



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 11:26 PM UTC

PDB ID : 5Y5Y / pdb_00005y5y
EMDB ID : EMD-6811
Title : V/A-type ATPase/synthase from *Thermus thermophilus*, peripheral domain, rotational state 1
Authors : Nakanishi, A.; Kishikawa, J.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2017-08-10
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

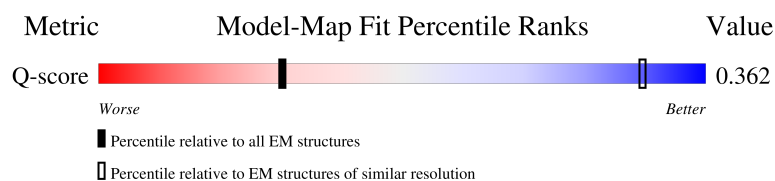
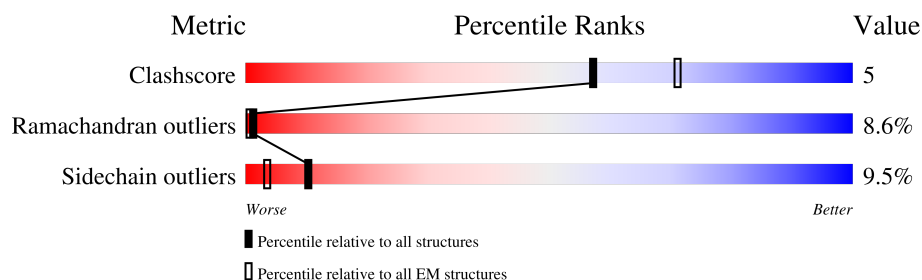
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.70 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	1989 (4.20 - 5.20)

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	578	 45% 44% 10% .
1	B	578	 48% 37% 12% .
1	C	578	 48% 38% 12% .
2	D	478	 42% 38% 12% . .

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Mol	Chain	Length	Quality of chain
2	E	478	42% 41% 11%
2	F	478	45% 38% 12%
3	G	223	16% 52% 30% 12% 6%
4	H	104	16% 47% 38% 10%
5	I	120	32% 39% 8% 49%
5	K	120	23% 41% 8% 49%
6	J	188	35% 63% 16% 19%
6	L	188	20% 63% 17% 19%
7	M	323	50% 72% 24%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32159 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		
1	B	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		
1	C	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		
2	E	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		
2	F	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	210	Total	C	N	O	S	0	0
			1642	1033	307	300	2		

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	100	Total	C	N	O	S	0	0
			758	479	131	145	3		

- Molecule 5 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	61	Total	C	N	O	0	0
			451	276	85	90		
5	K	61	Total	C	N	O	0	0
			451	276	85	90		

- Molecule 6 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	152	Total	C	N	O	0	0
			1043	646	203	194		
6	L	152	Total	C	N	O	0	0
			1043	646	203	194		

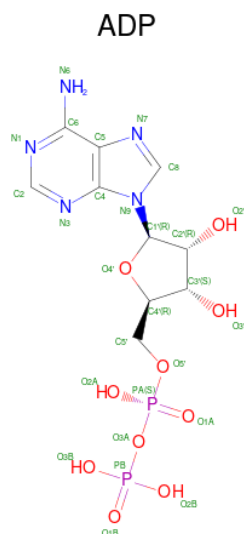
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	134	MET	LEU	conflict	UNP P74901
J	171	MET	LEU	conflict	UNP P74901
J	178	MET	LEU	conflict	UNP P74901
L	134	MET	LEU	conflict	UNP P74901
L	171	MET	LEU	conflict	UNP P74901
L	178	MET	LEU	conflict	UNP P74901

- Molecule 7 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	320	Total	C	N	O	S	0	0
			2513	1599	460	450	4		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

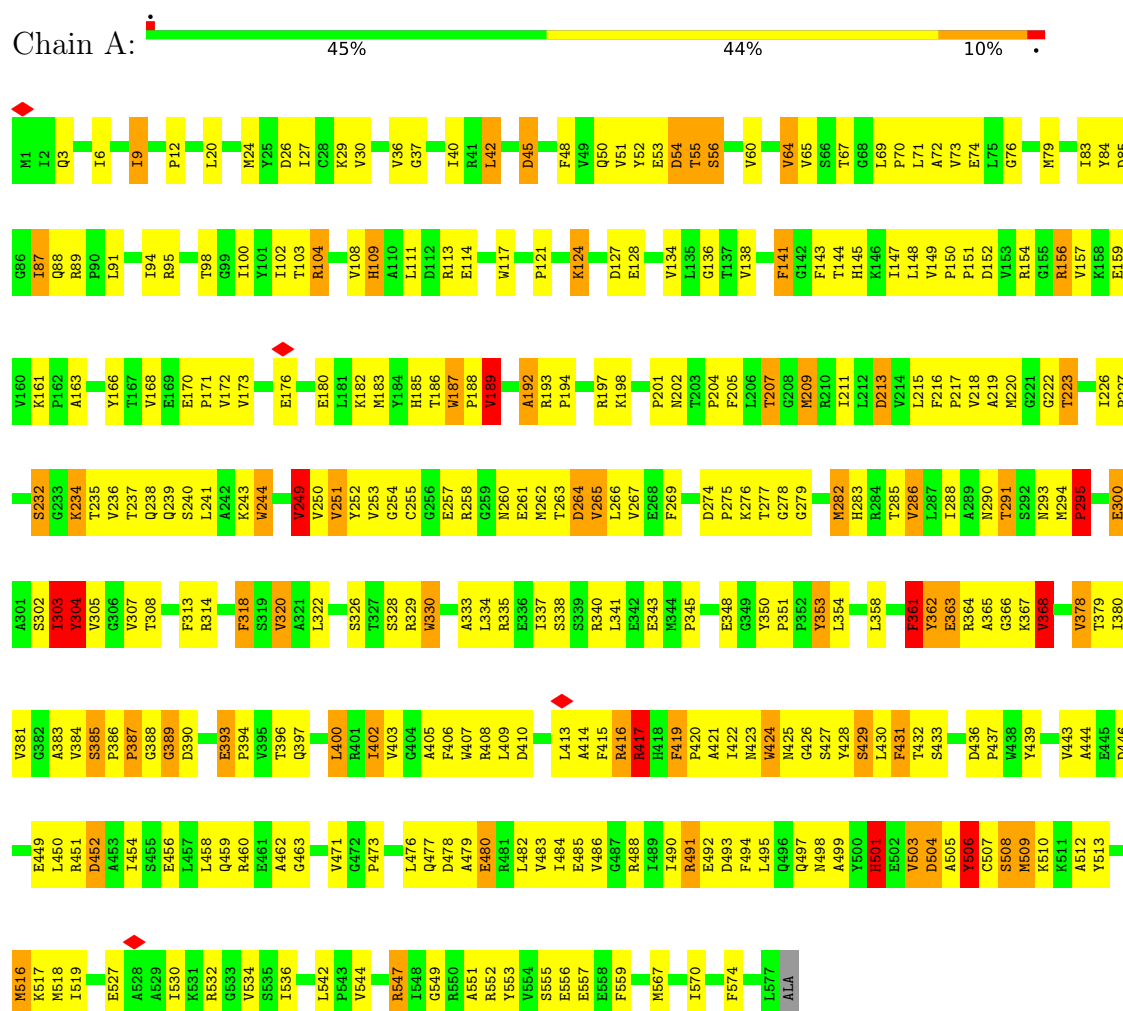


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 27	C 10	N 5	O 10	P 2	0
8	C	1	Total 27	C 10	N 5	O 10	P 2	0

3 Residue-property plots

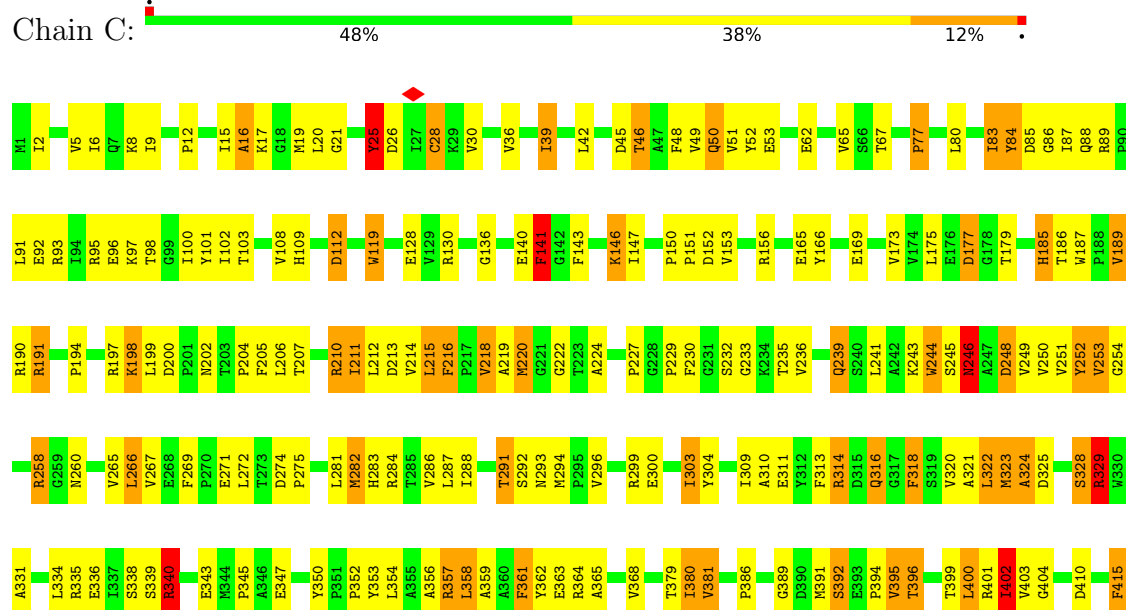
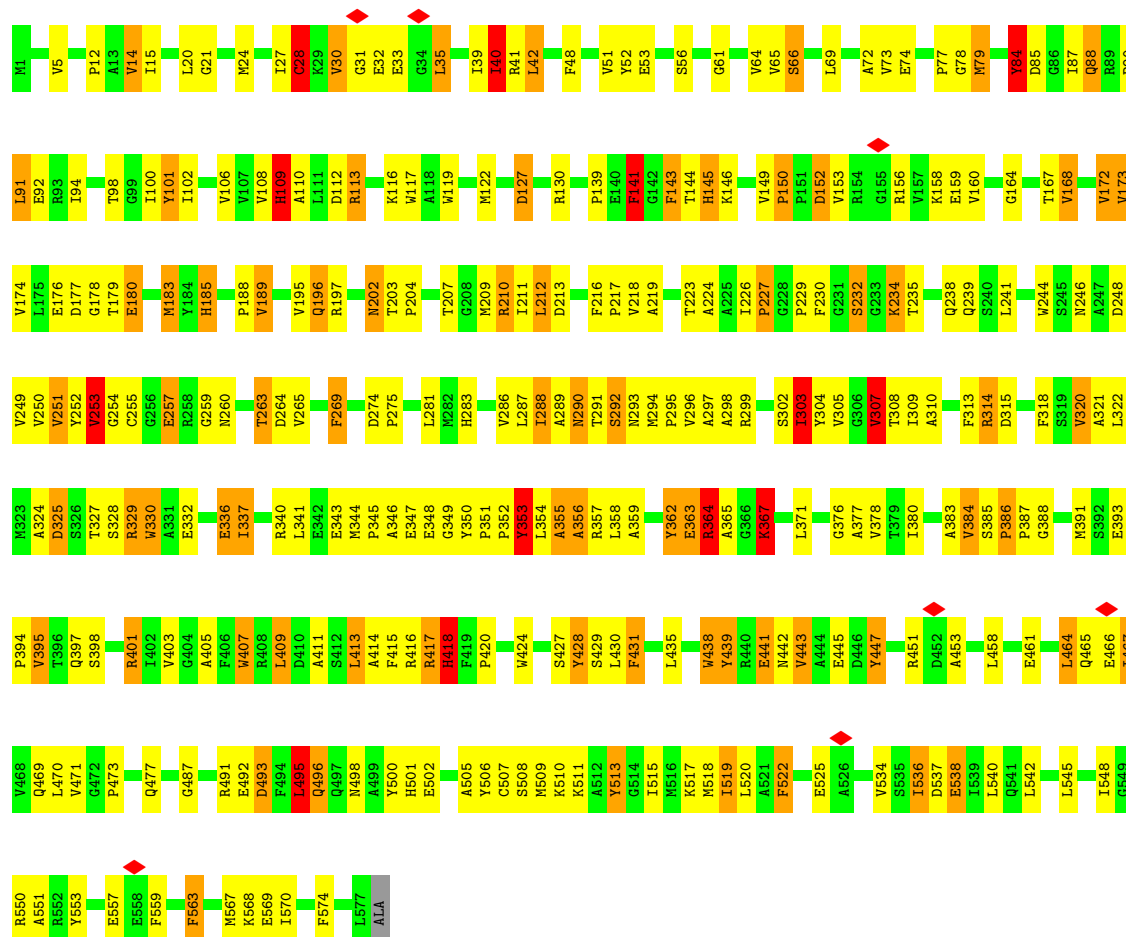
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

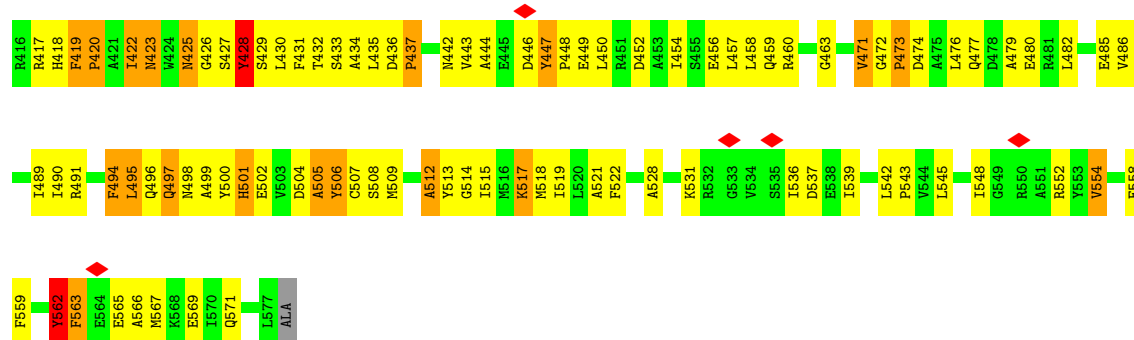
• Molecule 1: V-type ATP synthase alpha chain



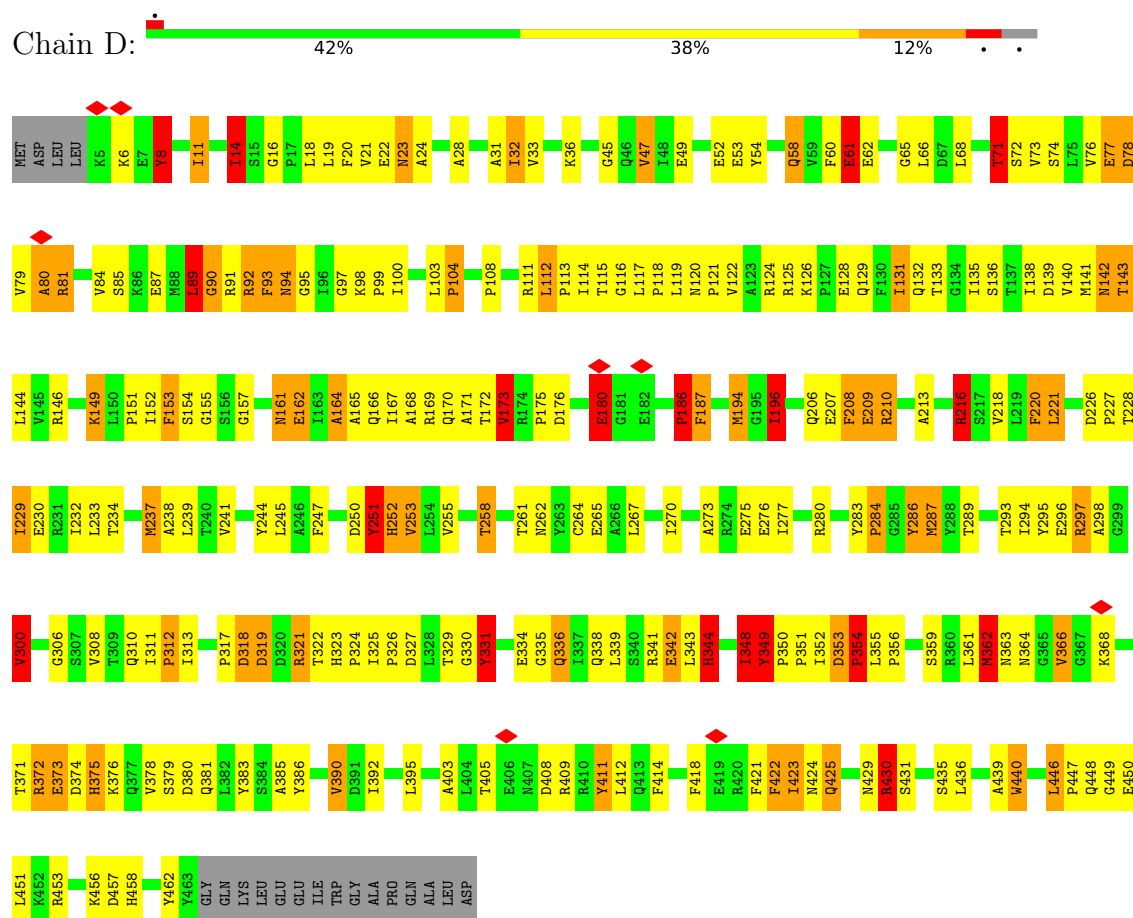
• Molecule 1: V-type ATP synthase alpha chain



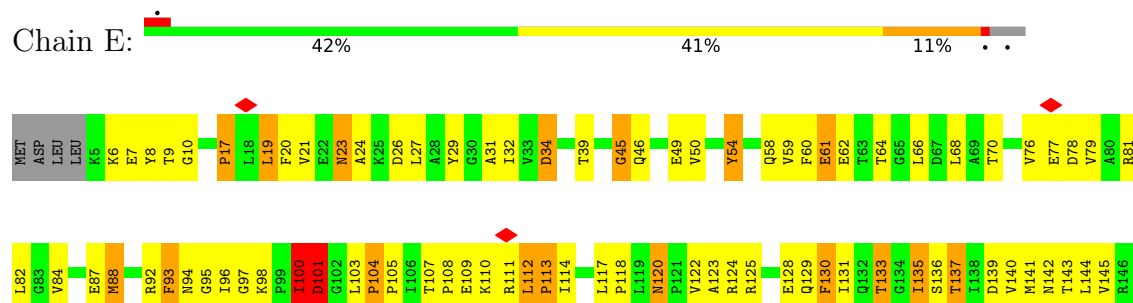


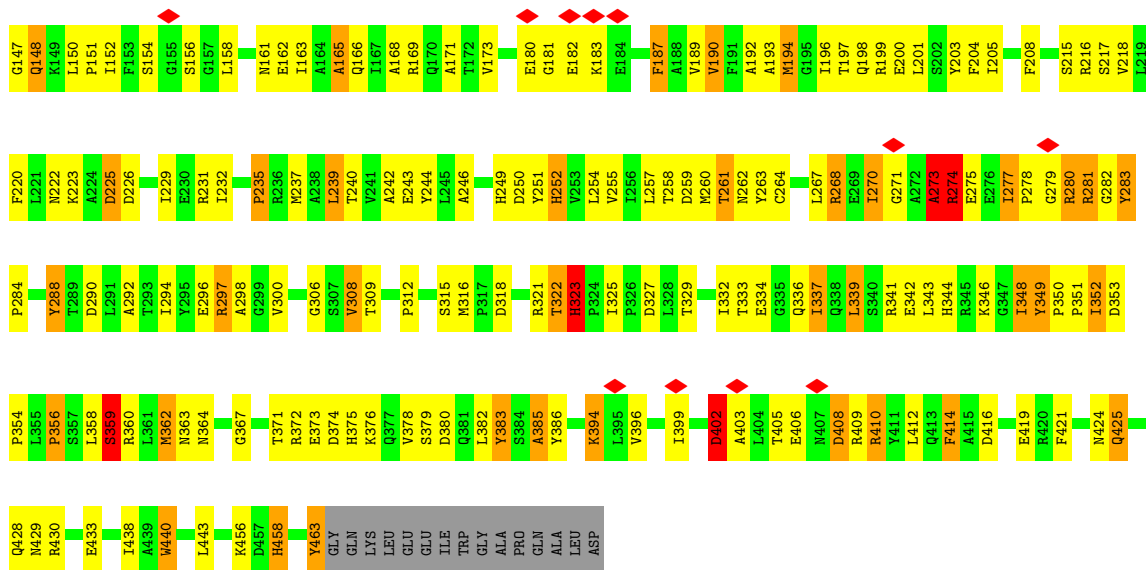


• Molecule 2: V-type ATP synthase beta chain

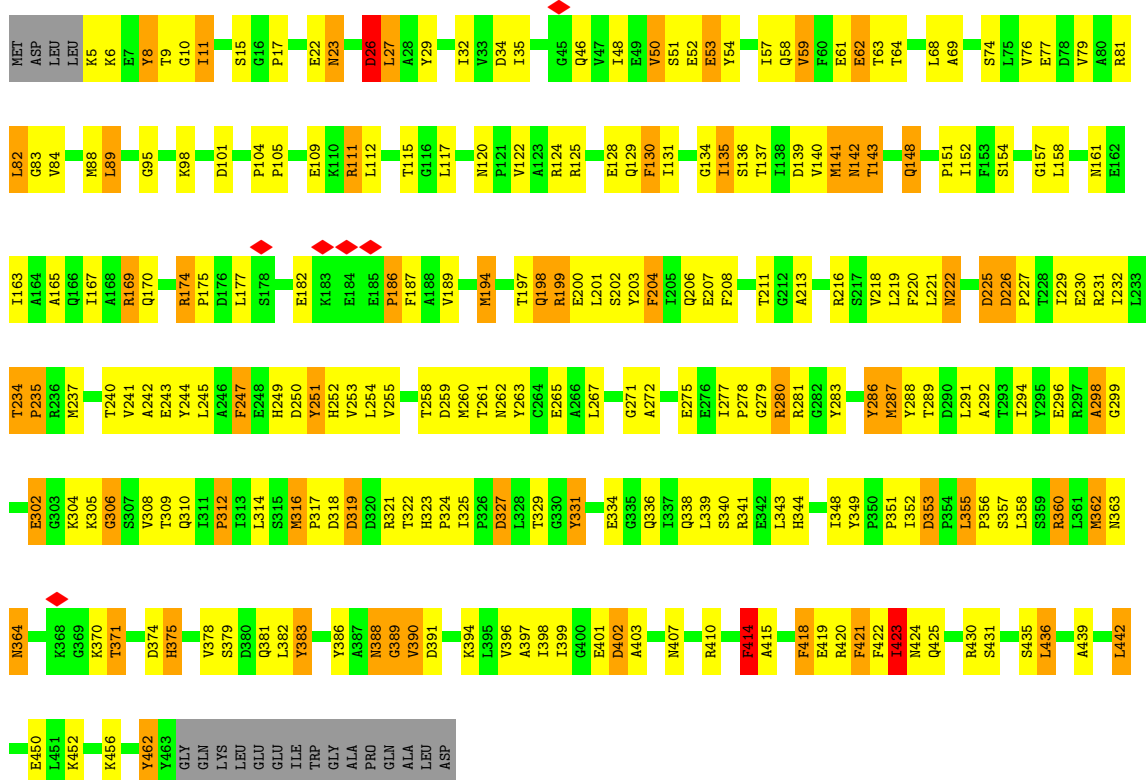


• Molecule 2: V-type ATP synthase beta chain



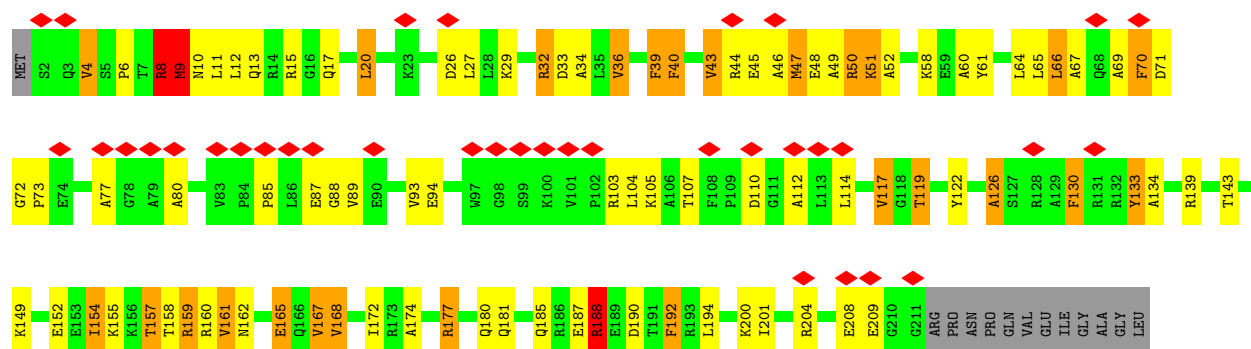


• Molecule 2: V-type ATP synthase beta chain

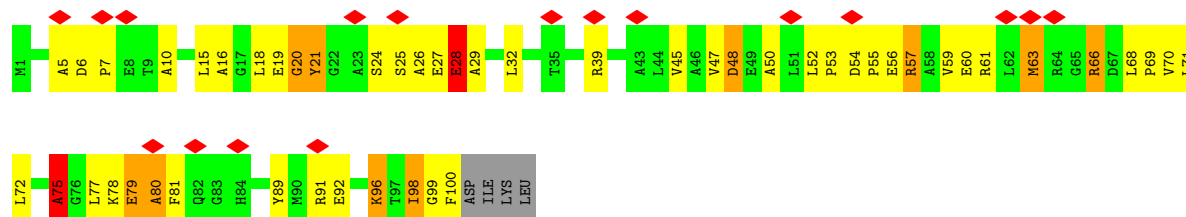


• Molecule 3: V-type ATP synthase subunit D

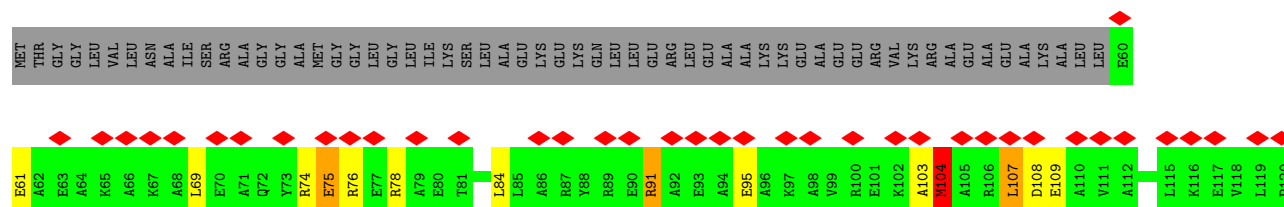
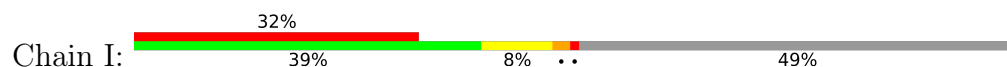




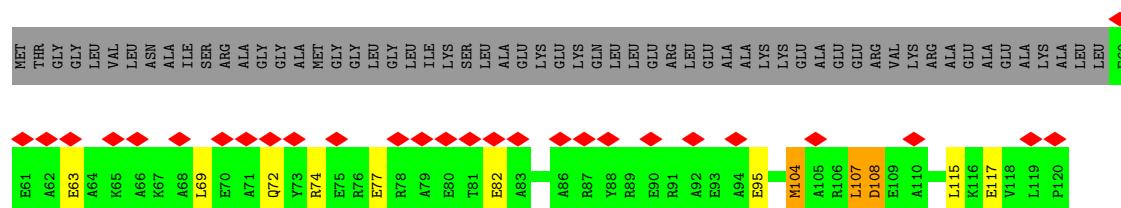
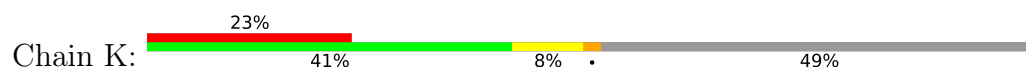
• Molecule 4: V-type ATP synthase subunit F



• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

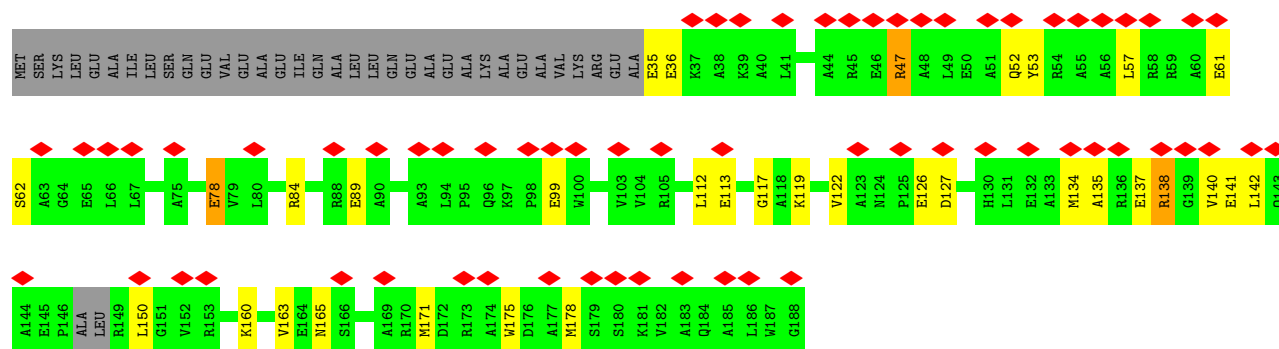


• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

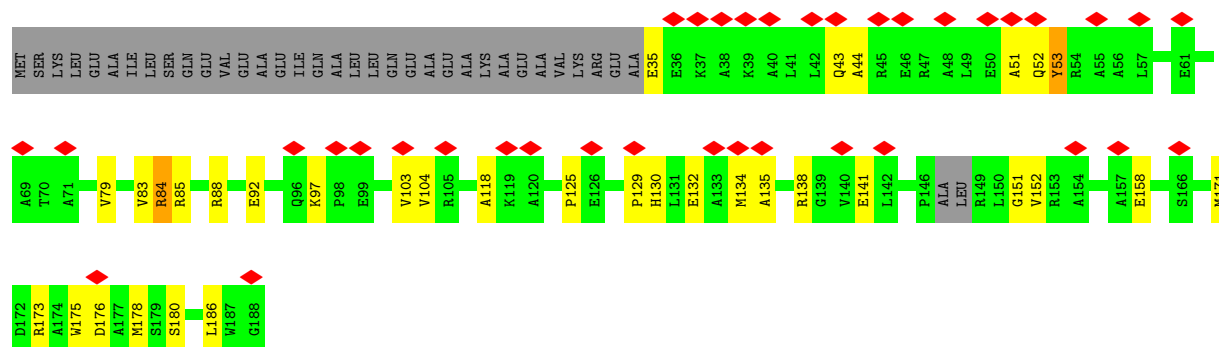


• Molecule 6: V-type ATP synthase subunit E

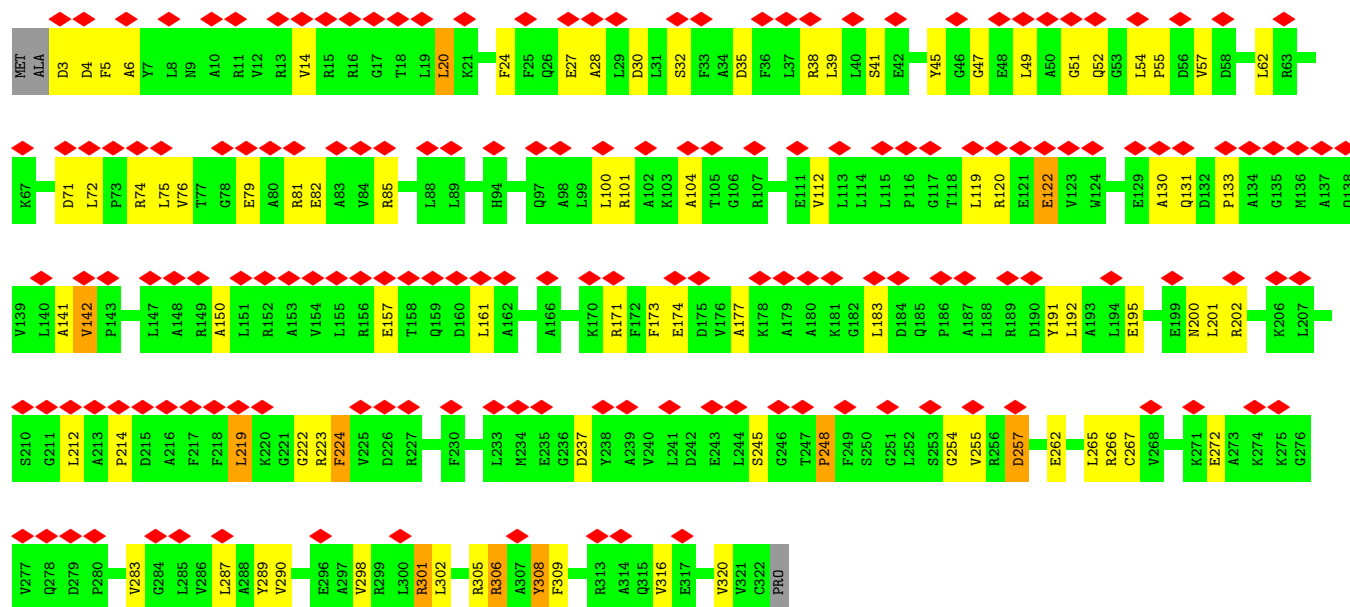




• Molecule 6: V-type ATP synthase subunit E



• Molecule 7: V-type ATP synthase subunit C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	117938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.778	Depositor
Minimum map value	-0.605	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	330.4, 330.4, 330.4	wwPDB
Map dimensions	236, 236, 236	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.11	152/4568 (3.3%)	1.93	140/6198 (2.3%)
1	B	2.02	136/4568 (3.0%)	1.90	139/6198 (2.2%)
1	C	2.09	151/4568 (3.3%)	1.92	131/6198 (2.1%)
2	D	2.03	109/3663 (3.0%)	1.92	123/4960 (2.5%)
2	E	2.05	118/3663 (3.2%)	1.97	138/4960 (2.8%)
2	F	2.13	138/3663 (3.8%)	1.94	120/4960 (2.4%)
3	G	1.89	30/1662 (1.8%)	2.04	57/2235 (2.6%)
4	H	1.67	7/769 (0.9%)	1.94	25/1039 (2.4%)
5	I	1.53	1/451 (0.2%)	1.90	14/608 (2.3%)
5	K	1.52	1/451 (0.2%)	1.79	7/608 (1.2%)
6	J	1.49	2/1053 (0.2%)	1.84	24/1439 (1.7%)
6	L	1.63	5/1053 (0.5%)	1.78	18/1439 (1.3%)
7	M	1.44	2/2552 (0.1%)	1.77	55/3446 (1.6%)
All	All	1.97	852/32684 (2.6%)	1.91	991/44288 (2.2%)

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	18
1	B	0	15
1	C	0	21
2	D	0	19
2	E	0	17
2	F	0	17
3	G	0	10
4	H	0	3
5	I	0	1
5	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	J	0	1
6	L	0	1
7	M	0	8
All	All	0	132

All (852) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	LEU	CA-C	-13.01	1.39	1.53
1	B	477	GLN	CA-C	-11.93	1.47	1.53
1	C	449	GLU	CA-C	-10.12	1.44	1.52
2	F	353	ASP	CA-C	-10.09	1.42	1.52
2	D	277	ILE	CA-C	-9.93	1.45	1.52
1	C	403	VAL	CA-C	-9.79	1.42	1.52
1	C	354	LEU	CA-C	-9.59	1.41	1.52
1	C	88	GLN	CA-C	-9.27	1.44	1.53
3	G	187	GLU	CA-C	-9.21	1.40	1.52
2	D	277	ILE	CA-CB	-9.11	1.47	1.54
2	F	323	HIS	C-N	-8.96	1.24	1.34
1	C	404	GLY	CA-C	-8.86	1.46	1.51
1	A	386	PRO	CA-C	-8.75	1.44	1.52
2	F	358	LEU	CA-C	-8.75	1.46	1.52
1	A	255	CYS	CA-C	-8.75	1.42	1.52
1	C	218	VAL	CA-C	-8.70	1.43	1.52
2	D	425	GLN	CA-C	-8.63	1.45	1.52
2	F	386	TYR	CA-C	-8.63	1.41	1.52
1	A	209	MET	CA-C	-8.57	1.42	1.52
1	B	461	GLU	CA-C	-8.54	1.44	1.52
2	D	133	THR	CA-C	-8.49	1.43	1.52
1	B	405	ALA	CA-C	-8.40	1.42	1.52
1	B	493	ASP	CA-C	-8.40	1.44	1.52
1	A	351	PRO	CA-C	-8.39	1.46	1.52
1	A	454	ILE	CA-C	-8.35	1.42	1.52
1	B	30	VAL	CA-C	-8.34	1.42	1.52
2	E	296	GLU	CA-C	-8.25	1.44	1.53
1	A	397	GLN	CA-C	-8.11	1.42	1.52
1	C	427	SER	CA-C	-8.10	1.43	1.52
1	A	430	LEU	CA-C	-8.06	1.43	1.52
1	C	227	PRO	CA-C	-8.01	1.45	1.53
1	C	361	PHE	CA-C	-7.98	1.42	1.52
1	A	322	LEU	CA-C	-7.98	1.43	1.52
1	A	495	LEU	CA-C	-7.96	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	412	LEU	CA-C	-7.96	1.44	1.53
1	C	296	VAL	CA-C	-7.94	1.43	1.52
1	C	559	PHE	N-CA	-7.93	1.40	1.46
1	B	332	GLU	CA-C	-7.85	1.41	1.52
2	E	348	ILE	CA-CB	-7.85	1.44	1.54
1	A	189	VAL	CA-C	-7.83	1.42	1.52
1	B	351	PRO	CA-C	-7.83	1.44	1.52
1	C	442	ASN	CA-C	-7.79	1.44	1.52
2	F	247	PHE	CA-C	-7.79	1.42	1.52
3	G	161	VAL	CA-C	-7.77	1.43	1.52
1	A	403	VAL	CA-C	-7.71	1.43	1.52
1	C	239	GLN	CA-C	-7.66	1.42	1.52
1	B	150	PRO	CA-C	-7.63	1.47	1.52
1	C	20	LEU	CA-C	-7.62	1.43	1.52
1	C	425	ASN	CA-C	-7.61	1.44	1.53
1	C	245	SER	CA-C	-7.61	1.43	1.52
1	B	427	SER	CA-C	-7.58	1.43	1.52
2	F	218	VAL	CA-C	-7.57	1.43	1.52
1	A	265	VAL	CA-C	-7.54	1.46	1.52
1	A	350	TYR	CA-C	-7.50	1.45	1.53
2	F	50	VAL	CA-C	-7.49	1.43	1.52
2	E	158	LEU	CA-C	-7.49	1.44	1.53
2	F	394	LYS	CA-C	-7.49	1.45	1.53
2	D	311	ILE	CA-C	-7.47	1.45	1.52
2	E	278	PRO	CA-C	-7.47	1.41	1.52
2	F	194	MET	CA-C	-7.43	1.44	1.52
2	E	246	ALA	CA-C	-7.40	1.43	1.52
2	E	290	ASP	CA-C	-7.37	1.43	1.52
2	F	418	PHE	CA-C	-7.37	1.42	1.52
2	E	327	ASP	CA-C	-7.37	1.43	1.52
1	C	458	LEU	CA-C	-7.37	1.42	1.52
1	C	211	ILE	CA-C	-7.36	1.44	1.52
1	B	327	THR	CA-C	-7.36	1.43	1.52
2	F	308	VAL	CA-C	-7.35	1.44	1.52
2	D	418	PHE	CA-C	-7.35	1.42	1.52
1	A	425	ASN	CA-C	-7.32	1.43	1.53
1	A	138	VAL	CA-C	-7.31	1.46	1.52
2	E	375	HIS	CA-C	-7.31	1.43	1.52
2	E	351	PRO	CA-C	-7.27	1.44	1.52
1	B	358	LEU	CA-C	-7.27	1.43	1.52
2	F	294	ILE	CA-C	-7.27	1.44	1.52
1	A	424	TRP	CA-C	-7.26	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	273	ALA	CA-C	-7.26	1.45	1.52
1	C	322	LEU	CA-C	-7.25	1.43	1.52
1	A	497	GLN	CA-C	-7.24	1.45	1.53
1	B	343	GLU	CA-C	-7.23	1.43	1.52
1	C	252	TYR	CA-C	-7.21	1.44	1.52
1	A	275	PRO	CA-C	-7.19	1.46	1.52
1	A	363	GLU	CA-C	-7.18	1.43	1.52
1	B	384	VAL	CA-C	-7.18	1.45	1.52
2	F	425	GLN	CA-C	-7.18	1.43	1.52
1	C	324	ALA	CA-C	-7.17	1.43	1.52
2	D	296	GLU	CA-C	-7.14	1.43	1.52
2	E	337	ILE	CA-C	-7.12	1.44	1.52
2	F	207	GLU	CA-C	-7.11	1.42	1.52
1	A	381	VAL	CA-C	-7.11	1.43	1.52
2	E	339	LEU	CA-C	-7.10	1.42	1.52
1	A	458	LEU	CA-C	-7.09	1.42	1.52
2	D	342	GLU	CA-C	-7.09	1.43	1.52
1	B	252	TYR	CA-C	-7.08	1.44	1.52
2	F	261	THR	CA-C	-7.08	1.43	1.52
1	B	336	GLU	CA-C	-7.06	1.43	1.52
1	C	391	MET	CA-C	-7.04	1.44	1.52
1	A	314	ARG	CA-C	-7.01	1.43	1.52
2	F	340	SER	CA-C	-7.01	1.43	1.52
1	C	314	ARG	CA-C	-7.00	1.43	1.52
2	D	167	ILE	CA-C	-6.99	1.43	1.52
2	D	142	ASN	CA-C	-6.99	1.46	1.53
2	E	325	ILE	CA-C	-6.98	1.45	1.52
1	C	358	LEU	CA-C	-6.98	1.44	1.52
1	B	325	ASP	CA-C	-6.98	1.43	1.52
1	C	336	GLU	CA-C	-6.98	1.44	1.52
2	D	381	GLN	CA-C	-6.96	1.43	1.52
2	D	252	HIS	CA-C	-6.93	1.44	1.52
2	E	137	THR	CA-CB	-6.93	1.41	1.53
1	C	402	ILE	CA-C	-6.92	1.44	1.52
1	B	156	ARG	CA-C	-6.91	1.44	1.52
2	F	240	THR	CA-C	-6.90	1.43	1.52
1	C	309	ILE	CA-C	-6.89	1.43	1.52
1	B	313	PHE	CA-C	-6.88	1.43	1.52
2	D	361	LEU	CA-C	-6.87	1.44	1.52
1	A	260	ASN	CA-C	-6.87	1.43	1.52
2	E	50	VAL	CA-C	-6.86	1.44	1.52
2	F	221	LEU	CA-C	-6.85	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	117	LEU	CA-C	-6.85	1.45	1.52
2	E	78	ASP	CA-C	-6.84	1.43	1.52
2	F	348	ILE	CA-CB	-6.83	1.45	1.54
1	C	28	CYS	CA-C	-6.82	1.44	1.52
1	A	338	SER	CA-C	-6.82	1.43	1.52
1	C	399	THR	CA-C	-6.81	1.45	1.53
1	B	501	HIS	CA-C	-6.81	1.44	1.52
2	F	423	ILE	CA-C	-6.81	1.44	1.52
2	F	272	ALA	CA-C	-6.80	1.42	1.52
1	C	554	VAL	CA-C	-6.80	1.44	1.52
2	F	360	ARG	CA-C	-6.79	1.44	1.52
2	E	161	ASN	CA-C	-6.79	1.44	1.52
2	E	264	CYS	CA-C	-6.78	1.44	1.52
1	A	303	ILE	CA-C	-6.78	1.44	1.52
1	A	213	ASP	CA-C	-6.77	1.43	1.52
1	B	407	TRP	CA-C	-6.77	1.46	1.53
1	C	386	PRO	CA-C	-6.75	1.45	1.52
1	A	509	MET	CA-C	-6.74	1.43	1.52
1	C	204	PRO	CA-C	-6.74	1.44	1.52
2	E	201	LEU	CA-C	-6.73	1.44	1.52
2	E	255	VAL	CA-C	-6.73	1.44	1.52
1	C	512	ALA	CA-C	-6.73	1.43	1.52
2	D	425	GLN	N-CA	-6.73	1.41	1.47
1	A	313	PHE	CA-C	-6.72	1.43	1.52
1	B	364	ARG	CA-C	-6.72	1.43	1.52
1	A	400	LEU	CA-C	-6.70	1.44	1.52
1	B	507	CYS	CA-C	-6.70	1.47	1.53
1	B	257	GLU	CA-C	-6.66	1.43	1.52
1	B	88	GLN	CA-C	-6.66	1.47	1.53
1	B	385	SER	CA-C	-6.65	1.44	1.52
2	F	378	VAL	CA-C	-6.65	1.45	1.52
2	E	169	ARG	CA-C	-6.65	1.44	1.52
1	C	108	VAL	CA-C	-6.64	1.45	1.52
4	H	16	ALA	CA-C	-6.63	1.44	1.52
2	D	270	ILE	CA-CB	-6.63	1.46	1.54
1	C	452	ASP	CA-C	-6.63	1.44	1.52
1	A	409	LEU	CA-C	-6.62	1.44	1.52
1	C	323	MET	CA-C	-6.62	1.45	1.53
2	D	21	VAL	CA-C	-6.62	1.44	1.52
2	D	325	ILE	CA-C	-6.62	1.46	1.52
2	E	438	ILE	CA-C	-6.61	1.44	1.52
1	C	350	TYR	CA-C	-6.60	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	399	ILE	CA-C	-6.60	1.44	1.52
1	C	423	ASN	CA-C	-6.60	1.44	1.52
1	C	199	LEU	CA-C	-6.59	1.44	1.52
2	D	300	VAL	CA-C	-6.58	1.45	1.52
2	E	277	ILE	CA-C	-6.58	1.46	1.52
2	F	148	GLN	CA-C	-6.57	1.44	1.52
2	F	129	GLN	CA-C	-6.57	1.44	1.52
2	E	323	HIS	CA-C	-6.56	1.45	1.53
2	F	339	LEU	CA-C	-6.56	1.44	1.52
1	C	30	VAL	CA-C	-6.56	1.44	1.52
1	A	456	GLU	CA-C	-6.55	1.44	1.52
2	F	435	SER	CA-C	-6.55	1.44	1.52
3	G	9	MET	CA-C	-6.55	1.44	1.52
1	B	229	PRO	CA-C	-6.54	1.44	1.52
3	G	157	THR	CA-C	-6.54	1.44	1.52
2	D	321	ARG	N-CA	-6.54	1.37	1.46
2	F	255	VAL	CA-C	-6.53	1.45	1.52
2	E	244	TYR	CA-C	-6.53	1.44	1.52
2	F	334	GLU	CA-C	-6.50	1.44	1.52
1	C	244	TRP	CA-C	-6.50	1.44	1.52
2	D	162	GLU	CA-C	-6.50	1.44	1.52
2	F	327	ASP	CA-C	-6.50	1.44	1.52
2	E	8	TYR	CA-C	-6.50	1.44	1.52
1	C	303	ILE	CA-C	-6.50	1.44	1.52
1	B	324	ALA	CA-C	-6.50	1.44	1.52
2	E	263	TYR	CA-C	-6.50	1.46	1.53
2	E	284	PRO	CA-C	-6.49	1.43	1.52
2	F	314	LEU	CA-C	-6.49	1.43	1.53
3	G	20	LEU	CA-C	-6.49	1.44	1.52
1	B	308	THR	CA-C	-6.48	1.44	1.52
5	I	74	ARG	CA-C	-6.48	1.43	1.52
1	B	250	VAL	CA-C	-6.47	1.44	1.52
1	C	519	ILE	CA-C	-6.47	1.44	1.52
2	F	82	LEU	CA-C	-6.47	1.44	1.52
2	E	353	ASP	CA-C	-6.46	1.44	1.52
2	E	364	ASN	CA-C	-6.46	1.44	1.52
2	D	313	ILE	CA-C	-6.46	1.44	1.52
1	A	241	LEU	CA-C	-6.45	1.44	1.52
1	B	173	VAL	CA-C	-6.44	1.44	1.52
3	G	43	VAL	CA-C	-6.42	1.45	1.52
2	D	47	VAL	CA-C	-6.42	1.45	1.52
2	E	108	PRO	CA-C	-6.42	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	113	PRO	CA-C	-6.41	1.44	1.52
1	A	499	ALA	N-CA	-6.40	1.39	1.46
1	B	251	VAL	CA-C	-6.40	1.44	1.52
1	C	432	THR	CA-C	-6.40	1.46	1.53
1	B	53	GLU	CA-C	-6.40	1.44	1.53
1	A	30	VAL	CA-C	-6.39	1.45	1.52
1	A	253	VAL	CA-C	-6.39	1.44	1.52
2	F	154	SER	CA-C	-6.38	1.44	1.52
1	C	381	VAL	CA-C	-6.38	1.44	1.52
1	C	404	GLY	N-CA	-6.38	1.40	1.45
1	C	220	MET	CA-C	-6.37	1.44	1.52
1	B	143	PHE	CA-C	-6.37	1.45	1.52
1	C	338	SER	CA-C	-6.37	1.44	1.52
1	A	498	ASN	CA-C	-6.36	1.44	1.52
1	A	413	LEU	CA-C	-6.36	1.45	1.52
2	F	362	MET	CA-C	-6.36	1.44	1.52
2	F	390	VAL	CA-C	-6.36	1.44	1.52
2	F	357	SER	CA-C	-6.35	1.45	1.52
3	G	27	LEU	CA-C	-6.35	1.43	1.52
2	E	152	ILE	CA-CB	-6.34	1.46	1.54
1	C	334	LEU	CA-C	-6.33	1.44	1.52
1	B	219	ALA	CA-C	-6.32	1.44	1.52
2	D	359	SER	CA-C	-6.31	1.44	1.52
2	E	232	ILE	CA-C	-6.31	1.44	1.53
2	F	260	MET	CA-C	-6.31	1.43	1.52
2	D	386	TYR	CA-C	-6.31	1.45	1.52
1	C	250	VAL	CA-C	-6.30	1.45	1.52
1	B	465	GLN	CA-C	-6.29	1.45	1.52
1	A	388	GLY	CA-C	-6.28	1.43	1.51
2	D	143	THR	CA-C	-6.28	1.45	1.52
1	C	296	VAL	CA-CB	-6.27	1.47	1.54
1	B	442	ASN	CA-C	-6.26	1.44	1.53
2	F	343	LEU	CA-C	-6.26	1.44	1.53
2	F	280	ARG	CA-C	-6.26	1.44	1.52
1	A	433	SER	CA-C	-6.25	1.44	1.52
1	C	236	VAL	CA-C	-6.25	1.44	1.52
2	E	192	ALA	CA-C	-6.24	1.45	1.52
1	A	368	VAL	CA-C	-6.24	1.45	1.52
2	E	316	MET	CA-C	-6.24	1.46	1.53
1	B	347	GLU	CA-C	-6.24	1.46	1.53
2	F	278	PRO	CA-C	-6.23	1.46	1.53
1	B	224	ALA	CA-C	-6.22	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	VAL	CA-C	-6.22	1.45	1.52
3	G	172	ILE	CA-C	-6.22	1.44	1.52
1	A	364	ARG	CA-C	-6.21	1.44	1.52
1	C	246	ASN	N-CA	-6.21	1.38	1.46
2	E	273	ALA	CA-C	-6.21	1.44	1.52
1	B	417	ARG	CA-C	-6.20	1.44	1.52
4	H	96	LYS	CA-C	-6.20	1.44	1.52
1	A	396	THR	CA-C	-6.20	1.45	1.52
1	C	558	GLU	CA-C	-6.20	1.44	1.52
2	D	170	GLN	CA-C	-6.20	1.44	1.52
2	F	88	MET	CA-C	-6.19	1.45	1.52
1	B	367	LYS	CA-C	-6.19	1.46	1.53
1	C	229	PRO	CA-C	-6.18	1.43	1.52
2	F	242	ALA	CA-C	-6.18	1.46	1.53
2	F	331	TYR	CA-C	-6.18	1.45	1.52
1	B	290	ASN	CA-C	-6.18	1.44	1.52
1	A	417	ARG	CA-C	-6.17	1.44	1.52
1	A	238	GLN	CA-C	-6.17	1.44	1.52
1	A	308	THR	CA-C	-6.16	1.44	1.52
2	E	292	ALA	CA-C	-6.16	1.44	1.52
6	J	165	ASN	CA-C	-6.15	1.47	1.53
2	E	348	ILE	CA-C	-6.14	1.45	1.52
1	C	300	GLU	CA-C	-6.14	1.44	1.52
1	B	253	VAL	CA-C	-6.13	1.45	1.52
2	F	237	MET	CA-C	-6.13	1.44	1.52
2	F	231	ARG	N-CA	-6.13	1.38	1.46
1	B	403	VAL	CA-C	-6.13	1.45	1.52
2	D	152	ILE	CA-C	-6.12	1.46	1.52
3	G	8	ARG	CA-C	-6.12	1.45	1.52
1	A	98	THR	CA-C	-6.12	1.48	1.52
2	E	9	THR	CA-C	-6.12	1.45	1.52
1	A	102	ILE	CA-C	-6.11	1.46	1.53
2	E	325	ILE	CA-CB	-6.11	1.46	1.54
1	C	345	PRO	CA-C	-6.11	1.43	1.52
2	E	359	SER	CA-C	-6.11	1.44	1.52
1	C	356	ALA	CA-C	-6.10	1.45	1.52
1	C	39	ILE	CA-C	-6.10	1.46	1.53
2	F	170	GLN	CA-C	-6.10	1.45	1.52
1	C	91	LEU	CA-C	-6.09	1.44	1.52
2	E	66	LEU	CA-C	-6.09	1.45	1.52
2	E	242	ALA	CA-C	-6.09	1.44	1.52
2	F	351	PRO	CA-C	-6.09	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	381	GLN	CA-C	-6.09	1.45	1.52
1	A	226	ILE	N-CA	-6.09	1.41	1.45
2	D	322	THR	CA-C	-6.09	1.45	1.52
2	F	58	GLN	CA-C	-6.08	1.45	1.53
1	A	29	LYS	CA-C	-6.08	1.45	1.52
3	G	133	TYR	CA-C	-6.08	1.44	1.52
2	E	386	TYR	CA-C	-6.07	1.45	1.52
2	F	64	THR	CA-C	-6.07	1.45	1.52
2	F	8	TYR	CA-C	-6.07	1.45	1.52
1	C	422	ILE	CA-CB	-6.06	1.47	1.54
1	B	563	PHE	CA-C	-6.06	1.45	1.52
1	A	353	TYR	CA-C	-6.05	1.44	1.52
1	A	483	VAL	CA-C	-6.05	1.45	1.52
1	B	362	TYR	CA-C	-6.05	1.44	1.52
1	A	6	ILE	CA-C	-6.05	1.46	1.52
2	F	277	ILE	CA-C	-6.05	1.46	1.52
1	B	363	GLU	CA-C	-6.05	1.45	1.52
1	A	220	MET	CA-C	-6.04	1.44	1.52
2	F	244	TYR	CA-C	-6.04	1.44	1.52
1	B	244	TRP	CA-C	-6.04	1.45	1.53
1	C	486	VAL	CA-CB	-6.04	1.47	1.54
1	C	321	ALA	CA-C	-6.03	1.45	1.52
2	D	131	ILE	CA-C	-6.03	1.45	1.52
1	B	185	HIS	CA-C	-6.03	1.45	1.52
1	B	211	ILE	CA-C	-6.03	1.45	1.52
6	L	53	TYR	CA-C	-6.03	1.47	1.52
2	E	379	SER	CA-C	-6.02	1.44	1.52
1	A	234	LYS	CA-C	-6.02	1.44	1.52
1	C	320	VAL	CA-C	-6.01	1.45	1.52
1	B	15	ILE	CA-C	-6.01	1.45	1.52
1	B	73	VAL	CA-C	-6.00	1.45	1.52
1	C	357	ARG	CA-C	-5.99	1.44	1.52
2	D	379	SER	CA-C	-5.99	1.44	1.52
1	B	500	TYR	CA-C	-5.98	1.44	1.52
1	A	425	ASN	N-CA	-5.98	1.40	1.46
2	E	156	SER	CA-C	-5.97	1.44	1.52
2	F	323	HIS	CA-C	-5.97	1.45	1.52
2	E	171	ALA	CA-C	-5.97	1.45	1.52
2	D	16	GLY	C-N	-5.97	1.28	1.33
2	E	32	ILE	CA-CB	-5.97	1.47	1.54
2	F	202	SER	CA-C	-5.96	1.45	1.52
1	C	454	ILE	CA-C	-5.95	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	THR	CA-C	-5.95	1.45	1.52
2	F	316	MET	CA-C	-5.94	1.46	1.53
1	B	441	GLU	CA-C	-5.93	1.45	1.52
1	C	292	SER	CA-C	-5.93	1.45	1.52
1	A	186	THR	CA-C	-5.93	1.45	1.52
1	C	343	GLU	CA-C	-5.93	1.45	1.52
2	E	193	ALA	CA-C	-5.93	1.45	1.52
2	D	237	MET	CA-C	-5.93	1.44	1.52
2	E	255	VAL	CA-CB	-5.93	1.46	1.54
1	A	482	LEU	CA-C	-5.92	1.45	1.52
2	F	292	ALA	CA-C	-5.92	1.46	1.52
2	E	378	VAL	CA-C	-5.92	1.45	1.52
2	D	241	VAL	CA-C	-5.91	1.44	1.52
1	C	336	GLU	N-CA	-5.91	1.38	1.46
1	B	287	LEU	CA-C	-5.90	1.45	1.52
2	D	436	LEU	CA-C	-5.90	1.45	1.52
2	F	364	ASN	N-CA	-5.90	1.38	1.46
1	C	216	PHE	CA-C	-5.90	1.45	1.52
2	E	412	LEU	CA-C	-5.90	1.44	1.52
1	A	421	ALA	N-CA	-5.89	1.38	1.46
1	C	271	GLU	CA-C	-5.89	1.45	1.52
2	F	287	MET	CA-C	-5.89	1.44	1.52
1	B	430	LEU	CA-C	-5.89	1.44	1.52
1	A	452	ASP	CA-C	-5.88	1.44	1.52
2	E	194	MET	N-CA	-5.88	1.39	1.46
1	C	500	TYR	CA-C	-5.88	1.46	1.53
2	E	376	LYS	N-CA	-5.88	1.38	1.46
2	F	189	VAL	CA-C	-5.88	1.45	1.52
1	B	519	ILE	CA-C	-5.88	1.45	1.52
1	C	542	LEU	C-N	-5.87	1.27	1.34
1	A	216	PHE	CA-C	-5.87	1.46	1.53
3	G	126	ALA	CA-C	-5.87	1.45	1.52
4	H	24	SER	CA-C	-5.87	1.46	1.53
1	B	20	LEU	CA-C	-5.86	1.45	1.52
2	F	152	ILE	CA-C	-5.86	1.45	1.52
2	E	59	VAL	CA-C	-5.86	1.46	1.52
1	C	251	VAL	CA-C	-5.86	1.45	1.52
1	B	354	LEU	CA-C	-5.85	1.42	1.52
1	C	50	GLN	CA-C	-5.85	1.45	1.52
2	F	375	HIS	CA-C	-5.85	1.45	1.52
3	G	107	THR	CA-C	-5.85	1.45	1.52
1	C	173	VAL	CA-C	-5.84	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	508	SER	CA-C	-5.84	1.45	1.53
2	D	136	SER	CA-C	-5.84	1.45	1.52
1	A	480	GLU	N-CA	-5.84	1.38	1.46
2	E	204	PHE	CA-C	-5.84	1.44	1.52
2	F	249	HIS	CA-C	-5.84	1.45	1.52
2	F	251	TYR	CA-C	-5.84	1.45	1.52
2	F	77	GLU	CA-C	-5.84	1.45	1.52
1	A	111	LEU	CA-C	-5.83	1.45	1.52
1	B	309	ILE	CA-CB	-5.83	1.48	1.54
2	E	135	ILE	CA-C	-5.83	1.46	1.52
2	F	135	ILE	CA-C	-5.82	1.45	1.52
1	A	56	SER	CA-C	-5.81	1.45	1.52
1	C	224	ALA	CA-C	-5.81	1.45	1.52
3	G	168	VAL	CA-C	-5.81	1.45	1.52
1	B	309	ILE	CA-C	-5.81	1.45	1.52
1	B	508	SER	CA-C	-5.80	1.45	1.52
2	E	267	LEU	CA-C	-5.80	1.45	1.52
3	G	29	LYS	CA-C	-5.80	1.45	1.52
2	E	165	ALA	CA-C	-5.80	1.45	1.52
1	B	354	LEU	N-CA	-5.79	1.39	1.46
1	C	205	PHE	CA-C	-5.79	1.45	1.52
2	E	268	ARG	CA-C	-5.79	1.45	1.52
2	F	51	SER	CA-C	-5.78	1.45	1.53
2	F	338	GLN	CA-C	-5.78	1.45	1.52
2	F	255	VAL	CA-CB	-5.78	1.47	1.54
1	C	294	MET	CA-C	-5.78	1.45	1.52
2	F	431	SER	CA-C	-5.78	1.45	1.52
2	D	80	ALA	CA-C	-5.78	1.45	1.53
1	B	536	ILE	CA-C	-5.77	1.45	1.52
2	F	167	ILE	CA-C	-5.77	1.44	1.52
1	A	239	GLN	CA-C	-5.77	1.45	1.52
2	F	348	ILE	CA-C	-5.76	1.46	1.52
1	B	358	LEU	N-CA	-5.76	1.39	1.46
1	B	341	LEU	CA-C	-5.76	1.45	1.52
1	A	491	ARG	CA-C	-5.75	1.45	1.52
1	A	507	CYS	CA-C	-5.75	1.45	1.52
2	D	267	LEU	CA-C	-5.75	1.45	1.52
1	C	403	VAL	N-CA	-5.74	1.39	1.46
1	B	195	VAL	CA-C	-5.74	1.46	1.52
1	A	51	VAL	CA-C	-5.74	1.45	1.52
4	H	10	ALA	CA-C	-5.74	1.45	1.52
2	D	53	GLU	CA-C	-5.74	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	333	THR	CA-C	-5.73	1.45	1.53
2	E	190	VAL	CA-C	-5.73	1.45	1.52
2	F	258	THR	CA-C	-5.73	1.45	1.52
1	C	328	SER	CA-C	-5.72	1.44	1.52
2	E	196	ILE	CA-C	-5.72	1.46	1.53
3	G	130	PHE	CA-C	-5.72	1.45	1.52
2	D	298	ALA	CA-C	-5.72	1.45	1.52
2	D	385	ALA	CA-C	-5.72	1.45	1.52
4	H	70	VAL	CA-C	-5.72	1.46	1.52
1	B	385	SER	C-N	-5.72	1.26	1.33
1	C	403	VAL	CA-CB	-5.72	1.46	1.54
1	C	340	ARG	CA-C	-5.71	1.45	1.52
2	D	448	GLN	CA-C	-5.71	1.45	1.53
1	A	303	ILE	CA-CB	-5.70	1.46	1.54
2	D	24	ALA	CA-C	-5.70	1.45	1.52
1	A	9	ILE	CA-CB	-5.70	1.47	1.54
1	A	334	LEU	CA-C	-5.70	1.45	1.52
1	C	151	PRO	CA-C	-5.70	1.45	1.52
1	A	384	VAL	CA-C	-5.70	1.46	1.52
2	F	26	ASP	CA-C	-5.70	1.45	1.52
1	A	305	VAL	CA-CB	-5.69	1.46	1.54
1	B	320	VAL	CA-C	-5.69	1.45	1.53
1	A	20	LEU	CA-C	-5.68	1.45	1.52
2	E	408	ASP	CA-C	-5.68	1.45	1.52
1	C	243	LYS	CA-C	-5.68	1.44	1.52
2	E	383	TYR	CA-C	-5.68	1.45	1.52
1	A	204	PRO	CA-C	-5.68	1.45	1.52
1	B	435	LEU	CA-C	-5.68	1.44	1.52
2	D	28	ALA	CA-C	-5.68	1.45	1.52
2	E	194	MET	CA-C	-5.68	1.46	1.52
2	E	114	ILE	CA-C	-5.67	1.45	1.52
2	F	298	ALA	CA-C	-5.67	1.45	1.52
1	C	250	VAL	N-CA	-5.67	1.39	1.46
2	E	141	MET	CA-C	-5.66	1.45	1.52
3	G	192	PHE	CA-C	-5.66	1.45	1.52
2	D	339	LEU	CA-C	-5.66	1.45	1.52
1	A	263	THR	CA-C	-5.65	1.45	1.52
2	F	220	PHE	CA-C	-5.65	1.45	1.52
1	B	356	ALA	CA-C	-5.65	1.45	1.52
3	G	13	GLN	CA-C	-5.64	1.45	1.52
2	F	309	THR	CA-CB	-5.64	1.45	1.53
2	D	166	GLN	CA-C	-5.64	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	24	ALA	CA-C	-5.64	1.45	1.52
1	A	215	LEU	N-CA	-5.64	1.39	1.46
1	C	51	VAL	CA-C	-5.64	1.45	1.52
1	B	511	LYS	CA-C	-5.64	1.46	1.53
1	C	42	LEU	CA-C	-5.63	1.46	1.52
2	F	229	ILE	CA-CB	-5.63	1.47	1.54
6	L	84	ARG	CA-C	-5.63	1.45	1.52
2	E	79	VAL	CA-C	-5.63	1.45	1.52
3	G	70	PHE	N-CA	-5.63	1.41	1.46
1	B	288	ILE	CA-C	-5.63	1.45	1.52
1	A	422	ILE	CA-CB	-5.62	1.46	1.54
2	D	245	LEU	N-CA	-5.62	1.40	1.46
2	F	253	VAL	CA-C	-5.62	1.45	1.52
1	C	415	PHE	CA-C	-5.62	1.45	1.52
2	F	291	LEU	CA-C	-5.61	1.45	1.52
1	A	381	VAL	N-CA	-5.61	1.39	1.46
2	D	126	LYS	CA-C	-5.61	1.47	1.53
1	C	95	ARG	CA-C	-5.61	1.45	1.52
2	D	90	GLY	CA-C	-5.61	1.44	1.51
1	A	361	PHE	CA-C	-5.60	1.45	1.52
1	B	263	THR	CA-C	-5.60	1.44	1.52
3	G	50	ARG	CA-C	-5.60	1.45	1.52
2	F	79	VAL	CA-C	-5.60	1.45	1.52
2	D	255	VAL	CA-CB	-5.60	1.47	1.54
2	D	270	ILE	N-CA	-5.59	1.40	1.46
2	E	425	GLN	CA-C	-5.59	1.46	1.52
4	H	21	TYR	CA-C	-5.59	1.45	1.52
1	A	380	ILE	CA-C	-5.59	1.45	1.52
2	D	251	TYR	CA-C	-5.59	1.45	1.52
2	E	143	THR	CA-C	-5.59	1.45	1.52
1	B	203	THR	CA-C	-5.58	1.46	1.52
1	C	53	GLU	CA-C	-5.58	1.45	1.52
2	F	112	LEU	CA-C	-5.58	1.45	1.52
1	A	148	LEU	CA-C	-5.58	1.45	1.52
1	A	267	VAL	CA-C	-5.58	1.45	1.52
2	F	115	THR	CA-C	-5.58	1.45	1.52
1	A	414	ALA	CA-C	-5.57	1.44	1.52
1	B	264	ASP	CA-C	-5.57	1.45	1.52
2	F	34	ASP	CA-C	-5.57	1.46	1.52
3	G	32	ARG	CA-C	-5.57	1.45	1.52
2	F	364	ASN	CA-C	-5.57	1.45	1.52
1	C	65	VAL	CA-C	-5.56	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	HIS	CA-C	-5.56	1.45	1.52
1	A	40	ILE	CA-C	-5.55	1.46	1.53
2	D	87	GLU	CA-C	-5.55	1.45	1.52
2	F	348	ILE	N-CA	-5.54	1.40	1.46
1	B	64	VAL	CA-C	-5.54	1.46	1.52
1	C	272	LEU	CA-C	-5.54	1.45	1.53
1	B	72	ALA	CA-C	-5.54	1.45	1.52
1	C	19	MET	CA-C	-5.54	1.45	1.52
1	C	175	LEU	CA-C	-5.54	1.45	1.52
1	A	55	THR	CA-C	-5.54	1.46	1.52
2	F	198	GLN	CA-C	-5.53	1.45	1.52
1	B	102	ILE	CA-C	-5.53	1.45	1.52
1	C	249	VAL	CA-C	-5.53	1.47	1.53
1	A	240	SER	CA-C	-5.52	1.45	1.52
2	E	380	ASP	N-CA	-5.52	1.39	1.46
1	B	110	ALA	CA-C	-5.52	1.45	1.52
2	F	59	VAL	CA-C	-5.52	1.45	1.52
1	B	84	TYR	CA-C	-5.52	1.45	1.52
2	F	267	LEU	CA-C	-5.52	1.45	1.52
2	D	338	GLN	CA-C	-5.51	1.45	1.53
1	A	421	ALA	CA-C	-5.51	1.45	1.52
1	C	153	VAL	N-CA	-5.51	1.39	1.46
1	A	390	ASP	N-CA	-5.50	1.39	1.46
1	A	429	SER	CA-C	-5.49	1.46	1.52
1	C	335	ARG	CA-C	-5.49	1.45	1.52
2	F	136	SER	CA-C	-5.48	1.45	1.52
2	D	114	ILE	CA-CB	-5.48	1.47	1.54
1	C	17	LYS	CA-C	-5.48	1.45	1.52
1	B	314	ARG	CA-C	-5.48	1.45	1.52
2	E	242	ALA	N-CA	-5.47	1.39	1.46
2	F	379	SER	N-CA	-5.47	1.40	1.46
1	A	390	ASP	CA-C	-5.46	1.45	1.52
2	D	262	ASN	CA-C	-5.46	1.45	1.52
1	C	507	CYS	CA-C	-5.46	1.46	1.52
1	C	109	HIS	CA-C	-5.45	1.45	1.53
1	C	146	LYS	CA-C	-5.45	1.46	1.52
1	B	106	VAL	CA-C	-5.45	1.46	1.52
1	B	515	ILE	CA-C	-5.45	1.45	1.52
2	E	260	MET	CA-C	-5.45	1.45	1.52
2	F	304	LYS	CA-C	-5.45	1.47	1.53
1	A	26	ASP	CA-C	-5.44	1.45	1.52
2	E	356	PRO	N-CA	-5.44	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	451	ARG	CA-C	-5.44	1.45	1.52
2	D	120	ASN	N-CA	-5.44	1.40	1.45
2	F	281	ARG	CA-C	-5.44	1.44	1.52
2	E	109	GLU	CA-C	-5.44	1.45	1.52
1	B	453	ALA	CA-C	-5.43	1.46	1.52
2	D	440	TRP	CA-C	-5.43	1.45	1.52
2	F	161	ASN	CA-C	-5.43	1.46	1.53
2	E	77	GLU	CA-C	-5.43	1.45	1.52
2	F	122	VAL	CA-C	-5.43	1.44	1.52
2	D	381	GLN	N-CA	-5.42	1.39	1.46
2	E	68	LEU	N-CA	-5.42	1.40	1.46
1	A	517	LYS	CA-C	-5.42	1.45	1.52
1	A	419	PHE	CA-C	-5.42	1.45	1.52
3	G	10	ASN	N-CA	-5.42	1.39	1.46
1	B	14	VAL	CA-C	-5.42	1.46	1.52
2	E	205	ILE	CA-CB	-5.42	1.48	1.54
1	C	450	LEU	CA-C	-5.41	1.45	1.52
1	B	355	ALA	CA-C	-5.41	1.45	1.52
1	C	169	GLU	CA-C	-5.41	1.46	1.52
2	D	354	PRO	N-CA	-5.41	1.40	1.47
2	E	144	LEU	CA-C	-5.41	1.47	1.53
2	F	62	GLU	CA-C	-5.41	1.45	1.53
3	G	34	ALA	CA-C	-5.41	1.46	1.52
2	D	431	SER	CA-C	-5.40	1.46	1.52
1	B	429	SER	CA-C	-5.40	1.46	1.52
2	E	351	PRO	N-CA	-5.40	1.40	1.47
2	D	14	ILE	CA-C	-5.40	1.46	1.52
1	A	24	MET	CA-C	-5.40	1.45	1.52
2	D	76	VAL	CA-C	-5.39	1.46	1.52
2	D	421	PHE	CA-C	-5.39	1.46	1.52
2	F	265	GLU	CA-C	-5.39	1.46	1.52
2	F	321	ARG	N-CA	-5.39	1.39	1.46
6	J	53	TYR	CA-C	-5.39	1.47	1.52
3	G	60	ALA	CA-C	-5.38	1.45	1.52
1	A	422	ILE	CA-C	-5.38	1.46	1.52
2	D	430	ARG	CA-C	-5.38	1.45	1.52
1	C	418	HIS	CA-C	-5.38	1.47	1.53
1	C	16	ALA	CA-C	-5.37	1.45	1.52
2	F	430	ARG	CA-C	-5.37	1.45	1.52
2	D	229	ILE	CA-C	-5.37	1.46	1.52
2	E	34	ASP	CA-C	-5.37	1.46	1.52
2	E	217	SER	CA-C	-5.37	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	32	ILE	CA-C	-5.37	1.46	1.52
1	C	89	ARG	CA-C	-5.36	1.47	1.53
1	C	324	ALA	N-CA	-5.36	1.39	1.46
3	G	185	GLN	CA-C	-5.36	1.45	1.52
1	A	250	VAL	CA-C	-5.36	1.45	1.52
3	G	167	VAL	CA-C	-5.36	1.46	1.52
2	D	373	GLU	CA-C	-5.35	1.46	1.53
2	E	249	HIS	CA-C	-5.35	1.45	1.52
2	E	288	TYR	CA-C	-5.35	1.45	1.52
1	A	449	GLU	CA-C	-5.35	1.45	1.52
2	D	392	ILE	CA-C	-5.35	1.46	1.52
1	C	210	ARG	CA-C	-5.34	1.45	1.52
2	F	283	TYR	CA-C	-5.34	1.45	1.52
1	A	252	TYR	CA-C	-5.34	1.46	1.52
1	C	419	PHE	C-N	-5.34	1.24	1.34
2	D	245	LEU	CA-C	-5.34	1.47	1.53
2	D	277	ILE	N-CA	-5.34	1.41	1.46
2	E	31	ALA	CA-C	-5.34	1.46	1.52
1	B	92	GLU	CA-C	-5.33	1.45	1.52
2	F	158	LEU	N-CA	-5.33	1.38	1.45
1	B	39	ILE	CA-CB	-5.33	1.47	1.54
1	A	145	HIS	CA-C	-5.33	1.46	1.53
1	B	330	TRP	CA-C	-5.33	1.45	1.52
2	D	54	TYR	CA-C	-5.33	1.45	1.52
2	E	62	GLU	CA-C	-5.33	1.46	1.52
1	A	519	ILE	CA-CB	-5.32	1.48	1.54
2	E	129	GLN	CA-C	-5.32	1.46	1.52
2	D	144	LEU	CA-C	-5.32	1.45	1.52
1	A	138	VAL	N-CA	-5.32	1.41	1.46
2	E	385	ALA	CA-C	-5.32	1.46	1.52
1	A	282	MET	CA-C	-5.31	1.45	1.52
2	D	228	THR	CA-C	-5.31	1.45	1.52
1	A	249	VAL	CA-C	-5.31	1.46	1.52
1	B	51	VAL	CA-C	-5.31	1.46	1.52
1	B	294	MET	CA-C	-5.31	1.47	1.53
1	A	254	GLY	CA-C	-5.31	1.46	1.51
1	A	257	GLU	CA-C	-5.31	1.46	1.52
1	A	407	TRP	CA-C	-5.31	1.46	1.52
1	B	380	ILE	CA-C	-5.30	1.46	1.52
1	C	189	VAL	CA-C	-5.30	1.46	1.52
2	E	337	ILE	CA-CB	-5.30	1.47	1.55
1	A	288	ILE	CA-C	-5.30	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	350	TYR	C-N	-5.30	1.27	1.33
2	E	124	ARG	CA-C	-5.30	1.46	1.52
2	E	321	ARG	N-CA	-5.30	1.39	1.46
1	B	291	THR	CA-C	-5.30	1.46	1.52
2	F	234	THR	CA-CB	-5.30	1.47	1.53
1	C	198	LYS	CA-C	-5.29	1.46	1.52
2	E	122	VAL	CA-C	-5.29	1.46	1.52
1	A	147	ILE	CA-C	-5.29	1.46	1.52
1	B	307	VAL	CA-CB	-5.29	1.48	1.54
1	A	226	ILE	CA-CB	-5.29	1.50	1.54
1	A	451	ARG	CA-C	-5.29	1.45	1.52
1	B	106	VAL	CA-CB	-5.29	1.47	1.54
1	C	214	VAL	CA-C	-5.29	1.46	1.52
2	F	423	ILE	CA-CB	-5.29	1.48	1.54
1	C	309	ILE	CA-CB	-5.29	1.47	1.54
1	B	274	ASP	CA-C	-5.28	1.47	1.53
1	C	434	ALA	N-CA	-5.28	1.42	1.47
1	A	385	SER	CA-C	-5.28	1.47	1.53
1	C	428	TYR	CA-C	-5.28	1.45	1.52
1	C	562	TYR	CA-C	-5.28	1.45	1.52
1	A	94	ILE	CA-C	-5.28	1.46	1.52
1	C	497	GLN	CA-C	-5.28	1.45	1.52
1	C	83	ILE	CA-C	-5.28	1.46	1.52
2	E	275	GLU	CA-C	-5.28	1.45	1.52
2	E	352	ILE	N-CA	-5.27	1.39	1.46
2	D	351	PRO	CA-C	-5.27	1.45	1.52
2	E	61	GLU	CA-C	-5.27	1.45	1.52
2	D	173	VAL	CA-C	-5.26	1.47	1.52
2	F	302	GLU	CA-C	-5.26	1.46	1.52
2	F	158	LEU	CA-C	-5.26	1.47	1.53
2	F	169	ARG	CA-C	-5.26	1.45	1.52
1	C	480	GLU	CA-C	-5.26	1.46	1.52
1	C	552	ARG	N-CA	-5.26	1.40	1.46
1	B	322	LEU	CA-C	-5.26	1.45	1.52
2	D	253	VAL	CA-C	-5.25	1.46	1.52
2	F	325	ILE	C-N	-5.25	1.27	1.33
2	D	196	ILE	CA-CB	-5.25	1.48	1.54
2	F	299	GLY	CA-C	-5.25	1.46	1.52
1	B	146	LYS	CA-C	-5.24	1.46	1.52
2	F	63	THR	CA-C	-5.24	1.46	1.52
1	A	305	VAL	CA-C	-5.24	1.46	1.52
1	C	232	SER	CA-C	-5.23	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	395	VAL	CA-CB	-5.23	1.47	1.54
2	D	323	HIS	CB-CG	-5.23	1.42	1.50
2	D	363	ASN	CA-C	-5.23	1.46	1.52
2	E	440	TRP	CA-C	-5.23	1.45	1.52
1	B	265	VAL	CA-C	-5.23	1.46	1.52
2	F	283	TYR	C-N	-5.22	1.26	1.33
1	C	352	PRO	CA-C	-5.22	1.44	1.52
2	F	452	LYS	CA-C	-5.22	1.45	1.52
1	B	329	ARG	CA-C	-5.22	1.45	1.52
2	F	442	LEU	CA-C	-5.22	1.45	1.52
6	L	151	GLY	CA-C	-5.22	1.46	1.51
1	A	53	GLU	CA-C	-5.22	1.46	1.53
1	B	35	LEU	CA-C	-5.22	1.46	1.52
2	D	220	PHE	CA-C	-5.22	1.45	1.52
1	C	186	THR	CA-C	-5.22	1.46	1.52
2	E	323	HIS	C-N	-5.21	1.27	1.33
2	E	341	ARG	CA-C	-5.21	1.45	1.52
2	E	380	ASP	CA-C	-5.21	1.46	1.52
6	L	88	ARG	CA-C	-5.21	1.46	1.52
1	B	149	VAL	CA-C	-5.21	1.47	1.52
3	G	160	ARG	CA-C	-5.21	1.46	1.52
2	E	218	VAL	CA-C	-5.21	1.46	1.52
1	C	429	SER	CA-C	-5.20	1.46	1.53
2	F	244	TYR	N-CA	-5.20	1.39	1.46
1	B	249	VAL	CA-CB	-5.20	1.48	1.54
2	D	376	LYS	CA-C	-5.20	1.45	1.52
2	F	130	PHE	CA-C	-5.20	1.46	1.52
1	A	138	VAL	CA-CB	-5.20	1.48	1.54
1	C	329	ARG	N-CA	-5.20	1.40	1.46
2	D	439	ALA	CA-C	-5.20	1.46	1.52
2	D	287	MET	CA-C	-5.20	1.46	1.52
1	B	160	VAL	CA-C	-5.20	1.46	1.52
1	B	507	CYS	N-CA	-5.20	1.41	1.46
2	E	199	ARG	N-CA	-5.20	1.40	1.46
2	D	52	GLU	CA-C	-5.19	1.45	1.52
1	C	274	ASP	CA-C	-5.19	1.47	1.53
2	D	79	VAL	CA-C	-5.19	1.46	1.52
6	L	118	ALA	CA-C	-5.19	1.46	1.52
1	A	463	GLY	CA-C	-5.19	1.45	1.52
2	E	145	VAL	CA-C	-5.19	1.46	1.52
1	B	218	VAL	CA-C	-5.19	1.45	1.52
1	B	66	SER	CA-C	-5.18	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	84	VAL	CA-CB	-5.18	1.50	1.55
1	A	262	MET	CA-C	-5.18	1.46	1.53
2	F	52	GLU	N-CA	-5.18	1.40	1.46
1	A	87	ILE	N-CA	-5.18	1.39	1.46
1	A	513	TYR	CA-C	-5.18	1.46	1.52
2	D	280	ARG	CA-C	-5.18	1.45	1.52
2	E	163	ILE	CA-CB	-5.17	1.48	1.54
1	C	179	THR	CA-C	-5.17	1.46	1.52
2	F	341	ARG	CA-C	-5.17	1.45	1.52
5	K	115	LEU	CA-C	-5.17	1.46	1.52
1	A	151	PRO	CA-C	-5.17	1.46	1.52
2	D	68	LEU	CA-C	-5.17	1.46	1.52
2	F	379	SER	CA-C	-5.17	1.46	1.52
2	F	389	GLY	CA-C	-5.17	1.44	1.51
2	D	33	VAL	CA-C	-5.16	1.46	1.52
2	D	78	ASP	CA-C	-5.16	1.45	1.52
2	D	414	PHE	CA-C	-5.16	1.46	1.52
2	F	424	ASN	CA-C	-5.16	1.46	1.52
1	A	83	ILE	N-CA	-5.16	1.40	1.46
1	C	517	LYS	CA-C	-5.16	1.45	1.52
1	B	517	LYS	CA-C	-5.16	1.46	1.52
3	G	12	LEU	CA-C	-5.16	1.45	1.52
1	A	144	THR	CA-C	-5.16	1.46	1.52
1	C	486	VAL	CA-C	-5.16	1.46	1.52
1	C	509	MET	CA-C	-5.15	1.46	1.52
1	A	431	PHE	CA-C	-5.15	1.45	1.52
1	A	488	ARG	CA-C	-5.15	1.46	1.52
1	A	518	MET	CA-C	-5.15	1.45	1.52
4	H	32	LEU	CA-C	-5.15	1.46	1.53
1	B	401	ARG	N-CA	-5.15	1.40	1.46
2	D	335	GLY	CA-C	-5.15	1.45	1.52
1	B	217	PRO	CA-C	-5.15	1.46	1.52
2	D	154	SER	CA-C	-5.15	1.46	1.53
3	G	172	ILE	CA-CB	-5.15	1.47	1.54
7	M	306	ARG	CA-C	-5.15	1.46	1.52
1	A	387	PRO	CA-C	-5.14	1.45	1.52
2	D	94	ASN	CA-C	-5.14	1.46	1.52
1	A	330	TRP	CA-C	-5.14	1.46	1.52
1	B	328	SER	CA-C	-5.14	1.45	1.52
2	D	89	LEU	CA-C	-5.14	1.45	1.52
1	A	194	PRO	CA-C	-5.14	1.45	1.52
1	B	178	GLY	CA-C	-5.14	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	352	ILE	CA-C	-5.14	1.46	1.52
2	E	59	VAL	CA-CB	-5.14	1.47	1.53
1	C	194	PRO	CA-C	-5.14	1.46	1.52
1	B	297	ALA	CA-C	-5.14	1.45	1.52
2	F	163	ILE	CA-CB	-5.14	1.48	1.54
2	D	353	ASP	CA-C	-5.13	1.46	1.52
2	F	226	ASP	CA-C	-5.13	1.46	1.52
3	G	104	LEU	CA-C	-5.13	1.45	1.52
1	B	299	ARG	CA-C	-5.13	1.45	1.52
1	C	396	THR	CA-CB	-5.13	1.46	1.53
2	D	66	LEU	CA-C	-5.13	1.46	1.52
1	B	498	ASN	N-CA	-5.12	1.40	1.46
2	E	81	ARG	CA-C	-5.12	1.46	1.52
2	F	9	THR	CA-C	-5.12	1.46	1.52
2	E	111	ARG	CA-C	-5.12	1.46	1.52
2	F	317	PRO	CA-C	-5.11	1.46	1.52
1	A	286	VAL	CA-CB	-5.11	1.47	1.54
1	C	437	PRO	CA-C	-5.11	1.44	1.52
1	A	232	SER	N-CA	-5.11	1.39	1.46
3	G	43	VAL	N-CA	-5.11	1.40	1.46
1	A	333	ALA	CA-C	-5.11	1.46	1.52
2	E	329	THR	CA-C	-5.11	1.46	1.52
1	B	94	ILE	CA-C	-5.10	1.46	1.52
1	A	343	GLU	CA-C	-5.10	1.46	1.52
2	E	297	ARG	N-CA	-5.10	1.39	1.46
2	F	363	ASN	CA-C	-5.10	1.46	1.52
1	C	39	ILE	N-CA	-5.10	1.40	1.46
2	D	458	HIS	CA-C	-5.10	1.46	1.52
1	A	192	ALA	CA-C	-5.10	1.46	1.52
1	B	239	GLN	CA-C	-5.10	1.46	1.52
1	C	329	ARG	CA-C	-5.09	1.46	1.52
2	D	334	GLU	CA-C	-5.09	1.46	1.52
2	F	291	LEU	N-CA	-5.09	1.40	1.46
2	F	355	LEU	CA-C	-5.09	1.46	1.52
2	D	14	ILE	N-CA	-5.09	1.40	1.46
1	C	528	ALA	CA-C	-5.09	1.46	1.52
1	C	506	TYR	CA-C	-5.09	1.46	1.52
2	D	435	SER	CA-C	-5.09	1.45	1.52
2	F	11	ILE	CA-CB	-5.09	1.47	1.54
1	C	396	THR	CA-C	-5.08	1.45	1.52
1	B	65	VAL	CA-CB	-5.08	1.50	1.55
1	B	438	TRP	CA-C	-5.08	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	TYR	CA-C	-5.08	1.46	1.52
2	D	18	LEU	CA-C	-5.08	1.46	1.52
2	D	289	THR	CA-C	-5.08	1.46	1.52
2	E	246	ALA	N-CA	-5.08	1.40	1.46
1	C	286	VAL	CA-C	-5.08	1.46	1.52
1	B	102	ILE	N-CA	-5.07	1.40	1.46
2	F	329	THR	CA-C	-5.07	1.46	1.52
2	F	35	ILE	CA-C	-5.07	1.46	1.52
1	B	477	GLN	N-CA	-5.07	1.42	1.46
1	B	548	ILE	CA-C	-5.07	1.45	1.52
2	F	245	LEU	CA-C	-5.07	1.45	1.52
2	D	234	THR	CA-C	-5.06	1.46	1.52
1	A	413	LEU	N-CA	-5.06	1.40	1.46
1	B	202	ASN	CA-C	-5.06	1.46	1.52
2	E	23	ASN	CA-C	-5.06	1.46	1.52
2	E	321	ARG	CA-C	-5.06	1.47	1.53
1	A	362	TYR	CA-C	-5.06	1.45	1.52
1	B	164	GLY	CA-C	-5.06	1.47	1.52
1	C	9	ILE	CA-CB	-5.06	1.47	1.54
1	C	239	GLN	N-CA	-5.06	1.40	1.46
2	F	254	LEU	CA-C	-5.06	1.46	1.52
2	E	79	VAL	N-CA	-5.06	1.40	1.46
1	A	519	ILE	CA-C	-5.05	1.46	1.52
1	B	39	ILE	N-CA	-5.05	1.40	1.46
2	D	210	ARG	CA-C	-5.05	1.46	1.52
2	F	105	PRO	CA-C	-5.05	1.46	1.52
1	A	197	ARG	CA-C	-5.05	1.46	1.52
1	C	542	LEU	CA-C	-5.05	1.47	1.53
1	A	444	ALA	CA-C	-5.05	1.46	1.52
1	B	141	PHE	CA-C	-5.05	1.46	1.52
1	C	190	ARG	CA-C	-5.05	1.46	1.52
1	A	364	ARG	N-CA	-5.05	1.39	1.46
1	A	236	VAL	CA-C	-5.05	1.45	1.52
1	C	401	ARG	CA-C	-5.05	1.46	1.52
1	C	92	GLU	CA-C	-5.05	1.46	1.52
2	D	218	VAL	CA-C	-5.05	1.46	1.52
1	A	149	VAL	N-CA	-5.04	1.42	1.47
1	A	136	GLY	CA-C	-5.03	1.47	1.51
1	A	42	LEU	CA-C	-5.03	1.46	1.52
1	A	138	VAL	C-N	-5.03	1.27	1.33
1	A	215	LEU	CA-C	-5.02	1.46	1.52
1	B	428	TYR	CA-C	-5.02	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	THR	CA-C	-5.02	1.46	1.52
2	E	382	LEU	CA-C	-5.02	1.46	1.52
2	D	297	ARG	N-CA	-5.02	1.39	1.46
1	B	28	CYS	CA-C	-5.02	1.46	1.52
1	B	251	VAL	CA-CB	-5.02	1.48	1.54
1	A	103	THR	CA-C	-5.01	1.46	1.52
1	B	309	ILE	N-CA	-5.01	1.41	1.46
2	E	356	PRO	CA-C	-5.01	1.45	1.52
2	F	289	THR	CA-C	-5.01	1.46	1.52
1	A	350	TYR	C-N	-5.01	1.28	1.33
1	B	102	ILE	CA-CB	-5.01	1.48	1.54
1	B	289	ALA	CA-C	-5.01	1.46	1.52
7	M	298	VAL	CA-C	-5.01	1.46	1.52
2	E	300	VAL	CA-C	-5.01	1.47	1.52
1	C	519	ILE	N-CA	-5.00	1.40	1.46
2	E	140	VAL	CA-C	-5.00	1.46	1.52
1	A	250	VAL	N-CA	-5.00	1.40	1.46
1	B	250	VAL	CA-CB	-5.00	1.48	1.54
2	F	319	ASP	CA-C	-5.00	1.46	1.53
1	C	454	ILE	N-CA	-5.00	1.40	1.46

All (991) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	46	ALA	N-CA-C	18.94	134.13	111.02
1	C	415	PHE	CA-CB-CG	-13.59	100.21	113.80
3	G	130	PHE	CA-CB-CG	-13.28	100.52	113.80
2	F	421	PHE	CA-CB-CG	-12.67	101.13	113.80
2	F	247	PHE	CA-CB-CG	-12.64	101.16	113.80
2	E	19	LEU	CA-C-N	12.23	138.54	121.05
2	E	19	LEU	C-N-CA	12.23	138.54	121.05
2	F	272	ALA	N-CA-C	-12.22	98.89	114.04
1	B	143	PHE	CA-CB-CG	-12.20	101.60	113.80
1	C	452	ASP	CA-CB-CG	-12.16	100.44	112.60
1	A	419	PHE	CA-CB-CG	-11.89	101.91	113.80
1	C	425	ASN	CA-CB-CG	-11.46	101.14	112.60
1	A	419	PHE	N-CA-C	-11.39	97.97	108.22
1	C	185	HIS	CA-C-N	11.26	139.22	121.66
1	C	185	HIS	C-N-CA	11.26	139.22	121.66
1	B	152	ASP	CA-CB-CG	-11.22	101.38	112.60
2	D	247	PHE	CA-CB-CG	-11.21	102.59	113.80
1	C	205	PHE	N-CA-C	-11.08	90.17	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	252	HIS	CA-CB-CG	-11.08	102.72	113.80
1	C	404	GLY	N-CA-C	-10.38	100.76	110.21
1	A	26	ASP	CA-CB-CG	-10.32	102.28	112.60
2	E	290	ASP	CA-CB-CG	-10.30	102.30	112.60
1	C	251	VAL	N-CA-C	-10.11	92.80	107.77
3	G	40	PHE	CA-CB-CG	-10.06	103.73	113.80
1	B	364	ARG	N-CA-C	-9.91	89.69	110.80
2	E	226	ASP	CA-CB-CG	-9.86	102.74	112.60
1	C	442	ASN	CA-CB-CG	-9.81	102.79	112.60
5	I	108	ASP	CA-CB-CG	-9.74	102.86	112.60
3	G	66	LEU	N-CA-C	-9.74	102.48	114.75
1	B	538	GLU	N-CA-C	-9.68	100.33	112.72
1	B	493	ASP	CA-CB-CG	-9.60	103.00	112.60
1	B	263	THR	N-CA-C	-9.55	102.20	114.04
2	F	226	ASP	CA-CB-CG	-9.47	103.13	112.60
2	E	93	PHE	N-CA-C	9.40	122.46	109.11
1	C	248	ASP	CA-CB-CG	-9.33	103.27	112.60
1	C	98	THR	N-CA-C	9.28	124.26	111.55
5	I	108	ASP	N-CA-C	9.26	122.53	111.33
3	G	77	ALA	CA-C-N	9.23	131.67	120.14
3	G	77	ALA	C-N-CA	9.23	131.67	120.14
6	J	36	GLU	N-CA-C	-9.19	101.21	111.14
1	A	478	ASP	CA-CB-CG	-9.03	103.57	112.60
1	C	143	PHE	CA-CB-CG	-8.97	104.83	113.80
5	K	117	GLU	N-CA-C	8.95	120.80	111.14
2	E	346	LYS	N-CA-C	-8.93	102.90	113.88
1	B	264	ASP	CA-CB-CG	-8.90	103.70	112.60
1	B	522	PHE	CA-CB-CG	8.89	122.69	113.80
1	C	216	PHE	CA-CB-CG	-8.82	104.98	113.80
2	E	133	THR	N-CA-C	-8.81	95.62	109.72
1	C	528	ALA	N-CA-C	-8.81	102.11	113.12
1	A	476	LEU	N-CA-C	-8.80	94.90	109.07
1	C	423	ASN	CA-CB-CG	-8.77	103.83	112.60
1	A	358	LEU	N-CA-C	-8.74	99.64	111.96
1	B	102	ILE	N-CA-C	-8.73	95.88	108.11
1	A	143	PHE	CA-CB-CG	-8.73	105.07	113.80
1	B	431	PHE	CA-CB-CG	-8.72	105.08	113.80
1	A	109	HIS	CA-CB-CG	-8.65	105.14	113.80
1	C	471	VAL	CB-CA-C	8.56	125.33	111.29
7	M	173	PHE	CA-CB-CG	-8.54	105.26	113.80
2	D	252	HIS	CA-CB-CG	-8.53	105.28	113.80
1	A	574	PHE	CA-CB-CG	-8.51	105.29	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	6	ASP	CA-C-N	8.49	128.48	119.05
4	H	6	ASP	C-N-CA	8.49	128.48	119.05
2	D	353	ASP	CA-CB-CG	-8.45	104.15	112.60
2	E	161	ASN	CA-CB-CG	-8.45	104.15	112.60
1	A	459	GLN	N-CA-C	-8.45	102.99	113.38
2	E	280	ARG	CA-C-N	8.43	137.63	121.54
2	E	280	ARG	C-N-CA	8.43	137.63	121.54
1	B	442	ASN	CA-CB-CG	-8.42	104.18	112.60
2	F	318	ASP	CA-CB-CG	-8.42	104.18	112.60
1	C	436	ASP	CA-CB-CG	-8.40	104.20	112.60
2	E	421	PHE	CA-CB-CG	-8.38	105.42	113.80
1	C	418	HIS	CB-CA-C	-8.37	100.74	111.70
6	L	43	GLN	N-CA-C	8.34	119.99	111.07
2	D	331	TYR	N-CA-C	-8.32	103.07	113.55
2	E	187	PHE	CA-CB-CG	-8.29	105.51	113.80
5	I	75	GLU	N-CA-C	-8.29	101.83	111.03
2	E	79	VAL	N-CA-C	-8.27	97.43	108.35
1	A	452	ASP	CA-CB-CG	-8.27	104.33	112.60
2	F	420	ARG	N-CA-C	8.26	121.10	111.02
1	C	506	TYR	N-CA-C	-8.25	93.23	110.80
1	A	419	PHE	N-CA-CB	8.22	119.74	111.10
2	E	364	ASN	N-CA-C	-8.19	96.87	109.24
7	M	30	ASP	CA-CB-CG	-8.15	104.45	112.60
1	A	555	SER	CA-C-N	8.12	131.51	120.38
1	A	555	SER	C-N-CA	8.12	131.51	120.38
2	E	220	PHE	CA-CB-CG	-8.10	105.70	113.80
2	E	429	ASN	CA-CB-CG	-8.09	104.51	112.60
2	F	222	ASN	CA-CB-CG	-8.07	104.53	112.60
2	E	416	ASP	CA-CB-CG	-8.05	104.55	112.60
3	G	190	ASP	CA-CB-CG	-8.03	104.57	112.60
1	A	425	ASN	N-CA-C	-8.02	100.43	112.54
1	C	554	VAL	N-CA-C	-8.02	97.29	108.27
2	F	291	LEU	N-CA-C	-8.01	102.82	112.59
2	F	292	ALA	N-CA-C	-8.00	102.04	112.68
2	E	252	HIS	CA-CB-CG	-7.99	105.81	113.80
2	D	169	ARG	N-CA-C	7.99	119.99	111.28
2	E	318	ASP	N-CA-C	-7.98	96.63	107.88
2	D	412	LEU	N-CA-C	-7.96	100.73	111.96
1	A	462	ALA	CA-C-N	7.94	128.92	120.03
1	A	462	ALA	C-N-CA	7.94	128.92	120.03
1	B	341	LEU	N-CA-C	-7.93	96.00	109.24
1	A	216	PHE	CA-CB-CG	-7.92	105.88	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	363	GLU	N-CA-C	7.92	119.60	110.97
1	A	431	PHE	CA-CB-CG	-7.91	105.89	113.80
2	E	344	HIS	CA-CB-CG	-7.90	105.90	113.80
2	D	24	ALA	N-CA-C	-7.86	97.79	109.81
1	C	141	PHE	CA-CB-CG	-7.84	105.96	113.80
1	A	420	PRO	N-CA-C	-7.84	91.72	112.10
2	D	78	ASP	CA-CB-CG	-7.84	104.76	112.60
1	C	48	PHE	CA-CB-CG	-7.84	105.96	113.80
2	D	378	VAL	CB-CA-C	-7.81	101.60	112.14
3	G	209	GLU	N-CA-C	-7.79	101.89	111.40
2	F	321	ARG	N-CA-C	-7.79	101.22	110.41
1	B	31	GLY	N-CA-C	-7.77	103.61	111.85
1	B	388	GLY	N-CA-C	-7.77	102.96	113.37
1	B	574	PHE	CA-CB-CG	-7.76	106.04	113.80
1	A	209	MET	N-CA-C	-7.74	95.91	108.52
2	E	323	HIS	N-CA-C	-7.74	100.33	109.93
2	F	98	LYS	N-CA-C	-7.73	92.72	109.81
2	F	398	ILE	N-CA-C	-7.71	105.53	111.62
1	B	377	ALA	N-CA-C	7.71	120.92	109.59
1	A	499	ALA	N-CA-C	-7.70	100.92	112.54
2	F	227	PRO	CA-C-N	7.70	130.93	120.54
2	F	227	PRO	C-N-CA	7.70	130.93	120.54
1	B	185	HIS	CA-CB-CG	-7.69	106.11	113.80
2	D	283	TYR	CA-C-N	7.69	129.46	119.84
2	D	283	TYR	C-N-CA	7.69	129.46	119.84
2	F	245	LEU	N-CA-C	-7.68	103.71	113.23
1	C	246	ASN	CA-CB-CG	-7.62	104.98	112.60
2	E	327	ASP	CA-CB-CG	-7.62	104.98	112.60
7	M	219	LEU	CA-C-N	7.60	132.00	120.82
7	M	219	LEU	C-N-CA	7.60	132.00	120.82
1	A	185	HIS	CA-C-N	7.59	131.66	120.87
1	A	185	HIS	C-N-CA	7.59	131.66	120.87
2	D	135	ILE	N-CA-C	-7.59	98.90	109.45
1	C	30	VAL	N-CA-C	-7.58	96.68	108.44
2	D	162	GLU	N-CA-C	-7.57	101.47	111.24
2	F	364	ASN	CA-CB-CG	-7.56	105.04	112.60
2	D	176	ASP	CA-CB-CG	-7.53	105.07	112.60
2	E	78	ASP	CA-CB-CG	-7.53	105.07	112.60
2	E	396	VAL	N-CA-CB	7.51	119.34	110.55
2	E	408	ASP	CA-CB-CG	-7.50	105.10	112.60
2	E	87	GLU	N-CA-C	-7.50	102.47	111.69
1	A	458	LEU	N-CA-C	7.49	121.33	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	364	ASN	N-CA-C	-7.49	95.95	108.75
3	G	45	GLU	N-CA-C	7.44	120.26	111.71
3	G	39	PHE	CA-CB-CG	7.43	121.23	113.80
2	E	372	ARG	CA-C-N	7.42	132.58	120.63
2	E	372	ARG	C-N-CA	7.42	132.58	120.63
1	A	473	PRO	N-CA-C	-7.42	104.25	114.27
2	D	161	ASN	CA-CB-CG	-7.42	105.18	112.60
2	E	20	PHE	N-CA-C	7.42	121.15	110.24
2	E	39	THR	N-CA-C	-7.42	103.53	112.59
3	G	208	GLU	N-CA-C	-7.42	102.48	112.94
2	D	77	GLU	CA-C-N	7.41	135.70	121.54
2	D	77	GLU	C-N-CA	7.41	135.70	121.54
2	E	218	VAL	N-CA-C	-7.40	97.50	108.45
2	F	283	TYR	N-CA-C	-7.40	100.10	110.31
1	B	461	GLU	N-CA-C	-7.39	103.10	112.93
2	E	76	VAL	CB-CA-C	-7.39	104.42	111.44
1	C	152	ASP	CA-CB-CG	-7.39	105.21	112.60
2	D	73	VAL	CA-C-N	7.38	132.24	122.42
2	D	73	VAL	C-N-CA	7.38	132.24	122.42
2	E	359	SER	N-CA-C	-7.36	95.13	110.80
7	M	283	VAL	CA-C-N	7.36	128.15	119.98
7	M	283	VAL	C-N-CA	7.36	128.15	119.98
1	A	553	TYR	N-CA-C	7.34	120.21	111.33
2	D	175	PRO	CA-C-N	7.32	131.80	120.82
2	D	175	PRO	C-N-CA	7.32	131.80	120.82
1	A	251	VAL	N-CA-C	-7.31	94.13	109.34
1	C	486	VAL	N-CA-C	-7.31	103.66	110.53
2	F	388	ASN	CA-CB-CG	-7.31	105.29	112.60
1	B	313	PHE	CA-CB-CG	-7.30	106.50	113.80
4	H	7	PRO	CA-C-N	7.28	130.76	120.28
4	H	7	PRO	C-N-CA	7.28	130.76	120.28
2	D	120	ASN	N-CA-C	-7.27	97.20	108.55
1	A	152	ASP	CA-CB-CG	-7.26	105.34	112.60
1	C	563	PHE	CA-CB-CG	-7.25	106.55	113.80
2	E	131	ILE	N-CA-C	7.23	117.80	108.12
2	F	111	ARG	N-CA-C	-7.21	98.11	109.50
1	B	563	PHE	N-CA-C	-7.21	102.61	111.40
1	A	446	ASP	CA-CB-CG	-7.20	105.40	112.60
3	G	119	THR	CA-C-O	-7.20	110.30	120.16
1	C	140	GLU	N-CA-C	-7.17	96.65	108.76
2	E	208	PHE	CA-CB-CG	-7.17	106.64	113.80
1	A	260	ASN	CA-CB-CG	-7.16	105.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	117	GLY	N-CA-C	-7.14	102.95	112.81
1	C	559	PHE	CA-CB-CG	-7.14	106.66	113.80
1	A	52	TYR	N-CA-C	7.12	119.04	111.28
1	A	388	GLY	N-CA-C	-7.11	96.34	113.18
4	H	39	ARG	N-CA-C	-7.10	103.48	112.93
4	H	99	GLY	N-CA-C	-7.10	100.50	111.64
1	A	141	PHE	CA-CB-CG	-7.09	106.71	113.80
2	E	130	PHE	CA-C-N	7.09	133.61	121.63
2	E	130	PHE	C-N-CA	7.09	133.61	121.63
1	B	257	GLU	N-CA-C	-7.08	95.71	110.80
1	B	269	PHE	CA-CB-CG	-7.08	106.72	113.80
2	F	208	PHE	CA-CB-CG	-7.07	106.73	113.80
2	E	364	ASN	CA-CB-CG	-7.06	105.54	112.60
2	F	234	THR	N-CA-C	7.06	122.43	113.25
1	C	415	PHE	CB-CA-C	7.04	122.02	110.90
2	D	187	PHE	N-CA-C	7.04	119.99	108.52
5	K	107	LEU	CA-C-N	7.03	134.96	121.54
5	K	107	LEU	C-N-CA	7.03	134.96	121.54
1	A	512	ALA	CA-C-N	7.01	130.01	120.54
1	A	512	ALA	C-N-CA	7.01	130.01	120.54
1	B	246	ASN	CA-CB-CG	-7.00	105.60	112.60
1	B	350	TYR	CA-C-N	7.00	127.59	120.38
1	B	350	TYR	C-N-CA	7.00	127.59	120.38
2	E	323	HIS	CA-CB-CG	-7.00	106.80	113.80
2	D	344	HIS	CA-CB-CG	-6.97	106.83	113.80
2	F	260	MET	N-CA-C	-6.95	104.07	114.64
3	G	105	LYS	N-CA-C	-6.95	97.64	109.24
1	C	425	ASN	N-CA-C	-6.94	94.91	107.60
5	K	108	ASP	CA-C-N	6.93	129.57	120.28
5	K	108	ASP	C-N-CA	6.93	129.57	120.28
1	A	127	ASP	CA-CB-CG	-6.93	105.67	112.60
2	F	48	ILE	CB-CA-C	-6.92	104.23	112.19
6	L	53	TYR	N-CA-C	-6.92	102.85	112.12
2	D	348	ILE	N-CA-C	-6.91	94.97	109.34
1	A	187	TRP	CA-C-N	6.89	128.46	119.84
1	A	187	TRP	C-N-CA	6.89	128.46	119.84
1	B	384	VAL	N-CA-C	-6.89	98.38	108.23
2	E	352	ILE	N-CA-C	-6.89	95.01	109.34
2	F	296	GLU	N-CA-C	6.89	120.79	112.38
1	B	196	GLN	N-CA-C	6.88	121.84	113.17
1	B	216	PHE	CA-CB-CG	-6.88	106.92	113.80
1	A	83	ILE	N-CA-C	-6.86	97.80	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	433	GLU	CA-C-N	6.85	129.77	120.38
2	E	433	GLU	C-N-CA	6.85	129.77	120.38
2	E	222	ASN	CA-CB-CG	-6.85	105.75	112.60
2	E	278	PRO	N-CA-C	-6.84	98.37	112.47
1	B	141	PHE	CA-CB-CG	-6.84	106.96	113.80
6	L	176	ASP	CA-CB-CG	6.84	119.44	112.60
1	A	433	SER	N-CA-C	-6.84	104.93	113.55
2	E	226	ASP	N-CA-C	-6.84	100.28	108.14
1	C	404	GLY	O-C-N	6.84	125.68	121.85
1	B	52	TYR	N-CA-C	6.83	119.59	111.33
1	B	153	VAL	N-CA-C	-6.83	98.46	107.88
1	A	506	TYR	N-CA-C	-6.82	96.27	110.80
2	F	34	ASP	CA-CB-CG	-6.82	105.78	112.60
1	C	316	GLN	CB-CG-CD	-6.80	101.04	112.60
1	B	227	PRO	N-CA-C	-6.79	98.48	112.47
1	C	266	LEU	CB-CA-C	-6.77	100.53	110.96
3	G	158	THR	N-CA-CB	6.77	120.84	110.14
2	E	410	ARG	N-CA-C	-6.77	104.66	113.12
2	D	375	HIS	N-CA-C	6.77	118.66	111.28
2	F	186	PRO	N-CA-C	-6.77	98.53	112.47
3	G	71	ASP	N-CA-C	-6.77	104.15	112.88
2	E	261	THR	N-CA-C	-6.74	103.86	111.07
2	E	433	GLU	N-CA-C	-6.74	103.55	111.03
1	B	32	GLU	N-CA-C	-6.74	103.94	111.28
6	L	135	ALA	N-CA-C	-6.73	104.08	112.90
1	C	381	VAL	CA-C-N	6.72	128.58	121.45
1	C	381	VAL	C-N-CA	6.72	128.58	121.45
1	B	310	ALA	N-CA-C	6.72	119.17	111.11
1	C	495	LEU	N-CA-C	-6.71	96.50	110.80
6	J	138	ARG	CA-C-N	6.70	134.54	121.41
6	J	138	ARG	C-N-CA	6.70	134.54	121.41
2	F	312	PRO	N-CA-C	-6.68	98.70	112.47
1	A	320	VAL	N-CA-C	6.68	118.05	109.30
2	D	66	LEU	N-CA-C	-6.68	98.46	107.88
6	L	44	ALA	N-CA-C	6.68	119.57	111.82
2	F	401	GLU	N-CA-C	-6.67	105.04	113.72
1	C	130	ARG	N-CA-C	-6.67	99.80	110.14
1	B	343	GLU	N-CA-C	-6.66	96.90	108.69
1	B	112	ASP	CA-CB-CG	-6.65	105.95	112.60
2	D	112	LEU	CA-C-O	-6.65	114.40	119.59
1	C	153	VAL	N-CA-C	-6.65	98.47	108.17
1	B	551	ALA	N-CA-C	6.64	119.37	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	MET	CG-SD-CE	-6.64	86.29	100.90
2	D	170	GLN	N-CA-C	6.63	118.51	111.28
2	D	355	LEU	CA-C-O	-6.63	112.23	118.33
2	E	375	HIS	CA-C-N	6.62	130.05	120.38
2	E	375	HIS	C-N-CA	6.62	130.05	120.38
2	D	186	PRO	CA-C-N	6.62	132.31	123.05
2	D	186	PRO	C-N-CA	6.62	132.31	123.05
2	D	74	SER	N-CA-C	6.62	119.06	108.41
2	F	177	LEU	N-CA-C	-6.60	104.36	112.88
2	D	277	ILE	CA-C-O	-6.59	115.42	119.51
2	E	270	ILE	CA-C-N	6.59	128.44	120.13
2	E	270	ILE	C-N-CA	6.59	128.44	120.13
1	B	127	ASP	CA-C-N	6.59	131.48	122.19
1	B	127	ASP	C-N-CA	6.59	131.48	122.19
2	D	90	GLY	N-CA-C	-6.58	97.58	113.18
2	F	204	PHE	CA-CB-CG	-6.58	107.22	113.80
2	F	422	PHE	N-CA-C	6.58	122.23	111.37
6	L	132	GLU	N-CA-C	-6.57	105.89	114.04
2	E	139	ASP	CA-CB-CG	-6.57	106.03	112.60
1	B	20	LEU	N-CA-C	-6.57	99.32	109.24
2	E	112	LEU	CA-C-N	6.57	126.53	120.03
2	E	112	LEU	C-N-CA	6.57	126.53	120.03
1	A	350	TYR	CA-CB-CG	-6.57	102.08	113.90
2	F	120	ASN	CA-CB-CG	-6.56	106.04	112.60
1	A	76	GLY	CA-C-N	6.56	126.92	119.83
1	A	76	GLY	C-N-CA	6.56	126.92	119.83
2	F	131	ILE	CA-C-N	6.56	131.44	122.19
2	F	131	ILE	C-N-CA	6.56	131.44	122.19
1	C	214	VAL	CB-CA-C	-6.55	103.30	112.14
2	D	104	PRO	N-CA-C	6.54	118.68	110.70
1	C	67	THR	N-CA-C	-6.54	104.91	114.39
2	D	103	LEU	CA-C-N	6.53	127.11	120.38
2	D	103	LEU	C-N-CA	6.53	127.11	120.38
2	D	111	ARG	N-CA-C	-6.53	99.18	109.50
1	A	337	ILE	CA-C-N	6.53	129.35	120.54
1	A	337	ILE	C-N-CA	6.53	129.35	120.54
2	D	321	ARG	N-CA-C	-6.53	96.90	110.80
6	J	36	GLU	CA-C-N	6.52	129.31	120.38
6	J	36	GLU	C-N-CA	6.52	129.31	120.38
6	J	53	TYR	N-CA-C	-6.52	103.38	112.12
1	B	557	GLU	N-CA-C	-6.51	104.37	112.90
3	G	188	ARG	N-CA-C	-6.51	103.80	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	VAL	N-CA-C	-6.51	98.98	108.87
1	A	430	LEU	N-CA-C	-6.50	104.03	112.68
2	E	34	ASP	CA-CB-CG	-6.49	106.11	112.60
2	D	115	THR	N-CA-C	-6.48	99.45	109.76
6	J	89	GLU	N-CA-C	6.48	118.89	111.11
1	B	85	ASP	CA-CB-CG	6.48	119.08	112.60
1	C	391	MET	N-CA-C	-6.48	97.12	108.20
2	F	249	HIS	CA-CB-CG	-6.47	107.33	113.80
1	C	50	GLN	N-CA-C	-6.47	99.63	109.85
1	B	386	PRO	N-CA-C	-6.47	102.81	110.70
1	A	290	ASN	CA-CB-CG	-6.46	106.14	112.60
2	E	147	GLY	CA-C-N	6.46	133.88	121.54
2	E	147	GLY	C-N-CA	6.46	133.88	121.54
1	A	488	ARG	N-CA-C	-6.46	103.14	111.02
2	D	273	ALA	N-CA-C	-6.45	104.35	112.93
2	F	104	PRO	N-CA-C	6.45	118.57	110.70
4	H	32	LEU	N-CA-C	-6.45	102.76	112.04
1	A	517	LYS	N-CA-C	-6.44	105.07	113.12
2	F	77	GLU	N-CA-C	-6.43	99.53	109.24
1	C	396	THR	N-CA-C	-6.42	105.98	113.88
2	E	183	LYS	CA-C-N	6.42	129.17	120.38
2	E	183	LYS	C-N-CA	6.42	129.17	120.38
7	M	214	PRO	CA-C-N	6.42	131.44	120.72
7	M	214	PRO	C-N-CA	6.42	131.44	120.72
2	D	374	ASP	N-CA-C	6.41	120.56	112.87
2	E	428	GLN	N-CA-C	-6.41	102.26	110.53
2	F	353	ASP	N-CA-C	-6.41	98.55	108.55
2	E	232	ILE	N-CA-C	-6.40	106.27	112.29
1	C	309	ILE	N-CA-C	-6.40	104.03	111.00
1	B	501	HIS	CA-CB-CG	-6.39	107.41	113.80
1	B	48	PHE	N-CA-C	-6.39	98.85	109.46
1	A	291	THR	CA-C-N	6.39	130.40	120.82
1	A	291	THR	C-N-CA	6.39	130.40	120.82
2	F	407	ASN	CA-CB-CG	-6.39	106.21	112.60
5	I	107	LEU	CA-C-N	6.39	129.13	120.38
5	I	107	LEU	C-N-CA	6.39	129.13	120.38
1	C	482	LEU	CA-C-N	6.38	129.53	120.53
1	C	482	LEU	C-N-CA	6.38	129.53	120.53
1	C	311	GLU	CB-CA-C	-6.37	100.88	110.88
2	D	429	ASN	N-CA-C	-6.37	101.03	110.46
1	C	103	THR	N-CA-C	-6.36	97.32	108.20
2	D	98	LYS	CA-C-N	6.35	127.78	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	98	LYS	C-N-CA	6.35	127.78	119.84
1	C	313	PHE	CA-CB-CG	-6.34	107.46	113.80
1	B	325	ASP	CA-CB-CG	6.33	118.93	112.60
2	E	430	ARG	N-CA-C	-6.33	100.00	108.74
2	F	240	THR	N-CA-C	-6.33	105.72	113.50
7	M	51	GLY	N-CA-C	-6.33	98.19	113.18
2	F	48	ILE	N-CA-C	6.32	117.54	111.91
6	L	103	VAL	N-CA-C	6.32	117.10	110.72
3	G	71	ASP	CB-CA-C	-6.31	100.05	110.72
4	H	28	GLU	N-CA-C	-6.31	107.43	114.62
3	G	4	VAL	N-CA-C	-6.30	101.42	109.30
1	B	337	ILE	N-CA-C	-6.29	104.39	110.42
3	G	52	ALA	N-CA-C	6.28	117.79	111.07
2	F	370	LYS	N-CA-C	-6.28	106.84	114.75
2	D	421	PHE	CA-CB-CG	-6.27	107.53	113.80
1	C	501	HIS	N-CA-C	-6.27	97.44	110.80
1	A	456	GLU	N-CA-CB	6.27	119.33	110.12
1	A	40	ILE	CB-CA-C	-6.26	103.78	112.36
1	B	477	GLN	CA-C-O	6.26	121.57	117.94
1	C	52	TYR	CB-CA-C	-6.26	103.16	111.74
2	E	142	ASN	CA-CB-CG	-6.26	106.34	112.60
1	C	97	LYS	CB-CA-C	-6.25	100.22	110.85
1	C	254	GLY	N-CA-C	-6.25	103.03	112.60
2	E	244	TYR	N-CA-C	-6.25	104.09	111.03
1	C	497	GLN	CB-CG-CD	-6.25	101.98	112.60
1	B	498	ASN	CA-CB-CG	-6.24	106.36	112.60
1	A	313	PHE	CA-CB-CG	-6.24	107.56	113.80
2	F	353	ASP	CB-CA-C	-6.23	98.66	109.32
1	A	50	GLN	N-CA-C	-6.23	99.04	109.07
2	D	92	ARG	N-CA-C	-6.22	97.28	108.48
2	D	139	ASP	CB-CA-C	-6.21	101.14	109.16
6	L	152	VAL	N-CA-C	-6.21	99.26	108.45
1	A	180	GLU	CB-CA-C	-6.20	101.18	110.24
1	C	267	VAL	N-CA-C	6.20	118.84	111.09
6	L	129	PRO	CA-C-N	6.20	128.59	120.28
6	L	129	PRO	C-N-CA	6.20	128.59	120.28
7	M	112	VAL	N-CA-C	-6.20	100.70	108.89
1	A	424	TRP	CB-CG-CD2	-6.20	118.13	126.80
2	F	148	GLN	N-CA-CB	6.20	119.97	109.87
2	D	221	LEU	CA-C-N	6.19	131.51	122.41
2	D	221	LEU	C-N-CA	6.19	131.51	122.41
2	E	201	LEU	N-CA-C	-6.19	103.26	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	100	PHE	CA-CB-CG	-6.18	107.62	113.80
4	H	68	LEU	CA-C-N	6.17	127.56	119.84
4	H	68	LEU	C-N-CA	6.17	127.56	119.84
3	G	17	GLN	N-CA-C	-6.17	104.47	111.14
2	D	61	GLU	CA-C-N	6.17	132.66	121.06
2	D	61	GLU	C-N-CA	6.17	132.66	121.06
6	L	92	GLU	N-CA-CB	-6.17	100.82	110.44
7	M	55	PRO	CA-C-N	6.17	129.68	120.31
7	M	55	PRO	C-N-CA	6.17	129.68	120.31
2	F	135	ILE	N-CA-CB	6.16	121.39	111.23
2	F	402	ASP	N-CA-C	-6.16	97.68	110.80
1	B	308	THR	N-CA-CB	6.15	120.89	110.49
1	A	156	ARG	CA-C-N	6.14	129.83	120.13
1	A	156	ARG	C-N-CA	6.14	129.83	120.13
1	A	361	PHE	CA-CB-CG	6.14	119.94	113.80
1	B	218	VAL	N-CA-C	-6.14	107.88	113.71
1	B	150	PRO	N-CA-C	-6.13	104.02	110.58
7	M	35	ASP	CA-C-N	6.13	128.41	120.44
7	M	35	ASP	C-N-CA	6.13	128.41	120.44
2	F	371	THR	N-CA-C	-6.12	100.11	108.38
1	C	504	ASP	CA-C-N	6.12	133.23	121.54
1	C	504	ASP	C-N-CA	6.12	133.23	121.54
1	A	419	PHE	CB-CA-C	-6.12	102.14	110.22
4	H	80	ALA	N-CA-C	-6.11	97.78	110.80
1	C	213	ASP	CA-CB-CG	-6.11	106.49	112.60
1	C	477	GLN	N-CA-C	-6.11	100.61	110.32
1	C	420	PRO	N-CA-C	-6.10	96.23	112.10
2	E	110	LYS	CA-C-N	6.10	130.54	122.30
2	E	110	LYS	C-N-CA	6.10	130.54	122.30
4	H	79	GLU	CA-C-N	6.10	133.20	121.54
4	H	79	GLU	C-N-CA	6.10	133.20	121.54
7	M	141	ALA	CA-C-N	6.10	126.28	120.43
7	M	141	ALA	C-N-CA	6.10	126.28	120.43
1	B	508	SER	N-CA-C	-6.09	99.48	108.79
3	G	119	THR	O-C-N	-6.09	114.32	121.32
6	J	112	LEU	CA-C-N	6.09	128.93	120.29
6	J	112	LEU	C-N-CA	6.09	128.93	120.29
2	F	174	ARG	N-CA-C	-6.08	101.91	110.31
1	A	144	THR	N-CA-C	-6.07	98.51	108.41
1	A	423	ASN	CA-CB-CG	-6.07	106.53	112.60
4	H	96	LYS	N-CA-C	-6.07	101.01	110.42
2	E	408	ASP	N-CA-C	-6.06	105.79	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	LEU	N-CA-C	6.06	117.58	110.97
7	M	267	CYS	CB-CA-C	-6.06	100.73	110.79
1	B	230	PHE	CA-CB-CG	-6.06	107.74	113.80
5	I	78	ARG	CA-C-N	6.06	128.40	120.28
5	I	78	ARG	C-N-CA	6.06	128.40	120.28
5	I	104	MET	CA-C-N	6.06	129.21	120.79
5	I	104	MET	C-N-CA	6.06	129.21	120.79
2	F	348	ILE	N-CA-CB	-6.05	104.17	110.95
3	G	165	GLU	CB-CA-C	-6.05	97.65	110.31
2	D	380	ASP	N-CA-C	-6.05	105.48	112.92
1	C	244	TRP	N-CA-C	-6.04	100.22	109.41
7	M	177	ALA	N-CA-C	6.04	117.54	111.07
2	D	129	GLN	CB-CG-CD	-6.03	102.35	112.60
1	B	98	THR	CB-CA-C	-6.03	101.26	109.28
1	B	563	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	67	THR	N-CA-C	-6.03	106.54	114.31
1	C	20	LEU	N-CA-C	-6.02	98.00	107.93
2	D	336	GLN	CA-C-N	6.02	132.81	121.97
2	D	336	GLN	C-N-CA	6.02	132.81	121.97
2	D	136	SER	CA-C-N	6.02	129.16	120.38
2	D	136	SER	C-N-CA	6.02	129.16	120.38
2	E	375	HIS	CB-CA-C	-6.01	101.41	110.90
1	B	464	LEU	CA-C-N	6.01	128.58	120.65
1	B	464	LEU	C-N-CA	6.01	128.58	120.65
2	E	316	MET	CA-C-N	6.00	126.78	120.12
2	E	316	MET	C-N-CA	6.00	126.78	120.12
7	M	100	LEU	N-CA-C	6.00	117.49	111.07
1	A	426	GLY	N-CA-C	-6.00	98.96	113.18
1	C	389	GLY	N-CA-C	-6.00	105.67	114.90
2	D	122	VAL	CB-CA-C	-5.98	104.07	112.14
1	B	487	GLY	CA-C-N	5.97	128.60	120.54
1	B	487	GLY	C-N-CA	5.97	128.60	120.54
1	A	55	THR	N-CA-C	-5.97	100.32	108.38
1	B	238	GLN	CB-CA-C	-5.97	100.53	110.68
6	J	78	GLU	N-CA-CB	5.97	119.41	110.22
1	C	485	GLU	CB-CA-C	-5.96	100.48	110.56
2	D	339	LEU	N-CA-C	-5.96	99.29	109.24
1	A	147	ILE	N-CA-C	-5.96	99.90	108.42
2	D	422	PHE	CA-CB-CG	-5.96	107.84	113.80
4	H	27	GLU	N-CA-C	-5.96	103.47	111.87
7	M	45	TYR	CA-C-N	5.95	130.97	120.74
7	M	45	TYR	C-N-CA	5.95	130.97	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	136	SER	CA-C-N	5.95	132.90	121.54
2	E	136	SER	C-N-CA	5.95	132.90	121.54
1	A	45	ASP	CA-CB-CG	-5.94	106.66	112.60
2	D	450	GLU	CB-CA-C	-5.94	99.41	109.03
3	G	29	LYS	N-CA-CB	5.94	118.68	110.07
1	A	353	TYR	CB-CA-C	-5.94	98.61	110.42
1	A	318	PHE	CA-CB-CG	-5.93	107.87	113.80
1	B	174	VAL	CB-CA-C	-5.92	103.05	111.40
1	A	559	PHE	CA-CB-CG	-5.92	107.89	113.80
2	F	213	ALA	CA-C-N	5.92	128.53	120.54
2	F	213	ALA	C-N-CA	5.92	128.53	120.54
1	A	182	LYS	N-CA-C	-5.91	101.18	109.69
1	B	525	GLU	N-CA-C	-5.91	106.41	113.97
1	C	281	LEU	N-CA-C	5.91	119.96	112.87
7	M	245	SER	N-CA-C	-5.90	100.94	110.32
1	C	97	LYS	N-CA-C	5.89	117.78	111.36
1	B	355	ALA	N-CA-C	-5.89	98.25	110.80
2	D	149	LYS	N-CA-C	-5.88	101.49	110.14
2	F	237	MET	CB-CA-C	-5.88	101.40	110.81
2	E	148	GLN	N-CA-C	5.87	123.31	110.80
1	A	64	VAL	N-CA-CB	5.87	120.91	111.23
2	F	378	VAL	CB-CA-C	-5.86	104.31	111.87
2	F	23	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	197	ARG	CA-C-N	5.85	129.79	121.42
1	A	197	ARG	C-N-CA	5.85	129.79	121.42
3	G	159	ARG	N-CA-C	5.85	118.13	111.11
1	B	212	LEU	N-CA-CB	5.85	120.38	110.49
2	F	167	ILE	CB-CA-C	-5.85	104.40	112.24
2	E	187	PHE	N-CA-C	5.85	118.43	108.90
1	C	429	SER	N-CA-C	-5.84	101.30	110.36
1	A	381	VAL	N-CA-C	-5.84	97.19	109.34
7	M	38	ARG	CB-CA-C	-5.84	101.72	110.88
2	F	339	LEU	N-CA-C	-5.83	100.78	110.17
1	C	531	LYS	CA-C-N	5.83	128.10	120.28
1	C	531	LYS	C-N-CA	5.83	128.10	120.28
2	D	312	PRO	N-CA-C	-5.83	100.46	112.47
1	B	150	PRO	CA-C-O	-5.83	116.13	120.73
3	G	160	ARG	CB-CA-C	-5.82	100.95	110.85
2	E	362	MET	N-CA-CB	5.82	120.33	110.49
2	E	279	GLY	N-CA-C	-5.82	107.44	114.66
2	E	169	ARG	CB-CA-C	-5.82	99.96	109.56
1	C	562	TYR	N-CA-C	-5.81	106.35	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	141	MET	CG-SD-CE	-5.81	88.12	100.90
2	E	315	SER	CB-CA-C	-5.80	99.68	109.72
2	F	104	PRO	CA-C-N	5.80	126.61	120.11
2	F	104	PRO	C-N-CA	5.80	126.61	120.11
2	F	253	VAL	CA-C-N	5.79	130.71	122.72
2	F	253	VAL	C-N-CA	5.79	130.71	122.72
1	A	111	LEU	N-CA-C	-5.79	99.97	109.40
1	A	274	ASP	CA-CB-CG	-5.78	106.82	112.60
2	E	251	TYR	N-CA-C	-5.78	100.76	108.74
2	F	424	ASN	N-CA-C	-5.78	101.12	110.32
1	A	381	VAL	CA-C-N	5.78	127.57	120.92
1	A	381	VAL	C-N-CA	5.78	127.57	120.92
2	D	139	ASP	N-CA-C	-5.78	107.47	114.75
1	A	351	PRO	CA-C-O	-5.78	116.17	120.73
3	G	60	ALA	N-CA-C	-5.78	104.42	112.45
2	E	374	ASP	N-CA-C	5.77	120.44	113.17
2	D	166	GLN	N-CA-CB	5.77	118.37	110.01
2	E	181	GLY	CA-C-N	5.76	128.48	120.29
2	E	181	GLY	C-N-CA	5.76	128.48	120.29
6	J	47	ARG	N-CA-C	5.76	118.05	111.02
2	D	372	ARG	N-CA-CB	5.76	120.22	110.49
1	C	446	ASP	CA-CB-CG	5.75	118.35	112.60
3	G	157	THR	N-CA-CB	5.75	118.30	109.91
1	B	290	ASN	CA-CB-CG	-5.75	106.85	112.60
1	B	176	GLU	CA-C-N	5.74	132.50	121.54
1	B	176	GLU	C-N-CA	5.74	132.50	121.54
2	E	165	ALA	N-CA-C	-5.74	104.66	111.03
1	A	172	VAL	N-CA-C	-5.74	106.72	112.17
2	E	131	ILE	N-CA-CB	5.73	117.59	111.46
1	B	461	GLU	CB-CA-C	-5.73	101.08	110.08
2	F	230	GLU	CA-C-N	5.73	130.29	120.72
2	F	230	GLU	C-N-CA	5.73	130.29	120.72
1	C	386	PRO	N-CA-C	-5.73	103.71	110.70
3	G	157	THR	CA-C-O	-5.72	115.00	121.00
7	M	224	PHE	CA-CB-CG	-5.72	108.08	113.80
3	G	160	ARG	CA-C-N	5.71	128.25	120.77
3	G	160	ARG	C-N-CA	5.71	128.25	120.77
1	A	53	GLU	CA-C-N	5.71	132.44	121.54
1	A	53	GLU	C-N-CA	5.71	132.44	121.54
1	A	264	ASP	CA-CB-CG	-5.71	106.89	112.60
1	B	358	LEU	N-CA-C	-5.71	104.98	111.14
2	F	50	VAL	CB-CA-C	-5.71	102.18	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	318	ASP	N-CA-C	-5.71	105.98	113.17
7	M	72	LEU	CA-C-N	5.70	125.32	119.56
7	M	72	LEU	C-N-CA	5.70	125.32	119.56
2	D	329	THR	N-CA-CB	5.70	119.41	109.72
7	M	142	VAL	N-CA-CB	5.70	114.34	110.52
4	H	66	ARG	N-CA-C	-5.70	98.67	110.80
7	M	130	ALA	CA-C-N	5.69	132.40	121.54
7	M	130	ALA	C-N-CA	5.69	132.40	121.54
1	B	492	GLU	N-CA-C	-5.69	106.69	113.97
2	D	449	GLY	N-CA-C	-5.69	107.40	115.30
2	F	82	LEU	N-CA-C	-5.68	100.66	109.24
1	A	73	VAL	CA-C-N	5.68	130.76	122.41
1	A	73	VAL	C-N-CA	5.68	130.76	122.41
2	D	208	PHE	CA-CB-CG	-5.68	108.12	113.80
2	D	453	ARG	N-CA-C	-5.68	104.47	111.40
1	B	431	PHE	N-CA-C	5.67	117.92	111.11
7	M	14	VAL	N-CA-C	5.66	115.86	110.42
2	E	68	LEU	N-CA-C	-5.66	104.25	113.19
2	F	374	ASP	CB-CA-C	-5.66	102.07	110.67
1	A	149	VAL	N-CA-C	-5.65	103.76	109.02
1	C	364	ARG	N-CA-C	5.65	118.17	111.33
1	B	52	TYR	CB-CA-C	-5.65	101.08	110.68
2	F	456	LYS	N-CA-C	5.65	118.16	111.33
3	G	94	GLU	N-CA-C	-5.65	99.92	107.88
1	B	158	LYS	N-CA-C	-5.64	100.49	109.23
1	A	415	PHE	CB-CA-C	-5.63	100.21	110.63
2	D	173	VAL	N-CA-CB	5.63	117.24	110.31
7	M	290	VAL	N-CA-C	5.63	115.83	110.42
1	A	536	ILE	CB-CA-C	-5.63	101.04	111.79
1	B	418	HIS	CA-CB-CG	5.62	119.42	113.80
2	E	21	VAL	CB-CA-C	-5.62	102.08	111.29
5	I	84	LEU	N-CA-C	5.62	117.40	111.28
1	A	180	GLU	CB-CG-CD	-5.61	103.06	112.60
1	B	292	SER	CA-C-N	5.61	132.26	121.54
1	B	292	SER	C-N-CA	5.61	132.26	121.54
2	D	372	ARG	N-CA-C	-5.61	98.84	110.80
1	C	96	GLU	CA-C-N	-5.61	112.32	120.29
1	C	96	GLU	C-N-CA	-5.61	112.32	120.29
1	A	150	PRO	N-CA-C	-5.61	103.86	110.70
1	C	86	GLY	N-CA-C	5.61	120.89	113.37
1	C	186	THR	N-CA-C	5.61	117.22	109.15
1	C	2	ILE	N-CA-C	-5.61	100.15	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	GLY	N-CA-C	-5.60	99.90	113.18
1	C	187	TRP	CA-C-N	5.60	126.84	119.84
1	C	187	TRP	C-N-CA	5.60	126.84	119.84
2	F	177	LEU	CA-C-N	5.60	131.06	121.87
2	F	177	LEU	C-N-CA	5.60	131.06	121.87
3	G	8	ARG	CA-C-N	5.60	132.24	121.54
3	G	8	ARG	C-N-CA	5.60	132.24	121.54
5	I	74	ARG	CB-CA-C	-5.60	98.95	110.38
6	J	113	GLU	N-CA-CB	-5.60	101.87	110.16
2	E	27	LEU	N-CA-C	-5.60	98.62	108.20
1	B	183	MET	CB-CA-C	-5.60	102.05	110.90
2	D	277	ILE	N-CA-C	-5.59	100.95	107.61
1	B	150	PRO	N-CA-CB	5.59	106.13	103.22
1	B	265	VAL	N-CA-CB	5.59	116.72	110.62
2	E	296	GLU	CB-CG-CD	-5.59	103.10	112.60
1	A	114	GLU	CB-CG-CD	-5.59	103.10	112.60
2	D	264	CYS	N-CA-C	-5.59	106.14	113.12
3	G	194	LEU	CA-C-N	5.59	128.08	120.54
3	G	194	LEU	C-N-CA	5.59	128.08	120.54
4	H	45	VAL	N-CA-C	-5.58	100.98	108.35
2	E	362	MET	N-CA-C	-5.58	98.91	110.80
1	B	362	TYR	N-CA-C	-5.58	106.14	113.12
2	E	380	ASP	CA-CB-CG	-5.58	107.02	112.60
2	F	76	VAL	CB-CA-C	-5.58	104.61	111.92
2	D	323	HIS	O-C-N	-5.58	115.56	121.30
1	C	379	THR	CA-CB-OG1	-5.58	101.24	109.60
2	E	237	MET	N-CA-C	-5.58	104.05	111.24
1	B	376	GLY	CA-C-N	5.57	129.26	121.24
1	B	376	GLY	C-N-CA	5.57	129.26	121.24
1	A	449	GLU	CB-CA-C	5.57	120.64	110.11
1	C	177	ASP	CA-CB-CG	-5.57	107.03	112.60
1	C	419	PHE	CB-CA-C	-5.56	100.49	109.67
1	B	61	GLY	N-CA-C	-5.56	107.69	114.92
1	B	189	VAL	CB-CA-C	-5.56	104.63	112.14
7	M	301	ARG	N-CA-C	5.56	117.42	111.36
4	H	91	ARG	N-CA-C	-5.56	105.76	112.54
1	C	354	LEU	N-CA-CB	5.56	118.24	110.07
2	F	390	VAL	CB-CA-C	-5.56	102.17	111.29
1	B	91	LEU	N-CA-C	5.56	119.56	112.34
6	J	137	GLU	CA-C-N	5.56	132.15	121.54
6	J	137	GLU	C-N-CA	5.56	132.15	121.54
1	B	353	TYR	CB-CA-C	-5.55	99.37	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	537	ASP	CA-CB-CG	-5.55	107.05	112.60
2	D	450	GLU	CB-CG-CD	-5.55	103.17	112.60
2	E	98	LYS	N-CA-C	-5.55	97.55	109.81
2	F	262	ASN	N-CA-C	-5.53	106.03	112.89
7	M	6	ALA	N-CA-C	5.53	117.00	110.97
1	C	459	GLN	N-CA-C	-5.53	104.94	110.97
2	D	153	PHE	CB-CA-C	-5.53	102.26	110.67
1	B	260	ASN	CA-CB-CG	-5.52	107.08	112.60
1	A	501	HIS	N-CA-CB	5.52	118.17	109.83
1	C	473	PRO	N-CA-C	-5.52	101.10	112.47
2	D	20	PHE	N-CA-C	-5.51	101.88	110.42
1	B	495	LEU	CA-C-N	5.51	132.07	121.54
1	B	495	LEU	C-N-CA	5.51	132.07	121.54
1	C	20	LEU	CB-CA-C	-5.51	102.62	110.34
1	A	238	GLN	N-CA-C	-5.51	105.92	113.30
2	F	319	ASP	CA-CB-CG	-5.51	107.09	112.60
2	E	54	TYR	CA-C-N	5.50	129.29	121.42
2	E	54	TYR	C-N-CA	5.50	129.29	121.42
2	D	113	PRO	CA-C-O	-5.50	115.34	121.23
2	D	220	PHE	N-CA-C	-5.50	99.08	110.80
4	H	63	MET	CA-C-N	5.50	130.18	122.36
4	H	63	MET	C-N-CA	5.50	130.18	122.36
1	B	174	VAL	CA-C-O	5.50	125.60	121.09
1	B	109	HIS	N-CA-C	-5.50	100.77	108.96
6	J	35	GLU	CA-C-N	5.49	127.91	120.44
6	J	35	GLU	C-N-CA	5.49	127.91	120.44
2	F	182	GLU	N-CA-C	-5.49	106.75	113.50
1	A	454	ILE	N-CA-C	-5.49	105.50	110.82
1	C	419	PHE	N-CA-C	-5.49	101.43	109.50
7	M	100	LEU	CB-CA-C	-5.49	102.27	110.88
2	E	249	HIS	CA-CB-CG	-5.48	108.32	113.80
2	E	394	LYS	N-CA-CB	5.47	117.92	109.98
2	F	46	GLN	N-CA-C	5.47	118.73	109.76
3	G	104	LEU	CB-CA-C	-5.47	99.53	110.42
1	A	547	ARG	N-CA-C	-5.47	104.96	111.69
2	F	165	ALA	N-CA-C	5.47	117.32	111.36
1	B	168	VAL	N-CA-C	5.47	116.19	110.62
1	B	352	PRO	CA-C-N	5.47	131.98	121.54
1	B	352	PRO	C-N-CA	5.47	131.98	121.54
1	A	85	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	459	GLN	CB-CG-CD	5.46	121.89	112.60
1	B	357	ARG	CA-C-N	5.46	127.87	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ARG	C-N-CA	5.46	127.87	120.44
3	G	47	MET	N-CA-C	5.46	119.94	113.28
1	A	490	ILE	N-CA-C	5.46	118.70	111.17
2	D	23	ASN	CA-CB-CG	-5.46	107.14	112.60
2	E	402	ASP	N-CA-C	-5.46	99.17	110.80
2	D	408	ASP	CA-CB-CG	-5.45	107.15	112.60
2	E	163	ILE	CB-CA-C	-5.45	104.99	111.97
3	G	72	GLY	CA-C-N	5.45	126.66	119.84
3	G	72	GLY	C-N-CA	5.45	126.66	119.84
3	G	177	ARG	N-CA-CB	5.45	118.06	109.94
1	B	74	GLU	CB-CG-CD	-5.45	103.34	112.60
6	L	83	VAL	CB-CA-C	-5.45	104.79	112.14
2	E	356	PRO	N-CA-C	-5.44	101.26	112.47
2	E	402	ASP	CA-C-N	5.44	131.93	121.54
2	E	402	ASP	C-N-CA	5.44	131.93	121.54
6	J	62	SER	CA-C-N	5.43	127.83	120.44
6	J	62	SER	C-N-CA	5.43	127.83	120.44
2	D	93	PHE	CB-CA-C	-5.43	98.78	110.45
1	B	451	ARG	N-CA-CB	5.42	118.02	109.94
2	D	418	PHE	N-CA-C	-5.42	104.91	112.45
2	E	262	ASN	CA-CB-CG	5.42	118.02	112.60
2	E	204	PHE	CB-CA-C	-5.42	99.11	110.17
7	M	81	ARG	CA-C-N	5.42	127.55	120.28
7	M	81	ARG	C-N-CA	5.42	127.55	120.28
1	A	48	PHE	CA-C-N	5.42	127.84	120.63
1	A	48	PHE	C-N-CA	5.42	127.84	120.63
2	E	101	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	21	GLY	N-CA-C	-5.40	107.79	115.30
6	J	61	GLU	CA-C-N	5.40	128.52	120.31
6	J	61	GLU	C-N-CA	5.40	128.52	120.31
1	A	408	ARG	N-CA-C	-5.40	101.08	109.72
2	E	403	ALA	N-CA-C	-5.40	99.30	110.80
1	B	78	GLY	N-CA-C	-5.40	107.66	115.27
6	L	141	GLU	N-CA-C	-5.39	100.54	108.79
1	C	402	ILE	N-CA-C	-5.39	98.12	109.34
1	C	363	GLU	N-CA-CB	5.39	117.78	109.91
1	B	42	LEU	CB-CA-C	-5.39	99.04	109.76
2	F	174	ARG	CB-CA-C	-5.38	101.20	108.68
1	A	491	ARG	N-CA-CB	5.38	118.15	110.67
1	C	26	ASP	CA-CB-CG	-5.38	107.22	112.60
2	D	209	GLU	N-CA-C	5.38	119.11	112.54
3	G	143	THR	N-CA-CB	5.38	118.53	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	141	MET	CB-CA-C	-5.37	102.41	110.90
1	B	520	LEU	N-CA-C	-5.37	104.31	111.24
1	B	464	LEU	N-CA-C	-5.37	105.54	112.68
2	F	391	ASP	CA-CB-CG	-5.37	107.23	112.60
3	G	40	PHE	N-CA-C	5.37	117.13	111.28
3	G	201	ILE	CB-CA-C	-5.37	105.01	112.04
2	D	133	THR	N-CA-C	-5.37	105.85	112.72
7	M	28	ALA	CA-C-N	5.37	128.01	120.28
7	M	28	ALA	C-N-CA	5.37	128.01	120.28
2	F	442	LEU	N-CA-C	-5.36	106.58	113.23
1	C	102	ILE	N-CA-C	-5.35	100.04	108.23
2	D	265	GLU	N-CA-C	-5.35	104.49	111.02
2	F	306	GLY	CA-C-O	-5.35	117.37	122.13
2	D	62	GLU	N-CA-C	-5.34	103.84	110.41
2	E	375	HIS	N-CA-CB	5.34	117.81	110.07
2	F	407	ASN	N-CA-C	-5.34	104.36	111.24
2	D	355	LEU	N-CA-C	5.33	120.86	113.45
2	E	252	HIS	N-CA-C	-5.33	99.72	108.41
2	E	70	THR	N-CA-CB	5.33	115.52	108.96
2	E	109	GLU	N-CA-C	-5.33	99.44	110.80
1	A	279	GLY	CA-C-N	5.33	125.58	119.83
1	A	279	GLY	C-N-CA	5.33	125.58	119.83
1	C	260	ASN	CB-CA-C	-5.33	100.44	110.67
1	A	209	MET	N-CA-CB	5.32	118.91	110.55
2	E	283	TYR	CA-CB-CG	-5.32	104.32	113.90
1	B	447	TYR	CA-C-N	5.32	124.77	119.24
1	B	447	TYR	C-N-CA	5.32	124.77	119.24
2	D	155	GLY	N-CA-C	-5.32	105.29	112.57
7	M	27	GLU	N-CA-C	5.32	117.08	111.28
1	B	553	TYR	CA-CB-CG	-5.31	104.33	113.90
2	D	375	HIS	CB-CA-C	-5.31	101.97	110.79
2	E	158	LEU	N-CA-C	-5.31	103.34	109.93
1	B	251	VAL	N-CA-C	-5.31	100.48	108.12
1	C	567	MET	N-CA-CB	5.31	118.43	109.78
2	D	165	ALA	N-CA-C	5.31	119.24	112.34
1	C	6	ILE	N-CA-CB	-5.31	101.72	111.91
2	D	58	GLN	CB-CG-CD	-5.31	103.58	112.60
1	A	89	ARG	CA-C-N	5.30	126.47	119.84
1	A	89	ARG	C-N-CA	5.30	126.47	119.84
1	C	230	PHE	CA-CB-CG	5.30	119.10	113.80
2	E	334	GLU	N-CA-C	-5.30	102.35	110.14
2	D	194	MET	N-CA-CB	5.29	119.61	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	LEU	N-CA-CB	5.29	119.75	110.27
1	C	472	GLY	N-CA-C	-5.29	101.54	112.34
1	A	56	SER	N-CA-CB	5.29	119.43	110.49
3	G	155	LYS	CA-C-N	5.29	127.62	120.38
3	G	155	LYS	C-N-CA	5.29	127.62	120.38
2	F	450	GLU	N-CA-C	-5.29	106.77	114.12
1	A	501	HIS	CA-CB-CG	-5.28	108.52	113.80
2	F	452	LYS	N-CA-C	-5.28	106.68	113.23
2	D	138	ILE	N-CA-C	-5.28	107.21	111.91
2	E	198	GLN	CA-C-N	5.28	127.62	120.65
2	E	198	GLN	C-N-CA	5.28	127.62	120.65
1	B	90	PRO	CA-C-N	5.28	129.13	120.63
1	B	90	PRO	C-N-CA	5.28	129.13	120.63
1	C	506	TYR	N-CA-CB	5.28	119.41	110.49
2	E	242	ALA	CB-CA-C	-5.27	102.04	110.79
5	I	103	ALA	CA-C-N	5.27	131.61	121.54
5	I	103	ALA	C-N-CA	5.27	131.61	121.54
5	I	75	GLU	N-CA-CB	5.27	117.62	109.98
1	B	545	LEU	CB-CA-C	-5.27	100.56	110.67
2	E	199	ARG	N-CA-CB	-5.27	102.22	109.91
6	J	135	ALA	N-CA-C	-5.27	106.00	112.90
3	G	49	ALA	CA-C-N	5.27	127.65	120.54
3	G	49	ALA	C-N-CA	5.27	127.65	120.54
2	E	273	ALA	N-CA-C	-5.26	99.58	110.80
1	A	479	ALA	N-CA-C	-5.26	106.37	112.89
1	B	411	ALA	N-CA-C	5.26	117.01	111.28
7	M	224	PHE	CB-CA-C	-5.26	101.28	110.17
1	B	234	LYS	N-CA-C	5.25	117.01	111.28
2	F	143	THR	CA-C-N	5.25	128.68	120.75
2	F	143	THR	C-N-CA	5.25	128.68	120.75
2	F	237	MET	CG-SD-CE	-5.25	89.34	100.90
2	F	382	LEU	CA-C-N	5.25	131.57	121.54
2	F	382	LEU	C-N-CA	5.25	131.57	121.54
2	F	109	GLU	N-CA-C	-5.24	105.21	113.02
2	E	255	VAL	N-CA-C	-5.24	100.52	108.17
2	D	327	ASP	CA-C-N	5.24	129.52	121.19
2	D	327	ASP	C-N-CA	5.24	129.52	121.19
2	F	305	LYS	N-CA-C	-5.24	100.76	108.99
4	H	19	GLU	CA-C-N	5.24	131.68	121.41
4	H	19	GLU	C-N-CA	5.24	131.68	121.41
2	D	457	ASP	CB-CA-C	-5.24	102.66	110.88
1	A	171	PRO	N-CA-C	-5.23	101.69	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	MET	CB-CA-C	-5.23	100.01	110.42
3	G	119	THR	CB-CA-C	5.23	120.48	110.17
1	A	492	GLU	N-CA-C	-5.23	105.64	112.23
2	D	180	GLU	CA-C-N	5.23	124.94	119.92
2	D	180	GLU	C-N-CA	5.23	124.94	119.92
1	B	537	ASP	CA-CB-CG	-5.23	107.37	112.60
1	A	397	GLN	CB-CA-C	-5.22	101.97	110.85
1	A	407	TRP	N-CA-C	-5.22	101.64	109.95
2	F	383	TYR	CA-CB-CG	5.22	123.30	113.90
2	F	319	ASP	N-CA-C	-5.22	105.37	112.26
3	G	36	VAL	CA-CB-CG2	5.22	119.28	110.40
1	A	394	PRO	N-CA-C	5.22	123.22	112.47
2	E	117	LEU	CA-C-N	5.22	125.21	119.89
2	E	117	LEU	C-N-CA	5.22	125.21	119.89
2	F	81	ARG	N-CA-C	-5.22	100.51	108.76
1	A	114	GLU	CB-CA-C	-5.21	101.02	110.56
1	B	130	ARG	N-CA-C	-5.21	101.37	109.24
1	C	324	ALA	N-CA-C	-5.21	101.28	109.25
2	E	201	LEU	N-CA-CB	5.21	117.72	110.07
7	M	57	VAL	CB-CA-C	-5.21	105.20	112.02
1	C	244	TRP	CA-CB-CG	-5.21	103.71	113.60
1	C	291	THR	CA-C-N	5.20	127.25	120.28
1	C	291	THR	C-N-CA	5.20	127.25	120.28
2	D	71	THR	N-CA-C	-5.20	99.72	110.80
1	B	336	GLU	N-CA-C	5.20	117.35	111.11
1	C	316	GLN	CB-CA-C	-5.20	104.79	111.50
2	F	414	PHE	N-CA-C	-5.19	107.12	113.50
3	G	32	ARG	N-CA-C	5.18	117.83	111.82
3	G	200	LYS	N-CA-C	-5.18	105.28	111.03
2	F	298	ALA	N-CA-C	-5.18	99.77	110.80
2	F	225	ASP	CA-CB-CG	-5.18	107.42	112.60
2	D	171	ALA	CA-C-N	5.17	129.96	121.58
2	D	171	ALA	C-N-CA	5.17	129.96	121.58
2	D	425	GLN	CB-CG-CD	-5.17	103.81	112.60
1	B	559	PHE	CA-CB-CG	-5.17	108.63	113.80
7	M	174	GLU	CB-CA-C	-5.17	102.21	110.79
1	B	407	TRP	CB-CA-C	-5.16	103.82	111.72
3	G	51	LYS	CB-CA-C	-5.16	102.22	110.79
1	B	362	TYR	CA-C-N	-5.16	114.24	121.72
1	B	362	TYR	C-N-CA	-5.16	114.24	121.72
3	G	11	LEU	CB-CA-C	-5.16	102.17	110.74
2	D	233	LEU	CB-CA-C	-5.16	100.76	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	287	LEU	CB-CA-C	-5.16	102.78	110.88
1	A	69	LEU	N-CA-C	-5.16	102.35	110.14
1	C	479	ALA	CA-C-N	5.16	127.46	120.44
1	C	479	ALA	C-N-CA	5.16	127.46	120.44
1	A	293	ASN	N-CA-C	5.16	117.57	111.33
1	B	119	TRP	N-CA-C	5.15	114.84	108.19
1	B	318	PHE	CA-CB-CG	-5.15	108.65	113.80
2	D	311	ILE	N-CA-C	-5.15	97.75	108.88
2	F	27	LEU	N-CA-C	-5.15	99.83	110.80
7	M	71	ASP	N-CA-C	5.15	116.89	111.28
2	E	103	LEU	CA-C-N	5.15	125.68	120.38
2	E	103	LEU	C-N-CA	5.15	125.68	120.38
6	L	97	LYS	CA-C-N	5.15	125.83	120.12
6	L	97	LYS	C-N-CA	5.15	125.83	120.12
1	B	40	ILE	N-CA-C	-5.14	98.64	109.34
1	B	371	LEU	N-CA-C	-5.14	106.51	112.89
1	C	84	TYR	N-CA-C	-5.14	108.27	114.75
1	C	542	LEU	CB-CA-C	-5.14	101.63	109.50
2	F	232	ILE	N-CA-C	-5.14	107.82	113.43
1	A	508	SER	N-CA-C	-5.14	102.91	110.52
1	C	109	HIS	N-CA-C	-5.14	103.90	110.53
2	F	316	MET	CG-SD-CE	-5.14	89.59	100.90
4	H	75	ALA	N-CA-CB	5.14	119.18	110.49
2	F	148	GLN	CB-CA-C	-5.14	101.86	110.29
1	B	364	ARG	N-CA-CB	5.14	119.17	110.49
2	E	180	GLU	CA-C-N	5.14	125.55	120.31
2	E	180	GLU	C-N-CA	5.14	125.55	120.31
2	D	265	GLU	N-CA-CB	5.13	117.62	109.82
6	L	35	GLU	CA-C-N	5.13	127.42	120.44
6	L	35	GLU	C-N-CA	5.13	127.42	120.44
1	A	161	LYS	CA-C-O	-5.13	114.84	120.17
1	A	454	ILE	N-CA-CB	5.12	117.90	110.52
2	D	258	THR	CA-C-N	5.12	130.01	122.63
2	D	258	THR	C-N-CA	5.12	130.01	122.63
7	M	79	GLU	CA-C-N	5.12	127.14	120.28
7	M	79	GLU	C-N-CA	5.12	127.14	120.28
1	A	189	VAL	CB-CA-C	-5.12	102.89	111.29
2	D	232	ILE	CA-C-O	-5.12	116.08	121.41
1	C	497	GLN	N-CA-CB	5.12	119.14	110.49
1	C	77	PRO	N-CA-C	-5.12	101.93	112.47
1	A	425	ASN	CA-CB-CG	-5.11	107.49	112.60
2	D	448	GLN	CB-CG-CD	-5.11	103.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	252	HIS	N-CA-C	-5.11	100.12	108.76
2	E	327	ASP	CB-CA-C	-5.11	103.09	110.96
2	D	138	ILE	N-CA-CB	-5.11	106.41	112.39
1	C	147	ILE	CA-C-N	5.11	128.10	120.95
1	C	147	ILE	C-N-CA	5.11	128.10	120.95
5	K	72	GLN	CB-CA-C	-5.11	102.31	110.79
3	G	133	TYR	CA-C-N	5.11	131.29	121.54
3	G	133	TYR	C-N-CA	5.11	131.29	121.54
1	C	457	LEU	N-CA-CB	5.10	117.58	109.82
2	D	424	ASN	CA-CB-CG	-5.10	107.50	112.60
1	B	235	THR	N-CA-C	5.09	117.57	111.71
7	M	62	LEU	CB-CA-C	-5.09	102.88	110.88
2	E	139	ASP	N-CA-C	5.09	118.98	112.87
1	A	351	PRO	N-CA-C	-5.09	105.13	110.58
2	F	74	SER	N-CA-C	5.09	116.89	108.13
2	F	211	THR	N-CA-C	-5.09	106.92	113.23
7	M	257	ASP	CA-CB-CG	5.09	117.69	112.60
2	F	142	ASN	CA-CB-CG	-5.09	107.51	112.60
1	C	310	ALA	N-CA-C	5.08	117.48	111.33
2	E	107	THR	N-CA-C	-5.08	103.63	109.93
2	F	462	TYR	CA-CB-CG	-5.08	104.75	113.90
4	H	5	ALA	N-CA-C	-5.08	101.52	108.38
7	M	248	PRO	N-CA-C	-5.08	107.51	113.86
6	J	160	LYS	N-CA-C	5.08	117.22	111.02
2	E	456	LYS	N-CA-C	5.08	116.81	111.28
2	F	22	GLU	CA-C-N	5.08	131.24	121.54
2	F	22	GLU	C-N-CA	5.08	131.24	121.54
1	A	389	GLY	N-CA-C	-5.07	101.15	113.18
1	A	485	GLU	N-CA-C	5.07	116.50	111.07
1	C	357	ARG	N-CA-C	-5.07	106.78	113.12
1	B	570	ILE	N-CA-C	-5.07	105.55	110.42
2	D	364	ASN	CA-CB-CG	-5.07	107.53	112.60
7	M	201	LEU	CB-CA-C	-5.07	102.92	110.88
1	A	530	ILE	N-CA-CB	5.07	118.18	110.58
2	D	323	HIS	CA-C-O	-5.06	114.91	120.17
2	F	310	GLN	CB-CA-C	-5.06	100.96	109.72
5	K	77	GLU	N-CA-C	5.06	116.49	111.07
1	B	542	LEU	CA-C-N	5.06	124.72	119.56
1	B	542	LEU	C-N-CA	5.06	124.72	119.56
1	C	512	ALA	CA-C-N	5.06	131.20	121.54
1	C	512	ALA	C-N-CA	5.06	131.20	121.54
1	C	521	ALA	CA-C-N	5.06	127.31	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	521	ALA	C-N-CA	5.06	127.31	120.38
2	E	458	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
2	F	243	GLU	CB-CA-C	-5.06	100.36	110.42
6	J	142	LEU	N-CA-C	-5.06	100.46	109.06
1	C	288	ILE	N-CA-C	-5.06	98.82	109.34
2	D	241	VAL	N-CA-C	-5.05	104.77	111.09
7	M	5	PHE	N-CA-C	-5.05	106.53	113.30
1	B	337	ILE	N-CA-CB	5.05	116.46	110.55
1	B	477	GLN	CB-CA-C	-5.05	109.79	117.07
2	D	350	PRO	N-CA-C	-5.05	98.96	112.10
6	L	125	PRO	N-CA-C	-5.05	107.81	114.03
1	A	436	ASP	CA-CB-CG	-5.05	107.55	112.60
1	B	188	PRO	CA-C-O	-5.05	115.27	121.03
1	B	281	LEU	N-CA-C	5.05	116.79	111.28
3	G	26	ASP	N-CA-CB	5.05	117.47	109.94
2	E	100	ILE	CA-C-N	5.05	131.18	121.54
2	E	100	ILE	C-N-CA	5.05	131.18	121.54
2	F	206	GLN	CB-CG-CD	-5.05	104.02	112.60
1	A	493	ASP	CA-CB-CG	-5.05	107.55	112.60
1	B	414	ALA	N-CA-C	-5.05	105.44	112.45
1	C	447	TYR	CA-C-O	-5.05	113.25	120.16
2	E	274	ARG	N-CA-C	-5.05	100.05	110.80
2	F	202	SER	CB-CA-C	-5.05	102.41	110.79
2	F	247	PHE	N-CA-C	5.05	117.56	111.40
2	D	456	LYS	N-CA-C	5.04	117.51	111.71
3	G	167	VAL	N-CA-CB	5.04	119.55	111.23
1	B	393	GLU	CA-C-O	-5.04	115.02	120.87
2	F	194	MET	N-CA-C	-5.03	105.20	113.50
7	M	266	ARG	N-CA-CB	-5.03	102.72	110.16
1	A	53	GLU	CB-CG-CD	-5.02	104.06	112.60
2	D	423	ILE	N-CA-C	-5.02	107.86	112.83
2	E	45	GLY	N-CA-C	5.02	117.77	111.09
2	F	286	TYR	CA-C-N	5.02	127.26	120.38
2	F	286	TYR	C-N-CA	5.02	127.26	120.38
7	M	212	LEU	CA-C-N	5.02	128.28	120.60
7	M	212	LEU	C-N-CA	5.02	128.28	120.60
1	C	334	LEU	N-CA-C	-5.02	106.00	111.82
7	M	47	GLY	N-CA-C	-5.02	109.15	114.67
1	C	354	LEU	N-CA-C	-5.02	104.77	111.24
2	E	280	ARG	O-C-N	5.01	128.55	122.94
2	D	411	TYR	CB-CA-C	-5.01	100.45	110.42
1	C	476	LEU	N-CA-C	-5.01	102.07	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	428	TYR	N-CA-CB	5.00	118.95	110.49
1	A	79	MET	CB-CA-C	-5.00	100.46	110.42
2	F	134	GLY	CA-C-N	5.00	130.97	121.97
2	F	134	GLY	C-N-CA	5.00	130.97	121.97
1	A	176	GLU	N-CA-C	-5.00	107.02	113.02
1	B	465	GLN	O-C-N	5.00	127.23	122.03
1	C	218	VAL	N-CA-C	-5.00	101.40	108.65

There are no chirality outliers.

All (132) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Sidechain
1	A	304	TYR	Sidechain
1	A	335	ARG	Sidechain
1	A	340	ARG	Sidechain
1	A	361	PHE	Sidechain
1	A	362	TYR	Sidechain
1	A	416	ARG	Sidechain
1	A	417	ARG	Sidechain
1	A	439	TYR	Sidechain
1	A	460	ARG	Sidechain
1	A	491	ARG	Sidechain
1	A	501	HIS	Sidechain
1	A	506	TYR	Sidechain
1	A	532	ARG	Sidechain
1	A	547	ARG	Sidechain
1	A	552	ARG	Sidechain
1	A	84	TYR	Sidechain
1	A	95	ARG	Sidechain
1	B	101	TYR	Sidechain
1	B	113	ARG	Sidechain
1	B	143	PHE	Sidechain
1	B	314	ARG	Sidechain
1	B	362	TYR	Sidechain
1	B	387	PRO	Mainchain
1	B	401	ARG	Sidechain
1	B	41	ARG	Sidechain
1	B	415	PHE	Sidechain
1	B	416	ARG	Sidechain
1	B	428	TYR	Sidechain
1	B	491	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	506	TYR	Sidechain
1	B	513	TYR	Sidechain
1	B	84	TYR	Sidechain
1	C	101	TYR	Sidechain
1	C	191	ARG	Sidechain
1	C	197	ARG	Sidechain
1	C	25	TYR	Sidechain
1	C	252	TYR	Sidechain
1	C	258	ARG	Sidechain
1	C	299	ARG	Sidechain
1	C	304	TYR	Sidechain
1	C	318	PHE	Sidechain
1	C	329	ARG	Sidechain
1	C	340	ARG	Sidechain
1	C	353	TYR	Sidechain
1	C	357	ARG	Sidechain
1	C	362	TYR	Sidechain
1	C	415	PHE	Sidechain
1	C	428	TYR	Sidechain
1	C	460	ARG	Sidechain
1	C	513	TYR	Sidechain
1	C	562	TYR	Sidechain
1	C	84	TYR	Sidechain
1	C	93	ARG	Sidechain
2	D	124	ARG	Sidechain
2	D	153	PHE	Sidechain
2	D	187	PHE	Sidechain
2	D	216	ARG	Sidechain
2	D	331	TYR	Sidechain
2	D	341	ARG	Sidechain
2	D	344	HIS	Sidechain
2	D	349	TYR	Sidechain
2	D	356	PRO	Mainchain
2	D	383	TYR	Sidechain
2	D	409	ARG	Sidechain
2	D	411	TYR	Sidechain
2	D	422	PHE	Sidechain
2	D	430	ARG	Sidechain
2	D	462	TYR	Sidechain
2	D	6	LYS	Peptide
2	D	8	TYR	Sidechain
2	D	91	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	93	PHE	Sidechain
2	E	125	ARG	Sidechain
2	E	130	PHE	Sidechain
2	E	187	PHE	Sidechain
2	E	231	ARG	Sidechain
2	E	268	ARG	Sidechain
2	E	274	ARG	Sidechain
2	E	280	ARG	Sidechain
2	E	288	TYR	Sidechain
2	E	29	TYR	Sidechain
2	E	349	TYR	Sidechain
2	E	383	TYR	Sidechain
2	E	414	PHE	Sidechain
2	E	458	HIS	Sidechain
2	E	463	TYR	Sidechain
2	E	6	LYS	Peptide
2	E	92	ARG	Peptide,Mainchain
2	F	111	ARG	Sidechain
2	F	124	ARG	Sidechain
2	F	169	ARG	Sidechain
2	F	203	TYR	Sidechain
2	F	216	ARG	Sidechain
2	F	247	PHE	Sidechain
2	F	271	GLY	Mainchain
2	F	288	TYR	Sidechain
2	F	29	TYR	Sidechain
2	F	331	TYR	Sidechain
2	F	349	TYR	Sidechain
2	F	383	TYR	Sidechain
2	F	421	PHE	Sidechain
2	F	462	TYR	Sidechain
2	F	54	TYR	Sidechain
2	F	6	LYS	Peptide
2	F	8	TYR	Sidechain
3	G	130	PHE	Sidechain
3	G	133	TYR	Sidechain
3	G	139	ARG	Sidechain
3	G	15	ARG	Sidechain
3	G	159	ARG	Sidechain
3	G	188	ARG	Sidechain
3	G	40	PHE	Sidechain
3	G	47	MET	Mainchain

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Mol	Chain	Res	Type	Group
3	G	50	ARG	Sidechain
3	G	8	ARG	Sidechain
4	H	21	TYR	Sidechain
4	H	61	ARG	Sidechain
4	H	89	TYR	Sidechain
5	I	76	ARG	Sidechain
6	J	47	ARG	Sidechain
5	K	74	ARG	Sidechain
6	L	85	ARG	Sidechain
7	M	120	ARG	Sidechain
7	M	183	LEU	Peptide
7	M	191	TYR	Sidechain
7	M	223	ARG	Sidechain
7	M	289	TYR	Sidechain
7	M	3	ASP	Peptide
7	M	308	TYR	Sidechain
7	M	85	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4472	0	4491	52	0
1	B	4472	0	4491	45	0
1	C	4472	0	4491	50	0
2	D	3596	0	3624	45	0
2	E	3596	0	3624	39	0
2	F	3596	0	3624	30	0
3	G	1642	0	1718	19	0
4	H	758	0	764	10	0
5	I	451	0	429	3	0
5	K	451	0	429	1	0
6	J	1043	0	936	4	0
6	L	1043	0	936	8	0
7	M	2513	0	2587	14	0
8	A	27	0	12	4	0
8	C	27	0	12	4	0
All	All	32159	0	32168	308	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 5.

All (308) 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:325:ASP:HA	1:B:383:ALA:HB3	1.65	0.77
6:L:178:MET:CG	6:L:178:MET:CE	2.63	0.77
1:B:234:LYS:HZ3	1:B:409:LEU:HD22	1.50	0.76
5:I:104:MET:CE	5:I:104:MET:CG	2.64	0.75
2:D:131:ILE:HG22	2:D:132:GLN:O	1.91	0.71
6:J:178:MET:CG	6:J:178:MET:CE	2.68	0.71
6:L:134:MET:CG	6:L:134:MET:CE	2.69	0.70
6:J:171:MET:CG	6:J:171:MET:CE	2.70	0.69
3:G:64:LEU:HD22	3:G:126:ALA:HB2	1.75	0.69
1:A:303:ILE:HD12	1:A:304:TYR:H	1.59	0.67
5:K:104:MET:CE	5:K:104:MET:CG	2.73	0.67
1:A:198:LYS:HA	1:A:368:VAL:HG12	1.77	0.66
2:D:22:GLU:CD	2:D:23:ASN:H	2.05	0.65
6:J:134:MET:CG	6:J:134:MET:CE	2.74	0.65
2:E:257:LEU:HD12	2:E:257:LEU:H	1.60	0.64
1:A:366:GLY:O	1:A:368:VAL:HG13	1.98	0.64
1:B:30:VAL:H	1:B:35:LEU:H	1.44	0.64
2:F:5:LYS:HG3	6:L:173:ARG:HH21	1.64	0.63
2:F:141:MET:HB2	2:F:142:ASN:HD22	1.62	0.63
2:E:373:GLU:CD	2:E:373:GLU:H	2.08	0.61
1:A:300:GLU:HG2	1:A:330:TRP:HE1	1.66	0.61
2:F:148:GLN:HE22	2:F:360:ARG:H	1.48	0.61
1:A:365:ALA:HB3	1:A:378:VAL:HB	1.84	0.60
1:B:367:LYS:HZ2	1:B:367:LYS:HA	1.66	0.60
1:C:235:THR:HG21	2:E:360:ARG:HH12	1.66	0.60
1:C:322:LEU:HD23	1:C:380:ILE:HD11	1.83	0.60
1:B:79:MET:HE3	1:B:88:GLN:HE21	1.68	0.59
1:A:141:PHE:CD2	1:A:283:HIS:CE1	2.90	0.59
1:A:419:PHE:CG	8:A:600:ADP:C5	2.91	0.58
1:A:91:LEU:H	1:A:91:LEU:HD12	1.68	0.58
1:A:419:PHE:CD2	8:A:600:ADP:C8	2.92	0.57
2:F:59:VAL:HG12	2:F:61:GLU:H	1.68	0.57
1:A:258:ARG:HA	1:A:291:THR:HG23	1.87	0.56
1:A:326:SER:H	1:A:383:ALA:HB3	1.68	0.56
1:A:501:HIS:CE1	1:A:503:VAL:H	2.24	0.56
1:B:251:VAL:HG13	1:B:286:VAL:HG13	1.88	0.56
1:C:266:LEU:HD21	1:C:287:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:PRO:HA	1:B:145:HIS:CE1	2.42	0.55
1:C:211:ILE:HG23	1:C:212:LEU:H	1.73	0.55
1:A:542:LEU:HB3	1:A:544:VAL:HG12	1.88	0.54
1:C:215:LEU:HD13	1:C:216:PHE:CE2	2.42	0.54
1:C:198:LYS:HA	1:C:368:VAL:HG12	1.89	0.54
1:A:124:LYS:HE3	1:A:124:LYS:H	1.72	0.54
3:G:8:ARG:NE	3:G:9:MET:H	2.05	0.54
2:D:344:HIS:CD2	2:D:344:HIS:C	2.86	0.53
1:A:556:GLU:CD	1:A:556:GLU:H	2.16	0.53
2:E:45:GLY:HA2	2:E:60:PHE:CE1	2.43	0.53
2:F:418:PHE:CE1	2:F:423:ILE:HD11	2.44	0.53
1:C:423:ASN:C	1:C:425:ASN:H	2.16	0.53
2:E:165:ALA:O	2:E:168:ALA:HB3	2.09	0.53
1:B:295:PRO:O	1:B:298:ALA:HB3	2.09	0.52
2:E:45:GLY:HA2	2:E:60:PHE:CD1	2.45	0.52
1:C:293:ASN:HD21	2:E:118:PRO:HA	1.74	0.52
2:D:11:ILE:HD13	2:D:11:ILE:H	1.73	0.52
6:L:171:MET:CG	6:L:171:MET:CE	2.88	0.52
1:C:146:LYS:H	1:C:316:GLN:NE2	2.06	0.52
2:E:194:MET:H	2:E:258:THR:HG22	1.74	0.52
1:C:219:ALA:HB2	1:C:431:PHE:CG	2.44	0.52
2:D:446:LEU:HD11	2:D:451:LEU:HD21	1.92	0.52
2:D:131:ILE:HA	2:D:173:VAL:HG12	1.92	0.52
5:I:109:GLU:H	5:I:109:GLU:CD	2.18	0.52
2:F:197:THR:HG22	2:F:198:GLN:H	1.75	0.52
1:A:419:PHE:CD1	8:A:600:ADP:C4	2.97	0.51
2:E:46:GLN:H	2:E:58:GLN:HB3	1.74	0.51
2:E:402:ASP:CG	2:E:409:ARG:HH22	2.18	0.51
1:B:418:HIS:CE1	1:B:495:LEU:HG	2.45	0.51
2:D:31:ALA:H	2:D:47:VAL:HB	1.76	0.51
2:D:239:LEU:HD21	2:D:310:GLN:HE22	1.76	0.51
2:E:203:TYR:C	2:E:203:TYR:CD2	2.89	0.51
1:B:439:TYR:CD1	1:B:447:TYR:CE2	2.98	0.50
1:B:168:VAL:HA	1:B:183:MET:SD	2.51	0.50
1:B:172:VAL:HG23	1:B:173:VAL:H	1.77	0.50
1:B:150:PRO:HB3	1:B:185:HIS:CG	2.47	0.50
2:E:197:THR:H	2:E:200:GLU:HB2	1.76	0.50
1:A:249:VAL:HG23	1:A:320:VAL:HA	1.94	0.50
2:E:440:TRP:CE3	2:E:443:LEU:HD12	2.47	0.50
7:M:224:PHE:CE2	7:M:248:PRO:HD2	2.47	0.50
3:G:161:VAL:HG12	3:G:165:GLU:CD	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:HB2	1:A:431:PHE:CD2	2.48	0.49
1:A:509:MET:N	1:A:509:MET:HE2	2.27	0.49
1:B:320:VAL:HG12	1:B:321:ALA:H	1.76	0.49
2:D:31:ALA:HB3	2:D:47:VAL:HG21	1.94	0.49
2:E:406:GLU:C	2:E:408:ASP:H	2.19	0.49
7:M:104:ALA:HB3	7:M:161:LEU:HD22	1.94	0.49
2:D:440:TRP:HA	2:D:440:TRP:CE3	2.47	0.49
2:E:17:PRO:HG3	2:E:273:ALA:HB1	1.95	0.49
1:B:568:LYS:H	1:B:568:LYS:HD2	1.77	0.49
3:G:8:ARG:HE	3:G:9:MET:H	1.59	0.49
5:I:91:ARG:HH21	5:I:95:GLU:HB2	1.77	0.49
2:E:150:LEU:O	2:E:312:PRO:HD2	2.12	0.49
1:C:328:SER:O	1:C:331:ALA:HB3	2.13	0.49
2:D:161:ASN:O	2:D:164:ALA:HB3	2.13	0.49
2:D:252:HIS:CE1	2:D:306:GLY:HA2	2.48	0.49
2:E:84:VAL:HG12	2:E:112:LEU:HD21	1.95	0.49
6:L:84:ARG:HH21	6:L:175:TRP:CG	2.31	0.49
2:D:196:ILE:HD13	2:D:196:ILE:H	1.76	0.48
2:E:349:TYR:CD1	2:E:350:PRO:HA	2.48	0.48
6:J:84:ARG:HH11	6:J:175:TRP:CD1	2.30	0.48
2:F:436:LEU:O	2:F:439:ALA:HB3	2.12	0.48
2:D:32:ILE:HD12	2:D:80:ALA:HB2	1.95	0.48
2:D:60:PHE:CD1	2:D:229:ILE:HG21	2.47	0.48
7:M:302:LEU:HD23	7:M:302:LEU:O	2.12	0.48
1:C:522:PHE:CZ	1:C:545:LEU:HD21	2.48	0.48
2:E:348:ILE:HG23	2:E:424:ASN:HB2	1.95	0.48
1:C:428:TYR:CE2	2:F:157:GLY:HA2	2.49	0.48
2:D:425:GLN:HB3	2:D:430:ARG:HH12	1.78	0.48
2:F:316:MET:HE1	2:F:319:ASP:HA	1.96	0.48
2:F:251:TYR:O	2:F:306:GLY:HA2	2.12	0.48
1:A:117:TRP:H	1:A:166:TYR:H	1.62	0.48
2:E:154:SER:HA	2:E:339:LEU:HD12	1.95	0.48
1:C:119:TRP:CZ3	1:C:136:GLY:HA3	2.49	0.48
6:L:130:HIS:CD2	6:L:130:HIS:N	2.81	0.48
1:B:536:ILE:C	1:B:538:GLU:H	2.20	0.48
2:E:323:HIS:CE1	3:G:181:GLN:CD	2.91	0.48
1:B:353:TYR:C	1:B:355:ALA:H	2.22	0.47
1:C:25:TYR:H	1:C:39:ILE:HB	1.78	0.47
3:G:65:LEU:HD12	3:G:69:ALA:HA	1.96	0.47
2:E:298:ALA:HB1	2:E:308:VAL:HB	1.96	0.47
2:D:390:VAL:HG12	2:D:390:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:VAL:HG13	1:A:269:PHE:CG	2.49	0.47
1:A:393:GLU:C	1:A:393:GLU:CD	2.82	0.47
1:B:303:ILE:HD11	1:B:330:TRP:CZ2	2.48	0.47
2:D:366:VAL:HG21	2:D:375:HIS:CG	2.50	0.47
1:A:243:LYS:O	1:A:244:TRP:CD2	2.68	0.47
2:F:199:ARG:C	2:F:199:ARG:HH11	2.23	0.46
1:A:294:MET:HB3	1:A:295:PRO:HD2	1.96	0.46
2:F:362:MET:C	2:F:364:ASN:H	2.23	0.46
1:A:251:VAL:HG22	1:A:286:VAL:HG21	1.98	0.46
1:A:109:HIS:CG	1:A:113:ARG:HE	2.33	0.46
1:C:314:ARG:HH11	1:C:368:VAL:HG21	1.79	0.46
2:D:220:PHE:CD2	2:D:238:ALA:HB2	2.50	0.46
4:H:56:GLU:HG3	4:H:71:LEU:HD11	1.96	0.46
1:B:141:PHE:CE2	1:B:283:HIS:CD2	3.04	0.46
1:C:419:PHE:CE1	8:C:600:ADP:C4	3.03	0.46
2:F:148:GLN:HE22	2:F:360:ARG:N	2.13	0.46
2:F:125:ARG:HB2	2:F:302:GLU:HA	1.97	0.46
2:F:352:ILE:HG22	2:F:353:ASP:N	2.31	0.46
1:B:418:HIS:O	1:B:418:HIS:CG	2.69	0.46
1:C:253:VAL:HG13	1:C:324:ALA:HB2	1.96	0.46
2:D:141:MET:HE1	2:D:354:PRO:HA	1.98	0.46
1:B:28:CYS:SG	1:B:66:SER:HA	2.56	0.46
2:D:146:ARG:HH11	2:D:252:HIS:CE1	2.34	0.46
1:C:489:ILE:C	1:C:491:ARG:H	2.23	0.45
1:A:168:VAL:HA	1:A:183:MET:SD	2.56	0.45
1:B:234:LYS:HZ3	1:B:409:LEU:CD2	2.25	0.45
1:C:100:ILE:C	2:E:120:ASN:HD21	2.25	0.45
1:B:42:LEU:H	1:B:42:LEU:HD12	1.80	0.45
1:C:419:PHE:CZ	8:C:600:ADP:C4	3.04	0.45
1:A:400:LEU:HD11	1:A:406:PHE:CE2	2.51	0.45
1:A:508:SER:C	1:A:509:MET:HE2	2.41	0.45
2:D:229:ILE:HG23	2:D:230:GLU:N	2.32	0.45
1:A:205:PHE:HB3	1:A:218:VAL:HG23	1.99	0.45
1:B:204:PRO:HG3	1:B:438:TRP:CZ2	2.51	0.45
1:C:359:ALA:HA	1:C:402:ILE:HD13	1.98	0.45
2:D:84:VAL:HG11	2:D:244:TYR:CD1	2.51	0.45
1:A:557:GLU:CD	1:A:557:GLU:H	2.25	0.45
2:D:162:GLU:CD	2:D:162:GLU:N	2.75	0.45
1:A:424:TRP:CD1	1:A:424:TRP:O	2.70	0.45
1:C:447:TYR:H	1:C:448:PRO:HD2	1.81	0.45
1:A:128:GLU:HB3	1:A:156:ARG:HE	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:HG22	1:B:286:VAL:HG12	1.99	0.44
1:B:307:VAL:HG12	1:B:364:ARG:HH21	1.82	0.44
3:G:161:VAL:HG12	3:G:165:GLU:OE2	2.16	0.44
4:H:18:LEU:C	4:H:20:GLY:H	2.24	0.44
4:H:71:LEU:HD12	4:H:71:LEU:O	2.16	0.44
7:M:41:SER:HB3	7:M:49:LEU:HD22	1.99	0.44
1:C:141:PHE:CE2	1:C:283:HIS:CE1	3.05	0.44
1:C:244:TRP:CE2	1:C:505:ALA:HB1	2.53	0.44
1:C:539:ILE:HD12	1:C:539:ILE:H	1.82	0.44
2:D:116:GLY:HA3	2:D:297:ARG:HH21	1.82	0.44
2:F:82:LEU:HD12	2:F:83:GLY:H	1.82	0.44
2:F:234:THR:HB	2:F:235:PRO:HD3	1.99	0.44
7:M:202:ARG:HH21	7:M:265:LEU:HD13	1.82	0.44
1:C:435:LEU:HD23	1:C:435:LEU:HA	1.82	0.44
2:D:94:ASN:HB2	2:D:100:ILE:HG13	2.00	0.44
4:H:59:VAL:HG12	4:H:63:MET:SD	2.57	0.44
1:A:428:TYR:CD2	2:D:157:GLY:HA3	2.52	0.44
1:C:253:VAL:O	1:C:324:ALA:HA	2.17	0.44
1:C:419:PHE:CE2	8:C:600:ADP:C8	3.05	0.44
2:D:81:ARG:HB2	2:D:112:LEU:O	2.18	0.44
2:D:143:THR:H	2:D:362:MET:HG3	1.82	0.44
2:D:446:LEU:HD12	2:D:447:PRO:O	2.17	0.44
2:D:14:ILE:HG23	2:D:19:LEU:HD13	1.99	0.44
3:G:66:LEU:HD13	3:G:66:LEU:O	2.18	0.44
1:A:400:LEU:HD21	1:A:406:PHE:CE1	2.53	0.44
1:C:314:ARG:NH1	1:C:368:VAL:HG21	2.33	0.44
7:M:200:ASN:HD21	7:M:219:LEU:H	1.66	0.44
1:B:320:VAL:HG12	1:B:321:ALA:N	2.33	0.43
1:C:21:GLY:H	2:F:68:LEU:HB2	1.81	0.43
3:G:48:GLU:HA	3:G:51:LYS:HE2	1.99	0.43
1:C:83:ILE:HA	1:C:287:LEU:HB2	1.99	0.43
2:F:396:VAL:HG13	2:F:397:ALA:N	2.33	0.43
3:G:33:ASP:O	3:G:36:VAL:HG22	2.18	0.43
1:A:3:GLN:HB3	1:A:65:VAL:HG13	2.00	0.43
1:B:251:VAL:HG13	1:B:286:VAL:CG1	2.48	0.43
1:B:513:TYR:C	1:B:513:TYR:CD2	2.95	0.43
1:C:219:ALA:HB2	1:C:431:PHE:CD2	2.53	0.43
2:D:186:PRO:HG2	2:D:251:TYR:CE2	2.54	0.43
2:D:294:ILE:O	2:D:295:TYR:CD1	2.71	0.43
1:B:116:LYS:HG2	1:B:167:THR:HG23	2.00	0.43
1:C:340:ARG:HD3	1:C:340:ARG:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:PRO:C	1:C:422:ILE:H	2.25	0.43
2:E:194:MET:SD	2:E:194:MET:C	3.02	0.43
2:F:442:LEU:HD23	2:F:442:LEU:HA	1.91	0.43
3:G:66:LEU:C	7:M:301:ARG:HH12	2.27	0.43
7:M:54:LEU:HD21	7:M:305:ARG:HG2	2.00	0.43
7:M:101:ARG:HA	7:M:161:LEU:HD21	2.00	0.43
1:B:443:VAL:HG21	1:B:447:TYR:CE2	2.54	0.43
3:G:103:ARG:HH21	3:G:149:LYS:HD3	1.83	0.43
1:B:363:GLU:OE2	1:B:363:GLU:HA	2.17	0.43
1:C:244:TRP:CD2	1:C:505:ALA:O	2.72	0.43
3:G:58:LYS:HA	3:G:61:TYR:CD2	2.54	0.43
1:A:354:LEU:HD12	1:A:354:LEU:H	1.83	0.42
2:F:174:ARG:HA	2:F:174:ARG:NE	2.34	0.42
2:D:140:VAL:O	2:D:375:HIS:HE1	2.01	0.42
4:H:98:ILE:HD13	4:H:98:ILE:H	1.82	0.42
1:A:424:TRP:O	1:A:424:TRP:CG	2.72	0.42
2:E:60:PHE:CD1	2:E:229:ILE:HG21	2.54	0.42
3:G:64:LEU:HD22	3:G:126:ALA:CB	2.45	0.42
7:M:150:ALA:HB1	7:M:171:ARG:HE	1.85	0.42
1:B:77:PRO:HB3	1:B:145:HIS:CE1	2.55	0.42
1:C:515:ILE:HA	1:C:518:MET:HG2	2.02	0.42
2:D:45:GLY:HA2	2:D:60:PHE:CE1	2.54	0.42
2:E:282:GLY:C	2:E:283:TYR:CD2	2.97	0.42
2:F:89:LEU:HD23	2:F:89:LEU:HA	1.87	0.42
1:C:16:ALA:O	1:C:46:THR:HA	2.19	0.42
1:C:265:VAL:HG13	1:C:269:PHE:CE2	2.54	0.42
2:D:32:ILE:CD1	2:D:80:ALA:HB2	2.50	0.42
1:A:27:ILE:HA	1:A:37:GLY:O	2.19	0.42
1:C:165:GLU:O	1:C:166:TYR:CD1	2.72	0.42
2:E:352:ILE:HD12	2:E:352:ILE:C	2.45	0.42
2:F:53:GLU:H	2:F:53:GLU:CD	2.26	0.42
2:F:414:PHE:CD1	2:F:414:PHE:C	2.97	0.42
1:A:235:THR:HG21	1:A:261:GLU:OE1	2.20	0.42
1:A:503:VAL:HG12	1:A:504:ASP:H	1.85	0.42
1:B:344:MET:HB2	3:G:192:PHE:CE1	2.55	0.42
2:D:125:ARG:NH2	2:D:300:VAL:HG11	2.34	0.42
2:E:281:ARG:H	2:E:281:ARG:HG3	1.54	0.42
2:F:199:ARG:NH1	2:F:200:GLU:HA	2.34	0.42
1:B:418:HIS:HB2	1:B:496:GLN:HE21	1.84	0.42
2:E:252:HIS:CE1	2:E:306:GLY:HA2	2.54	0.42
2:F:241:VAL:HG12	2:F:241:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:48:ASP:HB2	4:H:50:ALA:H	1.84	0.42
4:H:57:ARG:HE	4:H:57:ARG:H	1.67	0.42
7:M:308:TYR:CD2	7:M:309:PHE:CE1	3.08	0.42
2:E:194:MET:H	2:E:258:THR:CG2	2.33	0.41
2:E:385:ALA:HB1	2:E:414:PHE:CE1	2.53	0.41
2:F:26:ASP:C	2:F:27:LEU:HD22	2.44	0.41
3:G:20:LEU:HD23	3:G:20:LEU:HA	1.94	0.41
3:G:154:ILE:HD13	3:G:154:ILE:HA	1.93	0.41
6:L:51:ALA:C	6:L:53:TYR:H	2.28	0.41
1:B:109:HIS:CD2	1:B:113:ARG:HE	2.37	0.41
2:D:84:VAL:HG21	2:D:244:TYR:CD2	2.54	0.41
4:H:26:ALA:HB1	4:H:28:GLU:CD	2.46	0.41
4:H:48:ASP:HA	4:H:75:ALA:H	1.85	0.41
1:A:187:TRP:CE2	1:A:193:ARG:HG3	2.55	0.41
1:A:366:GLY:HA2	1:A:378:VAL:H	1.85	0.41
1:B:84:TYR:CD2	1:B:84:TYR:N	2.88	0.41
1:B:336:GLU:OE1	2:D:286:TYR:HA	2.20	0.41
2:F:199:ARG:HH11	2:F:199:ARG:HG2	1.85	0.41
7:M:122:GLU:CD	7:M:122:GLU:H	2.29	0.41
1:A:223:THR:O	1:A:405:ALA:HB3	2.20	0.41
1:B:424:TRP:NE1	1:B:458:LEU:HD13	2.36	0.41
1:C:128:GLU:HA	1:C:156:ARG:HE	1.86	0.41
2:D:342:GLU:O	2:D:343:LEU:C	2.62	0.41
2:D:368:LYS:HZ3	2:D:373:GLU:C	2.29	0.41
2:E:254:LEU:HD23	2:E:254:LEU:HA	1.90	0.41
1:A:209:MET:N	1:A:209:MET:SD	2.93	0.41
1:B:209:MET:HB2	1:B:212:LEU:HB2	2.02	0.41
1:C:150:PRO:HB3	1:C:185:HIS:CG	2.55	0.41
1:A:419:PHE:CD1	8:A:600:ADP:C5	3.08	0.41
1:B:212:LEU:HD22	1:B:407:TRP:CZ2	2.55	0.41
2:E:271:GLY:C	2:E:273:ALA:H	2.29	0.41
1:A:402:ILE:O	1:A:402:ILE:HG22	2.21	0.41
1:C:15:ILE:HG22	1:C:16:ALA:H	1.85	0.41
1:C:283:HIS:CD2	1:C:283:HIS:N	2.88	0.41
1:C:562:TYR:CD1	1:C:562:TYR:N	2.89	0.41
2:D:318:ASP:C	2:D:319:ASP:CG	2.89	0.41
2:F:11:ILE:H	2:F:11:ILE:HG12	1.60	0.41
7:M:20:LEU:HD23	7:M:24:PHE:CD2	2.55	0.41
7:M:306:ARG:HG3	7:M:316:VAL:HG21	2.03	0.41
1:A:494:PHE:CE2	1:A:516:MET:HG3	2.56	0.41
1:B:348:GLU:C	1:B:348:GLU:CD	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:THR:HG22	1:C:235:THR:O	2.20	0.41
3:G:192:PHE:N	3:G:192:PHE:CD1	2.88	0.41
1:A:235:THR:HG21	1:A:261:GLU:CD	2.46	0.40
1:A:328:SER:HB2	1:A:385:SER:H	1.85	0.40
1:B:329:ARG:HH21	2:D:331:TYR:HB3	1.86	0.40
1:C:361:PHE:CD2	1:C:361:PHE:C	2.99	0.40
2:E:94:ASN:HB2	2:E:100:ILE:HD11	2.03	0.40
2:E:100:ILE:HG22	2:E:101:ASP:H	1.86	0.40
2:E:104:PRO:HB2	2:E:105:PRO:HD2	2.02	0.40
2:E:135:ILE:HG23	2:E:425:GLN:OE1	2.21	0.40
1:A:405:ALA:HA	1:A:429:SER:HA	2.03	0.40
1:C:419:PHE:CD1	8:C:600:ADP:C5	3.09	0.40
2:E:95:GLY:C	2:E:97:GLY:H	2.29	0.40
1:A:113:ARG:HA	1:A:168:VAL:HG21	2.03	0.40
1:B:209:MET:HE2	1:B:420:PRO:HG3	2.04	0.40
1:C:206:LEU:H	1:C:246:ASN:ND2	2.20	0.40
2:D:45:GLY:HA2	2:D:58:GLN:O	2.21	0.40
2:E:112:LEU:HB2	2:E:113:PRO:CD	2.52	0.40
2:F:344:HIS:O	2:F:344:HIS:CG	2.75	0.40
3:G:64:LEU:HA	3:G:122:TYR:CD1	2.56	0.40
1:B:467:ILE:HD12	1:B:467:ILE:H	1.85	0.40
1:C:566:ALA:HA	1:C:569:GLU:CD	2.47	0.40
2:D:348:ILE:HG22	2:D:349:TYR:H	1.86	0.40
4:H:47:VAL:HG12	4:H:48:ASP:N	2.37	0.40
6:L:79:VAL:HG11	6:L:186:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	575/578 (100%)	423 (74%)	97 (17%)	55 (10%)	0 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	575/578 (100%)	408 (71%)	100 (17%)	67 (12%)	0	5
1	C	575/578 (100%)	426 (74%)	102 (18%)	47 (8%)	0	9
2	D	457/478 (96%)	317 (69%)	93 (20%)	47 (10%)	0	6
2	E	457/478 (96%)	321 (70%)	92 (20%)	44 (10%)	0	7
2	F	457/478 (96%)	337 (74%)	83 (18%)	37 (8%)	1	9
3	G	208/223 (93%)	157 (76%)	33 (16%)	18 (9%)	0	9
4	H	98/104 (94%)	65 (66%)	18 (18%)	15 (15%)	0	3
5	I	59/120 (49%)	57 (97%)	1 (2%)	1 (2%)	7	35
5	K	59/120 (49%)	55 (93%)	2 (3%)	2 (3%)	3	20
6	J	148/188 (79%)	115 (78%)	24 (16%)	9 (6%)	1	13
6	L	148/188 (79%)	129 (87%)	15 (10%)	4 (3%)	4	25
7	M	318/323 (98%)	293 (92%)	15 (5%)	10 (3%)	3	21
All	All	4134/4434 (93%)	3103 (75%)	675 (16%)	356 (9%)	1	9

All (356) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	56	SER
1	A	188	PRO
1	A	217	PRO
1	A	227	PRO
1	A	244	TRP
1	A	266	LEU
1	A	276	LYS
1	A	427	SER
1	A	471	VAL
1	A	480	GLU
1	B	27	ILE
1	B	101	TYR
1	B	122	MET
1	B	159	GLU
1	B	202	ASN
1	B	292	SER
1	B	303	ILE
1	B	304	TYR
1	B	305	VAL
1	B	353	TYR

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Mol	Chain	Res	Type
1	B	364	ARG
1	B	365	ALA
1	B	418	HIS
1	B	466	GLU
1	B	505	ALA
1	C	141	PHE
1	C	191	ARG
1	C	233	GLY
1	C	417	ARG
1	C	494	PHE
1	C	498	ASN
1	C	499	ALA
1	C	505	ALA
1	C	506	TYR
2	D	49	GLU
2	D	71	THR
2	D	72	SER
2	D	78	ASP
2	D	89	LEU
2	D	118	PRO
2	D	151	PRO
2	D	210	ARG
2	D	216	ARG
2	D	276	GLU
2	D	321	ARG
2	D	349	TYR
2	D	354	PRO
2	D	372	ARG
2	E	7	GLU
2	E	64	THR
2	E	96	ILE
2	E	100	ILE
2	E	137	THR
2	E	148	GLN
2	E	151	PRO
2	E	215	SER
2	E	281	ARG
2	E	354	PRO
2	E	362	MET
2	E	419	GLU
2	F	101	ASP
2	F	135	ILE

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Mol	Chain	Res	Type
2	F	139	ASP
2	F	143	THR
2	F	151	PRO
2	F	280	ARG
2	F	327	ASP
2	F	356	PRO
3	G	6	PRO
3	G	9	MET
3	G	67	ALA
4	H	66	ARG
4	H	69	PRO
4	H	75	ALA
4	H	80	ALA
6	J	138	ARG
6	J	141	GLU
6	L	138	ARG
7	M	4	ASP
7	M	32	SER
7	M	131	GLN
1	A	36	VAL
1	A	45	ASP
1	A	64	VAL
1	A	72	ALA
1	A	108	VAL
1	A	318	PHE
1	A	353	TYR
1	A	367	LYS
1	A	387	PRO
1	A	416	ARG
1	A	432	THR
1	A	506	TYR
1	A	551	ALA
1	B	28	CYS
1	B	100	ILE
1	B	139	PRO
1	B	152	ASP
1	B	180	GLU
1	B	210	ARG
1	B	255	CYS
1	B	259	GLY
1	B	275	PRO
1	B	293	ASN

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Mol	Chain	Res	Type
1	B	302	SER
1	B	340	ARG
1	B	397	GLN
1	B	443	VAL
1	B	467	ILE
1	B	469	GLN
1	B	471	VAL
1	B	495	LEU
1	C	45	ASP
1	C	112	ASP
1	C	177	ASP
1	C	202	ASN
1	C	210	ARG
1	C	222	GLY
1	C	246	ASN
1	C	347	GLU
1	C	392	SER
1	C	426	GLY
1	C	497	GLN
1	C	501	HIS
1	C	512	ALA
2	D	95	GLY
2	D	119	LEU
2	D	213	ALA
2	D	293	THR
2	D	330	GLY
2	D	366	VAL
2	E	10	GLY
2	E	216	ARG
2	E	239	LEU
2	E	259	ASP
2	E	274	ARG
2	E	322	THR
2	E	332	ILE
2	E	356	PRO
2	E	359	SER
2	E	363	ASN
2	E	367	GLY
2	F	15	SER
2	F	23	ASN
2	F	95	GLY
2	F	140	VAL

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Mol	Chain	Res	Type
2	F	186	PRO
2	F	275	GLU
2	F	298	ALA
2	F	389	GLY
2	F	402	ASP
3	G	112	ALA
3	G	117	VAL
3	G	119	THR
3	G	180	GLN
4	H	15	LEU
4	H	25	SER
4	H	48	ASP
4	H	54	ASP
6	J	99	GLU
6	J	163	VAL
5	K	107	LEU
6	L	180	SER
7	M	237	ASP
7	M	320	VAL
1	A	70	PRO
1	A	201	PRO
1	A	222	GLY
1	A	232	SER
1	A	278	GLY
1	A	282	MET
1	A	302	SER
1	A	304	TYR
1	A	389	GLY
1	A	417	ARG
1	B	56	SER
1	B	145	HIS
1	B	177	ASP
1	B	197	ARG
1	B	227	PRO
1	B	346	ALA
1	B	349	GLY
1	B	356	ALA
1	B	413	LEU
1	B	473	PRO
1	B	510	LYS
1	C	12	PRO
1	C	80	LEU

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Mol	Chain	Res	Type
1	C	85	ASP
1	C	318	PHE
1	C	365	ALA
1	C	400	LEU
1	C	410	ASP
1	C	463	GLY
1	C	473	PRO
1	C	496	GLN
2	D	97	GLY
2	D	164	ALA
2	D	168	ALA
2	D	180	GLU
2	D	284	PRO
2	D	317	PRO
2	D	326	PRO
2	D	362	MET
2	D	371	THR
2	E	17	PRO
2	E	88	MET
2	E	101	ASP
2	E	123	ALA
2	E	225	ASP
2	E	336	GLN
2	E	358	LEU
2	F	10	GLY
2	F	89	LEU
2	F	128	GLU
2	F	375	HIS
2	F	403	ALA
2	F	436	LEU
3	G	88	GLY
3	G	110	ASP
3	G	134	ALA
3	G	174	ALA
4	H	29	ALA
4	H	53	PRO
4	H	55	PRO
4	H	81	PHE
6	J	119	LYS
6	J	140	VAL
5	K	104	MET
1	A	71	LEU

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Mol	Chain	Res	Type
1	A	121	PRO
1	A	163	ALA
1	A	295	PRO
1	A	510	LYS
1	B	91	LEU
1	B	179	THR
1	B	232	SER
1	B	345	PRO
1	B	386	PRO
1	B	496	GLN
1	C	25	TYR
1	C	77	PRO
1	C	275	PRO
1	C	284	ARG
1	C	428	TYR
1	C	433	SER
1	C	444	ALA
2	D	77	GLU
2	D	108	PRO
2	D	117	LEU
2	D	237	MET
2	D	250	ASP
2	D	275	GLU
2	D	312	PRO
2	D	403	ALA
2	E	54	TYR
2	E	128	GLU
2	E	166	GLN
2	E	190	VAL
2	E	240	THR
2	E	277	ILE
2	E	297	ARG
2	F	69	ALA
2	F	222	ASN
2	F	263	TYR
2	F	312	PRO
2	F	415	ALA
3	G	80	ALA
3	G	85	PRO
3	G	87	GLU
3	G	168	VAL
4	H	79	GLU

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Mol	Chain	Res	Type
5	I	104	MET
6	J	52	GLN
6	J	126	GLU
6	L	52	GLN
7	M	254	GLY
1	A	202	ASN
1	A	277	THR
1	A	345	PRO
1	A	361	PHE
1	A	477	GLN
1	A	505	ALA
1	A	516	MET
1	B	108	VAL
1	B	141	PHE
1	B	248	ASP
1	B	257	GLU
1	B	315	ASP
1	B	359	ALA
1	B	395	VAL
1	B	417	ARG
1	B	445	GLU
1	B	540	LEU
1	C	402	ILE
1	C	563	PHE
2	D	8	TYR
2	D	61	GLU
2	D	336	GLN
2	E	23	ASN
2	E	49	GLU
2	E	250	ASP
2	F	137	THR
2	F	259	ASP
3	G	114	LEU
3	G	167	VAL
4	H	52	LEU
6	J	127	ASP
7	M	52	GLN
7	M	75	LEU
7	M	76	VAL
1	A	192	ALA
1	A	402	ILE
1	A	484	ILE

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Mol	Chain	Res	Type
1	B	253	VAL
1	B	296	VAL
1	B	509	MET
1	C	248	ASP
2	D	99	PRO
2	D	128	GLU
2	E	273	ALA
2	E	399	ILE
2	F	175	PRO
2	F	226	ASP
2	F	250	ASP
4	H	20	GLY
1	A	549	GLY
1	B	40	ILE
1	C	36	VAL
2	D	121	PRO
2	D	186	PRO
2	D	348	ILE
2	E	270	ILE
2	F	17	PRO
1	A	170	GLU
1	A	189	VAL
1	A	443	VAL
1	A	570	ILE
1	B	534	VAL
1	C	490	ILE
1	C	514	GLY
1	B	87	ILE
1	C	443	VAL
2	F	355	LEU
2	F	390	VAL
3	G	154	ILE
6	L	104	VAL
7	M	222	GLY
1	A	486	VAL
1	B	394	PRO
2	D	65	GLY
2	D	90	GLY
1	C	5	VAL
2	E	235	PRO
2	F	279	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/468 (100%)	421 (90%)	47 (10%)	7	24
1	B	468/468 (100%)	415 (89%)	53 (11%)	5	20
1	C	468/468 (100%)	418 (89%)	50 (11%)	6	22
2	D	386/401 (96%)	342 (89%)	44 (11%)	5	20
2	E	386/401 (96%)	351 (91%)	35 (9%)	9	28
2	F	386/401 (96%)	361 (94%)	25 (6%)	15	38
3	G	166/176 (94%)	148 (89%)	18 (11%)	6	22
4	H	76/80 (95%)	67 (88%)	9 (12%)	5	19
5	I	37/86 (43%)	32 (86%)	5 (14%)	4	16
5	K	37/86 (43%)	32 (86%)	5 (14%)	4	16
6	J	76/141 (54%)	72 (95%)	4 (5%)	20	42
6	L	76/141 (54%)	75 (99%)	1 (1%)	61	72
7	M	254/256 (99%)	239 (94%)	15 (6%)	18	40
All	All	3284/3573 (92%)	2973 (90%)	311 (10%)	10	26

All (311) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	12	PRO
1	A	42	LEU
1	A	54	ASP
1	A	55	THR
1	A	60	VAL
1	A	74	GLU
1	A	87	ILE
1	A	88	GLN
1	A	100	ILE
1	A	104	ARG
1	A	124	LYS

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Mol	Chain	Res	Type
1	A	134	VAL
1	A	154	ARG
1	A	157	VAL
1	A	159	GLU
1	A	173	VAL
1	A	189	VAL
1	A	207	THR
1	A	211	ILE
1	A	213	ASP
1	A	223	THR
1	A	234	LYS
1	A	237	THR
1	A	249	VAL
1	A	264	ASP
1	A	285	THR
1	A	295	PRO
1	A	300	GLU
1	A	303	ILE
1	A	307	VAL
1	A	329	ARG
1	A	341	LEU
1	A	348	GLU
1	A	363	GLU
1	A	368	VAL
1	A	378	VAL
1	A	393	GLU
1	A	410	ASP
1	A	437	PRO
1	A	450	LEU
1	A	452	ASP
1	A	503	VAL
1	A	504	ASP
1	A	527	GLU
1	A	534	VAL
1	A	567	MET
1	B	5	VAL
1	B	12	PRO
1	B	14	VAL
1	B	24	MET
1	B	33	GLU
1	B	40	ILE
1	B	69	LEU

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Mol	Chain	Res	Type
1	B	79	MET
1	B	109	HIS
1	B	117	TRP
1	B	127	ASP
1	B	144	THR
1	B	172	VAL
1	B	180	GLU
1	B	189	VAL
1	B	196	GLN
1	B	207	THR
1	B	210	ARG
1	B	213	ASP
1	B	223	THR
1	B	226	ILE
1	B	232	SER
1	B	241	LEU
1	B	253	VAL
1	B	263	THR
1	B	269	PHE
1	B	288	ILE
1	B	290	ASN
1	B	303	ILE
1	B	307	VAL
1	B	337	ILE
1	B	367	LYS
1	B	378	VAL
1	B	384	VAL
1	B	391	MET
1	B	395	VAL
1	B	398	SER
1	B	409	LEU
1	B	413	LEU
1	B	418	HIS
1	B	431	PHE
1	B	439	TYR
1	B	441	GLU
1	B	464	LEU
1	B	470	LEU
1	B	493	ASP
1	B	502	GLU
1	B	519	ILE
1	B	522	PHE

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Mol	Chain	Res	Type
1	B	550	ARG
1	B	563	PHE
1	B	567	MET
1	B	569	GLU
1	C	8	LYS
1	C	28	CYS
1	C	46	THR
1	C	49	VAL
1	C	50	GLN
1	C	62	GLU
1	C	87	ILE
1	C	112	ASP
1	C	119	TRP
1	C	189	VAL
1	C	200	ASP
1	C	207	THR
1	C	215	LEU
1	C	218	VAL
1	C	220	MET
1	C	239	GLN
1	C	241	LEU
1	C	253	VAL
1	C	258	ARG
1	C	282	MET
1	C	291	THR
1	C	303	ILE
1	C	323	MET
1	C	325	ASP
1	C	329	ARG
1	C	339	SER
1	C	358	LEU
1	C	380	ILE
1	C	381	VAL
1	C	392	SER
1	C	394	PRO
1	C	395	VAL
1	C	396	THR
1	C	400	LEU
1	C	402	ILE
1	C	430	LEU
1	C	437	PRO
1	C	456	GLU

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Mol	Chain	Res	Type
1	C	471	VAL
1	C	474	ASP
1	C	494	PHE
1	C	495	LEU
1	C	502	GLU
1	C	517	LYS
1	C	536	ILE
1	C	543	PRO
1	C	548	ILE
1	C	554	VAL
1	C	565	GLU
1	C	571	GLN
2	D	11	ILE
2	D	14	ILE
2	D	32	ILE
2	D	36	LYS
2	D	61	GLU
2	D	71	THR
2	D	81	ARG
2	D	85	SER
2	D	89	LEU
2	D	92	ARG
2	D	104	PRO
2	D	142	ASN
2	D	149	LYS
2	D	172	THR
2	D	173	VAL
2	D	180	GLU
2	D	194	MET
2	D	196	ILE
2	D	206	GLN
2	D	207	GLU
2	D	208	PHE
2	D	209	GLU
2	D	216	ARG
2	D	221	LEU
2	D	226	ASP
2	D	227	PRO
2	D	251	TYR
2	D	253	VAL
2	D	258	THR
2	D	261	THR

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Mol	Chain	Res	Type
2	D	284	PRO
2	D	286	TYR
2	D	287	MET
2	D	300	VAL
2	D	308	VAL
2	D	319	ASP
2	D	324	PRO
2	D	353	ASP
2	D	362	MET
2	D	390	VAL
2	D	395	LEU
2	D	405	THR
2	D	423	ILE
2	D	446	LEU
2	E	19	LEU
2	E	26	ASP
2	E	34	ASP
2	E	61	GLU
2	E	82	LEU
2	E	88	MET
2	E	93	PHE
2	E	104	PRO
2	E	120	ASN
2	E	133	THR
2	E	162	GLU
2	E	173	VAL
2	E	182	GLU
2	E	189	VAL
2	E	223	LYS
2	E	225	ASP
2	E	235	PRO
2	E	239	LEU
2	E	243	GLU
2	E	261	THR
2	E	294	ILE
2	E	308	VAL
2	E	309	THR
2	E	322	THR
2	E	323	HIS
2	E	337	ILE
2	E	342	GLU
2	E	343	LEU

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Mol	Chain	Res	Type
2	E	359	SER
2	E	371	THR
2	E	394	LYS
2	E	402	ASP
2	E	405	THR
2	E	410	ARG
2	E	463	TYR
2	F	26	ASP
2	F	50	VAL
2	F	53	GLU
2	F	57	ILE
2	F	62	GLU
2	F	130	PHE
2	F	187	PHE
2	F	194	MET
2	F	199	ARG
2	F	201	LEU
2	F	204	PHE
2	F	219	LEU
2	F	225	ASP
2	F	235	PRO
2	F	286	TYR
2	F	287	MET
2	F	322	THR
2	F	324	PRO
2	F	336	GLN
2	F	371	THR
2	F	388	ASN
2	F	410	ARG
2	F	414	PHE
2	F	419	GLU
2	F	423	ILE
3	G	4	VAL
3	G	8	ARG
3	G	9	MET
3	G	32	ARG
3	G	39	PHE
3	G	43	VAL
3	G	44	ARG
3	G	70	PHE
3	G	73	PRO
3	G	89	VAL

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Mol	Chain	Res	Type
3	G	93	VAL
3	G	117	VAL
3	G	152	GLU
3	G	157	THR
3	G	162	ASN
3	G	177	ARG
3	G	188	ARG
3	G	204	ARG
4	H	28	GLU
4	H	57	ARG
4	H	60	GLU
4	H	72	LEU
4	H	77	LEU
4	H	78	LYS
4	H	92	GLU
4	H	96	LYS
4	H	98	ILE
5	I	61	GLU
5	I	69	LEU
5	I	75	GLU
5	I	91	ARG
5	I	107	LEU
6	J	57	LEU
6	J	78	GLU
6	J	122	VAL
6	J	150	LEU
5	K	63	GLU
5	K	69	LEU
5	K	82	GLU
5	K	95	GLU
5	K	108	ASP
6	L	158	GLU
7	M	20	LEU
7	M	39	LEU
7	M	74	ARG
7	M	82	GLU
7	M	119	LEU
7	M	122	GLU
7	M	133	PRO
7	M	142	VAL
7	M	157	GLU
7	M	192	LEU

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Mol	Chain	Res	Type
7	M	195	GLU
7	M	255	VAL
7	M	257	ASP
7	M	262	GLU
7	M	272	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	185	HIS
1	A	283	HIS
1	A	316	GLN
1	A	459	GLN
1	B	109	HIS
1	B	145	HIS
1	B	185	HIS
1	B	239	GLN
1	B	260	ASN
1	B	283	HIS
1	B	316	GLN
1	B	418	HIS
1	B	496	GLN
1	C	3	GLN
1	C	316	GLN
2	D	58	GLN
2	D	161	ASN
2	D	170	GLN
2	D	198	GLN
2	D	249	HIS
2	D	252	HIS
2	D	323	HIS
2	D	344	HIS
2	D	363	ASN
2	D	427	GLN
2	E	249	HIS
2	E	323	HIS
2	E	336	GLN
2	E	381	GLN
2	E	437	GLN
2	E	458	HIS
2	F	132	GLN

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Mol	Chain	Res	Type
2	F	148	GLN
2	F	166	GLN
2	F	262	ASN
2	F	344	HIS
2	F	375	HIS
2	F	388	ASN
3	G	3	GLN
4	H	84	HIS
6	J	96	GLN
7	M	200	ASN
7	M	315	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	ADP	A	600	-	28,29,29	1.43	6 (21%)	43,45,45	1.14	5 (11%)
8	ADP	C	600	-	28,29,29	1.04	1 (3%)	43,45,45	1.09	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	A	600	-	-	8/16/32/32	0/3/3/3
8	ADP	C	600	-	-	10/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	600	ADP	C4-N9	-3.06	1.31	1.37
8	A	600	ADP	C5-N7	-2.61	1.34	1.39
8	A	600	ADP	C1'-N9	-2.51	1.39	1.46
8	A	600	ADP	C2'-C1'	-2.17	1.46	1.53
8	C	600	ADP	C5-N7	-2.17	1.35	1.39
8	A	600	ADP	PA-O2A	-2.01	1.46	1.55
8	A	600	ADP	O4'-C1'	-2.01	1.37	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	600	ADP	N6-C6-N1	3.74	126.72	118.38
8	A	600	ADP	N6-C6-N1	3.68	126.58	118.38
8	C	600	ADP	C5-C6-N6	-2.92	116.05	123.29
8	A	600	ADP	C1'-N9-C8	2.25	132.08	127.09
8	A	600	ADP	C2'-C1'-N9	-2.23	107.75	113.30
8	A	600	ADP	C4-N9-C1'	-2.23	121.43	126.63
8	A	600	ADP	C5-C6-N6	-2.02	118.27	123.29

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	600	ADP	PA-O3A-PB-O2B
8	A	600	ADP	C5'-O5'-PA-O1A
8	A	600	ADP	C5'-O5'-PA-O3A
8	C	600	ADP	PA-O3A-PB-O2B
8	C	600	ADP	PA-O3A-PB-O3B
8	C	600	ADP	PB-O3A-PA-O5'
8	C	600	ADP	C5'-O5'-PA-O2A
8	C	600	ADP	C5'-O5'-PA-O3A

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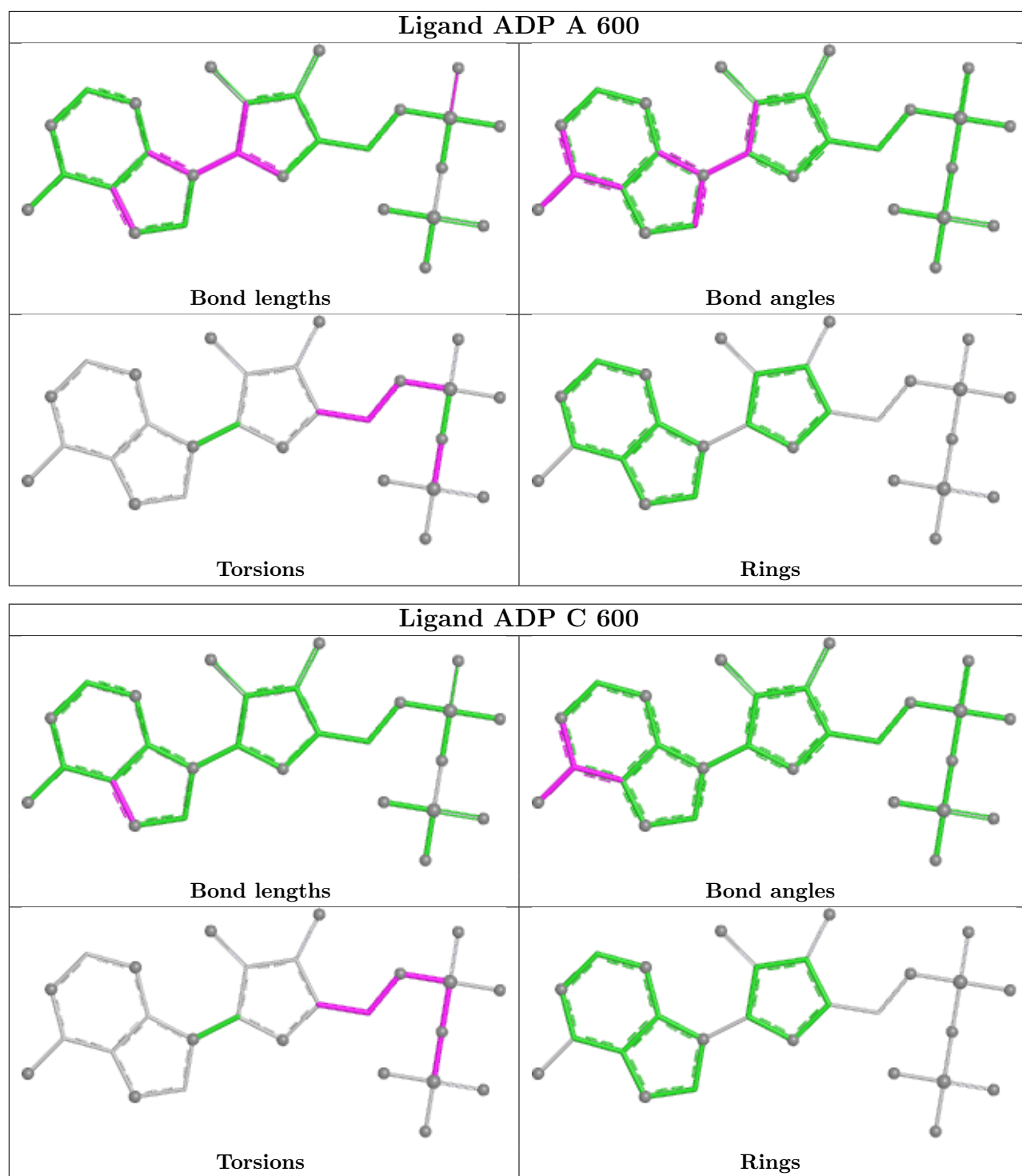
Mol	Chain	Res	Type	Atoms
8	C	600	ADP	O4'-C4'-C5'-O5'
8	C	600	ADP	C3'-C4'-C5'-O5'
8	A	600	ADP	O4'-C4'-C5'-O5'
8	A	600	ADP	C3'-C4'-C5'-O5'
8	C	600	ADP	C4'-C5'-O5'-PA
8	A	600	ADP	C5'-O5'-PA-O2A
8	C	600	ADP	C5'-O5'-PA-O1A
8	A	600	ADP	C4'-C5'-O5'-PA
8	A	600	ADP	PA-O3A-PB-O3B
8	C	600	ADP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	600	ADP	4	0
8	C	600	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

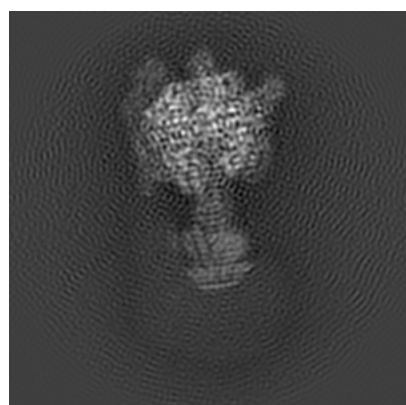
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6811. These allow visual inspection of the internal detail of the map and identification of artifacts.

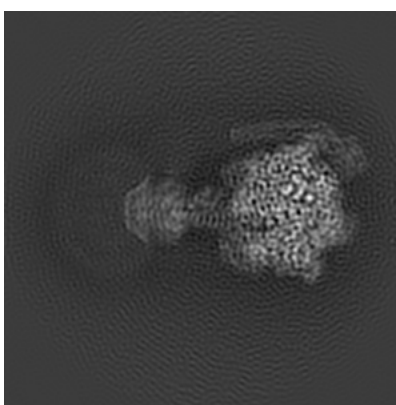
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

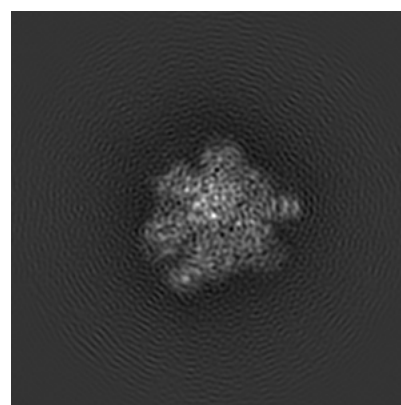
6.1.1 Primary map



X



Y

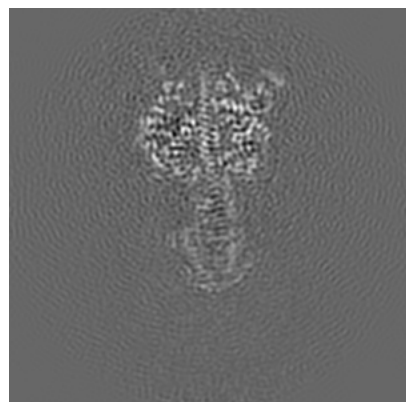


Z

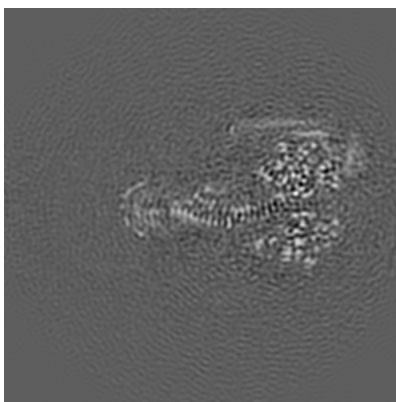
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

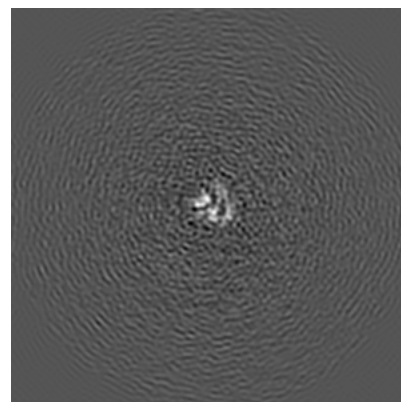
6.2.1 Primary map



X Index: 118



Y Index: 118

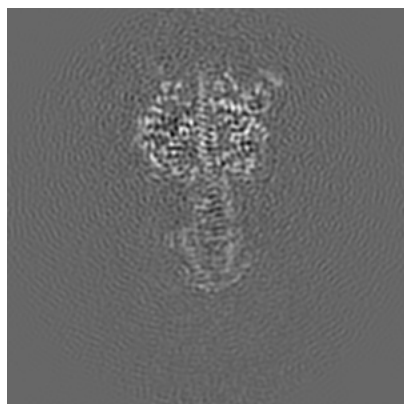


Z Index: 118

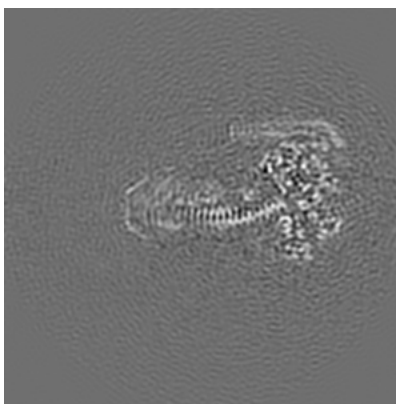
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

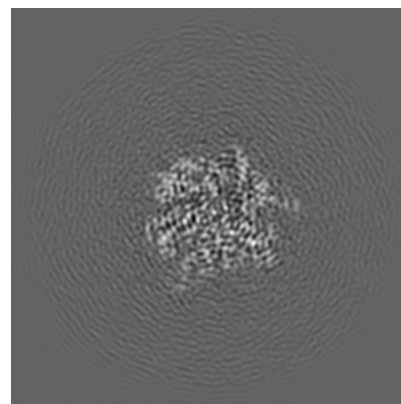
6.3.1 Primary map



X Index: 118



Y Index: 122

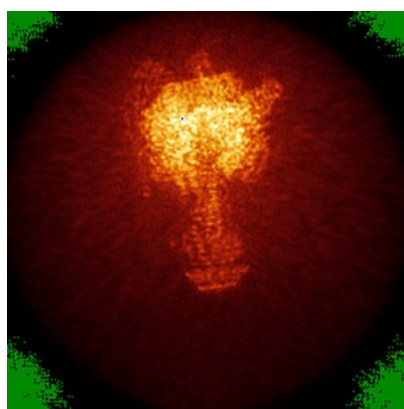


Z Index: 171

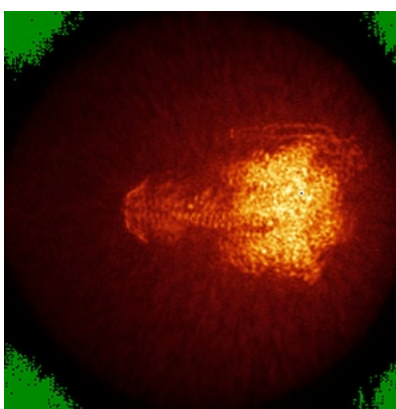
The images above show the largest variance slices of the map in three orthogonal directions.

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

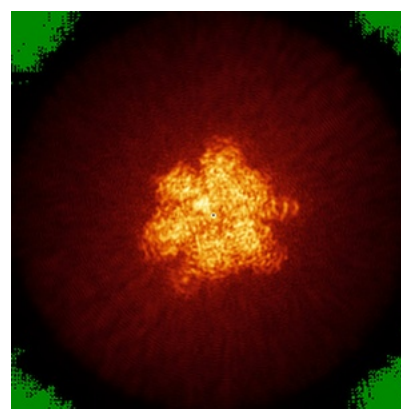
6.4.1 Primary map



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

This section was not generated.

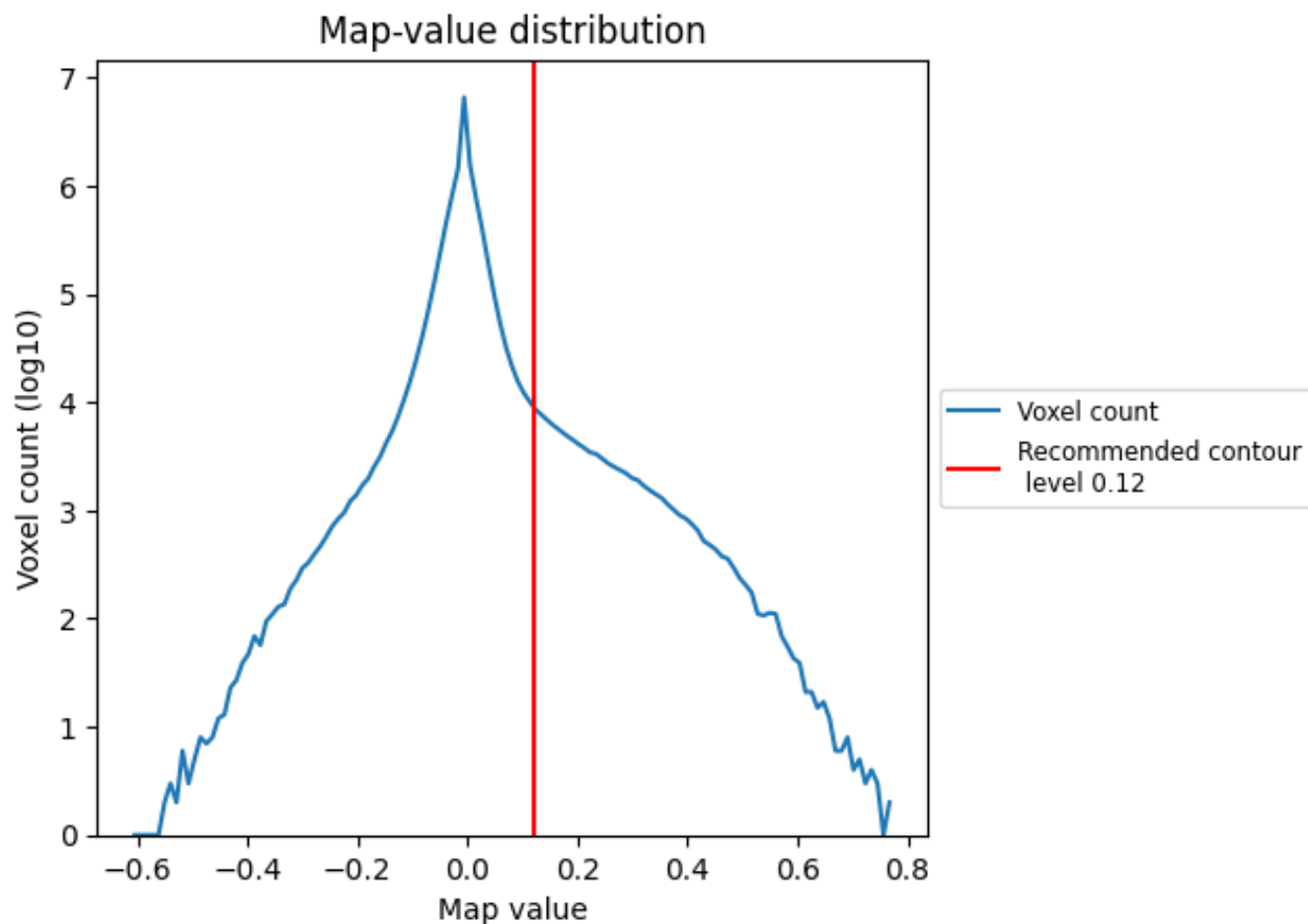
6.6 Mask visualisation

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

7 Map analysis [i](#)

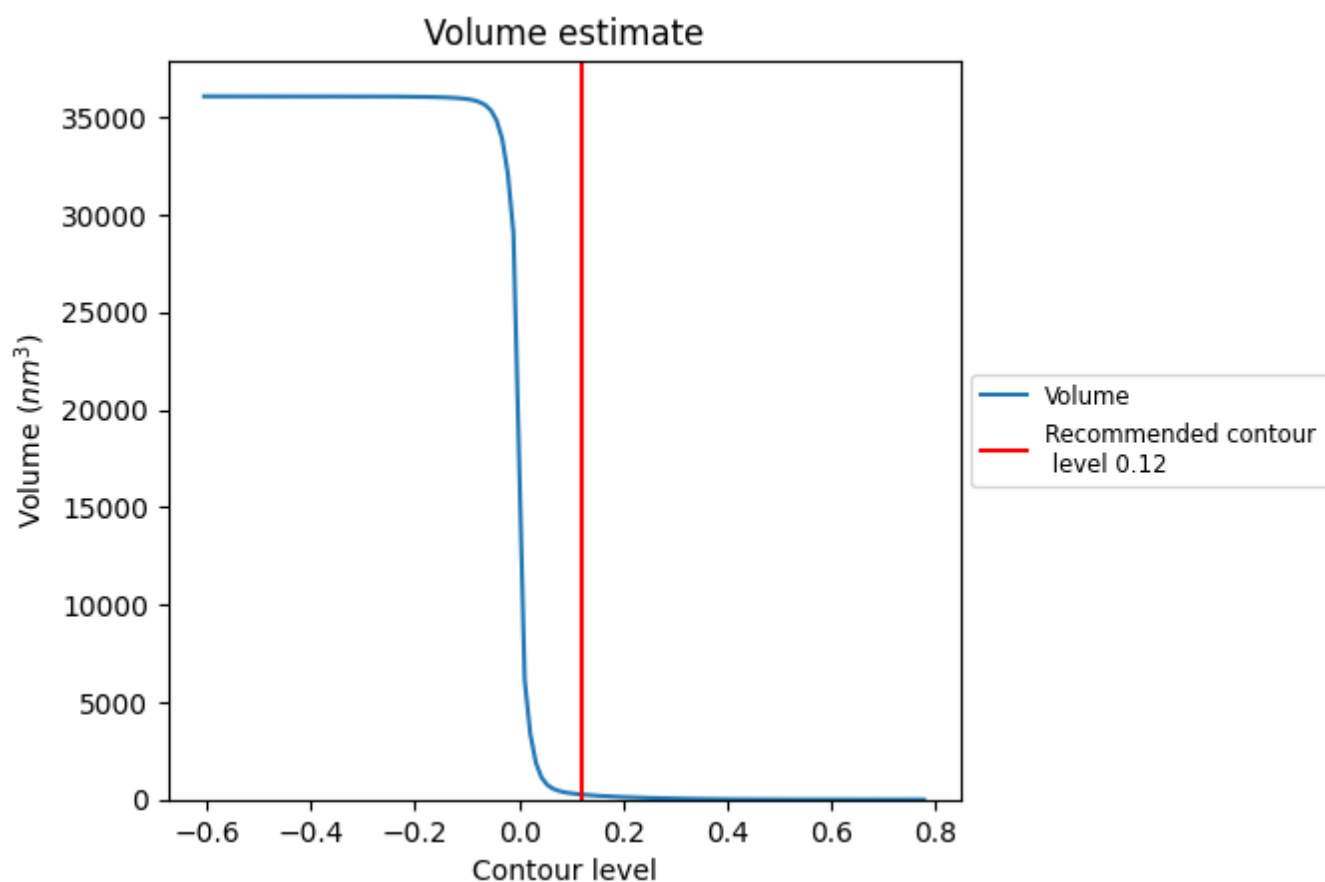
This section contains the results of statistical analysis of the map.

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.

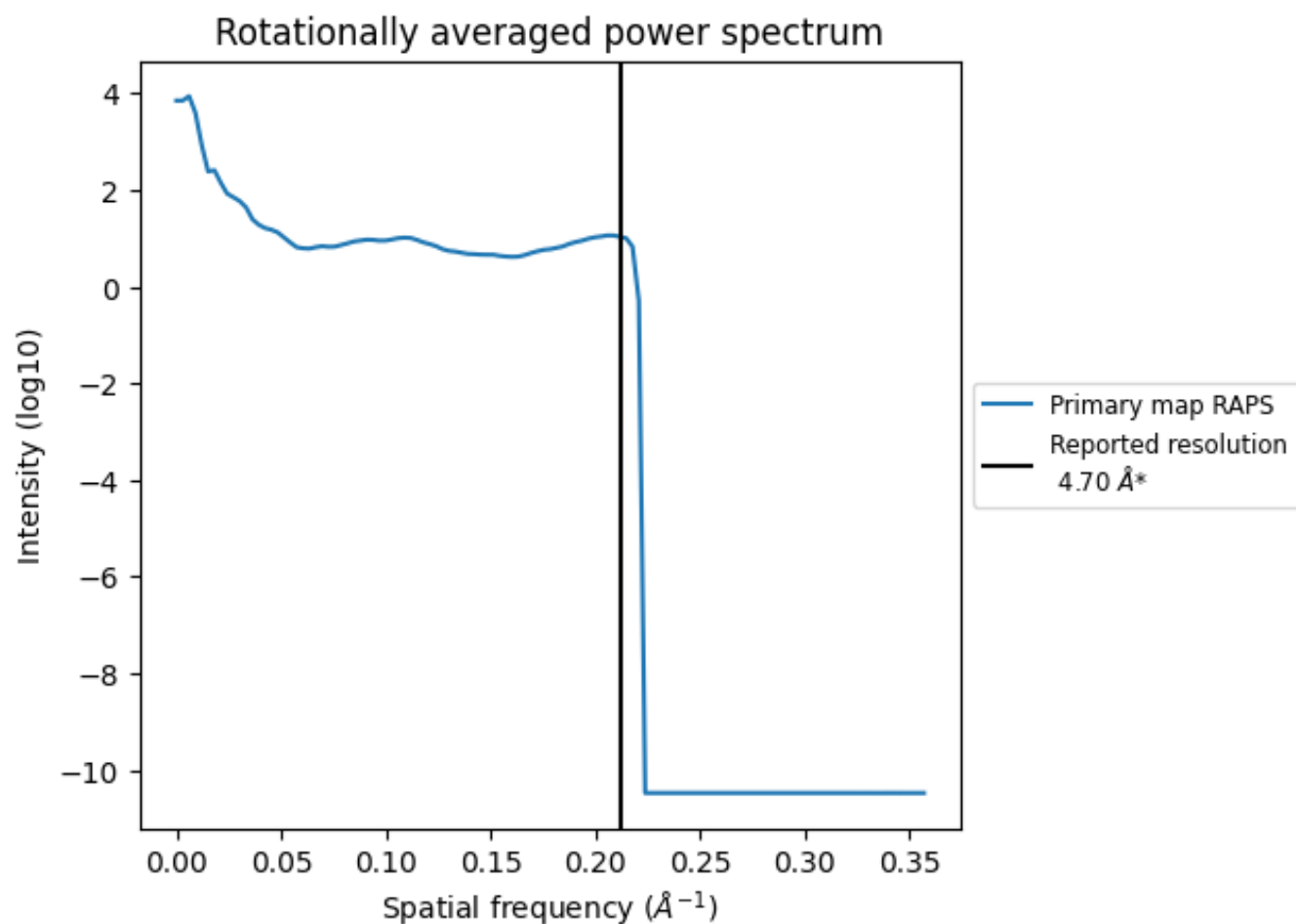
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 260 nm^3 ; this corresponds to an approximate mass of 234 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 ⓘ

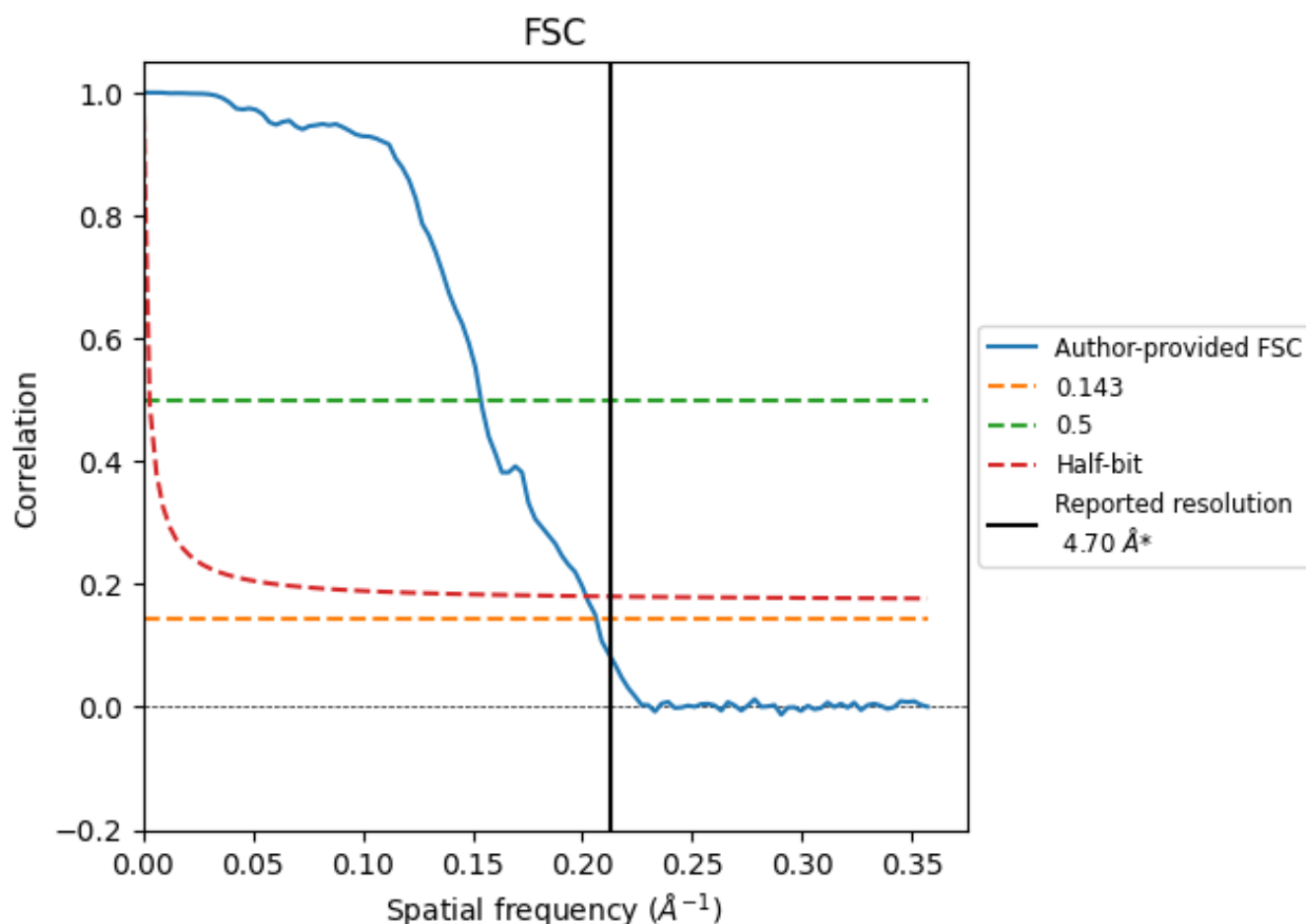


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

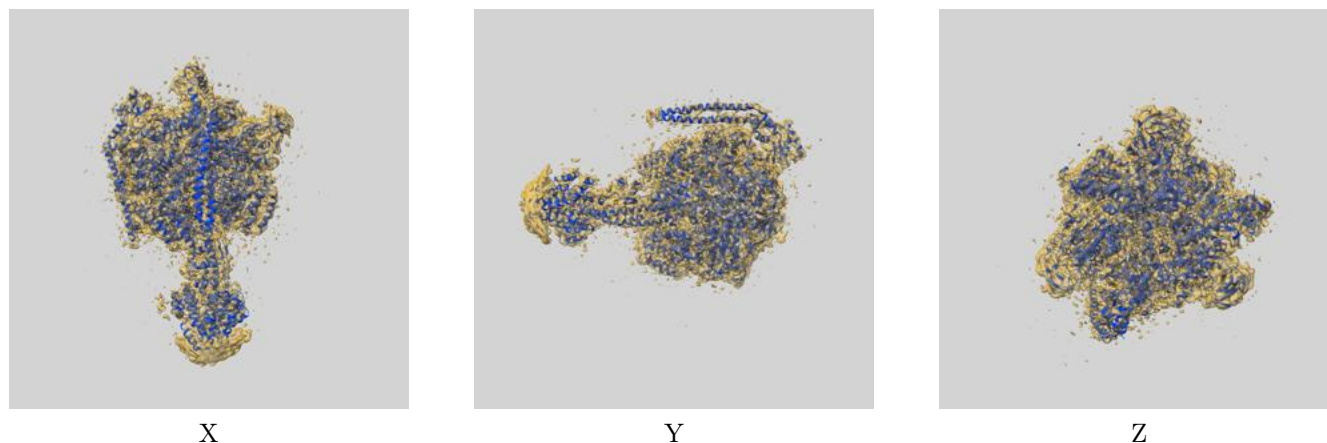
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.85	6.50	4.96
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

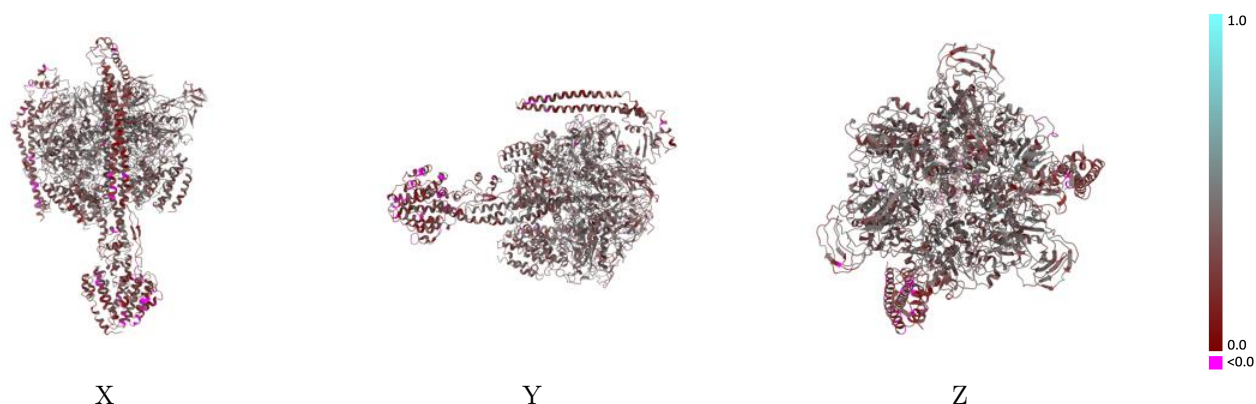
This section contains information regarding the fit between EMDB map EMD-6811 and PDB model 5Y5Y. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



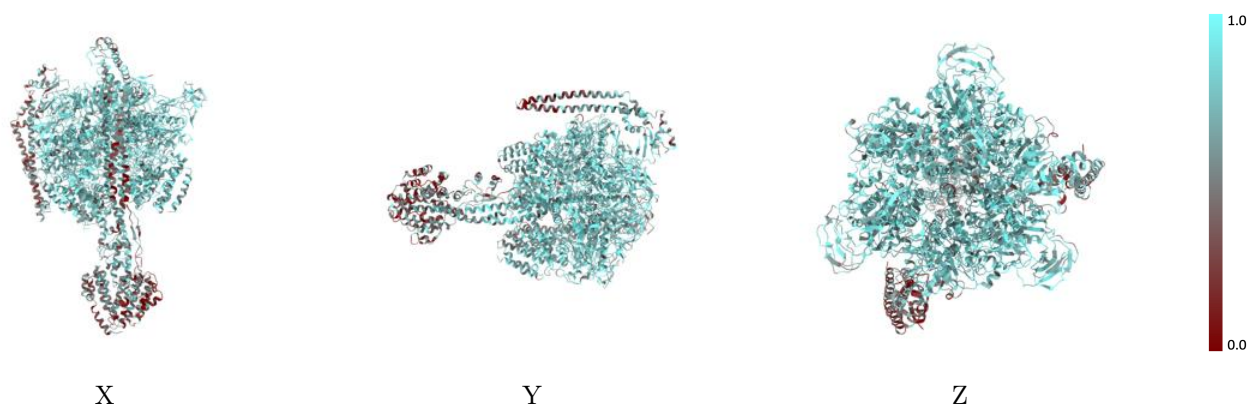
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



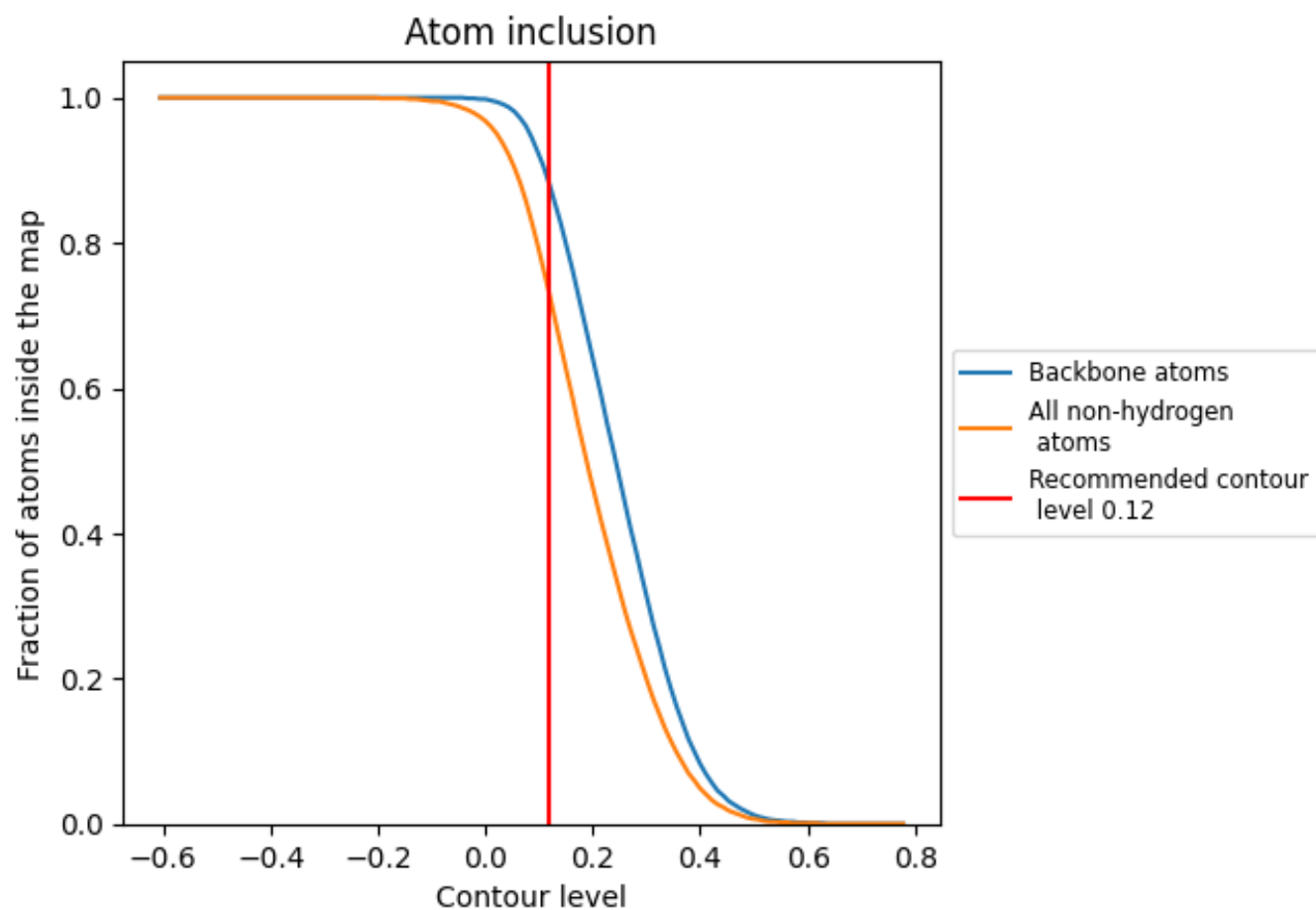
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.3620
A	0.7980	0.3940
B	0.7860	0.3910
C	0.8010	0.3920
D	0.8010	0.4010
E	0.7770	0.3880
F	0.8060	0.3970
G	0.6620	0.3330
H	0.6210	0.3170
I	0.3490	0.2250
J	0.4780	0.2370
K	0.4790	0.2140
L	0.6070	0.2880
M	0.4080	0.2290

