



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 04:21 PM UTC

PDB ID : 4BTQ / pdb_00004btq
EMDB ID : EMD-1206
Title : Coordinates of the bacteriophage phi6 capsid subunits fitted into the cryoEM map EMD-1206
Authors : Nemecek, D.; Boura, E.; Wu, W.; Cheng, N.; Plevka, P.; Qiao, J.; Mindich, L.; Heymann, J.B.; Hurley, J.H.; Steven, A.C.
Deposited on : 2013-06-18
Resolution : 7.50 Å (reported)
Based on initial model : 4K7H

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

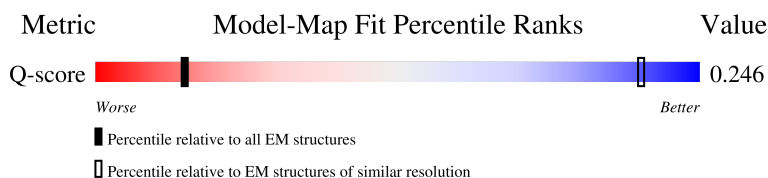
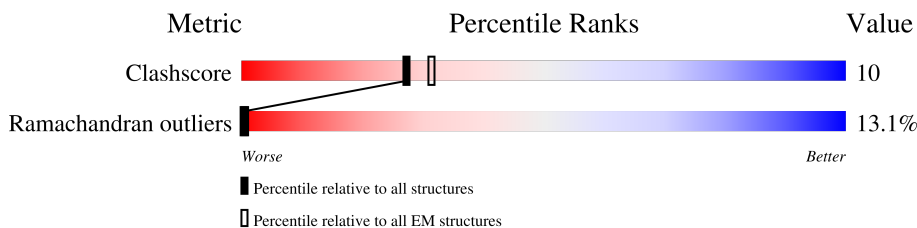
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	436 (7.00 - 8.00)

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	761	34% 27% 61% 12% .
1	B	761	27% 16% 65% 17% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6086 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 MAJOR INNER PROTEIN P1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	761	Total	C	N	O	0	0
			3043	1522	761	760		
1	B	761	Total	C	N	O	0	0
			3043	1522	761	760		

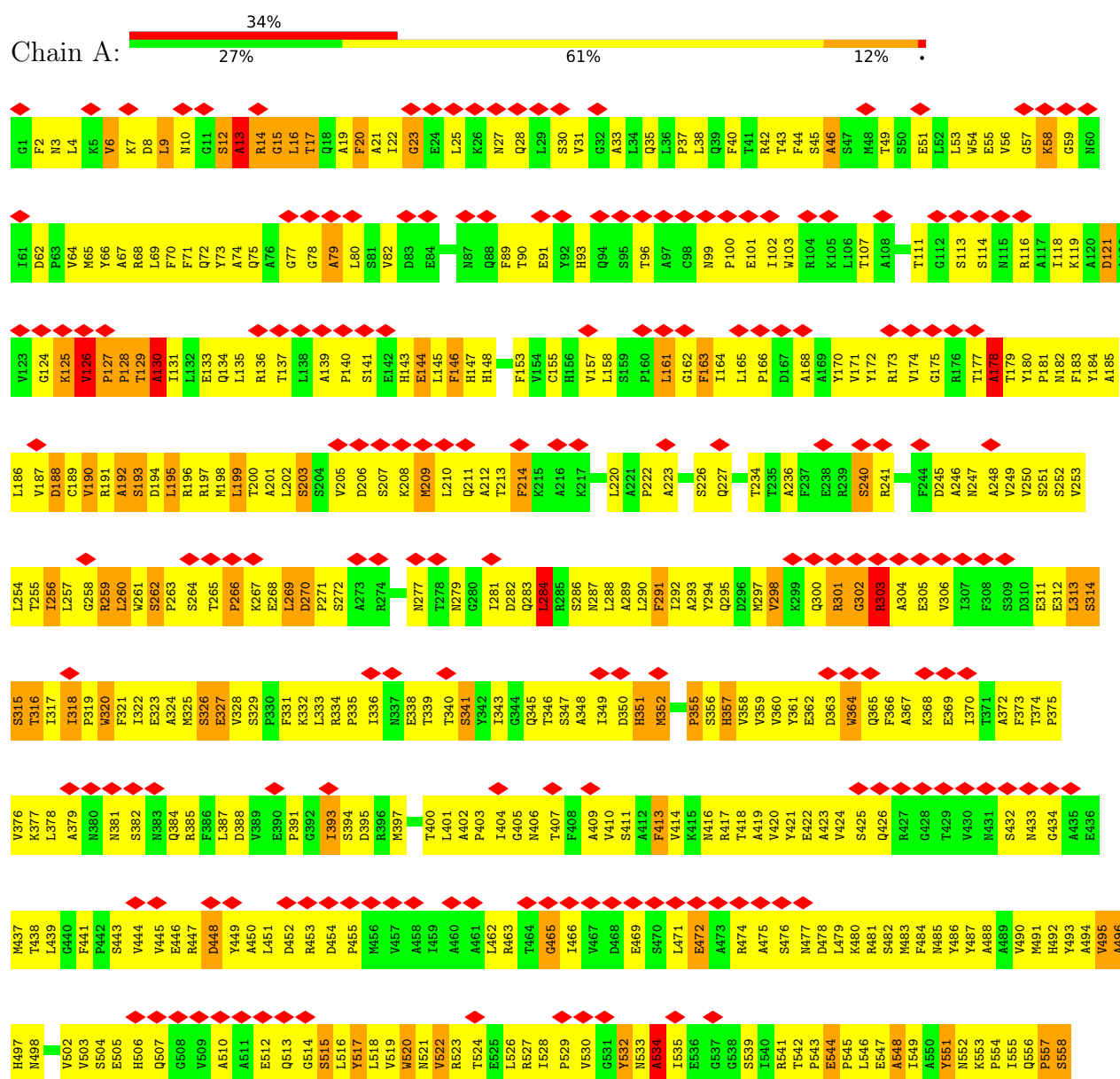
There are 2 discrepancies between the modelled and reference sequences:

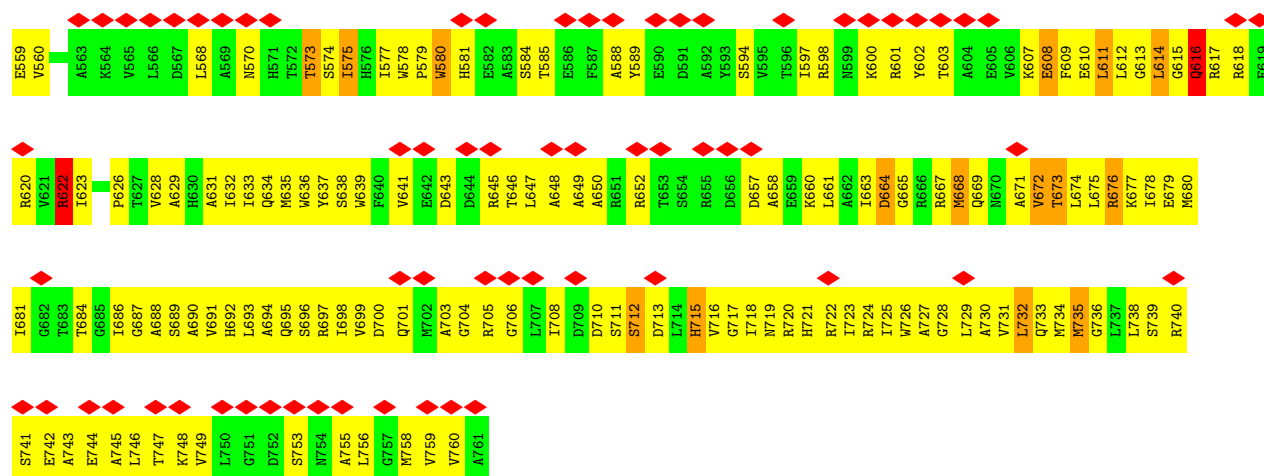
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P11126
B	1	GLY	-	expression tag	UNP P11126

3 Residue-property plots

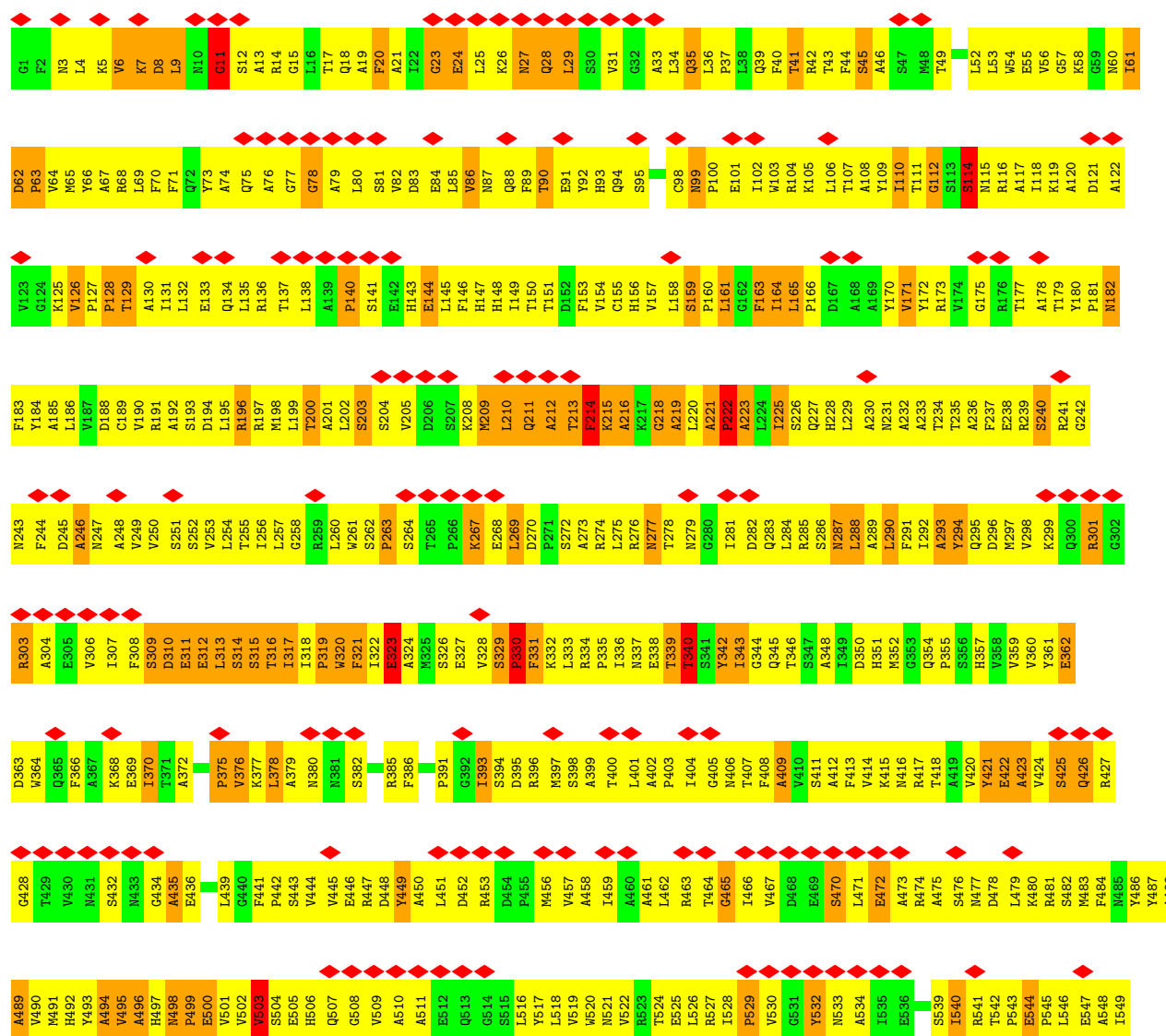
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

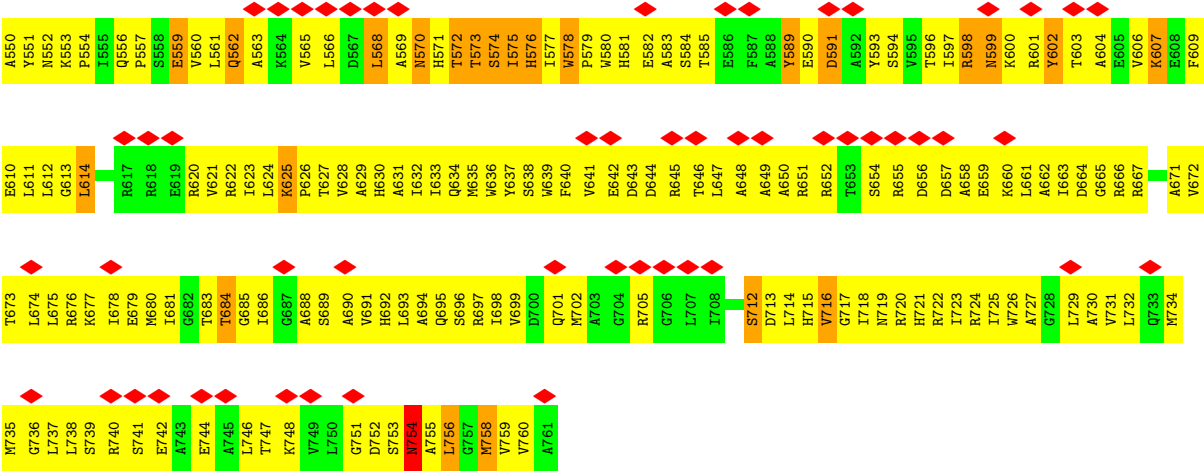
• Molecule 1: MAJOR INNER PROTEIN P1





• Molecule 1: MAJOR INNER PROTEIN P1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	10463	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	4406.000	Depositor
Minimum map value	-2373.000	Depositor
Average map value	108.317	Depositor
Map value standard deviation	931.766	Depositor
Recommended contour level	1800	Depositor
Map size ($\text{\AA}$)	589.4, 589.4, 589.4	wwPDB
Map dimensions	421, 421, 421	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	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	3.62	520/3042 (17.1%)	2.78	275/3801 (7.2%)
1	B	4.25	774/3041 (25.5%)	2.95	329/3798 (8.7%)
All	All	3.95	1294/6083 (21.3%)	2.87	604/7599 (7.9%)

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	31
1	B	0	42
All	All	0	73

All (1294) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	ILE	CA-C	-14.34	1.39	1.52
1	B	635	MET	CA-C	-14.22	1.34	1.52
1	B	54	TRP	CA-C	-13.85	1.39	1.53
1	B	104	ARG	CA-C	-13.28	1.35	1.52
1	B	288	LEU	CA-C	-13.18	1.35	1.52
1	A	721	HIS	CA-C	-13.03	1.35	1.52
1	B	484	PHE	CA-C	-13.02	1.36	1.52
1	B	126	VAL	CA-C	-12.91	1.39	1.52
1	B	359	VAL	CA-C	-12.28	1.37	1.52
1	A	332	LYS	CA-C	-12.20	1.38	1.52
1	A	498	ASN	CA-C	-11.97	1.39	1.52
1	A	315	SER	CA-C	-11.94	1.36	1.52
1	B	145	LEU	CA-C	-11.84	1.38	1.52
1	B	234	THR	CA-C	-11.64	1.38	1.52
1	B	721	HIS	CA-C	-11.60	1.36	1.52
1	B	84	GLU	CA-C	-11.57	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	720	ARG	CA-C	-11.54	1.38	1.52
1	B	70	PHE	CA-C	-11.46	1.37	1.52
1	B	492	HIS	CA-C	-11.44	1.38	1.52
1	A	44	PHE	N-CA	-11.37	1.36	1.46
1	B	719	ASN	N-CA	-11.35	1.32	1.46
1	B	297	MET	CA-C	-11.22	1.38	1.52
1	A	720	ARG	CA-C	-11.21	1.38	1.52
1	A	376	VAL	CA-C	-11.20	1.38	1.52
1	B	225	ILE	CA-C	-11.14	1.38	1.52
1	B	261	TRP	CA-C	-10.96	1.38	1.52
1	B	642	GLU	CA-C	-10.90	1.38	1.52
1	B	735	MET	CA-C	-10.89	1.40	1.52
1	B	692	HIS	CA-C	-10.88	1.39	1.52
1	A	636	TRP	CA-C	-10.80	1.38	1.52
1	B	42	ARG	CA-C	-10.78	1.39	1.52
1	A	180	TYR	CA-C	-10.77	1.41	1.53
1	B	313	LEU	CA-C	-10.72	1.40	1.53
1	A	260	LEU	CA-C	-10.64	1.38	1.52
1	B	154	VAL	CA-C	-10.63	1.39	1.52
1	B	88	GLN	CA-C	-10.61	1.39	1.52
1	B	53	LEU	CA-C	-10.57	1.39	1.52
1	A	333	LEU	CA-C	-10.40	1.39	1.52
1	B	507	GLN	CA-C	-10.37	1.39	1.53
1	B	334	ARG	CA-C	-10.36	1.41	1.52
1	B	192	ALA	CA-C	-10.35	1.38	1.52
1	B	633	ILE	CA-C	-10.34	1.39	1.52
1	A	495	VAL	N-CA	-10.31	1.33	1.46
1	A	495	VAL	CA-C	-10.28	1.39	1.52
1	B	89	PHE	N-CA	-10.27	1.33	1.46
1	B	197	ARG	CA-C	-10.22	1.39	1.52
1	B	600	LYS	CA-C	-10.20	1.40	1.52
1	A	721	HIS	N-CA	-10.18	1.33	1.46
1	B	674	LEU	CA-C	-10.18	1.39	1.52
1	B	159	SER	CA-C	-10.17	1.41	1.52
1	B	65	MET	CA-C	-10.12	1.40	1.52
1	B	330	PRO	CA-C	-10.11	1.42	1.52
1	B	685	GLY	CA-C	-10.07	1.41	1.52
1	A	481	ARG	CA-C	-10.06	1.39	1.52
1	B	488	ALA	CA-C	-10.05	1.40	1.52
1	A	20	PHE	CA-C	-10.04	1.39	1.52
1	B	639	TRP	CA-C	-10.04	1.39	1.52
1	B	318	ILE	N-CA	-10.02	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	718	ILE	CA-C	-10.02	1.40	1.52
1	B	52	LEU	CA-C	-10.01	1.40	1.52
1	B	506	HIS	CA-C	-9.99	1.40	1.52
1	A	629	ALA	CA-C	-9.99	1.39	1.52
1	B	155	CYS	CA-C	-9.97	1.40	1.52
1	A	416	ASN	CA-C	-9.97	1.39	1.52
1	B	13	ALA	CA-C	-9.96	1.42	1.53
1	B	393	ILE	CA-C	-9.91	1.39	1.52
1	B	194	ASP	CA-C	-9.91	1.39	1.52
1	B	725	ILE	CA-C	-9.91	1.40	1.52
1	A	199	LEU	CA-C	-9.88	1.40	1.52
1	A	691	VAL	CA-C	-9.85	1.40	1.52
1	A	692	HIS	CA-C	-9.81	1.40	1.52
1	B	503	VAL	CA-C	-9.79	1.40	1.52
1	A	517	TYR	CA-C	-9.79	1.40	1.52
1	B	521	ASN	CA-C	-9.79	1.40	1.52
1	B	676	ARG	CA-C	-9.79	1.40	1.52
1	A	413	PHE	CA-C	-9.77	1.40	1.52
1	B	689	SER	CA-C	-9.75	1.39	1.52
1	A	320	TRP	CA-C	-9.73	1.39	1.52
1	A	64	VAL	CA-C	-9.70	1.41	1.52
1	B	110	ILE	CA-C	-9.67	1.41	1.52
1	A	643	ASP	CA-C	-9.59	1.40	1.52
1	B	208	LYS	CA-C	-9.59	1.41	1.52
1	B	283	GLN	CA-C	-9.59	1.39	1.52
1	B	641	VAL	CA-C	-9.58	1.41	1.52
1	B	421	TYR	CA-C	-9.58	1.40	1.53
1	B	256	ILE	CA-C	-9.56	1.41	1.52
1	B	623	ILE	N-CA	-9.56	1.34	1.46
1	B	691	VAL	CA-C	-9.49	1.40	1.52
1	B	673	THR	CA-C	-9.46	1.40	1.52
1	A	633	ILE	N-CA	-9.43	1.34	1.46
1	B	44	PHE	CA-C	-9.42	1.41	1.52
1	A	491	MET	CA-C	-9.40	1.39	1.52
1	B	622	ARG	CA-C	-9.39	1.41	1.52
1	B	185	ALA	CA-C	-9.39	1.40	1.52
1	B	520	TRP	CA-C	-9.38	1.41	1.52
1	A	345	GLN	CA-C	-9.36	1.41	1.52
1	B	329	SER	C-N	-9.34	1.26	1.33
1	A	633	ILE	CA-C	-9.32	1.40	1.52
1	B	651	ARG	CA-C	-9.30	1.40	1.52
1	B	636	TRP	CA-C	-9.29	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	TRP	N-CA	-9.28	1.35	1.46
1	B	183	PHE	CA-C	-9.28	1.40	1.52
1	A	676	ARG	CA-C	-9.28	1.40	1.52
1	B	68	ARG	CA-C	-9.26	1.40	1.52
1	A	73	TYR	CA-C	-9.25	1.40	1.52
1	A	554	PRO	CA-C	-9.23	1.41	1.52
1	B	495	VAL	CA-C	-9.23	1.39	1.52
1	A	551	TYR	CA-C	-9.19	1.43	1.53
1	B	171	VAL	CA-C	-9.19	1.41	1.52
1	A	639	TRP	CA-C	-9.18	1.41	1.52
1	B	154	VAL	N-CA	-9.18	1.38	1.46
1	B	54	TRP	N-CA	-9.15	1.34	1.46
1	B	490	VAL	CA-C	-9.15	1.41	1.52
1	B	66	TYR	CA-C	-9.14	1.41	1.52
1	B	333	LEU	CA-C	-9.10	1.41	1.52
1	B	675	LEU	N-CA	-9.05	1.35	1.46
1	A	492	HIS	CA-C	-9.05	1.41	1.52
1	B	193	SER	CA-C	-9.03	1.40	1.52
1	A	185	ALA	CA-C	-9.03	1.41	1.52
1	A	465	GLY	CA-C	-9.03	1.39	1.51
1	B	660	LYS	CA-C	-9.02	1.41	1.52
1	B	228	HIS	CA-C	-9.01	1.41	1.52
1	B	100	PRO	CA-C	-9.00	1.39	1.52
1	B	385	ARG	CA-C	-8.99	1.41	1.52
1	B	43	THR	CA-C	-8.97	1.41	1.52
1	B	516	LEU	CA-C	-8.97	1.41	1.52
1	A	690	ALA	CA-C	-8.96	1.41	1.52
1	A	65	MET	CA-C	-8.94	1.41	1.52
1	B	252	SER	CA-C	-8.93	1.41	1.52
1	A	439	LEU	CA-C	-8.92	1.42	1.52
1	B	147	HIS	N-CA	-8.92	1.35	1.46
1	A	250	VAL	CA-C	-8.92	1.41	1.52
1	A	519	VAL	CA-C	-8.91	1.42	1.52
1	A	335	PRO	CA-C	-8.90	1.40	1.52
1	A	610	GLU	N-CA	-8.90	1.34	1.46
1	B	107	THR	CA-C	-8.90	1.41	1.52
1	A	247	ASN	CA-C	-8.85	1.41	1.52
1	B	331	PHE	CA-C	-8.84	1.41	1.52
1	A	739	SER	CA-C	-8.82	1.41	1.52
1	B	658	ALA	CA-C	-8.80	1.41	1.52
1	B	94	GLN	CA-C	-8.79	1.41	1.52
1	A	406	ASN	CA-C	-8.77	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	ILE	CA-C	-8.76	1.41	1.52
1	B	673	THR	N-CA	-8.75	1.35	1.46
1	B	415	LYS	CA-C	-8.74	1.41	1.52
1	B	699	VAL	N-CA	-8.74	1.36	1.46
1	B	105	LYS	CA-C	-8.72	1.41	1.52
1	B	91	GLU	N-CA	-8.71	1.35	1.46
1	B	64	VAL	CA-C	-8.71	1.42	1.52
1	B	735	MET	N-CA	-8.70	1.36	1.46
1	B	196	ARG	CA-C	-8.67	1.41	1.52
1	B	569	ALA	CA-C	-8.66	1.42	1.52
1	A	725	ILE	CA-C	-8.66	1.42	1.52
1	B	413	PHE	CA-C	-8.66	1.41	1.52
1	A	523	ARG	CA-C	-8.59	1.41	1.52
1	B	488	ALA	N-CA	-8.58	1.36	1.46
1	B	200	THR	CA-C	-8.56	1.41	1.52
1	A	437	MET	CA-C	-8.55	1.42	1.52
1	B	95	SER	CA-C	-8.54	1.41	1.52
1	A	672	VAL	CA-C	-8.53	1.40	1.52
1	B	71	PHE	CA-C	-8.53	1.41	1.52
1	B	102	ILE	CA-C	-8.53	1.42	1.52
1	B	83	ASP	N-CA	-8.52	1.36	1.46
1	B	343	ILE	N-CA	-8.52	1.35	1.46
1	B	582	GLU	CA-C	-8.50	1.41	1.52
1	A	332	LYS	N-CA	-8.50	1.36	1.46
1	B	296	ASP	CA-C	-8.49	1.42	1.52
1	B	411	SER	CA-C	-8.48	1.41	1.52
1	B	504	SER	CA-C	-8.48	1.42	1.52
1	A	358	VAL	CA-C	-8.47	1.42	1.52
1	B	478	ASP	CA-C	-8.46	1.42	1.52
1	A	44	PHE	CA-C	-8.46	1.43	1.52
1	A	518	LEU	CA-C	-8.46	1.42	1.52
1	A	248	ALA	N-CA	-8.44	1.35	1.46
1	A	585	THR	CA-C	-8.43	1.42	1.52
1	B	170	TYR	CA-C	-8.42	1.43	1.53
1	B	522	VAL	CA-C	-8.42	1.42	1.52
1	B	444	VAL	CA-C	-8.41	1.42	1.52
1	B	360	VAL	N-CA	-8.40	1.36	1.46
1	A	66	TYR	CA-C	-8.38	1.42	1.52
1	B	87	ASN	CA-C	-8.38	1.42	1.52
1	B	296	ASP	N-CA	-8.38	1.36	1.46
1	A	623	ILE	CA-C	-8.37	1.42	1.52
1	B	298	VAL	N-CA	-8.37	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	ASP	CA-C	-8.37	1.42	1.52
1	B	495	VAL	N-CA	-8.35	1.35	1.46
1	A	559	GLU	CA-C	-8.35	1.42	1.52
1	B	420	VAL	CA-C	-8.35	1.42	1.52
1	B	157	VAL	CA-C	-8.31	1.41	1.52
1	B	292	ILE	N-CA	-8.30	1.36	1.46
1	B	313	LEU	N-CA	-8.29	1.35	1.47
1	B	401	LEU	CA-C	-8.28	1.42	1.52
1	B	620	ARG	CA-C	-8.28	1.42	1.53
1	A	249	VAL	CA-C	-8.26	1.42	1.52
1	A	494	ALA	CA-C	-8.26	1.42	1.52
1	B	458	ALA	CA-C	-8.24	1.42	1.52
1	B	249	VAL	N-CA	-8.24	1.36	1.46
1	B	746	LEU	CA-C	-8.23	1.42	1.52
1	B	291	PHE	CA-C	-8.22	1.42	1.52
1	B	722	ARG	CA-C	-8.22	1.42	1.52
1	B	692	HIS	N-CA	-8.21	1.36	1.46
1	B	560	VAL	CA-C	-8.21	1.43	1.53
1	B	190	VAL	CA-C	-8.20	1.42	1.52
1	A	719	ASN	N-CA	-8.19	1.35	1.46
1	A	726	TRP	CA-C	-8.19	1.42	1.52
1	B	675	LEU	CA-C	-8.18	1.42	1.52
1	A	19	ALA	CA-C	-8.17	1.42	1.52
1	A	665	GLY	CA-C	-8.17	1.42	1.51
1	A	598	ARG	CA-C	-8.16	1.41	1.52
1	A	259	ARG	CA-C	-8.15	1.44	1.53
1	B	376	VAL	CA-C	-8.14	1.42	1.52
1	A	691	VAL	N-CA	-8.13	1.37	1.46
1	A	377	LYS	N-CA	-8.13	1.36	1.46
1	B	253	VAL	CA-C	-8.13	1.42	1.52
1	B	67	ALA	CA-C	-8.13	1.41	1.52
1	B	448	ASP	CA-C	-8.12	1.41	1.52
1	B	609	PHE	CA-C	-8.12	1.42	1.52
1	B	719	ASN	CA-C	-8.12	1.41	1.52
1	B	254	LEU	CA-C	-8.12	1.42	1.52
1	B	180	TYR	CA-C	-8.11	1.42	1.52
1	A	272	SER	CA-C	-8.11	1.42	1.52
1	B	698	ILE	CA-C	-8.10	1.43	1.52
1	B	742	GLU	CA-C	-8.10	1.42	1.52
1	A	422	GLU	N-CA	-8.09	1.35	1.45
1	B	676	ARG	N-CA	-8.09	1.36	1.46
1	B	286	SER	N-CA	-8.08	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	HIS	N-CA	-8.07	1.36	1.46
1	B	364	TRP	CA-C	-8.07	1.42	1.52
1	A	298	VAL	CA-C	-8.06	1.43	1.52
1	B	156	HIS	N-CA	-8.06	1.35	1.46
1	B	90	THR	CA-C	-8.06	1.42	1.52
1	B	293	ALA	N-CA	-8.06	1.36	1.46
1	A	522	VAL	CA-C	-8.05	1.42	1.52
1	B	480	LYS	CA-C	-8.05	1.42	1.52
1	B	672	VAL	CA-C	-8.04	1.41	1.52
1	A	404	ILE	N-CA	-8.04	1.36	1.46
1	B	404	ILE	CA-C	-8.03	1.42	1.52
1	B	463	ARG	CA-C	-8.03	1.43	1.52
1	B	132	LEU	N-CA	-8.03	1.36	1.46
1	B	292	ILE	CA-C	-8.03	1.41	1.52
1	B	235	THR	CA-C	-8.02	1.42	1.52
1	A	631	ALA	N-CA	-8.02	1.36	1.46
1	B	229	LEU	CA-C	-8.02	1.42	1.52
1	B	718	ILE	N-CA	-8.01	1.37	1.46
1	B	208	LYS	N-CA	-8.00	1.36	1.46
1	B	641	VAL	N-CA	-8.00	1.37	1.46
1	B	68	ARG	N-CA	-7.99	1.36	1.46
1	A	444	VAL	CA-C	-7.99	1.42	1.52
1	B	753	SER	CA-C	-7.98	1.42	1.52
1	A	719	ASN	CA-C	-7.97	1.42	1.52
1	A	637	TYR	N-CA	-7.97	1.37	1.46
1	A	515	SER	CA-C	-7.96	1.42	1.52
1	A	67	ALA	CA-C	-7.96	1.42	1.52
1	A	320	TRP	N-CA	-7.95	1.36	1.46
1	B	211	GLN	CA-C	-7.95	1.41	1.53
1	A	300	GLN	CA-C	-7.94	1.42	1.52
1	B	44	PHE	N-CA	-7.94	1.36	1.46
1	B	461	ALA	CA-C	-7.94	1.42	1.52
1	A	183	PHE	CA-C	-7.93	1.42	1.52
1	B	398	SER	CA-C	-7.93	1.42	1.52
1	B	601	ARG	CA-C	-7.93	1.43	1.52
1	B	134	GLN	CA-C	-7.92	1.42	1.52
1	A	184	TYR	CA-C	-7.91	1.42	1.52
1	B	581	HIS	CA-C	-7.91	1.42	1.52
1	A	177	THR	CA-C	-7.90	1.43	1.52
1	B	55	GLU	N-CA	-7.89	1.35	1.46
1	A	600	LYS	CA-C	-7.89	1.42	1.52
1	A	637	TYR	CA-C	-7.89	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	ALA	CA-C	-7.88	1.42	1.52
1	B	195	LEU	CA-C	-7.88	1.42	1.52
1	B	580	TRP	N-CA	-7.88	1.37	1.46
1	A	90	THR	CA-C	-7.88	1.42	1.52
1	A	635	MET	CA-C	-7.88	1.42	1.52
1	B	335	PRO	CA-C	-7.87	1.43	1.52
1	A	188	ASP	CA-C	-7.87	1.42	1.52
1	B	436	GLU	CA-C	-7.87	1.42	1.52
1	B	295	GLN	C-N	-7.85	1.23	1.33
1	B	725	ILE	N-CA	-7.85	1.37	1.46
1	B	267	LYS	CA-C	-7.85	1.42	1.52
1	B	647	LEU	CA-C	-7.84	1.42	1.52
1	B	276	ARG	CA-C	-7.84	1.42	1.52
1	B	665	GLY	CA-C	-7.84	1.43	1.52
1	B	86	VAL	CA-C	-7.83	1.41	1.52
1	B	165	LEU	CA-C	-7.83	1.43	1.52
1	B	694	ALA	CA-C	-7.83	1.43	1.52
1	B	645	ARG	N-CA	-7.82	1.37	1.46
1	A	673	THR	CA-C	-7.81	1.42	1.52
1	B	45	SER	CA-C	-7.80	1.43	1.52
1	B	533	ASN	CA-C	-7.80	1.42	1.53
1	A	422	GLU	CA-C	-7.80	1.42	1.52
1	A	712	SER	CA-C	-7.78	1.42	1.52
1	B	343	ILE	CA-C	-7.78	1.43	1.52
1	A	141	SER	CA-C	-7.78	1.42	1.52
1	A	271	PRO	CA-C	-7.76	1.44	1.52
1	B	546	LEU	CA-C	-7.76	1.42	1.52
1	B	360	VAL	CA-C	-7.75	1.43	1.52
1	B	494	ALA	CA-C	-7.75	1.42	1.52
1	B	53	LEU	N-CA	-7.74	1.36	1.45
1	B	483	MET	CA-C	-7.74	1.42	1.52
1	A	393	ILE	CA-C	-7.73	1.43	1.52
1	B	659	GLU	N-CA	-7.73	1.37	1.46
1	A	477	ASN	CA-C	-7.73	1.42	1.52
1	A	89	PHE	CA-C	-7.71	1.43	1.52
1	B	756	LEU	CA-C	-7.71	1.42	1.52
1	B	93	HIS	CA-C	-7.71	1.43	1.52
1	B	321	PHE	CA-C	-7.70	1.42	1.52
1	B	199	LEU	CA-C	-7.70	1.42	1.52
1	B	640	PHE	CA-C	-7.70	1.42	1.52
1	B	185	ALA	N-CA	-7.69	1.37	1.46
1	B	402	ALA	N-CA	-7.69	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	GLU	CA-C	-7.68	1.43	1.52
1	A	145	LEU	CA-C	-7.67	1.41	1.52
1	A	479	LEU	CA-C	-7.66	1.42	1.52
1	B	65	MET	N-CA	-7.66	1.37	1.46
1	B	491	MET	CA-C	-7.66	1.42	1.52
1	B	690	ALA	N-CA	-7.65	1.36	1.46
1	A	46	ALA	CA-C	-7.64	1.42	1.52
1	B	73	TYR	CA-C	-7.64	1.43	1.52
1	A	316	THR	CA-C	-7.63	1.42	1.52
1	B	306	VAL	CA-C	-7.63	1.43	1.52
1	B	316	THR	CA-C	-7.63	1.43	1.52
1	A	25	LEU	CA-C	-7.62	1.43	1.52
1	B	493	TYR	N-CA	-7.62	1.36	1.46
1	B	189	CYS	CA-C	-7.62	1.42	1.52
1	B	635	MET	N-CA	-7.61	1.36	1.46
1	A	385	ARG	CA-C	-7.59	1.43	1.52
1	B	643	ASP	CA-C	-7.59	1.43	1.52
1	B	397	MET	CA-C	-7.58	1.43	1.52
1	B	690	ALA	CA-C	-7.58	1.43	1.52
1	A	699	VAL	CA-C	-7.58	1.43	1.52
1	B	447	ARG	CA-C	-7.58	1.42	1.52
1	B	600	LYS	N-CA	-7.57	1.36	1.46
1	A	446	GLU	CA-C	-7.56	1.43	1.52
1	B	462	LEU	CA-C	-7.55	1.43	1.52
1	A	45	SER	CA-C	-7.55	1.43	1.52
1	A	360	VAL	CA-C	-7.54	1.43	1.52
1	A	321	PHE	N-CA	-7.54	1.36	1.46
1	B	645	ARG	CA-C	-7.54	1.43	1.52
1	B	328	VAL	CA-C	-7.53	1.43	1.52
1	A	93	HIS	CA-C	-7.53	1.43	1.52
1	B	695	GLN	CA-C	-7.53	1.43	1.52
1	A	547	GLU	CA-C	-7.52	1.43	1.52
1	B	568	LEU	CA-C	-7.52	1.42	1.52
1	A	355	PRO	CA-C	-7.52	1.41	1.52
1	A	727	ALA	CA-C	-7.51	1.43	1.52
1	B	19	ALA	CA-C	-7.51	1.43	1.52
1	B	147	HIS	CA-C	-7.51	1.43	1.52
1	B	414	VAL	CA-C	-7.51	1.42	1.52
1	B	104	ARG	N-CA	-7.51	1.37	1.46
1	A	496	ALA	CA-C	-7.49	1.43	1.52
1	A	716	VAL	CA-C	-7.49	1.44	1.52
1	B	295	GLN	N-CA	-7.49	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	PHE	CA-C	-7.49	1.42	1.52
1	B	99	ASN	C-N	-7.49	1.23	1.34
1	A	343	ILE	CA-C	-7.49	1.43	1.52
1	A	283	GLN	CA-C	-7.49	1.42	1.52
1	A	490	VAL	CA-C	-7.48	1.43	1.52
1	B	255	THR	N-CA	-7.47	1.36	1.46
1	A	609	PHE	CA-C	-7.46	1.43	1.52
1	B	136	ARG	CA-C	-7.46	1.43	1.52
1	B	317	ILE	CA-C	-7.46	1.42	1.52
1	B	377	LYS	CA-C	-7.46	1.42	1.52
1	B	629	ALA	CA-C	-7.46	1.42	1.52
1	B	482	SER	CA-C	-7.45	1.43	1.52
1	B	412	ALA	CA-C	-7.45	1.42	1.52
1	B	525	GLU	CA-C	-7.45	1.42	1.52
1	A	421	TYR	CA-C	-7.45	1.42	1.52
1	B	150	THR	N-CA	-7.44	1.36	1.46
1	B	517	TYR	CA-C	-7.44	1.43	1.52
1	B	161	LEU	N-CA	-7.44	1.37	1.46
1	A	486	TYR	CA-C	-7.43	1.43	1.52
1	B	332	LYS	CA-C	-7.42	1.43	1.52
1	B	198	MET	CA-C	-7.42	1.43	1.52
1	B	258	GLY	CA-C	-7.42	1.44	1.52
1	B	629	ALA	N-CA	-7.42	1.36	1.46
1	B	628	VAL	CA-C	-7.41	1.43	1.52
1	B	66	TYR	N-CA	-7.41	1.37	1.46
1	A	248	ALA	CA-C	-7.41	1.43	1.52
1	A	40	PHE	CA-C	-7.40	1.42	1.52
1	B	346	THR	CA-C	-7.39	1.43	1.52
1	B	696	SER	CA-C	-7.38	1.43	1.52
1	A	220	LEU	CA-C	-7.37	1.42	1.52
1	B	737	LEU	CA-C	-7.37	1.42	1.52
1	A	42	ARG	CA-C	-7.37	1.43	1.52
1	A	70	PHE	CA-C	-7.36	1.43	1.52
1	A	312	GLU	N-CA	-7.36	1.35	1.46
1	B	320	TRP	CA-C	-7.36	1.43	1.52
1	B	85	LEU	CA-C	-7.36	1.43	1.52
1	B	720	ARG	N-CA	-7.36	1.37	1.46
1	A	553	LYS	CA-C	-7.35	1.43	1.52
1	A	329	SER	CA-C	-7.35	1.45	1.52
1	A	649	ALA	CA-C	-7.35	1.42	1.52
1	A	203	SER	CA-C	-7.35	1.43	1.52
1	A	645	ARG	CA-C	-7.34	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	667	ARG	CA-C	-7.34	1.43	1.52
1	B	680	MET	CA-C	-7.32	1.43	1.52
1	A	315	SER	N-CA	-7.32	1.36	1.46
1	B	644	ASP	CA-C	-7.31	1.42	1.52
1	B	598	ARG	CA-C	-7.31	1.43	1.52
1	A	68	ARG	CA-C	-7.30	1.43	1.52
1	A	252	SER	CA-C	-7.30	1.43	1.52
1	B	255	THR	CA-C	-7.30	1.42	1.52
1	B	443	SER	N-CA	-7.29	1.37	1.46
1	B	688	ALA	CA-C	-7.29	1.43	1.52
1	B	357	HIS	CA-C	-7.29	1.43	1.52
1	B	230	ALA	CA-C	-7.28	1.43	1.52
1	B	234	THR	N-CA	-7.28	1.37	1.46
1	B	661	LEU	N-CA	-7.25	1.37	1.46
1	A	521	ASN	CA-C	-7.25	1.44	1.52
1	B	236	ALA	CA-C	-7.25	1.43	1.52
1	A	575	ILE	N-CA	-7.25	1.37	1.46
1	A	488	ALA	CA-C	-7.25	1.43	1.52
1	A	294	TYR	CA-C	-7.24	1.43	1.52
1	B	716	VAL	CA-C	-7.24	1.44	1.52
1	B	634	GLN	CA-C	-7.22	1.42	1.52
1	A	364	TRP	CA-C	-7.22	1.43	1.52
1	B	330	PRO	N-CA	-7.22	1.40	1.47
1	B	363	ASP	CA-C	-7.22	1.43	1.52
1	A	362	GLU	CA-C	-7.21	1.44	1.52
1	B	215	LYS	CA-C	-7.21	1.43	1.52
1	B	637	TYR	N-CA	-7.21	1.37	1.46
1	A	445	VAL	N-CA	-7.21	1.38	1.46
1	A	610	GLU	CA-C	-7.21	1.42	1.52
1	B	522	VAL	N-CA	-7.20	1.37	1.46
1	B	634	GLN	N-CA	-7.20	1.36	1.46
1	B	137	THR	CA-C	-7.20	1.43	1.52
1	B	284	LEU	N-CA	-7.20	1.36	1.46
1	B	310	ASP	N-CA	-7.19	1.39	1.46
1	B	543	PRO	N-CA	-7.19	1.38	1.47
1	B	94	GLN	N-CA	-7.19	1.37	1.46
1	B	403	PRO	CA-C	-7.17	1.40	1.52
1	A	700	ASP	CA-C	-7.16	1.43	1.52
1	B	569	ALA	N-CA	-7.16	1.37	1.46
1	A	441	PHE	CA-C	-7.16	1.45	1.52
1	A	319	PRO	CA-C	-7.16	1.39	1.52
1	A	343	ILE	N-CA	-7.15	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	648	ALA	CA-C	-7.15	1.43	1.52
1	A	400	THR	CA-C	-7.15	1.42	1.52
1	A	638	SER	CA-C	-7.13	1.43	1.52
1	A	186	LEU	CA-C	-7.12	1.43	1.52
1	B	111	THR	CA-C	-7.11	1.44	1.52
1	A	667	ARG	N-CA	-7.11	1.38	1.46
1	B	701	GLN	CA-C	-7.11	1.43	1.52
1	B	556	GLN	CA-C	-7.11	1.41	1.52
1	B	741	SER	N-CA	-7.11	1.38	1.46
1	A	194	ASP	CA-C	-7.11	1.43	1.52
1	A	674	LEU	CA-C	-7.10	1.43	1.52
1	A	693	LEU	CA-C	-7.10	1.43	1.52
1	B	64	VAL	N-CA	-7.10	1.38	1.46
1	B	667	ARG	CA-C	-7.10	1.43	1.52
1	A	555	ILE	CA-C	-7.09	1.43	1.52
1	A	253	VAL	N-CA	-7.09	1.37	1.46
1	A	649	ALA	N-CA	-7.09	1.37	1.46
1	B	548	ALA	CA-C	-7.08	1.43	1.52
1	B	190	VAL	N-CA	-7.08	1.38	1.46
1	B	203	SER	CA-C	-7.08	1.43	1.52
1	B	153	PHE	CA-C	-7.08	1.43	1.52
1	B	638	SER	CA-C	-7.08	1.43	1.52
1	B	268	GLU	CA-C	-7.07	1.45	1.53
1	B	664	ASP	CA-C	-7.07	1.43	1.52
1	B	233	ALA	CA-C	-7.07	1.43	1.52
1	B	498	ASN	N-CA	-7.06	1.37	1.46
1	B	43	THR	N-CA	-7.05	1.36	1.46
1	A	255	THR	CA-C	-7.05	1.43	1.52
1	B	380	ASN	CA-C	-7.05	1.43	1.52
1	B	237	PHE	N-CA	-7.05	1.37	1.46
1	B	724	ARG	CA-C	-7.04	1.43	1.52
1	A	584	SER	CA-C	-7.04	1.44	1.52
1	B	502	VAL	CA-C	-7.04	1.43	1.52
1	B	551	TYR	CA-C	-7.04	1.42	1.52
1	A	722	ARG	N-CA	-7.04	1.38	1.46
1	B	542	THR	CA-C	-7.03	1.44	1.52
1	B	680	MET	N-CA	-7.02	1.37	1.46
1	B	491	MET	N-CA	-7.01	1.36	1.46
1	A	492	HIS	N-CA	-7.01	1.37	1.46
1	A	338	GLU	CA-C	-7.01	1.42	1.52
1	A	493	TYR	N-CA	-7.01	1.37	1.46
1	B	238	GLU	N-CA	-7.01	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	ASN	CA-C	-7.00	1.43	1.52
1	B	319	PRO	N-CA	-7.00	1.38	1.47
1	A	119	LYS	CA-C	-7.00	1.44	1.53
1	A	497	HIS	CA-C	-7.00	1.43	1.52
1	B	337	ASN	CA-C	-6.99	1.42	1.52
1	A	289	ALA	CA-C	-6.99	1.43	1.52
1	B	274	ARG	CA-C	-6.99	1.43	1.52
1	A	548	ALA	CA-C	-6.98	1.43	1.52
1	B	172	TYR	N-CA	-6.98	1.37	1.46
1	B	198	MET	N-CA	-6.97	1.38	1.46
1	A	631	ALA	CA-C	-6.97	1.43	1.52
1	A	179	THR	CA-C	-6.97	1.44	1.52
1	A	10	ASN	CA-C	-6.97	1.46	1.53
1	A	20	PHE	N-CA	-6.97	1.38	1.46
1	B	55	GLU	CA-C	-6.95	1.43	1.52
1	B	570	ASN	CA-C	-6.95	1.43	1.52
1	A	414	VAL	N-CA	-6.94	1.37	1.46
1	B	9	LEU	CA-C	-6.94	1.43	1.52
1	A	741	SER	CA-C	-6.93	1.43	1.52
1	B	370	ILE	CA-C	-6.93	1.44	1.52
1	A	449	TYR	CA-C	-6.93	1.43	1.52
1	A	490	VAL	N-CA	-6.93	1.38	1.46
1	A	186	LEU	N-CA	-6.92	1.38	1.46
1	B	603	THR	CA-C	-6.92	1.44	1.52
1	B	643	ASP	N-CA	-6.92	1.37	1.46
1	B	263	PRO	CA-C	-6.92	1.42	1.52
1	A	673	THR	N-CA	-6.91	1.38	1.46
1	B	648	ALA	CA-C	-6.91	1.43	1.52
1	A	695	GLN	CA-C	-6.91	1.43	1.52
1	A	295	GLN	N-CA	-6.91	1.37	1.46
1	B	504	SER	N-CA	-6.90	1.37	1.46
1	B	748	LYS	N-CA	-6.89	1.38	1.46
1	A	746	LEU	CA-C	-6.88	1.43	1.52
1	A	13	ALA	CA-C	-6.87	1.43	1.52
1	A	686	ILE	CA-C	-6.86	1.42	1.52
1	B	694	ALA	N-CA	-6.86	1.38	1.46
1	A	523	ARG	N-CA	-6.86	1.37	1.46
1	B	5	LYS	CA-C	-6.86	1.44	1.52
1	B	184	TYR	CA-C	-6.86	1.43	1.52
1	B	209	MET	CA-C	-6.86	1.43	1.52
1	B	399	ALA	CA-C	-6.86	1.43	1.52
1	A	482	SER	CA-C	-6.85	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	ALA	CA-C	-6.85	1.43	1.52
1	B	199	LEU	N-CA	-6.85	1.36	1.46
1	A	519	VAL	N-CA	-6.85	1.38	1.46
1	A	195	LEU	N-CA	-6.84	1.37	1.46
1	A	336	ILE	N-CA	-6.84	1.38	1.46
1	A	679	GLU	CA-C	-6.84	1.43	1.52
1	B	289	ALA	N-CA	-6.84	1.38	1.46
1	A	325	MET	CA-C	-6.83	1.45	1.53
1	A	532	TYR	CA-C	-6.83	1.43	1.52
1	B	109	TYR	CA-C	-6.83	1.43	1.52
1	B	505	GLU	N-CA	-6.82	1.36	1.45
1	B	671	ALA	CA-C	-6.82	1.44	1.52
1	B	62	ASP	C-N	-6.82	1.25	1.34
1	A	290	LEU	N-CA	-6.82	1.37	1.46
1	B	238	GLU	CA-C	-6.82	1.44	1.52
1	B	298	VAL	CA-C	-6.82	1.43	1.52
1	A	402	ALA	N-CA	-6.81	1.40	1.46
1	B	293	ALA	CA-C	-6.81	1.44	1.52
1	B	445	VAL	N-CA	-6.81	1.37	1.46
1	B	623	ILE	CA-C	-6.81	1.44	1.52
1	B	310	ASP	CA-C	-6.81	1.44	1.53
1	A	732	LEU	CA-C	-6.81	1.43	1.52
1	B	377	LYS	N-CA	-6.81	1.37	1.46
1	B	193	SER	N-CA	-6.81	1.37	1.46
1	B	395	ASP	N-CA	-6.81	1.38	1.46
1	B	39	GLN	CA-C	-6.80	1.45	1.53
1	B	698	ILE	N-CA	-6.80	1.38	1.46
1	A	134	GLN	CA-C	-6.80	1.44	1.52
1	B	126	VAL	C-N	-6.80	1.25	1.33
1	B	446	GLU	CA-C	-6.80	1.44	1.52
1	B	539	SER	CA-C	-6.80	1.45	1.53
1	A	146	PHE	N-CA	-6.79	1.37	1.46
1	A	448	ASP	CA-C	-6.79	1.43	1.52
1	B	92	TYR	CA-C	-6.79	1.44	1.52
1	A	675	LEU	N-CA	-6.79	1.38	1.46
1	B	329	SER	CA-C	-6.77	1.44	1.52
1	B	666	ARG	N-CA	-6.77	1.38	1.46
1	B	295	GLN	CA-C	-6.76	1.44	1.52
1	B	345	GLN	CA-C	-6.76	1.44	1.52
1	A	290	LEU	CA-C	-6.76	1.43	1.52
1	A	295	GLN	CA-C	-6.76	1.43	1.52
1	A	462	LEU	CA-C	-6.75	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	483	MET	N-CA	-6.74	1.37	1.46
1	B	20	PHE	CA-C	-6.74	1.44	1.52
1	A	718	ILE	CA-C	-6.74	1.45	1.52
1	B	143	HIS	CA-C	-6.73	1.44	1.52
1	B	647	LEU	N-CA	-6.73	1.38	1.46
1	B	672	VAL	N-CA	-6.73	1.37	1.46
1	A	482	SER	N-CA	-6.72	1.38	1.46
1	B	201	ALA	N-CA	-6.72	1.38	1.46
1	A	313	LEU	CA-C	-6.72	1.44	1.52
1	A	185	ALA	N-CA	-6.71	1.38	1.46
1	B	451	LEU	N-CA	-6.71	1.37	1.46
1	B	188	ASP	CA-C	-6.71	1.43	1.52
1	B	596	THR	CA-C	-6.70	1.44	1.52
1	B	729	LEU	CA-C	-6.70	1.43	1.52
1	B	338	GLU	CA-C	-6.70	1.43	1.52
1	B	103	TRP	CA-C	-6.69	1.44	1.52
1	B	256	ILE	N-CA	-6.69	1.38	1.46
1	B	459	ILE	CA-C	-6.68	1.44	1.52
1	B	697	ARG	CA-C	-6.67	1.43	1.52
1	A	135	LEU	CA-C	-6.67	1.43	1.52
1	B	321	PHE	N-CA	-6.67	1.38	1.46
1	B	576	HIS	CA-C	-6.67	1.44	1.52
1	B	473	ALA	CA-C	-6.67	1.44	1.52
1	A	483	MET	CA-C	-6.66	1.43	1.52
1	B	549	ILE	N-CA	-6.66	1.37	1.46
1	B	559	GLU	CA-C	-6.65	1.43	1.52
1	A	608	GLU	CA-C	-6.64	1.44	1.52
1	B	214	PHE	N-CA	-6.64	1.37	1.46
1	A	401	LEU	N-CA	-6.64	1.38	1.46
1	B	681	ILE	CA-C	-6.63	1.43	1.52
1	B	572	THR	N-CA	-6.63	1.37	1.46
1	A	69	LEU	N-CA	-6.63	1.38	1.46
1	A	632	ILE	CA-C	-6.63	1.43	1.52
1	A	594	SER	CA-C	-6.63	1.44	1.52
1	B	418	THR	CA-C	-6.63	1.44	1.52
1	B	421	TYR	N-CA	-6.63	1.37	1.45
1	B	496	ALA	CA-C	-6.62	1.44	1.52
1	B	545	PRO	CA-C	-6.62	1.42	1.52
1	A	21	ALA	N-CA	-6.62	1.38	1.46
1	B	301	ARG	N-CA	-6.62	1.37	1.46
1	A	698	ILE	CA-C	-6.62	1.44	1.52
1	B	138	LEU	N-CA	-6.62	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	732	LEU	N-CA	-6.62	1.38	1.46
1	B	149	ILE	CA-C	-6.61	1.44	1.52
1	A	488	ALA	N-CA	-6.60	1.38	1.46
1	B	340	THR	CA-C	-6.60	1.44	1.52
1	B	444	VAL	N-CA	-6.60	1.38	1.46
1	B	646	THR	N-CA	-6.59	1.38	1.46
1	A	547	GLU	N-CA	-6.59	1.38	1.46
1	B	273	ALA	CA-C	-6.59	1.43	1.52
1	A	9	LEU	CA-C	-6.58	1.44	1.52
1	A	612	LEU	CA-C	-6.57	1.44	1.52
1	A	301	ARG	CA-C	-6.57	1.44	1.52
1	A	71	PHE	CA-C	-6.57	1.44	1.52
1	A	212	ALA	CA-C	-6.57	1.44	1.52
1	B	476	SER	CA-C	-6.56	1.44	1.52
1	B	705	ARG	CA-C	-6.56	1.44	1.52
1	B	737	LEU	N-CA	-6.56	1.37	1.46
1	A	658	ALA	CA-C	-6.55	1.44	1.52
1	B	56	VAL	CA-C	-6.55	1.44	1.52
1	A	158	LEU	CA-C	-6.54	1.44	1.52
1	B	631	ALA	CA-C	-6.53	1.43	1.52
1	B	416	ASN	CA-C	-6.53	1.43	1.52
1	A	292	ILE	N-CA	-6.53	1.38	1.46
1	B	689	SER	N-CA	-6.53	1.38	1.46
1	B	93	HIS	N-CA	-6.52	1.38	1.46
1	A	254	LEU	CA-C	-6.51	1.44	1.52
1	A	506	HIS	CA-C	-6.51	1.44	1.52
1	B	138	LEU	CA-C	-6.51	1.44	1.52
1	A	259	ARG	N-CA	-6.51	1.38	1.46
1	A	731	VAL	CA-C	-6.51	1.44	1.52
1	B	498	ASN	CA-C	-6.50	1.44	1.52
1	A	129	THR	CA-C	-6.50	1.44	1.52
1	A	258	GLY	CA-C	-6.50	1.44	1.51
1	B	311	GLU	CA-C	-6.50	1.44	1.52
1	B	145	LEU	N-CA	-6.50	1.38	1.46
1	A	148	HIS	CA-C	-6.49	1.44	1.52
1	B	699	VAL	CA-C	-6.49	1.44	1.52
1	A	493	TYR	CA-C	-6.48	1.44	1.52
1	B	679	GLU	CA-C	-6.48	1.43	1.52
1	A	203	SER	N-CA	-6.48	1.37	1.46
1	A	742	GLU	CA-C	-6.48	1.43	1.52
1	A	37	PRO	CA-C	-6.47	1.45	1.52
1	B	747	THR	CA-C	-6.47	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	GLU	N-CA	-6.47	1.37	1.46
1	A	256	ILE	N-CA	-6.47	1.39	1.46
1	B	610	GLU	CA-C	-6.47	1.43	1.52
1	A	136	ARG	CA-C	-6.46	1.44	1.52
1	A	443	SER	CA-C	-6.46	1.44	1.52
1	A	514	GLY	CA-C	-6.46	1.42	1.51
1	A	43	THR	CA-C	-6.46	1.44	1.52
1	A	647	LEU	CA-C	-6.46	1.44	1.52
1	B	195	LEU	N-CA	-6.46	1.38	1.46
1	B	60	ASN	CA-C	-6.46	1.44	1.52
1	B	319	PRO	CA-C	-6.46	1.43	1.52
1	A	447	ARG	N-CA	-6.46	1.38	1.46
1	B	754	ASN	CA-C	-6.46	1.44	1.52
1	B	20	PHE	N-CA	-6.45	1.38	1.46
1	A	727	ALA	N-CA	-6.45	1.38	1.46
1	B	108	ALA	CA-C	-6.45	1.44	1.52
1	B	417	ARG	CA-C	-6.45	1.43	1.52
1	A	4	LEU	CA-C	-6.44	1.44	1.52
1	A	555	ILE	N-CA	-6.44	1.38	1.46
1	B	129	THR	CA-C	-6.44	1.44	1.52
1	B	133	GLU	CA-C	-6.43	1.43	1.52
1	B	500	GLU	CA-C	-6.42	1.45	1.52
1	A	143	HIS	N-CA	-6.42	1.37	1.45
1	A	213	THR	CA-C	-6.42	1.46	1.53
1	B	69	LEU	CA-C	-6.42	1.44	1.52
1	B	581	HIS	N-CA	-6.42	1.38	1.46
1	B	493	TYR	CA-C	-6.40	1.44	1.52
1	B	544	GLU	C-N	-6.40	1.25	1.34
1	A	374	THR	CA-C	-6.40	1.44	1.52
1	B	585	THR	CA-C	-6.40	1.44	1.52
1	A	395	ASP	N-CA	-6.39	1.38	1.46
1	A	584	SER	N-CA	-6.39	1.37	1.45
1	B	227	GLN	N-CA	-6.38	1.38	1.46
1	A	570	ASN	CA-C	-6.38	1.44	1.52
1	A	74	ALA	CA-C	-6.37	1.44	1.52
1	B	379	ALA	CA-C	-6.37	1.44	1.52
1	B	731	VAL	CA-C	-6.37	1.44	1.52
1	A	65	MET	N-CA	-6.37	1.38	1.46
1	B	490	VAL	N-CA	-6.36	1.39	1.46
1	B	252	SER	N-CA	-6.35	1.38	1.46
1	B	662	ALA	N-CA	-6.35	1.38	1.46
1	B	146	PHE	CA-C	-6.34	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	477	ASN	CA-C	-6.34	1.44	1.52
1	A	257	LEU	N-CA	-6.34	1.38	1.46
1	A	90	THR	N-CA	-6.33	1.38	1.46
1	B	226	SER	CA-C	-6.33	1.44	1.52
1	A	684	THR	CA-C	-6.33	1.45	1.52
1	B	158	LEU	CA-C	-6.33	1.43	1.52
1	B	532	TYR	CA-C	-6.33	1.44	1.52
1	A	541	ARG	N-CA	-6.33	1.38	1.46
1	A	697	ARG	CA-C	-6.32	1.44	1.52
1	B	494	ALA	N-CA	-6.32	1.38	1.46
1	B	230	ALA	N-CA	-6.32	1.38	1.46
1	B	235	THR	N-CA	-6.32	1.38	1.46
1	A	384	GLN	N-CA	-6.32	1.38	1.46
1	A	602	TYR	CA-C	-6.32	1.45	1.52
1	A	694	ALA	N-CA	-6.32	1.38	1.46
1	B	439	LEU	CA-C	-6.31	1.45	1.52
1	B	723	ILE	N-CA	-6.31	1.38	1.46
1	A	417	ARG	CA-C	-6.31	1.43	1.52
1	B	107	THR	N-CA	-6.31	1.38	1.46
1	B	14	ARG	CA-C	-6.30	1.44	1.52
1	B	105	LYS	N-CA	-6.30	1.38	1.46
1	A	143	HIS	CA-C	-6.30	1.45	1.52
1	B	111	THR	N-CA	-6.30	1.38	1.46
1	A	171	VAL	N-CA	-6.29	1.38	1.46
1	A	713	ASP	CA-C	-6.29	1.43	1.52
1	B	553	LYS	N-CA	-6.28	1.39	1.46
1	B	229	LEU	N-CA	-6.28	1.38	1.46
1	B	394	SER	CA-C	-6.28	1.44	1.52
1	B	121	ASP	CA-C	-6.28	1.44	1.52
1	B	282	ASP	N-CA	-6.28	1.38	1.46
1	B	464	THR	CA-C	-6.28	1.44	1.52
1	B	528	ILE	CA-C	-6.28	1.46	1.52
1	B	696	SER	N-CA	-6.28	1.39	1.46
1	A	62	ASP	N-CA	-6.28	1.40	1.46
1	B	275	LEU	N-CA	-6.27	1.38	1.46
1	A	722	ARG	CA-C	-6.27	1.44	1.52
1	B	651	ARG	N-CA	-6.27	1.38	1.46
1	A	647	LEU	N-CA	-6.25	1.38	1.46
1	B	70	PHE	N-CA	-6.25	1.38	1.46
1	A	202	LEU	CA-C	-6.25	1.44	1.52
1	B	221	ALA	CA-C	-6.25	1.44	1.53
1	A	433	ASN	CA-C	-6.24	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	SER	CA-C	-6.23	1.44	1.52
1	A	377	LYS	CA-C	-6.23	1.45	1.52
1	B	232	ALA	CA-C	-6.22	1.44	1.52
1	A	321	PHE	CA-C	-6.22	1.44	1.52
1	B	497	HIS	CA-C	-6.22	1.44	1.52
1	A	129	THR	N-CA	-6.22	1.38	1.46
1	B	413	PHE	N-CA	-6.22	1.39	1.46
1	A	265	THR	N-CA	-6.21	1.40	1.46
1	A	438	THR	N-CA	-6.21	1.38	1.46
1	B	135	LEU	CA-C	-6.21	1.44	1.52
1	A	294	TYR	C-N	-6.20	1.25	1.34
1	B	748	LYS	CA-C	-6.20	1.44	1.52
1	B	108	ALA	N-CA	-6.20	1.38	1.46
1	A	62	ASP	CA-C	-6.20	1.45	1.52
1	B	474	ARG	CA-C	-6.20	1.45	1.52
1	B	115	ASN	CA-C	-6.20	1.44	1.52
1	B	552	ASN	CA-C	-6.19	1.46	1.53
1	B	131	ILE	CA-C	-6.19	1.45	1.52
1	B	467	VAL	CA-C	-6.19	1.43	1.52
1	A	79	ALA	CA-C	-6.18	1.44	1.52
1	A	102	ILE	CA-C	-6.18	1.45	1.52
1	A	718	ILE	N-CA	-6.18	1.39	1.46
1	A	597	ILE	CA-C	-6.17	1.45	1.52
1	B	386	PHE	CA-C	-6.17	1.45	1.52
1	B	194	ASP	N-CA	-6.17	1.38	1.46
1	B	318	ILE	C-O	-6.17	1.19	1.24
1	A	684	THR	N-CA	-6.16	1.39	1.46
1	A	723	ILE	CA-C	-6.16	1.45	1.52
1	B	103	TRP	N-CA	-6.16	1.39	1.46
1	A	677	LYS	N-CA	-6.16	1.39	1.46
1	A	628	VAL	CA-C	-6.16	1.45	1.52
1	B	471	LEU	N-CA	-6.16	1.39	1.46
1	B	227	GLN	CA-C	-6.15	1.44	1.52
1	B	628	VAL	N-CA	-6.15	1.39	1.46
1	A	479	LEU	N-CA	-6.14	1.39	1.46
1	A	480	LYS	N-CA	-6.14	1.38	1.46
1	B	120	ALA	CA-C	-6.14	1.44	1.52
1	A	739	SER	N-CA	-6.14	1.38	1.45
1	A	497	HIS	N-CA	-6.13	1.38	1.46
1	B	284	LEU	CA-C	-6.13	1.43	1.52
1	B	285	ARG	CA-C	-6.13	1.44	1.52
1	B	106	LEU	N-CA	-6.12	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	606	VAL	CA-C	-6.12	1.45	1.52
1	B	457	VAL	CA-C	-6.12	1.43	1.52
1	B	403	PRO	N-CA	-6.12	1.39	1.47
1	B	202	LEU	N-CA	-6.11	1.38	1.46
1	A	713	ASP	N-CA	-6.11	1.38	1.46
1	A	375	PRO	CA-C	-6.11	1.44	1.52
1	A	393	ILE	N-CA	-6.11	1.39	1.46
1	B	141	SER	CA-C	-6.11	1.46	1.53
1	A	661	LEU	N-CA	-6.11	1.39	1.46
1	B	58	LYS	CA-C	-6.11	1.44	1.52
1	A	317	ILE	CA-C	-6.10	1.45	1.52
1	A	601	ARG	CA-C	-6.10	1.45	1.52
1	A	348	ALA	CA-C	-6.10	1.46	1.53
1	B	322	ILE	N-CA	-6.10	1.38	1.46
1	B	151	THR	CA-C	-6.10	1.45	1.52
1	A	629	ALA	N-CA	-6.09	1.38	1.46
1	A	560	VAL	CA-C	-6.09	1.44	1.52
1	B	727	ALA	N-CA	-6.09	1.39	1.46
1	A	472	GLU	CA-C	-6.09	1.44	1.52
1	B	290	LEU	N-CA	-6.08	1.38	1.46
1	B	337	ASN	N-CA	-6.08	1.38	1.46
1	B	732	LEU	CA-C	-6.08	1.44	1.52
1	A	715	HIS	CA-C	-6.08	1.44	1.52
1	B	449	TYR	CA-C	-6.08	1.44	1.52
1	A	678	ILE	N-CA	-6.07	1.39	1.46
1	B	590	GLU	N-CA	-6.07	1.38	1.46
1	B	664	ASP	N-CA	-6.07	1.39	1.46
1	B	721	HIS	N-CA	-6.07	1.38	1.46
1	A	663	ILE	CA-C	-6.06	1.45	1.52
1	B	396	ARG	N-CA	-6.06	1.39	1.46
1	B	399	ALA	N-CA	-6.06	1.38	1.46
1	B	46	ALA	N-CA	-6.06	1.38	1.46
1	A	292	ILE	CA-C	-6.05	1.45	1.52
1	B	126	VAL	N-CA	-6.05	1.39	1.46
1	B	184	TYR	N-CA	-6.05	1.38	1.46
1	A	173	ARG	CA-C	-6.04	1.45	1.52
1	B	702	MET	N-CA	-6.04	1.38	1.46
1	B	125	LYS	CA-C	-6.04	1.45	1.53
1	A	724	ARG	N-CA	-6.03	1.39	1.46
1	B	7	LYS	CA-C	-6.03	1.44	1.52
1	A	641	VAL	CA-C	-6.02	1.45	1.52
1	B	612	LEU	N-CA	-6.02	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ALA	N-CA	-6.02	1.39	1.46
1	A	257	LEU	CA-C	-6.02	1.44	1.52
1	A	475	ALA	CA-C	-6.02	1.44	1.52
1	B	526	LEU	N-CA	-6.01	1.39	1.46
1	B	260	LEU	CA-C	-6.01	1.45	1.52
1	B	91	GLU	CA-C	-6.01	1.45	1.52
1	B	285	ARG	C-N	-6.00	1.25	1.33
1	B	497	HIS	N-CA	-6.00	1.38	1.46
1	B	597	ILE	CA-C	-6.00	1.45	1.52
1	A	147	HIS	N-CA	-6.00	1.39	1.46
1	B	546	LEU	N-CA	-5.99	1.39	1.46
1	A	725	ILE	N-CA	-5.99	1.39	1.46
1	B	67	ALA	N-CA	-5.99	1.38	1.46
1	B	173	ARG	CA-C	-5.99	1.44	1.52
1	A	323	GLU	CA-C	-5.99	1.44	1.52
1	B	161	LEU	CA-C	-5.99	1.45	1.52
1	B	85	LEU	N-CA	-5.99	1.39	1.46
1	B	201	ALA	CA-C	-5.98	1.45	1.52
1	B	396	ARG	CA-C	-5.98	1.45	1.52
1	A	657	ASP	N-CA	-5.97	1.39	1.46
1	B	332	LYS	N-CA	-5.97	1.38	1.46
1	A	199	LEU	N-CA	-5.97	1.39	1.46
1	B	474	ARG	N-CA	-5.97	1.39	1.46
1	B	652	ARG	CA-C	-5.96	1.45	1.52
1	B	404	ILE	N-CA	-5.96	1.39	1.46
1	B	458	ALA	N-CA	-5.96	1.39	1.46
1	B	579	PRO	CA-C	-5.96	1.44	1.52
1	A	187	VAL	CA-C	-5.96	1.45	1.52
1	B	443	SER	CA-C	-5.96	1.44	1.52
1	B	209	MET	N-CA	-5.96	1.38	1.46
1	A	192	ALA	N-CA	-5.95	1.38	1.46
1	B	589	TYR	CA-C	-5.95	1.44	1.52
1	B	323	GLU	CA-C	-5.95	1.44	1.52
1	A	503	VAL	N-CA	-5.95	1.39	1.46
1	B	249	VAL	CA-C	-5.95	1.45	1.52
1	B	412	ALA	N-CA	-5.95	1.38	1.46
1	B	157	VAL	N-CA	-5.94	1.38	1.46
1	B	575	ILE	CA-C	-5.94	1.45	1.52
1	B	661	LEU	CA-C	-5.94	1.45	1.52
1	B	466	ILE	CA-C	-5.94	1.45	1.52
1	A	133	GLU	N-CA	-5.93	1.38	1.46
1	B	136	ARG	N-CA	-5.93	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	ARG	CA-C	-5.93	1.44	1.52
1	A	297	MET	CA-C	-5.93	1.45	1.52
1	A	288	LEU	CA-C	-5.92	1.45	1.52
1	B	23	GLY	CA-C	-5.92	1.43	1.51
1	A	53	LEU	CA-C	-5.92	1.45	1.52
1	B	739	SER	CA-C	-5.92	1.45	1.53
1	B	611	LEU	CA-C	-5.92	1.44	1.52
1	B	407	THR	N-CA	-5.92	1.38	1.46
1	B	211	GLN	N-CA	-5.92	1.37	1.46
1	B	414	VAL	N-CA	-5.91	1.39	1.46
1	A	43	THR	N-CA	-5.90	1.38	1.46
1	B	734	MET	CA-C	-5.90	1.44	1.52
1	B	71	PHE	N-CA	-5.90	1.39	1.46
1	A	401	LEU	CA-C	-5.89	1.45	1.52
1	B	46	ALA	CA-C	-5.89	1.44	1.52
1	B	261	TRP	N-CA	-5.89	1.39	1.46
1	B	264	SER	N-CA	-5.89	1.38	1.46
1	B	150	THR	CA-C	-5.89	1.44	1.52
1	A	558	SER	CA-C	-5.88	1.44	1.52
1	B	269	LEU	CA-C	-5.88	1.44	1.52
1	A	724	ARG	CA-C	-5.87	1.45	1.52
1	B	62	ASP	CA-C	-5.87	1.45	1.52
1	B	197	ARG	N-CA	-5.86	1.38	1.46
1	B	130	ALA	CA-C	-5.86	1.45	1.52
1	B	487	TYR	CA-C	-5.86	1.45	1.52
1	A	255	THR	N-CA	-5.86	1.39	1.46
1	B	372	ALA	CA-C	-5.86	1.45	1.52
1	A	253	VAL	CA-C	-5.85	1.45	1.52
1	A	372	ALA	CA-C	-5.85	1.45	1.52
1	A	494	ALA	C-N	-5.85	1.26	1.33
1	B	488	ALA	C-O	-5.85	1.17	1.24
1	B	153	PHE	C-N	-5.85	1.27	1.33
1	B	395	ASP	CA-C	-5.85	1.45	1.52
1	B	6	VAL	CA-C	-5.85	1.46	1.52
1	A	549	ILE	N-CA	-5.84	1.38	1.46
1	B	127	PRO	CA-C	-5.84	1.46	1.52
1	A	22	ILE	CA-C	-5.84	1.44	1.52
1	B	521	ASN	N-CA	-5.84	1.39	1.45
1	B	344	GLY	CA-C	-5.84	1.46	1.52
1	B	480	LYS	N-CA	-5.84	1.39	1.46
1	A	341	SER	N-CA	-5.84	1.38	1.46
1	B	697	ARG	N-CA	-5.83	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	693	LEU	CA-C	-5.83	1.45	1.52
1	B	484	PHE	N-CA	-5.83	1.39	1.46
1	B	740	ARG	CA-C	-5.83	1.45	1.52
1	A	502	VAL	CA-C	-5.83	1.45	1.52
1	B	602	TYR	N-CA	-5.82	1.38	1.46
1	B	402	ALA	C-N	-5.82	1.26	1.33
1	B	702	MET	CA-C	-5.82	1.44	1.52
1	A	103	TRP	CA-C	-5.82	1.45	1.52
1	A	174	VAL	CA-C	-5.82	1.45	1.52
1	A	526	LEU	CA-C	-5.81	1.45	1.52
1	A	708	ILE	N-CA	-5.81	1.40	1.46
1	B	718	ILE	C-N	-5.81	1.26	1.34
1	A	614	LEU	CA-C	-5.81	1.45	1.52
1	B	686	ILE	N-CA	-5.81	1.38	1.46
1	B	210	LEU	CA-C	-5.81	1.45	1.52
1	A	705	ARG	CA-C	-5.80	1.46	1.53
1	A	611	LEU	CA-C	-5.80	1.45	1.52
1	B	499	PRO	CA-C	-5.80	1.44	1.52
1	A	30	SER	CA-C	-5.80	1.45	1.53
1	B	506	HIS	N-CA	-5.80	1.38	1.46
1	A	406	ASN	N-CA	-5.79	1.39	1.46
1	B	312	GLU	CA-C	-5.79	1.45	1.52
1	B	486	TYR	CA-C	-5.79	1.45	1.52
1	A	726	TRP	N-CA	-5.79	1.39	1.46
1	B	666	ARG	CA-C	-5.79	1.45	1.52
1	B	254	LEU	N-CA	-5.79	1.39	1.46
1	A	137	THR	CA-C	-5.78	1.45	1.52
1	B	212	ALA	CA-C	-5.78	1.45	1.52
1	B	405	GLY	CA-C	-5.78	1.45	1.52
1	B	450	ALA	N-CA	-5.78	1.38	1.46
1	B	691	VAL	N-CA	-5.78	1.39	1.46
1	B	642	GLU	N-CA	-5.77	1.39	1.46
1	A	668	MET	N-CA	-5.77	1.38	1.46
1	B	106	LEU	CA-C	-5.76	1.45	1.52
1	A	712	SER	N-CA	-5.76	1.39	1.46
1	B	151	THR	N-CA	-5.76	1.39	1.46
1	A	214	PHE	CA-C	-5.76	1.45	1.52
1	A	246	ALA	N-CA	-5.75	1.38	1.46
1	B	549	ILE	CA-C	-5.75	1.44	1.52
1	A	155	CYS	CA-C	-5.75	1.45	1.52
1	B	331	PHE	N-CA	-5.75	1.39	1.46
1	A	704	GLY	CA-C	-5.74	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	GLY	CA-C	-5.74	1.41	1.52
1	B	290	LEU	CA-C	-5.74	1.44	1.52
1	A	188	ASP	N-CA	-5.73	1.39	1.46
1	A	316	THR	N-CA	-5.73	1.38	1.46
1	B	610	GLU	N-CA	-5.73	1.38	1.46
1	A	187	VAL	N-CA	-5.72	1.39	1.46
1	A	556	GLN	N-CA	-5.72	1.38	1.46
1	B	326	SER	CA-C	-5.72	1.45	1.52
1	B	632	ILE	N-CA	-5.72	1.39	1.46
1	B	147	HIS	C-N	-5.71	1.26	1.34
1	A	426	GLN	N-CA	-5.71	1.38	1.46
1	A	99	ASN	CA-C	-5.70	1.45	1.52
1	A	266	PRO	N-CA	-5.70	1.43	1.47
1	A	639	TRP	N-CA	-5.70	1.39	1.46
1	A	652	ARG	CA-C	-5.70	1.45	1.52
1	A	42	ARG	N-CA	-5.70	1.38	1.45
1	A	227	GLN	CA-C	-5.70	1.45	1.52
1	A	505	GLU	CA-C	-5.69	1.45	1.53
1	B	49	THR	CA-C	-5.69	1.45	1.52
1	B	584	SER	CA-C	-5.69	1.45	1.52
1	B	475	ALA	CA-C	-5.69	1.45	1.52
1	A	677	LYS	CA-C	-5.69	1.45	1.52
1	B	327	GLU	CA-C	-5.69	1.45	1.52
1	B	457	VAL	N-CA	-5.69	1.39	1.46
1	A	476	SER	CA-C	-5.68	1.45	1.52
1	B	309	SER	CA-C	-5.68	1.45	1.53
1	B	231	ASN	N-CA	-5.68	1.39	1.46
1	A	729	LEU	CA-C	-5.67	1.45	1.52
1	A	503	VAL	CA-C	-5.67	1.45	1.52
1	B	368	LYS	CA-C	-5.67	1.45	1.52
1	A	249	VAL	N-CA	-5.67	1.39	1.46
1	B	481	ARG	N-CA	-5.66	1.39	1.46
1	A	546	LEU	C-N	-5.66	1.26	1.33
1	B	394	SER	C-N	-5.66	1.26	1.33
1	A	267	LYS	CA-C	-5.66	1.45	1.52
1	B	101	GLU	N-CA	-5.66	1.39	1.46
1	B	646	THR	CA-C	-5.66	1.45	1.52
1	B	52	LEU	N-CA	-5.66	1.39	1.46
1	B	131	ILE	C-N	-5.65	1.26	1.33
1	B	541	ARG	N-CA	-5.65	1.39	1.46
1	B	530	VAL	CA-C	-5.65	1.45	1.52
1	A	200	THR	N-CA	-5.64	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	PHE	CA-C	-5.64	1.45	1.52
1	B	525	GLU	N-CA	-5.64	1.39	1.46
1	B	406	ASN	CA-C	-5.64	1.45	1.52
1	A	8	ASP	CA-C	-5.64	1.45	1.52
1	A	700	ASP	N-CA	-5.63	1.39	1.46
1	A	418	THR	CA-C	-5.63	1.45	1.52
1	A	552	ASN	CA-C	-5.63	1.45	1.52
1	A	696	SER	CA-C	-5.63	1.45	1.52
1	B	144	GLU	CA-C	-5.62	1.45	1.52
1	A	17	THR	CA-C	-5.62	1.45	1.52
1	B	649	ALA	CA-C	-5.62	1.45	1.52
1	B	453	ARG	CA-C	-5.62	1.45	1.52
1	A	405	GLY	CA-C	-5.62	1.45	1.52
1	B	192	ALA	N-CA	-5.62	1.38	1.46
1	B	575	ILE	N-CA	-5.61	1.39	1.46
1	B	74	ALA	CA-C	-5.61	1.45	1.52
1	B	415	LYS	N-CA	-5.61	1.39	1.46
1	A	730	ALA	CA-C	-5.61	1.45	1.52
1	B	561	LEU	CA-C	-5.61	1.45	1.52
1	B	247	ASN	CA-C	-5.61	1.45	1.52
1	A	394	SER	CA-C	-5.60	1.45	1.52
1	B	129	THR	N-CA	-5.60	1.39	1.46
1	B	232	ALA	N-CA	-5.60	1.39	1.46
1	B	172	TYR	CA-C	-5.59	1.45	1.52
1	A	634	GLN	CA-C	-5.59	1.45	1.52
1	A	170	TYR	CA-C	-5.58	1.46	1.52
1	A	690	ALA	N-CA	-5.57	1.39	1.46
1	B	156	HIS	CA-C	-5.57	1.44	1.52
1	B	456	MET	CA-C	-5.57	1.44	1.52
1	A	192	ALA	CA-C	-5.57	1.45	1.52
1	A	699	VAL	N-CA	-5.57	1.39	1.46
1	B	451	LEU	CA-C	-5.57	1.44	1.52
1	B	470	SER	CA-C	-5.57	1.45	1.52
1	B	678	ILE	N-CA	-5.57	1.39	1.46
1	B	202	LEU	CA-C	-5.57	1.45	1.52
1	A	9	LEU	N-CA	-5.57	1.39	1.46
1	B	503	VAL	N-CA	-5.57	1.39	1.46
1	B	188	ASP	N-CA	-5.56	1.39	1.46
1	B	432	SER	CA-C	-5.56	1.45	1.52
1	B	727	ALA	CA-C	-5.56	1.45	1.52
1	A	236	ALA	CA-C	-5.56	1.45	1.52
1	A	381	ASN	CA-C	-5.56	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	731	VAL	N-CA	-5.56	1.39	1.46
1	B	526	LEU	CA-C	-5.55	1.46	1.52
1	A	213	THR	N-CA	-5.55	1.39	1.46
1	A	513	GLN	CA-C	-5.54	1.45	1.52
1	A	245	ASP	CA-C	-5.54	1.44	1.52
1	B	722	ARG	N-CA	-5.54	1.39	1.46
1	B	362	GLU	CA-C	-5.54	1.46	1.52
1	B	684	THR	CA-C	-5.53	1.45	1.52
1	A	484	PHE	CA-C	-5.53	1.45	1.52
1	A	474	ARG	CA-C	-5.53	1.45	1.52
1	A	193	SER	N-CA	-5.53	1.39	1.46
1	B	95	SER	N-CA	-5.53	1.39	1.46
1	B	543	PRO	CA-C	-5.53	1.44	1.52
1	B	459	ILE	N-CA	-5.52	1.40	1.46
1	B	236	ALA	N-CA	-5.51	1.39	1.46
1	A	486	TYR	N-CA	-5.51	1.40	1.46
1	A	747	THR	N-CA	-5.51	1.39	1.46
1	B	411	SER	N-CA	-5.50	1.39	1.46
1	A	728	GLY	CA-C	-5.50	1.46	1.52
1	B	12	SER	CA-C	-5.50	1.45	1.52
1	B	155	CYS	N-CA	-5.50	1.39	1.46
1	B	650	ALA	CA-C	-5.50	1.45	1.52
1	B	88	GLN	N-CA	-5.50	1.39	1.46
1	B	602	TYR	CA-C	-5.50	1.46	1.52
1	B	445	VAL	CA-C	-5.50	1.45	1.52
1	A	291	PHE	CA-C	-5.49	1.45	1.52
1	B	639	TRP	N-CA	-5.49	1.39	1.46
1	B	479	LEU	N-CA	-5.49	1.39	1.46
1	A	80	LEU	CA-C	-5.49	1.45	1.52
1	A	251	SER	N-CA	-5.49	1.39	1.46
1	A	294	TYR	N-CA	-5.49	1.39	1.46
1	B	339	THR	N-CA	-5.49	1.39	1.46
1	B	450	ALA	CA-C	-5.48	1.45	1.52
1	B	83	ASP	CA-C	-5.48	1.45	1.52
1	B	342	TYR	CA-C	-5.48	1.45	1.52
1	A	577	ILE	N-CA	-5.48	1.39	1.46
1	B	82	VAL	CA-C	-5.48	1.45	1.52
1	B	630	HIS	CA-C	-5.48	1.45	1.52
1	A	385	ARG	N-CA	-5.47	1.39	1.46
1	B	527	ARG	CA-C	-5.47	1.45	1.52
1	B	562	GLN	CA-C	-5.47	1.45	1.52
1	B	519	VAL	CA-C	-5.47	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	622	ARG	CA-C	-5.46	1.46	1.52
1	B	186	LEU	N-CA	-5.46	1.39	1.46
1	A	688	ALA	CA-C	-5.46	1.45	1.52
1	B	649	ALA	N-CA	-5.46	1.39	1.46
1	B	597	ILE	N-CA	-5.46	1.40	1.46
1	A	91	GLU	N-CA	-5.45	1.39	1.46
1	A	291	PHE	N-CA	-5.45	1.39	1.46
1	B	128	PRO	CA-C	-5.45	1.44	1.52
1	B	631	ALA	N-CA	-5.45	1.39	1.46
1	A	733	GLN	CA-C	-5.45	1.45	1.52
1	A	226	SER	CA-C	-5.44	1.45	1.52
1	B	132	LEU	CA-C	-5.44	1.45	1.52
1	A	645	ARG	N-CA	-5.43	1.40	1.46
1	B	547	GLU	CA-C	-5.43	1.45	1.52
1	B	8	ASP	CA-C	-5.43	1.45	1.52
1	B	565	VAL	N-CA	-5.43	1.40	1.46
1	A	287	ASN	CA-C	-5.42	1.46	1.52
1	A	680	MET	N-CA	-5.42	1.39	1.46
1	A	378	LEU	CA-C	-5.42	1.45	1.52
1	B	251	SER	CA-C	-5.42	1.45	1.52
1	B	4	LEU	CA-C	-5.41	1.45	1.52
1	A	365	GLN	N-CA	-5.41	1.39	1.45
1	B	3	ASN	CA-C	-5.41	1.46	1.52
1	A	179	THR	N-CA	-5.41	1.40	1.46
1	B	479	LEU	CA-C	-5.41	1.45	1.52
1	B	714	LEU	CA-C	-5.41	1.45	1.52
1	A	62	ASP	C-N	-5.41	1.26	1.33
1	A	190	VAL	N-CA	-5.41	1.39	1.46
1	B	435	ALA	CA-C	-5.41	1.45	1.52
1	B	741	SER	CA-C	-5.41	1.46	1.52
1	A	646	THR	CA-C	-5.41	1.45	1.52
1	A	672	VAL	C-O	-5.41	1.17	1.24
1	B	742	GLU	N-CA	-5.41	1.39	1.46
1	A	403	PRO	CA-C	-5.40	1.43	1.52
1	B	299	LYS	CA-C	-5.40	1.45	1.52
1	B	738	LEU	CA-C	-5.40	1.46	1.52
1	A	618	ARG	CA-C	-5.40	1.45	1.52
1	A	261	TRP	CA-C	-5.40	1.45	1.52
1	A	487	TYR	N-CA	-5.40	1.39	1.46
1	B	582	GLU	N-CA	-5.40	1.39	1.46
1	A	720	ARG	N-CA	-5.40	1.39	1.46
1	A	107	THR	CA-C	-5.39	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	GLU	CA-C	-5.39	1.45	1.52
1	B	518	LEU	N-CA	-5.39	1.39	1.45
1	B	686	ILE	CA-C	-5.39	1.44	1.52
1	B	118	ILE	N-CA	-5.39	1.39	1.46
1	A	416	ASN	N-CA	-5.39	1.39	1.46
1	A	668	MET	CA-C	-5.38	1.45	1.52
1	B	359	VAL	N-CA	-5.38	1.40	1.46
1	B	393	ILE	N-CA	-5.37	1.39	1.46
1	B	576	HIS	N-CA	-5.37	1.39	1.46
1	A	471	LEU	CA-C	-5.37	1.46	1.52
1	B	418	THR	N-CA	-5.37	1.39	1.46
1	A	696	SER	N-CA	-5.36	1.40	1.46
1	A	211	GLN	CA-C	-5.36	1.45	1.52
1	A	356	SER	N-CA	-5.36	1.42	1.47
1	B	98	CYS	N-CA	-5.36	1.39	1.46
1	B	179	THR	CA-C	-5.36	1.45	1.52
1	A	623	ILE	N-CA	-5.36	1.39	1.46
1	A	749	VAL	N-CA	-5.35	1.38	1.46
1	A	319	PRO	C-N	-5.35	1.26	1.33
1	B	397	MET	N-CA	-5.34	1.39	1.46
1	A	171	VAL	CA-C	-5.34	1.46	1.52
1	A	266	PRO	CA-C	-5.34	1.46	1.53
1	A	580	TRP	CA-C	-5.33	1.45	1.52
1	B	422	GLU	N-CA	-5.33	1.39	1.46
1	A	346	THR	CA-C	-5.33	1.46	1.52
1	B	61	ILE	CA-C	-5.33	1.46	1.52
1	A	254	LEU	N-CA	-5.33	1.40	1.46
1	A	293	ALA	N-CA	-5.33	1.39	1.46
1	B	723	ILE	CA-C	-5.32	1.45	1.52
1	A	423	ALA	N-CA	-5.32	1.38	1.45
1	B	5	LYS	N-CA	-5.32	1.39	1.46
1	A	394	SER	C-N	-5.32	1.26	1.33
1	A	694	ALA	CA-C	-5.31	1.45	1.52
1	B	119	LYS	CA-C	-5.31	1.45	1.52
1	B	301	ARG	CA-C	-5.31	1.45	1.52
1	B	218	GLY	CA-C	-5.31	1.44	1.51
1	A	135	LEU	N-CA	-5.31	1.39	1.46
1	A	483	MET	N-CA	-5.31	1.39	1.46
1	A	31	VAL	N-CA	-5.31	1.39	1.46
1	A	251	SER	CA-C	-5.31	1.45	1.52
1	A	447	ARG	CA-C	-5.31	1.45	1.52
1	B	101	GLU	CA-C	-5.31	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	638	SER	N-CA	-5.30	1.39	1.46
1	A	437	MET	N-CA	-5.30	1.39	1.46
1	B	348	ALA	CA-C	-5.30	1.46	1.52
1	B	17	THR	CA-C	-5.30	1.46	1.52
1	B	361	TYR	N-CA	-5.29	1.39	1.45
1	B	604	ALA	CA-C	-5.29	1.46	1.52
1	A	744	GLU	CA-C	-5.29	1.45	1.52
1	A	689	SER	CA-C	-5.28	1.45	1.52
1	A	366	PHE	CA-C	-5.28	1.45	1.52
1	B	329	SER	N-CA	-5.28	1.38	1.46
1	B	250	VAL	CA-C	-5.28	1.46	1.52
1	A	21	ALA	CA-C	-5.27	1.46	1.52
1	A	463	ARG	CA-C	-5.27	1.46	1.52
1	B	315	SER	N-CA	-5.27	1.36	1.46
1	A	261	TRP	N-CA	-5.27	1.39	1.46
1	B	541	ARG	CA-C	-5.26	1.45	1.52
1	B	200	THR	N-CA	-5.25	1.40	1.46
1	A	439	LEU	N-CA	-5.25	1.40	1.46
1	B	565	VAL	CA-C	-5.25	1.46	1.52
1	A	443	SER	N-CA	-5.24	1.40	1.46
1	B	171	VAL	N-CA	-5.24	1.40	1.46
1	B	652	ARG	N-CA	-5.24	1.40	1.46
1	A	650	ALA	CA-C	-5.24	1.46	1.52
1	B	274	ARG	N-CA	-5.24	1.39	1.46
1	A	534	ALA	N-CA	-5.23	1.39	1.46
1	A	660	LYS	CA-C	-5.23	1.46	1.52
1	A	478	ASP	N-CA	-5.23	1.40	1.46
1	B	269	LEU	N-CA	-5.23	1.39	1.46
1	A	334	ARG	CA-C	-5.22	1.47	1.52
1	A	54	TRP	CA-C	-5.22	1.46	1.52
1	B	730	ALA	CA-C	-5.22	1.45	1.52
1	B	637	TYR	CA-C	-5.22	1.46	1.52
1	B	677	LYS	CA-C	-5.22	1.46	1.52
1	B	196	ARG	N-CA	-5.21	1.39	1.46
1	A	481	ARG	N-CA	-5.21	1.40	1.46
1	B	400	THR	CA-C	-5.21	1.45	1.52
1	B	667	ARG	N-CA	-5.21	1.39	1.46
1	B	287	ASN	N-CA	-5.21	1.39	1.46
1	B	21	ALA	N-CA	-5.21	1.40	1.46
1	A	324	ALA	N-CA	-5.21	1.39	1.46
1	B	283	GLN	C-N	-5.21	1.26	1.33
1	B	86	VAL	N-CA	-5.20	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	ALA	N-CA	-5.20	1.40	1.46
1	A	397	MET	N-CA	-5.20	1.40	1.46
1	B	277	ASN	N-CA	-5.20	1.39	1.46
1	A	178	ALA	N-CA	-5.20	1.39	1.46
1	B	297	MET	N-CA	-5.20	1.40	1.46
1	B	524	THR	CA-C	-5.20	1.45	1.52
1	A	247	ASN	N-CA	-5.19	1.40	1.46
1	A	748	LYS	CA-C	-5.19	1.45	1.52
1	B	24	GLU	CA-C	-5.19	1.45	1.52
1	B	447	ARG	N-CA	-5.19	1.39	1.46
1	B	25	LEU	N-CA	-5.18	1.40	1.46
1	B	580	TRP	CA-C	-5.18	1.46	1.52
1	B	160	PRO	CA-C	-5.18	1.45	1.52
1	A	101	GLU	CA-C	-5.18	1.46	1.52
1	A	13	ALA	N-CA	-5.18	1.39	1.46
1	B	100	PRO	N-CA	-5.18	1.40	1.47
1	B	276	ARG	C-N	-5.17	1.26	1.34
1	B	659	GLU	CA-C	-5.17	1.46	1.52
1	A	706	GLY	CA-C	-5.17	1.44	1.51
1	A	650	ALA	N-CA	-5.17	1.40	1.46
1	B	3	ASN	N-CA	-5.16	1.39	1.46
1	A	698	ILE	N-CA	-5.16	1.40	1.46
1	A	197	ARG	CA-C	-5.16	1.45	1.52
1	A	198	MET	N-CA	-5.15	1.40	1.46
1	B	131	ILE	N-CA	-5.15	1.40	1.46
1	A	341	SER	CA-C	-5.14	1.45	1.52
1	B	149	ILE	C-N	-5.14	1.26	1.34
1	A	520	TRP	CA-C	-5.14	1.46	1.52
1	A	681	ILE	N-CA	-5.14	1.40	1.46
1	B	180	TYR	N-CA	-5.14	1.38	1.46
1	B	478	ASP	N-CA	-5.13	1.40	1.46
1	A	745	ALA	CA-C	-5.13	1.45	1.52
1	B	354	GLN	CA-C	-5.13	1.46	1.52
1	A	554	PRO	N-CA	-5.12	1.41	1.46
1	B	573	THR	CA-C	-5.12	1.46	1.52
1	A	79	ALA	N-CA	-5.12	1.39	1.46
1	A	189	CYS	CA-C	-5.12	1.46	1.52
1	A	284	LEU	CA-C	-5.12	1.46	1.52
1	A	214	PHE	N-CA	-5.12	1.39	1.46
1	B	35	GLN	CA-C	-5.11	1.46	1.52
1	B	607	LYS	CA-C	-5.11	1.46	1.52
1	A	265	THR	CA-C	-5.10	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	HIS	CA-C	-5.10	1.45	1.52
1	A	395	ASP	CA-C	-5.10	1.46	1.52
1	B	359	VAL	C-N	-5.10	1.26	1.33
1	A	111	THR	CA-C	-5.09	1.46	1.52
1	B	336	ILE	C-N	-5.09	1.27	1.33
1	B	268	GLU	N-CA	-5.09	1.40	1.46
1	B	550	ALA	CA-C	-5.09	1.45	1.52
1	A	125	LYS	C-N	5.09	1.39	1.33
1	A	485	ASN	N-CA	-5.09	1.39	1.46
1	A	131	ILE	N-CA	-5.08	1.40	1.46
1	B	540	ILE	CA-C	-5.08	1.46	1.52
1	A	184	TYR	N-CA	-5.08	1.39	1.46
1	A	663	ILE	N-CA	-5.08	1.40	1.46
1	B	759	VAL	CA-C	-5.08	1.46	1.52
1	A	198	MET	CA-C	-5.08	1.46	1.52
1	B	73	TYR	N-CA	-5.07	1.40	1.46
1	A	641	VAL	N-CA	-5.07	1.40	1.46
1	B	75	GLN	N-CA	-5.07	1.40	1.46
1	A	732	LEU	N-CA	-5.07	1.40	1.46
1	B	173	ARG	N-CA	-5.07	1.39	1.46
1	B	359	VAL	C-O	-5.07	1.18	1.24
1	B	561	LEU	N-CA	-5.07	1.39	1.46
1	A	3	ASN	CA-C	-5.07	1.46	1.52
1	A	594	SER	N-CA	-5.07	1.39	1.46
1	B	481	ARG	CA-C	-5.06	1.46	1.52
1	B	729	LEU	N-CA	-5.06	1.39	1.46
1	B	257	LEU	CA-C	-5.06	1.46	1.52
1	A	549	ILE	CA-C	-5.05	1.45	1.52
1	A	680	MET	CA-C	-5.05	1.46	1.52
1	B	33	ALA	CA-C	-5.05	1.46	1.52
1	B	11	GLY	N-CA	-5.04	1.38	1.45
1	B	64	VAL	C-N	-5.04	1.27	1.33
1	B	18	GLN	CA-C	-5.04	1.46	1.52
1	A	541	ARG	CA-C	-5.03	1.46	1.52
1	B	94	GLN	C-O	-5.03	1.18	1.24
1	B	572	THR	CA-C	-5.03	1.46	1.52
1	B	683	THR	N-CA	-5.03	1.39	1.46
1	A	480	LYS	CA-C	-5.03	1.46	1.52
1	B	233	ALA	N-CA	-5.03	1.40	1.46
1	B	311	GLU	N-CA	-5.03	1.39	1.46
1	B	63	PRO	CA-C	-5.03	1.45	1.52
1	B	219	ALA	CA-C	-5.03	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	LEU	CA-C	-5.03	1.46	1.52
1	A	277	ASN	CA-C	-5.02	1.46	1.52
1	B	606	VAL	N-CA	-5.02	1.40	1.46
1	B	294	TYR	C-N	-5.02	1.27	1.33
1	A	528	ILE	N-CA	-5.01	1.40	1.46
1	B	272	SER	CA-C	-5.01	1.46	1.53
1	A	496	ALA	N-CA	-5.01	1.40	1.46
1	B	688	ALA	N-CA	-5.01	1.40	1.46
1	B	730	ALA	N-CA	-5.01	1.40	1.46
1	A	318	ILE	N-CA	-5.01	1.40	1.46
1	A	743	ALA	CA-C	-5.01	1.46	1.52
1	B	186	LEU	CA-C	-5.00	1.46	1.52
1	A	560	VAL	N-CA	-5.00	1.40	1.46
1	A	711	SER	CA-C	-5.00	1.45	1.52
1	B	746	LEU	N-CA	-5.00	1.40	1.46
1	A	157	VAL	CA-C	-5.00	1.46	1.52
1	A	585	THR	N-CA	-5.00	1.39	1.45
1	B	583	ALA	CA-C	-5.00	1.45	1.52

All (604) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	ASN	CA-C-O	-21.37	97.14	120.43
1	B	408	PHE	N-CA-C	17.38	134.30	112.92
1	B	211	GLN	N-CA-C	-12.87	91.66	110.06
1	B	82	VAL	CA-C-N	12.74	137.74	120.54
1	B	82	VAL	C-N-CA	12.74	137.74	120.54
1	B	115	ASN	N-CA-C	12.10	125.63	111.71
1	B	313	LEU	N-CA-C	-12.08	82.37	107.37
1	B	715	HIS	N-CA-C	-12.01	98.65	113.18
1	B	351	HIS	N-CA-C	11.93	124.28	111.28
1	B	735	MET	N-CA-C	-11.91	87.20	107.80
1	A	201	ALA	N-CA-C	11.88	126.56	111.24
1	A	394	SER	CA-C-N	11.73	136.95	120.29
1	A	394	SER	C-N-CA	11.73	136.95	120.29
1	A	426	GLN	N-CA-C	-11.72	85.83	110.80
1	A	171	VAL	N-CA-C	-11.14	92.49	108.42
1	B	172	TYR	N-CA-C	-10.71	91.93	108.42
1	A	43	THR	N-CA-C	-10.53	94.21	108.74
1	B	500	GLU	N-CA-C	-10.49	89.66	108.02
1	A	15	GLY	N-CA-C	-10.42	88.48	113.18
1	B	336	ILE	CA-C-N	10.30	137.22	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	ILE	C-N-CA	10.30	137.22	120.63
1	B	627	THR	N-CA-C	10.26	122.46	111.28
1	B	350	ASP	CA-C-N	10.14	133.87	120.28
1	B	350	ASP	C-N-CA	10.14	133.87	120.28
1	B	163	PHE	CA-C-N	10.14	140.22	121.97
1	B	163	PHE	C-N-CA	10.14	140.22	121.97
1	A	143	HIS	N-CA-C	-10.11	93.53	109.50
1	B	202	LEU	N-CA-C	9.99	123.42	111.33
1	A	78	GLY	N-CA-C	-9.97	89.54	113.18
1	A	739	SER	N-CA-C	-9.91	94.16	109.52
1	B	716	VAL	N-CA-C	-9.73	95.79	108.93
1	B	330	PRO	N-CA-C	-9.69	103.39	114.92
1	B	522	VAL	N-CA-C	-9.64	94.23	108.12
1	B	64	VAL	CA-C-N	9.56	132.87	120.44
1	B	64	VAL	C-N-CA	9.56	132.87	120.44
1	B	111	THR	N-CA-C	-9.52	93.88	109.40
1	A	23	GLY	N-CA-C	-9.49	102.23	115.32
1	A	544	GLU	O-C-N	9.48	128.49	121.85
1	A	423	ALA	N-CA-C	-9.46	95.02	109.96
1	B	243	ASN	N-CA-C	9.43	121.56	111.28
1	A	257	LEU	CA-C-N	9.26	130.45	119.99
1	A	257	LEU	C-N-CA	9.26	130.45	119.99
1	A	704	GLY	N-CA-C	-9.21	100.98	112.77
1	B	131	ILE	CA-C-O	9.21	130.53	120.95
1	A	351	HIS	CA-C-N	9.17	139.06	121.54
1	A	351	HIS	C-N-CA	9.17	139.06	121.54
1	B	320	TRP	N-CA-C	-9.14	101.40	111.36
1	A	546	LEU	CA-C-O	9.13	130.23	120.55
1	A	31	VAL	N-CA-C	-9.06	94.36	107.77
1	B	678	ILE	N-CA-C	9.00	118.99	110.53
1	A	38	LEU	N-CA-C	8.97	121.70	108.60
1	B	131	ILE	CA-C-N	8.96	132.66	120.38
1	B	131	ILE	C-N-CA	8.96	132.66	120.38
1	B	342	TYR	N-CA-C	-8.95	101.31	113.30
1	A	258	GLY	N-CA-C	-8.90	101.87	112.64
1	A	71	PHE	N-CA-C	-8.90	101.58	111.28
1	B	175	GLY	N-CA-C	-8.88	100.55	112.81
1	B	247	ASN	N-CA-C	8.88	120.72	111.14
1	A	639	TRP	N-CA-C	-8.83	101.62	111.07
1	B	684	THR	CA-C-N	8.81	129.72	119.94
1	B	684	THR	C-N-CA	8.81	129.72	119.94
1	A	179	THR	N-CA-C	-8.79	104.60	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	711	SER	CA-C-N	8.78	132.92	120.28
1	A	711	SER	C-N-CA	8.78	132.92	120.28
1	A	2	PHE	N-CA-C	8.77	123.71	109.76
1	A	146	PHE	N-CA-C	-8.76	101.66	111.82
1	B	98	CYS	N-CA-C	8.76	120.91	111.36
1	A	664	ASP	CA-C-N	8.72	129.85	119.99
1	A	664	ASP	C-N-CA	8.72	129.85	119.99
1	A	377	LYS	N-CA-C	-8.71	94.39	108.41
1	B	327	GLU	N-CA-C	-8.52	101.89	113.30
1	B	553	LYS	N-CA-C	-8.51	97.13	108.11
1	B	740	ARG	N-CA-C	-8.45	102.07	111.28
1	A	252	SER	N-CA-C	-8.44	102.17	111.36
1	A	129	THR	N-CA-C	-8.43	92.85	110.80
1	A	452	ASP	CA-C-N	8.40	133.83	121.31
1	A	452	ASP	C-N-CA	8.40	133.83	121.31
1	B	510	ALA	CA-C-N	8.36	136.75	121.70
1	B	510	ALA	C-N-CA	8.36	136.75	121.70
1	B	344	GLY	N-CA-C	-8.36	98.18	112.06
1	A	616	GLN	N-CA-C	-8.36	87.60	111.00
1	A	127	PRO	N-CA-C	8.35	120.89	110.70
1	A	581	HIS	N-CA-C	-8.33	102.28	111.36
1	B	107	THR	CA-C-N	8.28	131.37	120.28
1	B	107	THR	C-N-CA	8.28	131.37	120.28
1	A	301	ARG	N-CA-C	-8.25	102.23	112.88
1	B	506	HIS	N-CA-C	-8.24	95.96	109.40
1	B	310	ASP	N-CA-C	-8.20	100.16	112.54
1	B	81	SER	N-CA-C	-8.19	100.32	111.55
1	A	202	LEU	CA-C-O	8.19	129.10	120.42
1	A	264	SER	N-CA-C	-8.19	88.06	111.00
1	A	753	SER	CA-C-N	8.17	136.41	121.70
1	A	753	SER	C-N-CA	8.17	136.41	121.70
1	A	425	SER	N-CA-C	-8.14	100.39	110.65
1	A	376	VAL	N-CA-C	-8.12	96.75	108.11
1	A	350	ASP	CA-C-N	8.09	136.99	121.54
1	A	350	ASP	C-N-CA	8.09	136.99	121.54
1	B	739	SER	CA-C-N	8.07	131.09	120.28
1	B	739	SER	C-N-CA	8.07	131.09	120.28
1	A	450	ALA	N-CA-C	-8.06	102.07	112.23
1	B	569	ALA	N-CA-C	-8.06	96.61	109.59
1	B	574	SER	CA-C-N	8.05	136.47	121.97
1	B	574	SER	C-N-CA	8.05	136.47	121.97
1	A	258	GLY	CA-C-N	8.04	134.61	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	GLY	C-N-CA	8.04	134.61	122.23
1	B	165	LEU	CA-C-N	8.02	129.87	119.84
1	B	165	LEU	C-N-CA	8.02	129.87	119.84
1	B	154	VAL	N-CA-C	-8.00	105.39	113.47
1	B	331	PHE	N-CA-C	-7.93	97.73	109.15
1	A	613	GLY	N-CA-C	-7.91	94.42	113.18
1	B	332	LYS	N-CA-C	-7.91	96.26	108.76
1	A	359	VAL	O-C-N	-7.89	114.84	123.20
1	B	755	ALA	CA-C-N	7.89	136.60	121.54
1	B	755	ALA	C-N-CA	7.89	136.60	121.54
1	A	130	ALA	CA-C-N	7.88	131.26	120.46
1	A	130	ALA	C-N-CA	7.88	131.26	120.46
1	B	78	GLY	N-CA-C	-7.84	94.61	113.18
1	B	287	ASN	N-CA-C	-7.83	96.47	109.24
1	A	405	GLY	CA-C-N	7.82	131.39	120.29
1	A	405	GLY	C-N-CA	7.82	131.39	120.29
1	A	545	PRO	N-CA-C	7.80	128.54	112.47
1	A	701	GLN	CA-C-N	-7.80	109.83	120.44
1	A	701	GLN	C-N-CA	-7.80	109.83	120.44
1	B	54	TRP	CA-C-N	7.79	132.56	121.42
1	B	54	TRP	C-N-CA	7.79	132.56	121.42
1	A	16	LEU	CA-C-N	7.76	136.36	121.54
1	A	16	LEU	C-N-CA	7.76	136.36	121.54
1	A	2	PHE	CA-C-N	7.76	133.57	122.09
1	A	2	PHE	C-N-CA	7.76	133.57	122.09
1	A	153	PHE	N-CA-C	7.75	119.36	111.07
1	A	96	THR	CA-C-N	7.74	131.43	120.28
1	A	96	THR	C-N-CA	7.74	131.43	120.28
1	B	161	LEU	N-CA-C	-7.71	97.97	108.38
1	B	744	GLU	N-CA-C	-7.71	102.88	111.82
1	B	286	SER	N-CA-C	-7.70	103.45	112.92
1	B	571	HIS	N-CA-C	-7.69	103.79	113.02
1	A	703	ALA	CA-C-N	7.65	128.41	120.00
1	A	703	ALA	C-N-CA	7.65	128.41	120.00
1	A	209	MET	CA-C-N	7.61	135.39	121.70
1	A	209	MET	C-N-CA	7.61	135.39	121.70
1	B	42	ARG	N-CA-C	-7.61	97.50	108.60
1	B	428	GLY	N-CA-C	-7.60	100.66	110.38
1	B	380	ASN	N-CA-C	-7.59	98.65	110.42
1	A	568	LEU	N-CA-C	-7.58	102.61	113.21
1	B	295	GLN	CA-C-O	7.57	128.58	120.55
1	A	203	SER	N-CA-C	-7.56	96.92	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	ILE	CA-C-N	7.54	130.90	120.49
1	B	466	ILE	C-N-CA	7.54	130.90	120.49
1	A	578	TRP	CA-C-N	7.54	129.26	119.84
1	A	578	TRP	C-N-CA	7.54	129.26	119.84
1	B	534	ALA	CA-C-N	7.54	135.27	121.70
1	B	534	ALA	C-N-CA	7.54	135.27	121.70
1	B	294	TYR	N-CA-C	7.53	119.12	111.07
1	B	149	ILE	CA-C-O	7.52	128.87	121.05
1	A	10	ASN	N-CA-C	-7.52	98.44	109.11
1	B	517	TYR	N-CA-C	-7.51	98.99	108.45
1	B	442	PRO	CA-C-N	7.49	130.64	120.38
1	B	442	PRO	C-N-CA	7.49	130.64	120.38
1	B	282	ASP	N-CA-C	-7.48	103.13	111.28
1	B	354	GLN	N-CA-C	-7.48	101.42	108.07
1	B	640	PHE	CA-C-N	7.48	129.98	120.56
1	B	640	PHE	C-N-CA	7.48	129.98	120.56
1	A	305	GLU	CA-C-N	7.43	135.34	121.97
1	A	305	GLU	C-N-CA	7.43	135.34	121.97
1	A	277	ASN	N-CA-C	-7.42	103.13	111.14
1	B	146	PHE	CA-C-O	7.41	128.46	120.24
1	A	172	TYR	N-CA-C	-7.40	97.87	109.72
1	B	504	SER	N-CA-C	-7.39	96.89	109.24
1	A	718	ILE	CA-C-N	7.37	131.52	120.31
1	A	718	ILE	C-N-CA	7.37	131.52	120.31
1	B	316	THR	N-CA-C	-7.37	103.38	113.18
1	B	329	SER	N-CA-C	-7.37	93.53	109.81
1	B	712	SER	CA-C-N	7.36	135.59	121.54
1	B	712	SER	C-N-CA	7.36	135.59	121.54
1	B	241	ARG	N-CA-C	7.35	119.29	111.28
1	A	58	LYS	CA-C-N	7.35	135.81	121.41
1	A	58	LYS	C-N-CA	7.35	135.81	121.41
1	B	221	ALA	CA-C-O	-7.32	112.37	121.01
1	B	222	PRO	N-CA-C	7.32	127.55	112.47
1	B	78	GLY	CA-C-N	7.32	135.52	121.54
1	B	78	GLY	C-N-CA	7.32	135.52	121.54
1	A	413	PHE	N-CA-C	-7.32	103.24	111.07
1	B	322	ILE	CA-C-N	7.30	135.49	121.54
1	B	322	ILE	C-N-CA	7.30	135.49	121.54
1	B	13	ALA	N-CA-C	-7.30	93.50	108.18
1	B	121	ASP	N-CA-C	-7.30	95.26	110.80
1	B	146	PHE	CA-C-N	7.29	130.05	120.28
1	B	146	PHE	C-N-CA	7.29	130.05	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	VAL	N-CA-C	-7.29	97.97	108.53
1	A	80	LEU	N-CA-C	-7.28	95.29	110.80
1	B	223	ALA	N-CA-C	-7.28	103.33	111.71
1	A	577	ILE	N-CA-C	-7.28	97.84	107.88
1	B	657	ASP	N-CA-C	7.27	118.99	111.14
1	B	753	SER	CA-C-N	7.27	135.42	121.54
1	B	753	SER	C-N-CA	7.27	135.42	121.54
1	B	422	GLU	N-CA-C	-7.26	95.34	110.80
1	A	615	GLY	N-CA-C	-7.25	100.88	111.03
1	A	622	ARG	N-CA-C	-7.24	98.42	109.85
1	A	183	PHE	N-CA-C	7.23	118.81	111.07
1	B	507	GLN	CA-C-N	7.22	135.55	121.41
1	B	507	GLN	C-N-CA	7.22	135.55	121.41
1	B	607	LYS	N-CA-C	-7.20	95.46	110.80
1	A	323	GLU	N-CA-C	-7.20	105.12	114.04
1	A	534	ALA	CA-C-N	7.19	134.64	121.70
1	A	534	ALA	C-N-CA	7.19	134.64	121.70
1	B	335	PRO	N-CA-C	-7.18	99.96	110.80
1	A	716	VAL	N-CA-C	-7.18	98.12	109.17
1	B	664	ASP	N-CA-C	7.17	119.10	111.28
1	A	44	PHE	N-CA-C	-7.17	101.68	113.50
1	A	749	VAL	CA-C-N	7.16	129.87	120.28
1	A	749	VAL	C-N-CA	7.16	129.87	120.28
1	A	303	ARG	N-CA-C	-7.15	95.56	110.80
1	A	609	PHE	CA-C-O	7.14	127.99	120.42
1	A	735	MET	N-CA-C	-7.14	104.45	113.02
1	B	319	PRO	N-CA-C	-7.13	97.78	112.47
1	B	606	VAL	N-CA-C	-7.13	97.06	108.90
1	B	114	SER	N-CA-C	7.12	125.97	110.80
1	B	262	SER	CA-C-N	-7.12	110.94	119.84
1	B	262	SER	C-N-CA	-7.12	110.94	119.84
1	B	639	TRP	N-CA-C	7.12	119.12	111.36
1	B	518	LEU	N-CA-C	-7.12	98.61	109.85
1	A	374	THR	N-CA-C	-7.11	97.27	109.15
1	A	365	GLN	N-CA-C	-7.11	97.83	108.99
1	B	43	THR	N-CA-C	-7.10	98.85	108.86
1	B	635	MET	N-CA-C	-7.10	102.74	111.40
1	B	736	GLY	N-CA-C	-7.09	101.10	111.03
1	A	208	LYS	N-CA-C	7.09	118.66	111.07
1	B	44	PHE	N-CA-C	-7.09	96.85	108.41
1	B	23	GLY	N-CA-C	-7.09	96.38	113.18
1	B	509	VAL	N-CA-C	-7.09	98.63	106.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	ASP	CA-C-N	7.08	126.78	119.56
1	A	454	ASP	C-N-CA	7.08	126.78	119.56
1	B	520	TRP	N-CA-C	-7.07	98.99	109.81
1	A	28	GLN	N-CA-C	-7.06	103.66	111.36
1	A	208	LYS	CA-C-N	7.02	134.33	121.70
1	A	208	LYS	C-N-CA	7.02	134.33	121.70
1	B	330	PRO	CA-C-N	7.00	132.59	121.66
1	B	330	PRO	C-N-CA	7.00	132.59	121.66
1	B	147	HIS	CA-C-O	6.99	127.96	120.55
1	A	534	ALA	N-CA-C	-6.96	95.97	110.80
1	B	221	ALA	O-C-N	-6.93	113.20	121.31
1	A	546	LEU	CA-C-N	6.91	129.54	120.28
1	A	546	LEU	C-N-CA	6.91	129.54	120.28
1	B	328	VAL	N-CA-C	-6.86	103.62	110.62
1	B	122	ALA	N-CA-C	-6.86	97.09	108.34
1	A	358	VAL	CA-C-O	-6.86	113.21	120.48
1	A	62	ASP	N-CA-C	-6.85	93.86	108.66
1	B	278	THR	N-CA-C	6.85	119.90	108.73
1	A	370	ILE	N-CA-C	6.85	119.49	109.63
1	B	464	THR	N-CA-C	-6.80	103.95	111.36
1	B	552	ASN	N-CA-C	-6.78	99.68	109.31
1	B	177	THR	CA-C-N	6.78	134.49	121.54
1	B	177	THR	C-N-CA	6.78	134.49	121.54
1	A	361	TYR	CA-C-N	6.77	132.75	122.93
1	A	361	TYR	C-N-CA	6.77	132.75	122.93
1	A	113	SER	N-CA-C	-6.74	104.53	112.89
1	B	281	ILE	CA-C-N	6.74	129.31	120.28
1	B	281	ILE	C-N-CA	6.74	129.31	120.28
1	A	77	GLY	CA-C-N	6.72	134.59	121.41
1	A	77	GLY	C-N-CA	6.72	134.59	121.41
1	A	357	HIS	N-CA-C	-6.68	96.57	110.80
1	A	320	TRP	N-CA-C	-6.68	104.27	112.88
1	A	78	GLY	CA-C-N	6.67	134.27	121.54
1	A	78	GLY	C-N-CA	6.67	134.27	121.54
1	B	313	LEU	CA-C-N	6.66	133.68	121.70
1	B	313	LEU	C-N-CA	6.66	133.68	121.70
1	A	20	PHE	N-CA-C	-6.65	104.03	111.28
1	A	82	VAL	CA-C-N	6.65	129.52	120.54
1	A	82	VAL	C-N-CA	6.65	129.52	120.54
1	A	195	LEU	N-CA-C	-6.64	103.87	112.23
1	B	208	LYS	N-CA-C	-6.61	98.96	109.59
1	B	488	ALA	CA-C-N	-6.59	111.44	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	488	ALA	C-N-CA	-6.59	111.44	120.28
1	B	458	ALA	N-CA-C	-6.59	104.17	111.36
1	B	295	GLN	CA-C-N	6.59	129.40	120.44
1	B	295	GLN	C-N-CA	6.59	129.40	120.44
1	B	656	ASP	CA-C-N	6.58	129.38	120.44
1	B	656	ASP	C-N-CA	6.58	129.38	120.44
1	A	720	ARG	CA-C-O	6.55	127.49	120.55
1	B	684	THR	N-CA-C	-6.54	96.87	110.80
1	A	510	ALA	N-CA-C	-6.54	100.01	110.14
1	B	545	PRO	N-CA-C	6.52	122.59	113.53
1	A	581	HIS	CA-C-N	6.52	129.01	120.28
1	A	581	HIS	C-N-CA	6.52	129.01	120.28
1	B	570	ASN	CA-C-N	6.50	133.75	122.56
1	B	570	ASN	C-N-CA	6.50	133.75	122.56
1	A	198	MET	N-CA-C	-6.50	104.12	111.14
1	A	375	PRO	CA-C-O	-6.49	113.75	121.67
1	A	402	ALA	CA-C-N	6.49	126.42	119.28
1	A	402	ALA	C-N-CA	6.49	126.42	119.28
1	A	211	GLN	N-CA-C	-6.49	96.98	110.80
1	B	386	PHE	N-CA-C	-6.48	100.10	110.14
1	A	367	ALA	CA-C-N	6.46	133.87	121.54
1	A	367	ALA	C-N-CA	6.46	133.87	121.54
1	B	336	ILE	N-CA-C	6.46	117.20	110.62
1	B	378	LEU	N-CA-C	-6.43	97.11	110.80
1	B	114	SER	CA-C-N	-6.43	111.03	120.28
1	B	114	SER	C-N-CA	-6.43	111.03	120.28
1	B	213	THR	N-CA-C	-6.40	104.36	111.71
1	B	737	LEU	N-CA-C	-6.39	97.19	110.80
1	A	56	VAL	CA-C-N	6.38	133.92	121.41
1	A	56	VAL	C-N-CA	6.38	133.92	121.41
1	B	394	SER	CA-C-N	6.37	129.11	120.44
1	B	394	SER	C-N-CA	6.37	129.11	120.44
1	B	153	PHE	CA-C-N	-6.36	115.08	122.14
1	B	153	PHE	C-N-CA	-6.36	115.08	122.14
1	B	27	ASN	CA-C-N	6.35	133.68	121.54
1	B	27	ASN	C-N-CA	6.35	133.68	121.54
1	A	375	PRO	N-CA-C	-6.33	101.32	111.38
1	B	465	GLY	N-CA-C	-6.32	106.52	115.30
1	A	258	GLY	O-C-N	6.31	128.38	122.13
1	A	573	THR	N-CA-C	-6.31	105.45	113.02
1	B	160	PRO	N-CA-C	-6.31	99.48	112.47
1	B	671	ALA	CA-C-O	6.30	127.10	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ILE	CA-C-N	6.28	133.54	121.54
1	A	281	ILE	C-N-CA	6.28	133.54	121.54
1	A	608	GLU	N-CA-C	6.28	117.93	111.14
1	B	418	THR	N-CA-C	-6.28	104.51	111.36
1	B	489	ALA	N-CA-C	6.28	118.13	111.28
1	A	311	GLU	N-CA-C	-6.28	103.00	111.54
1	B	44	PHE	CA-C-O	-6.26	113.60	120.30
1	A	260	LEU	N-CA-C	-6.25	97.48	110.80
1	B	82	VAL	CA-C-O	6.25	127.45	120.95
1	B	322	ILE	N-CA-C	-6.24	96.37	109.34
1	A	671	ALA	CA-C-O	6.23	127.02	120.42
1	B	504	SER	CA-C-O	6.23	127.83	120.66
1	B	279	ASN	N-CA-C	6.22	124.05	110.80
1	B	285	ARG	N-CA-C	-6.19	104.80	112.90
1	B	226	SER	N-CA-C	-6.15	104.58	111.28
1	A	6	VAL	N-CA-C	6.14	115.45	106.55
1	A	363	ASP	CA-C-N	6.14	133.26	121.54
1	A	363	ASP	C-N-CA	6.14	133.26	121.54
1	B	421	TYR	O-C-N	6.13	130.20	122.65
1	B	239	ARG	N-CA-C	-6.13	104.66	111.71
1	A	100	PRO	N-CA-C	-6.13	106.20	113.86
1	A	93	HIS	N-CA-C	6.12	117.96	111.28
1	B	45	SER	N-CA-C	-6.12	100.29	108.74
1	B	297	MET	N-CA-C	-6.11	104.53	111.07
1	A	306	VAL	CA-C-N	6.09	132.93	121.97
1	A	306	VAL	C-N-CA	6.09	132.93	121.97
1	B	61	ILE	CA-C-O	-6.09	113.17	120.78
1	A	328	VAL	N-CA-C	6.07	121.32	113.07
1	A	494	ALA	CA-C-O	6.06	126.98	120.55
1	B	484	PHE	O-C-N	6.06	128.63	122.09
1	B	77	GLY	N-CA-C	-6.06	107.53	115.47
1	A	469	GLU	N-CA-C	6.05	119.35	109.06
1	A	163	PHE	CA-C-N	6.05	132.86	121.97
1	A	163	PHE	C-N-CA	6.05	132.86	121.97
1	B	505	GLU	N-CA-C	-6.04	101.54	110.48
1	A	127	PRO	CA-C-O	-6.04	111.80	120.56
1	A	193	SER	CA-C-N	6.01	129.45	120.31
1	A	193	SER	C-N-CA	6.01	129.45	120.31
1	A	603	THR	CA-C-N	6.00	131.45	122.99
1	A	603	THR	C-N-CA	6.00	131.45	122.99
1	B	291	PHE	CA-C-O	5.99	126.87	120.70
1	A	578	TRP	O-C-N	5.99	127.29	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	CA-C-N	5.99	133.14	121.41
1	A	14	ARG	C-N-CA	5.99	133.14	121.41
1	A	575	ILE	N-CA-C	-5.97	96.92	109.34
1	A	678	ILE	N-CA-C	5.97	116.71	110.62
1	A	426	GLN	CA-C-N	5.95	132.42	121.70
1	A	426	GLN	C-N-CA	5.95	132.42	121.70
1	B	741	SER	N-CA-C	5.94	117.42	111.07
1	B	315	SER	N-CA-C	-5.93	94.38	111.00
1	A	552	ASN	N-CA-C	-5.93	100.37	108.38
1	B	655	ARG	N-CA-C	-5.92	106.06	113.28
1	A	684	THR	N-CA-C	-5.92	99.96	108.60
1	B	376	VAL	N-CA-C	-5.91	97.04	109.34
1	B	557	PRO	N-CA-C	-5.91	100.30	112.47
1	A	379	ALA	N-CA-C	-5.90	100.41	108.38
1	B	11	GLY	N-CA-C	-5.90	99.20	113.18
1	A	70	PHE	CA-C-N	5.87	128.15	120.28
1	A	70	PHE	C-N-CA	5.87	128.15	120.28
1	A	49	THR	N-CA-C	-5.87	99.63	108.96
1	B	377	LYS	N-CA-C	-5.87	98.31	110.80
1	B	409	ALA	N-CA-C	5.87	123.29	110.80
1	B	423	ALA	CA-C-N	5.87	132.53	121.97
1	B	423	ALA	C-N-CA	5.87	132.53	121.97
1	A	607	LYS	N-CA-C	5.86	118.60	109.52
1	B	165	LEU	O-C-N	5.86	126.33	121.35
1	B	198	MET	N-CA-C	-5.85	104.82	111.14
1	A	72	GLN	N-CA-C	5.85	118.44	111.71
1	B	108	ALA	N-CA-C	-5.84	104.91	111.28
1	B	436	GLU	N-CA-C	5.82	119.10	110.48
1	B	553	LYS	CA-C-N	5.82	127.11	119.84
1	B	553	LYS	C-N-CA	5.82	127.11	119.84
1	A	463	ARG	N-CA-C	-5.81	104.85	111.07
1	A	19	ALA	CA-C-N	5.80	128.05	120.28
1	A	19	ALA	C-N-CA	5.80	128.05	120.28
1	A	126	VAL	N-CA-C	5.79	121.39	108.88
1	B	663	ILE	N-CA-C	5.79	118.33	111.09
1	A	645	ARG	N-CA-C	-5.78	104.61	111.03
1	B	375	PRO	N-CA-C	-5.78	100.56	112.47
1	B	510	ALA	O-C-N	-5.78	114.91	122.59
1	B	658	ALA	CA-C-N	5.77	128.29	120.44
1	B	658	ALA	C-N-CA	5.77	128.29	120.44
1	A	240	SER	CA-C-N	5.77	132.56	121.54
1	A	240	SER	C-N-CA	5.77	132.56	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	SER	CA-C-N	5.76	132.55	121.54
1	A	326	SER	C-N-CA	5.76	132.55	121.54
1	B	359	VAL	CA-C-O	5.75	126.43	120.39
1	A	270	ASP	O-C-N	-5.75	114.71	121.32
1	A	55	GLU	N-CA-C	-5.74	102.40	110.50
1	B	35	GLN	N-CA-C	-5.73	98.59	110.80
1	B	450	ALA	N-CA-C	-5.73	105.01	112.23
1	A	222	PRO	CA-C-N	5.73	132.48	121.54
1	A	222	PRO	C-N-CA	5.73	132.48	121.54
1	B	425	SER	CA-C-N	5.73	132.48	121.54
1	B	425	SER	C-N-CA	5.73	132.48	121.54
1	B	293	ALA	CA-C-N	-5.72	113.01	120.44
1	B	293	ALA	C-N-CA	-5.72	113.01	120.44
1	B	361	TYR	CA-C-N	5.71	130.88	123.00
1	B	361	TYR	C-N-CA	5.71	130.88	123.00
1	A	347	SER	N-CA-C	5.71	116.93	108.60
1	B	352	MET	N-CA-C	5.70	119.05	111.75
1	B	240	SER	N-CA-C	5.70	117.49	111.28
1	B	496	ALA	N-CA-C	-5.69	104.28	111.11
1	A	75	GLN	N-CA-C	-5.69	105.08	111.28
1	B	180	TYR	CA-C-N	-5.69	112.73	119.84
1	B	180	TYR	C-N-CA	-5.69	112.73	119.84
1	B	560	VAL	N-CA-C	-5.69	105.85	111.77
1	B	159	SER	N-CA-C	-5.68	101.02	109.42
1	B	173	ARG	N-CA-C	-5.68	98.71	110.80
1	B	590	GLU	N-CA-C	-5.67	98.71	110.80
1	A	404	ILE	N-CA-C	5.65	116.43	110.72
1	B	716	VAL	CA-C-N	5.65	132.48	121.41
1	B	716	VAL	C-N-CA	5.65	132.48	121.41
1	A	703	ALA	CA-C-O	5.64	126.40	120.42
1	A	574	SER	N-CA-C	-5.64	106.25	113.02
1	B	624	LEU	CA-C-N	5.63	135.55	121.80
1	B	624	LEU	C-N-CA	5.63	135.55	121.80
1	A	401	LEU	N-CA-C	-5.63	105.22	111.36
1	B	31	VAL	N-CA-C	-5.62	99.76	107.75
1	A	202	LEU	CA-C-N	5.62	130.12	122.19
1	A	202	LEU	C-N-CA	5.62	130.12	122.19
1	B	34	LEU	CA-C-N	5.62	132.28	121.54
1	B	34	LEU	C-N-CA	5.62	132.28	121.54
1	B	41	THR	N-CA-C	5.61	122.76	110.80
1	A	711	SER	CA-C-O	5.61	126.28	119.38
1	B	65	MET	N-CA-C	-5.61	105.07	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	LEU	N-CA-C	-5.61	98.86	110.80
1	B	170	TYR	N-CA-C	-5.59	100.35	108.07
1	B	441	PHE	CA-C-N	5.58	125.41	119.28
1	B	441	PHE	C-N-CA	5.58	125.41	119.28
1	A	740	ARG	N-CA-C	-5.57	105.21	111.28
1	B	248	ALA	CA-C-O	5.57	126.37	119.97
1	A	407	THR	N-CA-C	-5.55	105.77	112.54
1	B	157	VAL	N-CA-C	-5.54	106.29	111.45
1	A	437	MET	N-CA-C	-5.54	99.64	109.06
1	A	14	ARG	N-CA-C	-5.54	103.83	111.81
1	B	519	VAL	N-CA-C	-5.53	97.83	109.34
1	B	270	ASP	N-CA-C	-5.52	103.17	110.40
1	B	656	ASP	N-CA-C	-5.51	100.97	109.52
1	A	382	SER	CA-C-N	5.51	129.50	120.63
1	A	382	SER	C-N-CA	5.51	129.50	120.63
1	B	471	LEU	N-CA-C	-5.50	99.78	108.14
1	A	21	ALA	N-CA-C	-5.50	105.29	111.28
1	A	610	GLU	N-CA-C	-5.49	106.08	112.89
1	A	615	GLY	CA-C-N	5.48	131.57	121.70
1	A	615	GLY	C-N-CA	5.48	131.57	121.70
1	B	74	ALA	CA-C-N	5.48	127.63	120.28
1	B	74	ALA	C-N-CA	5.48	127.63	120.28
1	B	191	ARG	CA-C-O	5.48	126.12	119.49
1	B	112	GLY	N-CA-C	-5.47	97.43	113.30
1	B	350	ASP	N-CA-C	5.47	116.97	110.19
1	B	99	ASN	N-CA-C	5.46	121.87	109.81
1	B	327	GLU	CA-C-N	5.46	127.94	120.46
1	B	327	GLU	C-N-CA	5.46	127.94	120.46
1	B	294	TYR	CA-C-O	5.45	126.55	120.82
1	A	116	ARG	N-CA-C	-5.43	101.24	108.74
1	A	270	ASP	CA-C-O	-5.43	112.72	120.16
1	A	411	SER	N-CA-C	-5.43	105.36	111.28
1	B	164	ILE	N-CA-C	-5.42	98.06	109.34
1	A	570	ASN	CA-C-O	-5.42	115.05	120.96
1	B	628	VAL	CA-C-O	5.41	126.58	120.95
1	A	340	THR	N-CA-C	-5.41	101.28	108.74
1	B	680	MET	CA-C-N	-5.41	111.78	120.64
1	B	680	MET	C-N-CA	-5.41	111.78	120.64
1	B	186	LEU	N-CA-C	5.40	116.85	111.07
1	B	426	GLN	CA-C-N	5.40	131.42	121.70
1	B	426	GLN	C-N-CA	5.40	131.42	121.70
1	A	302	GLY	N-CA-C	-5.39	108.41	115.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	GLY	N-CA-C	-5.39	100.40	113.18
1	A	124	GLY	CA-C-O	-5.39	117.38	122.39
1	A	352	MET	CA-C-N	5.39	131.40	121.70
1	A	352	MET	C-N-CA	5.39	131.40	121.70
1	B	578	TRP	N-CA-C	-5.38	97.91	109.81
1	A	518	LEU	CA-C-N	5.37	130.32	122.69
1	A	518	LEU	C-N-CA	5.37	130.32	122.69
1	B	184	TYR	CA-C-N	5.37	127.47	120.28
1	B	184	TYR	C-N-CA	5.37	127.47	120.28
1	B	252	SER	N-CA-C	-5.37	105.51	111.36
1	A	79	ALA	N-CA-C	-5.37	99.37	110.80
1	B	472	GLU	N-CA-C	5.36	122.22	110.80
1	A	111	THR	N-CA-C	-5.36	99.59	108.75
1	B	369	GLU	N-CA-C	-5.35	101.16	109.24
1	B	589	TYR	N-CA-C	-5.35	99.40	110.80
1	B	622	ARG	N-CA-C	-5.34	101.41	109.85
1	A	760	VAL	CA-C-N	5.34	131.32	121.70
1	A	760	VAL	C-N-CA	5.34	131.32	121.70
1	B	171	VAL	CA-C-N	5.34	132.75	121.91
1	B	171	VAL	C-N-CA	5.34	132.75	121.91
1	A	498	ASN	N-CA-C	-5.33	96.91	108.74
1	A	125	LYS	CA-C-N	5.33	131.99	122.13
1	A	125	LYS	C-N-CA	5.33	131.99	122.13
1	B	490	VAL	N-CA-C	5.33	115.54	110.42
1	A	546	LEU	N-CA-C	5.33	117.08	111.28
1	B	101	GLU	CA-C-N	-5.31	113.76	120.56
1	B	101	GLU	C-N-CA	-5.31	113.76	120.56
1	B	165	LEU	N-CA-C	-5.31	100.90	109.82
1	A	706	GLY	CA-C-N	5.31	131.68	121.54
1	A	706	GLY	C-N-CA	5.31	131.68	121.54
1	B	198	MET	CA-C-N	-5.30	110.68	121.18
1	B	198	MET	C-N-CA	-5.30	110.68	121.18
1	B	246	ALA	CA-C-N	-5.29	113.25	120.44
1	B	246	ALA	C-N-CA	-5.29	113.25	120.44
1	A	284	LEU	CA-C-N	5.28	131.63	121.54
1	A	284	LEU	C-N-CA	5.28	131.63	121.54
1	A	45	SER	CA-C-N	5.28	131.63	121.54
1	A	45	SER	C-N-CA	5.28	131.63	121.54
1	B	285	ARG	CA-C-O	5.28	125.78	119.60
1	B	18	GLN	N-CA-C	-5.28	105.70	111.82
1	B	352	MET	CA-C-N	5.28	131.19	121.70
1	B	352	MET	C-N-CA	5.28	131.19	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	SER	N-CA-C	5.27	122.03	110.80
1	A	378	LEU	N-CA-C	-5.26	105.53	112.94
1	B	140	PRO	N-CA-C	-5.26	101.64	112.47
1	B	185	ALA	CA-C-N	-5.25	113.61	120.44
1	B	185	ALA	C-N-CA	-5.25	113.61	120.44
1	A	175	GLY	CA-C-N	5.25	131.57	121.54
1	A	175	GLY	C-N-CA	5.25	131.57	121.54
1	A	234	THR	N-CA-C	-5.25	105.64	111.36
1	A	479	LEU	N-CA-C	-5.25	105.56	111.28
1	B	37	PRO	N-CA-C	5.25	123.28	112.47
1	B	276	ARG	CA-C-N	5.24	128.28	120.31
1	B	276	ARG	C-N-CA	5.24	128.28	120.31
1	B	594	SER	N-CA-C	5.24	117.35	109.23
1	A	268	GLU	N-CA-C	-5.24	105.05	113.28
1	A	359	VAL	N-CA-C	5.24	115.40	107.75
1	B	529	PRO	N-CA-C	-5.23	101.69	112.47
1	B	421	TYR	CA-C-N	5.23	131.53	121.54
1	B	421	TYR	C-N-CA	5.23	131.53	121.54
1	B	281	ILE	CA-C-O	5.23	127.32	120.78
1	B	758	MET	CA-C-N	5.23	131.38	121.97
1	B	758	MET	C-N-CA	5.23	131.38	121.97
1	B	200	THR	CA-C-O	5.19	126.06	120.55
1	A	411	SER	CA-C-O	5.19	126.05	120.55
1	A	497	HIS	CA-C-N	-5.19	115.68	122.74
1	A	497	HIS	C-N-CA	-5.19	115.68	122.74
1	A	316	THR	N-CA-C	-5.18	99.76	110.80
1	B	499	PRO	N-CA-C	-5.18	101.80	112.47
1	B	115	ASN	CA-C-O	-5.18	114.25	120.10
1	A	687	GLY	N-CA-C	-5.17	106.53	112.73
1	B	613	GLY	N-CA-C	-5.17	103.54	111.24
1	A	191	ARG	CA-C-O	5.16	125.72	119.38
1	A	492	HIS	N-CA-C	-5.16	105.74	111.36
1	B	614	LEU	CA-C-N	5.16	127.76	121.06
1	B	614	LEU	C-N-CA	5.16	127.76	121.06
1	B	89	PHE	O-C-N	-5.15	116.67	122.12
1	A	260	LEU	CA-C-N	-5.14	112.98	120.29
1	A	260	LEU	C-N-CA	-5.14	112.98	120.29
1	A	734	MET	N-CA-C	-5.14	106.78	113.16
1	A	318	ILE	N-CA-C	5.14	119.99	108.88
1	B	487	TYR	CA-C-O	5.14	126.00	120.55
1	A	555	ILE	CA-C-N	5.14	129.90	122.29
1	A	555	ILE	C-N-CA	5.14	129.90	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	PRO	N-CA-C	-5.13	98.76	112.10
1	A	526	LEU	CA-C-N	5.12	131.32	121.54
1	A	526	LEU	C-N-CA	5.12	131.32	121.54
1	A	168	ALA	N-CA-C	-5.12	105.78	111.36
1	B	314	SER	O-C-N	-5.11	114.83	123.00
1	A	246	ALA	CA-C-N	-5.11	113.49	120.44
1	A	246	ALA	C-N-CA	-5.11	113.49	120.44
1	B	565	VAL	CA-C-N	5.10	131.28	121.54
1	B	565	VAL	C-N-CA	5.10	131.28	121.54
1	B	116	ARG	CA-C-N	5.10	131.28	121.54
1	B	116	ARG	C-N-CA	5.10	131.28	121.54
1	B	372	ALA	N-CA-C	-5.09	100.11	108.41
1	B	639	TRP	CA-C-O	5.09	125.82	120.42
1	A	262	SER	O-C-N	-5.09	115.47	121.32
1	A	333	LEU	N-CA-C	-5.09	101.82	109.15
1	B	182	ASN	CA-C-N	5.08	127.08	120.28
1	B	182	ASN	C-N-CA	5.08	127.08	120.28
1	A	482	SER	N-CA-C	-5.07	105.83	111.36
1	B	456	MET	CA-C-O	5.07	125.62	119.38
1	A	422	GLU	O-C-N	5.07	128.74	123.06
1	B	581	HIS	CA-C-N	5.07	127.07	120.28
1	B	581	HIS	C-N-CA	5.07	127.07	120.28
1	B	225	ILE	N-CA-C	5.06	115.78	110.62
1	A	736	GLY	N-CA-C	-5.06	101.19	113.18
1	B	576	HIS	CA-C-N	5.06	131.07	121.97
1	B	576	HIS	C-N-CA	5.06	131.07	121.97
1	A	327	GLU	N-CA-C	5.05	121.56	110.80
1	B	81	SER	CA-C-N	5.05	127.38	120.46
1	B	81	SER	C-N-CA	5.05	127.38	120.46
1	B	560	VAL	CA-C-O	5.04	125.80	120.26
1	B	28	GLN	CA-C-N	5.04	131.16	121.54
1	B	28	GLN	C-N-CA	5.04	131.16	121.54
1	B	543	PRO	N-CA-C	-5.03	102.11	112.47
1	A	523	ARG	CA-C-N	5.02	131.13	121.54
1	A	523	ARG	C-N-CA	5.02	131.13	121.54
1	B	625	LYS	N-CA-C	5.02	120.91	109.81
1	A	298	VAL	CA-C-N	-5.01	113.63	120.44
1	A	298	VAL	C-N-CA	-5.01	113.63	120.44

There are no chirality outliers.

All (73) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	THR	Peptide
1	A	130	ALA	Mainchain
1	A	161	LEU	Peptide
1	A	162	GLY	Peptide
1	A	178	ALA	Peptide
1	A	182	ASN	Peptide,Mainchain
1	A	203	SER	Mainchain
1	A	284	LEU	Mainchain
1	A	291	PHE	Mainchain
1	A	314	SER	Peptide,Mainchain
1	A	339	THR	Mainchain
1	A	35	GLN	Peptide,Mainchain
1	A	357	HIS	Peptide,Mainchain
1	A	387	LEU	Mainchain
1	A	419	ALA	Mainchain
1	A	455	PRO	Peptide,Mainchain
1	A	516	LEU	Mainchain
1	A	520	TRP	Mainchain
1	A	544	GLU	Peptide,Mainchain
1	A	557	PRO	Mainchain
1	A	616	GLN	Mainchain
1	A	622	ARG	Mainchain
1	A	717	GLY	Peptide,Mainchain
1	A	758	MET	Peptide
1	B	110	ILE	Peptide,Mainchain
1	B	114	SER	Peptide,Mainchain
1	B	159	SER	Peptide
1	B	182	ASN	Mainchain
1	B	203	SER	Peptide
1	B	222	PRO	Peptide
1	B	240	SER	Mainchain
1	B	242	GLY	Peptide
1	B	277	ASN	Peptide,Mainchain
1	B	294	TYR	Peptide,Mainchain
1	B	330	PRO	Mainchain
1	B	340	THR	Peptide,Mainchain
1	B	343	ILE	Peptide
1	B	362	GLU	Mainchain
1	B	370	ILE	Peptide,Mainchain
1	B	393	ILE	Mainchain
1	B	40	PHE	Mainchain
1	B	421	TYR	Peptide
1	B	425	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	B	489	ALA	Peptide,Mainchain
1	B	500	GLU	Mainchain
1	B	503	VAL	Mainchain
1	B	532	TYR	Peptide,Mainchain
1	B	544	GLU	Peptide,Mainchain
1	B	591	ASP	Mainchain
1	B	599	ASN	Mainchain
1	B	602	TYR	Peptide,Mainchain
1	B	63	PRO	Peptide,Mainchain
1	B	716	VAL	Peptide
1	B	717	GLY	Peptide,Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3043	0	821	37	0
1	B	3043	0	820	39	0
All	All	6086	0	1641	76	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 (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:H	1:A:465:GLY:HA3	1.67	0.59
1:B:222:PRO:CA	1:B:225:ILE:H	2.17	0.58
1:A:504:SER:H	1:A:517:TYR:H	1.52	0.57
1:B:171:VAL:N	1:B:576:HIS:H	2.03	0.56
1:A:118:ILE:N	1:A:121:ASP:H	2.05	0.55
1:A:144:GLU:C	1:A:146:PHE:H	2.14	0.55
1:B:76:ALA:C	1:B:78:GLY:H	2.15	0.55
1:B:495:VAL:C	1:B:498:ASN:H	2.15	0.55
1:A:451:LEU:C	1:A:453:ARG:H	2.14	0.54
1:A:318:ILE:C	1:A:320:TRP:H	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:MET:H	1:B:214:PHE:N	2.06	0.53
1:A:9:LEU:C	1:A:12:SER:H	2.17	0.53
1:B:9:LEU:C	1:B:11:GLY:H	2.14	0.53
1:B:161:LEU:C	1:B:163:PHE:H	2.17	0.51
1:B:290:LEU:C	1:B:293:ALA:H	2.19	0.51
1:B:36:LEU:N	1:B:503:VAL:H	2.10	0.49
1:B:321:PHE:C	1:B:323:GLU:N	2.69	0.49
1:A:410:VAL:C	1:A:413:PHE:H	2.20	0.49
1:A:573:THR:C	1:A:575:ILE:H	2.17	0.48
1:A:672:VAL:O	1:A:676:ARG:N	2.46	0.48
1:B:126:VAL:C	1:B:165:LEU:H	2.22	0.47
1:A:732:LEU:C	1:A:735:MET:H	2.23	0.47
1:A:673:THR:C	1:A:676:ARG:H	2.23	0.46
1:A:13:ALA:C	1:A:15:GLY:H	2.24	0.46
1:A:608:GLU:C	1:A:611:LEU:H	2.24	0.46
1:B:6:VAL:H	1:B:435:ALA:H	1.64	0.46
1:B:287:ASN:C	1:B:288:LEU:N	2.74	0.45
1:A:313:LEU:O	1:A:315:SER:N	2.49	0.45
1:B:570:ASN:C	1:B:572:THR:H	2.23	0.45
1:B:211:GLN:C	1:B:215:LYS:O	2.60	0.45
1:B:15:GLY:H	1:B:465:GLY:HA3	1.82	0.45
1:B:45:SER:O	1:B:330:PRO:O	2.35	0.45
1:B:215:LYS:O	1:B:216:ALA:C	2.60	0.45
1:A:266:PRO:C	1:A:269:LEU:H	2.25	0.44
1:B:310:ASP:C	1:B:314:SER:H	2.25	0.44
1:B:221:ALA:O	1:B:223:ALA:N	2.51	0.44
1:A:298:VAL:O	1:A:302:GLY:C	2.61	0.44
1:B:86:VAL:O	1:B:90:THR:N	2.51	0.44
1:B:209:MET:H	1:B:213:THR:C	2.26	0.43
1:B:219:ALA:O	1:B:221:ALA:O	2.36	0.43
1:B:36:LEU:H	1:B:503:VAL:H	1.66	0.43
1:B:309:SER:C	1:B:313:LEU:O	2.62	0.43
1:B:312:GLU:O	1:B:316:THR:N	2.51	0.43
1:A:14:ARG:H	1:A:465:GLY:CA	2.31	0.43
1:A:548:ALA:C	1:A:551:TYR:H	2.27	0.43
1:A:188:ASP:O	1:A:192:ALA:N	2.52	0.42
1:B:311:GLU:C	1:B:314:SER:O	2.62	0.42
1:B:329:SER:C	1:B:331:PHE:N	2.72	0.42
1:A:318:ILE:C	1:A:320:TRP:N	2.77	0.42
1:A:712:SER:C	1:A:715:HIS:H	2.27	0.42
1:A:495:VAL:O	1:A:496:ALA:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:C	1:A:193:SER:H	2.28	0.42
1:A:448:ASP:C	1:A:451:LEU:H	2.27	0.42
1:B:494:ALA:O	1:B:498:ASN:N	2.53	0.42
1:A:391:PRO:C	1:A:393:ILE:H	2.28	0.42
1:B:752:ASP:C	1:B:754:ASN:H	2.27	0.42
1:A:6:VAL:O	1:A:434:GLY:HA2	2.20	0.42
1:A:504:SER:O	1:A:517:TYR:N	2.54	0.41
1:B:340:THR:C	1:B:342:TYR:H	2.28	0.41
1:A:373:PHE:O	1:A:622:ARG:O	2.39	0.41
1:B:301:ARG:C	1:B:303:ARG:H	2.28	0.41
1:A:195:LEU:O	1:A:199:LEU:N	2.53	0.41
1:A:256:ILE:O	1:A:259:ARG:O	2.39	0.41
1:B:495:VAL:O	1:B:496:ALA:C	2.63	0.41
1:A:20:PHE:C	1:A:23:GLY:H	2.29	0.41
1:A:301:ARG:C	1:A:303:ARG:N	2.79	0.41
1:A:532:TYR:C	1:A:534:ALA:H	2.29	0.41
1:A:126:VAL:CA	1:A:163:PHE:H	2.35	0.40
1:A:504:SER:N	1:A:517:TYR:H	2.17	0.40
1:B:449:TYR:C	1:B:452:ASP:H	2.28	0.40
1:B:20:PHE:C	1:B:23:GLY:H	2.28	0.40
1:B:196:ARG:O	1:B:200:THR:N	2.55	0.40
1:B:267:LYS:C	1:B:269:LEU:H	2.29	0.40
1:A:14:ARG:N	1:A:465:GLY:CA	2.84	0.40
1:B:317:ILE:C	1:B:320:TRP:H	2.29	0.40
1:B:495:VAL:O	1:B:498:ASN:N	2.54	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	759/761 (100%)	561 (74%)	98 (13%)	100 (13%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	757/761 (100%)	559 (74%)	100 (13%)	98 (13%)	0	4
All	All	1516/1522 (100%)	1120 (74%)	198 (13%)	198 (13%)	0	4

All (198) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ALA
1	A	16	LEU
1	A	17	THR
1	A	46	ALA
1	A	51	GLU
1	A	57	GLY
1	A	58	LYS
1	A	126	VAL
1	A	127	PRO
1	A	140	PRO
1	A	144	GLU
1	A	164	ILE
1	A	165	LEU
1	A	166	PRO
1	A	178	ALA
1	A	205	VAL
1	A	209	MET
1	A	210	LEU
1	A	240	SER
1	A	270	ASP
1	A	279	ASN
1	A	314	SER
1	A	326	SER
1	A	327	GLU
1	A	341	SER
1	A	349	ILE
1	A	351	HIS
1	A	368	LYS
1	A	369	GLU
1	A	424	VAL
1	A	432	SER
1	A	472	GLU
1	A	512	GLU
1	A	527	ARG
1	A	530	VAL
1	A	579	PRO

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Mol	Chain	Res	Type
1	A	580	TRP
1	A	588	ALA
1	A	589	TYR
1	A	614	LEU
1	A	617	ARG
1	A	620	ARG
1	A	668	MET
1	A	738	LEU
1	A	755	ALA
1	A	759	VAL
1	B	8	ASP
1	B	24	GLU
1	B	26	LYS
1	B	28	GLN
1	B	79	ALA
1	B	99	ASN
1	B	117	ALA
1	B	164	ILE
1	B	166	PRO
1	B	178	ALA
1	B	181	PRO
1	B	204	SER
1	B	205	VAL
1	B	222	PRO
1	B	246	ALA
1	B	263	PRO
1	B	303	ARG
1	B	304	ALA
1	B	378	LEU
1	B	382	SER
1	B	391	PRO
1	B	409	ALA
1	B	422	GLU
1	B	424	VAL
1	B	470	SER
1	B	508	GLY
1	B	554	PRO
1	B	563	ALA
1	B	566	LEU
1	B	575	ILE
1	B	577	ILE
1	B	578	TRP

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Mol	Chain	Res	Type
1	B	589	TYR
1	B	591	ASP
1	B	599	ASN
1	B	625	LYS
1	B	626	PRO
1	B	713	ASP
1	B	754	ASN
1	B	756	LEU
1	B	758	MET
1	B	760	VAL
1	A	27	ASN
1	A	59	GLY
1	A	79	ALA
1	A	130	ALA
1	A	206	ASP
1	A	207	SER
1	A	214	PHE
1	A	241	ARG
1	A	260	LEU
1	A	262	SER
1	A	304	ALA
1	A	322	ILE
1	A	409	ALA
1	A	420	VAL
1	A	466	ILE
1	A	515	SER
1	A	524	THR
1	A	535	ILE
1	A	539	SER
1	A	664	ASP
1	A	669	GLN
1	B	7	LYS
1	B	11	GLY
1	B	35	GLN
1	B	61	ILE
1	B	80	LEU
1	B	129	THR
1	B	210	LEU
1	B	323	GLU
1	B	366	PHE
1	B	423	ALA
1	B	426	GLN

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Mol	Chain	Res	Type
1	B	511	ALA
1	B	540	ILE
1	B	568	LEU
1	B	593	TYR
1	B	654	SER
1	B	684	THR
1	B	712	SER
1	A	33	ALA
1	A	114	SER
1	A	161	LEU
1	A	223	ALA
1	A	269	LEU
1	A	282	ASP
1	A	284	LEU
1	A	286	SER
1	A	303	ARG
1	A	352	MET
1	A	355	PRO
1	A	507	GLN
1	A	533	ASN
1	A	534	ALA
1	A	542	THR
1	A	557	PRO
1	A	626	PRO
1	A	710	ASP
1	A	756	LEU
1	B	27	ASN
1	B	41	THR
1	B	144	GLU
1	B	216	ALA
1	B	218	GLY
1	B	308	PHE
1	B	315	SER
1	B	324	ALA
1	B	559	GLU
1	B	562	GLN
1	B	573	THR
1	B	751	GLY
1	A	121	ASP
1	A	125	LYS
1	A	181	PRO
1	A	316	THR

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Mol	Chain	Res	Type
1	A	558	SER
1	A	616	GLN
1	B	214	PHE
1	B	245	ASP
1	B	375	PRO
1	B	499	PRO
1	B	574	SER
1	A	7	LYS
1	A	364	TRP
1	A	522	VAL
1	B	29	LEU
1	B	128	PRO
1	B	140	PRO
1	B	212	ALA
1	B	307	ILE
1	B	339	THR
1	B	376	VAL
1	B	427	ARG
1	B	472	GLU
1	B	529	PRO
1	B	598	ARG
1	B	607	LYS
1	B	614	LEU
1	A	543	PRO
1	B	114	SER
1	B	319	PRO
1	B	621	VAL
1	A	139	ALA
1	B	62	ASP
1	B	57	GLY
1	A	529	PRO
1	B	355	PRO
1	B	501	VAL
1	B	112	GLY
1	A	128	PRO
1	A	263	PRO

5.3.2 Protein sidechains ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	287:ASN	C	288:LEU	N	2.74

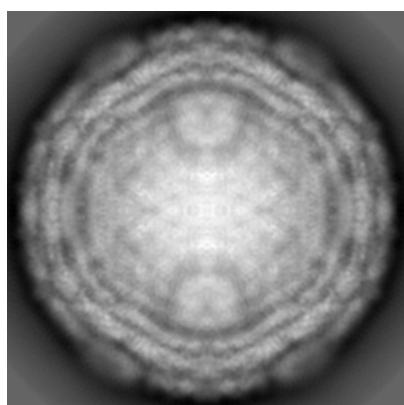
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1206. These allow visual inspection of the internal detail of the map and identification of artifacts.

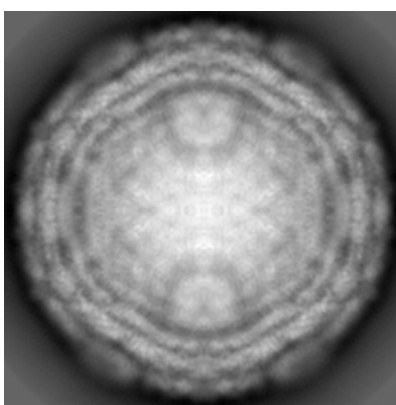
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

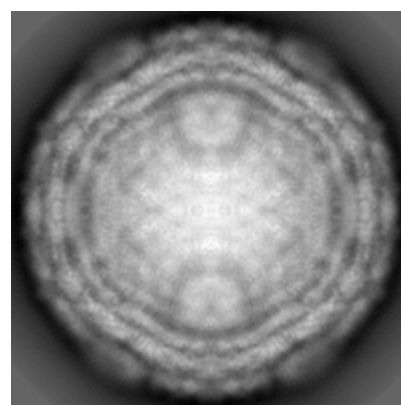
6.1.1 Primary map



X



Y

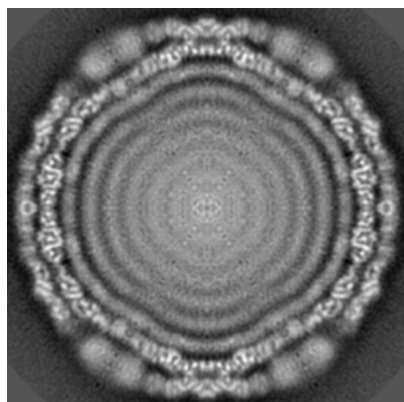


Z

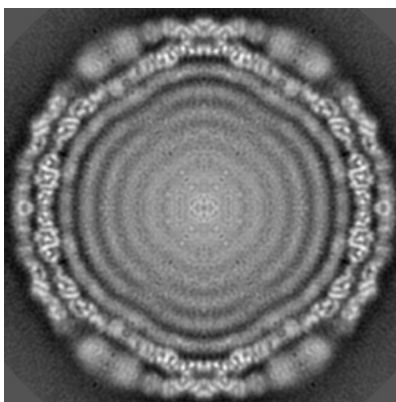
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

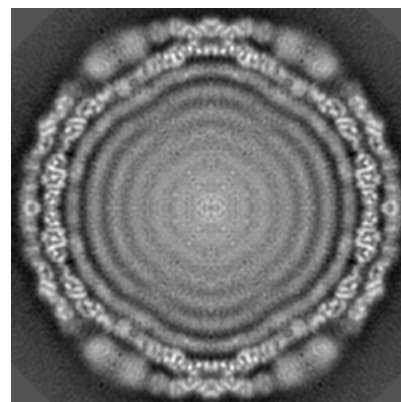
6.2.1 Primary map



X Index: 210



Y Index: 210

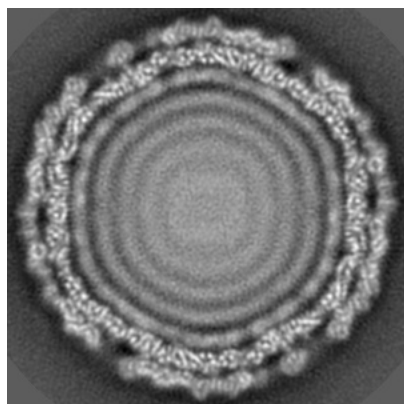


Z Index: 210

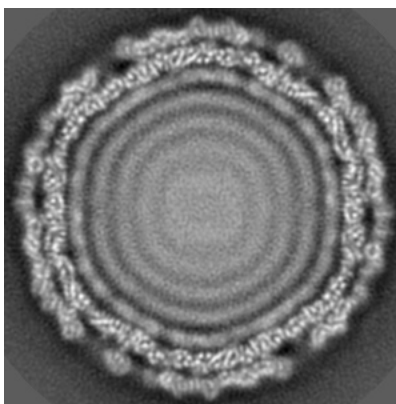
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

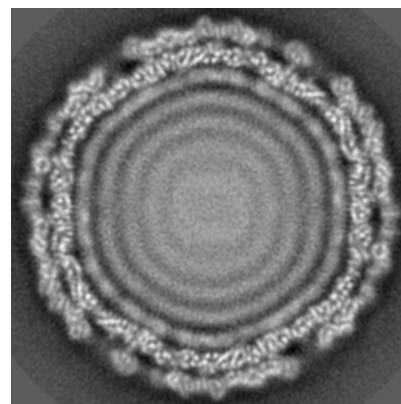
6.3.1 Primary map



X Index: 165



Y Index: 255

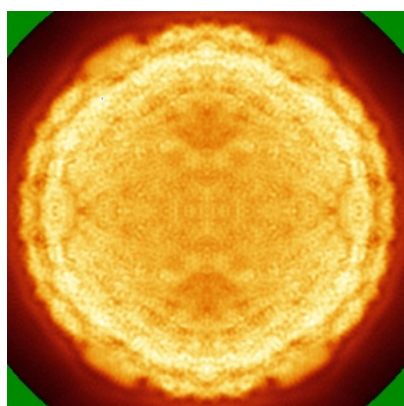


Z Index: 255

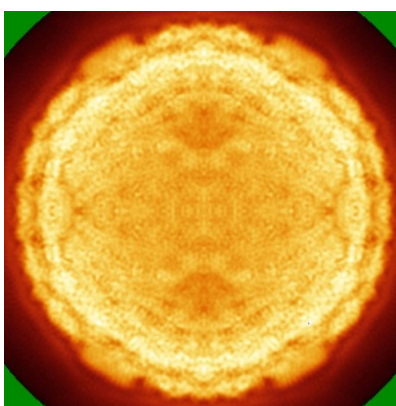
The images above show the largest variance slices of the map in three orthogonal directions.

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

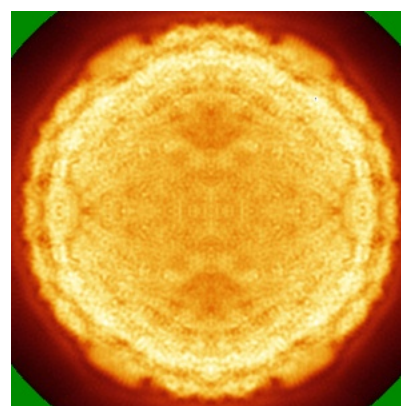
6.4.1 Primary map



X



Y



Z

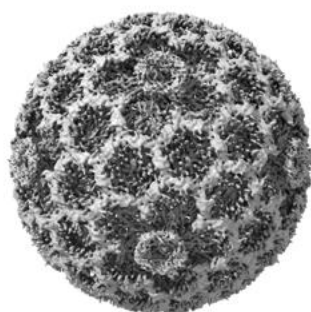
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

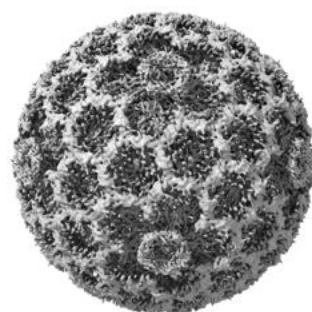
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1800.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

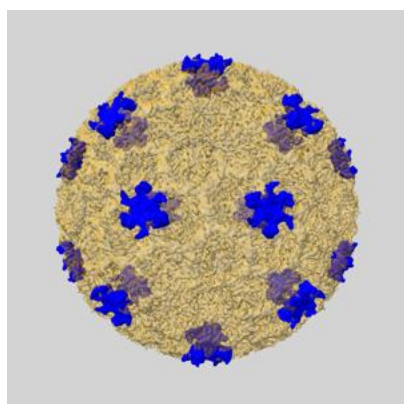
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

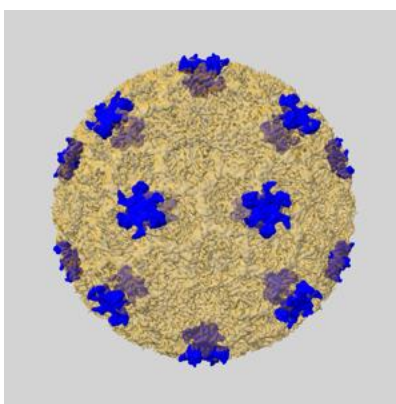
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

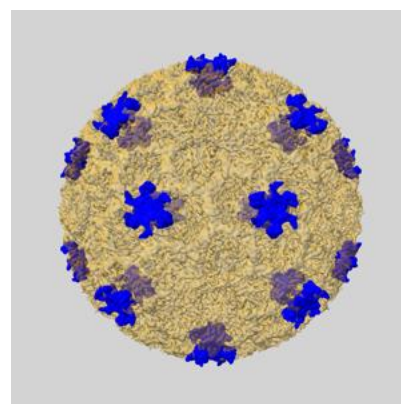
6.6.1 emd_1206_msk_6.map [i](#)



X

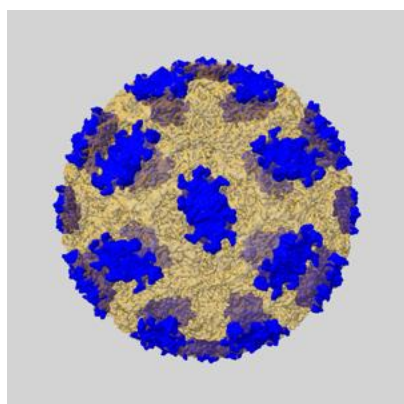


Y

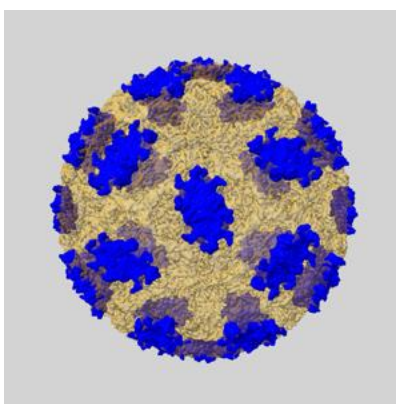


Z

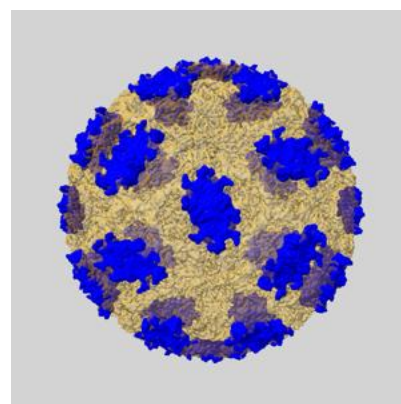
6.6.2 emd_1206_msk_5.map [i](#)



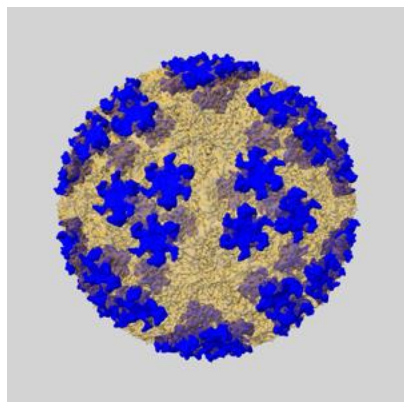
X



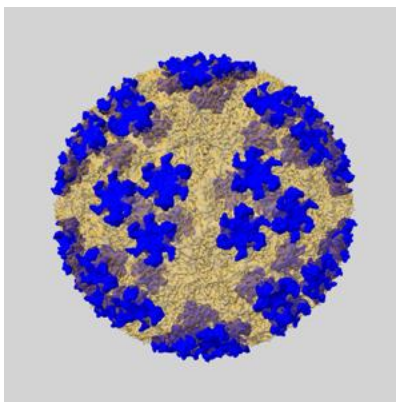
Y



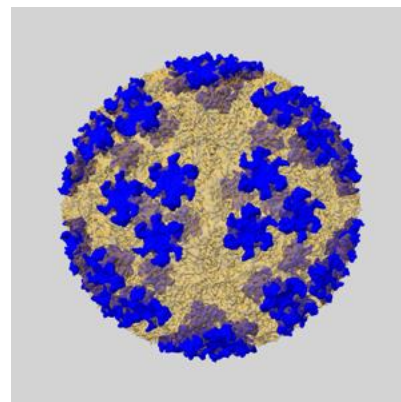
Z

6.6.3 emd_1206_msk_4.map [i](#)

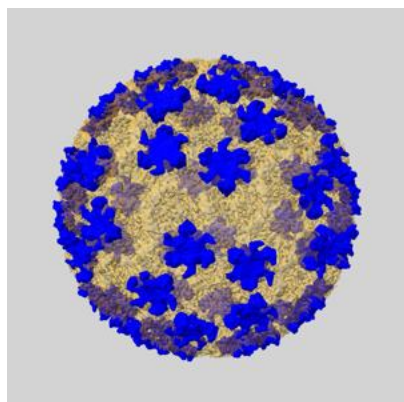
X



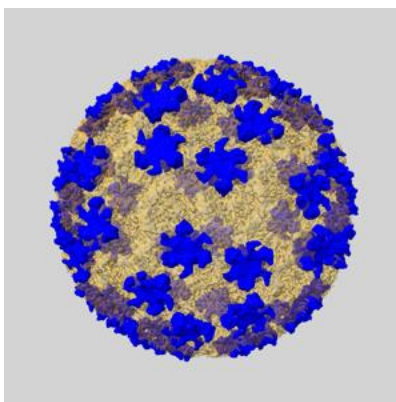
Y



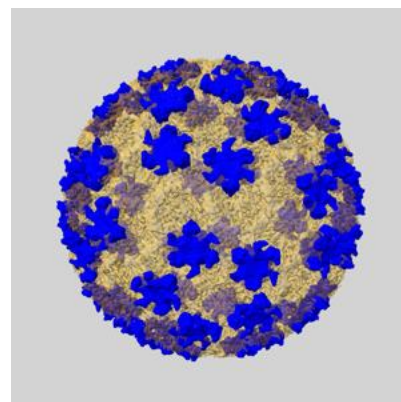
Z

6.6.4 emd_1206_msk_3.map [i](#)

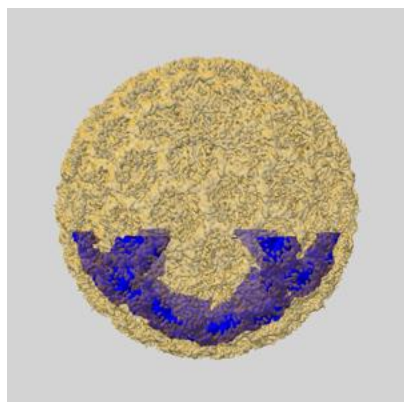
X



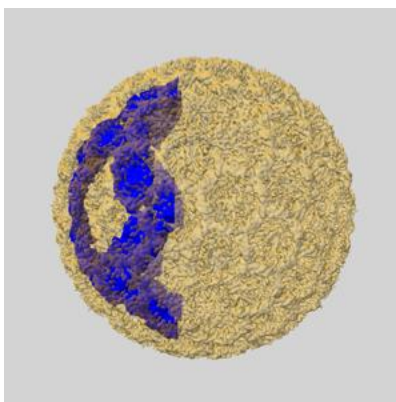
Y



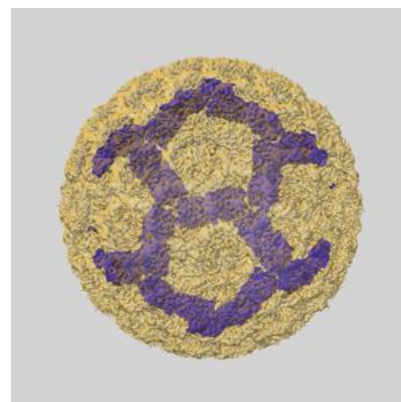
Z

6.6.5 emd_1206_msk_2.map [i](#)

X

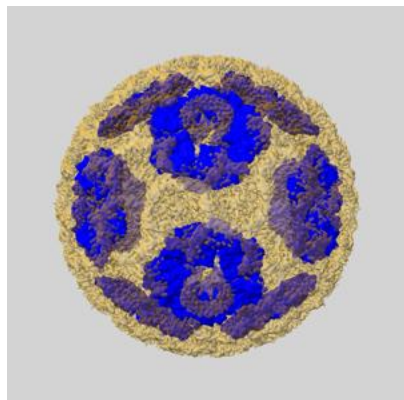


Y

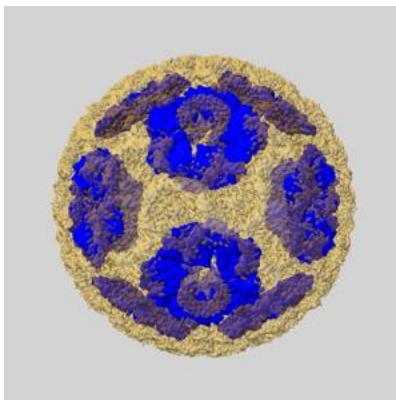


Z

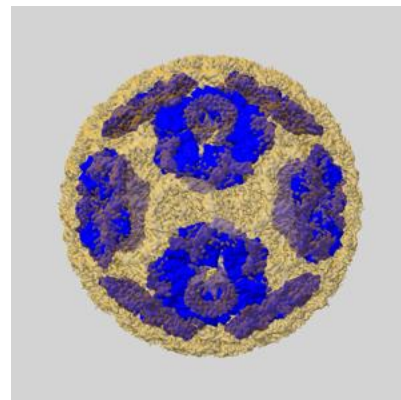
6.6.6 emd_1206_msk_1.map [i](#)



X



Y

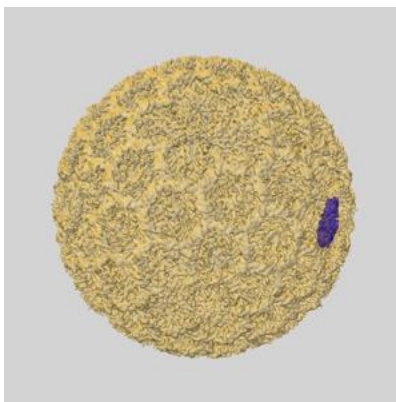


Z

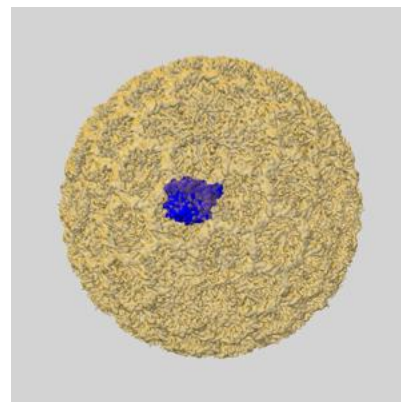
6.6.7 emd_1206_msk_7.map [i](#)



X



Y

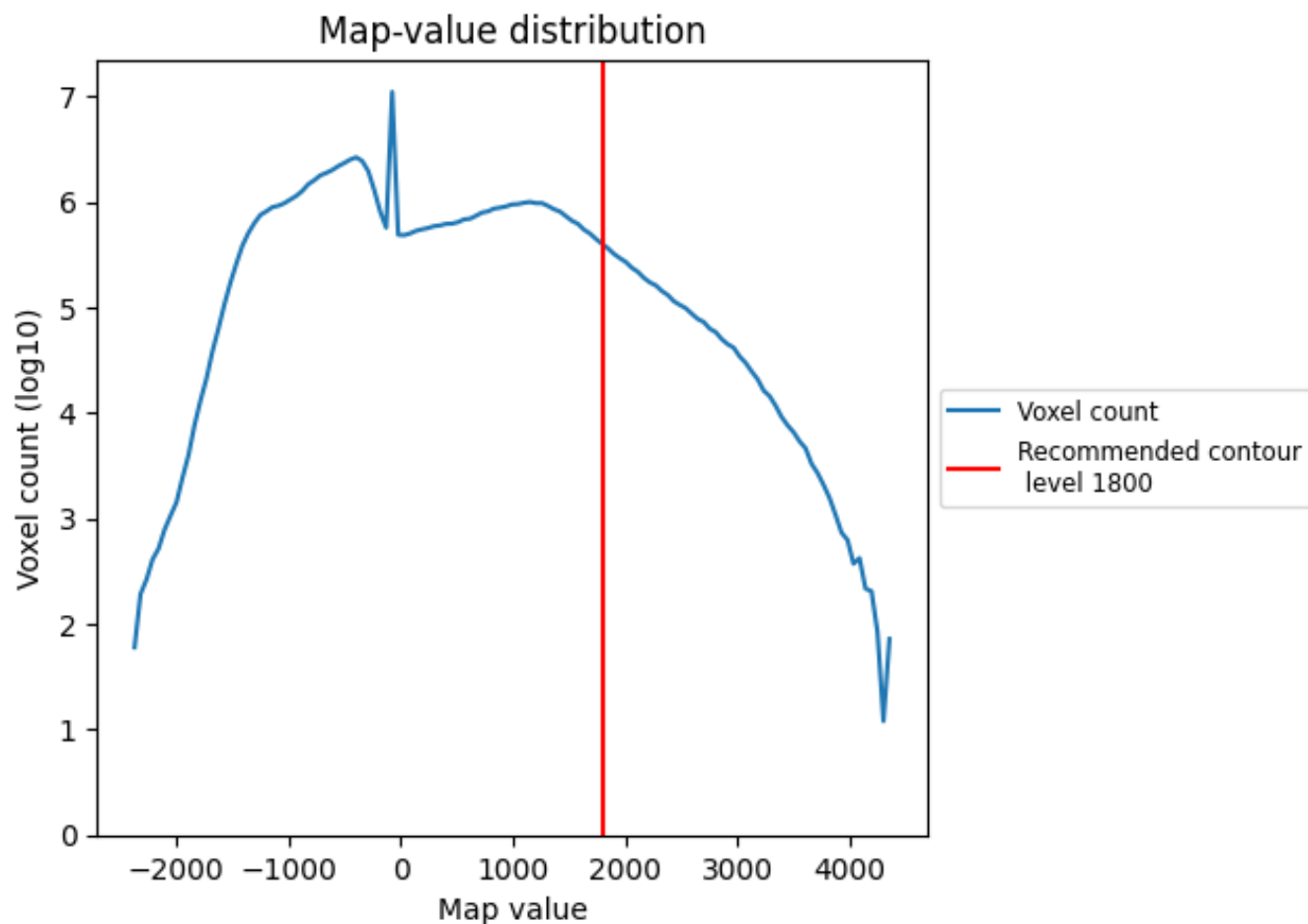


Z

7 Map analysis [i](#)

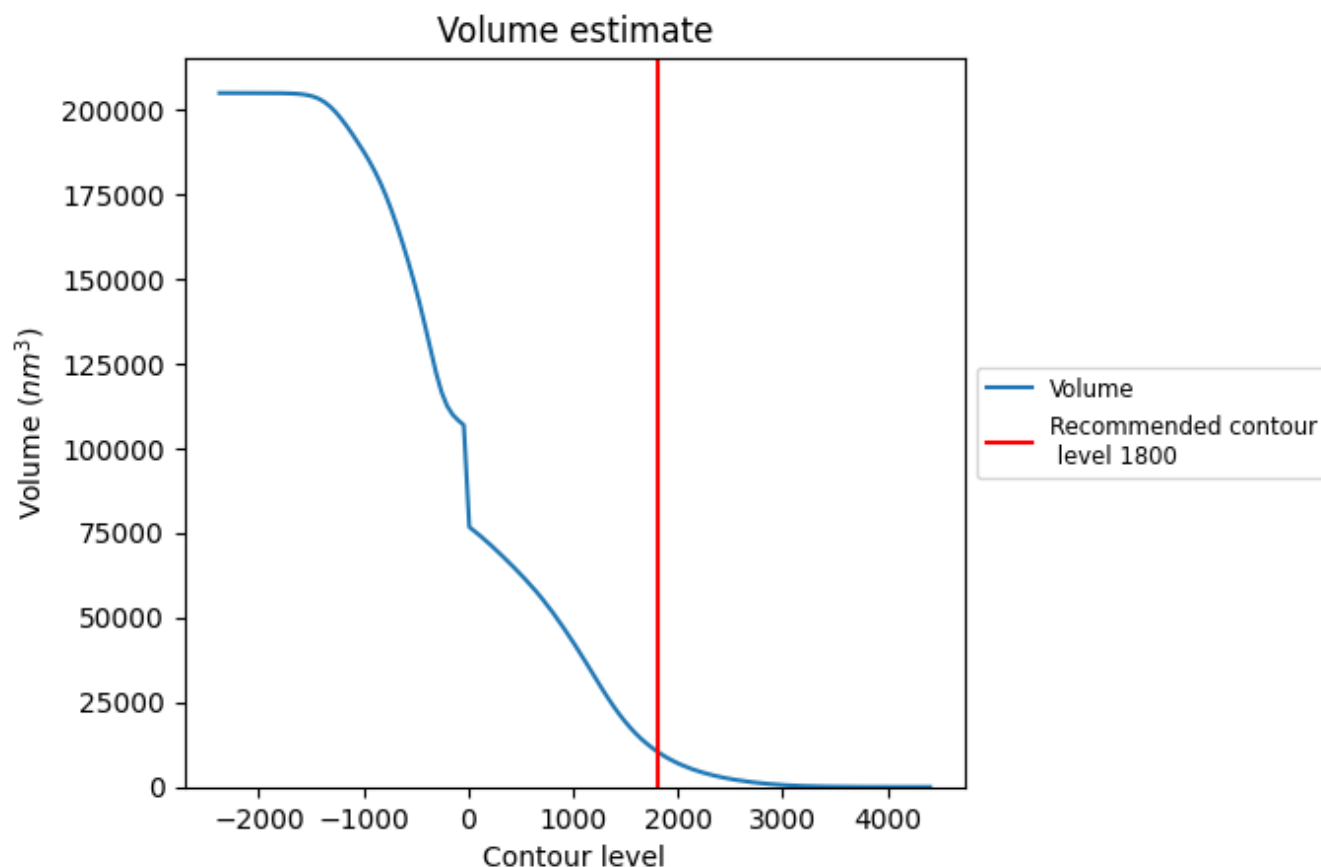
This section contains the results of statistical analysis of the map.

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.

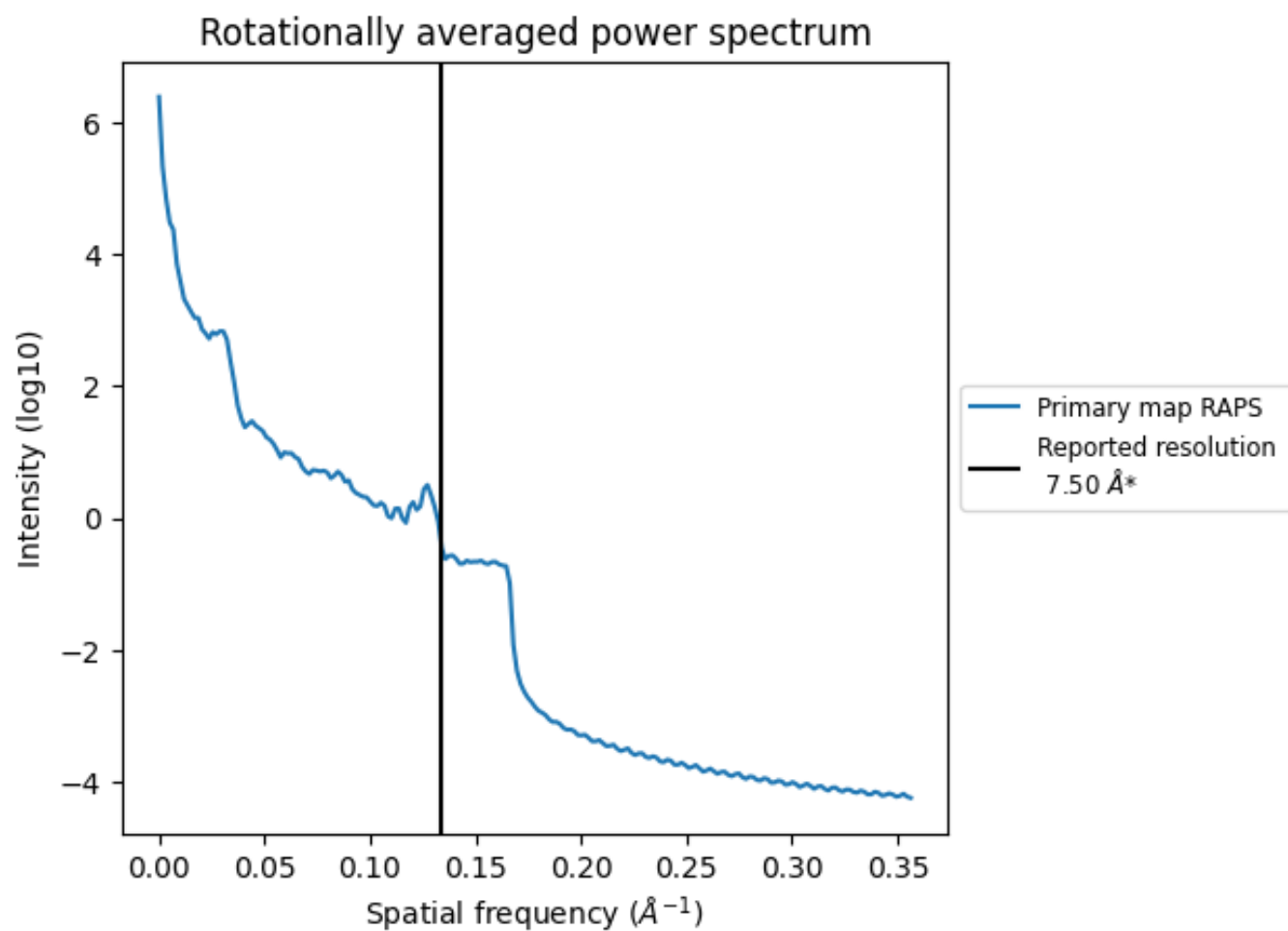
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10518 nm^3 ; this corresponds to an approximate mass of 9501 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 0.133 Å⁻¹

8 Fourier-Shell correlation ⓘ

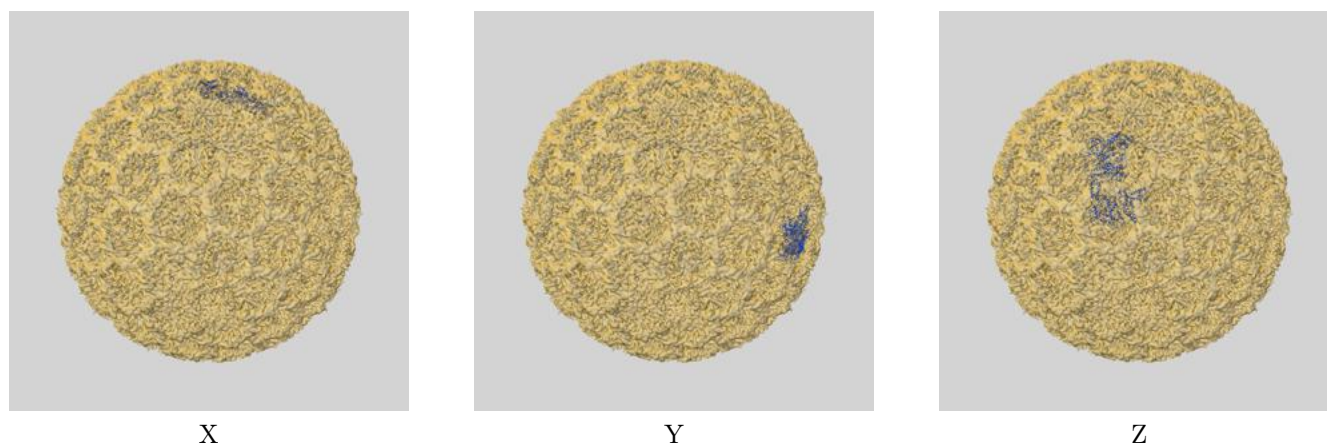
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

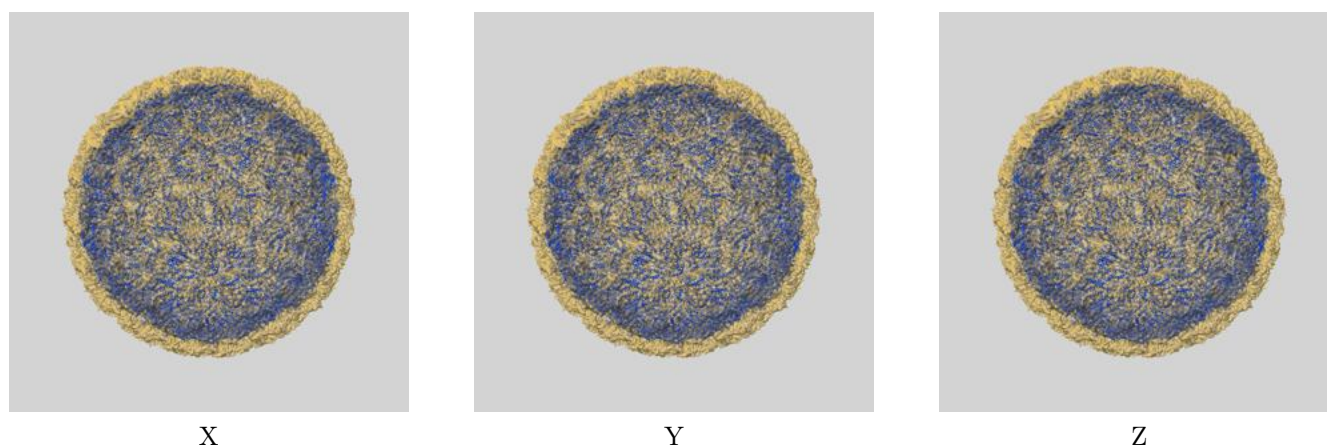
This section contains information regarding the fit between EMDB map EMD-1206 and PDB model 4BTQ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



9.1.2 Map-model assembly overlay [i](#)



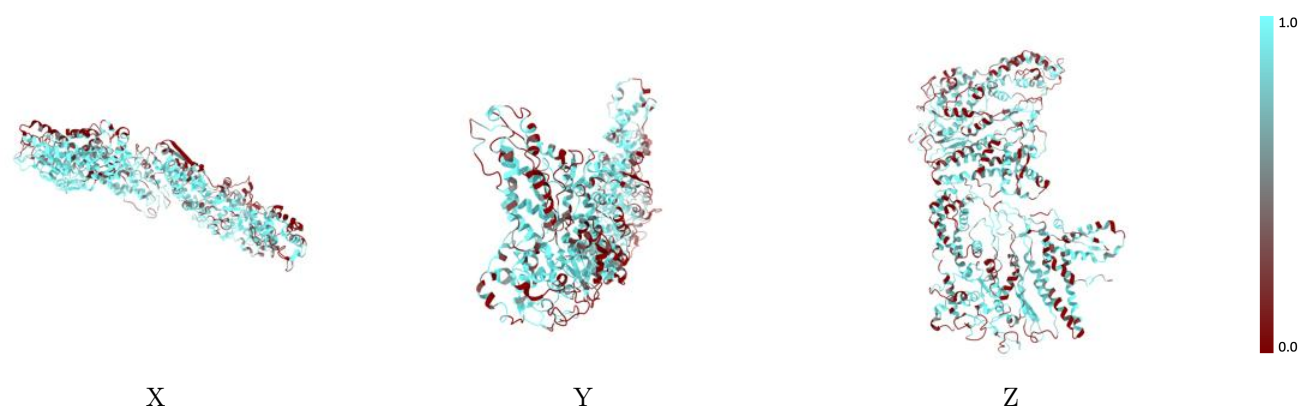
The images above show the 3D surface view of the map at the recommended contour level 1800.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



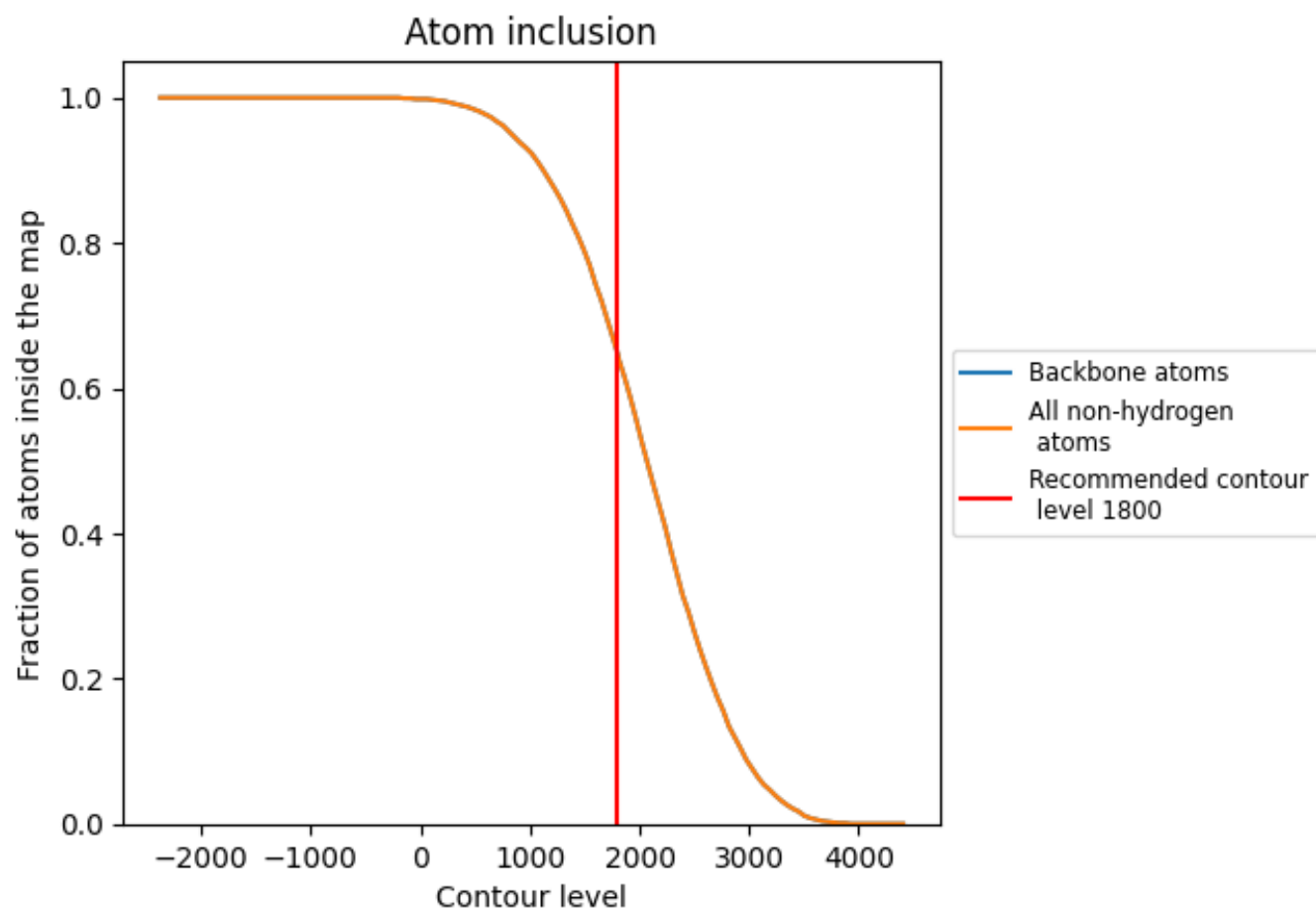
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1800).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 65% 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 (1800) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.2460
A	0.6130	0.2400
B	0.6830	0.2520

