



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:49 PM UTC

PDB ID : 5SV9 / pdb_00005sv9
EMDB ID : EMD-8313
Title : Structure of the SLC4 transporter Bor1p in an inward-facing conformation
Authors : Coudray, N.; Seyler, S.; Lasala, R.; Zhang, Z.; Clark, K.M.; Dumont, M.E.; Rohou, A.; Beckstein, O.; Stokes, D.L.; Transcontinental EM Initiative for Membrane Protein Structure (TEMIMPS)
Deposited on : 2016-08-05
Resolution : 5.90 Å(reported)
Based on initial model : 4YZF

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

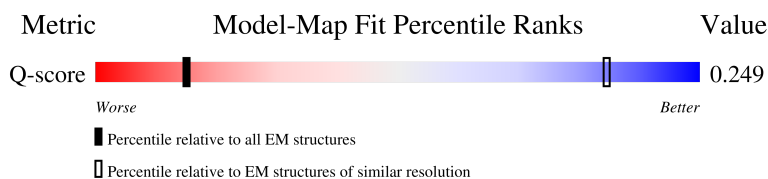
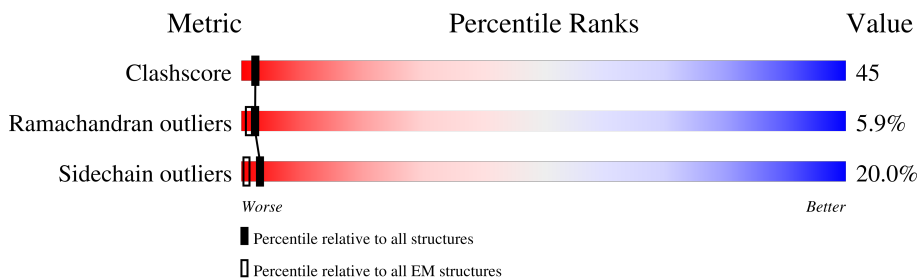
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	501 (5.40 - 6.40)

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	476	
1	B	476	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7612 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.

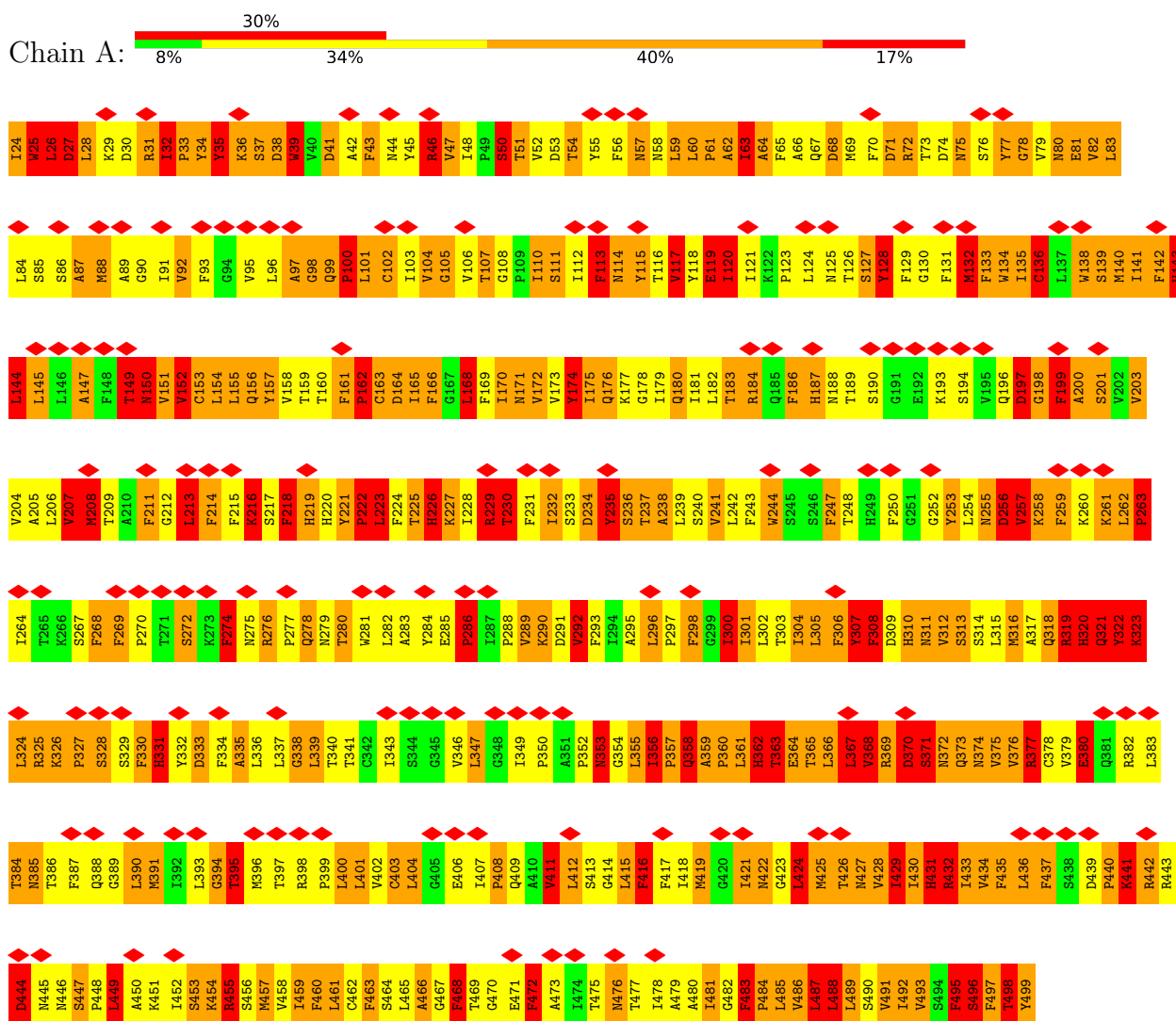
- Molecule 1 is a protein called Bor1p boron transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	476	Total	C	N	O	S	0	0
			3806	2527	608	652	19		
1	B	476	Total	C	N	O	S	0	0
			3806	2527	608	652	19		

3 Residue-property plots

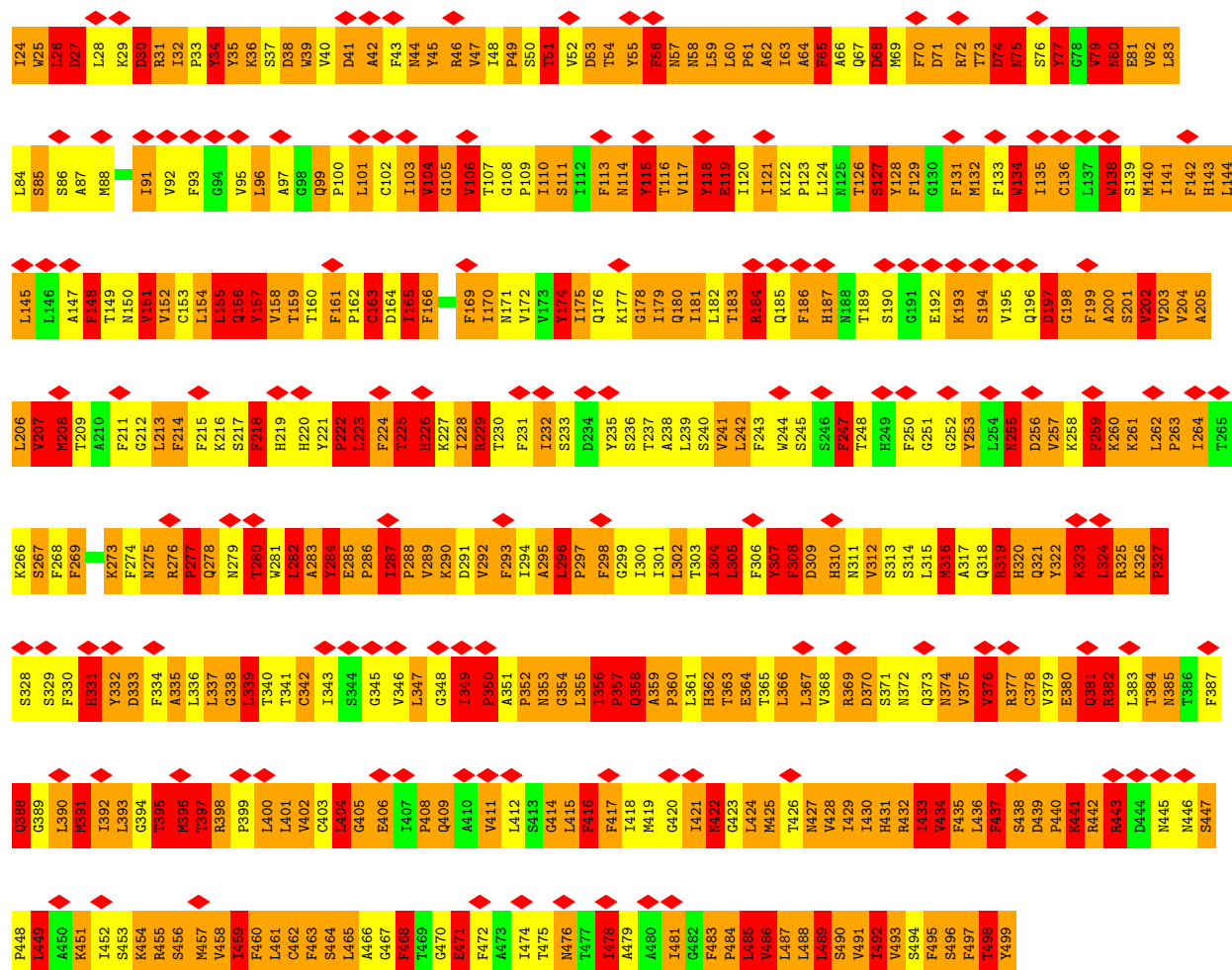
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Bor1p boron transporter



• Molecule 1: Bor1p boron transporter





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=37.35°, rise=4.8 Å, axial sym=C1	Depositor
Number of segments used	75	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	850	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	19000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	478.502	Depositor
Minimum map value	-365.121	Depositor
Average map value	0.789	Depositor
Map value standard deviation	24.341	Depositor
Recommended contour level	130	Depositor
Map size (Å)	183.82, 183.82, 183.82	wwPDB
Map dimensions	101, 101, 101	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.82, 1.82, 1.82	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	3.18	497/3917 (12.7%)	2.83	420/5333 (7.9%)
1	B	3.07	485/3917 (12.4%)	2.76	404/5333 (7.6%)
All	All	3.12	982/7834 (12.5%)	2.79	824/10666 (7.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	49
1	B	0	40
All	All	0	89

All (982) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	PHE	CA-C	-14.25	1.34	1.52
1	B	48	ILE	CA-CB	-14.11	1.46	1.54
1	B	309	ASP	CA-C	-13.70	1.35	1.52
1	A	432	ARG	CD-NE	12.99	1.64	1.46
1	A	430	ILE	CA-C	-12.79	1.36	1.52
1	A	460	PHE	CA-C	-12.75	1.36	1.52
1	B	430	ILE	CA-C	-12.59	1.36	1.52
1	A	359	ALA	N-CA	-12.29	1.35	1.46
1	B	356	ILE	CA-C	-12.12	1.40	1.52
1	A	274	PHE	CA-C	-12.08	1.38	1.52
1	A	366	LEU	CA-C	-12.06	1.39	1.53
1	A	462	CYS	CA-C	-11.77	1.37	1.52
1	B	358	GLN	CA-C	-11.74	1.37	1.52
1	B	218	PHE	CA-C	-11.46	1.37	1.52
1	A	239	LEU	CA-C	-11.37	1.38	1.52
1	A	226	HIS	CA-C	-11.35	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	496	SER	N-CA	-11.31	1.31	1.46
1	A	74	ASP	CA-C	-11.29	1.38	1.53
1	B	63	ILE	CA-C	-11.11	1.38	1.52
1	B	330	PHE	CA-CB	11.10	1.71	1.53
1	A	116	THR	CA-C	-11.04	1.38	1.52
1	B	374	ASN	CA-C	-11.02	1.39	1.52
1	A	108	GLY	CA-C	-10.87	1.44	1.51
1	A	490	SER	CA-C	-10.81	1.39	1.52
1	B	314	SER	CA-C	-10.78	1.38	1.52
1	B	134	TRP	CA-C	-10.77	1.39	1.52
1	A	229	ARG	CA-C	-10.76	1.38	1.52
1	A	25	TRP	CA-C	-10.76	1.38	1.52
1	A	158	VAL	CA-CB	-10.74	1.41	1.54
1	A	485	LEU	CA-C	-10.67	1.39	1.52
1	A	240	SER	CA-C	-10.66	1.39	1.52
1	A	314	SER	CA-C	-10.63	1.39	1.52
1	B	455	ARG	CA-C	-10.58	1.38	1.52
1	A	160	THR	CA-C	10.57	1.66	1.52
1	A	309	ASP	CA-C	-10.42	1.39	1.52
1	A	117	VAL	N-CA	-10.38	1.34	1.46
1	A	197	ASP	CA-C	-10.34	1.39	1.52
1	A	486	VAL	N-CA	-10.25	1.34	1.46
1	B	306	PHE	CA-C	-10.14	1.39	1.52
1	B	378	CYS	CA-C	-10.10	1.39	1.52
1	A	48	ILE	CA-CB	-10.09	1.49	1.54
1	B	59	LEU	CA-C	-10.08	1.39	1.52
1	B	239	LEU	CA-C	-10.08	1.39	1.52
1	A	61	PRO	CA-C	-9.95	1.36	1.52
1	A	491	VAL	N-CA	-9.94	1.34	1.46
1	B	307	TYR	CA-C	-9.93	1.40	1.52
1	B	65	PHE	CA-C	-9.92	1.39	1.52
1	B	61	PRO	CA-C	-9.87	1.36	1.52
1	A	99	GLN	N-CA	-9.86	1.36	1.46
1	A	465	LEU	CA-C	-9.85	1.39	1.52
1	A	163	CYS	CA-C	-9.84	1.40	1.52
1	A	355	LEU	CA-C	-9.84	1.39	1.52
1	A	207	VAL	CA-C	-9.84	1.40	1.52
1	A	372	ASN	CA-C	-9.84	1.44	1.53
1	B	338	GLY	CA-C	-9.82	1.39	1.51
1	A	141	ILE	CA-C	-9.81	1.40	1.52
1	B	359	ALA	N-CA	-9.80	1.37	1.46
1	B	485	LEU	CA-C	-9.79	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	TYR	CA-C	9.78	1.65	1.52
1	B	312	VAL	CA-C	-9.76	1.40	1.52
1	A	243	PHE	CA-C	-9.70	1.40	1.52
1	A	65	PHE	CA-C	-9.70	1.40	1.52
1	B	58	ASN	CA-C	-9.70	1.40	1.52
1	A	459	ILE	CA-C	-9.68	1.40	1.52
1	A	158	VAL	N-CA	-9.64	1.34	1.46
1	B	157	TYR	CA-C	-9.57	1.39	1.52
1	A	81	GLU	CA-C	-9.56	1.40	1.52
1	B	362	HIS	CA-C	-9.51	1.39	1.52
1	A	241	VAL	CA-C	-9.48	1.40	1.52
1	A	47	VAL	CA-C	-9.47	1.40	1.52
1	A	434	VAL	CA-C	-9.44	1.40	1.52
1	A	458	VAL	CA-C	-9.38	1.40	1.52
1	A	408	PRO	CA-C	-9.37	1.40	1.52
1	A	463	PHE	CA-C	-9.37	1.41	1.52
1	A	356	ILE	CA-C	-9.36	1.43	1.52
1	B	308	PHE	N-CA	-9.34	1.35	1.46
1	A	312	VAL	CA-C	-9.32	1.40	1.52
1	B	64	ALA	N-CA	-9.30	1.35	1.46
1	A	401	LEU	CA-C	-9.29	1.40	1.52
1	B	300	ILE	CA-C	-9.28	1.41	1.52
1	B	486	VAL	N-CA	-9.27	1.35	1.46
1	A	242	LEU	N-CA	-9.27	1.35	1.46
1	A	79	VAL	CA-C	-9.26	1.41	1.52
1	A	304	ILE	CA-C	-9.25	1.41	1.52
1	A	236	SER	N-CA	-9.23	1.35	1.46
1	A	428	VAL	CA-C	-9.23	1.39	1.52
1	A	310	HIS	CA-C	-9.22	1.41	1.52
1	B	310	HIS	N-CA	-9.22	1.35	1.46
1	B	69	MET	CA-C	-9.18	1.40	1.52
1	A	303	THR	CA-C	-9.18	1.40	1.52
1	A	369	ARG	CA-C	-9.16	1.42	1.52
1	A	304	ILE	N-CA	-9.16	1.35	1.46
1	B	305	LEU	CA-C	-9.14	1.41	1.52
1	A	227	LYS	N-CA	-9.12	1.35	1.46
1	A	318	GLN	CA-C	-9.11	1.40	1.52
1	A	111	SER	CA-C	-9.10	1.41	1.52
1	A	365	THR	CA-C	-9.07	1.41	1.52
1	A	311	ASN	CA-C	-9.06	1.41	1.52
1	B	208	MET	N-CA	-9.05	1.35	1.46
1	A	429	ILE	N-CA	-9.04	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	TRP	CA-C	-9.03	1.41	1.52
1	A	48	ILE	N-CA	-9.03	1.35	1.46
1	A	320	HIS	CB-CG	9.03	1.62	1.50
1	A	218	PHE	CA-C	-9.01	1.41	1.52
1	A	401	LEU	N-CA	-9.00	1.35	1.46
1	B	60	LEU	C-N	-9.00	1.23	1.34
1	B	163	CYS	CA-C	-9.00	1.41	1.52
1	A	240	SER	N-CA	-8.99	1.35	1.46
1	B	311	ASN	N-CA	-8.98	1.35	1.46
1	A	300	ILE	CA-C	-8.97	1.41	1.52
1	A	431	HIS	CA-C	-8.93	1.41	1.52
1	B	296	LEU	N-CA	-8.90	1.37	1.46
1	A	308	PHE	N-CA	-8.88	1.35	1.46
1	A	308	PHE	CA-C	-8.88	1.41	1.52
1	A	366	LEU	N-CA	-8.87	1.35	1.46
1	B	226	HIS	CA-C	-8.87	1.41	1.52
1	A	356	ILE	N-CA	-8.86	1.35	1.46
1	B	373	GLN	N-CA	-8.81	1.39	1.47
1	A	140	MET	CA-C	-8.78	1.41	1.52
1	B	45	TYR	CA-C	-8.76	1.41	1.52
1	A	488	LEU	CA-C	-8.74	1.41	1.52
1	A	313	SER	N-CA	-8.71	1.36	1.46
1	B	231	PHE	CA-C	-8.71	1.41	1.52
1	B	160	THR	CA-C	8.70	1.64	1.52
1	B	432	ARG	CD-NE	8.70	1.58	1.46
1	A	339	LEU	CA-C	-8.69	1.41	1.52
1	A	267	SER	CA-C	-8.69	1.41	1.52
1	A	60	LEU	C-N	-8.68	1.23	1.34
1	B	214	PHE	CA-C	-8.68	1.41	1.52
1	A	316	MET	CA-C	-8.68	1.41	1.52
1	A	415	LEU	CA-C	-8.67	1.41	1.52
1	A	377	ARG	CA-C	-8.66	1.41	1.52
1	A	470	GLY	CA-C	-8.66	1.42	1.52
1	A	247	PHE	CA-C	-8.64	1.41	1.52
1	A	373	GLN	CA-C	-8.60	1.41	1.52
1	A	204	VAL	CA-C	-8.60	1.41	1.52
1	B	141	ILE	CA-C	-8.59	1.42	1.52
1	A	208	MET	N-CA	-8.58	1.36	1.46
1	A	284	TYR	CA-C	-8.58	1.40	1.53
1	B	83	LEU	CA-C	-8.57	1.41	1.52
1	B	116	THR	CA-C	-8.55	1.42	1.52
1	A	237	THR	CA-C	-8.54	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	MET	CA-C	-8.54	1.41	1.52
1	A	451	LYS	CA-C	-8.53	1.41	1.52
1	B	59	LEU	N-CA	-8.53	1.36	1.46
1	A	59	LEU	CA-C	-8.51	1.41	1.52
1	B	47	VAL	CA-C	-8.51	1.42	1.52
1	A	487	LEU	CA-C	-8.50	1.41	1.52
1	A	306	PHE	CA-C	-8.49	1.41	1.52
1	B	470	GLY	CA-C	-8.49	1.42	1.52
1	A	433	ILE	CA-C	-8.47	1.42	1.52
1	A	157	TYR	CA-C	-8.47	1.41	1.52
1	A	369	ARG	N-CA	-8.46	1.38	1.46
1	A	390	LEU	CA-C	-8.45	1.42	1.52
1	A	162	PRO	CA-C	-8.45	1.40	1.52
1	B	81	GLU	CA-C	-8.43	1.41	1.52
1	A	498	THR	N-CA	-8.43	1.35	1.46
1	B	62	ALA	N-CA	-8.40	1.36	1.46
1	B	428	VAL	CA-C	-8.37	1.40	1.52
1	B	32	ILE	CA-CB	-8.36	1.48	1.53
1	A	317	ALA	N-CA	-8.36	1.36	1.46
1	B	140	MET	N-CA	-8.35	1.36	1.46
1	B	487	LEU	CA-C	-8.34	1.42	1.52
1	B	313	SER	N-CA	-8.34	1.36	1.46
1	B	460	PHE	CA-C	-8.33	1.42	1.52
1	B	242	LEU	N-CA	-8.31	1.36	1.46
1	B	60	LEU	N-CA	-8.30	1.37	1.46
1	B	304	ILE	CA-C	-8.29	1.42	1.52
1	A	422	ASN	CA-C	-8.29	1.42	1.52
1	B	373	GLN	CA-C	-8.28	1.45	1.52
1	B	433	ILE	CA-C	-8.27	1.42	1.52
1	B	401	LEU	CA-C	-8.26	1.41	1.52
1	B	339	LEU	CA-C	-8.24	1.42	1.52
1	B	56	PHE	CA-C	-8.23	1.42	1.52
1	B	437	PHE	CA-C	-8.22	1.42	1.52
1	B	495	PHE	CA-C	-8.22	1.41	1.52
1	A	290	LYS	N-CA	-8.19	1.36	1.46
1	A	274	PHE	N-CA	-8.19	1.35	1.46
1	B	366	LEU	CA-C	-8.18	1.44	1.53
1	B	401	LEU	N-CA	-8.18	1.36	1.46
1	A	183	THR	CA-C	-8.17	1.41	1.52
1	B	431	HIS	N-CA	-8.17	1.36	1.46
1	A	417	PHE	N-CA	-8.17	1.36	1.46
1	B	117	VAL	CA-C	-8.17	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	310	HIS	CA-C	-8.15	1.42	1.52
1	A	180	GLN	N-CA	-8.14	1.36	1.46
1	A	159	THR	N-CA	-8.14	1.35	1.46
1	B	57	ASN	CA-C	-8.14	1.41	1.52
1	B	400	LEU	CA-C	-8.12	1.41	1.52
1	B	48	ILE	N-CA	-8.11	1.37	1.46
1	B	157	TYR	N-CA	-8.11	1.36	1.46
1	B	315	LEU	CA-C	-8.10	1.42	1.52
1	A	322	TYR	CA-C	-8.09	1.43	1.53
1	B	134	TRP	N-CA	-8.09	1.36	1.46
1	A	291	ASP	CA-C	-8.07	1.42	1.52
1	B	179	ILE	CA-C	-8.06	1.42	1.52
1	B	356	ILE	N-CA	-8.06	1.36	1.46
1	B	405	GLY	CA-C	-8.05	1.43	1.52
1	A	320	HIS	CA-CB	8.05	1.65	1.53
1	B	182	LEU	CA-C	-8.05	1.42	1.52
1	B	44	ASN	CA-C	-8.04	1.43	1.52
1	A	293	PHE	N-CA	-8.02	1.36	1.46
1	B	99	GLN	CA-C	-8.02	1.42	1.52
1	B	85	SER	CA-C	-8.01	1.42	1.52
1	B	434	VAL	CA-C	-8.01	1.42	1.52
1	A	353	ASN	CA-C	-8.00	1.42	1.52
1	B	241	VAL	CA-C	-7.99	1.42	1.52
1	B	315	LEU	N-CA	-7.99	1.36	1.46
1	B	365	THR	CA-C	-7.98	1.42	1.52
1	A	176	GLN	CA-C	-7.96	1.42	1.52
1	A	495	PHE	CA-C	-7.95	1.41	1.52
1	A	275	ASN	N-CA	-7.95	1.36	1.46
1	B	140	MET	CA-C	-7.95	1.42	1.52
1	A	491	VAL	CA-CB	-7.94	1.45	1.54
1	A	358	GLN	CA-C	-7.93	1.42	1.52
1	A	429	ILE	CA-C	-7.93	1.42	1.52
1	B	158	VAL	CA-CB	-7.93	1.44	1.54
1	B	212	GLY	CA-C	-7.92	1.43	1.52
1	A	311	ASN	N-CA	-7.92	1.36	1.46
1	B	202	VAL	CA-C	-7.91	1.42	1.52
1	B	462	CYS	CA-C	-7.89	1.42	1.52
1	B	363	THR	N-CA	-7.89	1.36	1.46
1	B	369	ARG	CA-C	-7.88	1.42	1.52
1	B	358	GLN	N-CA	-7.88	1.36	1.46
1	B	379	VAL	N-CA	-7.86	1.37	1.46
1	A	236	SER	CA-C	-7.86	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	LEU	CA-C	-7.86	1.42	1.52
1	A	491	VAL	CA-C	-7.85	1.43	1.52
1	B	419	MET	N-CA	-7.85	1.36	1.46
1	A	338	GLY	CA-C	-7.84	1.43	1.52
1	B	491	VAL	CA-C	-7.82	1.43	1.52
1	B	390	LEU	CA-C	-7.81	1.43	1.52
1	B	28	LEU	CA-C	-7.81	1.42	1.52
1	A	307	TYR	CA-C	-7.80	1.43	1.52
1	B	142	PHE	CA-C	-7.79	1.42	1.52
1	B	418	ILE	CA-C	-7.79	1.42	1.52
1	A	36	LYS	N-CA	-7.78	1.36	1.46
1	B	486	VAL	CA-C	-7.76	1.43	1.52
1	B	142	PHE	N-CA	-7.75	1.36	1.46
1	A	427	ASN	CA-C	-7.75	1.40	1.53
1	A	432	ARG	NE-CZ	7.75	1.41	1.33
1	A	244	TRP	N-CA	-7.74	1.36	1.46
1	A	278	GLN	CA-C	-7.73	1.45	1.53
1	B	199	PHE	CA-C	-7.73	1.42	1.52
1	A	489	LEU	CA-C	-7.72	1.43	1.52
1	B	305	LEU	N-CA	-7.71	1.37	1.46
1	A	459	ILE	N-CA	-7.71	1.37	1.46
1	A	171	ASN	CA-C	-7.70	1.42	1.52
1	A	234	ASP	N-CA	-7.70	1.36	1.46
1	A	145	LEU	N-CA	-7.66	1.37	1.46
1	A	466	ALA	CA-C	-7.66	1.42	1.52
1	A	142	PHE	N-CA	-7.66	1.37	1.46
1	B	68	ASP	CA-C	-7.66	1.42	1.52
1	B	117	VAL	N-CA	-7.66	1.37	1.46
1	B	388	GLN	CA-C	-7.66	1.42	1.52
1	B	227	LYS	N-CA	-7.65	1.37	1.46
1	B	155	LEU	N-CA	-7.65	1.36	1.46
1	A	321	GLN	CA-C	-7.64	1.43	1.52
1	A	363	THR	N-CA	-7.64	1.36	1.46
1	B	70	PHE	N-CA	-7.63	1.37	1.46
1	B	67	GLN	CA-C	-7.63	1.43	1.52
1	A	69	MET	CA-C	-7.63	1.42	1.52
1	B	178	GLY	CA-C	-7.63	1.43	1.52
1	B	66	ALA	CA-C	-7.62	1.42	1.52
1	A	330	PHE	CA-C	-7.62	1.42	1.52
1	B	422	ASN	CA-C	-7.62	1.42	1.52
1	B	100	PRO	CA-C	-7.61	1.41	1.52
1	B	307	TYR	N-CA	-7.60	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	HIS	N-CA	-7.60	1.37	1.46
1	B	135	ILE	CA-C	-7.60	1.43	1.52
1	B	370	ASP	CA-C	-7.60	1.42	1.52
1	A	183	THR	N-CA	-7.59	1.36	1.46
1	A	360	PRO	CA-C	-7.59	1.41	1.52
1	A	177	LYS	CA-C	-7.59	1.43	1.52
1	A	142	PHE	CA-C	-7.58	1.43	1.52
1	A	177	LYS	N-CA	-7.58	1.37	1.46
1	A	59	LEU	N-CA	-7.58	1.37	1.46
1	B	67	GLN	N-CA	-7.56	1.37	1.46
1	A	497	PHE	CA-C	-7.56	1.43	1.52
1	B	384	THR	CA-C	-7.55	1.43	1.52
1	B	158	VAL	N-CA	-7.53	1.36	1.46
1	A	235	TYR	CA-C	-7.51	1.42	1.52
1	A	430	ILE	CA-CB	-7.51	1.45	1.54
1	A	214	PHE	CA-C	-7.50	1.43	1.52
1	B	156	GLN	CA-C	-7.50	1.42	1.52
1	B	333	ASP	N-CA	-7.50	1.37	1.46
1	A	488	LEU	N-CA	-7.50	1.37	1.46
1	B	51	THR	N-CA	-7.50	1.37	1.46
1	B	133	PHE	N-CA	-7.50	1.37	1.46
1	A	110	ILE	CA-C	-7.48	1.43	1.52
1	B	260	LYS	CA-C	-7.48	1.43	1.52
1	A	60	LEU	N-CA	-7.48	1.39	1.46
1	A	372	ASN	N-CA	-7.47	1.38	1.46
1	B	165	ILE	CA-C	-7.47	1.43	1.52
1	B	434	VAL	N-CA	-7.46	1.37	1.46
1	A	60	LEU	CA-C	-7.46	1.43	1.52
1	A	305	LEU	N-CA	-7.46	1.37	1.46
1	A	64	ALA	CA-C	-7.45	1.43	1.52
1	B	291	ASP	N-CA	-7.45	1.37	1.46
1	A	461	LEU	N-CA	-7.45	1.37	1.46
1	B	309	ASP	N-CA	-7.43	1.37	1.46
1	B	205	ALA	CA-C	-7.43	1.43	1.52
1	A	67	GLN	CA-C	-7.42	1.43	1.52
1	A	83	LEU	CA-C	-7.42	1.43	1.52
1	A	154	LEU	N-CA	-7.41	1.37	1.46
1	A	179	ILE	CA-C	-7.41	1.43	1.52
1	A	368	VAL	CA-C	-7.40	1.43	1.52
1	A	403	CYS	CA-C	-7.40	1.43	1.52
1	A	435	PHE	CA-C	-7.40	1.42	1.52
1	A	212	GLY	CA-C	-7.40	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	PHE	CA-C	-7.39	1.43	1.52
1	B	372	ASN	CA-C	-7.39	1.42	1.52
1	B	236	SER	CA-C	-7.38	1.43	1.52
1	A	70	PHE	CA-C	-7.38	1.43	1.52
1	B	127	SER	CA-C	-7.37	1.42	1.52
1	B	357	PRO	CA-C	-7.37	1.40	1.52
1	B	461	LEU	CA-C	-7.37	1.42	1.52
1	B	290	LYS	CA-C	-7.36	1.43	1.52
1	A	62	ALA	CA-C	-7.35	1.43	1.52
1	A	41	ASP	CA-C	-7.35	1.42	1.52
1	A	317	ALA	CA-C	-7.35	1.43	1.52
1	A	362	HIS	CA-C	-7.34	1.42	1.52
1	A	458	VAL	N-CA	-7.34	1.37	1.46
1	A	305	LEU	CA-C	-7.33	1.43	1.52
1	B	285	GLU	CA-C	7.33	1.62	1.52
1	A	84	LEU	CA-C	-7.32	1.43	1.52
1	B	301	ILE	N-CA	-7.32	1.37	1.46
1	A	330	PHE	N-CA	-7.31	1.37	1.46
1	A	230	THR	N-CA	-7.30	1.37	1.46
1	B	27	ASP	N-CA	-7.30	1.37	1.46
1	A	449	LEU	CA-C	-7.30	1.43	1.52
1	B	50	SER	CA-C	-7.30	1.43	1.52
1	A	80	ASN	N-CA	-7.29	1.37	1.46
1	A	292	VAL	CA-C	-7.29	1.42	1.52
1	A	481	ILE	N-CA	-7.28	1.37	1.46
1	B	382	ARG	CA-C	-7.27	1.42	1.52
1	B	165	ILE	N-CA	-7.27	1.37	1.46
1	B	26	LEU	CA-C	-7.27	1.43	1.52
1	B	356	ILE	C-N	-7.26	1.25	1.34
1	A	66	ALA	CA-C	-7.26	1.43	1.52
1	A	363	THR	CA-C	-7.26	1.43	1.52
1	A	157	TYR	N-CA	-7.24	1.37	1.46
1	A	469	THR	N-CA	-7.22	1.37	1.46
1	B	247	PHE	CA-C	-7.22	1.43	1.52
1	A	205	ALA	CA-C	-7.21	1.43	1.52
1	B	139	SER	CA-C	-7.21	1.43	1.52
1	A	64	ALA	N-CA	-7.19	1.37	1.46
1	A	156	GLN	N-CA	-7.19	1.37	1.46
1	B	84	LEU	N-CA	-7.18	1.37	1.46
1	A	383	LEU	CA-C	-7.18	1.43	1.52
1	B	425	MET	N-CA	-7.17	1.37	1.46
1	B	379	VAL	CA-C	-7.17	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	86	SER	N-CA	-7.16	1.37	1.46
1	B	174	TYR	CA-C	-7.13	1.43	1.52
1	B	201	SER	CA-C	-7.13	1.43	1.52
1	B	181	ILE	CA-C	-7.13	1.43	1.52
1	A	184	ARG	CA-C	-7.12	1.43	1.52
1	A	310	HIS	N-CA	-7.12	1.38	1.46
1	B	104	VAL	CA-CB	-7.12	1.46	1.54
1	B	183	THR	CA-C	-7.12	1.43	1.52
1	A	63	ILE	N-CA	-7.12	1.38	1.46
1	A	421	ILE	CA-C	-7.11	1.43	1.52
1	A	178	GLY	CA-C	-7.11	1.44	1.52
1	A	304	ILE	CA-CB	-7.11	1.45	1.54
1	A	315	LEU	CA-C	-7.10	1.43	1.52
1	A	340	THR	CA-C	-7.10	1.43	1.52
1	A	323	LYS	N-CA	-7.09	1.37	1.46
1	B	430	ILE	CA-CB	-7.08	1.45	1.54
1	A	277	PRO	CA-C	-7.07	1.45	1.52
1	B	171	ASN	CA-C	-7.07	1.43	1.52
1	B	63	ILE	N-CA	-7.06	1.38	1.46
1	A	139	SER	CA-C	-7.05	1.43	1.52
1	A	35	TYR	CA-C	-7.04	1.43	1.52
1	A	356	ILE	C-N	-7.04	1.25	1.34
1	B	385	ASN	CA-C	-7.04	1.43	1.52
1	A	283	ALA	CA-C	-7.03	1.43	1.53
1	A	496	SER	N-CA	-7.03	1.37	1.46
1	B	487	LEU	N-CA	-7.02	1.37	1.46
1	A	105	GLY	N-CA	-7.01	1.38	1.45
1	B	80	ASN	N-CA	-7.01	1.37	1.46
1	A	333	ASP	CA-C	-7.01	1.43	1.52
1	B	74	ASP	CA-C	-7.01	1.41	1.52
1	A	280	THR	CA-C	-7.01	1.44	1.52
1	A	432	ARG	N-CA	-7.01	1.37	1.46
1	B	336	LEU	N-CA	-7.00	1.37	1.46
1	A	57	ASN	N-CA	-7.00	1.37	1.46
1	B	360	PRO	CA-C	-6.99	1.42	1.52
1	B	416	PHE	CA-C	-6.99	1.44	1.52
1	B	433	ILE	N-CA	-6.98	1.38	1.46
1	B	242	LEU	CA-C	-6.98	1.43	1.52
1	A	67	GLN	N-CA	-6.97	1.38	1.46
1	B	222	PRO	CA-C	-6.97	1.42	1.52
1	A	319	ARG	N-CA	-6.97	1.37	1.46
1	A	181	ILE	CA-C	-6.96	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	367	LEU	CA-C	-6.96	1.44	1.52
1	B	201	SER	N-CA	-6.96	1.38	1.46
1	B	279	ASN	C-N	6.95	1.43	1.33
1	B	291	ASP	CA-C	-6.94	1.43	1.52
1	B	313	SER	CA-C	-6.94	1.44	1.52
1	B	462	CYS	N-CA	-6.94	1.38	1.46
1	A	140	MET	N-CA	-6.94	1.38	1.46
1	B	101	LEU	N-CA	-6.94	1.36	1.46
1	B	458	VAL	CA-C	-6.94	1.44	1.52
1	B	82	VAL	N-CA	-6.93	1.38	1.46
1	B	180	GLN	CA-C	-6.93	1.43	1.52
1	B	172	VAL	CA-C	-6.93	1.44	1.52
1	B	71	ASP	CA-C	-6.92	1.43	1.52
1	A	208	MET	CA-C	-6.91	1.44	1.52
1	B	229	ARG	N-CA	-6.89	1.38	1.46
1	B	463	PHE	CA-C	-6.88	1.44	1.52
1	A	56	PHE	CA-C	-6.87	1.43	1.52
1	A	62	ALA	N-CA	-6.87	1.38	1.46
1	B	322	TYR	N-CA	-6.86	1.38	1.46
1	B	493	VAL	CA-CB	-6.86	1.44	1.54
1	A	447	SER	N-CA	-6.85	1.39	1.46
1	A	244	TRP	CA-C	-6.84	1.44	1.52
1	A	123	PRO	CA-C	-6.84	1.45	1.52
1	B	273	LYS	CA-C	-6.83	1.45	1.53
1	A	29	LYS	N-CA	-6.83	1.38	1.46
1	A	400	LEU	CA-C	-6.83	1.43	1.52
1	A	63	ILE	CA-C	-6.81	1.44	1.52
1	B	415	LEU	CA-C	-6.80	1.44	1.52
1	A	238	ALA	CA-C	-6.80	1.44	1.52
1	A	58	ASN	CA-C	-6.80	1.44	1.52
1	A	302	LEU	CA-C	-6.80	1.44	1.52
1	A	485	LEU	C-N	-6.79	1.25	1.33
1	B	285	GLU	N-CA	6.79	1.55	1.46
1	A	316	MET	N-CA	-6.78	1.38	1.46
1	A	414	GLY	CA-C	-6.78	1.44	1.52
1	B	135	ILE	N-CA	-6.77	1.38	1.46
1	A	90	GLY	CA-C	-6.76	1.44	1.52
1	A	130	GLY	CA-C	-6.76	1.44	1.52
1	A	199	PHE	CA-C	-6.76	1.44	1.52
1	B	488	LEU	CA-C	-6.76	1.44	1.52
1	B	342	CYS	N-CA	-6.76	1.38	1.46
1	B	429	ILE	N-CA	-6.76	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	ALA	CA-C	-6.75	1.44	1.52
1	B	105	GLY	N-CA	-6.75	1.38	1.45
1	B	408	PRO	N-CA	-6.75	1.39	1.46
1	A	374	ASN	CA-C	-6.75	1.43	1.52
1	B	154	LEU	N-CA	-6.75	1.37	1.46
1	B	181	ILE	N-CA	-6.74	1.38	1.46
1	A	402	VAL	CA-C	-6.73	1.44	1.52
1	B	486	VAL	CA-CB	-6.73	1.46	1.54
1	A	355	LEU	N-CA	-6.72	1.37	1.45
1	B	321	GLN	CA-C	-6.71	1.43	1.52
1	B	175	ILE	N-CA	-6.70	1.38	1.46
1	A	108	GLY	C-N	-6.70	1.25	1.33
1	A	452	ILE	N-CA	-6.70	1.38	1.46
1	B	114	ASN	N-CA	-6.70	1.38	1.46
1	A	493	VAL	CA-CB	-6.70	1.44	1.54
1	B	133	PHE	CA-C	-6.69	1.44	1.52
1	A	71	ASP	CA-C	-6.69	1.44	1.52
1	A	313	SER	CA-C	-6.69	1.44	1.52
1	B	238	ALA	CA-C	-6.69	1.44	1.52
1	A	487	LEU	N-CA	-6.68	1.38	1.46
1	B	104	VAL	CA-C	-6.67	1.44	1.52
1	B	323	LYS	CA-C	-6.67	1.43	1.52
1	A	358	GLN	N-CA	-6.67	1.38	1.46
1	B	235	TYR	CA-C	-6.66	1.43	1.52
1	A	85	SER	CA-C	-6.66	1.44	1.52
1	A	334	PHE	N-CA	-6.66	1.38	1.46
1	B	341	THR	CA-C	-6.65	1.44	1.52
1	A	174	TYR	CA-C	-6.64	1.44	1.52
1	A	165	ILE	CA-C	-6.64	1.44	1.52
1	B	154	LEU	C-N	-6.63	1.25	1.34
1	A	301	ILE	N-CA	-6.63	1.38	1.46
1	B	79	VAL	CA-C	-6.63	1.44	1.52
1	B	330	PHE	CB-CG	6.62	1.65	1.50
1	A	250	PHE	CA-C	-6.62	1.45	1.52
1	B	457	MET	CA-C	-6.62	1.44	1.52
1	B	484	PRO	N-CA	-6.62	1.38	1.47
1	B	170	ILE	CA-C	-6.62	1.44	1.52
1	B	207	VAL	CA-C	-6.62	1.44	1.52
1	A	435	PHE	N-CA	-6.62	1.38	1.46
1	A	447	SER	CA-C	-6.62	1.44	1.52
1	B	46	ARG	CA-C	-6.62	1.43	1.52
1	A	203	VAL	CA-C	-6.61	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	ILE	CA-C	-6.61	1.44	1.52
1	A	158	VAL	CA-C	-6.61	1.43	1.52
1	B	54	THR	CA-C	-6.60	1.43	1.52
1	A	238	ALA	N-CA	-6.60	1.38	1.46
1	A	150	ASN	CA-C	-6.60	1.43	1.53
1	B	421	ILE	CA-C	-6.59	1.44	1.52
1	A	33	PRO	CA-C	-6.59	1.42	1.52
1	B	240	SER	CA-C	-6.59	1.44	1.52
1	A	118	TYR	CA-C	-6.59	1.44	1.52
1	A	411	VAL	CA-C	-6.59	1.44	1.52
1	A	92	VAL	CA-C	-6.58	1.44	1.52
1	A	32	ILE	CA-CB	-6.58	1.49	1.53
1	A	77	TYR	CA-C	-6.57	1.44	1.52
1	A	179	ILE	N-CA	-6.56	1.38	1.46
1	A	455	ARG	CA-C	-6.56	1.44	1.52
1	A	165	ILE	N-CA	-6.55	1.38	1.46
1	A	203	VAL	N-CA	-6.55	1.39	1.46
1	B	361	LEU	N-CA	-6.55	1.38	1.46
1	B	141	ILE	CA-CB	-6.55	1.46	1.54
1	B	316	MET	CA-C	-6.55	1.44	1.52
1	B	301	ILE	CA-CB	-6.54	1.46	1.54
1	B	363	THR	CA-C	-6.54	1.44	1.52
1	B	490	SER	CA-C	-6.54	1.44	1.52
1	B	62	ALA	CA-C	-6.53	1.44	1.52
1	A	457	MET	CA-C	-6.53	1.44	1.52
1	A	391	MET	CA-C	-6.52	1.44	1.52
1	A	73	THR	CA-C	-6.52	1.43	1.52
1	A	143	HIS	CB-CG	-6.52	1.41	1.50
1	B	81	GLU	N-CA	-6.51	1.38	1.46
1	A	80	ASN	CA-C	-6.50	1.44	1.52
1	A	143	HIS	N-CA	-6.50	1.38	1.46
1	B	282	LEU	CA-C	-6.49	1.44	1.52
1	A	486	VAL	CA-CB	-6.49	1.46	1.54
1	A	357	PRO	CA-C	-6.48	1.42	1.52
1	B	228	ILE	CA-C	-6.47	1.44	1.52
1	B	414	GLY	CA-C	-6.47	1.44	1.52
1	A	72	ARG	CA-C	-6.47	1.44	1.52
1	B	119	GLU	CA-C	-6.46	1.44	1.52
1	B	301	ILE	CA-C	-6.46	1.44	1.52
1	A	390	LEU	N-CA	-6.46	1.38	1.46
1	B	48	ILE	CA-C	-6.45	1.46	1.52
1	B	237	THR	N-CA	-6.45	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	LEU	N-CA	-6.45	1.38	1.46
1	B	256	ASP	N-CA	-6.45	1.38	1.46
1	A	175	ILE	CA-C	-6.44	1.44	1.52
1	A	60	LEU	C-O	-6.44	1.18	1.24
1	A	211	PHE	CA-C	-6.44	1.44	1.52
1	B	396	MET	CA-C	-6.44	1.44	1.52
1	A	307	TYR	N-CA	-6.44	1.38	1.46
1	B	458	VAL	N-CA	-6.43	1.38	1.46
1	B	80	ASN	CA-C	-6.42	1.44	1.52
1	B	203	VAL	N-CA	-6.42	1.39	1.46
1	A	498	THR	CA-C	-6.42	1.44	1.52
1	A	129	PHE	N-CA	-6.41	1.38	1.46
1	A	34	TYR	N-CA	-6.41	1.38	1.46
1	A	180	GLN	CA-C	-6.41	1.44	1.52
1	A	375	VAL	CA-C	-6.40	1.44	1.52
1	A	469	THR	CA-C	-6.40	1.44	1.52
1	B	468	PHE	N-CA	-6.40	1.38	1.46
1	B	49	PRO	CA-C	-6.39	1.41	1.52
1	A	170	ILE	CA-CB	-6.39	1.46	1.54
1	A	65	PHE	N-CA	-6.38	1.38	1.46
1	A	138	TRP	CA-C	-6.37	1.44	1.52
1	A	298	PHE	N-CA	-6.37	1.38	1.46
1	A	453	SER	CA-C	-6.37	1.46	1.53
1	B	476	ASN	N-CA	-6.36	1.38	1.46
1	B	353	ASN	C-N	-6.36	1.29	1.33
1	A	114	ASN	N-CA	-6.36	1.38	1.46
1	A	364	GLU	CA-C	-6.35	1.44	1.52
1	B	104	VAL	N-CA	-6.35	1.38	1.46
1	B	227	LYS	CA-C	-6.35	1.44	1.52
1	B	151	VAL	CA-CB	-6.34	1.45	1.54
1	B	60	LEU	CA-C	-6.33	1.44	1.52
1	B	496	SER	CA-C	-6.33	1.43	1.52
1	B	451	LYS	CA-C	-6.33	1.44	1.52
1	B	124	LEU	CA-C	-6.31	1.44	1.53
1	A	28	LEU	CA-C	-6.31	1.44	1.52
1	B	233	SER	CA-C	-6.31	1.44	1.52
1	B	489	LEU	N-CA	-6.31	1.38	1.46
1	A	174	TYR	N-CA	-6.30	1.38	1.46
1	B	113	PHE	CA-C	-6.30	1.44	1.52
1	B	495	PHE	C-N	-6.30	1.25	1.33
1	B	82	VAL	CA-C	-6.30	1.44	1.52
1	A	221	TYR	CA-CB	6.30	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	376	VAL	CA-C	-6.30	1.45	1.52
1	A	84	LEU	N-CA	-6.29	1.38	1.46
1	A	213	LEU	N-CA	-6.29	1.38	1.46
1	A	75	ASN	N-CA	-6.29	1.38	1.46
1	A	120	ILE	CA-C	-6.28	1.44	1.52
1	B	409	GLN	N-CA	-6.28	1.38	1.46
1	A	361	LEU	N-CA	-6.27	1.38	1.46
1	B	390	LEU	N-CA	-6.27	1.38	1.46
1	B	433	ILE	CA-CB	-6.27	1.46	1.54
1	A	367	LEU	CA-C	-6.27	1.44	1.52
1	B	279	ASN	CA-C	6.27	1.61	1.52
1	B	314	SER	N-CA	-6.27	1.38	1.46
1	A	302	LEU	N-CA	-6.26	1.38	1.46
1	A	289	VAL	CA-C	-6.26	1.44	1.52
1	B	60	LEU	C-O	-6.26	1.18	1.24
1	B	26	LEU	N-CA	-6.25	1.38	1.46
1	A	154	LEU	CA-C	-6.25	1.44	1.52
1	B	170	ILE	CA-CB	-6.25	1.46	1.54
1	A	209	THR	CA-C	-6.25	1.44	1.52
1	A	336	LEU	CA-C	-6.24	1.44	1.52
1	B	115	TYR	CA-C	-6.23	1.44	1.52
1	A	384	THR	CA-C	-6.23	1.45	1.52
1	A	413	SER	CA-C	-6.22	1.44	1.52
1	A	53	ASP	CA-C	-6.21	1.44	1.52
1	B	331	HIS	CA-C	-6.21	1.44	1.52
1	B	452	ILE	N-CA	-6.20	1.39	1.46
1	B	492	ILE	CA-C	-6.20	1.45	1.52
1	B	481	ILE	N-CA	-6.19	1.38	1.46
1	A	101	LEU	CA-C	-6.18	1.45	1.53
1	B	325	ARG	CA-C	6.17	1.61	1.52
1	A	32	ILE	CA-C	-6.16	1.47	1.52
1	A	264	ILE	C-N	6.16	1.42	1.33
1	B	455	ARG	N-CA	-6.15	1.38	1.46
1	A	38	ASP	CA-C	-6.15	1.44	1.52
1	A	471	GLU	N-CA	-6.15	1.39	1.46
1	A	156	GLN	CA-C	-6.15	1.44	1.52
1	B	157	TYR	C-N	-6.15	1.26	1.33
1	B	385	ASN	N-CA	-6.14	1.39	1.46
1	A	347	LEU	N-CA	-6.13	1.38	1.46
1	A	430	ILE	C-N	-6.13	1.25	1.33
1	A	471	GLU	CA-C	-6.13	1.44	1.52
1	B	391	MET	CA-C	-6.13	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	THR	N-CA	-6.13	1.39	1.46
1	B	304	ILE	N-CA	-6.13	1.39	1.46
1	B	303	THR	CA-C	-6.12	1.44	1.52
1	A	463	PHE	N-CA	-6.11	1.39	1.46
1	B	322	TYR	CA-C	-6.10	1.43	1.52
1	B	239	LEU	N-CA	-6.10	1.39	1.46
1	A	51	THR	N-CA	-6.09	1.39	1.46
1	A	346	VAL	CA-C	-6.09	1.45	1.52
1	A	160	THR	CA-CB	6.08	1.62	1.53
1	B	464	SER	N-CA	-6.08	1.39	1.46
1	B	176	GLN	CA-C	-6.08	1.44	1.52
1	A	196	GLN	CA-C	-6.08	1.45	1.52
1	B	325	ARG	CA-CB	6.08	1.63	1.53
1	B	411	VAL	CA-C	-6.08	1.45	1.52
1	B	417	PHE	CA-C	-6.08	1.45	1.52
1	B	213	LEU	N-CA	-6.07	1.39	1.46
1	B	216	LYS	N-CA	-6.07	1.39	1.46
1	A	459	ILE	CA-CB	-6.06	1.46	1.54
1	B	72	ARG	N-CA	-6.06	1.38	1.46
1	A	378	CYS	N-CA	-6.05	1.37	1.45
1	A	426	THR	CA-C	-6.04	1.44	1.53
1	A	54	THR	CA-C	-6.04	1.44	1.52
1	B	154	LEU	CA-C	-6.04	1.44	1.52
1	B	163	CYS	N-CA	-6.04	1.39	1.46
1	B	340	THR	CA-C	-6.03	1.45	1.52
1	A	42	ALA	N-CA	-6.03	1.39	1.46
1	A	144	LEU	CA-C	-6.03	1.45	1.52
1	B	359	ALA	C-N	-6.02	1.25	1.34
1	A	440	PRO	CA-C	-6.01	1.42	1.52
1	B	108	GLY	C-N	-6.01	1.26	1.33
1	A	298	PHE	CA-C	-6.00	1.45	1.52
1	A	454	LYS	CA-C	-6.00	1.45	1.52
1	B	361	LEU	CA-C	-6.00	1.44	1.52
1	B	474	ILE	CA-C	-5.99	1.45	1.52
1	A	112	ILE	N-CA	-5.99	1.39	1.46
1	A	427	ASN	N-CA	-5.99	1.38	1.47
1	A	493	VAL	CA-C	-5.99	1.43	1.52
1	B	336	LEU	CA-C	-5.98	1.45	1.52
1	A	341	THR	CA-C	-5.97	1.45	1.52
1	B	184	ARG	N-CA	-5.97	1.39	1.46
1	A	126	THR	CA-C	-5.96	1.44	1.52
1	A	327	PRO	C-N	5.96	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	LEU	CA-C	-5.96	1.45	1.52
1	A	466	ALA	N-CA	-5.96	1.39	1.46
1	B	41	ASP	N-CA	-5.96	1.38	1.46
1	A	404	LEU	N-CA	-5.95	1.39	1.46
1	A	111	SER	N-CA	-5.95	1.39	1.46
1	A	337	LEU	CA-C	-5.95	1.45	1.52
1	B	405	GLY	N-CA	-5.94	1.38	1.45
1	A	404	LEU	CA-C	-5.94	1.45	1.52
1	B	409	GLN	CA-C	-5.94	1.45	1.52
1	B	170	ILE	N-CA	-5.93	1.39	1.46
1	B	198	GLY	CA-C	-5.93	1.43	1.51
1	A	323	LYS	CA-C	-5.93	1.44	1.52
1	B	131	PHE	CA-C	-5.93	1.45	1.52
1	B	355	LEU	CA-C	-5.92	1.46	1.53
1	A	258	LYS	CA-C	-5.92	1.45	1.52
1	B	308	PHE	C-N	-5.92	1.26	1.33
1	A	100	PRO	CA-C	-5.92	1.44	1.52
1	B	432	ARG	N-CA	-5.91	1.38	1.46
1	A	368	VAL	N-CA	-5.91	1.39	1.46
1	A	495	PHE	C-N	-5.91	1.26	1.34
1	B	459	ILE	CA-C	-5.91	1.45	1.52
1	B	175	ILE	CA-C	-5.90	1.45	1.52
1	A	306	PHE	N-CA	-5.90	1.39	1.46
1	B	460	PHE	N-CA	-5.90	1.39	1.46
1	A	387	PHE	CA-C	-5.90	1.45	1.52
1	A	182	LEU	N-CA	-5.89	1.39	1.46
1	B	203	VAL	CA-C	-5.89	1.45	1.52
1	B	429	ILE	CA-C	-5.89	1.45	1.52
1	B	88	MET	CA-C	-5.88	1.45	1.52
1	A	418	ILE	CA-C	-5.87	1.45	1.52
1	B	404	LEU	CA-C	-5.87	1.45	1.52
1	B	119	GLU	N-CA	-5.87	1.39	1.46
1	B	488	LEU	N-CA	-5.87	1.39	1.46
1	A	378	CYS	CA-C	-5.87	1.45	1.53
1	B	229	ARG	CA-C	-5.87	1.45	1.52
1	A	98	GLY	CA-C	-5.86	1.45	1.51
1	A	412	LEU	CA-C	-5.86	1.44	1.52
1	B	84	LEU	CA-C	-5.86	1.45	1.52
1	A	50	SER	CA-C	-5.86	1.45	1.52
1	B	172	VAL	N-CA	-5.86	1.39	1.46
1	B	213	LEU	CA-C	-5.86	1.45	1.52
1	A	39	TRP	CA-C	-5.85	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	SER	N-CA	-5.85	1.39	1.46
1	A	225	THR	CA-C	-5.84	1.45	1.52
1	A	48	ILE	CA-C	-5.84	1.47	1.52
1	B	461	LEU	C-N	-5.84	1.26	1.33
1	A	430	ILE	N-CA	-5.84	1.39	1.46
1	B	243	PHE	CA-C	-5.84	1.45	1.52
1	A	492	ILE	CA-C	-5.82	1.45	1.52
1	A	141	ILE	CA-CB	-5.82	1.47	1.54
1	B	356	ILE	CA-CB	-5.82	1.46	1.54
1	A	95	VAL	CA-C	-5.81	1.45	1.52
1	A	170	ILE	CA-C	-5.80	1.45	1.52
1	B	475	THR	CA-C	-5.80	1.44	1.52
1	B	124	LEU	N-CA	-5.79	1.37	1.46
1	A	86	SER	N-CA	-5.79	1.39	1.46
1	B	465	LEU	N-CA	-5.79	1.38	1.46
1	B	38	ASP	CA-C	-5.79	1.44	1.52
1	A	239	LEU	N-CA	-5.78	1.39	1.46
1	A	153	CYS	N-CA	-5.78	1.39	1.46
1	A	428	VAL	N-CA	-5.77	1.38	1.46
1	B	397	THR	N-CA	-5.76	1.38	1.46
1	B	343	ILE	CA-CB	-5.75	1.47	1.54
1	A	301	ILE	CA-C	-5.75	1.45	1.52
1	B	30	ASP	CA-C	-5.75	1.45	1.52
1	B	61	PRO	N-CD	-5.75	1.39	1.47
1	A	155	LEU	CA-C	-5.75	1.45	1.52
1	A	179	ILE	CA-CB	-5.75	1.47	1.54
1	B	135	ILE	CA-CB	-5.74	1.47	1.54
1	A	46	ARG	CD-NE	5.74	1.54	1.46
1	B	131	PHE	N-CA	-5.74	1.39	1.46
1	B	114	ASN	CA-C	-5.73	1.45	1.52
1	B	432	ARG	NE-CZ	5.73	1.39	1.33
1	B	136	CYS	CA-C	-5.73	1.45	1.52
1	B	108	GLY	CA-C	-5.73	1.47	1.51
1	B	204	VAL	CA-C	-5.73	1.45	1.52
1	A	99	GLN	CA-C	-5.72	1.44	1.53
1	A	231	PHE	CA-CB	5.72	1.62	1.53
1	B	180	GLN	N-CA	-5.72	1.39	1.46
1	A	153	CYS	CA-C	-5.71	1.45	1.52
1	B	368	VAL	CA-CB	-5.71	1.47	1.54
1	B	45	TYR	N-CA	-5.71	1.39	1.46
1	B	387	PHE	CA-C	-5.71	1.45	1.52
1	B	183	THR	N-CA	-5.70	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	VAL	N-CA	-5.70	1.40	1.46
1	B	320	HIS	N-CA	-5.70	1.38	1.46
1	A	26	LEU	CA-C	-5.70	1.45	1.52
1	A	483	PHE	C-N	-5.70	1.26	1.33
1	A	234	ASP	CA-C	-5.69	1.45	1.52
1	B	64	ALA	CA-C	-5.69	1.45	1.52
1	B	337	LEU	CA-C	-5.68	1.45	1.52
1	B	484	PRO	CA-C	-5.68	1.43	1.52
1	A	119	GLU	CA-C	-5.68	1.45	1.52
1	B	419	MET	CA-C	-5.68	1.45	1.52
1	B	408	PRO	CA-C	-5.67	1.45	1.52
1	A	462	CYS	N-CA	-5.67	1.39	1.46
1	A	172	VAL	CA-C	-5.67	1.46	1.52
1	A	136	CYS	CA-C	-5.67	1.45	1.52
1	A	445	ASN	CA-C	-5.66	1.45	1.52
1	B	483	PHE	N-CA	-5.66	1.40	1.46
1	B	332	TYR	CA-C	-5.65	1.45	1.52
1	B	202	VAL	N-CA	-5.65	1.39	1.46
1	A	242	LEU	CA-C	-5.65	1.45	1.52
1	B	465	LEU	CA-C	-5.63	1.45	1.52
1	A	82	VAL	N-CA	-5.63	1.39	1.46
1	B	47	VAL	CA-CB	-5.62	1.47	1.54
1	B	162	PRO	CA-C	-5.62	1.44	1.52
1	A	489	LEU	N-CA	-5.62	1.39	1.46
1	A	26	LEU	N-CA	-5.62	1.39	1.46
1	A	336	LEU	N-CA	-5.62	1.39	1.46
1	B	181	ILE	CA-CB	-5.62	1.47	1.54
1	A	163	CYS	N-CA	-5.61	1.39	1.46
1	B	152	VAL	N-CA	-5.61	1.38	1.46
1	B	36	LYS	N-CA	-5.61	1.39	1.46
1	A	373	GLN	N-CA	-5.61	1.39	1.46
1	A	425	MET	N-CA	-5.61	1.38	1.46
1	A	155	LEU	C-N	-5.60	1.26	1.34
1	B	200	ALA	CA-C	-5.60	1.45	1.52
1	B	79	VAL	C-N	-5.60	1.26	1.33
1	B	353	ASN	C-O	-5.60	1.16	1.24
1	B	428	VAL	CA-CB	-5.60	1.46	1.54
1	B	278	GLN	C-N	5.59	1.41	1.33
1	A	57	ASN	CA-C	-5.59	1.45	1.52
1	B	197	ASP	CA-C	-5.58	1.46	1.52
1	A	78	GLY	CA-C	-5.58	1.44	1.52
1	A	72	ARG	N-CA	-5.57	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	LYS	N-CA	-5.57	1.39	1.46
1	B	75	ASN	N-CA	-5.57	1.39	1.46
1	A	364	GLU	N-CA	-5.57	1.39	1.46
1	B	365	THR	N-CA	-5.57	1.39	1.46
1	A	182	LEU	CA-C	-5.56	1.45	1.52
1	A	314	SER	N-CA	-5.56	1.39	1.46
1	B	341	THR	CA-CB	-5.56	1.44	1.53
1	B	343	ILE	N-CA	-5.55	1.40	1.46
1	A	428	VAL	CA-CB	-5.55	1.46	1.54
1	A	69	MET	N-CA	-5.54	1.39	1.46
1	B	302	LEU	N-CA	-5.54	1.39	1.46
1	A	283	ALA	N-CA	-5.54	1.40	1.46
1	B	95	VAL	CA-C	-5.53	1.46	1.52
1	B	37	SER	CA-C	-5.53	1.45	1.52
1	B	145	LEU	N-CA	-5.53	1.39	1.46
1	B	113	PHE	C-N	-5.52	1.26	1.33
1	B	491	VAL	N-CA	-5.51	1.40	1.46
1	B	206	LEU	CA-C	-5.51	1.45	1.52
1	B	365	THR	CA-CB	-5.51	1.44	1.53
1	B	375	VAL	CA-C	-5.51	1.45	1.52
1	B	70	PHE	CA-C	-5.50	1.45	1.52
1	A	200	ALA	CA-C	-5.49	1.45	1.52
1	B	179	ILE	N-CA	-5.49	1.40	1.46
1	A	135	ILE	CA-C	-5.49	1.45	1.52
1	A	255	ASN	CA-C	-5.49	1.45	1.52
1	B	284	TYR	C-N	5.49	1.45	1.33
1	B	430	ILE	N-CA	-5.49	1.40	1.46
1	B	177	LYS	N-CA	-5.48	1.39	1.46
1	A	434	VAL	N-CA	-5.47	1.40	1.46
1	B	57	ASN	N-CA	-5.47	1.39	1.46
1	B	116	THR	N-CA	-5.47	1.39	1.46
1	B	39	TRP	N-CA	-5.47	1.39	1.46
1	A	38	ASP	C-N	-5.47	1.26	1.33
1	B	174	TYR	N-CA	-5.46	1.39	1.46
1	B	317	ALA	N-CA	-5.46	1.39	1.46
1	B	156	GLN	C-N	-5.46	1.26	1.34
1	B	232	ILE	N-CA	-5.45	1.39	1.46
1	A	153	CYS	C-N	-5.44	1.26	1.34
1	A	204	VAL	N-CA	-5.44	1.40	1.46
1	B	40	VAL	CA-C	-5.43	1.45	1.52
1	B	393	LEU	CA-C	-5.43	1.46	1.52
1	B	240	SER	N-CA	-5.43	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	TYR	N-CA	-5.42	1.39	1.46
1	B	319	ARG	N-CA	-5.42	1.39	1.46
1	A	259	PHE	N-CA	-5.42	1.39	1.45
1	A	419	MET	N-CA	-5.41	1.39	1.46
1	A	329	SER	CA-C	-5.41	1.46	1.52
1	A	385	ASN	N-CA	-5.41	1.39	1.46
1	B	440	PRO	CA-C	-5.41	1.44	1.52
1	B	388	GLN	N-CA	-5.40	1.39	1.46
1	A	88	MET	CA-CB	5.40	1.61	1.53
1	A	113	PHE	CA-C	-5.40	1.45	1.52
1	B	317	ALA	CA-C	-5.39	1.46	1.52
1	A	485	LEU	N-CA	-5.39	1.39	1.46
1	B	298	PHE	N-CA	-5.39	1.39	1.46
1	A	257	VAL	CA-C	-5.38	1.46	1.52
1	B	69	MET	N-CA	-5.38	1.39	1.46
1	B	461	LEU	N-CA	-5.37	1.39	1.46
1	A	455	ARG	N-CA	-5.37	1.39	1.46
1	B	393	LEU	N-CA	-5.37	1.40	1.46
1	B	467	GLY	CA-C	-5.36	1.46	1.52
1	A	116	THR	C-N	-5.36	1.27	1.33
1	A	413	SER	N-CA	-5.36	1.39	1.46
1	B	428	VAL	N-CA	-5.36	1.39	1.46
1	B	318	GLN	CA-C	-5.35	1.45	1.52
1	A	104	VAL	CA-C	-5.34	1.46	1.52
1	B	417	PHE	N-CA	-5.34	1.40	1.46
1	A	107	THR	CA-C	-5.34	1.46	1.52
1	B	118	TYR	CA-C	-5.34	1.46	1.52
1	B	129	PHE	CA-C	-5.33	1.45	1.52
1	A	374	ASN	N-CA	-5.33	1.39	1.46
1	B	77	TYR	CA-CB	5.33	1.62	1.53
1	A	183	THR	CA-CB	-5.33	1.44	1.53
1	B	166	PHE	N-CA	-5.33	1.40	1.46
1	B	483	PHE	CA-C	-5.33	1.45	1.52
1	A	261	LYS	CA-C	-5.33	1.45	1.52
1	B	223	LEU	N-CA	-5.32	1.39	1.46
1	A	127	SER	CA-C	-5.31	1.45	1.52
1	B	434	VAL	CA-CB	-5.31	1.47	1.54
1	A	376	VAL	N-CA	-5.30	1.40	1.46
1	B	320	HIS	CB-CG	5.30	1.57	1.50
1	B	493	VAL	N-CA	-5.30	1.38	1.46
1	A	473	ALA	N-CA	-5.30	1.39	1.46
1	B	293	PHE	CA-C	-5.30	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	PHE	CA-C	-5.30	1.45	1.52
1	B	215	PHE	CA-C	-5.29	1.45	1.52
1	A	340	THR	N-CA	-5.29	1.40	1.46
1	A	141	ILE	N-CA	-5.29	1.40	1.46
1	A	386	THR	N-CA	-5.29	1.40	1.46
1	A	460	PHE	N-CA	-5.29	1.40	1.46
1	A	402	VAL	CA-CB	-5.28	1.48	1.54
1	A	492	ILE	CA-CB	-5.27	1.47	1.54
1	B	304	ILE	CA-CB	-5.27	1.47	1.54
1	B	456	SER	N-CA	-5.26	1.39	1.46
1	B	483	PHE	C-O	-5.26	1.19	1.24
1	A	419	MET	CA-C	-5.26	1.46	1.52
1	A	362	HIS	C-N	-5.26	1.26	1.34
1	B	269	PHE	CA-CB	5.25	1.60	1.54
1	B	299	GLY	CA-C	-5.25	1.46	1.52
1	B	96	LEU	CA-C	-5.25	1.45	1.52
1	A	175	ILE	N-CA	-5.25	1.40	1.46
1	A	379	VAL	CA-C	-5.25	1.46	1.52
1	B	353	ASN	CA-C	-5.25	1.45	1.52
1	A	301	ILE	CA-CB	-5.25	1.47	1.54
1	A	322	TYR	N-CA	-5.25	1.39	1.46
1	B	335	ALA	CA-C	-5.25	1.46	1.52
1	A	119	GLU	N-CA	-5.24	1.40	1.46
1	A	341	THR	CA-CB	-5.24	1.45	1.53
1	B	377	ARG	CA-C	-5.24	1.46	1.52
1	B	151	VAL	CA-C	-5.24	1.44	1.52
1	B	453	SER	CA-C	-5.23	1.48	1.53
1	A	415	LEU	N-CA	-5.22	1.40	1.46
1	A	296	LEU	N-CA	-5.22	1.41	1.46
1	B	236	SER	N-CA	-5.22	1.40	1.46
1	A	132	MET	CA-C	-5.21	1.46	1.52
1	B	205	ALA	N-CA	-5.21	1.40	1.46
1	A	484	PRO	N-CA	-5.21	1.40	1.47
1	A	375	VAL	N-CA	-5.21	1.40	1.46
1	A	168	LEU	N-CA	-5.21	1.40	1.46
1	A	215	PHE	CA-C	-5.21	1.46	1.52
1	B	51	THR	CA-C	-5.21	1.46	1.52
1	B	412	LEU	CA-C	-5.20	1.45	1.52
1	A	147	ALA	CA-C	-5.20	1.46	1.52
1	A	394	GLY	CA-C	-5.20	1.44	1.51
1	A	432	ARG	CA-CB	5.20	1.61	1.53
1	B	367	LEU	N-CA	-5.20	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	ARG	CA-C	-5.20	1.45	1.52
1	B	402	VAL	CA-C	-5.20	1.46	1.52
1	A	443	ARG	CA-C	-5.19	1.46	1.52
1	A	172	VAL	N-CA	-5.19	1.40	1.46
1	A	227	LYS	CA-C	-5.19	1.46	1.52
1	A	324	LEU	C-N	5.19	1.42	1.34
1	A	393	LEU	CA-C	-5.19	1.46	1.52
1	B	68	ASP	N-CA	-5.19	1.40	1.46
1	A	332	TYR	CA-C	-5.19	1.46	1.52
1	B	31	ARG	CA-C	-5.19	1.45	1.52
1	A	39	TRP	N-CA	-5.19	1.40	1.46
1	B	59	LEU	C-N	-5.18	1.26	1.33
1	B	177	LYS	CA-C	-5.18	1.46	1.52
1	B	428	VAL	C-O	-5.18	1.17	1.24
1	B	420	GLY	N-CA	-5.18	1.39	1.45
1	A	376	VAL	CA-CB	-5.17	1.47	1.54
1	A	152	VAL	N-CA	-5.17	1.39	1.46
1	B	401	LEU	C-O	-5.17	1.18	1.24
1	B	175	ILE	CA-CB	-5.17	1.47	1.54
1	B	34	TYR	N-CA	-5.16	1.39	1.46
1	B	120	ILE	CA-C	-5.16	1.45	1.52
1	A	367	LEU	N-CA	-5.15	1.39	1.45
1	B	490	SER	N-CA	-5.15	1.40	1.46
1	A	309	ASP	N-CA	-5.15	1.40	1.46
1	B	323	LYS	N-CA	-5.15	1.39	1.46
1	B	328	SER	CA-C	5.15	1.59	1.52
1	B	436	LEU	CA-C	-5.15	1.46	1.52
1	B	165	ILE	CA-CB	-5.14	1.48	1.54
1	B	283	ALA	N-CA	-5.14	1.40	1.46
1	A	386	THR	CA-C	-5.13	1.46	1.52
1	B	225	THR	CA-C	-5.13	1.45	1.52
1	B	368	VAL	CA-C	-5.13	1.46	1.52
1	A	87	ALA	CA-C	-5.13	1.46	1.52
1	B	110	ILE	CA-C	-5.13	1.46	1.52
1	B	394	GLY	CA-C	-5.13	1.44	1.51
1	A	201	SER	CA-C	-5.13	1.46	1.52
1	A	314	SER	C-O	-5.12	1.18	1.24
1	A	104	VAL	CA-CB	-5.12	1.48	1.54
1	B	425	MET	CA-C	-5.12	1.46	1.52
1	B	478	ILE	CA-C	-5.12	1.46	1.52
1	A	73	THR	N-CA	-5.12	1.40	1.46
1	B	414	GLY	N-CA	-5.11	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	PHE	N-CA	-5.11	1.40	1.46
1	A	353	ASN	C-O	-5.11	1.17	1.23
1	A	168	LEU	CA-C	-5.11	1.46	1.52
1	A	173	VAL	CA-C	-5.10	1.45	1.52
1	A	490	SER	N-CA	-5.09	1.40	1.46
1	B	53	ASP	CA-C	-5.09	1.46	1.52
1	B	341	THR	N-CA	-5.09	1.40	1.46
1	B	285	GLU	CA-CB	5.08	1.61	1.53
1	B	440	PRO	N-CA	-5.08	1.41	1.47
1	B	221	TYR	CA-CB	5.08	1.60	1.53
1	B	347	LEU	CA-C	-5.08	1.45	1.52
1	B	431	HIS	CA-C	-5.08	1.46	1.52
1	A	355	LEU	CA-CB	-5.07	1.45	1.53
1	A	483	PHE	N-CA	-5.07	1.41	1.46
1	A	395	THR	N-CA	-5.07	1.39	1.46
1	A	476	ASN	N-CA	-5.07	1.40	1.46
1	B	395	THR	CA-C	-5.07	1.46	1.52
1	A	291	ASP	N-CA	-5.07	1.40	1.46
1	B	230	THR	N-CA	-5.06	1.40	1.46
1	B	308	PHE	C-O	-5.06	1.18	1.24
1	B	27	ASP	CA-C	-5.05	1.46	1.52
1	B	258	LYS	CA-C	-5.05	1.46	1.52
1	B	458	VAL	CA-CB	-5.05	1.48	1.54
1	A	446	ASN	N-CA	-5.04	1.41	1.46
1	A	115	TYR	CA-C	-5.04	1.46	1.52
1	B	35	TYR	CA-C	-5.04	1.46	1.52
1	B	118	TYR	N-CA	-5.04	1.40	1.46
1	A	108	GLY	C-O	-5.04	1.19	1.24
1	A	206	LEU	N-CA	-5.03	1.40	1.46
1	A	239	LEU	C-N	-5.03	1.27	1.33
1	B	155	LEU	CA-C	-5.02	1.45	1.52
1	B	300	ILE	C-N	-5.02	1.27	1.33
1	A	354	GLY	CA-C	-5.02	1.44	1.52
1	A	461	LEU	CA-C	-5.02	1.45	1.52
1	B	289	VAL	N-CA	-5.02	1.40	1.46
1	A	467	GLY	CA-C	-5.02	1.46	1.52
1	A	166	PHE	N-CA	-5.01	1.40	1.46
1	B	143	HIS	N-CA	-5.01	1.40	1.46
1	A	93	PHE	CA-C	-5.01	1.46	1.52
1	A	73	THR	CA-CB	-5.00	1.46	1.53
1	A	454	LYS	C-N	-5.00	1.26	1.33
1	B	267	SER	CA-C	-5.00	1.46	1.52

All (824) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ILE	N-CA-C	26.50	135.44	110.53
1	B	330	PHE	CA-CB-CG	22.69	136.49	113.80
1	B	289	VAL	N-CA-C	18.29	129.19	110.72
1	B	218	PHE	CA-CB-CG	-17.49	96.31	113.80
1	A	320	HIS	CA-CB-CG	15.83	129.63	113.80
1	B	217	SER	N-CA-C	15.66	128.35	111.28
1	A	25	TRP	CB-CG-CD2	-15.58	104.99	126.80
1	B	437	PHE	CA-CB-CG	-15.55	98.25	113.80
1	A	160	THR	N-CA-C	15.50	128.26	111.36
1	A	219	HIS	CA-CB-CG	15.49	129.29	113.80
1	B	161	PHE	N-CA-C	15.33	133.60	112.75
1	A	161	PHE	N-CA-C	15.29	133.55	112.75
1	A	437	PHE	CA-CB-CG	-14.34	99.46	113.80
1	A	496	SER	N-CA-C	14.28	128.14	111.71
1	A	74	ASP	CA-CB-CG	-14.28	98.32	112.60
1	B	160	THR	N-CA-C	13.96	126.49	111.28
1	B	114	ASN	CA-CB-CG	-13.81	98.79	112.60
1	A	371	SER	N-CA-C	-13.57	94.76	112.41
1	A	290	LYS	N-CA-CB	-12.51	91.73	110.12
1	B	148	PHE	CA-CB-CG	-12.46	101.34	113.80
1	A	377	ARG	N-CA-CB	12.38	128.17	109.97
1	A	214	PHE	CA-CB-CG	-11.89	101.91	113.80
1	A	150	ASN	CA-CB-CG	-11.82	100.78	112.60
1	A	496	SER	N-CA-CB	-11.80	92.05	110.22
1	A	449	LEU	N-CA-C	-11.77	98.48	111.07
1	B	379	VAL	N-CA-C	-11.71	91.08	108.17
1	A	320	HIS	N-CA-C	-11.63	98.61	111.28
1	A	218	PHE	CA-CB-CG	-11.34	102.46	113.80
1	B	151	VAL	CA-C-N	11.28	139.69	120.86
1	B	151	VAL	C-N-CA	11.28	139.69	120.86
1	B	124	LEU	N-CA-C	-11.24	94.14	109.54
1	A	427	ASN	CA-CB-CG	-11.18	101.42	112.60
1	A	376	VAL	N-CA-C	-11.15	91.17	107.78
1	B	105	GLY	CA-C-N	10.99	141.76	121.97
1	B	105	GLY	C-N-CA	10.99	141.76	121.97
1	A	460	PHE	CA-CB-CG	-10.99	102.81	113.80
1	A	99	GLN	N-CA-C	-10.95	98.28	108.13
1	A	38	ASP	N-CA-C	10.93	124.28	111.71
1	B	374	ASN	CA-CB-CG	-10.91	101.69	112.60
1	A	231	PHE	CA-CB-CG	10.86	124.66	113.80
1	B	460	PHE	CA-CB-CG	-10.84	102.96	113.80
1	A	217	SER	N-CA-C	10.84	123.09	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	PHE	CA-CB-CG	-10.82	102.98	113.80
1	A	275	ASN	N-CA-C	-10.73	95.14	111.56
1	A	34	TYR	CA-C-N	10.60	134.90	120.38
1	A	34	TYR	C-N-CA	10.60	134.90	120.38
1	A	133	PHE	CA-CB-CG	10.54	124.34	113.80
1	A	427	ASN	N-CA-C	-10.52	85.69	107.67
1	A	293	PHE	CA-CB-CG	-10.48	103.32	113.80
1	A	235	TYR	CB-CA-C	-10.47	96.58	111.14
1	A	65	PHE	CA-CB-CG	-10.46	103.34	113.80
1	A	186	PHE	CA-CB-CG	-10.43	103.37	113.80
1	A	108	GLY	N-CA-C	-10.40	102.01	115.22
1	B	52	VAL	N-CA-C	10.38	120.28	110.53
1	B	253	TYR	N-CA-C	-10.34	100.34	113.16
1	B	424	LEU	N-CA-C	-10.11	101.61	112.93
1	A	486	VAL	N-CA-CB	-10.08	96.83	110.54
1	A	221	TYR	CA-C-N	10.04	132.39	119.84
1	A	221	TYR	C-N-CA	10.04	132.39	119.84
1	A	159	THR	N-CA-C	-9.96	89.59	110.80
1	B	259	PHE	CA-CB-CG	-9.91	103.89	113.80
1	B	214	PHE	CA-CB-CG	-9.89	103.91	113.80
1	A	289	VAL	CA-C-N	9.89	133.53	120.28
1	A	289	VAL	C-N-CA	9.89	133.53	120.28
1	B	166	PHE	CA-CB-CG	-9.87	103.93	113.80
1	A	369	ARG	N-CA-C	-9.85	97.25	113.50
1	B	372	ASN	N-CA-C	-9.85	89.82	110.80
1	A	479	ALA	CA-C-N	9.83	134.73	120.38
1	A	479	ALA	C-N-CA	9.83	134.73	120.38
1	A	194	SER	N-CA-C	9.81	121.74	111.14
1	A	52	VAL	N-CA-C	9.67	119.62	110.53
1	A	171	ASN	CB-CA-C	-9.65	94.77	110.79
1	A	194	SER	CA-C-N	9.64	139.05	121.70
1	A	194	SER	C-N-CA	9.64	139.05	121.70
1	B	432	ARG	N-CA-C	-9.62	100.67	111.82
1	A	88	MET	N-CA-C	-9.61	100.80	111.28
1	A	322	TYR	CA-C-N	9.57	139.82	121.54
1	A	322	TYR	C-N-CA	9.57	139.82	121.54
1	B	224	PHE	N-CA-C	9.53	124.29	109.52
1	B	159	THR	N-CA-CB	9.49	126.53	110.49
1	B	309	ASP	CA-CB-CG	-9.49	103.11	112.60
1	B	65	PHE	CA-CB-CG	-9.46	104.34	113.80
1	B	321	GLN	N-CA-C	-9.42	100.36	112.23
1	A	450	ALA	N-CA-C	9.34	121.55	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	HIS	CA-CB-CG	-9.32	104.48	113.80
1	B	65	PHE	N-CA-CB	9.32	124.57	110.22
1	B	74	ASP	N-CA-C	-9.30	101.52	112.86
1	B	231	PHE	CA-CB-CG	9.25	123.05	113.80
1	B	187	HIS	N-CA-C	9.21	121.31	111.28
1	A	233	SER	CA-C-N	9.20	134.29	120.31
1	A	233	SER	C-N-CA	9.20	134.29	120.31
1	B	373	GLN	N-CA-C	-9.18	100.36	113.21
1	A	135	ILE	CB-CA-C	-9.15	99.79	112.14
1	A	207	VAL	CA-CB-CG1	9.11	125.89	110.40
1	A	480	ALA	CA-C-N	9.11	135.55	120.62
1	A	480	ALA	C-N-CA	9.11	135.55	120.62
1	A	56	PHE	CA-CB-CG	-9.07	104.73	113.80
1	A	105	GLY	CA-C-N	9.05	138.26	121.97
1	A	105	GLY	C-N-CA	9.05	138.26	121.97
1	A	262	LEU	CA-C-N	9.03	131.13	119.84
1	A	262	LEU	C-N-CA	9.03	131.13	119.84
1	B	128	TYR	N-CA-C	-8.96	101.51	111.28
1	B	262	LEU	CB-CA-C	-8.96	96.58	110.02
1	A	417	PHE	N-CA-C	8.95	120.64	111.07
1	A	166	PHE	CA-CB-CG	-8.91	104.89	113.80
1	A	110	ILE	CB-CA-C	-8.84	100.20	112.14
1	A	264	ILE	CA-C-N	8.82	138.39	121.54
1	A	264	ILE	C-N-CA	8.82	138.39	121.54
1	A	419	MET	N-CA-CB	-8.81	97.17	110.12
1	B	427	ASN	CA-CB-CG	-8.76	103.84	112.60
1	B	293	PHE	CA-CB-CG	-8.72	105.08	113.80
1	B	269	PHE	CA-CB-CG	8.70	122.50	113.80
1	A	46	ARG	CA-C-N	8.67	132.34	120.46
1	A	46	ARG	C-N-CA	8.67	132.34	120.46
1	B	295	ALA	CA-C-N	8.66	132.01	120.58
1	B	295	ALA	C-N-CA	8.66	132.01	120.58
1	B	79	VAL	CA-C-O	8.65	130.34	121.17
1	A	221	TYR	CA-CB-CG	8.63	129.43	113.90
1	A	247	PHE	CA-CB-CG	-8.59	105.21	113.80
1	A	446	ASN	N-CA-C	-8.58	99.18	112.99
1	B	306	PHE	CA-CB-CG	8.56	122.36	113.80
1	B	329	SER	N-CA-C	8.55	123.12	107.99
1	B	108	GLY	N-CA-C	-8.49	104.43	115.22
1	A	79	VAL	N-CA-C	-8.47	102.29	110.42
1	A	156	GLN	N-CA-CB	-8.46	97.20	110.22
1	A	497	PHE	CA-C-N	8.46	132.46	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	PHE	C-N-CA	8.46	132.46	120.28
1	A	435	PHE	CA-CB-CG	-8.45	105.35	113.80
1	B	115	TYR	N-CA-C	-8.42	102.10	111.28
1	B	346	VAL	N-CA-C	8.41	118.49	110.42
1	A	346	VAL	CB-CA-C	-8.40	100.79	112.14
1	A	426	THR	N-CA-C	-8.39	98.06	110.06
1	A	428	VAL	CA-C-N	8.39	131.95	120.46
1	A	428	VAL	C-N-CA	8.39	131.95	120.46
1	A	400	LEU	CA-C-N	8.38	131.85	120.54
1	A	400	LEU	C-N-CA	8.38	131.85	120.54
1	B	159	THR	N-CA-C	-8.35	93.02	110.80
1	B	283	ALA	CA-C-N	8.35	137.48	121.54
1	B	283	ALA	C-N-CA	8.35	137.48	121.54
1	B	91	ILE	CB-CA-C	-8.32	101.12	112.02
1	B	416	PHE	CA-CB-CG	-8.28	105.52	113.80
1	B	499	TYR	N-CA-CB	-8.28	96.42	110.50
1	A	117	VAL	N-CA-CB	-8.26	99.31	110.54
1	B	79	VAL	CA-C-N	8.24	131.32	120.28
1	B	79	VAL	C-N-CA	8.24	131.32	120.28
1	B	425	MET	N-CA-C	-8.23	101.34	112.94
1	B	154	LEU	CA-C-O	8.18	129.35	120.10
1	A	88	MET	N-CA-CB	8.17	122.14	110.12
1	A	358	GLN	N-CA-C	-8.16	102.46	111.36
1	A	62	ALA	N-CA-C	-8.10	102.45	111.28
1	B	101	LEU	N-CA-C	-8.08	102.98	113.17
1	B	287	ILE	CA-C-N	8.08	129.94	119.84
1	B	287	ILE	C-N-CA	8.08	129.94	119.84
1	A	217	SER	CB-CA-C	-8.07	97.39	110.79
1	B	189	THR	CA-C-N	8.07	136.96	121.54
1	B	189	THR	C-N-CA	8.07	136.96	121.54
1	B	463	PHE	CA-C-O	8.04	129.26	120.82
1	B	333	ASP	N-CA-C	-8.03	102.53	111.28
1	A	449	LEU	N-CA-CB	8.03	121.65	110.01
1	A	151	VAL	N-CA-C	-8.02	101.07	111.09
1	B	417	PHE	N-CA-C	8.01	119.64	111.07
1	A	242	LEU	N-CA-CB	-8.00	98.41	110.01
1	A	470	GLY	N-CA-C	-7.96	103.27	112.50
1	A	391	MET	CG-SD-CE	-7.94	83.44	100.90
1	A	433	ILE	CB-CA-C	-7.93	101.44	112.14
1	B	366	LEU	CB-CA-C	-7.91	100.90	111.74
1	A	424	LEU	N-CA-C	-7.90	103.62	113.18
1	B	391	MET	CG-SD-CE	-7.88	83.56	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	THR	N-CA-CB	-7.87	98.56	110.12
1	B	362	HIS	CA-CB-CG	7.85	121.65	113.80
1	A	268	PHE	CA-CB-CG	-7.83	105.97	113.80
1	A	421	ILE	CA-C-N	7.79	132.92	121.31
1	A	421	ILE	C-N-CA	7.79	132.92	121.31
1	A	368	VAL	N-CA-C	-7.79	93.14	109.34
1	A	25	TRP	CA-C-N	7.78	130.71	120.28
1	A	25	TRP	C-N-CA	7.78	130.71	120.28
1	B	96	LEU	N-CA-CB	7.72	122.18	110.30
1	B	161	PHE	O-C-N	-7.70	113.63	120.48
1	A	95	VAL	CB-CA-C	-7.69	101.95	112.02
1	B	400	LEU	CA-C-N	7.67	130.89	120.38
1	B	400	LEU	C-N-CA	7.67	130.89	120.38
1	B	427	ASN	CA-C-N	7.67	132.88	120.30
1	B	427	ASN	C-N-CA	7.67	132.88	120.30
1	A	135	ILE	N-CA-C	7.66	118.44	110.62
1	B	308	PHE	CB-CA-C	-7.64	98.88	110.88
1	B	224	PHE	CA-CB-CG	-7.64	106.16	113.80
1	A	396	MET	CA-C-N	7.64	131.13	120.29
1	A	396	MET	C-N-CA	7.64	131.13	120.29
1	B	440	PRO	N-CA-C	-7.63	103.96	114.27
1	B	92	VAL	CB-CA-C	7.62	122.43	112.14
1	A	225	THR	CA-C-N	7.62	130.70	120.65
1	A	225	THR	C-N-CA	7.62	130.70	120.65
1	A	393	LEU	N-CA-C	-7.61	103.06	111.36
1	B	88	MET	N-CA-CB	7.61	121.31	110.12
1	B	280	THR	N-CA-C	7.60	119.57	108.86
1	B	158	VAL	N-CA-C	7.60	119.63	109.37
1	A	486	VAL	CB-CA-C	7.59	122.39	112.14
1	B	449	LEU	CB-CA-C	-7.59	98.86	110.92
1	A	472	PHE	CA-CB-CG	-7.58	106.22	113.80
1	A	401	LEU	N-CA-CB	-7.58	98.65	109.94
1	B	326	LYS	CB-CA-C	-7.58	97.65	109.85
1	B	253	TYR	CA-CB-CG	7.58	127.54	113.90
1	A	330	PHE	CA-CB-CG	-7.55	106.25	113.80
1	A	463	PHE	CB-CA-C	-7.55	99.03	110.88
1	A	307	TYR	N-CA-C	-7.54	103.00	111.07
1	A	35	TYR	CA-C-O	7.53	128.77	120.63
1	A	229	ARG	N-CA-CB	7.50	121.14	110.12
1	A	159	THR	CB-CA-C	7.50	125.34	110.42
1	A	284	TYR	CA-CB-CG	-7.49	100.42	113.90
1	A	250	PHE	CA-CB-CG	7.48	121.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	ARG	CD-NE-CZ	-7.46	113.95	124.40
1	A	161	PHE	CA-CB-CG	7.43	121.23	113.80
1	A	300	ILE	CA-CB-CG1	7.40	122.98	110.40
1	A	446	ASN	CA-CB-CG	-7.40	105.20	112.60
1	A	211	PHE	CA-C-N	7.39	128.18	119.98
1	A	211	PHE	C-N-CA	7.39	128.18	119.98
1	B	303	THR	CA-C-O	7.38	128.37	120.55
1	B	418	ILE	N-CA-CB	7.38	121.65	110.58
1	A	306	PHE	CA-CB-CG	7.38	121.18	113.80
1	B	80	ASN	N-CA-C	-7.37	103.25	111.28
1	A	492	ILE	N-CA-C	7.35	118.12	110.62
1	A	324	LEU	CA-C-N	7.35	134.41	122.14
1	A	324	LEU	C-N-CA	7.35	134.41	122.14
1	B	221	TYR	CA-CB-CG	7.34	127.12	113.90
1	B	430	ILE	CB-CA-C	-7.33	102.24	112.14
1	B	321	GLN	N-CA-CB	7.33	121.59	110.30
1	B	160	THR	O-C-N	-7.32	114.36	122.12
1	B	322	TYR	N-CA-C	-7.32	105.21	112.97
1	B	163	CYS	CA-C-N	-7.32	109.19	120.31
1	B	163	CYS	C-N-CA	-7.32	109.19	120.31
1	A	225	THR	N-CA-CB	7.31	124.42	111.69
1	B	134	TRP	CB-CA-C	-7.30	98.44	110.85
1	B	331	HIS	N-CA-C	7.30	119.32	111.36
1	B	296	LEU	CA-C-O	-7.30	111.62	118.33
1	A	157	TYR	N-CA-CB	-7.29	98.99	110.22
1	B	349	ILE	CA-C-N	7.29	128.95	119.84
1	B	349	ILE	C-N-CA	7.29	128.95	119.84
1	A	199	PHE	N-CA-C	-7.26	103.44	111.36
1	B	207	VAL	CA-C-O	7.26	128.54	120.85
1	A	325	ARG	N-CA-C	-7.23	102.47	112.30
1	A	439	ASP	CA-CB-CG	-7.23	105.37	112.60
1	A	116	THR	CB-CA-C	-7.22	99.55	110.88
1	A	219	HIS	CA-C-N	-7.21	110.06	120.29
1	A	219	HIS	C-N-CA	-7.21	110.06	120.29
1	A	216	LYS	N-CA-C	7.20	119.13	111.28
1	B	479	ALA	CA-C-N	7.19	130.88	120.38
1	B	479	ALA	C-N-CA	7.19	130.88	120.38
1	B	290	LYS	CA-C-N	7.17	130.48	120.29
1	B	290	LYS	C-N-CA	7.17	130.48	120.29
1	B	40	VAL	CB-CA-C	-7.17	102.33	112.22
1	B	71	ASP	CA-C-N	7.16	130.59	120.28
1	B	71	ASP	C-N-CA	7.16	130.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	SER	N-CA-C	-7.16	100.47	110.35
1	A	34	TYR	CA-CB-CG	-7.16	101.01	113.90
1	A	258	LYS	N-CA-CB	7.15	121.53	109.87
1	B	79	VAL	CB-CA-C	-7.15	102.81	111.97
1	A	142	PHE	CA-CB-CG	-7.14	106.66	113.80
1	A	199	PHE	CA-C-N	7.13	129.84	120.28
1	A	199	PHE	C-N-CA	7.13	129.84	120.28
1	B	171	ASN	CB-CA-C	-7.13	98.95	110.79
1	B	88	MET	N-CA-C	-7.13	103.51	111.28
1	B	346	VAL	CB-CA-C	-7.11	102.87	111.97
1	A	367	LEU	N-CA-C	-7.11	98.61	109.41
1	B	416	PHE	N-CA-C	-7.10	103.48	111.07
1	B	311	ASN	N-CA-CB	-7.07	99.76	110.01
1	B	217	SER	CB-CA-C	-7.06	99.06	110.79
1	B	161	PHE	CB-CA-C	-7.06	99.63	112.76
1	A	379	VAL	CA-C-N	-7.05	110.90	122.11
1	A	379	VAL	C-N-CA	-7.05	110.90	122.11
1	A	454	LYS	N-CA-C	7.05	118.61	111.07
1	B	166	PHE	N-CA-C	-7.04	103.53	111.07
1	B	43	PHE	N-CA-C	7.04	121.62	110.70
1	B	286	PRO	N-CA-C	7.03	126.96	112.47
1	A	485	LEU	CA-C-O	7.02	127.86	120.42
1	A	377	ARG	N-CA-C	-7.02	99.89	110.28
1	A	396	MET	N-CA-CB	7.00	120.41	109.83
1	B	208	MET	N-CA-CB	-7.00	99.82	110.12
1	B	221	TYR	CA-C-N	7.00	128.59	119.84
1	B	221	TYR	C-N-CA	7.00	128.59	119.84
1	A	497	PHE	CA-C-O	6.99	127.96	120.55
1	B	395	THR	CA-C-N	6.99	134.88	121.54
1	B	395	THR	C-N-CA	6.99	134.88	121.54
1	B	219	HIS	CA-C-N	-6.98	110.37	120.29
1	B	219	HIS	C-N-CA	-6.98	110.37	120.29
1	A	54	THR	CB-CA-C	-6.98	97.71	110.63
1	A	101	LEU	CA-C-N	6.98	134.87	121.54
1	A	101	LEU	C-N-CA	6.98	134.87	121.54
1	B	383	LEU	N-CA-C	6.97	118.88	111.28
1	B	293	PHE	N-CA-C	6.97	118.67	111.14
1	B	498	THR	CA-C-N	6.95	134.21	121.70
1	B	498	THR	C-N-CA	6.95	134.21	121.70
1	B	334	PHE	N-CA-C	6.93	118.48	111.07
1	B	442	ARG	N-CA-C	-6.92	98.79	109.24
1	B	335	ALA	CA-C-O	6.92	127.88	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470	GLY	N-CA-C	-6.91	104.44	112.73
1	A	48	ILE	N-CA-C	-6.91	104.06	112.35
1	A	331	HIS	CA-CB-CG	6.90	120.70	113.80
1	A	390	LEU	CA-C-O	-6.90	113.79	120.90
1	A	144	LEU	CB-CA-C	-6.90	99.34	110.79
1	A	379	VAL	N-CA-C	-6.88	95.03	109.34
1	A	479	ALA	N-CA-C	-6.88	104.84	113.23
1	B	332	TYR	CA-C-O	6.86	127.82	120.55
1	A	491	VAL	CB-CA-C	6.85	120.74	111.97
1	B	186	PHE	CA-CB-CG	-6.84	106.96	113.80
1	A	93	PHE	N-CA-C	-6.83	103.83	111.28
1	A	47	VAL	CA-C-N	6.82	125.78	120.33
1	A	47	VAL	C-N-CA	6.82	125.78	120.33
1	B	400	LEU	N-CA-CB	6.81	122.31	110.39
1	B	471	GLU	N-CA-C	6.81	118.71	111.28
1	A	91	ILE	N-CA-C	6.81	116.93	110.53
1	B	95	VAL	CB-CA-C	-6.80	103.11	112.02
1	B	446	ASN	CA-C-N	6.79	128.14	120.06
1	B	446	ASN	C-N-CA	6.79	128.14	120.06
1	B	449	LEU	N-CA-C	-6.79	102.74	111.02
1	A	38	ASP	CA-C-N	6.77	129.90	120.29
1	A	38	ASP	C-N-CA	6.77	129.90	120.29
1	B	290	LYS	CA-C-O	6.77	127.72	120.55
1	A	30	ASP	CA-CB-CG	-6.76	105.84	112.60
1	B	238	ALA	CB-CA-C	-6.76	99.57	110.79
1	B	430	ILE	N-CA-CB	6.75	119.72	110.54
1	B	142	PHE	CA-CB-CG	-6.75	107.05	113.80
1	B	485	LEU	N-CA-C	-6.75	104.01	111.36
1	A	79	VAL	CB-CA-C	-6.74	103.34	111.97
1	B	295	ALA	CA-C-O	6.74	127.67	119.38
1	A	274	PHE	CA-CB-CG	-6.73	107.07	113.80
1	A	366	LEU	N-CA-C	-6.72	102.18	110.65
1	B	356	ILE	CA-C-O	-6.72	110.94	119.95
1	A	462	CYS	CA-CB-SG	-6.70	99.00	114.40
1	B	380	GLU	N-CA-C	-6.70	99.16	109.14
1	A	156	GLN	CA-C-O	6.69	127.66	120.10
1	B	427	ASN	CB-CA-C	6.68	122.83	111.68
1	B	321	GLN	CB-CA-C	-6.68	96.76	110.38
1	B	200	ALA	CA-C-O	6.66	127.61	120.55
1	B	404	LEU	CA-C-N	6.65	127.32	120.00
1	B	404	LEU	C-N-CA	6.65	127.32	120.00
1	A	365	THR	CB-CA-C	-6.65	99.54	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	HIS	CA-C-O	6.65	127.61	119.97
1	A	120	ILE	N-CA-CB	6.64	120.54	110.58
1	A	343	ILE	N-CA-CB	6.63	119.55	110.54
1	B	353	ASN	O-C-N	-6.62	113.97	122.78
1	A	99	GLN	CB-CG-CD	-6.62	101.35	112.60
1	A	394	GLY	CA-C-N	6.62	134.18	121.54
1	A	394	GLY	C-N-CA	6.62	134.18	121.54
1	A	445	ASN	CB-CA-C	-6.61	100.50	110.88
1	A	78	GLY	CA-C-N	6.61	128.88	120.56
1	A	78	GLY	C-N-CA	6.61	128.88	120.56
1	B	491	VAL	N-CA-CB	6.60	118.28	110.55
1	A	48	ILE	N-CA-CB	-6.59	105.31	110.45
1	B	99	GLN	N-CA-C	-6.58	99.37	109.64
1	B	349	ILE	N-CA-CB	6.58	120.42	111.21
1	B	218	PHE	N-CA-CB	6.57	119.77	110.12
1	B	54	THR	N-CA-C	6.55	119.25	111.71
1	B	472	PHE	N-CA-CB	6.53	119.72	110.12
1	A	425	MET	N-CA-C	6.52	121.25	113.16
1	A	163	CYS	N-CA-CB	6.51	119.70	110.12
1	B	26	LEU	CA-C-N	6.51	129.01	120.28
1	B	26	LEU	C-N-CA	6.51	129.01	120.28
1	A	144	LEU	CA-C-O	6.51	127.45	120.55
1	B	296	LEU	N-CA-CB	-6.51	99.01	110.34
1	A	156	GLN	CA-C-N	6.51	129.65	120.28
1	A	156	GLN	C-N-CA	6.51	129.65	120.28
1	A	199	PHE	CA-CB-CG	-6.50	107.30	113.80
1	B	427	ASN	CA-C-O	6.50	128.67	121.39
1	B	158	VAL	CA-C-N	6.50	133.95	121.54
1	B	158	VAL	C-N-CA	6.50	133.95	121.54
1	B	454	LYS	CA-C-O	6.50	127.64	120.82
1	B	158	VAL	N-CA-CB	-6.49	101.43	110.13
1	B	110	ILE	N-CA-CB	6.49	119.36	110.54
1	B	220	HIS	CA-CB-CG	-6.49	107.31	113.80
1	B	144	LEU	CA-C-O	6.48	127.62	120.82
1	B	44	ASN	CA-C-N	6.46	129.26	120.54
1	B	44	ASN	C-N-CA	6.46	129.26	120.54
1	A	432	ARG	CB-CG-CD	6.46	126.16	111.30
1	B	43	PHE	CA-CB-CG	-6.46	107.34	113.80
1	A	100	PRO	N-CA-C	-6.45	99.19	112.47
1	A	226	HIS	N-CA-C	-6.45	103.94	110.97
1	A	237	THR	CA-CB-OG1	6.44	119.26	109.60
1	B	330	PHE	CA-C-O	6.44	127.44	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	PRO	CB-CA-C	-6.41	100.98	111.56
1	B	285	GLU	O-C-N	-6.41	113.95	121.32
1	A	43	PHE	CA-CB-CG	-6.40	107.40	113.80
1	A	160	THR	CA-C-O	6.40	127.20	120.42
1	B	48	ILE	O-C-N	-6.40	116.33	120.42
1	B	93	PHE	N-CA-C	-6.38	104.32	111.28
1	B	58	ASN	CA-CB-CG	-6.38	106.22	112.60
1	B	226	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	A	414	GLY	N-CA-C	-6.36	105.10	112.73
1	B	495	PHE	CA-C-O	6.33	127.25	120.10
1	A	187	HIS	N-CA-C	6.33	118.18	111.28
1	B	106	VAL	N-CA-C	6.33	122.50	109.34
1	B	279	ASN	N-CA-C	6.33	124.28	110.80
1	A	160	THR	O-C-N	-6.32	114.95	122.15
1	B	63	ILE	N-CA-C	-6.32	104.18	110.62
1	B	73	THR	CA-C-N	6.31	132.96	123.05
1	B	73	THR	C-N-CA	6.31	132.96	123.05
1	B	250	PHE	N-CA-C	-6.31	100.89	109.54
1	A	121	ILE	N-CA-CB	6.31	122.19	110.77
1	A	203	VAL	CB-CA-C	-6.31	103.90	111.97
1	A	244	TRP	N-CA-C	6.31	118.24	111.36
1	A	341	THR	CB-CA-C	6.31	121.26	110.79
1	B	62	ALA	N-CA-C	-6.31	104.40	111.28
1	B	381	GLN	N-CA-CB	6.29	121.13	110.49
1	A	354	GLY	CA-C-O	6.29	126.68	120.89
1	B	170	ILE	N-CA-CB	-6.28	102.01	110.54
1	B	194	SER	N-CA-CB	6.28	121.09	110.49
1	B	202	VAL	N-CA-C	-6.27	104.22	110.62
1	A	445	ASN	N-CA-C	6.27	117.78	111.07
1	B	354	GLY	O-C-N	-6.27	118.71	123.35
1	B	269	PHE	N-CA-C	-6.26	98.19	109.09
1	B	76	SER	CA-C-N	6.26	133.50	121.54
1	B	76	SER	C-N-CA	6.26	133.50	121.54
1	A	29	LYS	CA-C-N	-6.26	111.92	120.44
1	A	29	LYS	C-N-CA	-6.26	111.92	120.44
1	A	432	ARG	N-CA-C	-6.26	104.51	111.71
1	A	253	TYR	N-CA-C	-6.24	103.76	111.75
1	B	498	THR	N-CA-C	6.24	118.88	111.71
1	A	286	PRO	CA-N-CD	-6.23	103.28	112.00
1	A	89	ALA	CB-CA-C	-6.23	100.45	110.79
1	B	357	PRO	N-CA-CB	6.22	109.24	103.46
1	A	483	PHE	O-C-N	-6.21	114.55	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	VAL	CA-CB-CG1	6.21	120.96	110.40
1	B	140	MET	CG-SD-CE	-6.21	87.24	100.90
1	B	348	GLY	N-CA-C	-6.20	98.48	113.18
1	B	303	THR	CB-CA-C	-6.19	100.51	110.79
1	B	438	SER	CA-C-N	6.19	136.90	121.80
1	B	438	SER	C-N-CA	6.19	136.90	121.80
1	A	275	ASN	CA-CB-CG	-6.19	106.41	112.60
1	A	363	THR	N-CA-C	-6.18	104.65	111.82
1	B	291	ASP	N-CA-C	-6.18	104.62	111.36
1	A	45	TYR	N-CA-C	6.17	120.97	113.38
1	A	416	PHE	N-CA-C	-6.17	103.71	111.11
1	B	54	THR	CB-CA-C	-6.17	99.22	110.63
1	B	378	CYS	N-CA-CB	6.17	120.92	110.49
1	B	197	ASP	CA-C-N	6.16	133.49	121.41
1	B	197	ASP	C-N-CA	6.16	133.49	121.41
1	B	478	ILE	N-CA-C	-6.16	96.52	109.34
1	A	160	THR	CA-CB-OG1	6.16	118.84	109.60
1	A	378	CYS	O-C-N	6.16	129.81	122.79
1	B	441	LYS	N-CA-CB	6.16	119.90	110.79
1	A	234	ASP	CA-C-N	-6.15	112.75	122.95
1	A	234	ASP	C-N-CA	-6.15	112.75	122.95
1	B	491	VAL	N-CA-C	-6.14	104.52	110.42
1	A	421	ILE	CB-CA-C	-6.14	103.85	112.14
1	A	389	GLY	N-CA-C	-6.14	105.06	112.49
1	A	496	SER	CB-CA-C	-6.14	99.27	110.63
1	B	389	GLY	N-CA-C	-6.13	105.07	112.49
1	A	213	LEU	N-CA-C	-6.13	104.51	111.07
1	A	225	THR	CA-CB-OG1	6.13	118.79	109.60
1	A	325	ARG	CA-C-N	6.12	136.72	121.80
1	A	325	ARG	C-N-CA	6.12	136.72	121.80
1	A	53	ASP	N-CA-CB	6.11	119.11	110.12
1	A	220	HIS	N-CA-CB	6.11	119.21	110.16
1	A	142	PHE	CB-CA-C	6.11	120.94	110.79
1	A	395	THR	N-CA-C	-6.11	97.78	110.80
1	B	121	ILE	N-CA-CB	6.10	121.81	110.77
1	A	334	PHE	N-CA-CB	-6.09	101.18	110.01
1	B	216	LYS	CB-CA-C	6.09	120.89	110.79
1	B	441	LYS	CA-CB-CG	6.08	126.27	114.10
1	A	107	THR	CA-C-N	6.08	131.41	121.87
1	A	107	THR	C-N-CA	6.08	131.41	121.87
1	A	174	TYR	N-CA-CB	-6.07	101.20	110.01
1	A	290	LYS	N-CA-C	-6.07	104.66	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	TRP	CB-CG-CD2	-6.07	118.31	126.80
1	A	197	ASP	CB-CA-C	-6.06	97.42	110.45
1	B	235	TYR	CB-CA-C	-6.05	102.73	111.14
1	B	308	PHE	CA-CB-CG	-6.05	107.75	113.80
1	B	126	THR	CA-C-N	6.05	133.10	121.54
1	B	126	THR	C-N-CA	6.05	133.10	121.54
1	A	198	GLY	N-CA-C	-6.01	98.93	113.18
1	B	110	ILE	N-CA-C	-6.01	104.49	110.62
1	B	42	ALA	N-CA-C	6.00	118.61	111.71
1	A	133	PHE	CB-CA-C	-6.00	101.21	110.81
1	B	221	TYR	N-CA-C	-6.00	94.18	108.40
1	A	257	VAL	N-CA-CB	-6.00	104.12	112.52
1	A	396	MET	CA-C-O	5.99	127.78	121.19
1	A	114	ASN	CA-C-N	5.98	128.29	120.28
1	A	114	ASN	C-N-CA	5.98	128.29	120.28
1	B	145	LEU	CA-C-N	5.97	128.28	120.28
1	B	145	LEU	C-N-CA	5.97	128.28	120.28
1	A	160	THR	N-CA-CB	-5.97	101.32	110.16
1	B	141	ILE	CB-CA-C	-5.97	104.33	111.97
1	B	289	VAL	N-CA-CB	-5.97	101.63	110.58
1	B	164	ASP	CA-C-N	5.96	128.63	120.46
1	B	164	ASP	C-N-CA	5.96	128.63	120.46
1	B	221	TYR	CB-CG-CD1	5.96	129.75	120.80
1	B	282	LEU	N-CA-CB	5.96	120.56	110.49
1	B	152	VAL	N-CA-CB	-5.96	98.98	110.78
1	B	25	TRP	CA-C-N	5.95	128.26	120.28
1	B	25	TRP	C-N-CA	5.95	128.26	120.28
1	B	382	ARG	CA-C-N	-5.94	112.32	120.28
1	B	382	ARG	C-N-CA	-5.94	112.32	120.28
1	B	34	TYR	CA-CB-CG	-5.93	103.22	113.90
1	A	447	SER	CA-C-O	-5.92	112.59	118.34
1	A	277	PRO	N-CA-CB	5.92	109.00	102.72
1	B	228	ILE	CA-CB-CG1	5.92	120.47	110.40
1	B	433	ILE	N-CA-CB	-5.92	102.49	110.54
1	A	182	LEU	CA-C-O	5.92	127.03	120.82
1	B	207	VAL	CA-C-N	5.92	128.21	120.28
1	B	207	VAL	C-N-CA	5.92	128.21	120.28
1	A	247	PHE	N-CA-C	-5.91	104.84	111.28
1	A	416	PHE	CA-CB-CG	-5.91	107.89	113.80
1	B	247	PHE	CA-C-N	-5.89	112.38	120.28
1	B	247	PHE	C-N-CA	-5.89	112.38	120.28
1	B	395	THR	N-CA-C	-5.89	98.25	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	PRO	N-CA-CB	5.89	109.75	103.39
1	B	394	GLY	CA-C-N	5.89	132.78	121.54
1	B	394	GLY	C-N-CA	5.89	132.78	121.54
1	A	329	SER	N-CA-CB	5.88	120.46	110.71
1	B	200	ALA	CA-C-N	5.87	128.14	120.28
1	B	200	ALA	C-N-CA	5.87	128.14	120.28
1	A	264	ILE	N-CA-C	5.86	121.53	109.34
1	A	161	PHE	CB-CA-C	-5.86	101.86	112.76
1	B	164	ASP	CA-C-O	5.86	126.70	119.97
1	A	189	THR	N-CA-C	-5.85	101.82	110.48
1	A	96	LEU	CA-C-N	5.85	132.71	121.54
1	A	96	LEU	C-N-CA	5.85	132.71	121.54
1	A	159	THR	CA-C-O	-5.84	112.15	120.51
1	B	213	LEU	N-CA-C	-5.84	104.92	111.28
1	A	303	THR	CA-C-O	5.83	126.73	120.55
1	A	140	MET	N-CA-C	5.82	117.29	111.07
1	B	352	PRO	N-CA-C	-5.81	101.98	111.68
1	B	61	PRO	CB-CA-C	-5.80	103.63	112.11
1	A	149	THR	N-CA-C	5.80	123.15	110.80
1	A	220	HIS	CB-CA-C	-5.80	100.99	110.85
1	A	291	ASP	CB-CA-C	-5.80	100.99	110.85
1	A	128	TYR	N-CA-C	-5.80	104.87	111.07
1	B	93	PHE	CA-CB-CG	5.80	119.60	113.80
1	B	268	PHE	N-CA-C	-5.79	100.75	108.74
1	A	47	VAL	CB-CA-C	-5.79	104.32	112.14
1	A	353	ASN	CA-C-N	-5.79	114.26	120.92
1	A	353	ASN	C-N-CA	-5.79	114.26	120.92
1	A	445	ASN	CA-CB-CG	-5.79	106.81	112.60
1	A	496	SER	CA-C-N	-5.79	112.52	120.28
1	A	496	SER	C-N-CA	-5.79	112.52	120.28
1	B	114	ASN	CB-CA-C	5.79	120.39	110.79
1	A	221	TYR	CB-CG-CD1	5.78	129.47	120.80
1	B	163	CYS	N-CA-CB	5.78	118.72	110.16
1	A	236	SER	N-CA-CB	-5.78	101.63	110.01
1	A	25	TRP	CB-CA-C	-5.77	101.21	110.79
1	B	382	ARG	N-CA-CB	5.76	119.16	110.30
1	A	230	THR	CA-C-N	-5.75	112.81	120.63
1	A	230	THR	C-N-CA	-5.75	112.81	120.63
1	A	380	GLU	CB-CG-CD	5.74	122.36	112.60
1	A	325	ARG	CA-CB-CG	5.74	125.58	114.10
1	B	263	PRO	N-CA-C	-5.74	100.65	112.47
1	B	231	PHE	N-CA-C	-5.72	104.95	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ASP	N-CA-C	-5.71	104.96	111.07
1	B	475	THR	CB-CA-C	-5.70	100.08	110.63
1	A	441	LYS	N-CA-C	-5.70	106.66	113.21
1	B	393	LEU	N-CA-C	-5.67	105.01	111.14
1	A	491	VAL	CA-C-O	-5.67	115.16	121.17
1	B	119	GLU	N-CA-C	5.67	117.45	111.28
1	B	156	GLN	CA-C-N	5.66	128.44	120.28
1	B	156	GLN	C-N-CA	5.66	128.44	120.28
1	B	40	VAL	CA-C-O	5.65	126.84	120.85
1	A	416	PHE	CB-CA-C	-5.65	101.78	110.81
1	B	472	PHE	CA-CB-CG	-5.64	108.16	113.80
1	A	282	LEU	CB-CA-C	-5.64	99.19	110.42
1	B	133	PHE	CA-C-N	-5.64	112.28	120.29
1	B	133	PHE	C-N-CA	-5.64	112.28	120.29
1	A	90	GLY	CA-C-N	-5.64	113.34	120.56
1	A	90	GLY	C-N-CA	-5.64	113.34	120.56
1	A	335	ALA	CA-C-N	5.63	127.76	120.44
1	A	335	ALA	C-N-CA	5.63	127.76	120.44
1	A	155	LEU	N-CA-CB	-5.63	101.84	110.12
1	A	387	PHE	CA-C-N	5.63	127.82	120.28
1	A	387	PHE	C-N-CA	5.63	127.82	120.28
1	A	418	ILE	N-CA-CB	5.62	119.01	110.58
1	B	196	GLN	CA-C-N	-5.62	112.76	122.10
1	B	196	GLN	C-N-CA	-5.62	112.76	122.10
1	B	204	VAL	N-CA-C	5.62	116.36	110.62
1	B	228	ILE	CA-C-N	5.62	127.81	120.28
1	B	228	ILE	C-N-CA	5.62	127.81	120.28
1	B	322	TYR	CA-C-N	5.62	132.28	121.54
1	B	322	TYR	C-N-CA	5.62	132.28	121.54
1	B	54	THR	N-CA-CB	-5.62	101.56	110.22
1	A	125	ASN	CA-CB-CG	-5.62	106.98	112.60
1	A	145	LEU	CB-CA-C	5.62	119.70	110.88
1	A	477	THR	CA-C-N	5.62	132.08	121.97
1	A	477	THR	C-N-CA	5.62	132.08	121.97
1	A	293	PHE	CA-C-N	-5.61	111.86	121.97
1	A	293	PHE	C-N-CA	-5.61	111.86	121.97
1	A	454	LYS	N-CA-CB	-5.61	101.87	110.01
1	B	62	ALA	CA-C-N	5.61	128.14	120.46
1	B	62	ALA	C-N-CA	5.61	128.14	120.46
1	A	274	PHE	O-C-N	5.60	129.41	123.42
1	B	91	ILE	N-CA-C	5.59	115.79	110.53
1	B	179	ILE	CB-CA-C	-5.59	104.60	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ILE	CA-CB-CG1	5.58	119.89	110.40
1	B	496	SER	N-CA-CB	-5.58	100.83	110.32
1	B	247	PHE	N-CA-CB	5.58	118.11	110.01
1	B	420	GLY	CA-C-N	-5.58	112.49	120.42
1	B	420	GLY	C-N-CA	-5.58	112.49	120.42
1	B	401	LEU	N-CA-C	-5.58	104.58	111.33
1	B	424	LEU	CA-C-N	5.58	130.96	122.37
1	B	424	LEU	C-N-CA	5.58	130.96	122.37
1	B	498	THR	CB-CA-C	5.58	120.95	110.63
1	A	480	ALA	CA-C-O	5.57	126.44	120.20
1	B	325	ARG	N-CA-C	-5.57	98.93	110.80
1	A	115	TYR	N-CA-C	-5.57	105.21	111.28
1	B	301	ILE	CB-CA-C	5.57	119.90	112.22
1	A	276	ARG	CB-CA-C	-5.56	99.21	110.17
1	B	25	TRP	CA-CB-CG	-5.56	103.03	113.60
1	B	55	TYR	CA-C-O	5.56	126.66	120.82
1	B	378	CYS	CA-C-N	-5.56	114.69	122.75
1	B	378	CYS	C-N-CA	-5.56	114.69	122.75
1	A	188	ASN	CB-CA-C	-5.56	102.15	110.88
1	B	204	VAL	CB-CA-C	-5.56	104.64	112.14
1	A	222	PRO	N-CA-C	5.55	123.91	112.47
1	B	116	THR	CB-CA-C	-5.54	102.18	110.88
1	B	277	PRO	CA-C-N	5.54	131.66	121.85
1	B	277	PRO	C-N-CA	5.54	131.66	121.85
1	A	67	GLN	CA-C-N	-5.53	112.87	120.28
1	A	67	GLN	C-N-CA	-5.53	112.87	120.28
1	B	332	TYR	CA-C-N	5.53	127.69	120.28
1	B	332	TYR	C-N-CA	5.53	127.69	120.28
1	B	454	LYS	N-CA-C	5.53	116.99	111.07
1	B	57	ASN	CA-CB-CG	-5.53	107.07	112.60
1	B	276	ARG	N-CA-C	5.53	122.03	109.81
1	B	292	VAL	N-CA-CB	5.52	120.08	110.65
1	B	26	LEU	CA-C-O	5.50	126.38	120.55
1	A	197	ASP	N-CA-C	-5.50	100.72	109.07
1	A	188	ASN	CA-CB-CG	5.49	118.09	112.60
1	B	197	ASP	N-CA-C	5.49	115.79	108.38
1	A	229	ARG	CB-CA-C	-5.48	101.69	110.79
1	A	155	LEU	CA-C-O	5.48	126.36	120.55
1	A	231	PHE	CA-C-N	-5.48	113.55	120.56
1	A	231	PHE	C-N-CA	-5.48	113.55	120.56
1	A	145	LEU	N-CA-C	-5.48	105.21	111.07
1	A	409	GLN	N-CA-C	-5.48	105.31	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	THR	CB-CA-C	-5.48	100.50	110.63
1	B	324	LEU	CA-C-N	5.47	132.00	121.54
1	B	324	LEU	C-N-CA	5.47	132.00	121.54
1	B	406	GLU	N-CA-C	-5.47	105.42	111.71
1	A	427	ASN	CB-CA-C	5.47	119.91	112.09
1	B	312	VAL	CA-C-O	5.47	126.64	120.95
1	A	164	ASP	CA-CB-CG	-5.47	107.13	112.60
1	A	370	ASP	CA-CB-CG	-5.46	107.14	112.60
1	B	95	VAL	CA-C-N	-5.46	111.39	120.68
1	B	95	VAL	C-N-CA	-5.46	111.39	120.68
1	A	353	ASN	CA-CB-CG	-5.46	107.14	112.60
1	B	138	TRP	CA-C-O	5.46	126.34	120.55
1	A	254	LEU	N-CA-C	-5.46	101.21	108.74
1	A	436	LEU	CB-CA-C	-5.46	102.31	110.88
1	B	416	PHE	CB-CA-C	-5.45	102.33	110.88
1	B	181	ILE	N-CA-CB	-5.45	103.13	110.54
1	B	192	GLU	CA-C-N	5.44	131.93	121.54
1	B	192	GLU	C-N-CA	5.44	131.93	121.54
1	B	72	ARG	N-CA-C	-5.43	105.47	111.71
1	B	155	LEU	N-CA-CB	-5.42	101.87	110.22
1	A	452	ILE	N-CA-CB	-5.42	103.17	110.54
1	A	268	PHE	N-CA-C	-5.42	103.24	110.55
1	A	476	ASN	CA-CB-CG	-5.41	107.19	112.60
1	A	340	THR	CB-CA-C	-5.40	101.82	110.79
1	B	289	VAL	CB-CA-C	-5.40	104.77	112.22
1	A	320	HIS	CG-CD2-NE2	5.39	112.59	107.20
1	B	35	TYR	CA-C-O	5.39	126.67	120.90
1	B	73	THR	N-CA-C	-5.39	107.26	112.97
1	A	264	ILE	N-CA-CB	-5.38	102.35	111.23
1	A	467	GLY	N-CA-C	-5.38	106.27	112.73
1	B	220	HIS	N-CA-C	5.38	117.22	111.36
1	B	346	VAL	CA-C-N	-5.37	111.75	120.72
1	B	346	VAL	C-N-CA	-5.37	111.75	120.72
1	A	336	LEU	N-CA-CB	-5.37	102.23	110.01
1	B	158	VAL	O-C-N	5.37	128.14	122.67
1	A	151	VAL	CA-C-O	5.36	126.26	120.47
1	B	199	PHE	CB-CA-C	-5.36	101.74	110.85
1	A	126	THR	N-CA-CB	5.36	117.83	109.85
1	B	147	ALA	N-CA-C	-5.35	105.45	111.28
1	B	269	PHE	O-C-N	-5.35	117.38	121.55
1	B	406	GLU	CB-CG-CD	5.35	121.69	112.60
1	B	498	THR	N-CA-CB	-5.34	101.99	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	GLY	N-CA-C	-5.34	106.32	112.73
1	B	82	VAL	CB-CA-C	-5.34	104.94	112.14
1	B	275	ASN	CA-C-N	5.33	134.81	121.80
1	B	275	ASN	C-N-CA	5.33	134.81	121.80
1	A	432	ARG	CA-CB-CG	5.33	124.76	114.10
1	B	300	ILE	CB-CA-C	-5.32	105.16	111.97
1	A	310	HIS	CB-CA-C	-5.32	102.53	110.88
1	A	492	ILE	CB-CA-C	-5.32	104.96	112.14
1	B	461	LEU	CB-CA-C	-5.31	100.80	110.63
1	B	115	TYR	CA-CB-CG	5.31	123.46	113.90
1	A	372	ASN	N-CA-C	-5.31	102.39	108.49
1	A	73	THR	CA-C-N	5.31	129.89	122.36
1	A	73	THR	C-N-CA	5.31	129.89	122.36
1	B	100	PRO	N-CA-C	-5.31	101.54	112.47
1	B	85	SER	N-CA-C	-5.30	105.40	111.07
1	A	29	LYS	CA-C-O	-5.30	114.93	120.55
1	A	431	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
1	A	116	THR	CA-C-O	5.29	126.38	120.82
1	B	150	ASN	N-CA-CB	5.29	117.12	110.45
1	B	38	ASP	CA-C-N	5.28	127.79	120.29
1	B	38	ASP	C-N-CA	5.28	127.79	120.29
1	A	497	PHE	O-C-N	5.28	127.71	122.12
1	A	27	ASP	N-CA-C	-5.26	105.44	111.07
1	A	28	LEU	N-CA-C	-5.26	105.55	111.28
1	B	131	PHE	CA-CB-CG	-5.26	108.54	113.80
1	A	125	ASN	N-CA-C	5.25	121.99	110.80
1	B	247	PHE	N-CA-C	-5.25	105.45	111.07
1	A	269	PHE	CA-C-N	5.25	126.60	120.98
1	A	269	PHE	C-N-CA	5.25	126.60	120.98
1	A	289	VAL	CA-C-O	5.25	126.18	120.57
1	B	292	VAL	CA-CB-CG2	5.25	119.32	110.40
1	A	170	ILE	CB-CA-C	-5.25	105.06	112.14
1	A	377	ARG	CB-CA-C	-5.25	100.68	109.65
1	A	362	HIS	CB-CG-CD2	-5.24	124.38	131.20
1	B	159	THR	CA-CB-OG1	5.24	117.46	109.60
1	B	255	ASN	CA-C-N	5.24	130.88	122.86
1	B	255	ASN	C-N-CA	5.24	130.88	122.86
1	A	327	PRO	N-CA-C	5.24	123.26	112.47
1	A	346	VAL	CA-C-O	5.24	126.40	120.95
1	B	464	SER	CA-C-O	5.24	126.10	120.55
1	B	108	GLY	O-C-N	-5.23	119.19	121.07
1	A	129	PHE	CA-CB-CG	5.23	119.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	PHE	CB-CA-C	5.22	119.46	110.79
1	B	278	GLN	N-CA-C	-5.22	100.79	108.99
1	A	432	ARG	O-C-N	-5.22	116.11	122.22
1	B	323	LYS	CA-C-N	-5.22	114.71	122.74
1	B	323	LYS	C-N-CA	-5.22	114.71	122.74
1	B	496	SER	CA-C-N	-5.22	113.34	120.44
1	B	496	SER	C-N-CA	-5.22	113.34	120.44
1	A	446	ASN	CA-C-N	5.21	126.61	120.09
1	A	446	ASN	C-N-CA	5.21	126.61	120.09
1	A	171	ASN	N-CA-CB	5.21	117.78	110.12
1	A	492	ILE	CA-CB-CG1	5.21	119.26	110.40
1	A	233	SER	CA-C-O	5.21	125.79	119.38
1	A	338	GLY	N-CA-C	-5.21	106.11	112.77
1	B	468	PHE	O-C-N	-5.20	116.68	122.09
1	A	193	LYS	CA-C-N	5.20	127.51	120.44
1	A	193	LYS	C-N-CA	5.20	127.51	120.44
1	B	27	ASP	N-CA-C	-5.19	105.62	111.28
1	B	156	GLN	CA-C-O	5.19	125.97	120.10
1	A	233	SER	N-CA-C	5.19	118.87	112.54
1	A	491	VAL	CA-C-N	-5.19	113.35	120.46
1	A	491	VAL	C-N-CA	-5.19	113.35	120.46
1	A	230	THR	CA-C-O	-5.19	115.05	120.55
1	A	457	MET	CA-C-O	5.18	126.04	120.55
1	A	46	ARG	CB-CA-C	-5.18	100.73	110.67
1	A	371	SER	N-CA-CB	5.18	119.75	111.20
1	A	312	VAL	CA-C-O	5.17	126.33	120.85
1	A	334	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	489	LEU	CB-CA-C	-5.17	102.77	110.88
1	B	363	THR	N-CA-C	-5.16	105.83	111.82
1	B	440	PRO	N-CA-CB	5.15	108.10	103.20
1	A	194	SER	O-C-N	-5.15	116.53	122.09
1	A	139	SER	CA-C-N	-5.15	113.75	120.44
1	A	139	SER	C-N-CA	-5.15	113.75	120.44
1	B	157	TYR	N-CA-CB	-5.15	102.29	110.22
1	A	406	GLU	N-CA-C	5.15	117.79	111.82
1	B	280	THR	CB-CA-C	-5.14	99.31	111.65
1	B	196	GLN	CB-CA-C	-5.14	101.74	111.97
1	B	230	THR	CB-CA-C	-5.14	102.78	110.90
1	B	409	GLN	CB-CG-CD	-5.13	103.88	112.60
1	B	182	LEU	CB-CA-C	-5.13	102.83	110.88
1	B	215	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	247	PHE	CB-CA-C	-5.12	102.29	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	GLU	CB-CG-CD	5.12	121.31	112.60
1	A	207	VAL	N-CA-CB	-5.12	102.90	110.58
1	B	193	LYS	N-CA-C	5.12	121.70	110.80
1	A	187	HIS	CE1-NE2-CD2	-5.12	103.89	109.00
1	A	444	ASP	N-CA-C	5.12	121.69	110.80
1	B	117	VAL	CB-CA-C	-5.12	105.42	111.97
1	B	232	ILE	N-CA-C	5.12	115.89	110.72
1	A	499	TYR	CB-CG-CD1	5.11	128.46	120.80
1	A	194	SER	CA-C-O	-5.10	115.44	120.70
1	A	116	THR	N-CA-C	-5.10	105.61	111.07
1	B	370	ASP	CA-C-N	5.10	131.28	121.54
1	B	370	ASP	C-N-CA	5.10	131.28	121.54
1	B	333	ASP	CA-C-N	-5.09	113.82	120.44
1	B	333	ASP	C-N-CA	-5.09	113.82	120.44
1	A	223	LEU	O-C-N	-5.09	115.82	122.59
1	A	186	PHE	CA-C-N	5.09	127.10	120.28
1	A	186	PHE	C-N-CA	5.09	127.10	120.28
1	A	252	GLY	N-CA-C	-5.09	104.32	111.09
1	A	27	ASP	CA-C-N	5.08	127.09	120.28
1	A	27	ASP	C-N-CA	5.08	127.09	120.28
1	A	434	VAL	N-CA-C	-5.08	105.44	110.62
1	B	447	SER	N-CA-CB	5.08	118.57	110.39
1	A	60	LEU	O-C-N	-5.08	115.96	120.48
1	A	460	PHE	CB-CA-C	-5.08	102.91	110.88
1	A	46	ARG	N-CA-CB	5.07	118.14	110.28
1	A	74	ASP	N-CA-C	-5.07	104.39	111.39
1	A	77	TYR	CB-CA-C	-5.07	102.67	111.30
1	A	443	ARG	CA-C-O	-5.07	114.81	120.54
1	A	432	ARG	CG-CD-NE	5.07	123.15	112.00
1	A	104	VAL	N-CA-CB	5.07	118.14	111.25
1	B	267	SER	CA-C-N	5.07	130.16	122.11
1	B	267	SER	C-N-CA	5.07	130.16	122.11
1	A	419	MET	CA-CB-CG	5.06	124.23	114.10
1	B	290	LYS	O-C-N	5.06	127.49	122.12
1	A	309	ASP	CB-CA-C	-5.06	102.93	110.88
1	A	47	VAL	CA-C-O	5.06	126.21	120.95
1	B	447	SER	N-CA-C	-5.06	106.59	113.57
1	A	80	ASN	CB-CA-C	-5.06	102.39	110.79
1	A	263	PRO	N-CA-C	5.06	122.89	112.47
1	B	224	PHE	CA-C-N	5.05	131.19	121.54
1	B	224	PHE	C-N-CA	5.05	131.19	121.54
1	A	365	THR	CA-C-O	5.05	125.78	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	PHE	N-CA-C	-5.04	105.43	111.03
1	A	357	PRO	CA-C-N	5.04	127.45	120.29
1	A	357	PRO	C-N-CA	5.04	127.45	120.29
1	B	149	THR	N-CA-C	5.04	117.41	110.35
1	B	387	PHE	CA-C-N	5.04	127.04	120.28
1	B	387	PHE	C-N-CA	5.04	127.04	120.28
1	A	264	ILE	CA-CB-CG1	5.04	118.97	110.40
1	B	382	ARG	CB-CA-C	-5.04	100.11	110.38
1	B	161	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	150	ASN	CA-C-N	5.03	129.00	120.64
1	B	150	ASN	C-N-CA	5.03	129.00	120.64
1	B	157	TYR	CA-CB-CG	-5.03	104.84	113.90
1	B	174	TYR	CB-CG-CD2	-5.03	113.25	120.80
1	B	134	TRP	O-C-N	5.03	127.89	122.15
1	B	293	PHE	CB-CA-C	-5.03	102.96	110.90
1	B	226	HIS	CE1-NE2-CD2	-5.02	103.98	109.00
1	A	465	LEU	N-CA-C	-5.02	105.99	111.82
1	A	57	ASN	CA-CB-CG	-5.02	107.58	112.60
1	A	166	PHE	N-CA-C	-5.02	105.70	111.07
1	A	378	CYS	CA-C-N	5.01	131.00	121.97
1	A	378	CYS	C-N-CA	5.01	131.00	121.97
1	A	418	ILE	CA-C-N	5.01	127.00	120.28
1	A	418	ILE	C-N-CA	5.01	127.00	120.28
1	B	435	PHE	CA-CB-CG	-5.01	108.79	113.80
1	B	418	ILE	CB-CA-C	-5.00	105.31	112.22
1	A	163	CYS	CA-CB-SG	-5.00	102.89	114.40

There are no chirality outliers.

All (89) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	TYR	Sidechain
1	A	124	LEU	Mainchain
1	A	128	TYR	Sidechain
1	A	143	HIS	Sidechain
1	A	150	ASN	Mainchain
1	A	162	PRO	Peptide
1	A	174	TYR	Sidechain
1	A	197	ASP	Peptide,Mainchain
1	A	199	PHE	Sidechain
1	A	216	LYS	Mainchain
1	A	218	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	221	TYR	Sidechain
1	A	235	TYR	Sidechain
1	A	253	TYR	Peptide,Mainchain
1	A	263	PRO	Mainchain
1	A	268	PHE	Sidechain
1	A	274	PHE	Sidechain
1	A	306	PHE	Sidechain
1	A	31	ARG	Sidechain
1	A	320	HIS	Sidechain
1	A	322	TYR	Sidechain
1	A	326	LYS	Peptide
1	A	35	TYR	Sidechain
1	A	362	HIS	Sidechain
1	A	37	SER	Peptide,Mainchain
1	A	370	ASP	Peptide,Mainchain
1	A	374	ASN	Mainchain
1	A	375	VAL	Mainchain
1	A	377	ARG	Sidechain
1	A	398	ARG	Sidechain
1	A	416	PHE	Sidechain
1	A	423	GLY	Mainchain
1	A	43	PHE	Sidechain
1	A	432	ARG	Sidechain
1	A	442	ARG	Sidechain
1	A	455	ARG	Sidechain
1	A	46	ARG	Mainchain
1	A	468	PHE	Sidechain
1	A	472	PHE	Sidechain
1	A	476	ASN	Mainchain
1	A	483	PHE	Sidechain
1	A	496	SER	Peptide,Mainchain
1	A	55	TYR	Sidechain
1	A	72	ARG	Sidechain
1	B	104	VAL	Mainchain
1	B	115	TYR	Sidechain
1	B	118	TYR	Sidechain
1	B	148	PHE	Sidechain
1	B	156	GLN	Mainchain
1	B	157	TYR	Sidechain
1	B	158	VAL	Mainchain
1	B	174	TYR	Sidechain
1	B	218	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	B	226	HIS	Sidechain
1	B	229	ARG	Sidechain
1	B	247	PHE	Sidechain
1	B	253	TYR	Sidechain
1	B	259	PHE	Sidechain
1	B	297	PRO	Peptide,Mainchain
1	B	307	TYR	Sidechain
1	B	308	PHE	Sidechain
1	B	319	ARG	Sidechain
1	B	320	HIS	Mainchain
1	B	325	ARG	Sidechain
1	B	331	HIS	Peptide,Sidechain,Mainchain
1	B	332	TYR	Sidechain
1	B	34	TYR	Sidechain
1	B	357	PRO	Peptide,Mainchain
1	B	398	ARG	Sidechain
1	B	416	PHE	Sidechain
1	B	435	PHE	Sidechain
1	B	437	PHE	Sidechain
1	B	441	LYS	Mainchain
1	B	443	ARG	Sidechain
1	B	468	PHE	Sidechain
1	B	497	PHE	Peptide,Sidechain,Mainchain
1	B	498	THR	Mainchain
1	B	56	PHE	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3806	0	3851	333	0
1	B	3806	0	3851	366	0
All	All	7612	0	7702	693	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 45.

All (693) 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:B:107:THR:HG23	1:B:110:ILE:H	1.40	0.87
1:B:331:HIS:HE1	1:B:335:ALA:HB2	1.40	0.86
1:A:184:ARG:HA	1:A:187:HIS:CD2	2.12	0.84
1:A:39:TRP:H	1:A:39:TRP:CD1	1.93	0.82
1:B:143:HIS:CE1	1:B:338:GLY:HA3	2.16	0.79
1:B:331:HIS:CE1	1:B:335:ALA:HB2	2.20	0.77
1:B:154:LEU:HA	1:B:157:TYR:CE2	2.20	0.77
1:A:25:TRP:HA	1:A:25:TRP:CE2	2.19	0.76
1:A:60:LEU:HD13	1:A:412:LEU:HB3	1.65	0.76
1:A:459:ILE:HG22	1:A:463:PHE:CE1	2.21	0.76
1:B:105:GLY:C	1:B:353:ASN:H	1.93	0.76
1:B:288:PRO:O	1:B:292:VAL:HG13	1.85	0.75
1:A:496:SER:HA	1:A:499:TYR:CZ	2.23	0.74
1:A:203:VAL:HG22	1:B:203:VAL:HG22	1.69	0.74
1:A:140:MET:HA	1:A:143:HIS:CD2	2.24	0.72
1:A:262:LEU:HD12	1:A:404:LEU:O	1.89	0.72
1:A:207:VAL:HG13	1:A:211:PHE:CE2	2.24	0.72
1:A:138:TRP:HE1	1:A:295:ALA:HB3	1.54	0.72
1:A:496:SER:HA	1:A:499:TYR:CE2	2.25	0.72
1:A:356:ILE:N	1:A:358:GLN:HE22	1.87	0.72
1:A:261:LYS:HA	1:A:408:PRO:HA	1.71	0.71
1:B:199:PHE:O	1:B:203:VAL:HG23	1.90	0.71
1:B:113:PHE:O	1:B:117:VAL:HG23	1.90	0.71
1:A:223:LEU:H	1:A:229:ARG:HH12	1.38	0.71
1:B:218:PHE:CD1	1:B:223:LEU:HB2	2.25	0.71
1:B:497:PHE:CD2	1:B:498:THR:HA	2.26	0.70
1:A:431:HIS:CD2	1:A:431:HIS:N	2.57	0.70
1:B:198:GLY:O	1:B:202:VAL:HG23	1.91	0.70
1:B:140:MET:HE1	1:B:143:HIS:CD2	2.26	0.70
1:B:154:LEU:HA	1:B:157:TYR:CZ	2.27	0.69
1:B:319:ARG:HG3	1:B:322:TYR:H	1.57	0.69
1:B:72:ARG:HH22	1:B:111:SER:HB3	1.57	0.69
1:B:359:ALA:HA	1:B:362:HIS:CD2	2.27	0.69
1:A:134:TRP:CD1	1:A:295:ALA:HB2	2.28	0.68
1:B:169:PHE:CE2	1:B:483:PHE:CD1	2.82	0.68
1:A:460:PHE:HA	1:A:463:PHE:CE2	2.29	0.67
1:B:455:ARG:O	1:B:458:VAL:HG22	1.93	0.67
1:B:135:ILE:HA	1:B:138:TRP:CD1	2.29	0.67
1:B:184:ARG:HH11	1:B:185:GLN:HG3	1.59	0.67
1:A:428:VAL:HA	1:A:431:HIS:ND1	2.09	0.67
1:B:280:THR:HG22	1:B:281:TRP:H	1.60	0.66
1:A:183:THR:HB	1:A:187:HIS:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:GLY:C	1:B:425:MET:H	2.02	0.65
1:A:441:LYS:HD3	1:A:442:ARG:HH11	1.60	0.65
1:B:104:VAL:HG12	1:B:352:PRO:HB2	1.78	0.65
1:B:430:ILE:O	1:B:433:ILE:HB	1.96	0.65
1:B:25:TRP:CD2	1:B:25:TRP:N	2.61	0.65
1:B:359:ALA:O	1:B:362:HIS:CG	2.50	0.65
1:A:415:LEU:O	1:A:419:MET:HB3	1.97	0.65
1:A:216:LYS:O	1:A:219:HIS:CD2	2.50	0.65
1:B:178:GLY:HA3	1:B:416:PHE:CG	2.32	0.64
1:B:226:HIS:CE1	1:B:370:ASP:O	2.49	0.64
1:A:356:ILE:HD12	1:A:356:ILE:H	1.63	0.64
1:A:138:TRP:HE1	1:A:295:ALA:CB	2.10	0.64
1:A:154:LEU:HA	1:A:157:TYR:CE2	2.32	0.64
1:A:38:ASP:HB2	1:A:382:ARG:HH11	1.62	0.64
1:A:218:PHE:HB3	1:A:229:ARG:HH11	1.63	0.64
1:A:134:TRP:HB2	1:A:138:TRP:CZ2	2.33	0.64
1:A:278:GLN:HA	1:A:281:TRP:CE3	2.33	0.64
1:A:307:TYR:CD1	1:A:307:TYR:C	2.75	0.63
1:A:359:ALA:HA	1:A:362:HIS:CD2	2.33	0.63
1:A:31:ARG:HH22	1:A:100:PRO:HD3	1.63	0.63
1:B:126:THR:HG22	1:B:127:SER:H	1.63	0.63
1:A:278:GLN:HA	1:A:281:TRP:CZ3	2.35	0.62
1:B:211:PHE:HA	1:B:214:PHE:CD2	2.35	0.62
1:A:207:VAL:HG13	1:A:211:PHE:CZ	2.34	0.62
1:A:226:HIS:CD2	1:A:370:ASP:O	2.53	0.62
1:A:223:LEU:H	1:A:229:ARG:NH1	1.98	0.62
1:B:483:PHE:CD1	1:B:484:PRO:HD3	2.34	0.61
1:A:154:LEU:HA	1:A:157:TYR:CZ	2.34	0.61
1:A:261:LYS:O	1:A:262:LEU:HD23	2.01	0.61
1:B:24:ILE:HB	1:B:25:TRP:CE2	2.36	0.61
1:B:443:ARG:HA	1:B:443:ARG:HH11	1.65	0.61
1:B:460:PHE:HA	1:B:463:PHE:CE2	2.36	0.61
1:A:487:LEU:O	1:A:491:VAL:HG22	2.01	0.61
1:A:134:TRP:CE2	1:A:292:VAL:HA	2.36	0.61
1:A:216:LYS:HD2	1:A:219:HIS:CE1	2.36	0.61
1:A:135:ILE:HA	1:A:138:TRP:CD1	2.36	0.60
1:B:107:THR:HG23	1:B:110:ILE:N	2.15	0.60
1:B:53:ASP:HA	1:B:56:PHE:CZ	2.36	0.60
1:A:391:MET:HG2	1:A:394:GLY:H	1.67	0.60
1:B:135:ILE:HG23	1:B:295:ALA:HB1	1.84	0.60
1:B:138:TRP:HZ2	1:B:295:ALA:HB3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLN:C	1:B:323:LYS:H	2.09	0.60
1:B:80:ASN:HA	1:B:83:LEU:HD12	1.84	0.60
1:B:305:LEU:HA	1:B:308:PHE:CD2	2.36	0.60
1:A:24:ILE:HG12	1:A:331:HIS:CE1	2.37	0.59
1:A:432:ARG:HA	1:A:435:PHE:CD2	2.37	0.59
1:B:496:SER:HA	1:B:499:TYR:CE2	2.36	0.59
1:A:150:ASN:HA	1:A:152:VAL:HG22	1.84	0.59
1:A:224:PHE:H	1:A:229:ARG:NH1	2.00	0.59
1:B:432:ARG:HH21	1:B:449:LEU:HD13	1.66	0.59
1:A:26:LEU:HD23	1:A:26:LEU:H	1.68	0.59
1:A:455:ARG:HE	1:A:456:SER:H	1.49	0.59
1:B:154:LEU:O	1:B:157:TYR:CD2	2.56	0.59
1:B:38:ASP:HA	1:B:41:ASP:OD2	2.03	0.59
1:B:161:PHE:CE2	1:B:491:VAL:HG12	2.38	0.59
1:B:493:VAL:HA	1:B:495:PHE:CE2	2.36	0.59
1:A:258:LYS:HD3	1:A:260:LYS:HZ3	1.67	0.58
1:A:169:PHE:HD2	1:A:170:ILE:HD13	1.67	0.58
1:B:38:ASP:HB2	1:B:39:TRP:CE3	2.37	0.58
1:B:38:ASP:HB3	1:B:382:ARG:H	1.67	0.58
1:B:319:ARG:HD3	1:B:322:TYR:CE2	2.38	0.58
1:A:416:PHE:HA	1:A:419:MET:SD	2.44	0.58
1:B:45:TYR:O	1:B:49:PRO:HD2	2.03	0.58
1:B:307:TYR:CD1	1:B:307:TYR:C	2.78	0.58
1:A:427:ASN:O	1:A:431:HIS:CE1	2.56	0.58
1:B:24:ILE:HB	1:B:25:TRP:CZ2	2.38	0.58
1:B:72:ARG:HH22	1:B:111:SER:CB	2.16	0.58
1:B:331:HIS:O	1:B:331:HIS:CD2	2.57	0.58
1:A:169:PHE:CZ	1:A:483:PHE:CE2	2.92	0.58
1:B:462:CYS:HA	1:B:465:LEU:HD12	1.85	0.58
1:A:149:THR:HG23	1:A:151:VAL:H	1.69	0.58
1:A:175:ILE:HA	1:A:416:PHE:CD1	2.39	0.57
1:B:307:TYR:CD2	1:B:308:PHE:CD1	2.93	0.57
1:B:497:PHE:O	1:B:497:PHE:CD1	2.57	0.57
1:A:174:TYR:HB3	1:A:416:PHE:CZ	2.39	0.57
1:A:367:LEU:HD13	1:A:368:VAL:H	1.69	0.57
1:A:140:MET:HA	1:A:143:HIS:NE2	2.19	0.57
1:A:429:ILE:HA	1:A:432:ARG:HB2	1.86	0.57
1:A:430:ILE:HB	1:A:431:HIS:CD2	2.40	0.57
1:A:427:ASN:H	1:A:431:HIS:CE1	2.22	0.57
1:A:24:ILE:HB	1:A:25:TRP:CZ3	2.40	0.57
1:A:135:ILE:HA	1:A:138:TRP:NE1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:HIS:CE1	1:B:370:ASP:C	2.83	0.57
1:A:421:ILE:HG22	1:A:425:MET:HE1	1.87	0.57
1:A:186:PHE:CE1	1:A:197:ASP:HB3	2.39	0.56
1:B:174:TYR:HB3	1:B:416:PHE:CZ	2.40	0.56
1:A:98:GLY:HA3	1:A:333:ASP:HB3	1.88	0.56
1:A:203:VAL:CG2	1:B:203:VAL:HG22	2.34	0.56
1:A:226:HIS:O	1:A:230:THR:HB	2.04	0.56
1:A:460:PHE:HA	1:A:463:PHE:CD2	2.40	0.56
1:A:257:VAL:HB	1:A:259:PHE:CE1	2.40	0.56
1:B:126:THR:HG22	1:B:127:SER:N	2.21	0.56
1:A:211:PHE:HA	1:A:214:PHE:CD2	2.41	0.56
1:A:457:MET:HA	1:A:460:PHE:CD2	2.41	0.56
1:A:31:ARG:HE	1:A:98:GLY:HA2	1.71	0.56
1:B:154:LEU:HD22	1:B:307:TYR:OH	2.05	0.56
1:A:26:LEU:H	1:A:26:LEU:CD2	2.17	0.56
1:B:331:HIS:O	1:B:331:HIS:CG	2.58	0.56
1:B:451:LYS:HG3	1:B:454:LYS:HZ3	1.70	0.55
1:A:39:TRP:CZ2	1:A:382:ARG:NH1	2.74	0.55
1:A:104:VAL:HA	1:A:353:ASN:O	2.06	0.55
1:B:282:LEU:HD12	1:B:283:ALA:H	1.70	0.55
1:B:485:LEU:O	1:B:489:LEU:HD23	2.05	0.55
1:A:78:GLY:HA3	1:A:269:PHE:CD2	2.41	0.55
1:A:135:ILE:HG12	1:A:295:ALA:HB1	1.88	0.55
1:A:369:ARG:O	1:A:373:GLN:HA	2.07	0.55
1:B:324:LEU:HD13	1:B:326:LYS:H	1.71	0.55
1:B:287:ILE:HD12	1:B:288:PRO:HD2	1.89	0.55
1:A:68:ASP:HA	1:A:71:ASP:OD2	2.06	0.55
1:A:263:PRO:O	1:A:404:LEU:HD11	2.05	0.55
1:A:388:GLN:HA	1:A:391:MET:HE1	1.87	0.55
1:A:416:PHE:CD1	1:A:416:PHE:C	2.84	0.55
1:B:38:ASP:HB2	1:B:39:TRP:CZ3	2.41	0.55
1:B:356:ILE:HB	1:B:357:PRO:HD3	1.89	0.55
1:A:99:GLN:HG3	1:A:101:LEU:H	1.72	0.55
1:B:170:ILE:CG2	1:B:174:TYR:CZ	2.90	0.55
1:A:493:VAL:C	1:A:495:PHE:H	2.15	0.55
1:A:99:GLN:HA	1:A:99:GLN:OE1	2.06	0.54
1:A:319:ARG:HD2	1:A:321:GLN:HG3	1.87	0.54
1:B:38:ASP:HB2	1:B:39:TRP:CD2	2.43	0.54
1:B:260:LYS:C	1:B:409:GLN:H	2.15	0.54
1:A:455:ARG:NE	1:A:456:SER:H	2.05	0.54
1:B:156:GLN:HB2	1:B:157:TYR:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PRO:C	1:A:442:ARG:H	2.15	0.54
1:B:36:LYS:O	1:B:39:TRP:CD1	2.60	0.54
1:B:68:ASP:HA	1:B:71:ASP:OD2	2.07	0.54
1:B:87:ALA:HB1	1:B:395:THR:HA	1.88	0.54
1:A:153:CYS:O	1:A:157:TYR:CE1	2.61	0.54
1:B:218:PHE:O	1:B:222:PRO:HA	2.08	0.54
1:B:319:ARG:HD3	1:B:322:TYR:CZ	2.42	0.54
1:B:104:VAL:HG13	1:B:353:ASN:O	2.07	0.54
1:B:170:ILE:HG22	1:B:174:TYR:CE2	2.43	0.54
1:B:44:ASN:CG	1:B:45:TYR:H	2.15	0.54
1:B:104:VAL:HA	1:B:353:ASN:O	2.07	0.54
1:A:421:ILE:O	1:A:425:MET:SD	2.66	0.54
1:A:60:LEU:HD12	1:A:60:LEU:O	2.07	0.53
1:B:421:ILE:O	1:B:425:MET:SD	2.66	0.53
1:B:161:PHE:CD2	1:B:491:VAL:HG12	2.43	0.53
1:B:170:ILE:HG23	1:B:174:TYR:CZ	2.44	0.53
1:A:105:GLY:O	1:A:355:LEU:HD21	2.08	0.53
1:A:408:PRO:HG2	1:A:411:VAL:HG23	1.91	0.53
1:A:139:SER:O	1:A:143:HIS:CD2	2.60	0.53
1:B:260:LYS:HB3	1:B:409:GLN:HB2	1.91	0.53
1:A:436:LEU:HD23	1:A:437:PHE:CZ	2.43	0.53
1:B:34:TYR:CE2	1:B:327:PRO:HB3	2.43	0.53
1:B:416:PHE:CD1	1:B:416:PHE:C	2.85	0.53
1:A:421:ILE:O	1:A:424:LEU:HD13	2.08	0.53
1:B:205:ALA:O	1:B:208:MET:SD	2.67	0.53
1:A:138:TRP:NE1	1:A:295:ALA:HB3	2.23	0.53
1:A:38:ASP:HA	1:A:41:ASP:OD2	2.08	0.53
1:B:138:TRP:CZ2	1:B:295:ALA:HB3	2.43	0.53
1:B:186:PHE:CE2	1:B:197:ASP:HB3	2.44	0.53
1:B:283:ALA:C	1:B:284:TYR:CD1	2.87	0.53
1:B:495:PHE:O	1:B:499:TYR:CZ	2.62	0.53
1:B:129:PHE:CE1	1:B:273:LYS:HB3	2.44	0.52
1:B:359:ALA:O	1:B:362:HIS:CD2	2.61	0.52
1:A:105:GLY:C	1:A:355:LEU:HD21	2.34	0.52
1:B:81:GLU:HB3	1:B:350:PRO:HD3	1.91	0.52
1:B:169:PHE:CZ	1:B:483:PHE:CE1	2.98	0.52
1:A:280:THR:HA	1:A:347:LEU:HA	1.91	0.52
1:A:280:THR:HA	1:A:347:LEU:O	2.08	0.52
1:B:455:ARG:HA	1:B:455:ARG:NE	2.25	0.52
1:A:162:PRO:HB3	1:A:491:VAL:HG11	1.91	0.52
1:B:39:TRP:CD2	1:B:39:TRP:N	2.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LEU:HG	1:B:224:PHE:CZ	2.44	0.52
1:B:262:LEU:HD11	1:B:404:LEU:C	2.35	0.52
1:B:463:PHE:N	1:B:463:PHE:CD1	2.73	0.52
1:A:304:ILE:O	1:A:307:TYR:CD2	2.63	0.52
1:A:319:ARG:HD2	1:A:322:TYR:CG	2.44	0.52
1:A:138:TRP:CD1	1:A:296:LEU:HA	2.45	0.52
1:B:432:ARG:HH21	1:B:449:LEU:HD22	1.75	0.52
1:A:483:PHE:O	1:A:486:VAL:HB	2.10	0.52
1:B:99:GLN:HG3	1:B:101:LEU:H	1.75	0.51
1:A:134:TRP:CD2	1:A:292:VAL:HA	2.45	0.51
1:A:432:ARG:HA	1:A:435:PHE:CE2	2.46	0.51
1:A:197:ASP:HB2	1:A:199:PHE:CD1	2.44	0.51
1:B:51:THR:HG23	1:B:384:THR:OG1	2.11	0.51
1:A:368:VAL:HG21	1:A:376:VAL:H	1.75	0.51
1:A:457:MET:HA	1:A:460:PHE:CE2	2.46	0.51
1:A:495:PHE:O	1:A:499:TYR:CE1	2.64	0.51
1:B:106:VAL:HA	1:B:353:ASN:OD1	2.10	0.51
1:B:241:VAL:O	1:B:245:SER:HB2	2.10	0.51
1:A:105:GLY:C	1:A:353:ASN:H	2.19	0.51
1:B:324:LEU:HD13	1:B:326:LYS:N	2.26	0.51
1:A:24:ILE:HA	1:A:27:ASP:CG	2.36	0.51
1:B:153:CYS:O	1:B:157:TYR:CE1	2.63	0.51
1:B:439:ASP:HB3	1:B:442:ARG:HG2	1.92	0.51
1:A:218:PHE:CD1	1:A:222:PRO:C	2.89	0.51
1:A:232:ILE:HA	1:A:235:TYR:CD2	2.46	0.51
1:A:320:HIS:CE1	1:A:325:ARG:HB2	2.46	0.51
1:A:463:PHE:O	1:A:466:ALA:HB3	2.11	0.51
1:B:77:TYR:CZ	1:B:269:PHE:CZ	2.98	0.51
1:A:324:LEU:HD13	1:A:377:ARG:HH21	1.76	0.51
1:B:118:TYR:CZ	1:B:128:TYR:CZ	2.98	0.51
1:B:135:ILE:HG22	1:B:295:ALA:O	2.10	0.51
1:A:50:SER:OG	1:A:365:THR:HG21	2.11	0.51
1:B:72:ARG:C	1:B:74:ASP:H	2.18	0.51
1:B:138:TRP:CE2	1:B:296:LEU:HA	2.46	0.51
1:A:31:ARG:HH22	1:A:100:PRO:CD	2.23	0.50
1:A:132:MET:SD	1:A:132:MET:C	2.94	0.50
1:A:485:LEU:O	1:A:488:LEU:HB3	2.11	0.50
1:B:468:PHE:HA	1:B:471:GLU:OE2	2.10	0.50
1:B:356:ILE:HB	1:B:357:PRO:CD	2.41	0.50
1:B:460:PHE:HA	1:B:463:PHE:CD2	2.46	0.50
1:B:62:ALA:HA	1:B:65:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:TYR:CE1	1:B:132:MET:SD	3.05	0.50
1:A:131:PHE:HA	1:A:134:TRP:CZ2	2.46	0.50
1:A:87:ALA:CB	1:A:395:THR:HA	2.42	0.50
1:A:280:THR:HB	1:A:347:LEU:HA	1.94	0.50
1:A:358:GLN:H	1:A:358:GLN:NE2	2.09	0.50
1:A:484:PRO:HA	1:A:487:LEU:HB2	1.94	0.50
1:B:443:ARG:CZ	1:B:447:SER:HB2	2.41	0.50
1:A:258:LYS:HZ2	1:A:260:LYS:HD3	1.76	0.50
1:B:364:GLU:C	1:B:364:GLU:CD	2.79	0.50
1:A:113:PHE:CD1	1:A:113:PHE:C	2.89	0.50
1:A:289:VAL:O	1:A:292:VAL:HG22	2.11	0.50
1:B:436:LEU:HB3	1:B:437:PHE:CZ	2.47	0.50
1:A:175:ILE:HA	1:A:416:PHE:CE1	2.46	0.50
1:A:382:ARG:HA	1:A:385:ASN:HD21	1.76	0.50
1:A:488:LEU:HD13	1:A:489:LEU:N	2.25	0.50
1:B:81:GLU:HB3	1:B:350:PRO:CD	2.42	0.50
1:B:136:CYS:SG	1:B:345:GLY:HA3	2.52	0.50
1:B:289:VAL:O	1:B:292:VAL:HG22	2.11	0.50
1:A:497:PHE:CG	1:A:498:THR:N	2.80	0.49
1:B:255:ASN:HA	1:B:259:PHE:CE2	2.47	0.49
1:B:497:PHE:O	1:B:497:PHE:CG	2.65	0.49
1:A:134:TRP:CD1	1:A:295:ALA:CB	2.94	0.49
1:A:435:PHE:N	1:A:435:PHE:CD1	2.75	0.49
1:B:319:ARG:HG2	1:B:322:TYR:CD2	2.48	0.49
1:A:307:TYR:CG	1:A:308:PHE:N	2.80	0.49
1:A:356:ILE:HB	1:A:357:PRO:HD3	1.93	0.49
1:B:319:ARG:CG	1:B:322:TYR:CG	2.95	0.49
1:A:154:LEU:O	1:A:157:TYR:CD2	2.65	0.49
1:A:262:LEU:HD11	1:A:407:ILE:HB	1.93	0.49
1:A:359:ALA:O	1:A:362:HIS:CG	2.66	0.49
1:B:175:ILE:HA	1:B:416:PHE:CE1	2.48	0.49
1:A:244:TRP:CZ3	1:A:247:PHE:CE1	3.00	0.49
1:A:428:VAL:HA	1:A:431:HIS:HD1	1.78	0.49
1:B:432:ARG:NH2	1:B:449:LEU:HD22	2.28	0.49
1:B:484:PRO:HA	1:B:487:LEU:HB3	1.95	0.49
1:A:166:PHE:O	1:A:169:PHE:HB3	2.13	0.49
1:A:25:TRP:CE3	1:A:25:TRP:N	2.80	0.49
1:B:397:THR:HA	1:B:400:LEU:HB2	1.94	0.49
1:A:131:PHE:HA	1:A:134:TRP:CE2	2.48	0.49
1:A:218:PHE:HA	1:A:222:PRO:HA	1.94	0.49
1:B:443:ARG:HH22	1:B:451:LYS:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASN:O	1:A:117:VAL:HB	2.13	0.48
1:B:32:ILE:N	1:B:33:PRO:HD2	2.28	0.48
1:B:104:VAL:HG22	1:B:354:GLY:HA2	1.93	0.48
1:B:290:LYS:HA	1:B:293:PHE:CE2	2.48	0.48
1:B:426:THR:O	1:B:428:VAL:HG23	2.14	0.48
1:B:483:PHE:CE1	1:B:484:PRO:HG3	2.49	0.48
1:A:359:ALA:HA	1:A:362:HIS:NE2	2.28	0.48
1:A:364:GLU:HA	1:A:367:LEU:HB2	1.95	0.48
1:B:455:ARG:HA	1:B:455:ARG:CZ	2.43	0.48
1:A:432:ARG:HH21	1:A:449:LEU:HG	1.77	0.48
1:B:428:VAL:O	1:B:432:ARG:N	2.43	0.48
1:A:140:MET:HA	1:A:143:HIS:CE1	2.48	0.48
1:A:368:VAL:CG2	1:A:376:VAL:H	2.27	0.48
1:B:161:PHE:O	1:B:165:ILE:HG13	2.14	0.48
1:B:377:ARG:CZ	1:B:378:CYS:O	2.62	0.48
1:A:498:THR:HG23	1:A:499:TYR:CD1	2.49	0.48
1:B:157:TYR:CD1	1:B:157:TYR:N	2.76	0.48
1:A:226:HIS:CE1	1:A:372:ASN:O	2.67	0.48
1:B:68:ASP:C	1:B:72:ARG:HE	2.22	0.48
1:B:431:HIS:O	1:B:434:VAL:HB	2.13	0.48
1:A:161:PHE:CE2	1:A:491:VAL:HG12	2.49	0.48
1:B:155:LEU:CD1	1:B:155:LEU:H	2.27	0.48
1:A:274:PHE:CD1	1:A:276:ARG:HB2	2.48	0.48
1:A:447:SER:HB3	1:A:448:PRO:HD3	1.96	0.48
1:A:468:PHE:CE1	1:A:472:PHE:HB2	2.49	0.48
1:B:199:PHE:O	1:B:202:VAL:HB	2.13	0.48
1:A:119:GLU:OE2	1:A:120:ILE:HG23	2.13	0.47
1:A:143:HIS:CE1	1:A:335:ALA:O	2.67	0.47
1:A:300:ILE:HG13	1:A:301:ILE:HG23	1.96	0.47
1:A:424:LEU:HB2	1:A:425:MET:SD	2.54	0.47
1:B:356:ILE:CB	1:B:357:PRO:HD3	2.44	0.47
1:B:153:CYS:SG	1:B:154:LEU:HD13	2.53	0.47
1:B:42:ALA:O	1:B:47:VAL:HG21	2.14	0.47
1:B:153:CYS:SG	1:B:154:LEU:CD1	3.02	0.47
1:A:482:GLY:C	1:A:484:PRO:HD2	2.38	0.47
1:B:38:ASP:HB2	1:B:39:TRP:CH2	2.49	0.47
1:A:47:VAL:O	1:A:51:THR:HG23	2.15	0.47
1:A:223:LEU:N	1:A:229:ARG:HH12	2.09	0.47
1:A:321:GLN:CD	1:A:322:TYR:CE1	2.93	0.47
1:B:114:ASN:HA	1:B:117:VAL:HB	1.95	0.47
1:B:169:PHE:CZ	1:B:483:PHE:CD1	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:THR:HA	1:B:255:ASN:CG	2.39	0.47
1:B:261:LYS:HA	1:B:408:PRO:HA	1.96	0.47
1:A:369:ARG:O	1:A:369:ARG:HG2	2.14	0.47
1:B:226:HIS:HA	1:B:229:ARG:HE	1.79	0.47
1:B:241:VAL:HG23	1:B:242:LEU:HG	1.95	0.47
1:B:485:LEU:HG	1:B:486:VAL:N	2.29	0.47
1:A:36:LYS:C	1:A:39:TRP:HE1	2.23	0.47
1:A:430:ILE:O	1:A:433:ILE:HB	2.15	0.47
1:A:459:ILE:O	1:A:463:PHE:CD1	2.68	0.47
1:B:38:ASP:CB	1:B:382:ARG:H	2.27	0.47
1:B:61:PRO:O	1:B:64:ALA:HB3	2.15	0.47
1:B:157:TYR:CD2	1:B:492:ILE:HG22	2.49	0.47
1:B:307:TYR:CG	1:B:308:PHE:N	2.83	0.47
1:B:356:ILE:H	1:B:356:ILE:HD12	1.78	0.47
1:A:168:LEU:C	1:A:168:LEU:HD13	2.40	0.47
1:A:218:PHE:HD1	1:A:222:PRO:C	2.23	0.47
1:A:431:HIS:O	1:A:435:PHE:CD1	2.67	0.47
1:A:485:LEU:HD22	1:A:488:LEU:HD12	1.97	0.47
1:B:46:ARG:C	1:B:49:PRO:HD2	2.39	0.47
1:B:110:ILE:O	1:B:113:PHE:HB3	2.15	0.47
1:B:118:TYR:CE1	1:B:128:TYR:CE1	3.02	0.47
1:A:31:ARG:NH1	1:A:328:SER:HB2	2.30	0.47
1:A:369:ARG:O	1:A:370:ASP:CG	2.58	0.47
1:B:104:VAL:HG13	1:B:353:ASN:N	2.30	0.47
1:B:209:THR:HG21	1:B:417:PHE:HB3	1.97	0.47
1:B:316:MET:SD	1:B:319:ARG:HD2	2.55	0.47
1:A:312:VAL:HG23	1:A:313:SER:N	2.29	0.46
1:A:364:GLU:O	1:A:367:LEU:HB2	2.14	0.46
1:B:38:ASP:HB2	1:B:39:TRP:CE2	2.51	0.46
1:B:186:PHE:CD1	1:B:186:PHE:C	2.93	0.46
1:A:226:HIS:CG	1:A:371:SER:HA	2.50	0.46
1:A:244:TRP:CE2	1:A:247:PHE:HB2	2.50	0.46
1:B:439:ASP:OD2	1:B:441:LYS:HG2	2.15	0.46
1:A:143:HIS:NE2	1:A:338:GLY:C	2.72	0.46
1:A:358:GLN:CD	1:A:359:ALA:N	2.74	0.46
1:B:68:ASP:HB2	1:B:72:ARG:HE	1.81	0.46
1:B:140:MET:HB2	1:B:342:CYS:SG	2.55	0.46
1:B:319:ARG:O	1:B:322:TYR:C	2.59	0.46
1:B:391:MET:SD	1:B:391:MET:N	2.89	0.46
1:B:51:THR:HG23	1:B:384:THR:HA	1.97	0.46
1:B:54:THR:HB	1:B:388:GLN:HE22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:MET:SD	1:B:338:GLY:O	2.74	0.46
1:B:443:ARG:HH22	1:B:451:LYS:CD	2.29	0.46
1:B:128:TYR:CZ	1:B:132:MET:SD	3.08	0.46
1:B:218:PHE:CD1	1:B:223:LEU:CB	2.96	0.46
1:B:223:LEU:HB3	1:B:224:PHE:CE2	2.51	0.46
1:B:443:ARG:NH2	1:B:451:LYS:HD3	2.30	0.46
1:A:297:PRO:HA	1:A:300:ILE:HG23	1.97	0.46
1:A:431:HIS:O	1:A:434:VAL:HB	2.16	0.46
1:B:277:PRO:CD	1:B:278:GLN:H	2.29	0.46
1:B:395:THR:O	1:B:397:THR:HG23	2.16	0.46
1:B:128:TYR:O	1:B:132:MET:SD	2.74	0.46
1:B:323:LYS:HE2	1:B:375:VAL:HG11	1.98	0.46
1:B:367:LEU:HD21	1:B:375:VAL:HG13	1.98	0.46
1:A:147:ALA:HB2	1:A:335:ALA:HB2	1.98	0.46
1:A:186:PHE:CD1	1:A:197:ASP:HA	2.51	0.46
1:A:390:LEU:O	1:A:391:MET:C	2.58	0.46
1:A:483:PHE:CD2	1:A:484:PRO:HD3	2.50	0.46
1:B:38:ASP:HB2	1:B:39:TRP:CZ2	2.51	0.46
1:B:175:ILE:O	1:B:179:ILE:HG13	2.16	0.46
1:B:377:ARG:HH11	1:B:377:ARG:HB2	1.80	0.46
1:B:459:ILE:O	1:B:463:PHE:CE1	2.69	0.46
1:A:77:TYR:HA	1:A:81:GLU:HG3	1.98	0.46
1:A:161:PHE:CE2	1:A:491:VAL:HA	2.51	0.46
1:A:199:PHE:CE2	1:B:195:VAL:HB	2.51	0.46
1:A:227:LYS:HA	1:A:230:THR:HG22	1.98	0.46
1:B:273:LYS:O	1:B:274:PHE:CG	2.68	0.46
1:B:366:LEU:HD22	1:B:381:GLN:HE22	1.81	0.46
1:A:304:ILE:HA	1:A:307:TYR:HD2	1.81	0.45
1:B:36:LYS:HA	1:B:39:TRP:HE1	1.81	0.45
1:B:60:LEU:O	1:B:63:ILE:HB	2.16	0.45
1:B:129:PHE:CD1	1:B:273:LYS:HB3	2.51	0.45
1:B:170:ILE:O	1:B:174:TYR:CG	2.69	0.45
1:B:175:ILE:HG22	1:B:416:PHE:HE1	1.81	0.45
1:B:492:ILE:HG13	1:B:493:VAL:HG13	1.98	0.45
1:A:27:ASP:OD2	1:A:331:HIS:CD2	2.70	0.45
1:A:481:ILE:O	1:A:484:PRO:HD3	2.16	0.45
1:B:35:TYR:O	1:B:39:TRP:CZ2	2.70	0.45
1:A:330:PHE:CD1	1:A:330:PHE:N	2.81	0.45
1:B:59:LEU:O	1:B:62:ALA:HB3	2.16	0.45
1:A:165:ILE:O	1:A:168:LEU:HB3	2.17	0.45
1:A:180:GLN:O	1:A:180:GLN:CD	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:HIS:O	1:A:435:PHE:CE1	2.69	0.45
1:B:38:ASP:OD2	1:B:382:ARG:HB2	2.16	0.45
1:B:319:ARG:HD3	1:B:322:TYR:CD2	2.52	0.45
1:A:280:THR:CA	1:A:347:LEU:HA	2.46	0.45
1:A:324:LEU:HD13	1:A:377:ARG:NH2	2.32	0.45
1:B:257:VAL:O	1:B:259:PHE:CD2	2.70	0.45
1:B:283:ALA:O	1:B:284:TYR:CD1	2.70	0.45
1:A:157:TYR:N	1:A:157:TYR:CD1	2.78	0.45
1:A:323:LYS:O	1:A:324:LEU:HG	2.16	0.45
1:A:356:ILE:O	1:A:359:ALA:HB3	2.17	0.45
1:B:126:THR:CG2	1:B:127:SER:H	2.27	0.45
1:B:443:ARG:HH21	1:B:448:PRO:HG3	1.82	0.45
1:A:141:ILE:HG13	1:A:142:PHE:CG	2.52	0.45
1:A:349:ILE:HG23	1:A:350:PRO:HD2	1.99	0.45
1:B:55:TYR:CE2	1:B:393:LEU:HB3	2.52	0.45
1:B:103:ILE:HB	1:B:355:LEU:HD12	1.99	0.45
1:B:443:ARG:HH22	1:B:451:LYS:HD3	1.81	0.45
1:B:490:SER:O	1:B:493:VAL:HG22	2.17	0.45
1:A:218:PHE:CE1	1:A:223:LEU:HB2	2.52	0.45
1:B:115:TYR:O	1:B:119:GLU:CD	2.60	0.45
1:A:99:GLN:C	1:A:102:CYS:SG	3.00	0.45
1:A:144:LEU:HG	1:A:145:LEU:N	2.30	0.45
1:A:455:ARG:NE	1:A:455:ARG:H	2.14	0.45
1:B:114:ASN:O	1:B:117:VAL:HB	2.17	0.45
1:B:140:MET:SD	1:B:338:GLY:C	3.00	0.45
1:B:155:LEU:C	1:B:157:TYR:H	2.24	0.45
1:B:323:LYS:CE	1:B:375:VAL:HG11	2.47	0.45
1:A:34:TYR:CZ	1:A:327:PRO:HG2	2.52	0.44
1:A:186:PHE:CD1	1:A:186:PHE:N	2.77	0.44
1:B:53:ASP:O	1:B:57:ASN:CG	2.60	0.44
1:B:208:MET:SD	1:B:414:GLY:HA3	2.57	0.44
1:B:310:HIS:CG	1:B:337:LEU:HD22	2.51	0.44
1:A:25:TRP:HA	1:A:25:TRP:CZ2	2.52	0.44
1:A:425:MET:O	1:A:431:HIS:CE1	2.70	0.44
1:B:155:LEU:CD1	1:B:155:LEU:N	2.81	0.44
1:A:59:LEU:O	1:A:62:ALA:HB3	2.18	0.44
1:A:224:PHE:CD1	1:A:225:THR:HG23	2.52	0.44
1:A:234:ASP:OD2	1:A:235:TYR:CD1	2.69	0.44
1:A:436:LEU:CD2	1:A:437:PHE:CZ	3.00	0.44
1:A:493:VAL:HA	1:A:495:PHE:CZ	2.53	0.44
1:B:77:TYR:CE1	1:B:269:PHE:CE2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:O	1:B:85:SER:HB2	2.18	0.44
1:B:166:PHE:CZ	1:B:312:VAL:HG21	2.52	0.44
1:B:432:ARG:HH21	1:B:449:LEU:CD1	2.30	0.44
1:A:319:ARG:CZ	1:A:322:TYR:CE2	3.01	0.44
1:A:472:PHE:CD2	1:A:472:PHE:C	2.95	0.44
1:B:208:MET:SD	1:B:414:GLY:C	3.01	0.44
1:B:257:VAL:H	1:B:259:PHE:HE2	1.65	0.44
1:B:274:PHE:CZ	1:B:285:GLU:OE2	2.71	0.44
1:B:460:PHE:O	1:B:460:PHE:CD1	2.70	0.44
1:B:489:LEU:O	1:B:492:ILE:HG12	2.18	0.44
1:A:60:LEU:O	1:A:63:ILE:HB	2.18	0.44
1:A:363:THR:O	1:A:366:LEU:C	2.61	0.44
1:A:463:PHE:CD1	1:A:463:PHE:N	2.83	0.44
1:A:497:PHE:CD2	1:A:497:PHE:C	2.95	0.44
1:B:24:ILE:HD12	1:B:148:PHE:CE1	2.53	0.44
1:A:147:ALA:O	1:A:331:HIS:CE1	2.71	0.44
1:A:288:PRO:HB2	1:A:290:LYS:HB3	2.00	0.44
1:A:326:LYS:HB3	1:A:327:PRO:HD3	1.99	0.44
1:B:55:TYR:HA	1:B:58:ASN:HD21	1.82	0.44
1:B:138:TRP:O	1:B:142:PHE:CD2	2.70	0.44
1:B:198:GLY:O	1:B:202:VAL:N	2.50	0.44
1:B:402:VAL:O	1:B:406:GLU:HG3	2.17	0.44
1:B:57:ASN:O	1:B:61:PRO:HD2	2.18	0.44
1:B:161:PHE:CD2	1:B:491:VAL:HA	2.53	0.44
1:B:211:PHE:CD1	1:B:211:PHE:N	2.85	0.44
1:B:487:LEU:O	1:B:491:VAL:HG22	2.18	0.44
1:A:150:ASN:HD22	1:A:152:VAL:HG22	1.82	0.44
1:A:166:PHE:CE1	1:A:312:VAL:HG21	2.53	0.44
1:A:319:ARG:HB3	1:A:322:TYR:HB2	2.00	0.44
1:B:55:TYR:HA	1:B:58:ASN:ND2	2.33	0.44
1:B:289:VAL:HG23	1:B:290:LYS:N	2.33	0.44
1:B:460:PHE:CD2	1:B:463:PHE:CE2	3.06	0.44
1:A:171:ASN:O	1:A:174:TYR:HB2	2.18	0.43
1:A:280:THR:CB	1:A:347:LEU:HA	2.48	0.43
1:B:82:VAL:C	1:B:85:SER:H	2.26	0.43
1:B:218:PHE:HD1	1:B:222:PRO:C	2.26	0.43
1:B:225:THR:O	1:B:229:ARG:HB3	2.18	0.43
1:B:468:PHE:O	1:B:471:GLU:OE1	2.36	0.43
1:A:211:PHE:CD1	1:A:211:PHE:N	2.82	0.43
1:A:224:PHE:CD1	1:B:437:PHE:O	2.71	0.43
1:A:298:PHE:CD1	1:A:298:PHE:N	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:PHE:CD1	1:A:484:PRO:N	2.86	0.43
1:B:140:MET:O	1:B:143:HIS:HB3	2.17	0.43
1:B:322:TYR:N	1:B:322:TYR:CD1	2.79	0.43
1:B:61:PRO:C	1:B:64:ALA:H	2.26	0.43
1:B:105:GLY:H	1:B:355:LEU:HG	1.82	0.43
1:B:208:MET:SD	1:B:414:GLY:CA	3.07	0.43
1:B:484:PRO:HA	1:B:487:LEU:CB	2.49	0.43
1:A:305:LEU:O	1:A:308:PHE:HB2	2.19	0.43
1:A:459:ILE:HG22	1:A:463:PHE:CZ	2.54	0.43
1:B:105:GLY:N	1:B:353:ASN:O	2.51	0.43
1:B:151:VAL:O	1:B:154:LEU:HB2	2.18	0.43
1:B:170:ILE:O	1:B:174:TYR:CD1	2.71	0.43
1:B:183:THR:O	1:B:187:HIS:CG	2.71	0.43
1:B:280:THR:HG22	1:B:281:TRP:N	2.32	0.43
1:B:293:PHE:O	1:B:296:LEU:HB3	2.19	0.43
1:B:304:ILE:O	1:B:308:PHE:CG	2.71	0.43
1:B:181:ILE:HG23	1:B:184:ARG:HH12	1.83	0.43
1:B:229:ARG:HG2	1:B:229:ARG:HH11	1.84	0.43
1:B:356:ILE:CB	1:B:357:PRO:CD	2.95	0.43
1:B:430:ILE:C	1:B:433:ILE:HB	2.43	0.43
1:A:107:THR:HG23	1:A:110:ILE:H	1.83	0.43
1:A:285:GLU:N	1:A:286:PRO:HD3	2.32	0.43
1:B:260:LYS:O	1:B:408:PRO:HA	2.18	0.43
1:B:324:LEU:HD21	1:B:380:GLU:OE2	2.19	0.43
1:B:134:TRP:HA	1:B:134:TRP:CE3	2.53	0.43
1:B:161:PHE:CE2	1:B:491:VAL:HA	2.54	0.43
1:B:163:CYS:SG	1:B:316:MET:HB2	2.58	0.43
1:A:31:ARG:HH21	1:A:97:ALA:C	2.27	0.43
1:B:31:ARG:NH2	1:B:327:PRO:C	2.77	0.43
1:B:39:TRP:CH2	1:B:382:ARG:HB2	2.53	0.43
1:B:91:ILE:HG12	1:B:390:LEU:HA	2.01	0.43
1:B:134:TRP:HB3	1:B:138:TRP:CE2	2.54	0.43
1:B:267:SER:C	1:B:398:ARG:HH21	2.26	0.43
1:B:267:SER:HA	1:B:398:ARG:HH21	1.84	0.43
1:B:287:ILE:HG23	1:B:288:PRO:HD2	2.01	0.43
1:B:297:PRO:HD2	1:B:298:PHE:CD2	2.53	0.43
1:B:374:ASN:O	1:B:376:VAL:HG23	2.19	0.43
1:B:423:GLY:H	1:B:425:MET:HB2	1.83	0.43
1:A:169:PHE:CD1	1:A:483:PHE:CD1	3.07	0.43
1:A:216:LYS:O	1:A:219:HIS:CG	2.72	0.43
1:A:224:PHE:CG	1:B:437:PHE:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LYS:HZ1	1:A:377:ARG:HH11	1.65	0.43
1:B:135:ILE:HA	1:B:138:TRP:NE1	2.33	0.43
1:B:154:LEU:O	1:B:157:TYR:CG	2.72	0.43
1:B:207:VAL:HG13	1:B:211:PHE:CE2	2.54	0.43
1:A:32:ILE:HA	1:A:35:TYR:HB2	2.01	0.43
1:A:46:ARG:HH11	1:A:366:LEU:C	2.27	0.43
1:A:105:GLY:C	1:A:352:PRO:HA	2.44	0.43
1:A:139:SER:O	1:A:143:HIS:CG	2.72	0.43
1:A:234:ASP:C	1:A:236:SER:H	2.27	0.43
1:A:319:ARG:HB3	1:A:322:TYR:H	1.83	0.43
1:A:324:LEU:HD21	1:A:377:ARG:NE	2.34	0.43
1:A:399:PRO:C	1:A:401:LEU:H	2.27	0.43
1:B:290:LYS:HA	1:B:293:PHE:CD2	2.53	0.43
1:A:132:MET:SD	1:A:136:CYS:SG	3.17	0.42
1:A:368:VAL:HG21	1:A:376:VAL:N	2.34	0.42
1:A:391:MET:N	1:A:391:MET:SD	2.91	0.42
1:A:493:VAL:O	1:A:495:PHE:CD1	2.72	0.42
1:B:106:VAL:HG12	1:B:107:THR:H	1.83	0.42
1:B:391:MET:SD	1:B:391:MET:O	2.77	0.42
1:B:483:PHE:CG	1:B:484:PRO:N	2.87	0.42
1:A:120:ILE:HD11	1:A:298:PHE:CZ	2.54	0.42
1:A:150:ASN:O	1:A:153:CYS:HB2	2.19	0.42
1:A:238:ALA:HA	1:A:241:VAL:HG22	2.01	0.42
1:A:324:LEU:CD1	1:A:377:ARG:HH21	2.32	0.42
1:A:384:THR:HG23	1:A:385:ASN:N	2.34	0.42
1:A:453:SER:HA	1:A:455:ARG:CZ	2.49	0.42
1:B:211:PHE:HA	1:B:214:PHE:CE2	2.54	0.42
1:A:46:ARG:NH1	1:A:368:VAL:HG22	2.34	0.42
1:A:324:LEU:HD22	1:A:326:LYS:HB2	2.00	0.42
1:B:118:TYR:CE2	1:B:128:TYR:CZ	3.07	0.42
1:B:262:LEU:HG	1:B:405:GLY:HA2	2.01	0.42
1:A:133:PHE:CE2	1:A:285:GLU:OE2	2.72	0.42
1:B:73:THR:C	1:B:75:ASN:N	2.73	0.42
1:B:180:GLN:HA	1:B:183:THR:OG1	2.19	0.42
1:B:200:ALA:O	1:B:204:VAL:HG23	2.20	0.42
1:A:244:TRP:CE3	1:A:244:TRP:HA	2.55	0.42
1:A:468:PHE:CD1	1:A:468:PHE:C	2.96	0.42
1:A:361:LEU:C	1:A:364:GLU:H	2.28	0.42
1:B:25:TRP:HE3	1:B:26:LEU:HD21	1.84	0.42
1:B:25:TRP:CE3	1:B:26:LEU:HD21	2.54	0.42
1:B:226:HIS:O	1:B:229:ARG:CZ	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:C	1:A:157:TYR:H	2.27	0.42
1:A:359:ALA:N	1:A:360:PRO:HD2	2.34	0.42
1:A:459:ILE:HG22	1:A:463:PHE:HE1	1.78	0.42
1:B:30:ASP:HB2	1:B:31:ARG:HH11	1.85	0.42
1:B:79:VAL:HB	1:B:264:ILE:HD13	2.01	0.42
1:B:152:VAL:CA	1:B:155:LEU:HD13	2.50	0.42
1:B:396:MET:SD	1:B:399:PRO:HD2	2.60	0.42
1:A:168:LEU:O	1:A:172:VAL:HG23	2.20	0.42
1:B:204:VAL:O	1:B:208:MET:HB3	2.19	0.42
1:B:260:LYS:HB3	1:B:409:GLN:CB	2.49	0.42
1:A:33:PRO:HA	1:A:36:LYS:HD2	2.02	0.42
1:A:166:PHE:CD1	1:A:166:PHE:C	2.98	0.42
1:B:25:TRP:O	1:B:29:LYS:HG3	2.20	0.42
1:B:226:HIS:CG	1:B:229:ARG:HH21	2.37	0.42
1:B:244:TRP:O	1:B:244:TRP:CD1	2.72	0.42
1:A:153:CYS:HA	1:A:156:GLN:CD	2.45	0.41
1:A:169:PHE:CE2	1:A:483:PHE:CZ	3.08	0.41
1:A:208:MET:HA	1:A:211:PHE:CD2	2.55	0.41
1:A:355:LEU:C	1:A:358:GLN:HE22	2.27	0.41
1:A:397:THR:HA	1:A:400:LEU:HB3	2.02	0.41
1:B:287:ILE:HG23	1:B:288:PRO:N	2.35	0.41
1:B:401:LEU:HA	1:B:404:LEU:HD12	2.01	0.41
1:B:447:SER:N	1:B:448:PRO:CD	2.83	0.41
1:A:200:ALA:O	1:A:203:VAL:HB	2.20	0.41
1:A:428:VAL:O	1:A:431:HIS:HB2	2.20	0.41
1:A:431:HIS:CD2	1:A:431:HIS:H	2.28	0.41
1:B:97:ALA:HB1	1:B:382:ARG:HE	1.85	0.41
1:B:305:LEU:O	1:B:309:ASP:CG	2.62	0.41
1:A:31:ARG:HH22	1:A:100:PRO:HG3	1.85	0.41
1:A:213:LEU:HG	1:A:214:PHE:CE1	2.55	0.41
1:A:262:LEU:HG	1:A:407:ILE:O	2.20	0.41
1:A:311:ASN:N	1:A:311:ASN:HD22	2.17	0.41
1:B:68:ASP:OD2	1:B:72:ARG:NH2	2.54	0.41
1:B:244:TRP:CD1	1:B:244:TRP:C	2.96	0.41
1:B:355:LEU:C	1:B:358:GLN:HG2	2.45	0.41
1:B:440:PRO:C	1:B:442:ARG:H	2.27	0.41
1:A:80:ASN:HA	1:A:83:LEU:HB3	2.02	0.41
1:A:198:GLY:C	1:A:201:SER:H	2.28	0.41
1:B:415:LEU:O	1:B:416:PHE:C	2.61	0.41
1:A:226:HIS:CE1	1:A:372:ASN:N	2.89	0.41
1:B:27:ASP:OD1	1:B:27:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:THR:O	1:B:110:ILE:HG22	2.20	0.41
1:B:402:VAL:HG13	1:B:403:CYS:N	2.35	0.41
1:A:105:GLY:HA2	1:A:352:PRO:HA	2.02	0.41
1:A:164:ASP:HA	1:A:316:MET:SD	2.60	0.41
1:A:176:GLN:CD	1:A:176:GLN:C	2.89	0.41
1:A:357:PRO:C	1:A:360:PRO:HD2	2.46	0.41
1:B:277:PRO:HB2	1:B:278:GLN:OE1	2.21	0.41
1:B:356:ILE:O	1:B:360:PRO:HD2	2.21	0.41
1:B:484:PRO:C	1:B:487:LEU:H	2.28	0.41
1:A:101:LEU:HD21	1:A:380:GLU:HB2	2.02	0.41
1:A:163:CYS:C	1:A:316:MET:SD	3.03	0.41
1:A:274:PHE:CG	1:A:276:ARG:HB2	2.56	0.41
1:A:324:LEU:HD22	1:A:326:LYS:CG	2.51	0.41
1:A:416:PHE:CE1	1:A:416:PHE:O	2.74	0.41
1:A:428:VAL:O	1:A:432:ARG:N	2.51	0.41
1:A:499:TYR:CD1	1:A:499:TYR:N	2.86	0.41
1:B:64:ALA:O	1:B:68:ASP:OD1	2.38	0.41
1:B:206:LEU:C	1:B:209:THR:H	2.29	0.41
1:B:292:VAL:HG22	1:B:293:PHE:CE1	2.55	0.41
1:B:326:LYS:HD2	1:B:378:CYS:HB3	2.02	0.41
1:B:481:ILE:O	1:B:484:PRO:HD3	2.20	0.41
1:A:34:TYR:O	1:A:38:ASP:OD1	2.39	0.41
1:A:169:PHE:CE1	1:A:483:PHE:CG	3.09	0.41
1:B:118:TYR:CZ	1:B:128:TYR:CE1	3.08	0.41
1:B:143:HIS:ND1	1:B:338:GLY:HA3	2.34	0.41
1:B:339:LEU:O	1:B:342:CYS:HB3	2.21	0.41
1:B:425:MET:SD	1:B:425:MET:N	2.94	0.41
1:B:427:ASN:O	1:B:430:ILE:HB	2.21	0.41
1:A:261:LYS:C	1:A:262:LEU:HG	2.46	0.41
1:A:321:GLN:HG3	1:A:322:TYR:CD1	2.55	0.41
1:A:323:LYS:O	1:A:324:LEU:HD23	2.21	0.41
1:A:485:LEU:HD13	1:A:485:LEU:C	2.45	0.41
1:A:493:VAL:C	1:A:495:PHE:N	2.75	0.41
1:B:55:TYR:CZ	1:B:393:LEU:HB3	2.56	0.41
1:B:141:ILE:O	1:B:144:LEU:HB3	2.20	0.41
1:B:263:PRO:C	1:B:264:ILE:HG22	2.46	0.41
1:B:324:LEU:HD22	1:B:324:LEU:HA	1.91	0.41
1:B:430:ILE:HG22	1:B:434:VAL:HG23	2.02	0.41
1:A:255:ASN:C	1:A:256:ASP:CG	2.89	0.41
1:A:270:PRO:HB3	1:A:274:PHE:HB3	2.03	0.41
1:A:492:ILE:O	1:A:495:PHE:CD2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:HA	1:A:495:PHE:CE1	2.56	0.41
1:B:33:PRO:HG2	1:B:34:TYR:CD1	2.55	0.41
1:B:297:PRO:HB2	1:B:298:PHE:CD1	2.56	0.41
1:B:457:MET:O	1:B:461:LEU:HG	2.21	0.41
1:A:61:PRO:C	1:A:64:ALA:H	2.29	0.40
1:A:88:MET:O	1:A:92:VAL:HG22	2.21	0.40
1:A:180:GLN:CD	1:A:180:GLN:C	2.89	0.40
1:A:296:LEU:HB3	1:A:297:PRO:HD3	2.03	0.40
1:B:169:PHE:CE1	1:B:483:PHE:CE1	3.09	0.40
1:B:358:GLN:OE1	1:B:358:GLN:CA	2.69	0.40
1:B:369:ARG:HA	1:B:374:ASN:C	2.46	0.40
1:B:487:LEU:O	1:B:491:VAL:HG13	2.21	0.40
1:A:168:LEU:HA	1:A:171:ASN:CG	2.46	0.40
1:A:199:PHE:CD2	1:B:195:VAL:HB	2.56	0.40
1:A:307:TYR:O	1:A:310:HIS:HB3	2.20	0.40
1:A:368:VAL:HG21	1:A:376:VAL:O	2.21	0.40
1:A:483:PHE:CG	1:A:484:PRO:HD3	2.56	0.40
1:A:483:PHE:HA	1:A:486:VAL:HB	2.03	0.40
1:B:263:PRO:O	1:B:264:ILE:HB	2.21	0.40
1:B:369:ARG:HA	1:B:374:ASN:O	2.21	0.40
1:B:70:PHE:O	1:B:75:ASN:HA	2.21	0.40
1:B:183:THR:O	1:B:187:HIS:CD2	2.74	0.40
1:B:289:VAL:O	1:B:293:PHE:CE2	2.75	0.40
1:B:304:ILE:O	1:B:307:TYR:HB3	2.21	0.40
1:A:37:SER:HB2	1:A:41:ASP:OD2	2.21	0.40
1:A:54:THR:HA	1:A:57:ASN:ND2	2.36	0.40
1:A:203:VAL:O	1:A:207:VAL:HB	2.21	0.40
1:A:415:LEU:O	1:A:416:PHE:C	2.60	0.40
1:B:247:PHE:CZ	1:B:252:GLY:HA2	2.56	0.40
1:B:356:ILE:C	1:B:358:GLN:H	2.26	0.40
1:A:82:VAL:HA	1:A:350:PRO:HG2	2.04	0.40
1:B:110:ILE:HG12	1:B:351:ALA:HB3	2.02	0.40
1:B:122:LYS:N	1:B:123:PRO:HD2	2.36	0.40
1:B:166:PHE:CD2	1:B:487:LEU:HD23	2.56	0.40
1:B:294:ILE:O	1:B:298:PHE:CE2	2.75	0.40
1:B:440:PRO:HA	1:B:451:LYS:NZ	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/476 (100%)	408 (86%)	45 (10%)	21 (4%)	2	17
1	B	474/476 (100%)	392 (83%)	47 (10%)	35 (7%)	1	10
All	All	948/952 (100%)	800 (84%)	92 (10%)	56 (6%)	2	13

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ALA
1	A	100	PRO
1	A	102	CYS
1	A	106	VAL
1	A	190	SER
1	A	256	ASP
1	A	263	PRO
1	A	279	ASN
1	A	286	PRO
1	A	319	ARG
1	A	323	LYS
1	A	368	VAL
1	A	395	THR
1	A	444	ASP
1	B	77	TYR
1	B	106	VAL
1	B	190	SER
1	B	193	LYS
1	B	194	SER
1	B	264	ILE
1	B	319	ARG
1	B	327	PRO
1	B	371	SER
1	B	395	THR
1	B	439	ASP

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Mol	Chain	Res	Type
1	B	478	ILE
1	A	149	THR
1	A	223	LEU
1	B	127	SER
1	B	223	LEU
1	B	257	VAL
1	B	277	PRO
1	B	376	VAL
1	B	391	MET
1	B	445	ASN
1	B	251	GLY
1	B	255	ASN
1	B	261	LYS
1	B	282	LEU
1	B	323	LYS
1	B	422	ASN
1	A	127	SER
1	B	159	THR
1	B	286	PRO
1	B	381	GLN
1	A	356	ILE
1	A	478	ILE
1	B	222	PRO
1	B	276	ARG
1	B	350	PRO
1	B	356	ILE
1	B	494	SER
1	A	76	SER
1	A	222	PRO
1	B	392	ILE
1	B	349	ILE

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/424 (100%)	350 (82%)	74 (18%)	2	9
1	B	424/424 (100%)	328 (77%)	96 (23%)	1	6
All	All	848/848 (100%)	678 (80%)	170 (20%)	3	7

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	25	TRP
1	A	26	LEU
1	A	27	ASP
1	A	28	LEU
1	A	32	ILE
1	A	39	TRP
1	A	44	ASN
1	A	50	SER
1	A	63	ILE
1	A	68	ASP
1	A	75	ASN
1	A	103	ILE
1	A	111	SER
1	A	113	PHE
1	A	117	VAL
1	A	119	GLU
1	A	120	ILE
1	A	128	TYR
1	A	132	MET
1	A	134	TRP
1	A	136	CYS
1	A	144	LEU
1	A	149	THR
1	A	152	VAL
1	A	168	LEU
1	A	207	VAL
1	A	208	MET
1	A	213	LEU
1	A	222	PRO
1	A	226	HIS
1	A	229	ARG

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Mol	Chain	Res	Type
1	A	230	THR
1	A	237	THR
1	A	248	THR
1	A	256	ASP
1	A	257	VAL
1	A	263	PRO
1	A	272	SER
1	A	292	VAL
1	A	300	ILE
1	A	307	TYR
1	A	308	PHE
1	A	318	GLN
1	A	321	GLN
1	A	328	SER
1	A	331	HIS
1	A	339	LEU
1	A	353	ASN
1	A	356	ILE
1	A	358	GLN
1	A	363	THR
1	A	367	LEU
1	A	368	VAL
1	A	371	SER
1	A	380	GLU
1	A	403	CYS
1	A	411	VAL
1	A	422	ASN
1	A	424	LEU
1	A	426	THR
1	A	429	ILE
1	A	431	HIS
1	A	441	LYS
1	A	444	ASP
1	A	449	LEU
1	A	454	LYS
1	A	455	ARG
1	A	461	LEU
1	A	468	PHE
1	A	487	LEU
1	A	488	LEU
1	A	495	PHE
1	A	498	THR

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Mol	Chain	Res	Type
1	B	24	ILE
1	B	26	LEU
1	B	27	ASP
1	B	30	ASP
1	B	51	THR
1	B	65	PHE
1	B	68	ASP
1	B	74	ASP
1	B	75	ASN
1	B	79	VAL
1	B	80	ASN
1	B	96	LEU
1	B	102	CYS
1	B	103	ILE
1	B	106	VAL
1	B	109	PRO
1	B	111	SER
1	B	115	TYR
1	B	116	THR
1	B	119	GLU
1	B	121	ILE
1	B	131	PHE
1	B	134	TRP
1	B	138	TRP
1	B	145	LEU
1	B	151	VAL
1	B	155	LEU
1	B	163	CYS
1	B	165	ILE
1	B	184	ARG
1	B	197	ASP
1	B	201	SER
1	B	202	VAL
1	B	207	VAL
1	B	208	MET
1	B	213	LEU
1	B	222	PRO
1	B	223	LEU
1	B	225	THR
1	B	228	ILE
1	B	232	ILE
1	B	256	ASP

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Mol	Chain	Res	Type
1	B	266	LYS
1	B	275	ASN
1	B	280	THR
1	B	284	TYR
1	B	287	ILE
1	B	288	PRO
1	B	296	LEU
1	B	302	LEU
1	B	304	ILE
1	B	305	LEU
1	B	307	TYR
1	B	316	MET
1	B	324	LEU
1	B	327	PRO
1	B	333	ASP
1	B	339	LEU
1	B	347	LEU
1	B	349	ILE
1	B	350	PRO
1	B	358	GLN
1	B	363	THR
1	B	364	GLU
1	B	376	VAL
1	B	381	GLN
1	B	382	ARG
1	B	385	ASN
1	B	388	GLN
1	B	391	MET
1	B	392	ILE
1	B	395	THR
1	B	396	MET
1	B	397	THR
1	B	404	LEU
1	B	411	VAL
1	B	422	ASN
1	B	424	LEU
1	B	429	ILE
1	B	433	ILE
1	B	434	VAL
1	B	438	SER
1	B	441	LYS
1	B	443	ARG

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Mol	Chain	Res	Type
1	B	449	LEU
1	B	456	SER
1	B	459	ILE
1	B	464	SER
1	B	471	GLU
1	B	476	ASN
1	B	478	ILE
1	B	485	LEU
1	B	486	VAL
1	B	488	LEU
1	B	489	LEU
1	B	492	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	187	HIS
1	A	219	HIS
1	A	311	ASN
1	A	318	GLN
1	A	358	GLN
1	A	431	HIS
1	B	187	HIS
1	B	219	HIS
1	B	226	HIS
1	B	310	HIS
1	B	331	HIS
1	B	381	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8313. 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](#)

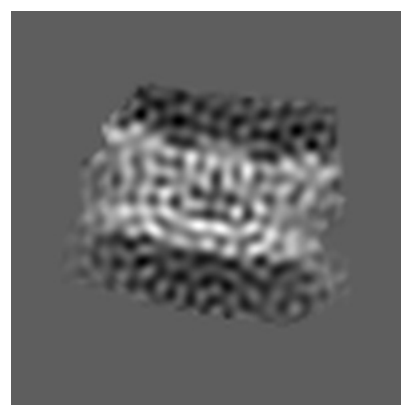
6.1.1 Primary map



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: 50



Y Index: 50



Z Index: 50

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: 39



Y Index: 46

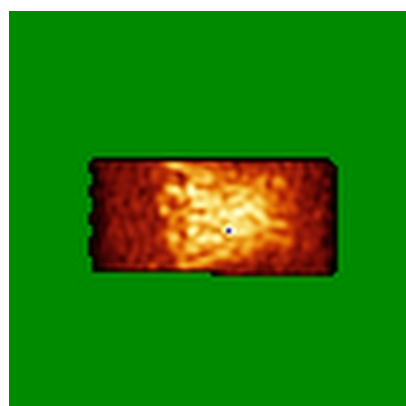


Z Index: 50

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

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

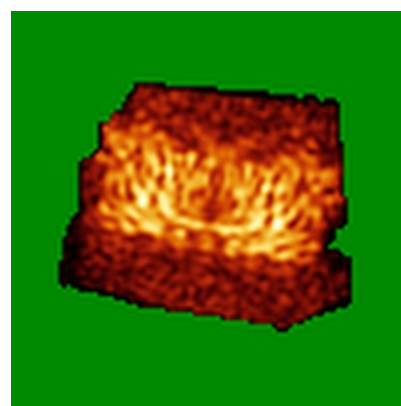
6.4.1 Primary map



X



Y

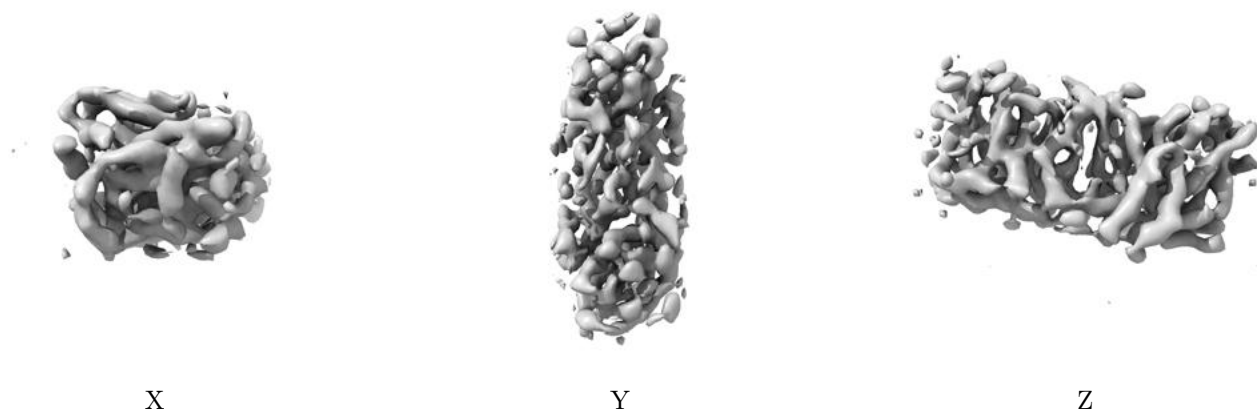


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 130.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

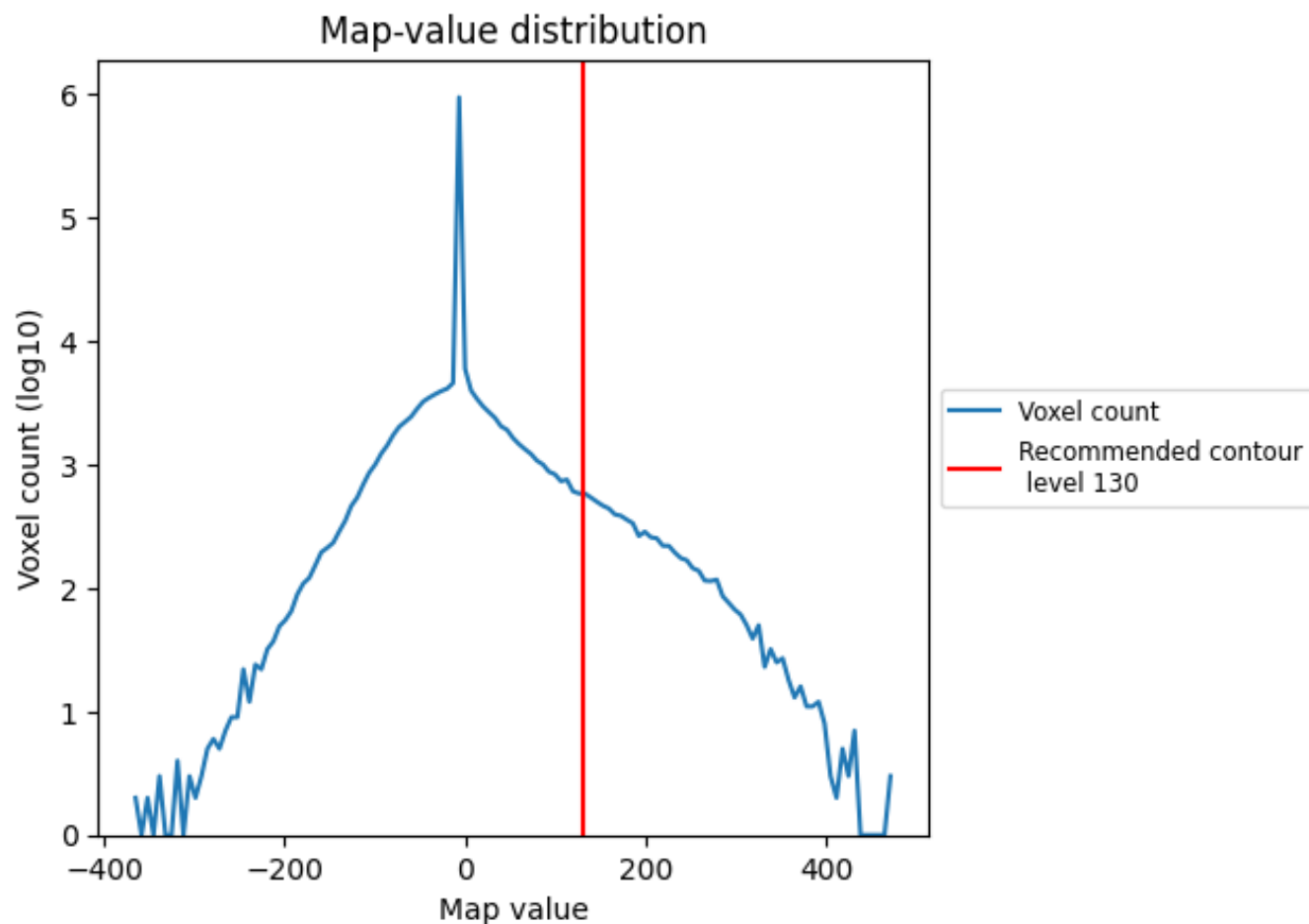
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

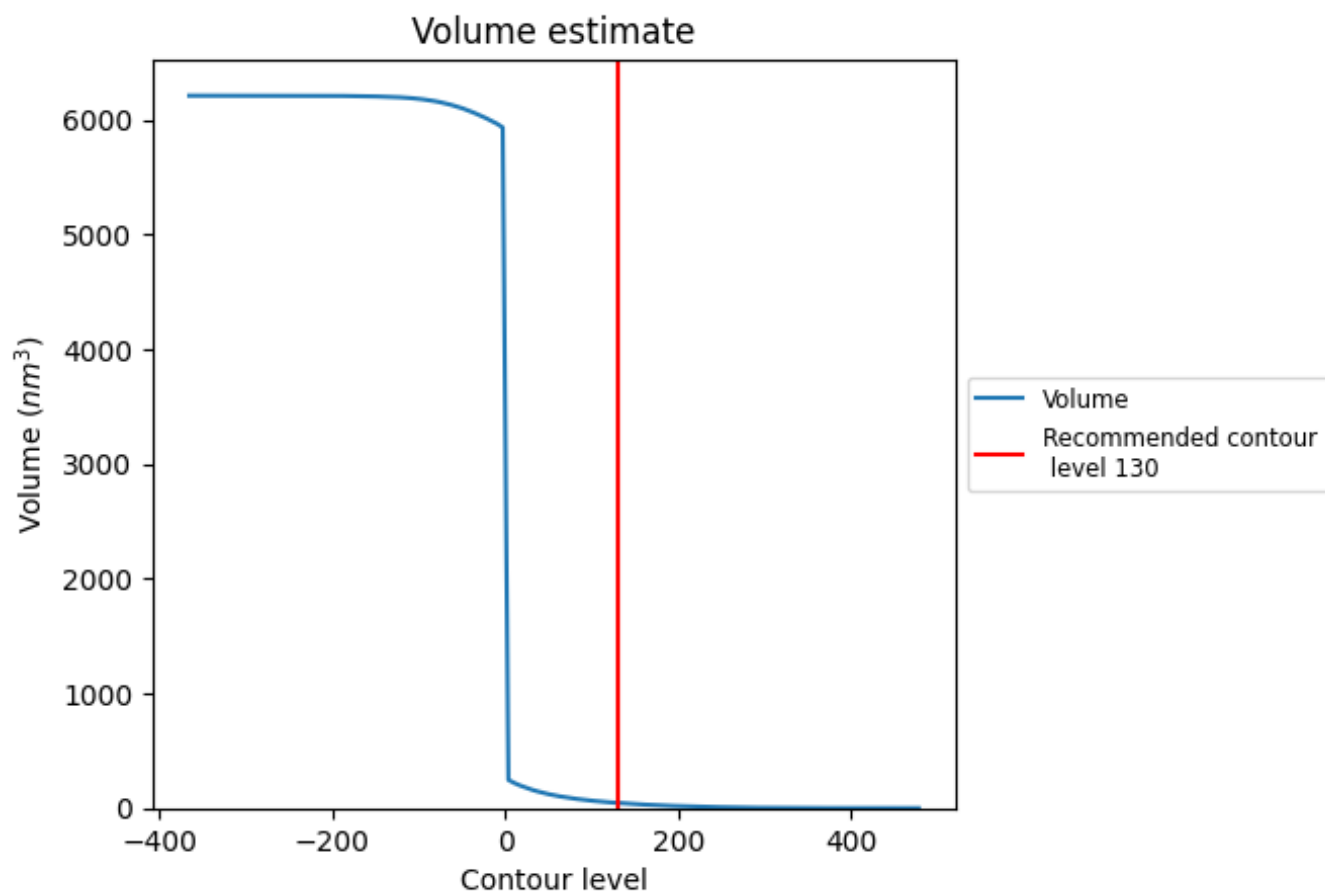
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

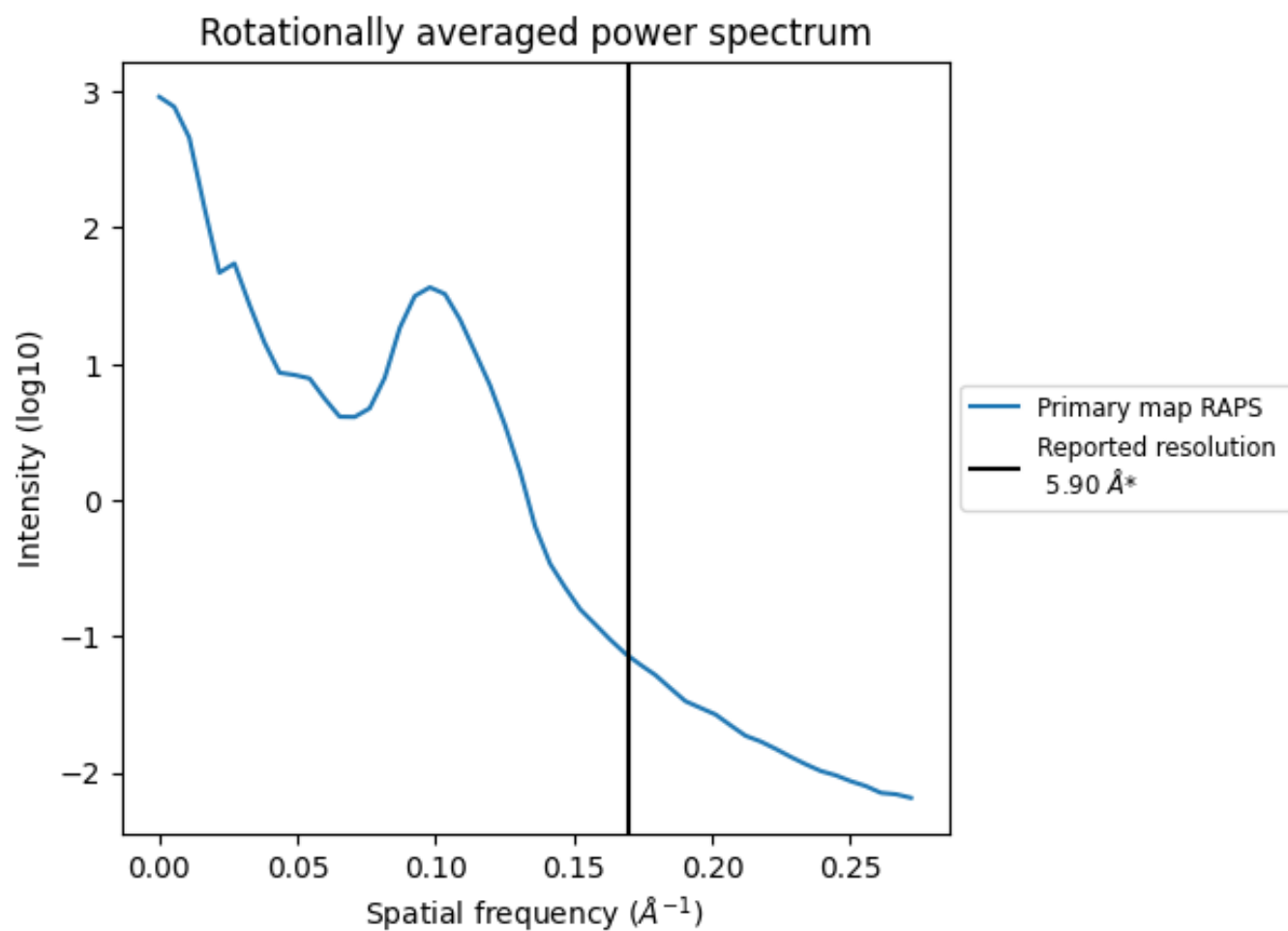
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm^3 ; this corresponds to an approximate mass of 41 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 ⓘ

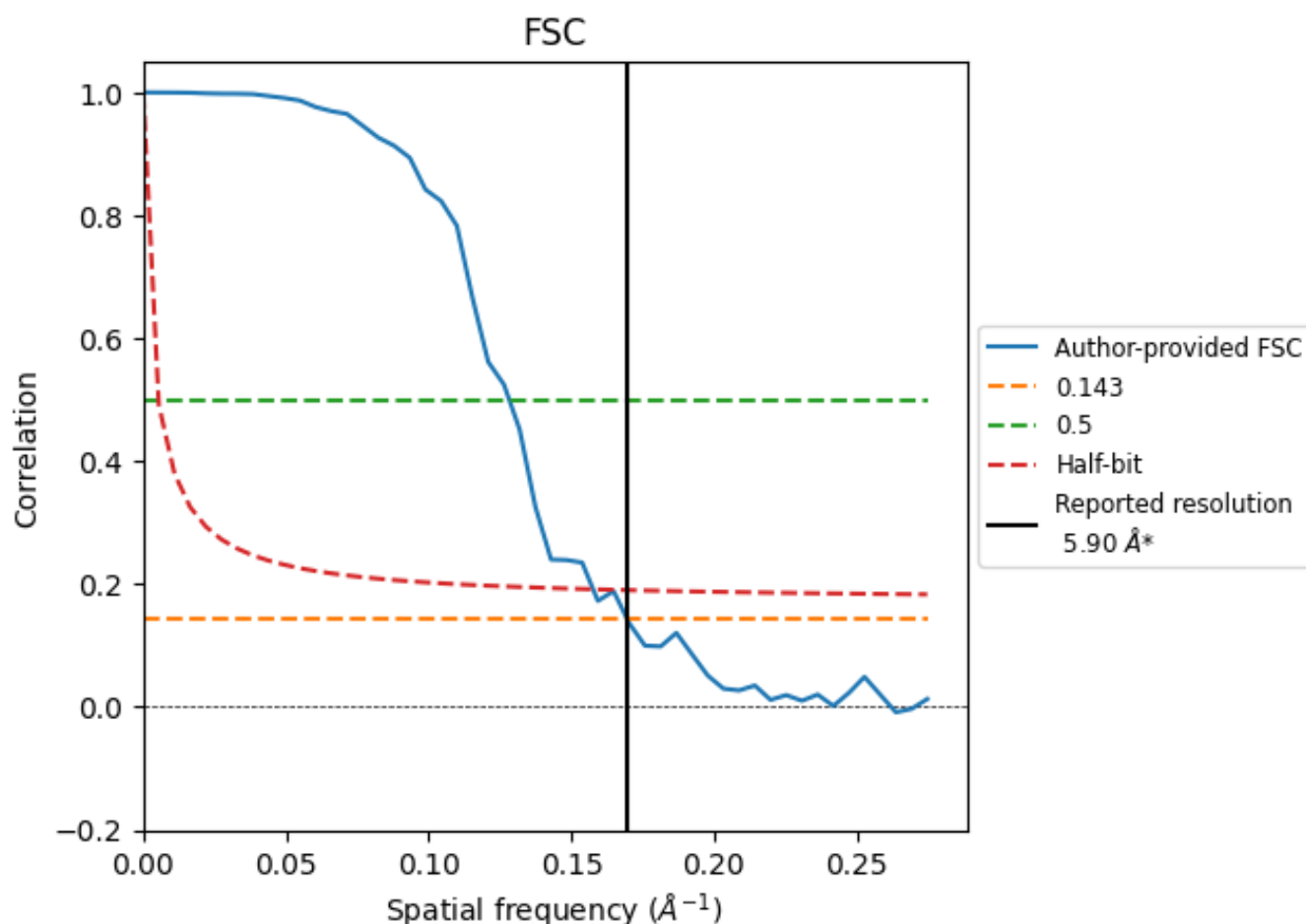


*Reported resolution corresponds to spatial frequency of 0.169 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.169 Å⁻¹

8.2 Resolution estimates [i](#)

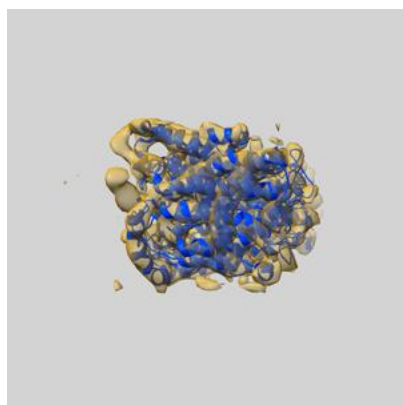
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	5.90	7.80	6.34
Unmasked-calculated*	-	-	-

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

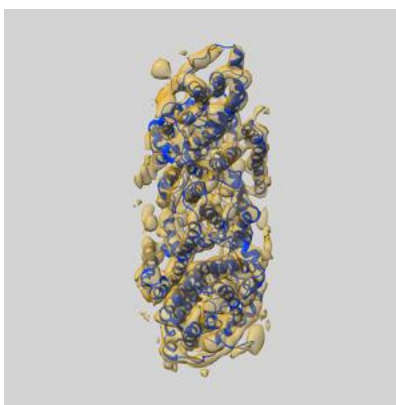
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8313 and PDB model 5SV9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

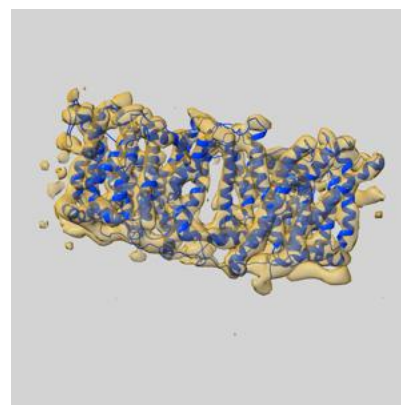
9.1 Map-model overlay [i](#)



X



Y



Z

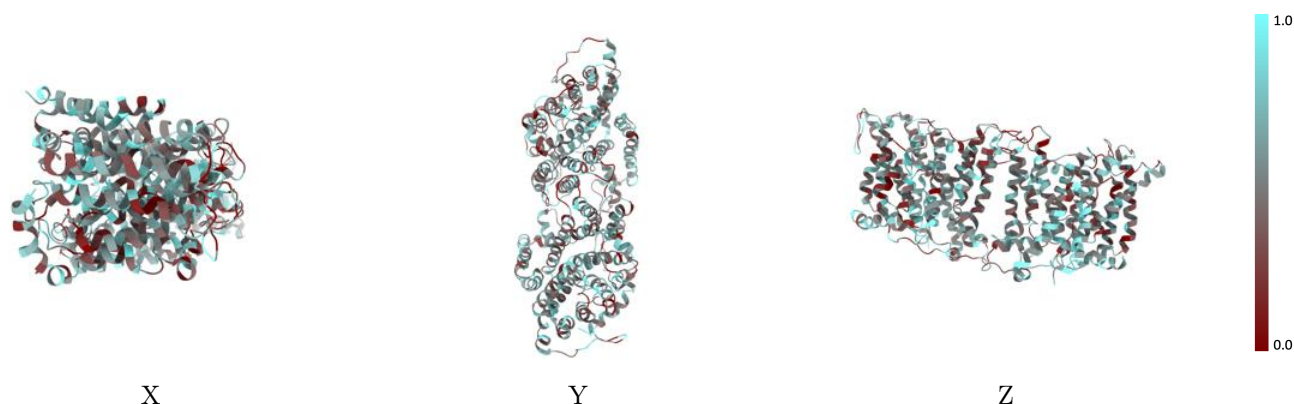
The images above show the 3D surface view of the map at the recommended contour level 130.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



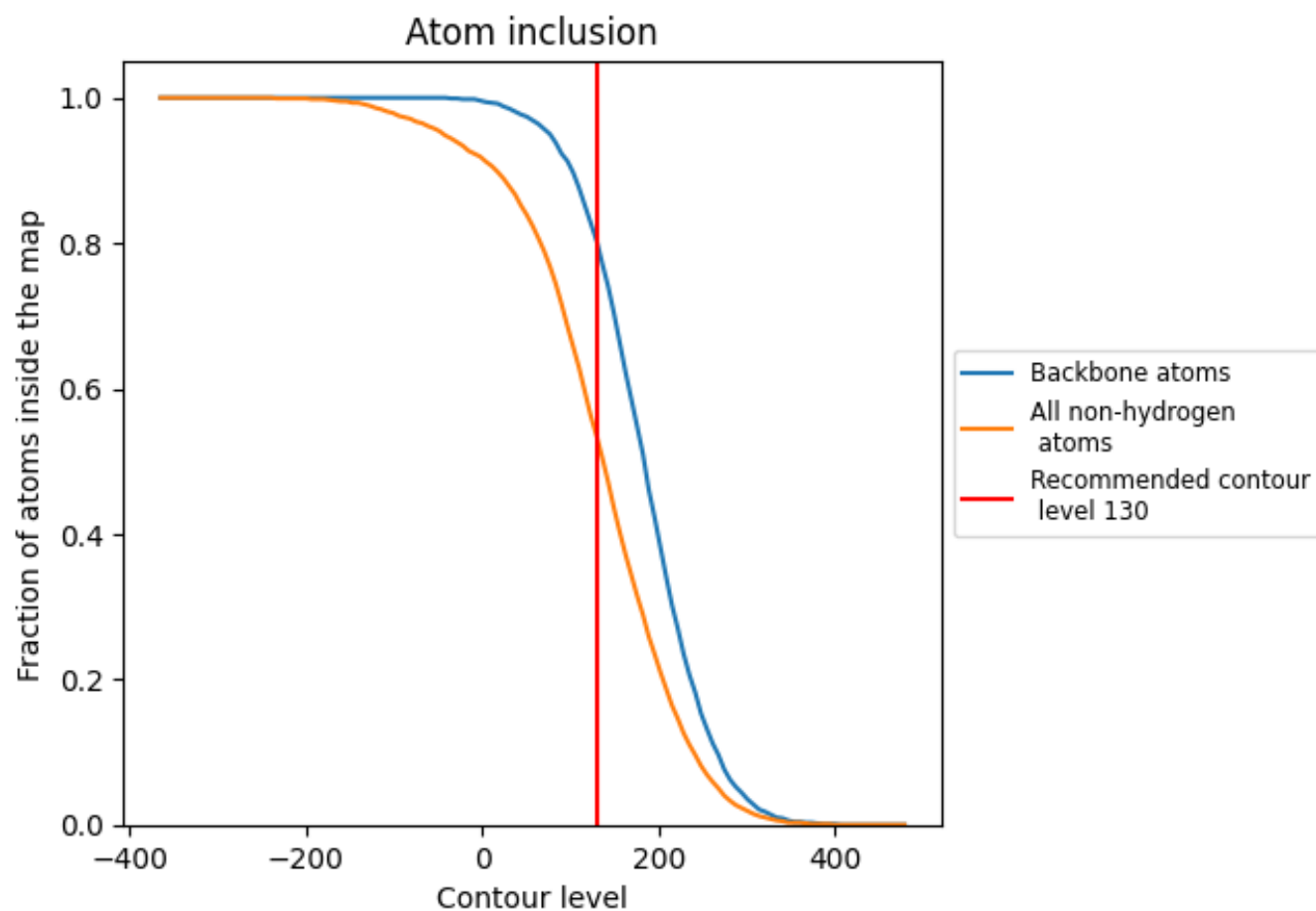
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (130).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 53% 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 (130) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5320	0.2490
A	0.5260	0.2440
B	0.5370	0.2540

