	119.97
3	D	889	ASP	N-CA-CB	6.45	119.62	109.82
3	D	473	THR	N-CA-C	6.43	121.16	109.32
2	C	667	LEU	CA-C-N	-6.43	118.23	122.60
2	C	667	LEU	C-N-CA	-6.43	118.23	122.60
3	D	914	ALA	N-CA-C	6.42	121.00	111.04
2	C	705	GLU	O-C-N	6.42	129.73	122.22
3	D	105	ILE	CB-CA-C	6.42	121.81	110.71
2	C	519	ASN	CB-CA-C	6.41	122.80	110.17
4	E	4	VAL	N-CA-CB	-6.41	103.39	110.51
1	A	144	ILE	N-CA-CB	-6.40	100.62	110.86
2	C	144	VAL	O-C-N	6.40	129.20	122.67
2	C	446	ASP	N-CA-C	6.40	120.19	112.38
3	D	355	ILE	CA-C-O	-6.40	113.48	120.71
3	D	375	GLU	N-CA-C	-6.40	103.54	112.12
2	C	1176	LEU	N-CA-C	6.39	120.69	113.02
2	C	1334	GLY	CA-C-N	-6.38	114.78	123.14
2	C	1334	GLY	C-N-CA	-6.38	114.78	123.14
2	C	72	SER	CB-CA-C	-6.38	108.20	115.79
2	C	555	TYR	CB-CA-C	6.37	120.77	110.96
5	M	269	GLU	CA-C-N	6.37	125.99	119.56
5	M	269	GLU	C-N-CA	6.37	125.99	119.56
3	D	253	VAL	O-C-N	6.36	128.35	121.10
2	C	1072	ASN	CA-C-O	-6.36	114.90	120.88
3	D	19	ALA	O-C-N	-6.36	114.14	122.59
2	C	97	ARG	CA-C-O	-6.35	113.84	120.70
2	C	886	LYS	CB-CA-C	6.35	121.79	110.16
2	C	758	ARG	CA-C-O	6.35	128.28	121.55
2	C	788	SER	CB-CA-C	6.35	120.91	111.89
2	C	1081	PRO	N-CA-CB	-6.34	96.59	103.25
3	D	485	MET	CA-C-N	-6.34	109.21	121.58
3	D	485	MET	C-N-CA	-6.34	109.21	121.58
3	D	1323	ALA	CA-C-O	-6.34	113.77	120.55
3	D	459	ALA	CA-C-O	6.34	127.20	120.36
3	D	637	ALA	CA-C-O	-6.33	113.23	120.58
2	C	1100	PRO	CB-CA-C	-6.33	101.69	112.26
3	D	356	THR	CA-C-N	-6.33	111.90	120.95
3	D	356	THR	C-N-CA	-6.33	111.90	120.95
4	E	40	PRO	CB-CA-C	-6.33	103.67	111.64
5	M	259	PRO	N-CA-CB	6.32	109.89	103.25
1	A	72	GLU	CB-CA-C	-6.32	98.85	109.53
2	C	514	PHE	N-CA-C	-6.29	100.97	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600	ALA	N-CA-C	-6.29	104.42	111.28
3	D	629	PHE	CA-C-O	-6.29	114.17	120.90
3	D	915	ILE	O-C-N	6.28	130.43	122.57
3	D	359	PRO	N-CA-CB	6.28	109.85	103.25
2	C	1269	ARG	N-CA-CB	6.26	119.18	109.85
3	D	438	GLU	N-CA-C	-6.25	100.56	109.62
2	C	818	VAL	N-CA-CB	6.25	121.69	111.44
3	D	488	ASN	O-C-N	6.25	129.73	122.17
3	D	1348	LYS	CB-CA-C	-6.25	100.42	110.79
3	D	729	GLY	N-CA-C	-6.24	106.53	115.64
5	M	276	ASP	N-CA-CB	6.23	121.02	110.49
2	C	144	VAL	CA-C-O	-6.22	113.91	121.13
2	C	1308	ILE	N-CA-C	-6.22	104.22	111.00
2	C	657	THR	N-CA-C	6.20	120.45	113.01
1	B	28	LEU	N-CA-CB	-6.19	100.85	110.57
2	C	1056	VAL	N-CA-CB	-6.19	101.29	111.44
1	A	182	ARG	CA-C-O	-6.18	114.18	121.16
2	C	1273	MET	N-CA-CB	-6.16	100.73	110.22
4	E	55	GLU	N-CA-C	-6.16	104.64	111.36
2	C	1061	GLN	CA-C-N	-6.16	113.60	121.91
2	C	1061	GLN	C-N-CA	-6.16	113.60	121.91
2	C	716	ALA	CA-C-N	-6.15	115.16	123.10
2	C	716	ALA	C-N-CA	-6.15	115.16	123.10
3	D	443	GLU	N-CA-CB	6.15	119.49	109.95
2	C	818	VAL	O-C-N	6.15	129.68	123.10
2	C	518	ASN	O-C-N	-6.15	116.21	123.22
3	D	467	ALA	CB-CA-C	-6.14	99.08	109.83
2	C	1210	ILE	N-CA-C	-6.14	99.64	108.42
3	D	900	GLY	N-CA-C	6.14	122.90	114.92
3	D	1280	VAL	N-CA-C	-6.14	104.52	110.72
3	D	1280	VAL	N-CA-CB	6.13	119.78	110.58
3	D	372	MET	CA-C-O	-6.13	112.92	119.97
3	D	401	VAL	N-CA-C	-6.11	104.34	111.00
2	C	529	ARG	N-CA-C	-6.11	99.40	108.99
3	D	927	GLY	N-CA-C	-6.11	107.42	114.69
1	A	51	MET	N-CA-CB	6.10	121.23	110.37
2	C	817	LEU	N-CA-CB	-6.10	100.48	110.43
3	D	702	GLN	N-CA-C	-6.10	100.96	110.17
3	D	1363	TYR	CA-C-O	-6.10	114.42	120.82
3	D	442	ILE	CA-C-O	-6.09	114.38	120.90
2	C	921	PRO	CA-C-O	-6.09	114.40	121.34
3	D	627	THR	CB-CA-C	6.08	122.35	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	632	ALA	CB-CA-C	-6.08	100.51	110.85
2	C	690	VAL	N-CA-CB	6.08	119.72	111.21
3	D	361	LEU	CA-C-N	6.08	129.75	120.82
3	D	361	LEU	C-N-CA	6.08	129.75	120.82
3	D	1328	THR	N-CA-CB	6.08	119.34	110.47
3	D	894	VAL	CB-CA-C	6.08	121.25	111.29
3	D	1317	GLU	N-CA-C	6.07	118.40	111.11
3	D	434	ILE	CB-CA-C	6.07	119.19	110.33
2	C	661	VAL	N-CA-C	6.07	117.41	109.58
3	D	112	ALA	CB-CA-C	-6.07	108.98	117.23
2	C	787	PRO	CB-CA-C	6.06	118.96	110.17
3	D	455	ALA	N-CA-C	-6.06	104.36	110.97
2	C	578	TYR	O-C-N	6.05	129.90	122.34
2	C	1115	THR	N-CA-CB	6.05	118.84	110.07
2	C	79	VAL	N-CA-C	6.04	116.78	110.62
3	D	599	LYS	O-C-N	6.04	128.38	122.09
3	D	421	VAL	N-CA-CB	-6.02	105.20	112.07
2	C	705	GLU	N-CA-C	6.02	118.63	111.71
3	D	78	LEU	CB-CA-C	6.02	122.40	110.42
3	D	1365	TYR	O-C-N	-6.02	114.57	122.39
1	A	88	LEU	CA-C-N	-6.02	113.92	122.94
1	A	88	LEU	C-N-CA	-6.02	113.92	122.94
1	B	179	PRO	CA-C-O	-6.02	116.86	121.31
2	C	1291	LEU	N-CA-C	-6.01	104.29	111.69
2	C	1192	GLU	CB-CA-C	-6.01	98.46	110.42
3	D	620	PHE	CB-CA-C	-6.01	100.64	110.85
2	C	676	ALA	CA-C-N	-6.01	110.47	121.52
2	C	676	ALA	C-N-CA	-6.01	110.47	121.52
2	C	814	ASP	N-CA-C	-6.01	105.13	112.88
2	C	1102	GLY	CA-C-O	6.00	127.23	121.05
3	D	802	ASP	N-CA-C	6.00	118.61	111.71
3	D	895	CYS	CB-CA-C	-6.00	98.88	109.62
5	M	183	GLN	N-CA-C	-5.99	105.23	112.54
2	C	752	ASN	CA-C-O	5.99	126.91	120.38
2	C	520	PRO	CA-C-N	-5.97	111.81	120.29
2	C	520	PRO	C-N-CA	-5.97	111.81	120.29
2	C	453	ILE	N-CA-C	5.96	116.89	108.36
2	C	770	CYS	N-CA-CB	5.96	118.71	110.07
2	C	1266	GLY	CA-C-N	-5.96	109.73	121.41
2	C	1266	GLY	C-N-CA	-5.96	109.73	121.41
4	E	58	LEU	N-CA-C	5.95	118.73	111.82
5	M	185	PHE	CA-C-O	-5.95	112.00	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ILE	CB-CA-C	5.95	119.85	110.81
2	C	1075	VAL	CA-C-N	-5.95	114.93	122.37
2	C	1075	VAL	C-N-CA	-5.95	114.93	122.37
3	D	115	TRP	CA-C-N	5.94	130.27	120.94
3	D	115	TRP	C-N-CA	5.94	130.27	120.94
3	D	834	PRO	CA-C-O	-5.93	114.48	122.08
2	C	1079	ILE	N-CA-C	5.93	116.34	107.51
1	A	310	ARG	CA-C-N	5.93	126.67	120.03
1	A	310	ARG	C-N-CA	5.93	126.67	120.03
2	C	801	ARG	N-CA-C	-5.92	99.58	109.24
2	C	1070	HIS	N-CA-CB	5.92	118.74	110.56
3	D	378	LYS	N-CA-C	5.92	122.90	109.81
3	D	917	VAL	CA-C-N	-5.92	111.11	120.47
3	D	917	VAL	C-N-CA	-5.92	111.11	120.47
1	A	94	GLY	CA-C-O	5.92	126.79	120.40
3	D	908	ILE	CB-CA-C	-5.91	103.33	111.49
2	C	1191	LYS	CA-C-O	-5.91	115.12	121.56
2	C	827	ARG	CA-C-N	-5.91	110.25	121.54
2	C	827	ARG	C-N-CA	-5.91	110.25	121.54
3	D	17	PHE	CB-CA-C	5.91	122.00	110.30
5	M	141	ALA	N-CA-C	-5.91	104.76	111.14
2	C	1225	VAL	CA-C-O	-5.91	114.26	120.76
3	D	897	HIS	CA-C-O	-5.91	112.36	119.27
2	C	654	ASP	N-CA-C	5.90	120.10	113.02
2	C	1281	TYR	CB-CA-C	-5.90	99.34	110.67
2	C	1071	GLY	CA-C-N	5.90	132.18	121.97
2	C	1071	GLY	C-N-CA	5.90	132.18	121.97
3	D	38	VAL	N-CA-CB	5.90	118.78	111.41
3	D	509	GLY	CA-C-N	-5.89	112.78	120.44
3	D	509	GLY	C-N-CA	-5.89	112.78	120.44
3	D	1321	SER	O-C-N	-5.89	115.40	122.65
2	C	707	ALA	N-CA-C	5.89	117.70	111.28
2	C	832	HIS	CB-CA-C	-5.88	102.11	110.34
2	C	567	PRO	N-CA-C	-5.88	107.00	114.35
2	C	1309	VAL	N-CA-C	-5.88	103.75	111.09
3	D	474	LEU	O-C-N	5.88	130.40	122.59
3	D	738	ARG	N-CA-C	-5.88	104.95	111.71
3	D	898	CYS	N-CA-C	-5.88	102.95	110.53
1	A	130	ILE	CA-C-N	-5.87	110.32	121.54
1	A	130	ILE	C-N-CA	-5.87	110.32	121.54
3	D	629	PHE	O-C-N	5.87	128.19	122.09
3	D	587	LEU	CA-C-N	5.87	125.82	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	587	LEU	C-N-CA	5.87	125.82	119.78
3	D	1352	ILE	O-C-N	-5.87	116.18	121.87
3	D	115	TRP	N-CA-C	-5.86	104.80	111.07
2	C	1225	VAL	CA-C-N	-5.86	112.81	121.24
2	C	1225	VAL	C-N-CA	-5.86	112.81	121.24
2	C	1172	LEU	N-CA-CB	5.85	118.72	110.12
3	D	914	ALA	CA-C-N	-5.84	111.45	121.97
3	D	914	ALA	C-N-CA	-5.84	111.45	121.97
2	C	762	ASN	CB-CA-C	-5.84	103.59	111.89
2	C	1321	GLU	N-CA-CB	5.84	118.82	110.06
2	C	563	THR	O-C-N	5.84	126.38	121.83
3	D	255	LEU	N-CA-C	5.84	119.41	110.36
2	C	1294	LYS	CB-CA-C	-5.83	100.39	110.72
6	N	-17	DT	C5'-C4'-O4'	5.83	118.15	109.40
3	D	806	ASP	N-CA-CB	-5.83	100.19	110.39
1	A	69	SER	CA-C-O	-5.83	115.11	121.87
2	C	453	ILE	N-CA-CB	5.83	117.98	110.99
2	C	1072	ASN	CA-C-N	-5.82	113.04	122.36
2	C	1072	ASN	C-N-CA	-5.82	113.04	122.36
3	D	506	VAL	CB-CA-C	-5.82	104.41	112.04
2	C	1226	THR	CA-C-O	-5.82	113.83	120.58
5	M	264	SER	CB-CA-C	5.81	119.91	110.96
3	D	261	ALA	CA-C-O	-5.80	114.43	121.28
1	A	146	VAL	CA-C-O	-5.80	114.32	120.53
3	D	1344	LEU	N-CA-C	5.80	119.40	111.39
1	A	182	ARG	N-CA-CB	5.80	120.13	110.85
2	C	816	ILE	N-CA-CB	5.80	120.80	111.23
2	C	1194	GLU	CA-C-O	5.79	126.51	119.38
3	D	738	ARG	CA-C-O	-5.79	113.55	120.10
2	C	721	GLY	N-CA-C	5.79	121.45	112.60
3	D	246	PRO	CA-C-N	5.79	125.16	118.85
3	D	246	PRO	C-N-CA	5.79	125.16	118.85
3	D	539	SER	O-C-N	-5.79	110.31	121.42
2	C	537	GLY	N-CA-C	5.78	118.42	110.56
2	C	1099	ASN	CA-C-N	5.78	126.17	119.47
2	C	1099	ASN	C-N-CA	5.78	126.17	119.47
3	D	438	GLU	CB-CA-C	5.78	116.42	109.31
3	D	640	GLY	N-CA-C	-5.77	101.98	110.87
2	C	700	VAL	N-CA-C	-5.77	99.87	108.46
3	D	858	VAL	N-CA-CB	5.77	119.28	111.21
3	D	476	ALA	CA-C-N	-5.76	112.49	120.38
3	D	476	ALA	C-N-CA	-5.76	112.49	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	793	SER	CA-C-N	-5.76	113.08	120.34
3	D	793	SER	C-N-CA	-5.76	113.08	120.34
1	A	230	ALA	N-CA-C	-5.76	105.52	112.54
7	T	2	DG	N9-C1'-C2'	-5.75	104.87	113.50
2	C	1265	PHE	CB-CA-C	-5.75	101.71	112.30
2	C	836	LEU	CA-C-O	-5.75	113.94	120.32
3	D	92	VAL	CA-C-O	5.73	127.95	120.78
3	D	385	LEU	CB-CA-C	-5.73	101.28	110.79
3	D	809	VAL	N-CA-C	5.73	121.25	109.34
2	C	1244	HIS	O-C-N	-5.72	115.18	121.76
3	D	741	ALA	CA-C-N	-5.72	115.21	122.19
3	D	741	ALA	C-N-CA	-5.72	115.21	122.19
5	M	111	VAL	N-CA-C	-5.72	103.75	110.21
2	C	10	ARG	CA-C-N	-5.72	116.10	123.19
2	C	10	ARG	C-N-CA	-5.72	116.10	123.19
2	C	818	VAL	CA-C-O	-5.72	114.27	120.67
2	C	1324	ASN	CA-C-N	-5.72	113.36	120.56
2	C	1324	ASN	C-N-CA	-5.72	113.36	120.56
2	C	551	HIS	N-CA-C	-5.71	102.97	110.39
3	D	767	LEU	O-C-N	-5.71	115.00	122.59
3	D	1328	THR	N-CA-C	-5.71	106.45	113.41
2	C	1129	ASN	N-CA-C	-5.70	104.97	111.07
2	C	11	ILE	N-CA-CB	-5.70	103.50	111.25
1	A	183	ILE	N-CA-C	5.69	117.02	107.18
2	C	149	LEU	CA-C-O	5.69	126.27	120.24
2	C	673	HIS	N-CA-CB	-5.68	100.43	110.42
2	C	688	GLN	N-CA-C	-5.68	105.94	112.92
2	C	1263	ALA	CB-CA-C	-5.68	99.12	110.42
5	M	190	VAL	CA-C-N	-5.68	110.70	121.54
5	M	190	VAL	C-N-CA	-5.68	110.70	121.54
3	D	810	THR	N-CA-C	5.67	120.24	111.56
3	D	547	ARG	CA-C-O	5.67	128.42	121.84
2	C	75	LEU	CA-C-N	-5.67	117.43	122.47
2	C	75	LEU	C-N-CA	-5.67	117.43	122.47
3	D	464	ASP	N-CA-C	5.66	117.60	110.24
1	A	175	ALA	CA-C-N	-5.66	112.13	122.38
1	A	175	ALA	C-N-CA	-5.66	112.13	122.38
3	D	40	LYS	N-CA-CB	5.66	121.38	111.19
3	D	768	ASN	N-CA-C	-5.66	101.64	110.42
3	D	925	GLU	O-C-N	5.66	126.03	120.71
3	D	635	SER	N-CA-C	-5.66	105.20	111.71
1	A	101	THR	CA-C-O	-5.66	114.50	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1261	LEU	N-CA-CB	5.65	118.86	110.49
2	C	729	ALA	N-CA-C	5.65	117.91	111.02
2	C	5	TYR	CA-C-O	-5.65	112.43	120.51
3	D	801	VAL	N-CA-CB	5.65	116.78	110.51
3	D	34	SER	N-CA-C	5.64	118.43	109.96
2	C	575	LEU	CB-CA-C	-5.64	100.35	109.72
2	C	1314	GLN	N-CA-CB	-5.64	101.87	111.69
3	D	1147	ALA	N-CA-C	-5.64	103.66	111.28
2	C	559	CYS	CA-C-N	-5.64	112.79	119.84
2	C	559	CYS	C-N-CA	-5.64	112.79	119.84
2	C	560	PRO	CA-C-N	-5.63	115.92	122.63
2	C	560	PRO	C-N-CA	-5.63	115.92	122.63
2	C	1295	SER	N-CA-CB	5.63	120.01	110.49
2	C	1223	ARG	CA-C-N	-5.63	114.96	120.98
2	C	1223	ARG	C-N-CA	-5.63	114.96	120.98
3	D	627	THR	N-CA-C	-5.63	105.29	111.82
3	D	456	ALA	CA-C-O	-5.63	114.91	120.70
2	C	884	VAL	CA-C-N	-5.62	115.75	122.16
2	C	884	VAL	C-N-CA	-5.62	115.75	122.16
3	D	300	GLN	CB-CA-C	-5.62	101.46	110.79
3	D	540	GLY	N-CA-C	-5.62	108.28	115.42
5	M	125	MET	CB-CA-C	5.62	120.41	110.85
2	C	928	VAL	N-CA-CB	5.62	117.41	111.00
3	D	624	ILE	N-CA-C	-5.62	104.89	110.62
2	C	651	ASP	N-CA-C	5.61	120.12	113.16
2	C	1099	ASN	CB-CA-C	-5.61	103.95	110.17
3	D	495	ASN	N-CA-C	-5.60	105.17	112.23
3	D	1310	THR	N-CA-CB	5.58	118.84	110.19
1	B	182	ARG	CA-C-O	5.58	127.29	120.60
3	D	253	VAL	N-CA-CB	5.58	119.02	111.21
2	C	801	ARG	CA-C-N	-5.57	113.31	122.67
2	C	801	ARG	C-N-CA	-5.57	113.31	122.67
2	C	1255	THR	N-CA-CB	5.57	119.90	110.49
2	C	445	ILE	N-CA-C	-5.56	105.11	110.72
2	C	932	GLN	N-CA-C	5.56	119.80	111.96
2	C	589	THR	CA-C-N	-5.55	114.61	120.66
2	C	589	THR	C-N-CA	-5.55	114.61	120.66
2	C	681	MET	CA-C-O	-5.54	115.00	120.70
3	D	349	TYR	CB-CA-C	-5.52	99.44	110.42
3	D	354	VAL	N-CA-CB	-5.52	100.69	110.95
3	D	631	TYR	CA-C-N	-5.52	112.45	120.29
3	D	631	TYR	C-N-CA	-5.52	112.45	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	198	CYS	N-CA-CB	5.52	118.23	110.12
2	C	771	VAL	O-C-N	5.51	128.22	122.54
3	D	57	PHE	CB-CA-C	5.51	121.39	110.42
3	D	1327	GLU	CA-C-N	-5.51	112.23	122.09
3	D	1327	GLU	C-N-CA	-5.51	112.23	122.09
1	A	10	LYS	CB-CA-C	5.50	116.08	109.31
2	C	1246	ARG	N-CA-C	5.50	118.55	109.85
3	D	598	LYS	N-CA-C	5.50	117.08	111.14
2	C	699	LEU	N-CA-CB	-5.50	101.44	110.40
3	D	892	PHE	N-CA-CB	-5.50	101.83	110.46
2	C	721	GLY	CA-C-O	-5.50	114.77	122.36
2	C	688	GLN	N-CA-CB	5.50	118.58	110.56
1	A	182	ARG	CB-CA-C	-5.49	99.33	109.37
2	C	525	THR	CA-C-N	-5.48	112.50	120.29
2	C	525	THR	C-N-CA	-5.48	112.50	120.29
3	D	442	ILE	CB-CA-C	-5.48	101.16	111.30
2	C	873	ILE	CA-C-N	-5.48	115.68	123.08
2	C	873	ILE	C-N-CA	-5.48	115.68	123.08
2	C	516	ASP	CA-C-N	-5.48	114.06	122.60
2	C	516	ASP	C-N-CA	-5.48	114.06	122.60
2	C	563	THR	CA-C-N	-5.47	114.08	119.99
2	C	563	THR	C-N-CA	-5.47	114.08	119.99
3	D	794	GLY	O-C-N	5.47	128.63	122.34
3	D	486	SER	CA-C-O	5.47	126.11	119.11
2	C	4	SER	CA-C-O	-5.46	113.53	120.20
3	D	908	ILE	O-C-N	5.46	129.63	122.47
2	C	1083	GLU	N-CA-C	5.45	119.03	112.38
2	C	1324	ASN	CA-C-O	5.45	126.33	120.55
2	C	1265	PHE	CA-C-N	-5.44	114.39	120.53
2	C	1265	PHE	C-N-CA	-5.44	114.39	120.53
3	D	1354	GLY	CA-C-O	5.44	125.87	119.46
3	D	92	VAL	N-CA-C	5.43	120.64	109.34
5	M	263	GLN	N-CA-C	-5.43	106.71	113.55
2	C	771	VAL	CB-CA-C	-5.42	105.38	111.45
3	D	7	PHE	CB-CA-C	5.42	119.08	110.19
3	D	1329	THR	O-C-N	5.42	127.94	122.09
3	D	427	PRO	CB-CA-C	-5.41	102.63	111.56
3	D	316	ILE	N-CA-C	5.41	120.60	109.34
1	A	181	GLU	CA-C-O	-5.40	112.78	120.51
2	C	857	VAL	O-C-N	5.40	129.03	123.20
2	C	1327	LEU	CB-CA-C	-5.40	101.83	110.79
2	C	1256	GLN	CB-CA-C	-5.39	104.64	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1301	ARG	N-CA-C	5.39	118.07	111.82
2	C	667	LEU	N-CA-CB	-5.39	102.04	110.44
3	D	304	ASP	CB-CA-C	-5.38	100.34	110.67
3	D	605	LEU	CB-CA-C	-5.38	100.68	110.63
2	C	553	THR	N-CA-C	-5.38	106.40	113.17
3	D	451	PRO	CA-C-N	-5.36	112.55	120.38
3	D	451	PRO	C-N-CA	-5.36	112.55	120.38
3	D	783	LEU	CA-C-N	-5.36	111.23	121.94
3	D	783	LEU	C-N-CA	-5.36	111.23	121.94
2	C	127	ILE	CA-C-N	-5.35	114.21	119.99
2	C	127	ILE	C-N-CA	-5.35	114.21	119.99
3	D	721	SER	CA-C-O	-5.35	115.38	121.00
2	C	682	GLY	N-CA-C	-5.35	105.93	112.77
2	C	712	SER	CB-CA-C	-5.35	100.41	110.67
2	C	1111	GLN	CA-C-N	-5.35	113.72	120.56
2	C	1111	GLN	C-N-CA	-5.35	113.72	120.56
3	D	469	HIS	O-C-N	5.35	129.47	123.27
2	C	133	ASN	N-CA-C	-5.34	106.44	113.17
2	C	1175	ASN	CB-CA-C	5.34	119.93	110.85
3	D	884	SER	CA-C-O	-5.34	115.70	121.36
3	D	1355	ARG	CB-CA-C	5.34	120.27	110.24
3	D	639	VAL	CA-C-O	5.33	126.61	120.90
3	D	1327	GLU	N-CA-CB	-5.33	102.19	110.55
2	C	531	SER	CA-C-O	5.32	126.35	120.71
2	C	1222	GLU	N-CA-C	-5.32	101.79	110.20
3	D	362	ARG	N-CA-CB	-5.32	101.42	109.92
3	D	834	PRO	CB-CA-C	-5.30	104.00	110.95
1	A	56	VAL	N-CA-C	5.30	116.85	109.80
2	C	704	MET	O-C-N	-5.30	115.50	122.39
3	D	245	LEU	N-CA-C	-5.30	102.98	110.29
3	D	926	PRO	N-CA-C	-5.29	103.24	111.13
2	C	1121	ALA	CA-C-O	-5.29	114.37	120.24
2	C	720	ARG	CA-C-N	-5.29	115.59	121.83
2	C	720	ARG	C-N-CA	-5.29	115.59	121.83
3	D	807	LEU	CA-C-O	5.29	127.55	121.47
2	C	524	ILE	N-CA-C	5.28	115.73	110.23
2	C	1243	MET	N-CA-C	5.28	122.05	110.80
3	D	499	ILE	CA-C-N	-5.28	112.46	121.97
3	D	499	ILE	C-N-CA	-5.28	112.46	121.97
5	M	277	VAL	N-CA-CB	-5.28	103.81	111.52
2	C	1297	ASP	CA-C-N	-5.28	114.44	120.88
2	C	1297	ASP	C-N-CA	-5.28	114.44	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1222	GLU	CA-C-O	-5.27	115.04	121.05
3	D	783	LEU	O-C-N	5.27	128.16	122.15
2	C	784	ALA	N-CA-C	5.27	118.17	109.85
2	C	1095	ASP	CA-C-N	-5.27	112.49	121.97
2	C	1095	ASP	C-N-CA	-5.27	112.49	121.97
1	A	55	ALA	CA-C-N	-5.26	113.07	120.75
1	A	55	ALA	C-N-CA	-5.26	113.07	120.75
2	C	920	VAL	N-CA-C	5.26	114.75	108.96
2	C	920	VAL	CB-CA-C	-5.26	105.73	110.88
3	D	1256	ILE	CA-C-O	5.25	126.74	121.17
3	D	551	ARG	N-CA-C	-5.25	101.16	109.76
2	C	1279	GLU	N-CA-C	-5.25	105.56	111.28
4	E	19	LEU	CB-CA-C	-5.24	102.08	110.79
2	C	1050	VAL	CB-CA-C	-5.24	102.43	110.50
3	D	528	THR	N-CA-C	5.24	117.61	108.76
2	C	1230	MET	O-C-N	-5.24	116.34	123.10
3	D	467	ALA	CA-C-N	-5.24	115.66	122.94
3	D	467	ALA	C-N-CA	-5.24	115.66	122.94
3	D	1144	LEU	N-CA-C	-5.24	106.04	112.90
2	C	1267	GLY	N-CA-C	5.23	125.58	113.18
2	C	520	PRO	N-CA-C	5.23	122.25	113.78
3	D	803	VAL	CB-CA-C	-5.23	105.35	111.94
3	D	1264	ALA	N-CA-C	5.23	117.57	110.35
4	E	17	PHE	CB-CA-C	-5.23	100.02	110.42
3	D	808	VAL	O-C-N	-5.22	116.05	122.57
2	C	19	PRO	CA-C-N	-5.21	114.47	122.87
2	C	19	PRO	C-N-CA	-5.21	114.47	122.87
2	C	517	GLN	CA-C-N	-5.21	114.84	122.19
2	C	517	GLN	C-N-CA	-5.21	114.84	122.19
2	C	1046	VAL	CB-CA-C	-5.21	101.48	110.65
3	D	725	MET	N-CA-C	-5.21	105.52	111.14
1	B	230	ALA	CB-CA-C	-5.20	101.83	110.68
1	B	56	VAL	N-CA-CB	-5.20	105.36	111.39
2	C	1304	MET	CB-CA-C	-5.20	102.95	110.96
3	D	430	HIS	CA-C-O	-5.20	115.31	121.60
3	D	888	CYS	CA-C-N	-5.20	113.56	120.79
3	D	888	CYS	C-N-CA	-5.20	113.56	120.79
3	D	243	PRO	CB-CA-C	-5.20	103.20	110.63
2	C	1101	LEU	CA-C-N	5.19	125.86	119.99
2	C	1101	LEU	C-N-CA	5.19	125.86	119.99
2	C	608	ALA	N-CA-C	5.19	117.68	111.71
3	D	832	LYS	N-CA-C	5.19	116.75	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1131	MET	CB-CA-C	5.19	119.10	110.90
2	C	141	THR	N-CA-C	-5.19	101.19	109.23
3	D	481	ARG	N-CA-CB	5.19	117.93	110.20
5	M	131	THR	CA-C-N	5.19	126.33	119.84
5	M	131	THR	C-N-CA	5.19	126.33	119.84
2	C	1205	PRO	CA-C-N	5.18	127.47	120.38
2	C	1205	PRO	C-N-CA	5.18	127.47	120.38
3	D	428	THR	CA-C-N	-5.18	112.87	122.60
3	D	428	THR	C-N-CA	-5.18	112.87	122.60
2	C	170	VAL	N-CA-CB	-5.17	105.38	111.90
3	D	1330	ARG	O-C-N	5.17	127.47	122.09
7	T	-1	DC	O5'-P-OP1	-5.17	93.49	109.00
3	D	619	ILE	O-C-N	5.16	128.65	121.84
3	D	621	ALA	O-C-N	5.16	127.39	122.07
3	D	123	ARG	CA-C-O	5.16	125.90	119.97
2	C	452	ARG	O-C-N	5.16	129.89	123.19
7	T	0	DC	O5'-P-OP2	-5.15	92.55	108.00
2	C	176	ILE	CB-CA-C	5.15	118.24	110.98
2	C	1129	ASN	O-C-N	5.14	127.37	122.07
3	D	899	TYR	N-CA-CB	5.14	119.19	110.49
3	D	1355	ARG	CA-C-O	-5.14	115.61	121.68
3	D	436	ALA	CA-C-N	-5.14	113.44	121.87
3	D	436	ALA	C-N-CA	-5.14	113.44	121.87
3	D	777	HIS	CA-C-N	-5.14	113.86	120.34
3	D	777	HIS	C-N-CA	-5.14	113.86	120.34
3	D	472	LEU	CB-CA-C	-5.14	107.98	114.40
3	D	63	GLY	CA-C-N	5.13	126.47	120.98
3	D	63	GLY	C-N-CA	5.13	126.47	120.98
3	D	502	PRO	CA-C-N	-5.12	113.86	123.03
3	D	502	PRO	C-N-CA	-5.12	113.86	123.03
3	D	536	LEU	N-CA-CB	5.12	117.39	109.91
2	C	1231	TYR	N-CA-CB	5.12	118.97	110.47
3	D	538	ARG	N-CA-C	-5.12	106.72	113.17
5	M	126	TRP	CA-C-O	5.12	125.89	120.10
3	D	800	LEU	N-CA-C	-5.12	105.78	111.36
2	C	552	PRO	CA-C-N	-5.12	114.10	122.54
2	C	552	PRO	C-N-CA	-5.12	114.10	122.54
2	C	143	ARG	CA-C-N	5.12	127.43	120.63
2	C	143	ARG	C-N-CA	5.12	127.43	120.63
3	D	767	LEU	N-CA-C	5.12	121.70	110.80
2	C	715	THR	O-C-N	5.11	128.74	122.96
2	C	758	ARG	N-CA-CB	-5.11	102.52	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1264	GLN	O-C-N	5.11	129.39	122.59
3	D	1260	MET	N-CA-CB	-5.11	102.43	110.46
3	D	366	CYS	O-C-N	5.11	129.39	122.59
3	D	1363	TYR	CA-C-N	-5.11	113.07	121.19
3	D	1363	TYR	C-N-CA	-5.11	113.07	121.19
3	D	111	THR	CA-C-O	-5.10	115.66	121.58
2	C	1073	LYS	O-C-N	-5.10	116.53	122.96
2	C	1227	VAL	CA-C-O	-5.10	114.92	121.40
2	C	562	GLU	N-CA-CB	5.10	118.10	109.94
3	D	8	LEU	CA-C-N	5.10	129.29	120.58
3	D	8	LEU	C-N-CA	5.10	129.29	120.58
3	D	1319	PHE	N-CA-CB	5.09	118.70	110.40
2	C	520	PRO	N-CA-CB	5.09	108.70	103.15
2	C	824	GLN	CB-CA-C	-5.09	102.34	110.79
2	C	918	LEU	N-CA-C	5.09	118.52	112.72
3	D	397	ALA	O-C-N	5.09	127.31	122.07
5	M	458	VAL	N-CA-C	-5.09	105.53	110.42
3	D	20	ILE	CB-CA-C	-5.09	102.95	111.29
1	A	35	PHE	O-C-N	5.08	129.43	122.46
3	D	504	GLN	CA-C-N	-5.08	112.59	120.31
3	D	504	GLN	C-N-CA	-5.08	112.59	120.31
1	A	86	LYS	O-C-N	5.07	127.50	122.12
2	C	1067	ALA	N-CA-CB	-5.07	101.75	110.87
2	C	590	PRO	CA-C-O	-5.06	115.90	122.13
1	B	35	PHE	O-C-N	5.06	129.45	122.46
2	C	1112	ILE	N-CA-C	5.06	115.29	110.53
3	D	824	PRO	O-C-N	-5.06	116.97	123.04
2	C	532	ALA	CB-CA-C	-5.06	100.01	109.72
3	D	375	GLU	O-C-N	5.06	127.87	121.95
7	T	3	DG	C5'-C4'-C3'	5.05	122.48	114.90
1	A	29	GLU	CA-C-N	5.05	126.15	119.84
1	A	29	GLU	C-N-CA	5.05	126.15	119.84
7	T	1	DA	C4'-C3'-O3'	5.04	117.56	110.00
3	D	345	LYS	O-C-N	-5.04	117.42	123.06
3	D	911	LYS	N-CA-CB	-5.04	102.56	109.97
2	C	1184	THR	CB-CA-C	-5.04	104.58	110.17
3	D	520	ALA	CA-C-O	5.04	127.71	120.51
1	A	231	PHE	N-CA-CB	5.03	118.08	110.28
2	C	693	LEU	CA-C-N	-5.03	115.63	122.93
2	C	693	LEU	C-N-CA	-5.03	115.63	122.93
3	D	1340	LYS	CA-C-O	-5.03	115.69	121.47
3	D	93	THR	CA-C-N	5.02	131.13	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	93	THR	C-N-CA	5.02	131.13	121.54
2	C	564	PRO	N-CA-C	-5.01	102.74	111.32
2	C	875	ALA	CB-CA-C	-5.01	101.08	109.65
3	D	497	GLU	N-CA-C	-5.01	103.64	110.36
3	D	602	SER	N-CA-C	-5.01	105.70	111.07
5	M	185	PHE	CB-CA-C	-5.01	100.44	110.42
3	D	1257	VAL	O-C-N	5.01	126.73	121.87
2	C	1159	VAL	N-CA-CB	5.01	116.66	110.05
2	C	691	PRO	CB-CA-C	-5.01	103.79	110.85
3	D	478	LEU	N-CA-CB	-5.01	102.52	110.28
2	C	7	GLU	N-CA-CB	5.00	117.47	110.12

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	CYS	Mainchain
1	A	151	GLY	Mainchain,Peptide
1	A	47	LEU	Mainchain
1	A	63	GLY	Peptide
1	A	93	GLN	Peptide
2	C	1070	HIS	Mainchain
2	C	1085	MET	Mainchain
2	C	1098	LEU	Mainchain
2	C	1102	GLY	Peptide
2	C	1185	PRO	Peptide
2	C	1210	ILE	Mainchain
2	C	1230	MET	Mainchain
2	C	1266	GLY	Mainchain,Peptide
2	C	1270	PHE	Peptide
2	C	1333	LEU	Mainchain
2	C	452	ARG	Mainchain
2	C	519	ASN	Peptide
2	C	548	ARG	Mainchain
2	C	681	MET	Mainchain
2	C	687	ARG	Mainchain
2	C	709	ALA	Mainchain
2	C	788	SER	Mainchain
2	C	815	SER	Mainchain,Peptide
2	C	821	ARG	Mainchain
2	C	840	SER	Peptide
2	C	851	THR	Peptide

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Mol	Chain	Res	Type	Group
2	C	852	ALA	Peptide
3	D	1178	THR	Peptide
3	D	1349	GLU	Mainchain
3	D	19	ALA	Peptide
3	D	345	LYS	Mainchain
3	D	352	ARG	Mainchain
3	D	358	GLY	Peptide
3	D	361	LEU	Mainchain
3	D	365	GLN	Mainchain
3	D	369	PRO	Mainchain
3	D	372	MET	Mainchain
3	D	374	LEU	Mainchain
3	D	425	ARG	Peptide
3	D	435	GLN	Mainchain
3	D	455	ALA	Mainchain
3	D	5	LEU	Peptide
3	D	503	SER	Peptide
3	D	510	LEU	Mainchain
3	D	577	ALA	Mainchain
3	D	802	ASP	Mainchain
3	D	808	VAL	Mainchain
3	D	894	VAL	Mainchain
3	D	90	VAL	Mainchain
3	D	91	GLU	Peptide
3	D	92	VAL	Peptide
4	E	15	ASN	Mainchain
5	M	185	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1526	0	684	7	0
1	B	1160	0	526	4	0
2	C	6599	0	2971	53	0
3	D	6619	0	3083	85	0
4	E	371	0	172	5	0
5	M	1570	0	692	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	946	0	518	61	0
7	T	842	0	457	60	0
All	All	19633	0	9103	287	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 (287) 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)
6:N:14:DT:H2''	6:N:15:DT:C7	1.31	1.56
5:M:378:GLU:CB	6:N:-16:DT:H73	1.64	1.26
6:N:14:DT:C2'	6:N:15:DT:C7	2.22	1.18
2:C:1262:LYS:O	2:C:1263:ALA:HB3	1.44	1.15
5:M:378:GLU:CB	6:N:-16:DT:C7	2.24	1.15
5:M:379:SER:CB	6:N:-15:DT:C6	2.29	1.15
5:M:379:SER:CB	6:N:-15:DT:C5	2.20	1.15
7:T:4:DG:C1'	7:T:5:DC:H5'	1.79	1.12
7:T:4:DG:H1'	7:T:5:DC:H5'	1.28	1.12
6:N:14:DT:H2''	6:N:15:DT:H73	1.30	1.11
7:T:-9:DA:H2''	7:T:-8:DT:H71	1.26	1.09
6:N:14:DT:H2''	6:N:15:DT:H71	1.08	1.02
7:T:4:DG:H4'	7:T:5:DC:OP1	1.57	1.01
7:T:-9:DA:C2'	7:T:-8:DT:H71	1.90	1.01
2:C:1262:LYS:O	2:C:1263:ALA:CB	2.11	0.99
6:N:8:DA:H2''	6:N:9:DT:H71	1.44	0.99
6:N:14:DT:C2'	6:N:15:DT:H73	1.90	0.98
5:M:415:ALA:HB3	5:M:419:ALA:HB2	1.44	0.96
6:N:14:DT:C2'	6:N:15:DT:H71	1.88	0.93
7:T:12:DT:OP2	7:T:12:DT:H3'	1.68	0.93
6:N:14:DT:H2''	6:N:15:DT:C5	2.05	0.92
7:T:12:DT:H3'	7:T:12:DT:P	2.09	0.92
5:M:366:VAL:HA	6:N:-17:DT:P	2.09	0.92
6:N:-10:DT:H3'	6:N:-9:DC:H5''	1.53	0.89
5:M:447:SER:HA	5:M:452:MET:H	1.38	0.89
7:T:-9:DA:H2''	7:T:-8:DT:C7	2.02	0.89
6:N:8:DA:C2'	6:N:9:DT:H71	2.03	0.88
5:M:389:TYR:HA	5:M:398:GLU:HA	1.53	0.87
3:D:311:ARG:O	3:D:312:ARG:CB	2.23	0.86
6:N:13:DG:H2''	6:N:14:DT:C5	2.13	0.83
2:C:1267:GLY:HA3	3:D:347:VAL:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:378:GLU:CB	6:N:-16:DT:H71	2.11	0.80
5:M:379:SER:CB	6:N:-15:DT:H6	1.96	0.79
6:N:8:DA:H2''	6:N:9:DT:C7	2.13	0.78
7:T:20:DT:H2''	7:T:21:DC:C5	2.18	0.78
2:C:179:TYR:H	2:C:397:LEU:HA	1.48	0.77
7:T:-1:DC:P	7:T:-1:DC:H3'	2.25	0.76
6:N:-8:DG:H3'	6:N:-7:DA:H5''	1.66	0.75
2:C:833:ILE:HA	2:C:1054:LEU:O	1.88	0.74
3:D:348:ASP:O	3:D:349:TYR:C	2.30	0.74
3:D:117:LEU:O	3:D:118:LYS:CB	2.34	0.73
7:T:13:DG:H2'	7:T:14:DC:C6	2.24	0.72
7:T:-1:DC:H3'	7:T:-1:DC:OP2	1.89	0.72
5:M:109:LEU:CB	7:T:2:DG:O6	2.38	0.72
5:M:366:VAL:CB	6:N:-17:DT:OP2	2.32	0.72
1:A:304:LYS:O	1:A:308:ALA:HB2	1.90	0.71
5:M:447:SER:HA	5:M:452:MET:N	2.05	0.71
5:M:389:TYR:CA	5:M:398:GLU:HA	2.21	0.71
7:T:-3:DG:C2'	7:T:-2:DC:H5'	2.22	0.70
6:N:8:DA:C2'	6:N:9:DT:C7	2.70	0.69
7:T:-9:DA:C2'	7:T:-8:DT:C7	2.65	0.69
2:C:1272:GLU:HA	3:D:343:LEU:CB	2.23	0.69
7:T:4:DG:OP2	7:T:4:DG:H3'	1.93	0.67
6:N:15:DT:H3	7:T:-15:DA:H61	1.42	0.67
5:M:190:VAL:O	5:M:191:ALA:HB3	1.93	0.66
5:M:457:THR:HA	5:M:460:LYS:CB	2.26	0.66
6:N:3:DC:H2''	6:N:4:DG:H5''	1.78	0.66
2:C:540:ARG:C	2:C:542:ARG:H	2.04	0.65
5:M:457:THR:N	7:T:23:DT:H71	2.12	0.65
5:M:392:SER:H	5:M:396:ILE:CB	2.10	0.65
4:E:14:GLY:O	4:E:15:ASN:C	2.36	0.64
2:C:1253:LEU:CB	5:M:113:GLN:O	2.46	0.64
3:D:529:GLY:N	3:D:530:PRO:HA	2.13	0.64
6:N:-13:DC:H2''	6:N:-12:DA:O4'	1.98	0.64
6:N:-7:DA:H2'	6:N:-6:DC:C2	2.33	0.63
7:T:11:DG:H2'	7:T:12:DT:H71	1.81	0.63
3:D:898:CYS:O	3:D:899:TYR:CB	2.46	0.63
2:C:256:GLU:HA	2:C:261:VAL:HA	1.82	0.62
5:M:366:VAL:HA	6:N:-17:DT:OP1	1.99	0.62
6:N:-8:DG:H3'	6:N:-7:DA:C5'	2.28	0.61
3:D:914:ALA:O	3:D:915:ILE:CB	2.42	0.61
7:T:1:DA:H2'	7:T:1:DA:N3	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:59:ALA:O	3:D:60:ARG:CB	2.49	0.60
6:N:-21:DG:C2	6:N:-20:DA:C2	2.90	0.60
6:N:-5:DT:H1'	6:N:-4:DA:C8	2.37	0.60
3:D:1321:SER:C	3:D:1323:ALA:H	2.10	0.60
3:D:373:ALA:C	3:D:375:GLU:H	2.08	0.60
6:N:-21:DG:H2''	6:N:-20:DA:C8	2.38	0.59
7:T:-9:DA:H2'	7:T:-8:DT:H71	1.82	0.59
6:N:-10:DT:H3'	6:N:-9:DC:C5'	2.29	0.59
5:M:213:LEU:O	5:M:217:ARG:CB	2.51	0.58
6:N:-17:DT:C6	6:N:-16:DT:H72	2.38	0.58
6:N:-7:DA:H4'	6:N:-7:DA:OP1	2.03	0.58
7:T:0:DC:OP2	7:T:0:DC:H4'	2.03	0.58
7:T:0:DC:OP2	7:T:0:DC:C4'	2.50	0.58
3:D:1262:ARG:O	3:D:1263:LYS:CB	2.49	0.58
7:T:-9:DA:H2''	7:T:-8:DT:C5	2.38	0.58
3:D:885:VAL:C	3:D:887:SER:H	2.12	0.58
3:D:19:ALA:HA	3:D:1343:GLU:H	1.69	0.57
3:D:765:GLU:O	3:D:766:GLY:C	2.42	0.57
6:N:8:DA:H2''	6:N:9:DT:C5	2.38	0.57
6:N:-10:DT:H2'	6:N:-9:DC:H4'	1.85	0.57
2:C:918:LEU:O	2:C:919:ARG:C	2.46	0.57
5:M:362:MET:O	5:M:415:ALA:HB1	2.04	0.57
6:N:-5:DT:H4'	6:N:-4:DA:OP1	2.04	0.57
6:N:-9:DC:H4'	6:N:-8:DG:OP1	2.05	0.57
2:C:1155:VAL:O	2:C:1157:GLN:N	2.38	0.57
3:D:123:ARG:O	3:D:127:LEU:CB	2.53	0.56
5:M:366:VAL:CA	6:N:-17:DT:P	2.78	0.56
2:C:1267:GLY:O	3:D:347:VAL:O	2.22	0.56
6:N:13:DG:H2''	6:N:14:DT:C6	2.39	0.56
7:T:-7:DG:H2''	7:T:-6:DC:C6	2.40	0.56
7:T:-11:DG:H2''	7:T:-10:DC:C5	2.40	0.56
1:A:130:ILE:O	1:A:131:CYS:C	2.46	0.56
3:D:546:ALA:O	3:D:547:ARG:C	2.48	0.56
2:C:64:GLY:C	2:C:66:SER:H	2.14	0.56
3:D:289:ASP:O	3:D:293:ARG:CB	2.54	0.56
1:A:53:GLY:O	1:A:148:ARG:HA	2.06	0.55
2:C:28:LEU:O	2:C:30:ILE:N	2.39	0.55
2:C:1222:GLU:O	2:C:1223:ARG:CB	2.51	0.55
3:D:56:LEU:O	3:D:57:PHE:CB	2.50	0.55
3:D:884:SER:C	3:D:885:VAL:O	2.48	0.55
7:T:-3:DG:H2'	7:T:-2:DC:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:-11:DG:H2''	7:T:-10:DC:C6	2.42	0.55
3:D:185:ILE:O	3:D:189:LEU:CB	2.54	0.55
3:D:366:CYS:O	3:D:439:PRO:HA	2.07	0.55
3:D:585:LYS:O	3:D:587:LEU:N	2.40	0.55
3:D:179:LYS:CB	3:D:184:ALA:HB2	2.38	0.54
2:C:540:ARG:O	2:C:542:ARG:N	2.33	0.54
7:T:15:DA:H2''	7:T:16:DA:C8	2.43	0.54
2:C:346:TYR:C	2:C:348:SER:H	2.16	0.54
5:M:457:THR:O	5:M:461:TYR:N	2.34	0.54
7:T:-3:DG:H4'	7:T:-2:DC:OP1	2.08	0.54
7:T:3:DG:H2'	7:T:4:DG:C8	2.43	0.54
5:M:456:ARG:CB	7:T:23:DT:H73	2.37	0.54
5:M:460:LYS:O	5:M:464:SER:N	2.41	0.54
2:C:1252:SER:O	2:C:1256:GLN:HA	2.07	0.53
6:N:15:DT:O2	7:T:-15:DA:N1	2.40	0.53
7:T:12:DT:H2''	7:T:13:DG:H5''	1.90	0.53
3:D:551:ARG:HA	3:D:569:LEU:HA	1.89	0.53
5:M:457:THR:H	7:T:23:DT:H71	1.73	0.53
3:D:92:VAL:O	3:D:94:GLN:N	2.37	0.53
6:N:8:DA:H2''	6:N:9:DT:C6	2.44	0.53
7:T:-9:DA:H2''	7:T:-8:DT:C6	2.44	0.53
7:T:3:DG:H3'	7:T:4:DG:H3'	1.91	0.53
7:T:20:DT:H2''	7:T:21:DC:H5	1.74	0.53
7:T:4:DG:O4'	7:T:5:DC:H5'	2.08	0.52
3:D:809:VAL:HA	3:D:893:GLY:O	2.09	0.52
3:D:499:ILE:O	3:D:500:ILE:CB	2.54	0.52
3:D:902:ASP:O	3:D:903:LEU:CB	2.56	0.52
2:C:1263:ALA:O	2:C:1264:GLN:CB	2.57	0.52
2:C:159:SER:C	2:C:161:LYS:H	2.18	0.52
7:T:4:DG:C2'	7:T:5:DC:H5'	2.40	0.52
7:T:-15:DA:H2'	7:T:-14:DA:C8	2.45	0.51
3:D:226:ALA:O	3:D:230:SER:CB	2.59	0.51
4:E:16:ARG:O	4:E:17:PHE:C	2.48	0.51
6:N:-14:DG:H2''	6:N:-13:DC:O4'	2.10	0.51
3:D:893:GLY:O	3:D:894:VAL:CB	2.52	0.51
3:D:902:ASP:C	3:D:903:LEU:O	2.44	0.51
3:D:92:VAL:C	3:D:94:GLN:H	2.18	0.51
2:C:500:ALA:O	2:C:504:GLU:CB	2.59	0.51
2:C:701:GLY:O	2:C:1184:THR:N	2.39	0.51
7:T:4:DG:H3'	7:T:4:DG:P	2.50	0.51
5:M:417:SER:CB	7:T:21:DC:H3'	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:523:GLU:HA	3:D:546:ALA:HB1	1.93	0.50
4:E:16:ARG:O	4:E:19:LEU:N	2.44	0.50
7:T:24:DG:H2''	7:T:25:DC:C6	2.47	0.50
3:D:1161:GLY:HA3	3:D:1203:ARG:HA	1.93	0.50
6:N:8:DA:H2'	6:N:9:DT:H71	1.88	0.50
2:C:1254:VAL:O	2:C:1255:THR:CB	2.59	0.50
6:N:13:DG:H2''	6:N:14:DT:C7	2.41	0.50
7:T:3:DG:H2''	7:T:4:DG:H5'	1.93	0.50
2:C:1267:GLY:O	2:C:1268:GLN:CB	2.52	0.50
3:D:530:PRO:CB	3:D:531:LYS:C	2.84	0.50
5:M:470:SER:N	6:N:-26:DG:H5''	2.25	0.50
5:M:366:VAL:CB	6:N:-17:DT:P	3.00	0.50
6:N:14:DT:H2'	6:N:15:DT:H73	1.83	0.49
2:C:1:MET:C	2:C:3:TYR:H	2.20	0.49
3:D:350:SER:HA	3:D:468:VAL:O	2.12	0.49
2:C:851:THR:CB	2:C:869:GLY:HA3	2.41	0.49
3:D:530:PRO:N	3:D:531:LYS:HA	2.27	0.49
3:D:1321:SER:C	3:D:1323:ALA:N	2.69	0.49
7:T:-7:DG:H2''	7:T:-6:DC:H6	1.77	0.49
5:M:398:GLU:C	5:M:400:LYS:H	2.21	0.49
1:A:103:ASN:HA	1:A:140:ILE:O	2.12	0.49
3:D:1058:SER:HA	3:D:1108:GLN:HA	1.94	0.49
5:M:447:SER:HA	5:M:452:MET:CA	2.42	0.49
6:N:13:DG:H2''	6:N:14:DT:H72	1.94	0.49
3:D:342:LEU:C	3:D:344:GLY:N	2.68	0.49
7:T:23:DT:H2''	7:T:24:DG:C8	2.47	0.49
2:C:540:ARG:C	2:C:542:ARG:N	2.71	0.48
3:D:914:ALA:C	3:D:916:GLY:H	2.21	0.48
2:C:767:GLN:HA	2:C:785:ASP:O	2.13	0.48
3:D:155:GLU:O	3:D:156:ARG:C	2.57	0.48
7:T:11:DG:C4	7:T:12:DT:H73	2.49	0.48
3:D:362:ARG:O	3:D:363:LEU:C	2.55	0.48
7:T:27:DA:H2''	7:T:28:DG:C8	2.49	0.48
3:D:1321:SER:O	3:D:1323:ALA:N	2.47	0.48
2:C:257:ALA:N	2:C:260:LYS:O	2.43	0.47
5:M:152:GLY:O	5:M:154:LEU:N	2.45	0.47
1:B:5:VAL:C	1:B:7:GLU:H	2.23	0.47
3:D:373:ALA:O	3:D:375:GLU:N	2.48	0.47
7:T:1:DA:OP2	7:T:1:DA:O3'	2.33	0.47
3:D:893:GLY:O	3:D:894:VAL:C	2.53	0.47
2:C:186:PHE:HA	2:C:195:PHE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:391:ALA:HB1	3:D:396:ALA:HB3	1.97	0.46
2:C:1167:GLU:O	2:C:1168:GLU:CB	2.61	0.46
2:C:1244:HIS:O	2:C:1245:ALA:HB3	2.15	0.46
2:C:1006:GLU:O	2:C:1010:GLN:CB	2.63	0.46
2:C:91:THR:HA	2:C:139:ASN:H	1.81	0.46
5:M:457:THR:CB	7:T:23:DT:O4	2.64	0.46
6:N:-19:DC:H2''	6:N:-18:DT:C6	2.51	0.46
1:A:192:VAL:C	1:A:194:GLN:H	2.24	0.46
2:C:187:GLU:O	2:C:194:LEU:HA	2.16	0.46
3:D:352:ARG:HA	3:D:466:MET:O	2.16	0.46
1:B:55:ALA:HB2	1:B:176:CYS:O	2.15	0.46
2:C:46:GLN:HA	2:C:51:ALA:HB2	1.98	0.46
7:T:0:DC:O4'	7:T:0:DC:P	2.73	0.46
4:E:15:ASN:O	4:E:16:ARG:C	2.57	0.46
6:N:-11:DC:H2''	6:N:-10:DT:C5'	2.46	0.46
2:C:1334:GLY:C	3:D:25:ALA:HB3	2.41	0.45
6:N:8:DA:H2'	6:N:9:DT:C7	2.44	0.45
1:B:25:LYS:HA	1:B:203:ILE:O	2.15	0.45
2:C:816:ILE:O	2:C:1076:ILE:HA	2.16	0.45
2:C:885:GLY:HA2	2:C:917:SER:CB	2.46	0.45
2:C:363:LEU:CB	2:C:381:ALA:HB1	2.47	0.45
7:T:0:DC:H2''	7:T:1:DA:H5'	1.98	0.45
2:C:1340:GLU:O	3:D:18:ASP:O	2.35	0.45
7:T:1:DA:OP2	7:T:1:DA:H3'	2.17	0.45
2:C:137:VAL:HA	2:C:141:THR:O	2.16	0.45
3:D:709:ARG:C	3:D:711:GLY:H	2.25	0.45
3:D:584:PRO:O	3:D:585:LYS:CB	2.65	0.45
5:M:415:ALA:CB	5:M:419:ALA:HB2	2.32	0.45
6:N:-23:DA:H2''	6:N:-22:DC:C6	2.51	0.45
6:N:10:DG:H2''	6:N:11:DC:C6	2.52	0.45
2:C:156:PHE:O	2:C:174:ALA:HA	2.17	0.44
4:E:10:VAL:O	4:E:13:ILE:O	2.35	0.44
7:T:4:DG:C4'	7:T:5:DC:C5'	2.95	0.44
3:D:322:ARG:C	3:D:324:LEU:H	2.25	0.44
2:C:1259:LEU:O	2:C:1266:GLY:HA2	2.18	0.44
3:D:529:GLY:N	3:D:530:PRO:CA	2.81	0.44
3:D:373:ALA:C	3:D:375:GLU:N	2.75	0.44
5:M:397:PHE:C	5:M:399:LEU:H	2.25	0.44
6:N:13:DG:C2'	6:N:14:DT:H72	2.48	0.44
3:D:133:ARG:O	3:D:137:ARG:CB	2.66	0.44
1:B:109:PRO:HA	1:B:132:HIS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1267:GLY:CA	3:D:347:VAL:O	2.59	0.44
3:D:704:GLU:O	3:D:705:THR:C	2.61	0.44
6:N:-24:DC:H2''	6:N:-23:DA:C8	2.53	0.43
5:M:447:SER:HA	5:M:452:MET:HA	2.01	0.43
5:M:397:PHE:C	5:M:399:LEU:N	2.76	0.43
3:D:342:LEU:C	3:D:344:GLY:H	2.24	0.43
3:D:322:ARG:O	3:D:324:LEU:N	2.52	0.43
3:D:545:HIS:O	3:D:546:ALA:HB3	2.17	0.43
3:D:1133:ASP:C	3:D:1135:THR:H	2.26	0.43
7:T:-1:DC:H6	7:T:-1:DC:H2'	1.63	0.43
3:D:132:LEU:O	3:D:136:GLU:CB	2.66	0.43
3:D:161:THR:O	3:D:165:TYR:N	2.46	0.43
7:T:12:DT:H1'	7:T:13:DG:C8	2.54	0.43
3:D:520:ALA:HB3	3:D:545:HIS:CB	2.48	0.43
3:D:968:ASN:HA	3:D:1118:GLY:HA3	2.01	0.42
7:T:1:DA:H3'	7:T:1:DA:P	2.58	0.42
2:C:1012:GLU:O	2:C:1016:GLU:CB	2.66	0.42
3:D:19:ALA:CB	3:D:1343:GLU:H	2.33	0.42
3:D:61:ILE:O	3:D:62:PHE:CB	2.67	0.42
3:D:323:PRO:O	3:D:324:LEU:CB	2.63	0.42
3:D:932:MET:O	3:D:1137:GLY:HA3	2.19	0.42
5:M:175:VAL:O	5:M:179:LEU:CB	2.68	0.42
6:N:-16:DT:C6	6:N:-15:DT:H72	2.54	0.42
2:C:480:SER:O	2:C:481:LEU:CB	2.68	0.42
3:D:702:GLN:O	3:D:703:THR:C	2.63	0.42
2:C:1269:ARG:HA	3:D:346:ARG:HA	2.02	0.42
3:D:77:ARG:C	3:D:79:LYS:H	2.28	0.42
5:M:438:SER:HA	6:N:-27:DT:H3'	2.01	0.42
1:A:136:GLU:O	1:A:137:ASN:CB	2.67	0.42
7:T:2:DG:H2''	7:T:3:DG:H1'	2.02	0.42
6:N:-28:DC:H2'	6:N:-27:DT:H72	2.01	0.42
5:M:436:PRO:O	5:M:469:PRO:HA	2.20	0.41
6:N:4:DG:C4	6:N:5:DC:C5	3.08	0.41
2:C:1222:GLU:O	3:D:635:SER:O	2.37	0.41
3:D:19:ALA:HB2	3:D:1343:GLU:HA	2.02	0.41
2:C:174:ALA:O	2:C:185:ASP:HA	2.20	0.41
3:D:329:ASP:C	3:D:331:ILE:H	2.28	0.41
2:C:346:TYR:C	2:C:348:SER:N	2.79	0.41
2:C:553:THR:C	2:C:555:TYR:H	2.29	0.41
3:D:1314:LEU:HA	3:D:1322:ALA:HB1	2.01	0.41
7:T:-3:DG:C4'	7:T:-2:DC:OP1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:O	1:A:180:VAL:C	2.64	0.40
3:D:253:VAL:HA	5:M:112:TYR:CB	2.51	0.40
5:M:194:ASP:C	5:M:196:ARG:H	2.29	0.40
3:D:147:ILE:O	3:D:149:GLY:N	2.54	0.40
3:D:329:ASP:C	3:D:331:ILE:N	2.79	0.40
3:D:554:GLU:N	3:D:566:LYS:O	2.54	0.40
2:C:1008:GLN:O	2:C:1012:GLU:CB	2.69	0.40
3:D:365:GLN:HA	3:D:438:GLU:O	2.21	0.40
3:D:373:ALA:O	3:D:374:LEU:CB	2.69	0.40
6:N:-4:DA:H2''	6:N:-3:DA:H8	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/329 (93%)	269 (88%)	32 (10%)	4 (1%)	10	42
1	B	233/329 (71%)	209 (90%)	22 (9%)	2 (1%)	14	51
2	C	1339/1342 (100%)	1183 (88%)	128 (10%)	28 (2%)	5	30
3	D	1335/1407 (95%)	1133 (85%)	163 (12%)	39 (3%)	3	23
4	E	73/91 (80%)	68 (93%)	3 (4%)	2 (3%)	4	26
5	M	310/497 (62%)	254 (82%)	41 (13%)	15 (5%)	2	17
All	All	3595/3995 (90%)	3116 (87%)	389 (11%)	90 (2%)	7	27

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ILE
2	C	29	SER

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Mol	Chain	Res	Type
2	C	347	ILE
2	C	541	GLU
2	C	1155	VAL
3	D	118	LYS
3	D	158	GLN
3	D	312	ARG
3	D	426	ALA
3	D	500	ILE
3	D	521	LYS
3	D	586	GLY
3	D	886	VAL
3	D	1134	ILE
4	E	15	ASN
5	M	153	TYR
5	M	259	PRO
5	M	260	ARG
5	M	261	PRO
5	M	274	ILE
5	M	275	PRO
2	C	2	VAL
2	C	228	VAL
2	C	570	GLY
2	C	728	ASP
2	C	773	LEU
2	C	919	ARG
2	C	1156	ARG
2	C	1189	GLY
2	C	1264	GLN
2	C	1268	GLN
3	D	94	GLN
3	D	349	TYR
3	D	574	VAL
3	D	915	ILE
3	D	1159	ILE
3	D	1309	ILE
5	M	169	GLU
5	M	282	VAL
1	A	98	VAL
1	A	177	TYR
1	B	168	ILE
2	C	481	LEU
2	C	509	SER

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Mol	Chain	Res	Type
2	C	852	ALA
2	C	1255	THR
3	D	360	TYR
3	D	363	LEU
3	D	585	LYS
3	D	594	GLN
3	D	767	LEU
3	D	787	ALA
3	D	1210	ILE
4	E	14	GLY
5	M	156	ILE
5	M	167	ASP
5	M	188	VAL
1	A	131	CYS
2	C	519	ASN
2	C	655	VAL
2	C	720	ARG
3	D	20	ILE
3	D	316	ILE
3	D	320	ASN
3	D	520	ALA
3	D	899	TYR
2	C	643	SER
2	C	1223	ARG
3	D	67	ASP
3	D	323	PRO
3	D	546	ALA
3	D	1180	VAL
5	M	185	PHE
2	C	892	GLU
2	C	1245	ALA
3	D	92	VAL
3	D	260	PHE
5	M	257	ASP
5	M	265	ILE
3	D	83	VAL
3	D	809	VAL
3	D	885	VAL
2	C	229	ILE
3	D	673	VAL
5	M	170	ILE
1	B	159	ILE

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Mol	Chain	Res	Type
2	C	558	VAL
2	C	1186	VAL
3	D	145	VAL
3	D	894	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

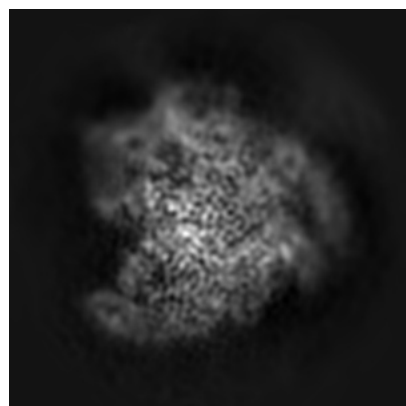
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52919. These allow visual inspection of the internal detail of the map and identification of artifacts.

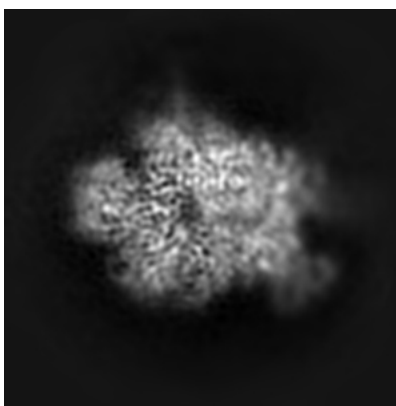
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

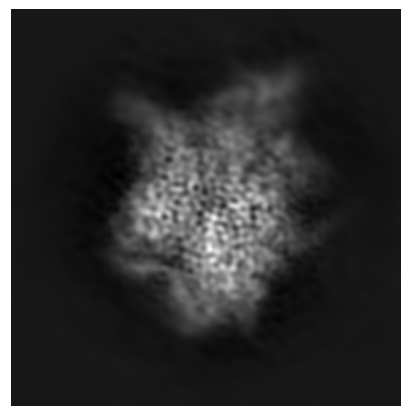
6.1.1 Primary map



X

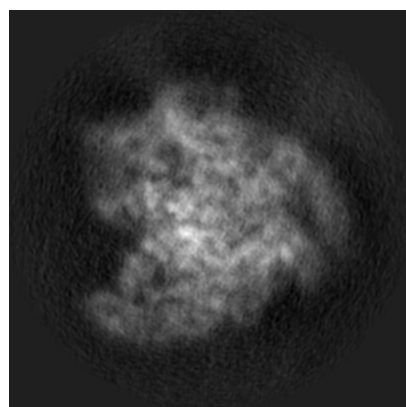


Y

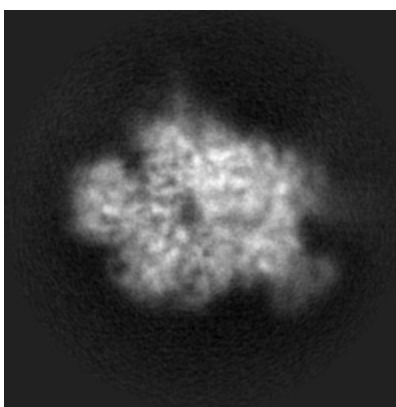


Z

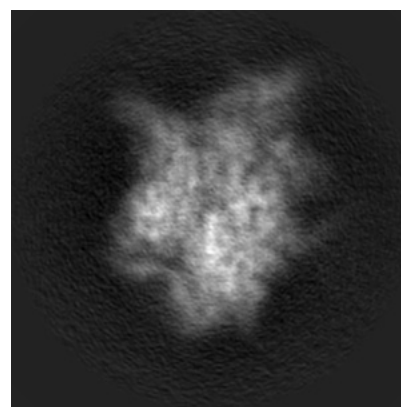
6.1.2 Raw map



X



Y

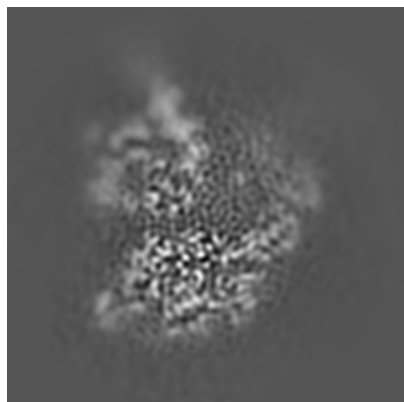


Z

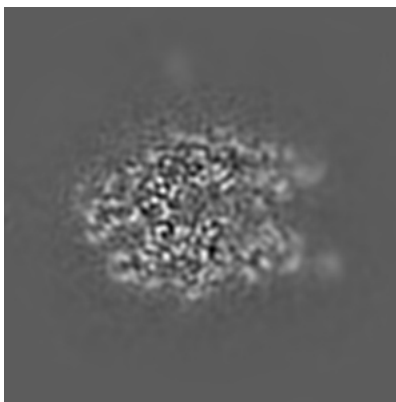
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

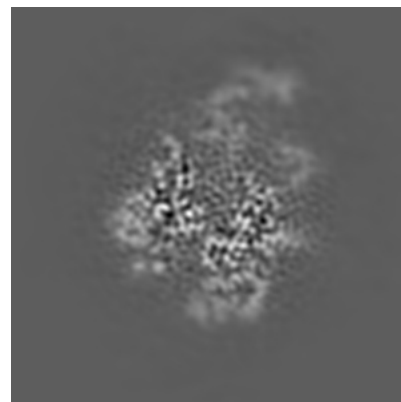
6.2.1 Primary map



X Index: 100

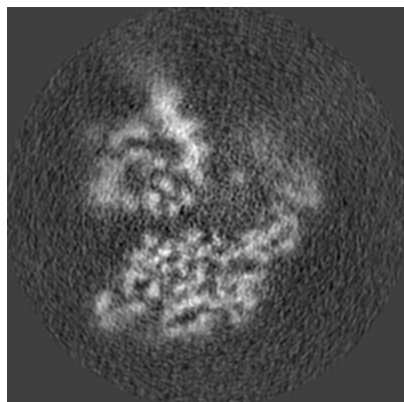


Y Index: 100

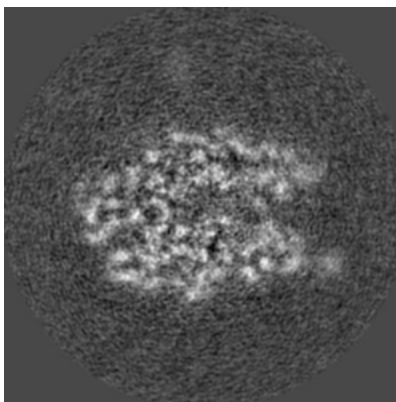


Z Index: 100

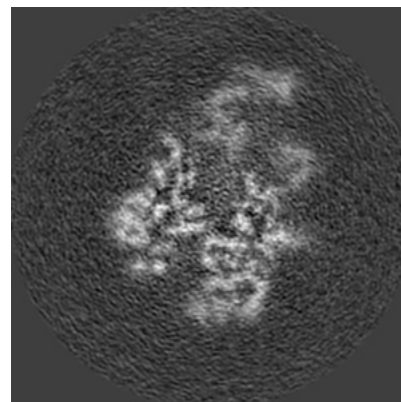
6.2.2 Raw map



X Index: 100



Y Index: 100

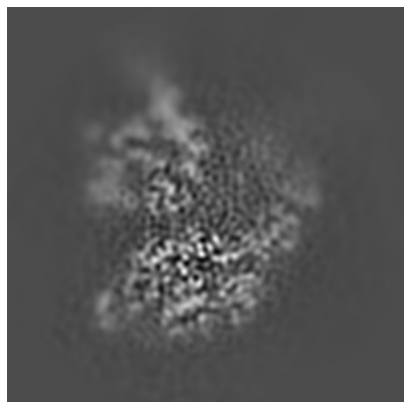


Z Index: 100

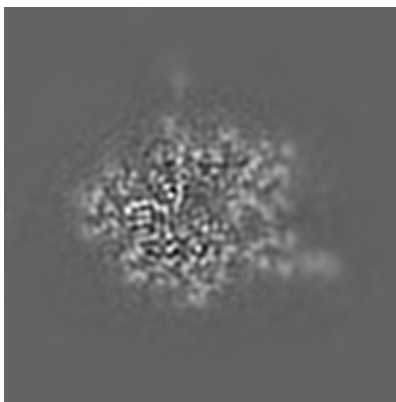
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

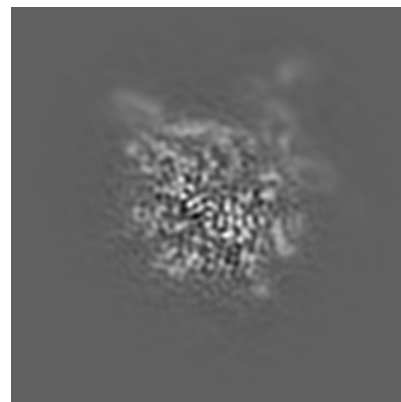
6.3.1 Primary map



X Index: 99

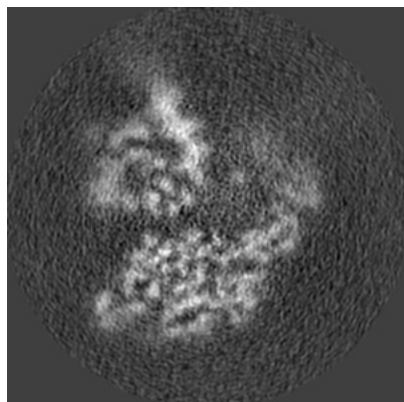


Y Index: 96

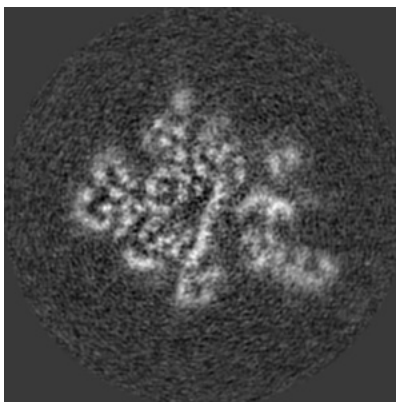


Z Index: 79

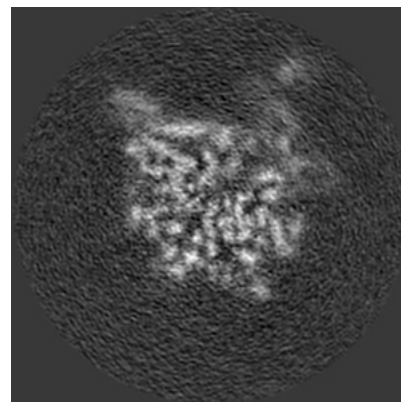
6.3.2 Raw map



X Index: 100



Y Index: 88

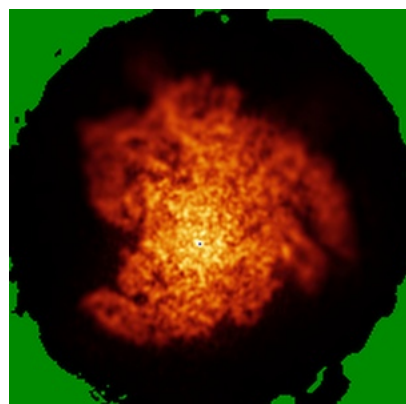


Z Index: 78

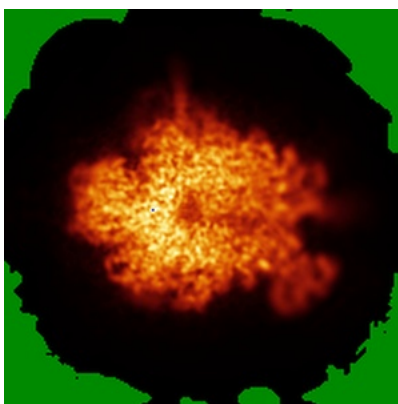
The images above show the largest variance slices of the map in three orthogonal directions.

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

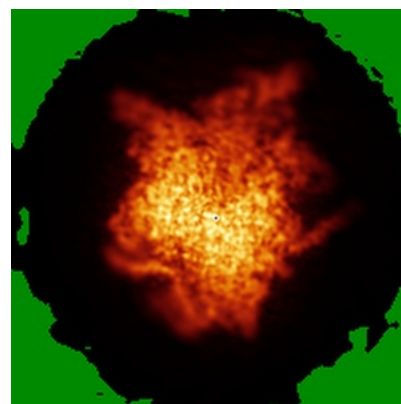
6.4.1 Primary map



X

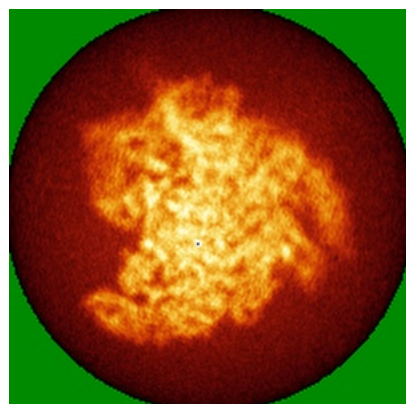


Y

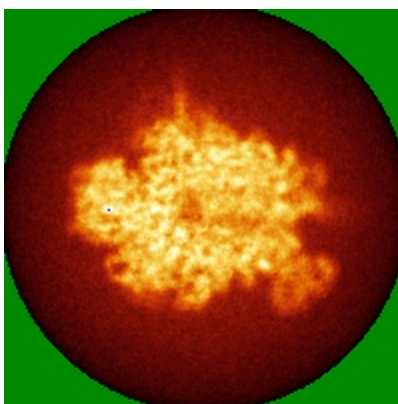


Z

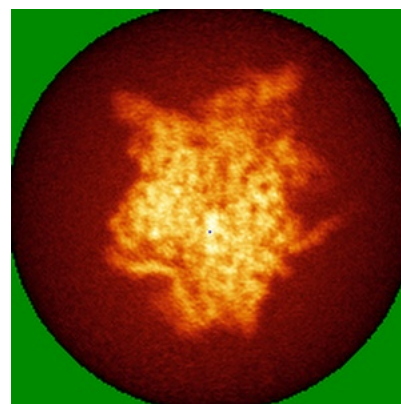
6.4.2 Raw map



X



Y

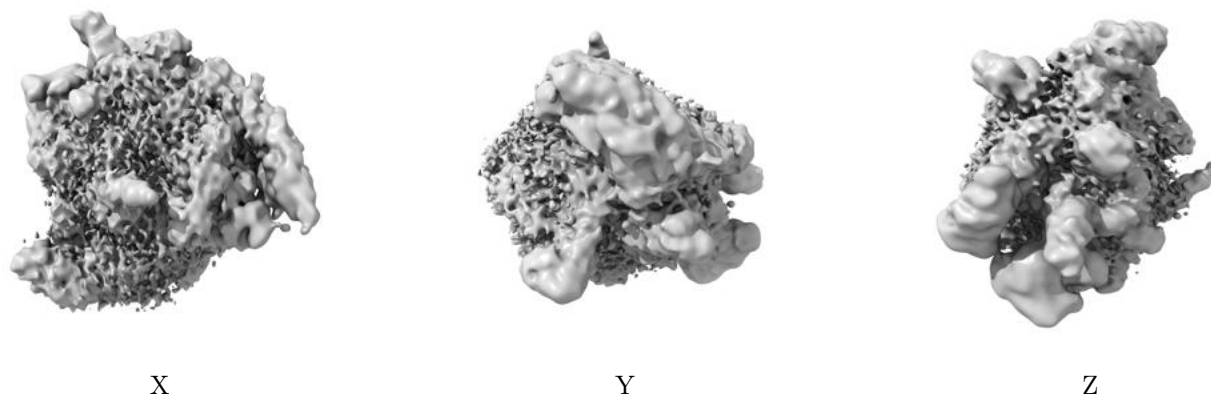


Z

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

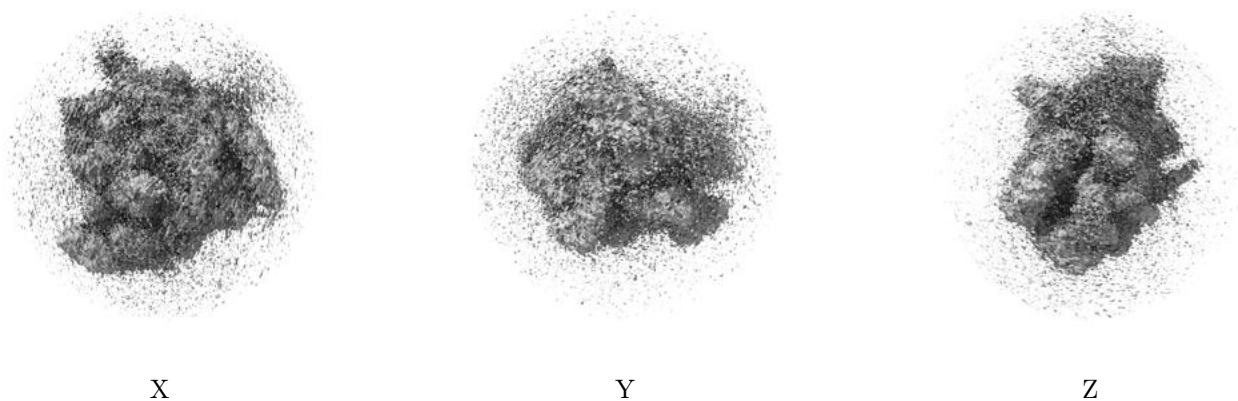
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

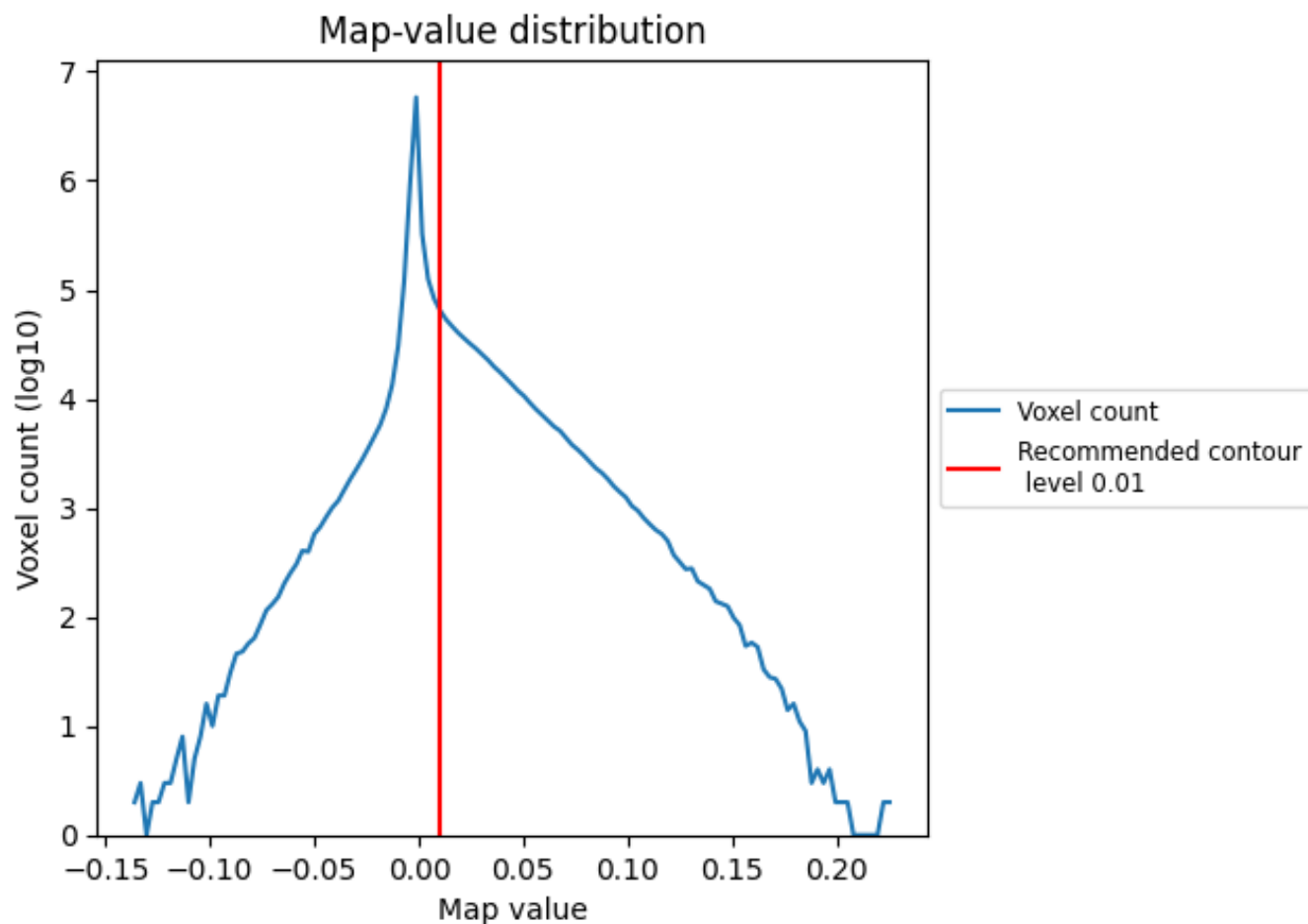
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

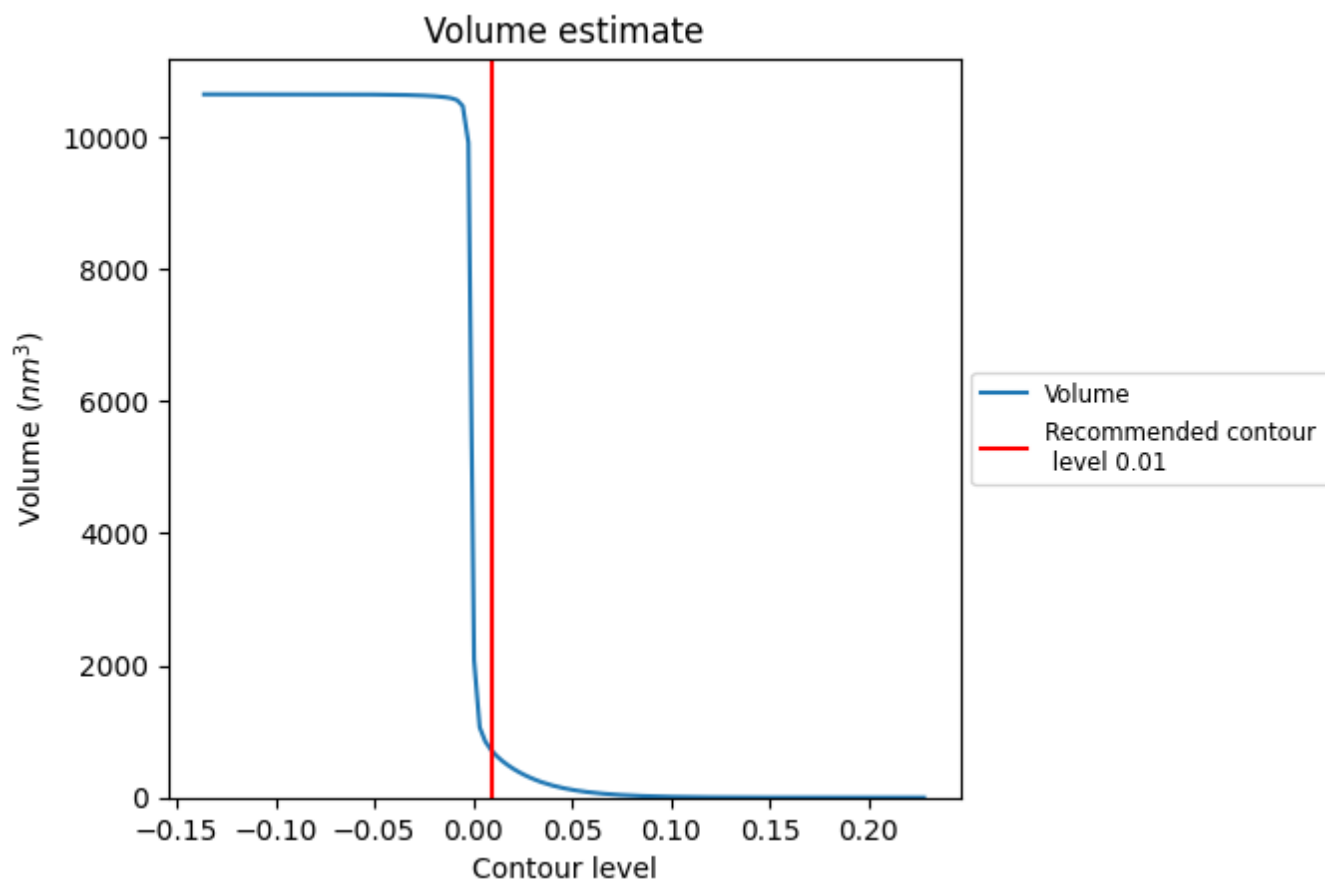
This section contains the results of statistical analysis of the map.

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.

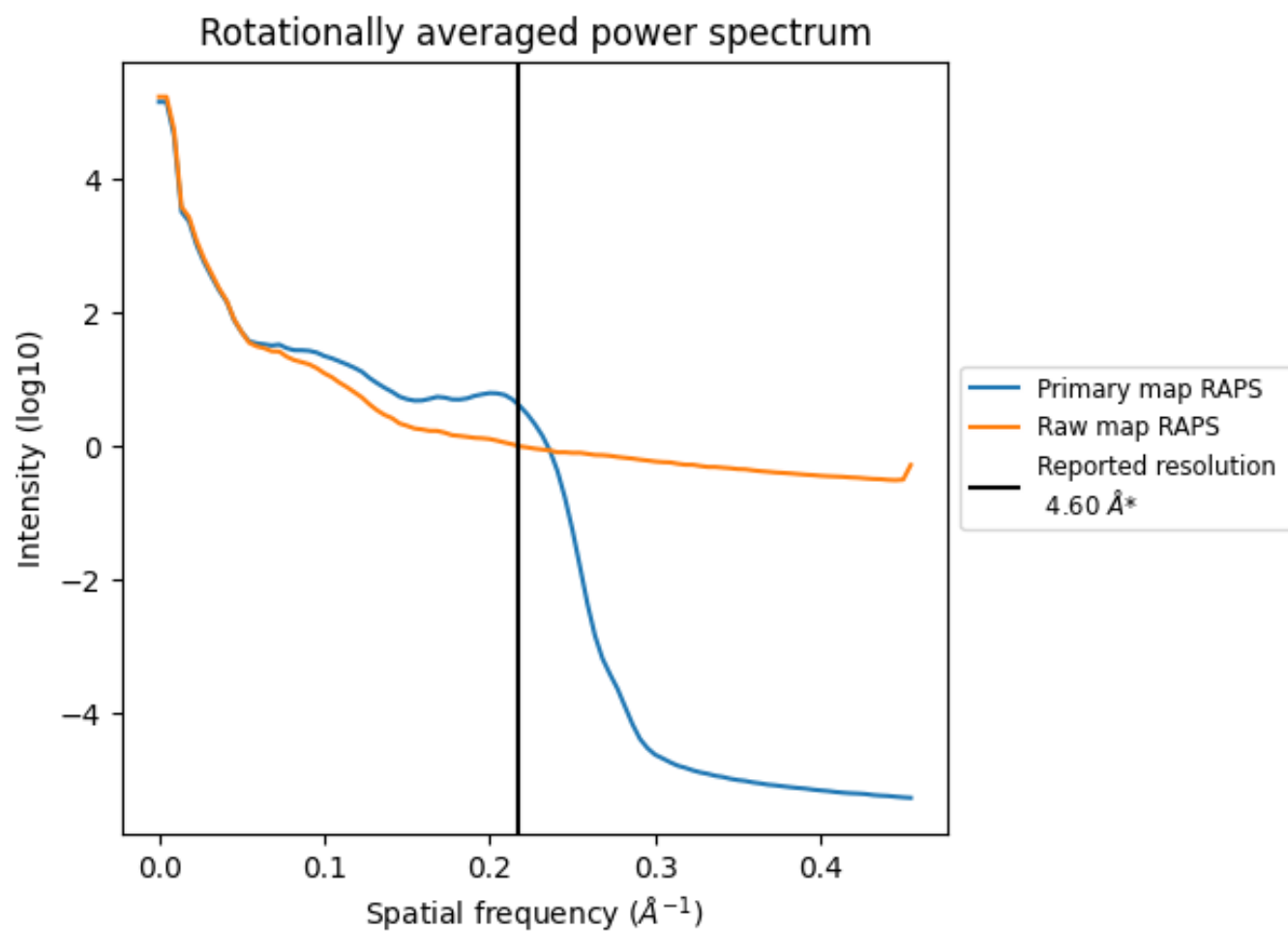
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 694 nm^3 ; this corresponds to an approximate mass of 627 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 ⓘ

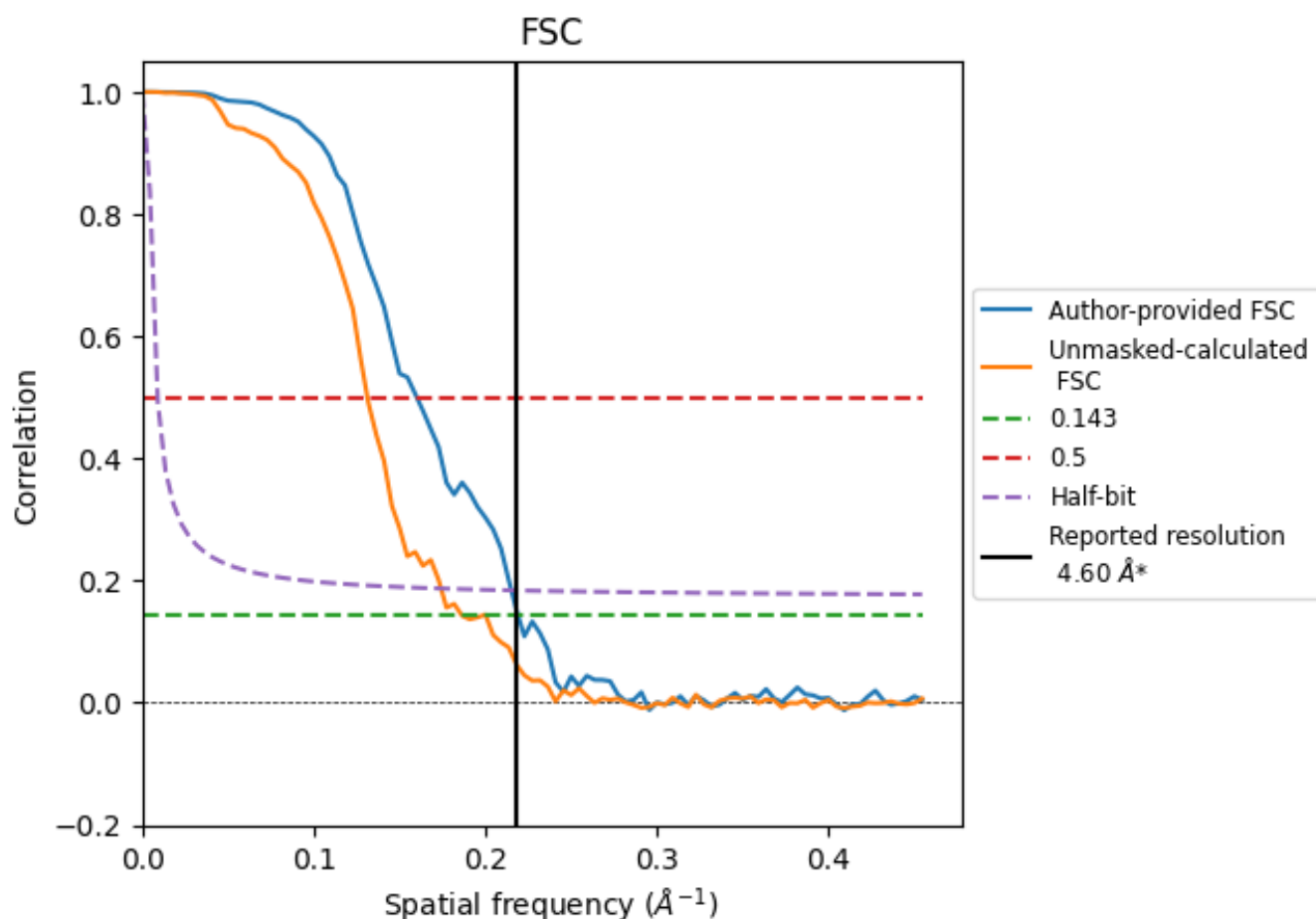


*Reported resolution corresponds to spatial frequency of 0.217 \AA^{-1}

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 0.217 \AA^{-1}

8.2 Resolution estimates [i](#)

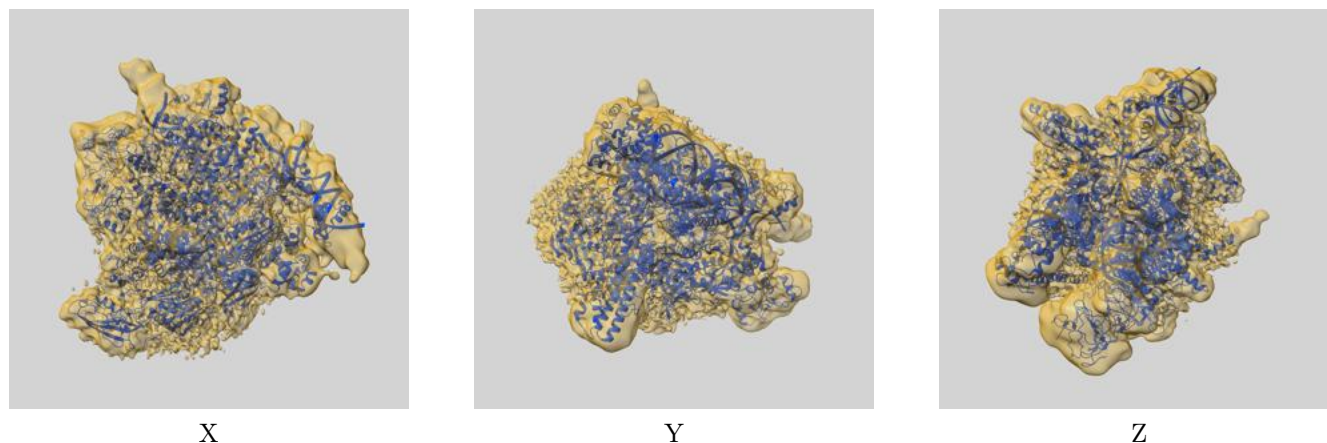
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	4.57	6.25	4.65
Unmasked-calculated*	5.37	7.62	5.74

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

9 Map-model fit [i](#)

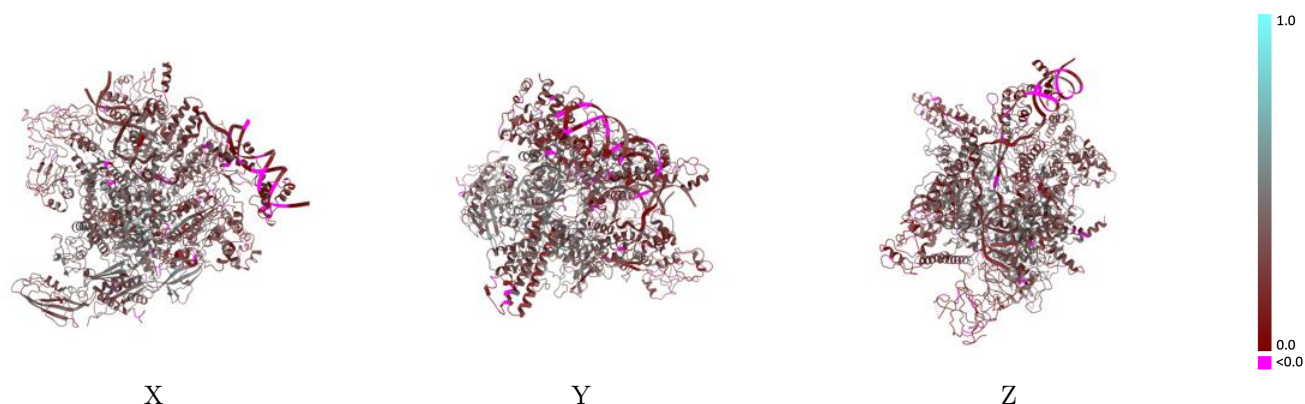
This section contains information regarding the fit between EMDB map EMD-52919 and PDB model 9Q96. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



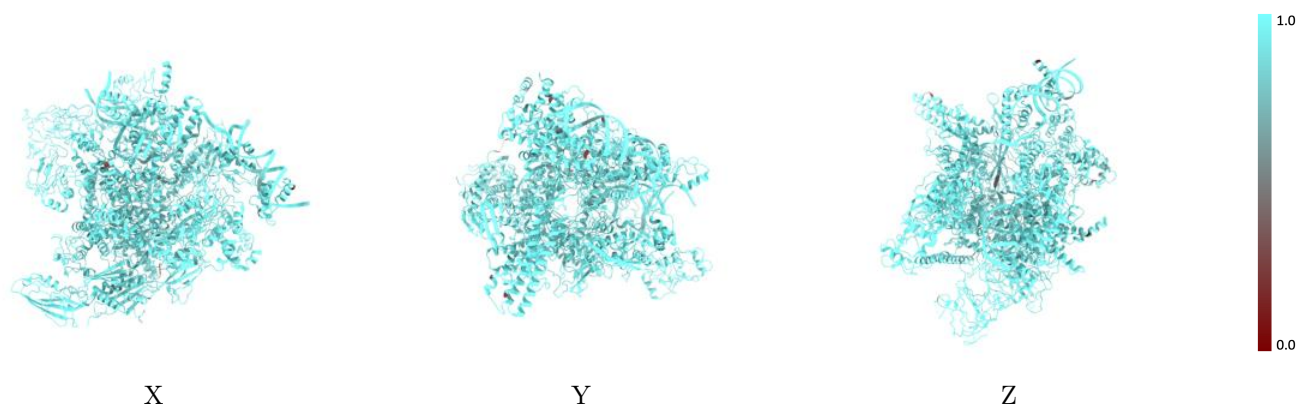
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



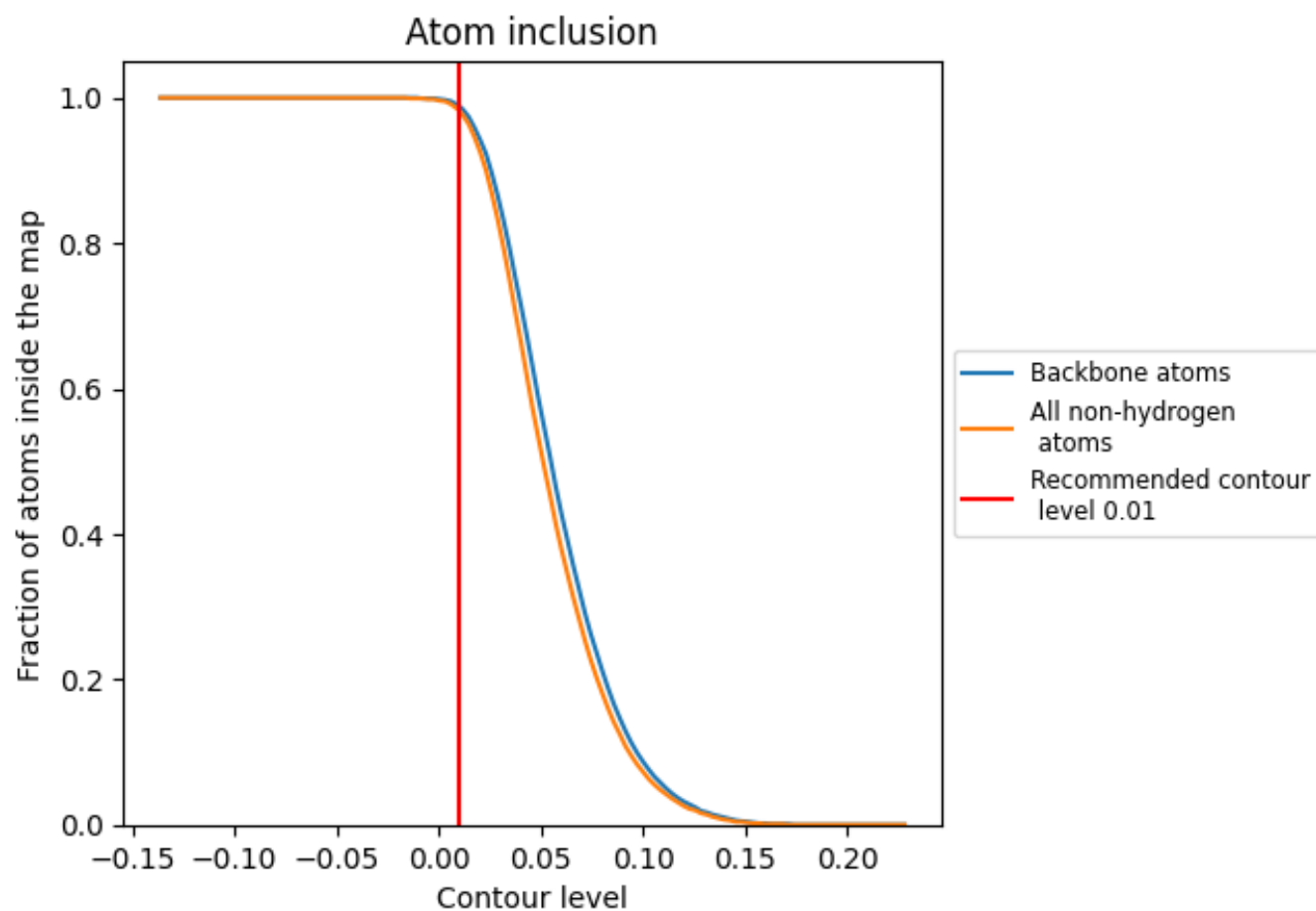
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9830</div>	<div><div></div>0.3070</div>
A	<div><div></div>0.9740</div>	<div><div></div>0.3460</div>
B	<div><div></div>0.9940</div>	<div><div></div>0.3430</div>
C	<div><div></div>0.9910</div>	<div><div></div>0.3410</div>
D	<div><div></div>0.9890</div>	<div><div></div>0.3200</div>
E	<div><div></div>0.9810</div>	<div><div></div>0.3400</div>
M	<div><div></div>0.9780</div>	<div><div></div>0.2350</div>
N	<div><div></div>0.9490</div>	<div><div></div>0.1450</div>
T	<div><div></div>0.9180</div>	<div><div></div>0.1270</div>

1.0

0.0

<0.0