



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 03:34 AM UTC

PDB ID : 6O22 / pdb_00006o22
BMRB ID : 30576
Title : Structure of Asf1-H3:H4-Rtt109-Vps75 histone chaperone-lysine acetyltransferase complex with the histone substrate.
Authors : Danilenko, N.; Carlomagno, T.; Kirkpatrick, J.P.
Deposited on : 2019-02-22

This is a Full wwPDB NMR Structure 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/NMRValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

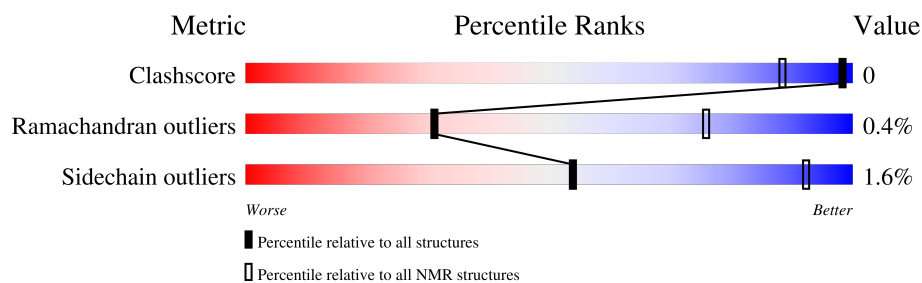
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLUTION SCATTERING

The overall completeness of chemical shifts assignment is 2%.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	264	51% 34% . 13%
1	B	264	48% 30% . 18%
2	C	442	55% 39% . .
3	D	279	34% 24% . 41%
4	E	136	27% 25% . 45%
5	F	103	44% 34% . . 20%

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19411 atoms, of which 9680 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Vacuolar protein sorting-associated protein 75.

Mol	Chain	Residues	Atoms						Trace
1	A	230	Total	C	H	N	O	S	0
			3733	1221	1825	309	372	6	
1	B	217	Total	C	H	N	O	S	0
			3562	1168	1752	294	343	5	

- Molecule 2 is a protein called Histone acetyltransferase RTT109.

Mol	Chain	Residues	Atoms						Trace
2	C	424	Total	C	H	N	O	S	0
			6917	2205	3480	585	637	10	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q07794
C	-4	MET	-	expression tag	UNP Q07794
C	-3	ASP	-	expression tag	UNP Q07794
C	-2	PRO	-	expression tag	UNP Q07794
C	-1	ASN	-	expression tag	UNP Q07794
C	0	SER	-	expression tag	UNP Q07794

- Molecule 3 is a protein called Histone chaperone ASF1.

Mol	Chain	Residues	Atoms						Trace
3	D	164	Total	C	H	N	O	S	0
			2592	840	1280	212	258	2	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	SER	-	expression tag	UNP P32447

- Molecule 4 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms						Trace
4	E	75	Total	C	H	N	O	S	0
			1243	384	636	114	106	3	

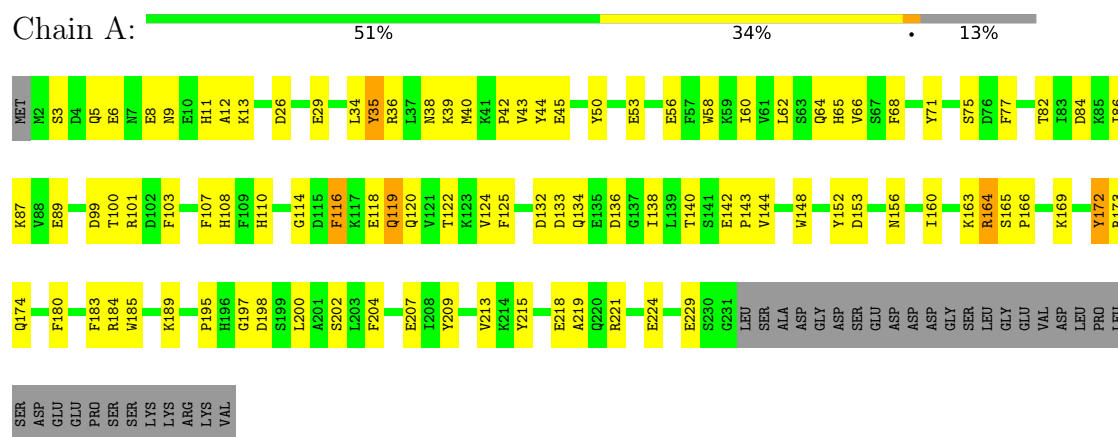
- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						Trace
5	F	82	Total	C	H	N	O	S	0
			1364	416	707	128	112	1	

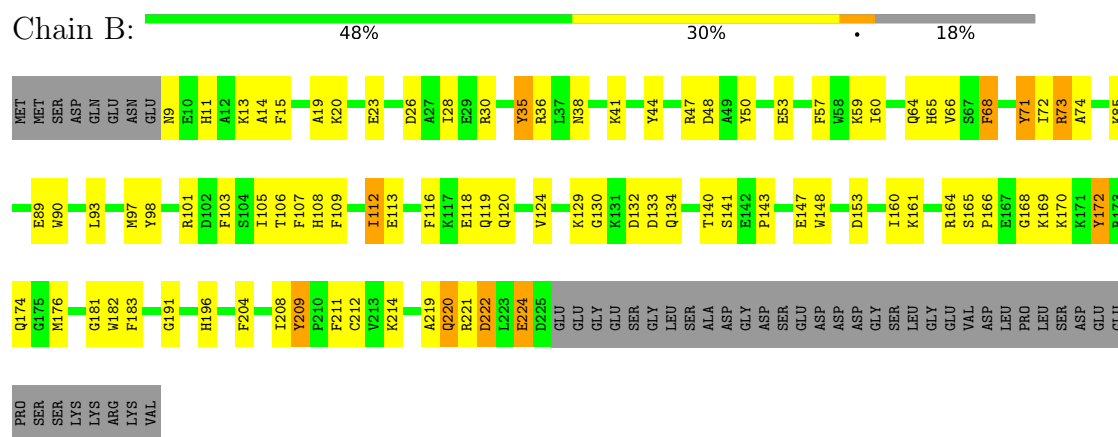
4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Vacuolar protein sorting-associated protein 75

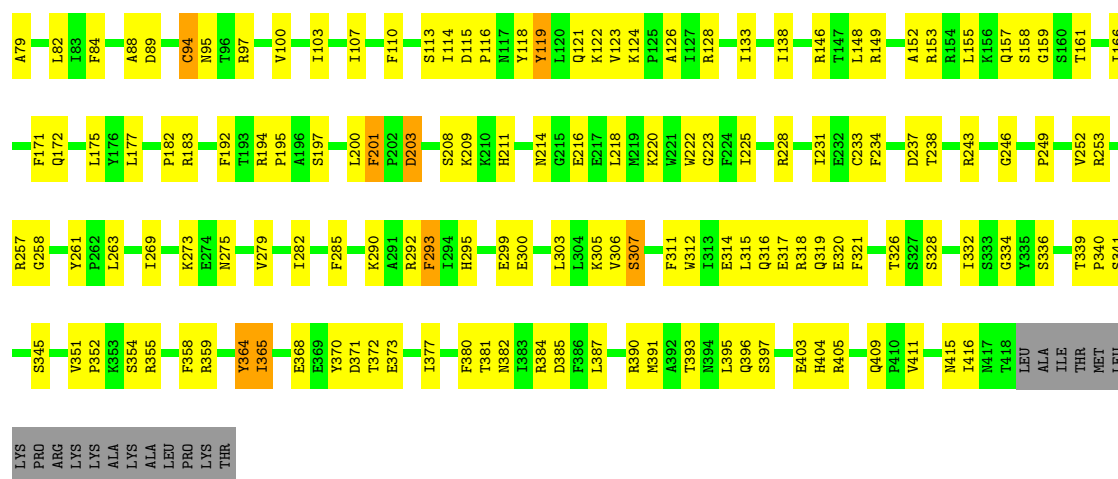


• Molecule 1: Vacuolar protein sorting-associated protein 75

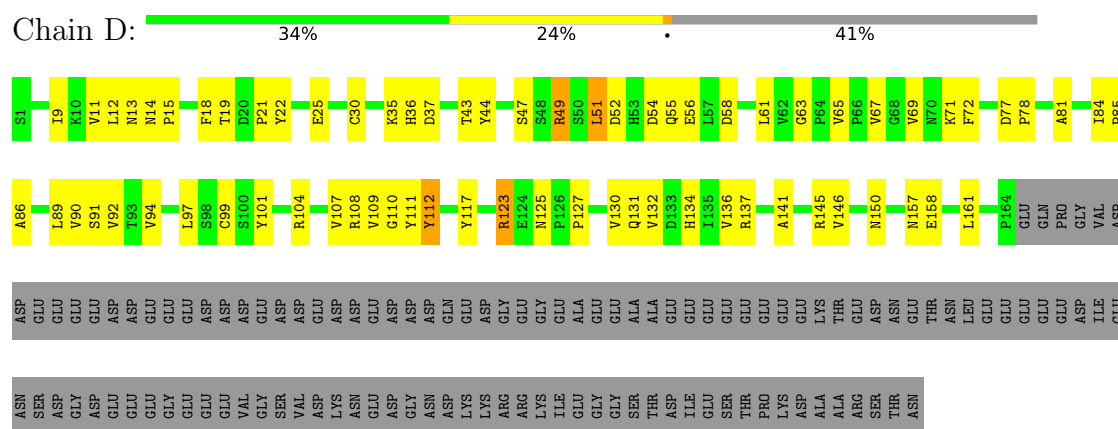


• Molecule 2: Histone acetyltransferase RTT109

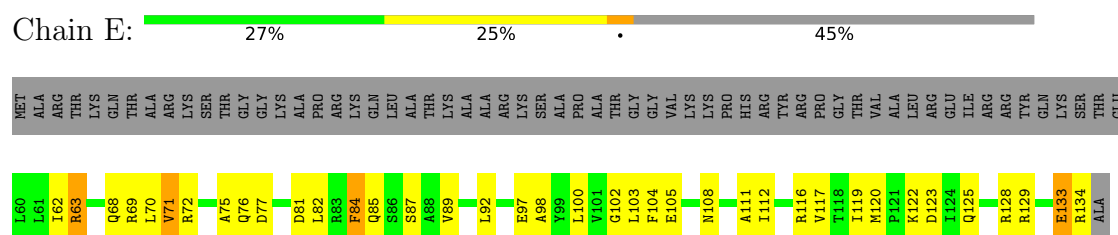




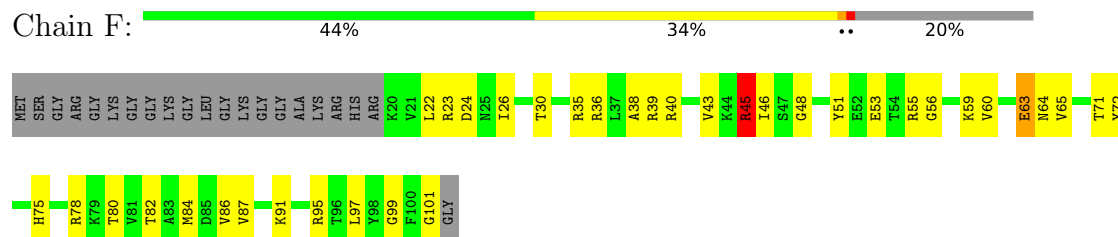
• Molecule 3: Histone chaperone ASF1



• Molecule 4: Histone H3.2



• Molecule 5: Histone H4



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 150 calculated structures, 1 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	structure calculation	
Amber	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	368
Number of shifts mapped to atoms	368
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	2%

6 Model quality (i)

6.1 Standard geometry (i)

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 (average) 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	1.94	39/1956 (2.0%)	2.32	99/2633 (3.8%)
1	B	1.96	37/1858 (2.0%)	2.35	101/2503 (4.0%)
2	C	1.97	74/3515 (2.1%)	2.35	184/4758 (3.9%)
3	D	2.01	27/1344 (2.0%)	2.32	67/1835 (3.7%)
4	E	2.10	15/614 (2.4%)	2.44	36/823 (4.4%)
5	F	2.06	16/664 (2.4%)	2.40	39/889 (4.4%)
All	All	1.99	208/9951 (2.1%)	2.35	526/13441 (3.9%)

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

Mol	Chain	Chirality	Planarity
1	A	0	4
1	B	0	8
2	C	0	9
3	D	0	4
4	E	0	3
5	F	0	4
All	All	0	32

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	130	VAL	N-CA	9.93	1.58	1.46
1	B	103	PHE	CA-C	9.05	1.63	1.52
1	A	118	GLU	N-CA	8.83	1.57	1.46
1	B	196	HIS	CD2-NE2	-8.61	1.28	1.37
1	B	209	TYR	CA-C	8.53	1.63	1.52
1	B	165	SER	CA-C	8.25	1.62	1.53
2	C	306	VAL	C-O	-8.09	1.15	1.24
2	C	336	SER	CA-C	7.96	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	ILE	N-CA	7.77	1.56	1.46
2	C	94	CYS	CA-C	7.76	1.62	1.52
2	C	381	THR	N-CA	7.62	1.55	1.46
1	A	229	GLU	CA-C	7.58	1.61	1.52
1	A	42	PRO	N-CD	-7.52	1.37	1.47
5	F	35	ARG	N-CA	7.49	1.55	1.46
1	B	74	ALA	CA-C	7.45	1.62	1.52
3	D	108	ARG	N-CA	-7.25	1.37	1.46
4	E	62	ILE	N-CA	7.19	1.54	1.46
2	C	47	ILE	N-CA	7.14	1.54	1.46
1	A	156	ASN	CA-C	7.11	1.61	1.52
2	C	23	GLN	CA-C	7.08	1.60	1.52
5	F	56	GLY	CA-C	7.05	1.60	1.52
3	D	15	PRO	N-CD	-6.96	1.38	1.47
1	B	112	ILE	CA-CB	6.90	1.62	1.54
1	B	101	ARG	CZ-NH2	-6.84	1.24	1.33
1	B	108	HIS	CE1-NE2	6.83	1.39	1.32
2	C	252	VAL	CA-C	6.79	1.61	1.52
1	B	153	ASP	N-CA	6.76	1.55	1.46
2	C	21	SER	N-CA	6.76	1.54	1.46
3	D	89	LEU	CA-CB	6.76	1.63	1.53
2	C	122	LYS	N-CA	6.74	1.54	1.46
2	C	315	LEU	N-CA	6.69	1.54	1.46
5	F	65	VAL	N-CA	6.66	1.54	1.46
2	C	128	ARG	NE-CZ	-6.66	1.25	1.33
1	A	133	ASP	N-CA	6.62	1.54	1.45
3	D	137	ARG	CD-NE	6.58	1.55	1.46
4	E	129	ARG	CZ-NH2	-6.58	1.24	1.33
2	C	285	PHE	CA-C	6.55	1.61	1.52
4	E	123	ASP	CA-C	6.50	1.61	1.52
1	A	58	TRP	CA-C	6.49	1.61	1.52
1	A	120	GLN	N-CA	6.49	1.53	1.46
1	A	26	ASP	CA-C	6.48	1.61	1.52
1	B	118	GLU	CA-CB	-6.47	1.43	1.53
1	A	116	PHE	CA-CB	6.45	1.65	1.53
1	A	53	GLU	N-CA	6.44	1.54	1.46
2	C	273	LYS	CA-C	-6.43	1.44	1.52
2	C	194	ARG	CA-C	6.41	1.59	1.52
2	C	233	CYS	CA-C	6.41	1.60	1.52
4	E	89	VAL	CA-CB	6.38	1.62	1.54
1	B	169	LYS	CA-C	6.37	1.61	1.52
2	C	253	ARG	CZ-NH1	-6.34	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	380	PHE	CA-C	6.29	1.60	1.52
2	C	234	PHE	CA-C	6.29	1.60	1.52
2	C	393	THR	CA-C	6.28	1.60	1.52
4	E	62	ILE	CA-C	6.28	1.60	1.52
1	B	66	VAL	CA-C	6.27	1.60	1.52
1	A	110	HIS	CE1-NE2	6.25	1.38	1.32
2	C	177	LEU	N-CA	6.24	1.53	1.45
5	F	99	GLY	C-O	6.23	1.30	1.23
2	C	97	ARG	C-N	6.20	1.41	1.33
2	C	65	LEU	C-N	6.20	1.41	1.33
4	E	75	ALA	N-CA	6.19	1.54	1.46
1	B	11	HIS	C-O	-6.19	1.16	1.24
2	C	115	ASP	C-N	6.18	1.41	1.33
2	C	303	LEU	N-CA	6.13	1.54	1.46
1	A	3	SER	CA-C	6.12	1.60	1.52
1	A	62	LEU	N-CA	6.12	1.54	1.46
1	B	106	THR	N-CA	6.12	1.53	1.46
5	F	55	ARG	N-CA	6.12	1.53	1.46
2	C	148	LEU	CA-C	6.10	1.61	1.52
1	A	215	TYR	N-CA	6.05	1.54	1.46
5	F	30	THR	N-CA	6.05	1.53	1.45
5	F	101	GLY	N-CA	6.04	1.55	1.45
5	F	26	ILE	N-CA	6.04	1.53	1.46
1	B	133	ASP	N-CA	6.04	1.53	1.46
2	C	183	ARG	CZ-NH2	-6.04	1.25	1.33
5	F	64	ASN	CA-C	6.01	1.60	1.52
3	D	12	LEU	N-CA	6.00	1.54	1.46
4	E	82	LEU	CA-C	5.96	1.60	1.52
3	D	123	ARG	CZ-NH2	-5.96	1.25	1.33
2	C	218	LEU	CA-C	5.95	1.60	1.52
3	D	67	VAL	CA-C	5.95	1.59	1.52
2	C	172	GLN	N-CA	5.92	1.53	1.46
2	C	14	SER	CA-C	5.91	1.60	1.52
1	B	224	GLU	CA-C	5.91	1.59	1.52
1	B	23	GLU	CA-C	5.90	1.60	1.52
2	C	340	PRO	CA-C	5.89	1.59	1.52
2	C	397	SER	N-CA	5.89	1.53	1.46
3	D	84	ILE	CA-C	5.87	1.57	1.53
2	C	124	LYS	C-N	5.87	1.40	1.33
3	D	123	ARG	CA-C	5.86	1.60	1.52
2	C	290	LYS	N-CA	5.86	1.53	1.46
1	A	6	GLU	N-CA	5.84	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	25	ILE	C-O	-5.84	1.17	1.25
2	C	33	VAL	CA-C	5.83	1.59	1.52
4	E	120	MET	N-CA	5.82	1.50	1.46
2	C	119	TYR	N-CA	5.77	1.53	1.46
2	C	40	LYS	CA-C	5.76	1.60	1.52
4	E	98	ALA	CA-C	5.76	1.60	1.52
3	D	145	ARG	N-CA	-5.76	1.39	1.46
4	E	70	LEU	CA-CB	5.76	1.62	1.53
1	B	222	ASP	N-CA	5.75	1.53	1.45
2	C	97	ARG	N-CA	5.75	1.53	1.46
2	C	233	CYS	N-CA	5.75	1.53	1.46
3	D	107	VAL	CA-C	5.75	1.59	1.52
3	D	99	CYS	CA-C	5.71	1.59	1.52
1	A	8	GLU	N-CA	5.70	1.53	1.45
1	A	110	HIS	CG-CD2	5.69	1.42	1.35
1	A	204	PHE	CA-CB	-5.68	1.44	1.53
3	D	78	PRO	CA-C	5.68	1.57	1.52
2	C	71	VAL	CA-CB	-5.67	1.47	1.54
3	D	55	GLN	CA-C	5.67	1.59	1.52
5	F	87	VAL	CA-CB	5.66	1.62	1.54
2	C	159	GLY	C-N	5.66	1.40	1.33
1	A	64	GLN	CA-C	5.64	1.60	1.52
1	A	34	LEU	CA-C	5.63	1.60	1.52
2	C	220	LYS	C-N	-5.63	1.26	1.33
2	C	326	THR	N-CA	5.62	1.55	1.46
2	C	395	LEU	C-N	5.61	1.40	1.33
2	C	258	GLY	CA-C	-5.60	1.45	1.52
2	C	377	ILE	CB-CG1	5.60	1.64	1.53
2	C	47	ILE	C-N	5.59	1.41	1.33
1	A	75	SER	CA-C	5.59	1.60	1.52
1	B	220	GLN	CA-C	5.58	1.60	1.52
1	A	108	HIS	N-CA	5.58	1.52	1.46
2	C	30	HIS	CG-ND1	5.58	1.44	1.38
5	F	43	VAL	N-CA	5.58	1.52	1.46
2	C	365	ILE	N-CA	5.58	1.54	1.46
1	B	26	ASP	CA-C	5.57	1.60	1.52
3	D	11	VAL	CA-C	5.56	1.59	1.52
2	C	243	ARG	C-N	-5.53	1.27	1.33
1	A	219	ALA	N-CA	5.52	1.53	1.46
1	B	143	PRO	N-CA	-5.51	1.40	1.47
1	A	36	ARG	CZ-NH2	-5.51	1.26	1.33
1	B	48	ASP	N-CA	5.49	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	404	HIS	ND1-CE1	5.48	1.38	1.32
1	B	66	VAL	CA-CB	5.47	1.61	1.54
2	C	175	LEU	N-CA	5.45	1.53	1.46
1	A	140	THR	CB-OG1	5.45	1.52	1.43
1	A	71	TYR	C-N	5.42	1.41	1.33
2	C	341	SER	N-CA	5.42	1.53	1.46
1	A	207	GLU	N-CA	5.41	1.53	1.46
5	F	22	LEU	C-O	-5.41	1.17	1.24
1	B	85	LYS	N-CA	5.40	1.52	1.45
1	B	181	GLY	CA-C	5.40	1.58	1.51
2	C	390	ARG	CZ-NH1	-5.39	1.25	1.32
3	D	150	ASN	CA-CB	5.39	1.61	1.53
1	B	19	ALA	CA-C	5.39	1.60	1.52
1	B	120	GLN	CA-CB	5.38	1.61	1.53
2	C	391	MET	CA-C	5.37	1.59	1.52
1	B	153	ASP	CA-C	5.36	1.60	1.52
1	A	218	GLU	CA-C	5.36	1.60	1.52
2	C	332	ILE	N-CA	5.35	1.51	1.46
4	E	133	GLU	N-CA	5.35	1.53	1.46
1	A	209	TYR	CA-CB	-5.34	1.45	1.53
2	C	279	VAL	C-O	-5.33	1.18	1.24
1	A	221	ARG	CA-C	5.33	1.59	1.52
2	C	243	ARG	N-CA	5.32	1.52	1.45
1	A	53	GLU	C-N	5.32	1.40	1.33
2	C	225	ILE	CA-C	5.30	1.60	1.52
1	A	174	GLN	C-O	-5.29	1.17	1.24
1	B	191	GLY	CA-C	5.29	1.58	1.51
4	E	102	GLY	N-CA	-5.29	1.39	1.45
4	E	71	VAL	CA-C	-5.28	1.46	1.52
2	C	152	ALA	CA-CB	5.28	1.62	1.53
1	B	35	TYR	CA-CB	5.27	1.62	1.53
2	C	9	SER	C-O	5.26	1.30	1.24
3	D	65	VAL	CA-C	5.26	1.57	1.53
3	D	104	ARG	CZ-NH2	-5.25	1.26	1.33
1	B	38	ASN	N-CA	5.25	1.52	1.46
5	F	97	LEU	N-CA	5.24	1.52	1.46
1	B	93	LEU	N-CA	5.21	1.53	1.46
2	C	261	TYR	CA-C	5.20	1.58	1.53
3	D	97	LEU	C-O	-5.18	1.17	1.24
1	A	163	LYS	CA-C	5.18	1.59	1.52
1	B	204	PHE	N-CA	5.17	1.52	1.46
2	C	231	ILE	N-CA	5.17	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	ASN	C-N	-5.16	1.26	1.33
3	D	52	ASP	CA-CB	5.16	1.62	1.53
5	F	23	ARG	CZ-NH2	-5.16	1.26	1.33
3	D	19	THR	N-CA	5.16	1.52	1.46
2	C	42	VAL	CA-C	5.15	1.58	1.52
4	E	85	GLN	CA-C	5.15	1.59	1.52
2	C	387	LEU	CA-C	5.14	1.59	1.52
3	D	110	GLY	N-CA	5.14	1.51	1.45
5	F	45	ARG	N-CA	5.14	1.52	1.46
5	F	84	MET	N-CA	5.13	1.52	1.46
1	A	29	GLU	CA-C	5.12	1.59	1.52
3	D	14	ASN	CA-C	5.12	1.57	1.52
2	C	385	ASP	CA-C	5.11	1.59	1.52
1	A	60	ILE	CA-CB	5.11	1.60	1.54
2	C	49	THR	CB-OG1	-5.10	1.35	1.43
2	C	114	ILE	CA-CB	5.09	1.60	1.54
2	C	114	ILE	N-CA	5.08	1.52	1.46
2	C	352	PRO	CA-C	5.08	1.59	1.52
4	E	129	ARG	CZ-NH1	-5.08	1.25	1.32
2	C	370	TYR	N-CA	5.08	1.53	1.46
3	D	47	SER	N-CA	5.07	1.52	1.46
1	A	156	ASN	C-O	-5.06	1.17	1.24
1	A	184	ARG	N-CA	5.06	1.52	1.46
1	B	176	MET	CA-C	5.06	1.59	1.52
2	C	118	TYR	N-CA	5.05	1.52	1.46
2	C	195	PRO	C-O	-5.05	1.17	1.24
1	B	124	VAL	CA-CB	-5.05	1.48	1.54
3	D	51	LEU	CA-CB	5.05	1.62	1.53
3	D	69	VAL	N-CA	5.04	1.52	1.46
1	A	143	PRO	N-CD	-5.04	1.40	1.47
1	B	11	HIS	CE1-NE2	5.02	1.37	1.32
2	C	318	ARG	CZ-NH2	-5.02	1.26	1.33

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	84	PHE	CA-CB-CG	12.83	126.63	113.80
1	B	222	ASP	CA-CB-CG	11.01	123.61	112.60
1	A	164	ARG	NE-CZ-NH2	10.24	128.42	119.20
1	B	72	ILE	CA-C-N	10.08	135.18	120.87
1	B	72	ILE	C-N-CA	10.08	135.18	120.87
1	A	103	PHE	CA-CB-CG	10.06	123.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	13	ASN	OD1-CG-ND2	-9.51	113.09	122.60
2	C	97	ARG	NE-CZ-NH2	9.49	127.75	119.20
3	D	131	GLN	OE1-CD-NE2	-9.47	113.13	122.60
2	C	201	PHE	CA-CB-CG	9.46	123.26	113.80
2	C	121	GLN	OE1-CD-NE2	-9.28	113.33	122.60
2	C	19	TYR	CA-C-N	9.14	135.09	122.19
2	C	19	TYR	C-N-CA	9.14	135.09	122.19
1	A	65	HIS	CA-CB-CG	-8.95	104.85	113.80
1	B	60	ILE	O-C-N	-8.55	113.18	122.07
3	D	30	CYS	CA-C-O	-8.46	111.25	120.30
5	F	53	GLU	N-CA-C	8.45	120.49	111.28
1	B	59	LYS	CA-C-N	8.40	130.81	122.66
1	B	59	LYS	C-N-CA	8.40	130.81	122.66
2	C	352	PRO	N-CA-CB	8.35	111.10	103.33
5	F	39	ARG	NE-CZ-NH2	8.34	126.71	119.20
4	E	125	GLN	OE1-CD-NE2	-8.28	114.32	122.60
3	D	86	ALA	N-CA-C	8.28	122.35	111.75
4	E	81	ASP	CA-CB-CG	8.26	120.86	112.60
5	F	80	THR	CA-C-N	8.24	132.19	120.98
5	F	80	THR	C-N-CA	8.24	132.19	120.98
2	C	25	ILE	CB-CA-C	8.23	118.94	110.88
1	A	136	ASP	CA-CB-CG	8.14	120.74	112.60
2	C	26	PRO	N-CA-CB	8.13	110.52	103.36
2	C	-3	ASP	CA-CB-CG	8.01	120.61	112.60
2	C	321	PHE	CA-CB-CG	7.98	121.78	113.80
1	B	105	ILE	CA-C-N	7.96	133.98	123.00
1	B	105	ILE	C-N-CA	7.96	133.98	123.00
2	C	214	ASN	OD1-CG-ND2	-7.86	114.74	122.60
5	F	78	ARG	O-C-N	-7.83	114.28	123.06
2	C	382	ASN	OD1-CG-ND2	-7.77	114.83	122.60
5	F	39	ARG	NH1-CZ-NH2	-7.73	109.25	119.30
2	C	345	SER	CA-C-N	7.70	131.36	120.28
2	C	345	SER	C-N-CA	7.70	131.36	120.28
2	C	312	TRP	N-CA-C	7.69	121.92	112.54
1	A	119	GLN	N-CA-C	7.67	120.04	108.46
1	B	89	GLU	CA-C-O	7.62	129.43	120.14
1	A	114	GLY	CA-C-O	-7.59	110.58	119.01
1	A	38	ASN	OD1-CG-ND2	-7.58	115.02	122.60
2	C	295	HIS	O-C-N	-7.54	113.05	122.17
3	D	134	HIS	CB-CG-CD2	-7.53	121.41	131.20
1	B	20	LYS	CA-C-N	7.51	130.65	120.44
1	B	20	LYS	C-N-CA	7.51	130.65	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	64	ASN	OD1-CG-ND2	-7.49	115.11	122.60
5	F	60	VAL	N-CA-C	7.48	118.28	110.72
2	C	321	PHE	CA-C-N	7.48	133.68	122.68
2	C	321	PHE	C-N-CA	7.48	133.68	122.68
2	C	303	LEU	CD1-CG-CD2	-7.48	94.35	110.80
4	E	63	ARG	NE-CZ-NH1	7.45	128.95	121.50
1	B	68	PHE	CA-C-N	7.42	130.55	120.38
1	B	68	PHE	C-N-CA	7.42	130.55	120.38
1	A	110	HIS	ND1-CG-CD2	7.41	113.51	106.10
2	C	228	ARG	NE-CZ-NH2	7.38	125.84	119.20
1	B	129	LYS	O-C-N	-7.35	115.55	123.26
2	C	58	GLN	CA-CB-CG	7.33	128.76	114.10
2	C	192	PHE	CA-CB-CG	7.31	121.11	113.80
4	E	100	LEU	CA-C-O	-7.31	112.67	120.42
1	A	138	ILE	CA-CB-CG1	7.30	122.81	110.40
2	C	246	GLY	CA-C-N	7.29	131.85	121.42
2	C	246	GLY	C-N-CA	7.29	131.85	121.42
2	C	5	ASP	O-C-N	-7.26	113.73	122.22
5	F	23	ARG	CA-C-N	7.24	130.71	120.28
5	F	23	ARG	C-N-CA	7.24	130.71	120.28
2	C	194	ARG	CA-C-N	7.23	127.56	119.32
2	C	194	ARG	C-N-CA	7.23	127.56	119.32
2	C	252	VAL	O-C-N	7.23	128.99	121.91
1	B	119	GLN	OE1-CD-NE2	-7.22	115.38	122.60
1	B	65	HIS	CA-C-O	-7.20	112.53	120.81
4	E	76	GLN	OE1-CD-NE2	-7.20	115.40	122.60
3	D	77	ASP	CA-CB-CG	7.20	119.80	112.60
1	B	134	GLN	CB-CA-C	7.19	120.14	111.22
2	C	11	LEU	CA-C-N	7.18	127.15	119.76
2	C	11	LEU	C-N-CA	7.18	127.15	119.76
1	A	101	ARG	NH1-CZ-NH2	-7.15	110.00	119.30
1	A	39	LYS	N-CA-C	7.14	119.15	111.36
1	A	180	PHE	CA-C-N	7.13	127.90	119.98
1	A	180	PHE	C-N-CA	7.13	127.90	119.98
1	A	185	TRP	CE2-CD2-CE3	-7.13	111.67	118.80
1	A	224	GLU	CB-CG-CD	7.12	124.71	112.60
2	C	171	PHE	CA-CB-CG	-7.11	106.69	113.80
1	A	198	ASP	CA-C-O	-7.10	113.39	120.70
2	C	238	THR	CA-CB-CG2	7.09	122.56	110.50
1	B	119	GLN	O-C-N	-7.08	114.76	123.33
2	C	355	ARG	NE-CZ-NH2	-7.05	112.85	119.20
4	E	75	ALA	N-CA-C	7.04	119.99	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	PHE	CA-CB-CG	-7.02	106.78	113.80
1	B	119	GLN	N-CA-C	6.99	120.95	109.06
2	C	157	GLN	OE1-CD-NE2	-6.99	115.61	122.60
2	C	269	ILE	CA-CB-CG2	6.98	122.36	110.50
1	B	89	GLU	O-C-N	-6.96	115.49	123.42
1	B	11	HIS	CA-C-N	6.93	131.22	120.82
1	B	11	HIS	C-N-CA	6.93	131.22	120.82
2	C	359	ARG	NE-CZ-NH2	-6.93	112.96	119.20
2	C	126	ALA	CA-C-N	6.93	132.53	122.69
2	C	126	ALA	C-N-CA	6.93	132.53	122.69
2	C	182	PRO	N-CA-CB	6.92	109.37	103.35
1	A	183	PHE	CA-C-N	6.91	132.43	120.68
1	A	183	PHE	C-N-CA	6.91	132.43	120.68
1	B	168	GLY	O-C-N	-6.91	115.49	122.19
4	E	108	ASN	CA-C-O	-6.89	113.25	120.55
2	C	32	VAL	CA-CB-CG1	6.88	122.09	110.40
3	D	145	ARG	CD-NE-CZ	6.87	134.02	124.40
2	C	396	GLN	OE1-CD-NE2	-6.84	115.76	122.60
4	E	117	VAL	CA-CB-CG2	6.84	122.03	110.40
1	A	107	PHE	CA-CB-CG	6.80	120.60	113.80
2	C	334	GLY	N-CA-C	6.78	119.26	110.45
2	C	203	ASP	CA-C-N	6.77	130.26	120.38
2	C	203	ASP	C-N-CA	6.77	130.26	120.38
2	C	158	SER	CA-C-N	6.75	132.93	122.20
2	C	158	SER	C-N-CA	6.75	132.93	122.20
1	A	185	TRP	NE1-CE2-CD2	-6.72	98.66	107.40
1	B	161	LYS	CA-C-O	6.72	127.67	120.55
2	C	328	SER	N-CA-C	6.71	120.23	108.75
2	C	293	PHE	CA-CB-CG	6.69	120.49	113.80
1	B	44	TYR	CA-CB-CG	6.68	125.93	113.90
2	C	415	ASN	CA-CB-CG	6.68	119.28	112.60
2	C	25	ILE	N-CA-CB	-6.66	102.14	110.33
4	E	68	GLN	OE1-CD-NE2	-6.65	115.95	122.60
5	F	24	ASP	CA-C-N	6.63	132.95	122.60
5	F	24	ASP	C-N-CA	6.63	132.95	122.60
1	A	144	VAL	O-C-N	-6.61	113.57	121.10
3	D	108	ARG	CB-CA-C	6.61	121.80	109.71
4	E	71	VAL	O-C-N	6.60	128.63	121.83
3	D	55	GLN	CB-CA-C	6.60	121.97	109.37
5	F	40	ARG	CD-NE-CZ	6.58	133.61	124.40
1	B	73	ARG	CA-C-O	-6.56	113.81	121.16
2	C	138	ILE	N-CA-C	6.56	116.91	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	45	ARG	NE-CZ-NH2	-6.56	113.30	119.20
1	B	140	THR	CA-CB-OG1	6.54	119.42	109.60
2	C	275	ASN	CA-CB-CG	6.54	119.14	112.60
1	A	75	SER	CA-C-O	6.54	127.49	119.97
4	E	123	ASP	CA-CB-CG	6.51	119.11	112.60
2	C	-3	ASP	CA-C-N	6.48	126.05	119.19
2	C	-3	ASP	C-N-CA	6.48	126.05	119.19
3	D	101	TYR	CA-C-O	-6.45	113.34	120.38
5	F	65	VAL	N-CA-CB	6.44	119.30	110.54
1	A	11	HIS	CB-CG-CD2	-6.42	122.86	131.20
2	C	372	THR	CA-CB-OG1	6.41	119.21	109.60
2	C	409	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	B	28	ILE	CA-C-N	6.40	129.15	120.38
1	B	28	ILE	C-N-CA	6.40	129.15	120.38
3	D	14	ASN	OD1-CG-ND2	-6.38	116.22	122.60
2	C	11	LEU	CA-C-O	-6.37	113.75	120.70
4	E	92	LEU	CA-C-N	6.37	129.10	120.44
4	E	92	LEU	C-N-CA	6.37	129.10	120.44
3	D	36	HIS	CB-CG-CD2	-6.34	122.95	131.20
3	D	132	VAL	CA-C-N	6.34	132.23	121.14
3	D	132	VAL	C-N-CA	6.34	132.23	121.14
1	B	64	GLN	OE1-CD-NE2	-6.32	116.28	122.60
5	F	55	ARG	CA-C-N	6.31	126.94	120.00
5	F	55	ARG	C-N-CA	6.31	126.94	120.00
1	A	66	VAL	CA-CB-CG2	6.30	121.12	110.40
1	B	90	TRP	CE2-CD2-CE3	-6.30	112.50	118.80
2	C	249	PRO	N-CA-CB	6.30	110.35	103.30
5	F	84	MET	O-C-N	-6.29	114.86	122.22
3	D	85	PRO	N-CA-CB	6.29	109.85	103.25
1	B	174	GLN	CA-C-N	6.28	127.06	120.03
1	B	174	GLN	C-N-CA	6.28	127.06	120.03
1	A	86	ILE	O-C-N	-6.28	116.74	123.14
1	A	43	VAL	CA-C-O	-6.27	113.70	120.47
3	D	91	SER	CA-C-N	6.27	128.90	120.50
3	D	91	SER	C-N-CA	6.27	128.90	120.50
2	C	299	GLU	O-C-N	-6.25	115.34	122.09
1	A	204	PHE	CA-CB-CG	-6.25	107.55	113.80
2	C	249	PRO	CA-C-O	-6.25	109.77	119.64
1	A	110	HIS	CG-CD2-NE2	-6.22	100.98	107.20
2	C	411	VAL	CA-CB-CG1	6.22	120.98	110.40
2	C	146	ARG	CA-C-O	-6.22	112.82	119.97
4	E	69	ARG	CD-NE-CZ	6.22	133.10	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	292	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	A	172	TYR	CA-C-N	6.21	128.60	120.28
1	A	172	TYR	C-N-CA	6.21	128.60	120.28
1	B	208	ILE	O-C-N	-6.21	115.43	121.83
1	A	42	PRO	N-CD-CG	6.21	112.51	103.20
3	D	99	CYS	CB-CA-C	6.20	121.05	109.71
4	E	103	LEU	N-CA-C	6.19	118.83	111.71
1	A	221	ARG	NE-CZ-NH1	6.18	127.68	121.50
3	D	134	HIS	ND1-CG-CD2	6.18	112.28	106.10
2	C	-2	PRO	CB-CA-C	-6.18	103.09	112.11
1	A	89	GLU	CA-C-O	-6.17	113.19	120.60
1	B	120	GLN	CA-C-N	6.17	131.59	122.71
1	B	120	GLN	C-N-CA	6.17	131.59	122.71
1	B	147	GLU	N-CA-CB	-6.16	101.31	110.24
2	C	128	ARG	NE-CZ-NH1	6.15	127.65	121.50
5	F	23	ARG	CA-C-O	6.14	127.08	120.20
3	D	132	VAL	N-CA-C	6.13	119.63	111.17
5	F	63	GLU	CA-C-N	6.12	128.73	120.65
5	F	63	GLU	C-N-CA	6.12	128.73	120.65
1	A	202	SER	N-CA-C	6.11	118.02	111.36
2	C	97	ARG	CD-NE-CZ	6.09	132.93	124.40
3	D	58	ASP	O-C-N	-6.07	117.45	123.46
1	A	35	TYR	CA-C-N	6.06	128.32	120.44
1	A	35	TYR	C-N-CA	6.06	128.32	120.44
1	B	221	ARG	CD-NE-CZ	6.05	132.88	124.40
2	C	339	THR	CA-CB-CG2	6.04	120.76	110.50
1	B	124	VAL	CA-C-N	6.03	132.74	122.37
1	B	124	VAL	C-N-CA	6.03	132.74	122.37
2	C	153	ARG	CA-C-O	-6.03	114.10	120.55
2	C	355	ARG	NH1-CZ-NH2	6.03	127.13	119.30
2	C	282	ILE	CA-CB-CG1	6.02	120.64	110.40
5	F	82	THR	CA-CB-OG1	-5.99	100.61	109.60
4	E	112	ILE	O-C-N	5.98	127.77	121.91
1	B	60	ILE	CA-C-O	5.97	125.91	120.30
2	C	223	GLY	O-C-N	-5.97	116.40	122.19
3	D	49	ARG	CA-CB-CG	5.97	126.04	114.10
5	F	86	VAL	CA-C-O	-5.95	114.45	121.05
3	D	127	PRO	CA-C-N	5.94	128.17	120.44
3	D	127	PRO	C-N-CA	5.94	128.17	120.44
1	B	209	TYR	CB-CG-CD1	-5.94	111.89	120.80
1	B	112	ILE	N-CA-CB	-5.93	103.98	111.46
2	C	146	ARG	N-CA-C	5.92	118.69	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	GLN	CA-CB-CG	-5.91	102.28	114.10
2	C	28	GLU	N-CA-C	5.91	118.76	109.96
5	F	23	ARG	N-CA-C	5.91	119.31	111.75
2	C	55	LEU	CA-C-N	5.90	131.14	123.00
2	C	55	LEU	C-N-CA	5.90	131.14	123.00
3	D	94	VAL	N-CA-C	5.89	117.93	108.85
2	C	316	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	A	38	ASN	CB-CG-ND2	5.88	125.22	116.40
2	C	3	LEU	CD1-CG-CD2	-5.88	97.87	110.80
1	A	165	SER	CA-C-O	-5.87	114.08	121.01
1	B	141	SER	O-C-N	-5.87	117.10	123.26
2	C	95	ASN	OD1-CG-ND2	-5.87	116.73	122.60
3	D	136	VAL	O-C-N	-5.87	116.26	122.95
2	C	249	PRO	CA-N-CD	-5.86	103.79	112.00
1	A	144	VAL	CG1-CB-CG2	-5.86	97.91	110.80
1	A	86	ILE	CA-C-O	5.86	127.40	120.72
1	A	26	ASP	CA-C-O	5.85	126.97	120.82
4	E	70	LEU	CA-C-O	5.85	126.95	120.63
2	C	279	VAL	N-CA-C	5.85	116.59	110.62
1	A	125	PHE	CA-C-N	5.84	131.57	121.64
1	A	125	PHE	C-N-CA	5.84	131.57	121.64
1	B	183	PHE	N-CA-C	5.84	117.32	111.07
3	D	69	VAL	CA-CB-CG1	5.84	120.33	110.40
2	C	261	TYR	CA-C-O	-5.84	113.94	120.25
1	B	9	ASN	OD1-CG-ND2	-5.83	116.77	122.60
3	D	63	GLY	O-C-N	-5.83	115.94	121.77
1	A	39	LYS	CA-C-N	5.83	128.41	120.54
1	A	39	LYS	C-N-CA	5.83	128.41	120.54
1	A	110	HIS	CB-CG-CD2	-5.82	123.64	131.20
2	C	416	ILE	N-CA-C	5.82	121.44	109.34
1	A	40	MET	CA-C-N	5.80	129.55	120.97
1	A	40	MET	C-N-CA	5.80	129.55	120.97
2	C	115	ASP	CA-CB-CG	5.80	118.40	112.60
5	F	91	LYS	CA-C-N	5.79	129.12	120.31
5	F	91	LYS	C-N-CA	5.79	129.12	120.31
2	C	23	GLN	O-C-N	-5.77	116.34	123.44
3	D	92	VAL	CA-CB-CG1	5.77	120.21	110.40
1	A	119	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	B	109	PHE	N-CA-CB	5.75	119.80	110.43
2	C	371	ASP	CA-CB-CG	5.74	118.33	112.60
1	B	65	HIS	CA-CB-CG	5.73	119.53	113.80
3	D	161	LEU	O-C-N	-5.72	115.52	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	PHE	O-C-N	-5.72	116.81	123.27
3	D	146	VAL	N-CA-CB	-5.71	104.74	111.60
1	B	211	PHE	CA-CB-CG	5.71	119.51	113.80
1	A	189	LYS	CA-C-O	-5.71	115.00	121.28
1	B	15	PHE	CA-CB-CG	5.71	119.50	113.80
2	C	113	SER	N-CA-C	5.70	119.85	113.01
1	A	173	ARG	NH1-CZ-NH2	-5.68	111.91	119.30
2	C	33	VAL	CA-CB-CG1	5.68	120.05	110.40
1	B	71	TYR	N-CA-C	5.67	120.48	112.93
3	D	72	PHE	CA-CB-CG	5.67	119.47	113.80
1	B	30	ARG	N-CA-C	5.66	117.53	111.36
2	C	67	VAL	CB-CA-C	-5.65	103.10	111.80
2	C	332	ILE	CA-C-O	-5.65	115.74	121.67
2	C	390	ARG	N-CA-C	5.64	122.08	113.61
2	C	166	ILE	CA-CB-CG1	5.64	119.99	110.40
5	F	80	THR	CA-CB-CG2	5.63	120.08	110.50
3	D	107	VAL	N-CA-C	5.63	115.27	108.06
3	D	109	VAL	N-CA-CB	5.63	118.91	111.25
1	B	212	CYS	CA-C-O	-5.62	114.59	120.55
2	C	351	VAL	CA-C-N	5.62	125.53	119.85
2	C	351	VAL	C-N-CA	5.62	125.53	119.85
3	D	56	GLU	CB-CG-CD	5.62	122.16	112.60
5	F	95	ARG	CA-C-O	5.62	127.46	121.11
1	A	84	ASP	CA-C-O	-5.62	113.06	119.41
3	D	36	HIS	CB-CG-ND1	5.62	131.12	122.70
2	C	197	SER	O-C-N	-5.60	115.38	122.27
1	B	66	VAL	N-CA-CB	-5.59	103.48	110.47
2	C	107	ILE	N-CA-CB	5.59	118.14	110.54
1	A	213	VAL	CB-CA-C	5.59	119.34	112.02
2	C	373	GLU	CA-C-O	5.58	126.24	119.49
2	C	326	THR	CB-CA-C	5.58	119.94	111.80
3	D	43	THR	CA-C-N	5.58	130.69	123.00
3	D	43	THR	C-N-CA	5.58	130.69	123.00
2	C	4	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	A	164	ARG	CB-CA-C	5.57	118.98	109.24
2	C	317	GLU	CA-C-O	-5.57	114.52	120.42
1	B	160	ILE	CA-C-N	5.56	127.73	120.28
1	B	160	ILE	C-N-CA	5.56	127.73	120.28
5	F	65	VAL	CA-C-N	5.56	127.57	120.56
5	F	65	VAL	C-N-CA	5.56	127.57	120.56
4	E	119	ILE	CA-CB-CG1	5.56	119.85	110.40
2	C	352	PRO	CA-C-O	5.54	128.43	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	316	GLN	CA-C-N	5.53	128.15	120.29
2	C	316	GLN	C-N-CA	5.53	128.15	120.29
1	A	166	PRO	CA-C-N	5.53	127.63	120.44
1	A	166	PRO	C-N-CA	5.53	127.63	120.44
4	E	111	ALA	CA-C-O	5.53	126.62	120.82
4	E	71	VAL	CA-C-O	-5.52	115.00	120.85
2	C	228	ARG	CD-NE-CZ	5.52	132.12	124.40
2	C	116	PRO	N-CA-CB	5.51	108.99	103.48
2	C	299	GLU	CA-C-O	5.51	126.38	120.70
2	C	352	PRO	CA-N-CD	-5.51	104.29	112.00
3	D	112	TYR	CA-C-N	5.50	130.42	123.10
3	D	112	TYR	C-N-CA	5.50	130.42	123.10
2	C	89	ASP	CA-CB-CG	5.50	118.10	112.60
2	C	358	PHE	N-CA-C	5.50	116.96	111.07
3	D	157	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	77	PHE	N-CA-C	5.49	117.27	111.28
1	A	134	GLN	OE1-CD-NE2	-5.49	117.11	122.60
2	C	27	LEU	CA-C-N	5.49	129.15	121.02
2	C	27	LEU	C-N-CA	5.49	129.15	121.02
3	D	71	LYS	CB-CA-C	5.49	120.23	109.35
1	A	99	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	195	PRO	N-CA-CB	5.48	108.19	103.31
2	C	253	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	B	148	TRP	CA-C-O	-5.48	114.51	120.87
3	D	141	ALA	N-CA-C	5.48	119.45	112.87
1	A	100	THR	CA-C-N	5.48	129.37	120.60
1	A	100	THR	C-N-CA	5.48	129.37	120.60
1	A	185	TRP	CD2-CE2-CZ2	5.47	127.87	122.40
1	B	124	VAL	CG1-CB-CG2	-5.46	98.78	110.80
2	C	216	GLU	O-C-N	-5.46	116.33	122.12
3	D	125	ASN	N-CA-CB	-5.46	103.50	111.20
3	D	54	ASP	CA-C-O	-5.46	115.61	121.56
1	A	152	TYR	CA-CB-CG	5.46	123.72	113.90
3	D	35	LYS	N-CA-CB	-5.45	101.74	110.19
4	E	134	ARG	NE-CZ-NH2	-5.45	114.29	119.20
2	C	295	HIS	ND1-CG-CD2	5.44	111.54	106.10
3	D	84	ILE	N-CA-C	5.44	113.31	108.63
2	C	6	PHE	CA-CB-CG	5.44	119.24	113.80
3	D	22	TYR	CA-C-N	5.43	129.63	122.30
3	D	22	TYR	C-N-CA	5.43	129.63	122.30
1	A	5	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	82	THR	CA-CB-CG2	5.43	119.72	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	97	LEU	CA-C-O	5.42	126.16	120.36
2	C	61	VAL	N-CA-CB	5.42	118.04	110.56
2	C	67	VAL	CA-C-O	-5.42	115.86	120.96
4	E	129	ARG	CD-NE-CZ	5.42	131.99	124.40
2	C	208	SER	N-CA-C	5.41	118.67	111.75
2	C	292	ARG	CA-C-O	-5.41	115.14	120.82
4	E	104	PHE	CA-CB-CG	-5.40	108.40	113.80
5	F	26	ILE	CB-CA-C	5.40	118.56	111.33
1	A	153	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	44	TYR	N-CA-CB	5.39	117.97	109.94
2	C	88	ALA	O-C-N	-5.38	117.45	123.48
1	B	41	LYS	CA-C-O	-5.38	112.78	120.16
2	C	30	HIS	CA-CB-CG	5.38	119.18	113.80
1	A	173	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	B	172	TYR	CA-C-O	-5.38	115.18	120.82
1	A	164	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	A	189	LYS	O-C-N	5.37	125.58	121.23
1	A	77	PHE	CB-CG-CD2	-5.36	111.58	120.70
5	F	65	VAL	CG1-CB-CG2	-5.36	99.00	110.80
2	C	79	ALA	N-CA-C	5.36	116.99	108.79
3	D	14	ASN	CA-CB-CG	5.36	117.96	112.60
4	E	122	LYS	N-CA-C	5.36	122.21	110.80
1	B	219	ALA	N-CA-CB	-5.35	101.50	110.39
1	B	170	LYS	CA-C-O	-5.35	115.19	120.70
1	B	98	TYR	CA-C-N	5.35	129.34	120.94
1	B	98	TYR	C-N-CA	5.35	129.34	120.94
2	C	403	GLU	N-CA-C	5.34	118.39	110.48
5	F	38	ALA	CA-C-N	5.34	127.44	120.28
5	F	38	ALA	C-N-CA	5.34	127.44	120.28
1	B	53	GLU	CB-CA-C	5.34	117.68	109.03
1	B	72	ILE	N-CA-C	5.34	116.00	108.36
3	D	134	HIS	CA-C-O	-5.34	113.18	119.05
2	C	368	GLU	O-C-N	-5.34	116.77	122.85
2	C	-1	ASN	CA-CB-CG	-5.33	107.27	112.60
2	C	314	GLU	O-C-N	-5.33	116.47	122.12
2	C	320	GLU	CA-C-N	5.33	129.62	120.72
2	C	320	GLU	C-N-CA	5.33	129.62	120.72
1	A	11	HIS	CG-CD2-NE2	-5.33	101.88	107.20
1	A	45	GLU	CB-CA-C	5.32	119.16	110.96
1	A	143	PRO	CA-C-O	-5.32	115.36	121.86
1	B	36	ARG	O-C-N	5.32	127.55	122.07
2	C	263	LEU	CA-C-N	5.32	128.32	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	263	LEU	C-N-CA	5.32	128.32	120.82
1	B	166	PRO	N-CD-CG	5.32	111.17	103.20
4	E	98	ALA	N-CA-C	5.32	118.23	111.69
2	C	253	ARG	CA-C-O	5.31	126.10	120.10
2	C	209	LYS	CA-C-O	-5.30	112.15	119.05
1	A	124	VAL	O-C-N	-5.30	116.83	122.61
2	C	319	GLN	CB-CG-CD	5.30	121.61	112.60
1	B	73	ARG	NE-CZ-NH1	5.29	126.79	121.50
2	C	34	THR	CA-C-N	5.29	125.23	119.78
2	C	34	THR	C-N-CA	5.29	125.23	119.78
2	C	103	ILE	N-CA-C	5.28	116.64	110.62
2	C	405	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	C	222	TRP	N-CA-C	5.28	117.94	111.82
1	A	122	THR	O-C-N	-5.28	117.07	123.29
2	C	305	LYS	N-CA-C	-5.28	107.86	114.56
1	B	130	GLY	CA-C-O	-5.27	115.92	120.30
2	C	26	PRO	CA-C-N	5.27	131.27	122.73
2	C	26	PRO	C-N-CA	5.27	131.27	122.73
1	B	120	GLN	OE1-CD-NE2	-5.27	117.33	122.60
2	C	100	VAL	CA-CB-CG2	5.27	119.36	110.40
4	E	72	ARG	N-CA-C	5.27	116.71	111.07
1	A	213	VAL	CA-C-N	5.26	127.64	120.54
1	A	213	VAL	C-N-CA	5.26	127.64	120.54
2	C	68	TYR	O-C-N	-5.26	116.53	123.16
1	B	209	TYR	CD1-CG-CD2	5.25	125.98	118.10
2	C	364	TYR	N-CA-C	5.25	121.99	110.80
1	A	56	GLU	CA-C-N	5.25	128.09	120.79
1	A	56	GLU	C-N-CA	5.25	128.09	120.79
2	C	282	ILE	CA-C-N	5.25	125.15	119.85
2	C	282	ILE	C-N-CA	5.25	125.15	119.85
2	C	43	PRO	CA-C-N	5.24	128.28	120.31
2	C	43	PRO	C-N-CA	5.24	128.28	120.31
1	A	60	ILE	CA-C-N	5.24	127.36	120.60
1	A	60	ILE	C-N-CA	5.24	127.36	120.60
1	A	11	HIS	ND1-CG-CD2	5.24	111.34	106.10
2	C	161	THR	O-C-N	5.24	128.71	122.27
2	C	292	ARG	NE-CZ-NH1	5.24	126.73	121.50
2	C	13	VAL	CA-C-N	5.23	131.53	121.54
2	C	13	VAL	C-N-CA	5.23	131.53	121.54
5	F	60	VAL	CG1-CB-CG2	-5.23	99.30	110.80
5	F	71	THR	CA-C-O	-5.23	115.01	120.55
1	A	148	TRP	CA-C-N	5.23	125.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	TRP	C-N-CA	5.23	125.23	119.90
2	C	214	ASN	CA-CB-CG	5.22	117.82	112.60
4	E	105	GLU	CA-C-O	-5.22	114.89	120.42
2	C	65	LEU	CA-C-N	5.21	131.09	122.33
2	C	65	LEU	C-N-CA	5.21	131.09	122.33
4	E	70	LEU	N-CA-C	5.21	117.64	111.33
5	F	75	HIS	CB-CG-CD2	-5.21	124.43	131.20
2	C	222	TRP	CD2-CE3-CZ3	-5.21	111.83	118.60
2	C	234	PHE	CA-C-N	5.21	129.12	120.94
2	C	234	PHE	C-N-CA	5.21	129.12	120.94
1	B	153	ASP	CA-C-N	5.20	130.24	121.14
1	B	153	ASP	C-N-CA	5.20	130.24	121.14
2	C	365	ILE	CA-CB-CG2	5.20	119.34	110.50
3	D	11	VAL	CA-C-O	-5.20	114.58	120.66
3	D	14	ASN	N-CA-C	5.20	114.28	108.25
1	A	13	LYS	O-C-N	-5.20	116.72	122.07
1	A	89	GLU	CB-CA-C	5.20	119.93	109.38
2	C	305	LYS	CA-C-N	5.20	129.07	121.80
2	C	305	LYS	C-N-CA	5.20	129.07	121.80
1	B	209	TYR	CA-C-N	5.19	126.33	119.84
1	B	209	TYR	C-N-CA	5.19	126.33	119.84
3	D	18	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	200	LEU	CD1-CG-CD2	-5.19	99.38	110.80
1	B	170	LYS	CA-C-N	5.19	127.23	120.28
1	B	170	LYS	C-N-CA	5.19	127.23	120.28
3	D	81	ALA	N-CA-C	5.18	118.39	111.75
1	B	141	SER	CA-C-O	5.18	126.87	121.38
1	B	172	TYR	O-C-N	5.18	127.40	122.07
1	A	87	LYS	CB-CA-C	5.17	120.38	109.79
1	B	38	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	B	97	MET	N-CA-C	5.17	118.84	112.54
2	C	194	ARG	CB-CA-C	5.17	117.98	109.97
1	A	101	ARG	NE-CZ-NH1	5.16	126.66	121.50
3	D	44	TYR	N-CA-CB	-5.16	102.46	110.57
1	B	164	ARG	CD-NE-CZ	5.16	131.63	124.40
4	E	105	GLU	CA-C-N	5.16	127.46	120.44
4	E	105	GLU	C-N-CA	5.16	127.46	120.44
2	C	354	SER	CA-C-N	5.16	127.71	120.28
2	C	354	SER	C-N-CA	5.16	127.71	120.28
4	E	87	SER	CA-C-N	5.16	129.40	120.58
4	E	87	SER	C-N-CA	5.16	129.40	120.58
1	B	107	PHE	CA-C-O	-5.15	115.29	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	155	LEU	O-C-N	-5.14	116.29	122.15
1	A	142	GLU	CA-C-N	5.13	125.58	120.14
1	A	142	GLU	C-N-CA	5.13	125.58	120.14
2	C	194	ARG	CA-C-O	-5.13	115.62	120.34
1	A	12	ALA	N-CA-CB	-5.13	102.63	110.33
1	A	110	HIS	CA-CB-CG	5.13	118.93	113.80
2	C	307	SER	O-C-N	-5.13	116.81	122.86
2	C	14	SER	O-C-N	-5.13	115.77	122.59
2	C	416	ILE	N-CA-CB	-5.12	102.78	111.23
2	C	172	GLN	N-CA-CB	5.12	118.21	110.28
1	B	113	GLU	CB-CA-C	5.12	117.53	110.16
2	C	50	GLN	N-CA-C	5.11	117.73	109.40
2	C	211	HIS	CA-C-O	-5.11	114.56	120.49
3	D	22	TYR	O-C-N	-5.11	116.59	122.87
1	B	182	TRP	O-C-N	-5.11	116.71	122.12
1	B	14	ALA	N-CA-CB	-5.10	102.61	110.16
1	B	116	PHE	CB-CA-C	5.10	118.06	110.62
3	D	25	GLU	CA-C-N	5.10	129.35	122.93
3	D	25	GLU	C-N-CA	5.10	129.35	122.93
3	D	158	GLU	CA-C-O	5.10	125.98	120.32
5	F	48	GLY	N-CA-C	5.09	120.50	113.99
3	D	55	GLN	OE1-CD-NE2	-5.08	117.52	122.60
4	E	77	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	124	VAL	CA-CB-CG2	5.08	119.03	110.40
2	C	31	ALA	N-CA-CB	-5.08	101.62	109.69
5	F	46	ILE	N-CA-C	5.08	115.43	108.12
1	A	183	PHE	O-C-N	-5.07	115.46	122.46
2	C	84	PHE	CA-CB-CG	-5.07	108.73	113.80
2	C	110	PHE	CB-CG-CD2	-5.07	112.09	120.70
1	B	211	PHE	N-CA-CB	-5.06	104.17	110.90
1	B	13	LYS	CA-C-N	5.06	127.47	120.29
1	B	13	LYS	C-N-CA	5.06	127.47	120.29
1	A	75	SER	N-CA-CB	-5.05	102.45	110.28
1	B	133	ASP	CA-C-N	5.05	131.46	122.31
1	B	133	ASP	C-N-CA	5.05	131.46	122.31
1	A	160	ILE	CA-C-O	-5.05	115.28	121.04
2	C	200	LEU	CA-C-N	5.05	131.77	123.08
2	C	200	LEU	C-N-CA	5.05	131.77	123.08
1	B	65	HIS	CB-CG-CD2	-5.05	124.64	131.20
2	C	89	ASP	CA-C-N	5.05	131.30	122.82
2	C	89	ASP	C-N-CA	5.05	131.30	122.82
1	A	213	VAL	CA-C-O	-5.04	115.45	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	121	GLN	CG-CD-NE2	5.04	123.96	116.40
2	C	115	ASP	CA-C-O	-5.04	114.76	119.80
3	D	130	VAL	CG1-CB-CG2	-5.03	99.73	110.80
4	E	71	VAL	CB-CA-C	5.03	119.16	112.22
4	E	97	GLU	CB-CG-CD	5.03	121.15	112.60
2	C	35	PRO	CB-CA-C	5.03	117.66	111.23
2	C	153	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	B	47	ARG	O-C-N	5.02	127.24	122.07
2	C	67	VAL	O-C-N	5.02	128.01	123.19
2	C	216	GLU	N-CA-CB	5.01	117.49	110.12
3	D	9	ILE	N-CA-C	5.01	115.87	108.45
3	D	21	PRO	CA-C-N	5.01	129.81	122.85
3	D	21	PRO	C-N-CA	5.01	129.81	122.85
1	B	148	TRP	N-CA-CB	-5.01	102.77	110.03
3	D	37	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	214	LYS	O-C-N	5.00	127.29	122.09

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	35	TYR	Sidechain
1	A	50	TYR	Sidechain
1	A	172	TYR	Sidechain
1	A	197	GLY	Mainchain
1	B	35	TYR	Sidechain
1	B	50	TYR	Sidechain
1	B	57	PHE	Sidechain
1	B	68	PHE	Sidechain
1	B	71	TYR	Sidechain
1	B	73	ARG	Sidechain
1	B	172	TYR	Sidechain
1	B	209	TYR	Sidechain
2	C	119	TYR	Sidechain
2	C	123	VAL	Mainchain
2	C	133	ILE	Peptide
2	C	149	ARG	Sidechain
2	C	201	PHE	Sidechain
2	C	257	ARG	Sidechain
2	C	307	SER	Mainchain
2	C	364	TYR	Sidechain
2	C	384	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	D	111	TYR	Sidechain
3	D	112	TYR	Sidechain
3	D	117	TYR	Sidechain
3	D	123	ARG	Sidechain
4	E	63	ARG	Sidechain
4	E	116	ARG	Sidechain
4	E	128	ARG	Sidechain
5	F	36	ARG	Sidechain
5	F	45	ARG	Sidechain
5	F	51	TYR	Sidechain
5	F	72	TYR	Sidechain

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1908	1825	1824	2
2	C	3437	3480	3480	2
4	E	607	636	634	1
All	All	9731	9680	9675	5

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 0.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:C:365:ILE:N	2:C:365:ILE:HD12	0.52	2.19
1:A:164:ARG:O	1:A:169:LYS:HE3	0.44	2.12
4:E:71:VAL:HG12	4:E:84:PHE:CZ	0.43	2.49
1:A:116:PHE:CE1	1:A:119:GLN:NE2	0.40	2.88
2:C:293:PHE:CD1	2:C:311:PHE:CE1	0.40	3.10

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR 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	228/264 (86%)	209 (92%)	19 (8%)	0 (0%)	100	100
1	B	215/264 (81%)	203 (94%)	11 (5%)	1 (0%)	26	74
2	C	422/442 (95%)	389 (92%)	31 (7%)	2 (0%)	26	74
3	D	162/279 (58%)	155 (96%)	6 (4%)	1 (1%)	23	72
4	E	73/136 (54%)	67 (92%)	5 (7%)	1 (1%)	11	58
5	F	80/103 (78%)	78 (98%)	2 (2%)	0 (0%)	100	100
All	All	1180/1488 (79%)	1101 (93%)	74 (6%)	5 (0%)	31	76

All 5 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	B	132	ASP
2	C	14	SER
2	C	203	ASP
3	D	90	VAL
4	E	133	GLU

6.3.2 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 NMR 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	205/235 (87%)	203 (99%)	2 (1%)	65	95
1	B	194/235 (83%)	190 (98%)	4 (2%)	46	90
2	C	388/403 (96%)	383 (99%)	5 (1%)	59	94
3	D	151/252 (60%)	148 (98%)	3 (2%)	48	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	64/111 (58%)	64 (100%)	0 (0%)	100	100
5	F	68/79 (86%)	65 (96%)	3 (4%)	27	77
All	All	1070/1315 (81%)	1053 (98%)	17 (2%)	54	92

All 17 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	68	PHE
1	A	132	ASP
1	B	112	ILE
1	B	220	GLN
1	B	222	ASP
1	B	224	GLU
2	C	62	PHE
2	C	82	LEU
2	C	94	CYS
2	C	237	ASP
2	C	300	GLU
3	D	49	ARG
3	D	51	LEU
3	D	61	LEU
5	F	45	ARG
5	F	59	LYS
5	F	63	GLU

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 2% for the well-defined parts and 2% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	368
Number of shifts mapped to atoms	368
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 2%, i.e. 368 atoms were assigned a chemical shift out of a possible 16842. 0 out of 181 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/5901 (0%)	0/2382 (0%)	0/2384 (0%)	0/1135 (0%)
Sidechain	368/9499 (4%)	276/6138 (4%)	92/2970 (3%)	0/391 (0%)
Aromatic	0/1442 (0%)	0/707 (0%)	0/697 (0%)	0/38 (0%)
Overall	368/16842 (2%)	276/9227 (3%)	92/6051 (2%)	0/1564 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 368 atoms were assigned a chemical shift out of a possible 16842. 0 out of 181 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/5901 (0%)	0/2382 (0%)	0/2384 (0%)	0/1135 (0%)
Sidechain	368/9499 (4%)	276/6138 (4%)	92/2970 (3%)	0/391 (0%)
Aromatic	0/1442 (0%)	0/707 (0%)	0/697 (0%)	0/38 (0%)
Overall	368/16842 (2%)	276/9227 (3%)	92/6051 (2%)	0/1564 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

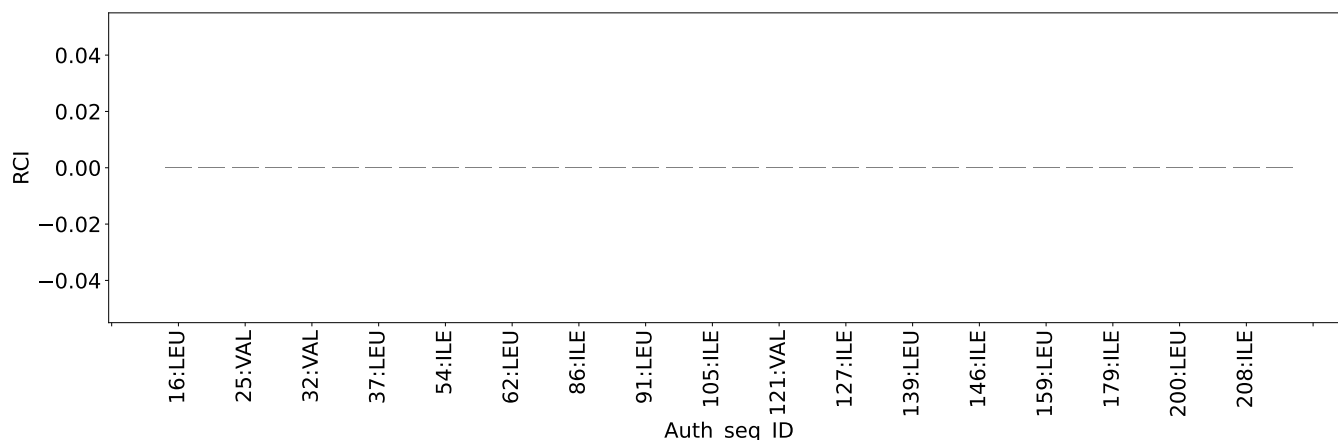
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	200	LEU	HD21	-0.69	-0.65 – 2.13	-5.1
1	A	200	LEU	HD22	-0.69	-0.65 – 2.13	-5.1
1	A	200	LEU	HD23	-0.69	-0.65 – 2.13	-5.1
1	B	200	LEU	HD21	-0.68	-0.65 – 2.13	-5.1
1	B	200	LEU	HD22	-0.68	-0.65 – 2.13	-5.1
1	B	200	LEU	HD23	-0.68	-0.65 – 2.13	-5.1

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

