



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 01:36 AM UTC

PDB ID : 2IXQ / pdb_00002ixq
Title : The solution structure of the invasive tip complex from Afa-Dr fibrils
Authors : Cota, E.; Jones, C.; Simpson, P.; Altroff, H.; Anderson, K.L.; du Merle, L.;
Guignot, J.; Servin, A.; Le Bouguenec, C.; Mardon, H.; Matthews, S.
Deposited on : 2006-07-10

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

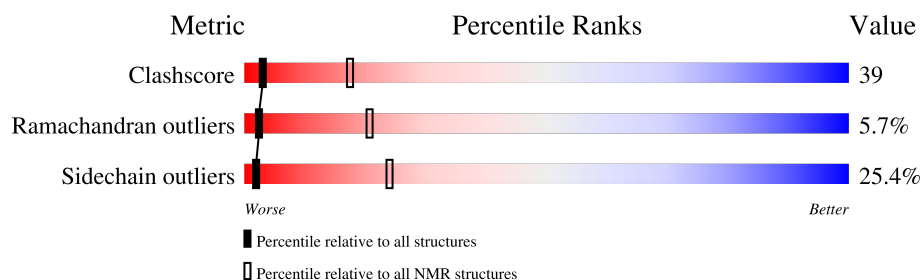
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	142	
2	B	143	

2 Ensemble composition and analysis ⓘ

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4179 atoms, of which 2016 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein AfaD.

Mol	Chain	Residues	Atoms						Trace
1	A	142	Total	C	H	N	O	S	0
			2061	653	986	205	213	4	

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	ALA	conflict	UNP Q47038
A	123	ASP	-	expression tag	UNP Q47038
A	124	ASN	-	expression tag	UNP Q47038
A	125	LYS	-	expression tag	UNP Q47038
A	126	GLN	-	expression tag	UNP Q47038
A	127	GLY	-	expression tag	UNP Q47038
A	128	PHE	-	expression tag	UNP Q47038
A	129	THR	-	expression tag	UNP Q47038
A	130	PRO	-	expression tag	UNP Q47038
A	131	SER	-	expression tag	UNP Q47038
A	132	GLY	-	expression tag	UNP Q47038
A	133	THR	-	expression tag	UNP Q47038
A	134	THR	-	expression tag	UNP Q47038
A	135	GLY	-	expression tag	UNP Q47038
A	136	THR	-	expression tag	UNP Q47038
A	137	THR	-	expression tag	UNP Q47038
A	138	LYS	-	expression tag	UNP Q47038
A	139	LEU	-	expression tag	UNP Q47038
A	140	THR	-	expression tag	UNP Q47038
A	141	VAL	-	expression tag	UNP Q47038
A	142	THR	-	expression tag	UNP Q47038

- Molecule 2 is a protein called Afimbrial adhesin AFA-III.

Mol	Chain	Residues	Atoms						Trace
2	B	143	Total	C	H	N	O	S	0
			2118	677	1030	188	220	3	

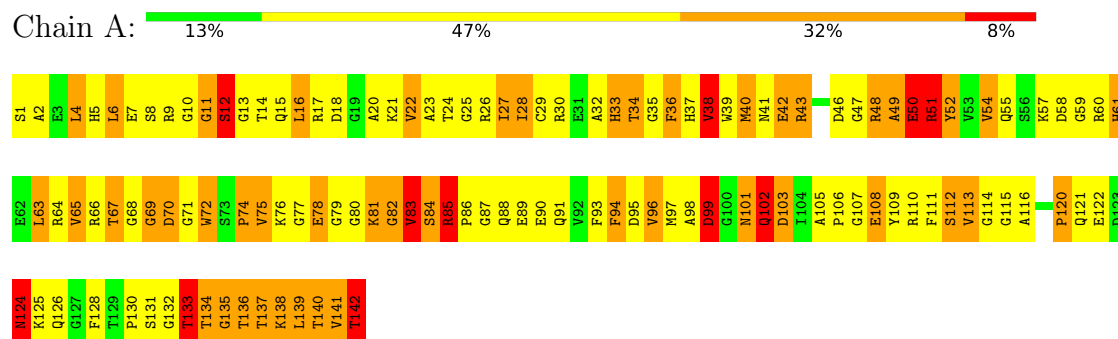
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	124	ASP	-	expression tag	UNP Q57254
B	125	ASN	-	expression tag	UNP Q57254
B	126	LYS	-	expression tag	UNP Q57254
B	127	GLN	-	expression tag	UNP Q57254
B	128	GLY	-	expression tag	UNP Q57254
B	129	PHE	-	expression tag	UNP Q57254
B	130	THR	-	expression tag	UNP Q57254
B	131	PRO	-	expression tag	UNP Q57254
B	132	SER	-	expression tag	UNP Q57254
B	133	GLY	-	expression tag	UNP Q57254
B	134	THR	-	expression tag	UNP Q57254
B	135	THR	-	expression tag	UNP Q57254
B	136	GLY	-	expression tag	UNP Q57254
B	137	THR	-	expression tag	UNP Q57254
B	138	THR	-	expression tag	UNP Q57254
B	139	LYS	-	expression tag	UNP Q57254
B	140	LEU	-	expression tag	UNP Q57254
B	141	THR	-	expression tag	UNP Q57254
B	142	VAL	-	expression tag	UNP Q57254
B	143	THR	-	expression tag	UNP Q57254

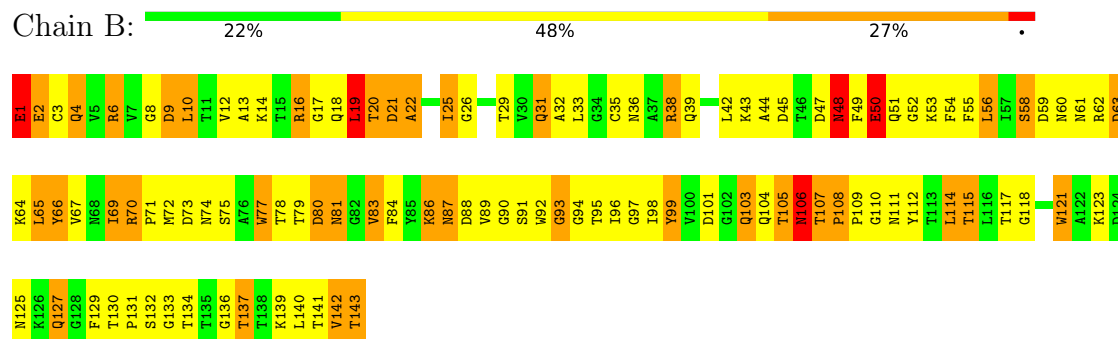
4 Residue-property plots

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: Protein AfaD



• Molecule 2: Afimbrial adhesin AFA-III



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
CNS	refinement	

No chemical shift data was provided.

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	8.87	374/1094 (34.2%)	4.04	145/1471 (9.9%)
2	B	7.86	272/1109 (24.5%)	4.16	130/1510 (8.6%)
All	All	8.38	646/2203 (29.3%)	4.10	275/2981 (9.2%)

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	Planarity
1	A	4	0
2	B	1	0
All	All	5	0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLU	CA-CB	-63.02	0.27	1.53
1	A	142	THR	C-O	-51.45	0.20	1.23
1	A	142	THR	CB-OG1	-49.53	0.64	1.43
1	A	58	ASP	C-O	-47.95	0.60	1.24
1	A	141	VAL	C-O	-46.56	0.69	1.23
2	B	1	GLU	CG-CD	-46.51	0.35	1.52
1	A	13	GLY	C-O	-46.48	0.67	1.23
1	A	141	VAL	C-N	-44.42	0.71	1.33
1	A	67	THR	CB-OG1	-43.90	0.73	1.43
2	B	2	GLU	N-CA	-41.75	0.97	1.45
2	B	2	GLU	CD-OE2	-39.58	0.50	1.25
2	B	4	GLN	CD-NE2	-39.57	0.50	1.33
1	A	70	ASP	C-O	-39.42	0.74	1.24
1	A	142	THR	CA-CB	-39.20	0.48	1.54
1	A	140	THR	CB-OG1	-38.82	0.81	1.43
2	B	2	GLU	CA-CB	-37.91	0.93	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLU	CB-CG	-37.73	0.39	1.52
2	B	63	ASP	CG-OD2	-36.77	0.55	1.25
1	A	99	ASP	CG-OD2	-36.46	0.56	1.25
2	B	1	GLU	C-N	-35.78	0.83	1.33
2	B	50	GLU	CD-OE2	-34.97	0.58	1.25
1	A	94	PHE	C-O	-34.88	0.84	1.23
2	B	50	GLU	CD-OE1	-33.92	0.60	1.25
2	B	1	GLU	C-O	-33.84	0.55	1.23
2	B	4	GLN	CD-OE1	-33.44	0.60	1.23
1	A	142	THR	C-OXT	-32.46	0.58	1.23
1	A	114	GLY	C-O	-32.09	0.88	1.24
1	A	142	THR	CA-C	-32.06	0.85	1.52
1	A	49	ALA	C-N	-32.03	0.88	1.33
2	B	2	GLU	CB-CG	-31.96	0.56	1.52
1	A	77	GLY	C-O	-31.55	0.92	1.23
1	A	49	ALA	C-O	-31.34	0.82	1.24
2	B	74	ASN	C-O	-30.31	0.85	1.24
1	A	138	LYS	CE-NZ	-30.23	0.58	1.49
2	B	2	GLU	CD-OE1	-29.34	0.69	1.25
1	A	68	GLY	C-O	-28.96	0.84	1.23
2	B	16	ARG	CZ-NH1	-28.81	0.92	1.32
2	B	1	GLU	CD-OE2	-28.71	0.70	1.25
2	B	92	TRP	C-O	-28.30	0.90	1.23
2	B	63	ASP	CG-OD1	-27.52	0.73	1.25
2	B	1	GLU	N-CA	-27.33	0.94	1.46
1	A	115	GLY	C-O	-27.25	0.94	1.24
1	A	30	ARG	CZ-NH1	-26.80	0.95	1.32
2	B	48	ASN	CG-ND2	-26.42	0.77	1.33
2	B	58	SER	CB-OG	-26.31	0.89	1.42
1	A	68	GLY	CA-C	-26.12	1.15	1.51
2	B	2	GLU	CG-CD	-25.77	0.87	1.52
2	B	1	GLU	CA-C	-25.56	0.99	1.52
2	B	2	GLU	C-O	-25.34	0.90	1.23
1	A	58	ASP	C-N	-25.26	0.96	1.33
1	A	83	VAL	C-O	-25.10	0.96	1.23
1	A	70	ASP	C-N	-24.98	0.97	1.33
1	A	26	ARG	CZ-NH1	-24.89	0.97	1.32
1	A	85	ARG	CZ-NH1	-24.81	0.98	1.32
1	A	108	GLU	CD-OE1	-24.56	0.78	1.25
2	B	105	THR	C-O	-24.51	0.93	1.24
2	B	16	ARG	CZ-NH2	-24.33	1.01	1.33
1	A	11	GLY	C-O	-24.12	0.91	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	PHE	C-O	-24.04	0.94	1.23
1	A	102	GLN	C-O	-23.93	0.93	1.24
1	A	99	ASP	CB-CG	-23.87	0.92	1.52
1	A	12	SER	CA-CB	-23.70	1.13	1.53
2	B	83	VAL	C-O	-23.26	0.96	1.24
2	B	48	ASN	CG-OD1	-23.23	0.79	1.23
2	B	19	LEU	CG-CD1	-23.08	0.76	1.52
1	A	69	GLY	N-CA	-23.07	1.13	1.45
1	A	14	THR	C-O	-22.83	0.90	1.23
1	A	12	SER	C-O	-22.79	0.95	1.24
1	A	101	ASN	C-O	-22.51	0.95	1.24
2	B	66	TYR	CG-CD2	-22.33	0.92	1.39
2	B	53	LYS	C-O	-22.31	0.98	1.23
2	B	66	TYR	CG-CD1	-22.28	0.92	1.39
2	B	87	ASN	CG-OD1	-21.93	0.81	1.23
2	B	1	GLU	CD-OE1	-21.91	0.83	1.25
2	B	51	GLN	C-O	-21.86	0.88	1.24
2	B	16	ARG	CD-NE	-21.81	1.15	1.46
2	B	94	GLY	C-O	-21.80	0.98	1.23
1	A	12	SER	CB-OG	-21.65	0.98	1.42
2	B	19	LEU	CG-CD2	-21.50	0.81	1.52
1	A	77	GLY	C-N	-21.45	1.04	1.33
1	A	101	ASN	C-N	-21.43	1.03	1.33
2	B	2	GLU	C-N	-21.13	1.03	1.33
1	A	132	GLY	C-O	-20.91	0.98	1.23
1	A	23	ALA	C-O	-20.89	0.97	1.23
1	A	13	GLY	C-N	-20.84	0.97	1.33
1	A	141	VAL	CB-CG1	-20.82	0.83	1.52
1	A	52	TYR	C-O	-20.66	0.96	1.23
1	A	67	THR	C-O	-20.61	0.97	1.24
1	A	52	TYR	C-N	-20.60	1.12	1.33
2	B	36	ASN	CG-ND2	-20.41	0.90	1.33
1	A	96	VAL	CB-CG2	-20.35	0.85	1.52
1	A	141	VAL	CB-CG2	-19.98	0.86	1.52
2	B	75	SER	CB-OG	-19.94	1.02	1.42
1	A	142	THR	CB-CG2	-19.92	0.86	1.52
2	B	66	TYR	CE1-CZ	-19.92	0.90	1.38
1	A	120	PRO	C-O	-19.87	0.98	1.24
2	B	66	TYR	CE2-CZ	-19.85	0.90	1.38
1	A	94	PHE	C-N	-19.73	1.04	1.33
2	B	106	ASN	CG-OD1	-19.65	0.86	1.23
2	B	105	THR	C-N	-19.65	1.06	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	ASN	CG-ND2	-19.64	0.92	1.33
1	A	16	LEU	CB-CG	-19.56	1.14	1.53
1	A	24	THR	C-O	-19.40	1.02	1.23
1	A	50	GLU	C-O	-19.28	0.97	1.23
2	B	18	GLN	C-O	-19.23	1.02	1.24
1	A	64	ARG	CZ-NH1	-19.13	1.05	1.32
1	A	102	GLN	C-N	-19.09	1.07	1.33
2	B	56	LEU	CG-CD2	-19.07	0.89	1.52
2	B	74	ASN	C-N	-18.80	1.07	1.33
2	B	31	GLN	CD-NE2	-18.71	0.94	1.33
1	A	140	THR	CB-CG2	-18.68	0.91	1.52
1	A	14	THR	C-N	-18.52	1.11	1.33
1	A	50	GLU	CG-CD	-18.51	1.05	1.52
1	A	82	GLY	C-O	-18.46	0.99	1.23
2	B	36	ASN	CG-OD1	-18.45	0.88	1.23
1	A	99	ASP	CG-OD1	-18.42	0.90	1.25
1	A	79	GLY	C-O	-18.40	0.99	1.23
1	A	57	LYS	C-O	-18.33	1.02	1.24
2	B	87	ASN	CG-ND2	-18.26	0.94	1.33
2	B	14	LYS	C-O	-18.24	1.03	1.23
1	A	50	GLU	C-N	-18.15	1.08	1.33
1	A	70	ASP	N-CA	-18.12	1.22	1.46
1	A	67	THR	CB-CG2	-18.06	0.93	1.52
1	A	28	ILE	CB-CG1	-18.00	1.17	1.53
1	A	96	VAL	CB-CG1	-18.00	0.93	1.52
2	B	81	ASN	CG-OD1	-17.98	0.89	1.23
2	B	87	ASN	CB-CG	-17.70	1.07	1.52
1	A	69	GLY	CA-C	-17.68	1.26	1.51
2	B	56	LEU	CB-CG	-17.58	1.18	1.53
2	B	38	ARG	CZ-NH2	-17.57	1.10	1.33
1	A	108	GLU	CD-OE2	-17.23	0.92	1.25
2	B	106	ASN	CG-ND2	-17.20	0.97	1.33
1	A	50	GLU	CB-CG	-17.15	1.01	1.52
2	B	6	ARG	CZ-NH1	-17.14	1.08	1.32
1	A	40	MET	SD-CE	-16.86	1.37	1.79
1	A	93	PHE	C-N	-16.78	1.11	1.33
1	A	103	ASP	CG-OD1	-16.77	0.93	1.25
2	B	111	ASN	C-O	-16.76	1.03	1.23
2	B	104	GLN	C-O	-16.70	1.11	1.23
1	A	51	ARG	C-O	-16.69	1.02	1.24
2	B	38	ARG	CZ-NH1	-16.59	1.09	1.32
2	B	38	ARG	CD-NE	-16.47	1.23	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	51	GLN	C-N	-16.44	1.09	1.33
2	B	83	VAL	C-N	-16.42	1.11	1.33
2	B	103	GLN	CD-OE1	-16.21	0.92	1.23
1	A	138	LYS	CG-CD	-16.16	1.03	1.52
2	B	70	ARG	CZ-NH1	-16.09	1.10	1.32
2	B	9	ASP	CG-OD1	-16.06	0.94	1.25
1	A	70	ASP	CA-CB	-16.02	1.26	1.53
1	A	50	GLU	CD-OE1	-15.96	0.95	1.25
2	B	21	ASP	C-O	-15.85	1.06	1.23
1	A	30	ARG	CZ-NH2	-15.76	1.12	1.33
2	B	48	ASN	CB-CG	-15.71	1.12	1.52
1	A	140	THR	C-O	-15.68	1.04	1.24
1	A	43	ARG	CZ-NH1	-15.61	1.10	1.32
1	A	42	GLU	CD-OE1	-15.54	0.95	1.25
1	A	134	THR	C-O	-15.47	1.03	1.23
1	A	69	GLY	C-O	-15.30	1.02	1.24
1	A	17	ARG	NE-CZ	-15.26	1.16	1.33
2	B	94	GLY	C-N	-15.22	1.12	1.33
2	B	45	ASP	CG-OD1	-15.22	0.96	1.25
1	A	68	GLY	C-N	-15.14	1.10	1.33
1	A	83	VAL	CA-CB	-15.09	1.29	1.55
1	A	101	ASN	CG-OD1	-15.08	0.94	1.23
2	B	81	ASN	CG-ND2	-15.04	1.01	1.33
1	A	122	GLU	CD-OE2	-15.02	0.96	1.25
1	A	13	GLY	N-CA	-15.02	1.31	1.45
1	A	17	ARG	CZ-NH1	-15.01	1.11	1.32
2	B	67	VAL	C-O	-14.92	1.09	1.24
1	A	140	THR	C-N	-14.77	1.16	1.33
1	A	50	GLU	CD-OE2	-14.76	0.97	1.25
2	B	103	GLN	CD-NE2	-14.72	1.02	1.33
2	B	47	ASP	CG-OD1	-14.63	0.97	1.25
1	A	97	MET	C-O	-14.63	1.06	1.24
2	B	13	ALA	C-O	-14.42	1.02	1.23
2	B	109	PRO	C-O	-14.41	1.05	1.24
2	B	73	ASP	CG-OD2	-14.39	0.98	1.25
1	A	16	LEU	CG-CD1	-14.38	1.05	1.52
1	A	46	ASP	C-O	-14.35	1.11	1.24
1	A	85	ARG	NE-CZ	-14.35	1.17	1.33
1	A	47	GLY	C-O	-14.29	1.04	1.23
1	A	78	GLU	CD-OE1	-14.25	0.98	1.25
2	B	6	ARG	NE-CZ	-14.14	1.17	1.33
1	A	12	SER	C-N	-14.07	1.15	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	THR	C-N	-14.00	1.13	1.33
1	A	30	ARG	CD-NE	-13.88	1.26	1.46
2	B	4	GLN	C-N	-13.82	1.19	1.33
2	B	99	TYR	C-O	-13.81	1.04	1.24
2	B	18	GLN	CB-CG	-13.77	1.11	1.52
1	A	78	GLU	CD-OE2	-13.72	0.99	1.25
2	B	140	LEU	CB-CG	-13.71	1.26	1.53
2	B	106	ASN	CB-CG	-13.51	1.18	1.52
1	A	141	VAL	CA-CB	-13.51	1.38	1.53
1	A	69	GLY	C-N	-13.38	1.15	1.33
1	A	65	VAL	C-O	-13.35	1.10	1.24
2	B	64	LYS	CD-CE	-13.33	1.12	1.52
1	A	120	PRO	C-N	-13.17	1.16	1.33
1	A	103	ASP	CG-OD2	-13.07	1.00	1.25
2	B	31	GLN	CD-OE1	-13.01	0.98	1.23
1	A	49	ALA	CA-CB	-12.85	1.34	1.53
2	B	88	ASP	CG-OD2	-12.83	1.00	1.25
1	A	70	ASP	CG-OD2	-12.79	1.01	1.25
1	A	114	GLY	CA-C	-12.72	1.38	1.51
2	B	4	GLN	C-O	-12.67	1.09	1.23
2	B	25	ILE	C-O	-12.67	1.08	1.24
2	B	92	TRP	C-N	-12.66	1.15	1.33
1	A	64	ARG	CZ-NH2	-12.64	1.17	1.33
2	B	88	ASP	CG-OD1	-12.60	1.01	1.25
1	A	78	GLU	C-O	-12.57	1.08	1.24
2	B	4	GLN	CB-CG	-12.53	1.14	1.52
1	A	17	ARG	CZ-NH2	-12.52	1.17	1.33
1	A	51	ARG	CD-NE	-12.49	1.28	1.46
2	B	129	PHE	C-O	-12.46	1.07	1.23
2	B	62	ARG	CZ-NH1	-12.41	1.15	1.32
1	A	16	LEU	CG-CD2	-12.38	1.11	1.52
1	A	26	ARG	NE-CZ	-12.37	1.19	1.33
1	A	64	ARG	NE-CZ	-12.34	1.19	1.33
2	B	9	ASP	CG-OD2	-12.30	1.01	1.25
2	B	18	GLN	C-N	-12.27	1.16	1.33
1	A	11	GLY	CA-C	-12.19	1.34	1.51
2	B	53	LYS	C-N	-12.20	1.16	1.33
2	B	50	GLU	CB-CG	-12.07	1.16	1.52
1	A	51	ARG	C-N	-12.06	1.18	1.33
2	B	86	LYS	CD-CE	-12.04	1.16	1.52
2	B	14	LYS	C-N	-12.02	1.17	1.33
1	A	132	GLY	C-N	-12.00	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	THR	C-N	-11.98	1.19	1.33
1	A	43	ARG	CZ-NH2	-11.98	1.17	1.33
1	A	51	ARG	CZ-NH2	-11.91	1.18	1.33
1	A	72	TRP	C-O	-11.81	1.08	1.23
1	A	10	GLY	C-O	-11.77	1.08	1.23
2	B	19	LEU	CB-CG	-11.77	1.29	1.53
2	B	80	ASP	C-O	-11.74	1.09	1.24
1	A	17	ARG	CD-NE	-11.73	1.29	1.46
1	A	42	GLU	CD-OE2	-11.72	1.03	1.25
1	A	133	THR	C-O	-11.70	1.08	1.23
2	B	140	LEU	C-O	-11.69	1.09	1.24
1	A	10	GLY	C-N	-11.67	1.16	1.33
1	A	72	TRP	NE1-CE2	-11.66	1.24	1.37
2	B	73	ASP	CG-OD1	-11.64	1.03	1.25
2	B	107	THR	CB-OG1	-11.64	1.25	1.43
1	A	22	VAL	CB-CG1	-11.59	1.14	1.52
1	A	64	ARG	CD-NE	-11.56	1.30	1.46
2	B	125	ASN	C-O	-11.56	1.05	1.24
1	A	101	ASN	CG-ND2	-11.54	1.09	1.33
1	A	108	GLU	CG-CD	-11.51	1.23	1.52
1	A	28	ILE	C-O	-11.51	1.10	1.23
1	A	88	GLN	C-O	-11.45	1.08	1.24
2	B	43	LYS	CB-CG	-11.38	1.18	1.52
2	B	140	LEU	CG-CD1	-11.37	1.15	1.52
1	A	33	HIS	CE1-NE2	-11.33	1.21	1.32
1	A	137	THR	CB-OG1	-11.30	1.25	1.43
1	A	40	MET	CG-SD	-11.27	1.52	1.80
1	A	90	GLU	CD-OE2	-11.26	1.03	1.25
2	B	45	ASP	CG-OD2	-11.25	1.03	1.25
1	A	8	SER	CB-OG	-11.20	1.19	1.42
1	A	12	SER	CA-C	-11.15	1.37	1.52
2	B	4	GLN	CG-CD	-11.13	1.24	1.52
1	A	78	GLU	C-N	-11.08	1.17	1.33
2	B	62	ARG	NE-CZ	-11.08	1.20	1.33
2	B	12	VAL	C-O	-11.02	1.09	1.24
2	B	89	VAL	C-O	-10.98	1.10	1.24
2	B	48	ASN	C-O	-10.92	1.09	1.24
2	B	47	ASP	CB-CG	-10.90	1.24	1.52
2	B	31	GLN	CB-CG	-10.89	1.19	1.52
1	A	30	ARG	NE-CZ	-10.87	1.21	1.33
2	B	43	LYS	CE-NZ	-10.87	1.16	1.49
1	A	70	ASP	CB-CG	-10.85	1.25	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	GLY	C-N	-10.84	1.18	1.33
2	B	6	ARG	CZ-NH2	-10.81	1.19	1.33
1	A	30	ARG	CB-CG	-10.77	1.20	1.52
1	A	24	THR	CB-OG1	-10.77	1.26	1.43
1	A	43	ARG	CD-NE	-10.74	1.31	1.46
1	A	37	HIS	CE1-NE2	-10.73	1.21	1.32
1	A	114	GLY	C-N	-10.69	1.18	1.33
1	A	81	LYS	CE-NZ	-10.68	1.17	1.49
1	A	64	ARG	C-O	-10.68	1.10	1.23
1	A	115	GLY	N-CA	-10.64	1.34	1.45
1	A	138	LYS	C-O	-10.64	1.10	1.23
1	A	83	VAL	C-N	-10.60	1.19	1.33
1	A	47	GLY	C-N	-10.60	1.18	1.33
1	A	122	GLU	CD-OE1	-10.48	1.05	1.25
1	A	134	THR	C-N	-10.47	1.19	1.34
1	A	20	ALA	C-O	-10.36	1.11	1.24
1	A	89	GLU	CD-OE2	-10.33	1.05	1.25
2	B	84	PHE	CG-CD1	-10.32	1.17	1.38
1	A	85	ARG	CZ-NH2	-10.31	1.20	1.33
2	B	70	ARG	CZ-NH2	-10.31	1.20	1.33
1	A	102	GLN	CD-NE2	-10.25	1.11	1.33
1	A	12	SER	N-CA	-10.23	1.32	1.46
2	B	103	GLN	CB-CG	-10.22	1.21	1.52
1	A	66	ARG	NE-CZ	-10.21	1.21	1.33
1	A	37	HIS	CG-ND1	-10.18	1.27	1.38
1	A	46	ASP	CG-OD1	-10.12	1.06	1.25
2	B	6	ARG	CD-NE	-10.06	1.32	1.46
1	A	89	GLU	CD-OE1	-9.99	1.06	1.25
1	A	48	ARG	C-O	-9.93	1.12	1.24
2	B	142	VAL	CB-CG1	-9.88	1.20	1.52
2	B	93	GLY	C-O	-9.85	1.10	1.23
1	A	79	GLY	CA-C	-9.82	1.38	1.51
2	B	81	ASN	CB-CG	-9.82	1.27	1.52
2	B	87	ASN	C-O	-9.81	1.11	1.24
2	B	90	GLY	C-O	-9.80	1.09	1.23
1	A	80	GLY	C-O	-9.73	1.10	1.23
2	B	110	GLY	C-O	-9.71	1.10	1.23
2	B	112	TYR	C-O	-9.71	1.12	1.23
1	A	51	ARG	NE-CZ	-9.69	1.22	1.33
1	A	21	LYS	CE-NZ	-9.68	1.20	1.49
1	A	41	ASN	CG-OD1	-9.66	1.05	1.23
2	B	59	ASP	CG-OD2	-9.65	1.07	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	VAL	CB-CG2	-9.63	1.20	1.52
1	A	46	ASP	CG-OD2	-9.61	1.07	1.25
1	A	110	ARG	CB-CG	-9.61	1.23	1.52
1	A	15	GLN	CD-NE2	-9.60	1.13	1.33
1	A	83	VAL	N-CA	-9.60	1.35	1.46
2	B	141	THR	C-O	-9.60	1.12	1.24
1	A	94	PHE	CB-CG	-9.56	1.28	1.50
2	B	112	TYR	CG-CD2	-9.51	1.19	1.39
1	A	71	GLY	C-O	-9.49	1.11	1.23
1	A	141	VAL	CA-C	-9.48	1.41	1.52
1	A	38	VAL	CB-CG2	-9.48	1.21	1.52
2	B	106	ASN	C-O	-9.48	1.12	1.24
1	A	70	ASP	CA-C	-9.47	1.40	1.52
2	B	97	GLY	C-O	-9.45	1.11	1.23
2	B	97	GLY	C-N	-9.43	1.21	1.33
1	A	85	ARG	CD-NE	-9.43	1.33	1.46
2	B	70	ARG	NE-CZ	-9.42	1.22	1.33
1	A	41	ASN	CB-CG	-9.39	1.28	1.52
1	A	95	ASP	CG-OD1	-9.39	1.07	1.25
1	A	48	ARG	NE-CZ	-9.37	1.22	1.33
1	A	82	GLY	C-N	-9.37	1.21	1.33
1	A	18	ASP	C-O	-9.35	1.12	1.23
1	A	132	GLY	CA-C	-9.34	1.45	1.52
1	A	48	ARG	CZ-NH2	-9.33	1.21	1.33
2	B	84	PHE	CG-CD2	-9.33	1.19	1.38
1	A	70	ASP	CG-OD1	-9.31	1.07	1.25
2	B	109	PRO	C-N	-9.31	1.20	1.33
1	A	88	GLN	C-N	-9.31	1.20	1.33
2	B	13	ALA	C-N	-9.29	1.21	1.33
2	B	47	ASP	CG-OD2	-9.28	1.07	1.25
2	B	104	GLN	CD-NE2	-9.23	1.13	1.33
1	A	130	PRO	C-O	-9.22	1.14	1.23
1	A	97	MET	C-N	-9.21	1.20	1.33
2	B	69	ILE	CB-CG1	-9.20	1.35	1.53
2	B	70	ARG	CD-NE	-9.17	1.33	1.46
1	A	76	LYS	CB-CG	-9.10	1.25	1.52
1	A	64	ARG	CB-CG	-9.09	1.25	1.52
1	A	134	THR	CB-OG1	-9.07	1.29	1.43
2	B	111	ASN	C-N	-9.04	1.20	1.33
2	B	131	PRO	C-O	-8.95	1.12	1.24
2	B	142	VAL	CB-CG2	-8.94	1.23	1.52
1	A	76	LYS	CD-CE	-8.93	1.25	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	LEU	CB-CG	-8.90	1.35	1.53
2	B	35	CYS	C-O	-8.90	1.14	1.23
1	A	102	GLN	CD-OE1	-8.87	1.06	1.23
1	A	103	ASP	C-O	-8.82	1.13	1.24
2	B	125	ASN	C-N	-8.82	1.22	1.33
1	A	38	VAL	CB-CG1	-8.79	1.23	1.52
2	B	47	ASP	C-O	-8.79	1.12	1.24
1	A	79	GLY	C-N	-8.73	1.20	1.33
1	A	50	GLU	CA-CB	-8.70	1.41	1.53
1	A	131	SER	C-N	-8.66	1.27	1.33
1	A	138	LYS	CD-CE	-8.66	1.26	1.52
1	A	90	GLU	CD-OE1	-8.65	1.08	1.25
1	A	48	ARG	CD-NE	-8.64	1.34	1.46
1	A	81	LYS	CD-CE	-8.64	1.26	1.52
1	A	80	GLY	N-CA	-8.61	1.32	1.45
1	A	59	GLY	C-O	-8.60	1.12	1.23
1	A	32	ALA	C-O	-8.59	1.13	1.24
2	B	137	THR	C-O	-8.58	1.14	1.24
1	A	48	ARG	CZ-NH1	-8.57	1.20	1.32
1	A	33	HIS	CG-CD2	-8.55	1.26	1.35
2	B	18	GLN	CG-CD	-8.55	1.30	1.52
2	B	43	LYS	CD-CE	-8.55	1.26	1.52
2	B	104	GLN	CD-OE1	-8.54	1.07	1.23
2	B	106	ASN	CA-CB	-8.54	1.39	1.53
1	A	15	GLN	CG-CD	-8.52	1.30	1.52
1	A	7	GLU	CD-OE2	-8.51	1.09	1.25
1	A	21	LYS	C-O	-8.51	1.12	1.23
1	A	84	SER	CB-OG	-8.50	1.25	1.42
1	A	23	ALA	C-N	-8.50	1.21	1.33
2	B	62	ARG	CG-CD	-8.49	1.26	1.52
1	A	75	VAL	CB-CG1	-8.47	1.24	1.52
2	B	9	ASP	CB-CG	-8.47	1.30	1.52
2	B	118	GLY	C-O	-8.47	1.12	1.23
1	A	23	ALA	CA-C	-8.43	1.42	1.52
1	A	28	ILE	CB-CG2	-8.41	1.24	1.52
2	B	112	TYR	CE1-CZ	-8.41	1.18	1.38
1	A	136	THR	CB-OG1	-8.37	1.30	1.43
1	A	29	CYS	C-O	-8.36	1.13	1.23
2	B	59	ASP	CG-OD1	-8.33	1.09	1.25
1	A	55	GLN	C-O	-8.31	1.13	1.23
1	A	71	GLY	N-CA	-8.31	1.33	1.45
2	B	54	PHE	CG-CD2	-8.31	1.21	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	LYS	C-N	-8.29	1.21	1.33
1	A	48	ARG	C-N	-8.27	1.22	1.33
1	A	96	VAL	C-O	-8.20	1.12	1.23
2	B	99	TYR	C-N	-8.20	1.21	1.33
2	B	16	ARG	C-O	-8.19	1.14	1.24
1	A	122	GLU	CB-CG	-8.18	1.27	1.52
1	A	133	THR	CB-OG1	-8.17	1.30	1.43
1	A	72	TRP	C-N	-8.14	1.22	1.33
1	A	63	LEU	C-O	-8.13	1.14	1.24
2	B	67	VAL	C-N	-8.12	1.21	1.33
1	A	58	ASP	CG-OD1	-8.08	1.09	1.25
2	B	93	GLY	C-N	-8.07	1.23	1.33
2	B	104	GLN	C-N	-8.07	1.22	1.33
2	B	143	THR	CB-OG1	-8.06	1.30	1.43
1	A	26	ARG	CZ-NH2	-8.05	1.23	1.33
1	A	24	THR	N-CA	-8.04	1.36	1.47
1	A	17	ARG	CB-CG	-8.03	1.28	1.52
1	A	15	GLN	CB-CG	-8.02	1.28	1.52
1	A	59	GLY	C-N	-8.01	1.22	1.33
1	A	81	LYS	C-O	-8.01	1.13	1.24
2	B	140	LEU	C-N	-8.00	1.22	1.33
1	A	66	ARG	C-O	-7.97	1.12	1.23
1	A	72	TRP	CD2-CE3	-7.92	1.27	1.40
1	A	67	THR	CA-CB	-7.91	1.41	1.53
1	A	133	THR	C-N	-7.88	1.22	1.33
2	B	43	LYS	CG-CD	-7.88	1.28	1.52
2	B	90	GLY	C-N	-7.86	1.23	1.33
2	B	18	GLN	CD-OE1	-7.85	1.08	1.23
2	B	25	ILE	C-N	-7.85	1.21	1.33
2	B	80	ASP	C-N	-7.83	1.21	1.33
2	B	114	LEU	CB-CG	-7.81	1.37	1.53
1	A	67	THR	CA-C	-7.79	1.41	1.52
1	A	94	PHE	CG-CD2	-7.76	1.22	1.38
1	A	33	HIS	CG-ND1	-7.74	1.29	1.38
2	B	121	TRP	C-O	-7.74	1.14	1.23
2	B	139	LYS	CD-CE	-7.69	1.29	1.52
1	A	96	VAL	C-N	-7.68	1.22	1.33
2	B	60	ASN	CG-OD1	-7.65	1.09	1.23
1	A	13	GLY	CA-C	-7.63	1.42	1.52
2	B	42	LEU	CG-CD2	-7.63	1.27	1.52
1	A	52	TYR	CG-CD1	-7.63	1.23	1.39
2	B	60	ASN	CG-ND2	-7.62	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	GLU	CG-CD	-7.58	1.33	1.52
1	A	15	GLN	CD-OE1	-7.58	1.09	1.23
2	B	49	PHE	CG-CD2	-7.57	1.23	1.38
1	A	27	ILE	C-O	-7.53	1.14	1.23
1	A	82	GLY	CA-C	-7.53	1.41	1.51
2	B	77	TRP	C-O	-7.52	1.14	1.23
2	B	21	ASP	C-N	-7.51	1.23	1.33
1	A	68	GLY	N-CA	-7.50	1.34	1.45
2	B	20	THR	CB-OG1	-7.49	1.31	1.43
1	A	110	ARG	CZ-NH1	-7.49	1.22	1.32
2	B	32	ALA	C-O	-7.48	1.14	1.23
2	B	141	THR	C-N	-7.45	1.24	1.33
1	A	5	HIS	CE1-NE2	-7.41	1.25	1.32
1	A	71	GLY	C-N	-7.38	1.23	1.33
2	B	125	ASN	CG-OD1	-7.38	1.09	1.23
2	B	33	LEU	CG-CD2	-7.31	1.28	1.52
1	A	28	ILE	C-N	-7.31	1.24	1.33
2	B	58	SER	C-O	-7.31	1.14	1.23
2	B	73	ASP	C-O	-7.28	1.15	1.23
2	B	136	GLY	C-O	-7.28	1.12	1.23
2	B	48	ASN	C-N	-7.27	1.23	1.33
2	B	110	GLY	C-N	-7.26	1.24	1.33
1	A	66	ARG	CZ-NH1	-7.25	1.22	1.32
2	B	56	LEU	CG-CD1	-7.25	1.28	1.52
1	A	121	GLN	CD-NE2	-7.24	1.18	1.33
2	B	10	LEU	CB-CG	-7.23	1.39	1.53
2	B	86	LYS	CE-NZ	-7.20	1.27	1.49
1	A	65	VAL	C-N	-7.18	1.24	1.33
1	A	83	VAL	CB-CG2	-7.13	1.29	1.52
1	A	63	LEU	CG-CD1	-7.11	1.29	1.52
1	A	21	LYS	C-N	-7.08	1.24	1.33
1	A	6	LEU	CB-CG	-7.08	1.39	1.53
1	A	24	THR	CA-CB	-7.07	1.43	1.52
1	A	106	PRO	C-N	-7.07	1.25	1.33
2	B	8	GLY	C-O	-7.04	1.14	1.23
1	A	93	PHE	CG-CD1	-7.01	1.24	1.38
2	B	36	ASN	CB-CG	-7.00	1.34	1.52
2	B	49	PHE	CG-CD1	-7.00	1.24	1.38
2	B	18	GLN	CD-NE2	-6.97	1.18	1.33
1	A	29	CYS	C-N	-6.96	1.25	1.34
1	A	24	THR	CB-CG2	-6.95	1.29	1.52
1	A	103	ASP	CB-CG	-6.92	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	58	SER	C-N	-6.91	1.24	1.34
1	A	18	ASP	C-N	-6.89	1.23	1.33
1	A	97	MET	SD-CE	-6.84	1.62	1.79
1	A	94	PHE	CG-CD1	-6.84	1.24	1.38
1	A	115	GLY	CA-C	-6.82	1.44	1.51
2	B	33	LEU	CG-CD1	-6.82	1.30	1.52
1	A	94	PHE	CD1-CE1	-6.80	1.18	1.38
1	A	75	VAL	CB-CG2	-6.79	1.30	1.52
1	A	94	PHE	CD2-CE2	-6.79	1.18	1.38
1	A	11	GLY	C-N	-6.76	1.24	1.33
1	A	52	TYR	CE2-CZ	-6.75	1.22	1.38
2	B	31	GLN	C-O	-6.72	1.16	1.24
1	A	90	GLU	C-O	-6.71	1.15	1.24
1	A	46	ASP	C-N	-6.71	1.23	1.33
1	A	106	PRO	C-O	-6.66	1.14	1.23
2	B	87	ASN	C-N	-6.65	1.24	1.33
2	B	69	ILE	CB-CG2	-6.65	1.30	1.52
2	B	89	VAL	C-N	-6.65	1.25	1.32
2	B	8	GLY	C-N	-6.64	1.24	1.33
2	B	111	ASN	CG-ND2	-6.63	1.19	1.33
2	B	88	ASP	CB-CG	-6.63	1.35	1.52
1	A	63	LEU	C-N	-6.62	1.24	1.33
2	B	39	GLN	CD-NE2	-6.59	1.19	1.33
1	A	110	ARG	CZ-NH2	-6.59	1.24	1.33
2	B	125	ASN	CG-ND2	-6.58	1.19	1.33
2	B	98	ILE	CB-CG1	-6.56	1.40	1.53
2	B	59	ASP	CA-CB	-6.53	1.42	1.53
2	B	59	ASP	CB-CG	-6.53	1.35	1.52
1	A	110	ARG	NE-CZ	-6.51	1.25	1.33
1	A	72	TRP	CZ2-CH2	-6.50	1.24	1.37
2	B	17	GLY	C-O	-6.50	1.15	1.23
1	A	121	GLN	CD-OE1	-6.48	1.11	1.23
2	B	59	ASP	C-O	-6.48	1.16	1.24
2	B	98	ILE	CG1-CD1	-6.47	1.26	1.51
1	A	26	ARG	CD-NE	-6.47	1.37	1.46
1	A	50	GLU	N-CA	-6.46	1.38	1.46
2	B	137	THR	C-N	-6.41	1.24	1.33
1	A	32	ALA	C-N	-6.35	1.25	1.33
2	B	62	ARG	C-O	-6.35	1.16	1.24
1	A	52	TYR	CA-CB	-6.34	1.43	1.53
2	B	136	GLY	C-N	-6.33	1.24	1.33
1	A	57	LYS	CE-NZ	-6.32	1.30	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	44	ALA	C-O	-6.32	1.16	1.23
1	A	139	LEU	CG-CD1	-6.30	1.31	1.52
1	A	61	HIS	CE1-NE2	-6.29	1.26	1.32
1	A	142	THR	N-CA	-6.28	1.34	1.46
1	A	126	GLN	C-O	-6.27	1.17	1.24
2	B	130	THR	CB-OG1	-6.27	1.33	1.43
1	A	84	SER	CA-CB	-6.26	1.44	1.53
2	B	140	LEU	CG-CD2	-6.25	1.31	1.52
2	B	53	LYS	CG-CD	-6.25	1.33	1.52
1	A	64	ARG	C-N	-6.23	1.25	1.33
2	B	112	TYR	CG-CD1	-6.22	1.26	1.39
2	B	54	PHE	CG-CD1	-6.20	1.25	1.38
1	A	15	GLN	C-O	-6.19	1.15	1.23
1	A	5	HIS	CG-ND1	-6.19	1.31	1.38
2	B	63	ASP	CB-CG	-6.19	1.36	1.52
1	A	27	ILE	C-N	-6.18	1.25	1.33
2	B	50	GLU	CG-CD	-6.16	1.36	1.52
1	A	43	ARG	NE-CZ	-6.15	1.26	1.33
2	B	77	TRP	C-N	-6.14	1.24	1.33
2	B	52	GLY	C-O	-6.10	1.15	1.23
1	A	15	GLN	C-N	-6.10	1.24	1.33
2	B	65	LEU	C-O	-6.09	1.17	1.24
1	A	66	ARG	CZ-NH2	-6.09	1.25	1.33
1	A	66	ARG	CG-CD	-6.07	1.34	1.52
1	A	37	HIS	CD2-NE2	-6.07	1.31	1.37
2	B	91	SER	C-O	-6.06	1.16	1.23
1	A	88	GLN	CD-OE1	-6.03	1.12	1.23
2	B	17	GLY	C-N	-6.00	1.26	1.33
1	A	107	GLY	C-O	-5.99	1.17	1.23
1	A	83	VAL	CA-C	-5.98	1.45	1.52
1	A	6	LEU	CG-CD2	-5.98	1.32	1.52
2	B	118	GLY	C-N	-5.97	1.24	1.33
2	B	54	PHE	CE1-CZ	-5.95	1.20	1.38
1	A	135	GLY	C-O	-5.93	1.14	1.23
2	B	79	THR	C-O	-5.93	1.16	1.23
2	B	90	GLY	N-CA	-5.90	1.39	1.45
2	B	53	LYS	CE-NZ	-5.90	1.31	1.49
1	A	83	VAL	CB-CG1	-5.89	1.33	1.52
2	B	89	VAL	CA-CB	-5.89	1.47	1.54
1	A	66	ARG	CD-NE	-5.87	1.38	1.46
1	A	23	ALA	CA-CB	-5.84	1.39	1.54
1	A	78	GLU	CA-C	-5.82	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	51	GLN	CD-OE1	-5.82	1.12	1.23
1	A	34	THR	CB-OG1	-5.80	1.34	1.43
2	B	96	ILE	C-O	-5.80	1.17	1.24
2	B	112	TYR	C-N	-5.80	1.24	1.33
1	A	88	GLN	CD-NE2	-5.79	1.21	1.33
1	A	66	ARG	C-N	-5.78	1.25	1.33
1	A	58	ASP	CG-OD2	-5.78	1.14	1.25
2	B	127	GLN	CD-NE2	-5.78	1.21	1.33
1	A	111	PHE	CG-CD2	-5.77	1.26	1.38
1	A	74	PRO	C-O	-5.74	1.16	1.24
1	A	7	GLU	C-O	-5.73	1.16	1.23
1	A	110	ARG	CD-NE	-5.72	1.38	1.46
2	B	47	ASP	C-N	-5.70	1.25	1.33
1	A	138	LYS	C-N	-5.68	1.23	1.34
2	B	84	PHE	CD1-CE1	-5.67	1.21	1.38
1	A	55	GLN	C-N	-5.63	1.25	1.33
1	A	25	GLY	N-CA	-5.63	1.39	1.44
2	B	132	SER	C-N	-5.62	1.25	1.33
2	B	133	GLY	C-O	-5.62	1.16	1.23
2	B	84	PHE	CD2-CE2	-5.62	1.21	1.38
1	A	80	GLY	C-N	-5.61	1.25	1.33
1	A	76	LYS	C-N	-5.60	1.25	1.33
1	A	4	LEU	CB-CG	-5.58	1.42	1.53
2	B	73	ASP	C-N	-5.56	1.25	1.33
1	A	7	GLU	CD-OE1	-5.55	1.14	1.25
2	B	3	CYS	C-O	-5.54	1.17	1.24
2	B	112	TYR	CE2-CZ	-5.53	1.25	1.38
1	A	20	ALA	C-N	-5.52	1.25	1.33
2	B	42	LEU	CG-CD1	-5.49	1.34	1.52
2	B	131	PRO	C-N	-5.49	1.23	1.34
1	A	49	ALA	N-CA	-5.49	1.39	1.46
1	A	94	PHE	CE1-CZ	-5.49	1.22	1.38
1	A	36	PHE	C-O	-5.43	1.17	1.23
2	B	101	ASP	CG-OD2	-5.43	1.15	1.25
2	B	49	PHE	CE1-CZ	-5.43	1.22	1.38
1	A	48	ARG	CA-C	-5.42	1.45	1.52
2	B	107	THR	C-O	-5.42	1.16	1.24
2	B	115	THR	CB-OG1	-5.42	1.35	1.43
2	B	29	THR	CB-OG1	-5.41	1.35	1.43
2	B	81	ASN	C-O	-5.39	1.17	1.24
2	B	84	PHE	C-O	-5.37	1.18	1.24
1	A	40	MET	CB-CG	-5.36	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	GLU	C-N	-5.35	1.25	1.33
1	A	110	ARG	CG-CD	-5.34	1.36	1.52
1	A	51	ARG	CZ-NH1	-5.34	1.25	1.32
1	A	37	HIS	CG-CD2	-5.33	1.29	1.35
1	A	61	HIS	CG-ND1	-5.32	1.32	1.38
1	A	109	TYR	C-O	-5.31	1.17	1.24
2	B	109	PRO	N-CD	-5.30	1.40	1.47
1	A	128	PHE	CG-CD1	-5.30	1.27	1.38
2	B	81	ASN	C-N	-5.29	1.25	1.33
1	A	14	THR	CB-OG1	-5.28	1.35	1.43
1	A	116	ALA	CA-CB	-5.28	1.44	1.53
1	A	49	ALA	CA-C	-5.28	1.45	1.52
1	A	141	VAL	N-CA	-5.28	1.40	1.46
2	B	139	LYS	CE-NZ	-5.28	1.33	1.49
2	B	59	ASP	N-CA	-5.27	1.39	1.46
1	A	137	THR	CB-CG2	-5.27	1.35	1.52
2	B	121	TRP	C-N	-5.25	1.25	1.33
1	A	65	VAL	CA-CB	-5.24	1.47	1.54
1	A	111	PHE	CG-CD1	-5.24	1.27	1.38
2	B	107	THR	CB-CG2	-5.23	1.35	1.52
1	A	30	ARG	CG-CD	-5.21	1.36	1.52
2	B	143	THR	CB-CG2	-5.19	1.35	1.52
2	B	39	GLN	CD-OE1	-5.19	1.13	1.23
2	B	64	LYS	CE-NZ	-5.18	1.33	1.49
1	A	71	GLY	CA-C	-5.15	1.44	1.51
1	A	112	SER	C-O	-5.15	1.17	1.24
1	A	55	GLN	CD-NE2	-5.15	1.22	1.33
1	A	94	PHE	CA-CB	-5.14	1.44	1.53
1	A	28	ILE	CG1-CD1	-5.13	1.31	1.51
1	A	93	PHE	CG-CD2	-5.13	1.28	1.38
1	A	136	THR	CB-CG2	-5.12	1.35	1.52
1	A	72	TRP	N-CA	-5.12	1.40	1.45
1	A	131	SER	C-O	-5.09	1.18	1.23
2	B	108	PRO	CA-CB	-5.09	1.47	1.54
1	A	55	GLN	CD-OE1	-5.06	1.14	1.23
1	A	72	TRP	CG-CD2	-5.05	1.34	1.43
2	B	89	VAL	CA-C	-5.05	1.46	1.52
1	A	33	HIS	ND1-CE1	-5.05	1.27	1.32
1	A	124	ASN	CG-ND2	-5.04	1.22	1.33
1	A	133	THR	CA-CB	-5.04	1.45	1.53
2	B	139	LYS	CB-CG	-5.04	1.37	1.52
1	A	140	THR	CA-C	-5.03	1.46	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	GLN	OE1-CD-NE2	-74.16	48.44	122.60
1	A	141	VAL	O-C-N	-40.60	72.42	122.77
1	A	99	ASP	CA-CB-CG	37.75	150.35	112.60
1	A	69	GLY	N-CA-C	35.03	164.66	115.27
1	A	50	GLU	CB-CG-CD	34.86	171.85	112.60
2	B	50	GLU	OE1-CD-OE2	-30.81	48.95	122.90
1	A	58	ASP	O-C-N	-29.05	82.28	122.37
1	A	142	THR	CA-CB-OG1	-28.96	66.15	109.60
2	B	2	GLU	CA-CB-CG	26.88	167.85	114.10
2	B	66	TYR	CD1-CG-CD2	-25.77	79.44	118.10
2	B	1	GLU	CB-CG-CD	25.40	155.78	112.60
2	B	63	ASP	OD1-CG-OD2	-23.91	65.53	122.90
2	B	4	GLN	CG-CD-NE2	23.88	152.22	116.40
2	B	48	ASN	CA-CB-CG	23.72	136.32	112.60
1	A	13	GLY	O-C-N	-23.08	92.00	122.47
2	B	1	GLU	CB-CA-C	-22.21	67.89	110.10
2	B	87	ASN	CA-CB-CG	21.83	134.43	112.60
1	A	141	VAL	CA-C-O	20.46	145.71	120.75
2	B	1	GLU	CG-CD-OE2	-19.94	72.55	118.40
1	A	49	ALA	O-C-N	-19.76	94.31	122.36
1	A	142	THR	OG1-CB-CG2	19.48	148.26	109.30
2	B	4	GLN	CG-CD-OE1	19.27	159.34	120.80
2	B	66	TYR	CE1-CZ-CE2	-19.20	81.90	120.30
1	A	70	ASP	O-C-N	-18.42	98.09	122.59
2	B	16	ARG	NH1-CZ-NH2	-18.12	95.74	119.30
2	B	36	ASN	OD1-CG-ND2	-17.78	104.82	122.60
2	B	103	GLN	OE1-CD-NE2	-17.74	104.86	122.60
2	B	16	ARG	NE-CZ-NH2	17.67	135.10	119.20
1	A	142	THR	CB-CA-C	-17.13	71.42	109.10
2	B	1	GLU	N-CA-C	16.90	158.31	111.00
1	A	77	GLY	O-C-N	-16.71	104.29	123.51
2	B	31	GLN	OE1-CD-NE2	-16.70	105.89	122.60
2	B	2	GLU	O-C-N	-16.54	103.66	122.84
1	A	142	THR	CA-CB-CG2	16.45	138.47	110.50
2	B	50	GLU	CG-CD-OE1	16.45	156.23	118.40
2	B	1	GLU	OE1-CD-OE2	15.98	161.26	122.90
2	B	50	GLU	CG-CD-OE2	15.83	154.82	118.40
1	A	67	THR	CA-CB-CG2	15.59	137.00	110.50
1	A	138	LYS	CD-CE-NZ	15.54	161.62	111.90
1	A	101	ASN	OD1-CG-ND2	-15.26	107.34	122.60
1	A	142	THR	N-CA-C	15.04	153.12	111.00
2	B	63	ASP	CB-CG-OD1	14.87	152.59	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	74	ASN	O-C-N	-14.67	103.07	122.59
1	A	108	GLU	CB-CG-CD	14.66	137.53	112.60
1	A	96	VAL	CA-CB-CG1	14.52	135.08	110.40
2	B	59	ASP	CA-CB-CG	14.50	127.10	112.60
1	A	26	ARG	NE-CZ-NH2	14.45	132.21	119.20
1	A	96	VAL	CG1-CB-CG2	-14.37	79.18	110.80
1	A	30	ARG	NE-CZ-NH2	14.32	132.09	119.20
2	B	48	ASN	OD1-CG-ND2	-14.29	108.31	122.60
2	B	94	GLY	O-C-N	-14.29	110.64	123.36
1	A	58	ASP	CA-C-N	14.20	149.25	121.41
1	A	58	ASP	C-N-CA	14.20	149.25	121.41
1	A	94	PHE	O-C-N	-14.00	101.71	122.99
1	A	85	ARG	NE-CZ-NH2	13.72	131.55	119.20
1	A	49	ALA	CA-C-O	13.46	134.62	119.41
2	B	9	ASP	CA-CB-CG	13.33	125.93	112.60
2	B	106	ASN	CA-CB-CG	13.30	125.90	112.60
2	B	92	TRP	O-C-N	-13.19	109.41	123.26
1	A	13	GLY	CA-C-N	13.19	145.76	122.42
1	A	13	GLY	C-N-CA	13.19	145.76	122.42
2	B	18	GLN	CB-CG-CD	13.13	134.92	112.60
2	B	66	TYR	CB-CG-CD2	13.01	140.31	120.80
2	B	66	TYR	CB-CG-CD1	12.97	140.25	120.80
1	A	101	ASN	O-C-N	-12.88	105.46	122.59
2	B	66	TYR	CG-CD1-CE1	12.83	140.44	121.20
2	B	66	TYR	CG-CD2-CE2	12.73	140.30	121.20
1	A	141	VAL	CA-C-N	12.49	144.18	121.70
1	A	141	VAL	C-N-CA	12.49	144.18	121.70
1	A	140	THR	CA-CB-CG2	12.48	131.71	110.50
1	A	132	GLY	O-C-N	-12.42	114.05	123.61
1	A	96	VAL	CA-CB-CG2	12.37	131.43	110.40
1	A	102	GLN	O-C-N	-12.37	106.13	122.59
2	B	1	GLU	N-CA-CB	12.33	131.46	110.50
1	A	138	LYS	CB-CG-CD	11.97	138.83	111.30
1	A	67	THR	OG1-CB-CG2	-11.79	85.73	109.30
1	A	14	THR	O-C-N	-11.52	108.43	122.25
1	A	140	THR	OG1-CB-CG2	-11.43	86.44	109.30
2	B	50	GLU	CB-CG-CD	11.26	131.74	112.60
2	B	105	THR	O-C-N	-11.11	107.82	122.59
2	B	47	ASP	CA-CB-CG	10.90	123.50	112.60
1	A	52	TYR	O-C-N	-10.77	111.21	123.48
2	B	66	TYR	CD1-CE1-CZ	10.76	138.96	119.60
2	B	66	TYR	CZ-CE2-CD2	10.76	138.97	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	PHE	CA-C-N	10.62	137.81	122.09
1	A	94	PHE	C-N-CA	10.62	137.81	122.09
2	B	2	GLU	N-CA-C	10.60	126.14	110.46
1	A	30	ARG	CB-CG-CD	10.59	135.66	111.30
2	B	83	VAL	O-C-N	-10.57	109.36	122.57
1	A	115	GLY	O-C-N	-10.50	113.80	123.56
1	A	99	ASP	CB-CG-OD2	-10.49	94.26	118.40
2	B	1	GLU	CA-CB-CG	-10.46	93.19	114.10
2	B	16	ARG	CD-NE-CZ	10.28	138.79	124.40
1	A	140	THR	CA-CB-OG1	10.22	124.93	109.60
2	B	63	ASP	CB-CG-OD2	10.21	141.88	118.40
2	B	50	GLU	CA-CB-CG	10.10	134.30	114.10
1	A	99	ASP	CB-CG-OD1	10.08	141.58	118.40
1	A	93	PHE	O-C-N	-10.02	110.53	123.16
2	B	1	GLU	CA-C-N	10.00	139.96	122.67
2	B	1	GLU	C-N-CA	10.00	139.96	122.67
2	B	86	LYS	CD-CE-NZ	9.97	143.80	111.90
1	A	138	LYS	CG-CD-CE	9.81	133.87	111.30
1	A	114	GLY	O-C-N	-9.74	114.70	123.76
1	A	110	ARG	CB-CG-CD	9.72	133.67	111.30
1	A	50	GLU	O-C-N	-9.68	108.90	121.97
1	A	58	ASP	CA-C-O	9.65	130.96	119.28
2	B	2	GLU	CB-CG-CD	9.54	128.82	112.60
1	A	26	ARG	NE-CZ-NH1	-9.38	112.11	121.50
2	B	19	LEU	CD1-CG-CD2	-9.33	90.28	110.80
2	B	31	GLN	CB-CG-CD	9.32	128.45	112.60
1	A	16	LEU	CD1-CG-CD2	-9.26	90.44	110.80
1	A	70	ASP	CA-C-N	9.25	139.54	121.41
1	A	70	ASP	C-N-CA	9.25	139.54	121.41
2	B	19	LEU	CB-CG-CD2	9.24	138.42	110.70
2	B	2	GLU	N-CA-CB	-9.21	96.19	110.46
2	B	51	GLN	O-C-N	-9.17	105.31	122.09
2	B	84	PHE	CE1-CZ-CE2	-9.06	103.69	120.00
2	B	53	LYS	O-C-N	-9.02	112.34	123.44
1	A	141	VAL	CG1-CB-CG2	-8.99	91.02	110.80
1	A	15	GLN	CB-CG-CD	8.95	127.81	112.60
2	B	49	PHE	CA-CB-CG	8.92	122.72	113.80
1	A	67	THR	CA-CB-OG1	8.88	122.92	109.60
2	B	38	ARG	NH1-CZ-NH2	-8.87	107.77	119.30
1	A	85	ARG	NE-CZ-NH1	-8.81	112.69	121.50
1	A	120	PRO	O-C-N	-8.72	110.87	122.64
2	B	31	GLN	CA-CB-CG	8.70	131.50	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	THR	N-CA-CB	8.60	126.12	111.50
2	B	58	SER	CA-CB-OG	8.53	128.16	111.10
2	B	81	ASN	OD1-CG-ND2	-8.52	114.08	122.60
2	B	4	GLN	CB-CG-CD	8.51	127.07	112.60
2	B	2	GLU	CG-CD-OE1	8.42	137.77	118.40
2	B	74	ASN	CA-C-N	8.36	135.99	122.53
2	B	74	ASN	C-N-CA	8.36	135.99	122.53
1	A	64	ARG	NE-CZ-NH2	8.35	126.72	119.20
1	A	50	GLU	CA-CB-CG	8.33	130.77	114.10
2	B	43	LYS	CA-CB-CG	8.28	130.65	114.10
2	B	38	ARG	NE-CZ-NH2	8.26	126.64	119.20
1	A	102	GLN	OE1-CD-NE2	-8.25	114.35	122.60
1	A	30	ARG	CD-NE-CZ	8.23	135.92	124.40
1	A	134	THR	CA-C-N	8.15	128.66	121.82
1	A	134	THR	C-N-CA	8.15	128.66	121.82
1	A	68	GLY	N-CA-C	8.08	132.32	113.18
1	A	26	ARG	CD-NE-CZ	8.04	135.65	124.40
2	B	94	GLY	CA-C-N	7.98	132.07	120.82
2	B	94	GLY	C-N-CA	7.98	132.07	120.82
1	A	141	VAL	CA-CB-CG1	7.85	123.75	110.40
1	A	114	GLY	CA-C-N	7.84	134.19	121.17
1	A	114	GLY	C-N-CA	7.84	134.19	121.17
2	B	14	LYS	O-C-N	-7.79	113.86	123.36
1	A	22	VAL	CA-CB-CG2	7.70	123.48	110.40
2	B	62	ARG	NE-CZ-NH1	-7.66	113.84	121.50
2	B	16	ARG	NE-CZ-NH1	7.66	129.16	121.50
1	A	30	ARG	NH1-CZ-NH2	-7.65	109.35	119.30
1	A	14	THR	CA-C-N	7.64	134.73	123.12
1	A	14	THR	C-N-CA	7.64	134.73	123.12
1	A	24	THR	O-C-N	-7.57	114.50	123.28
1	A	43	ARG	NE-CZ-NH2	7.51	125.96	119.20
2	B	1	GLU	O-C-N	-7.48	111.03	123.00
1	A	83	VAL	O-C-N	-7.47	114.58	123.02
2	B	70	ARG	NE-CZ-NH2	7.41	125.87	119.20
2	B	104	GLN	OE1-CD-NE2	-7.36	115.24	122.60
1	A	101	ASN	CB-CG-ND2	7.32	127.37	116.40
1	A	17	ARG	CB-CG-CD	7.25	127.98	111.30
1	A	114	GLY	CA-C-O	-7.24	113.83	121.29
1	A	85	ARG	CD-NE-CZ	7.17	134.44	124.40
2	B	16	ARG	CG-CD-NE	7.17	127.78	112.00
1	A	141	VAL	CA-CB-CG2	7.17	122.59	110.40
1	A	122	GLU	CB-CG-CD	7.16	124.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	ASN	CA-CB-CG	7.06	119.66	112.60
1	A	52	TYR	CA-C-N	7.00	131.94	122.01
1	A	52	TYR	C-N-CA	7.00	131.94	122.01
1	A	102	GLN	CA-C-N	6.97	133.04	122.93
1	A	102	GLN	C-N-CA	6.97	133.04	122.93
2	B	103	GLN	CG-CD-NE2	6.96	126.85	116.40
1	A	11	GLY	CA-C-N	6.88	134.68	121.54
1	A	11	GLY	C-N-CA	6.88	134.68	121.54
2	B	18	GLN	CA-CB-CG	6.87	127.85	114.10
2	B	60	ASN	OD1-CG-ND2	-6.76	115.84	122.60
2	B	6	ARG	NE-CZ-NH2	6.71	125.24	119.20
1	A	49	ALA	CA-C-N	6.67	133.11	123.17
1	A	49	ALA	C-N-CA	6.67	133.11	123.17
1	A	101	ASN	CA-C-O	6.67	130.05	120.51
2	B	92	TRP	CA-C-N	6.67	134.48	121.41
2	B	92	TRP	C-N-CA	6.67	134.48	121.41
2	B	111	ASN	O-C-N	-6.66	115.80	123.33
1	A	77	GLY	CA-C-N	6.66	132.58	122.93
1	A	77	GLY	C-N-CA	6.66	132.58	122.93
2	B	51	GLN	CA-C-N	6.57	134.29	121.41
2	B	51	GLN	C-N-CA	6.57	134.29	121.41
1	A	140	THR	O-C-N	-6.54	115.76	123.22
1	A	81	LYS	CD-CE-NZ	6.53	132.78	111.90
2	B	64	LYS	CG-CD-CE	6.52	126.29	111.30
2	B	53	LYS	CA-C-N	6.43	131.60	122.72
2	B	53	LYS	C-N-CA	6.43	131.60	122.72
1	A	28	ILE	CA-CB-CG2	6.39	121.36	110.50
2	B	66	TYR	CE1-CZ-OH	6.39	139.06	119.90
2	B	66	TYR	OH-CZ-CE2	6.38	139.05	119.90
2	B	140	LEU	CD1-CG-CD2	-6.38	96.77	110.80
2	B	62	ARG	NE-CZ-NH2	6.37	124.93	119.20
2	B	18	GLN	O-C-N	-6.29	115.09	122.32
2	B	31	GLN	CG-CD-OE1	6.26	133.31	120.80
1	A	93	PHE	CA-C-N	6.25	131.95	122.95
1	A	93	PHE	C-N-CA	6.25	131.95	122.95
2	B	64	LYS	CD-CE-NZ	6.24	131.87	111.90
1	A	134	THR	O-C-N	-6.23	114.31	122.97
1	A	132	GLY	CA-C-N	6.20	130.67	120.94
1	A	132	GLY	C-N-CA	6.20	130.67	120.94
1	A	41	ASN	CB-CG-OD1	6.14	133.09	120.80
2	B	106	ASN	OD1-CG-ND2	-6.13	116.47	122.60
2	B	125	ASN	OD1-CG-ND2	-6.13	116.47	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	90	GLY	O-C-N	-6.10	117.86	123.78
1	A	57	LYS	O-C-N	-6.10	115.66	122.12
2	B	2	GLU	CA-C-N	6.09	131.96	123.07
2	B	2	GLU	C-N-CA	6.09	131.96	123.07
1	A	97	MET	O-C-N	-6.08	115.54	123.02
1	A	83	VAL	CA-C-N	6.05	131.53	123.00
1	A	83	VAL	C-N-CA	6.05	131.53	123.00
1	A	47	GLY	O-C-N	-6.01	114.89	122.70
2	B	56	LEU	CB-CG-CD1	6.00	128.71	110.70
2	B	54	PHE	CA-CB-CG	6.00	119.80	113.80
2	B	67	VAL	O-C-N	-5.99	116.60	123.00
1	A	68	GLY	CA-C-O	-5.97	110.19	120.57
2	B	86	LYS	CG-CD-CE	5.96	125.00	111.30
1	A	83	VAL	N-CA-C	5.91	118.70	108.90
1	A	22	VAL	CG1-CB-CG2	-5.87	97.88	110.80
1	A	12	SER	N-CA-C	5.85	123.25	110.80
1	A	10	GLY	O-C-N	-5.85	115.10	122.70
2	B	105	THR	CA-C-N	5.84	132.69	121.54
2	B	105	THR	C-N-CA	5.84	132.69	121.54
2	B	109	PRO	O-C-N	-5.81	114.80	122.64
2	B	98	ILE	CB-CG1-CD1	5.77	125.92	113.80
2	B	73	ASP	OD1-CG-OD2	-5.76	109.08	122.90
2	B	39	GLN	OE1-CD-NE2	-5.72	116.88	122.60
2	B	62	ARG	CB-CG-CD	5.71	124.43	111.30
1	A	15	GLN	CA-CB-CG	5.67	125.45	114.10
1	A	120	PRO	CA-C-N	5.67	130.67	122.16
1	A	120	PRO	C-N-CA	5.67	130.67	122.16
2	B	99	TYR	O-C-N	-5.64	114.92	122.14
1	A	11	GLY	CA-C-O	-5.64	110.76	120.57
1	A	16	LEU	CA-CB-CG	5.62	135.98	116.30
1	A	82	GLY	CA-C-N	5.61	130.65	122.69
1	A	82	GLY	C-N-CA	5.61	130.65	122.69
1	A	115	GLY	CA-C-N	5.60	132.24	121.54
1	A	115	GLY	C-N-CA	5.60	132.24	121.54
2	B	103	GLN	CB-CG-CD	5.59	122.11	112.60
1	A	51	ARG	O-C-N	-5.53	115.23	122.59
1	A	108	GLU	CG-CD-OE2	5.53	131.12	118.40
2	B	107	THR	CA-C-N	5.52	126.07	120.38
2	B	107	THR	C-N-CA	5.52	126.07	120.38
1	A	23	ALA	O-C-N	-5.50	116.48	123.24
1	A	24	THR	CA-C-N	5.49	127.95	122.30
1	A	24	THR	C-N-CA	5.49	127.95	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	45	ASP	OD1-CG-OD2	-5.46	109.79	122.90
2	B	140	LEU	O-C-N	-5.45	116.86	123.29
1	A	64	ARG	CB-CG-CD	5.44	123.81	111.30
1	A	115	GLY	N-CA-C	5.42	120.90	111.14
1	A	46	ASP	CB-CA-C	-5.34	109.96	117.23
1	A	67	THR	O-C-N	-5.31	114.82	122.36
2	B	36	ASN	CB-CG-OD1	5.22	131.24	120.80
1	A	23	ALA	CA-C-N	5.21	131.40	121.87
1	A	23	ALA	C-N-CA	5.21	131.40	121.87
1	A	75	VAL	CA-CB-CG2	5.20	119.24	110.40
2	B	38	ARG	CD-NE-CZ	5.18	131.66	124.40
1	A	72	TRP	O-C-N	-5.17	116.85	122.84
2	B	25	ILE	O-C-N	-5.15	116.13	122.57
1	A	121	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	A	41	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	108	GLU	OE1-CD-OE2	-5.08	110.70	122.90
2	B	48	ASN	CB-CG-OD1	5.07	130.94	120.80
2	B	83	VAL	CA-C-N	5.05	130.12	123.00
2	B	83	VAL	C-N-CA	5.05	130.12	123.00
2	B	36	ASN	CB-CG-ND2	5.03	123.95	116.40
2	B	56	LEU	CA-CB-CG	5.03	133.90	116.30
1	A	50	GLU	CA-C-O	5.01	127.38	121.17
2	B	6	ARG	NE-CZ-NH1	-5.00	116.50	121.50

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	67	THR	CB
1	A	140	THR	CB
1	A	142	THR	CB,CA
2	B	1	GLU	CA

There are no planarity outliers.

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	1075	986	1003	100
2	B	1088	1030	1037	68
All	All	2163	2016	2040	163

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:19:LEU:CD1	2:B:19:LEU:CB	1.58	1.80
2:B:4:GLN:NE2	2:B:4:GLN:CG	1.48	1.69
1:A:141:VAL:CG1	1:A:141:VAL:CA	1.41	1.97
1:A:138:LYS:NZ	1:A:138:LYS:CD	1.39	1.82
1:A:141:VAL:CA	1:A:141:VAL:CG2	1.38	1.98
1:A:141:VAL:C	1:A:142:THR:CA	1.38	1.96
2:B:66:TYR:CZ	2:B:66:TYR:CD2	1.35	2.14
2:B:66:TYR:CZ	2:B:66:TYR:CD1	1.34	2.13
2:B:66:TYR:CG	2:B:66:TYR:CE1	1.33	2.16
2:B:66:TYR:CG	2:B:66:TYR:CE2	1.31	2.16
1:A:142:THR:OXT	2:B:1:GLU:N	1.30	1.64
2:B:4:GLN:CG	2:B:4:GLN:OE1	1.29	1.81
2:B:63:ASP:OD2	2:B:63:ASP:CB	1.26	1.83
2:B:19:LEU:CB	2:B:19:LEU:CD2	1.25	1.98
1:A:141:VAL:C	1:A:142:THR:OG1	1.24	1.80
1:A:96:VAL:CG2	1:A:96:VAL:CA	1.24	2.16
1:A:141:VAL:CA	1:A:142:THR:N	1.22	2.02
1:A:140:THR:CG2	1:A:140:THR:CA	1.20	2.19
1:A:67:THR:CG2	1:A:67:THR:CA	1.19	2.18
2:B:50:GLU:OE2	2:B:50:GLU:CG	1.17	1.91
1:A:67:THR:CA	1:A:67:THR:OG1	1.17	1.91
2:B:66:TYR:CD1	2:B:66:TYR:CB	1.16	2.29
2:B:50:GLU:CG	2:B:50:GLU:OE1	1.15	1.93
2:B:66:TYR:CD2	2:B:66:TYR:CB	1.14	2.29
1:A:96:VAL:CA	1:A:96:VAL:CG1	1.12	2.26
1:A:67:THR:CG2	1:A:67:THR:HB	1.07	1.61
2:B:63:ASP:CB	2:B:63:ASP:OD1	1.06	2.03
1:A:142:THR:OXT	2:B:1:GLU:OE1	1.05	1.72
1:A:140:THR:CG2	1:A:140:THR:HB	1.04	1.62
1:A:140:THR:CA	1:A:140:THR:OG1	1.03	2.05
1:A:96:VAL:CG2	1:A:96:VAL:HB	1.02	1.66
1:A:141:VAL:CG1	1:A:141:VAL:HB	1.02	1.56
2:B:66:TYR:CE2	2:B:66:TYR:OH	1.01	2.13
1:A:140:THR:CB	1:A:140:THR:HG22	0.99	1.53

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:67:THR:CB	1:A:67:THR:HG23	0.99	1.55
1:A:140:THR:CB	1:A:140:THR:HG23	0.99	1.53
2:B:66:TYR:CE1	2:B:66:TYR:OH	0.99	2.13
1:A:67:THR:CB	1:A:67:THR:HG21	0.98	1.55
1:A:96:VAL:CB	1:A:96:VAL:HG12	0.98	1.55
1:A:96:VAL:CB	1:A:96:VAL:HG13	0.98	1.55
1:A:141:VAL:CA	1:A:141:VAL:O	0.98	2.02
2:B:63:ASP:OD1	2:B:63:ASP:CG	0.98	0.73
1:A:67:THR:CB	1:A:67:THR:HG22	0.97	1.55
1:A:96:VAL:CB	1:A:96:VAL:HG11	0.96	1.55
1:A:142:THR:HG22	2:B:1:GLU:N	0.96	1.71
1:A:140:THR:CB	1:A:140:THR:HG21	0.96	1.53
1:A:141:VAL:CB	1:A:141:VAL:HG23	0.95	1.50
1:A:96:VAL:CG1	1:A:96:VAL:HB	0.95	1.70
1:A:96:VAL:CB	1:A:96:VAL:HG23	0.94	1.49
1:A:141:VAL:CB	1:A:141:VAL:HG11	0.94	1.48
1:A:96:VAL:CB	1:A:96:VAL:HG22	0.94	1.49
1:A:101:ASN:O	1:A:102:GLN:HB2	0.94	1.59
1:A:141:VAL:CG2	1:A:141:VAL:HB	0.93	1.59
1:A:141:VAL:CB	1:A:141:VAL:HG21	0.93	1.50
1:A:96:VAL:CB	1:A:96:VAL:HG21	0.93	1.49
2:B:19:LEU:CG	2:B:19:LEU:HD22	0.93	1.46
1:A:96:VAL:CG1	1:A:96:VAL:CB	0.92	0.93
1:A:141:VAL:CB	1:A:141:VAL:HG22	0.92	1.50
1:A:141:VAL:CB	1:A:141:VAL:HG13	0.92	1.48
1:A:67:THR:CG2	1:A:67:THR:CB	0.92	0.93
2:B:66:TYR:CD2	2:B:66:TYR:CG	0.92	0.92
2:B:66:TYR:CD1	2:B:66:TYR:CG	0.92	0.92
1:A:141:VAL:C	1:A:142:THR:HA	0.91	1.39
2:B:19:LEU:CG	2:B:19:LEU:HD21	0.91	1.46
1:A:140:THR:CG2	1:A:140:THR:CB	0.90	0.90
1:A:141:VAL:CB	1:A:141:VAL:HG12	0.90	1.48
2:B:66:TYR:CZ	2:B:66:TYR:CE2	0.90	0.90
2:B:66:TYR:CZ	2:B:66:TYR:CE1	0.90	0.90
2:B:19:LEU:CD2	2:B:19:LEU:HG	0.89	1.47
2:B:19:LEU:CG	2:B:19:LEU:HD23	0.89	1.46
2:B:19:LEU:CG	2:B:19:LEU:HD11	0.89	1.42
1:A:50:GLU:O	1:A:51:ARG:HB2	0.88	1.66
2:B:19:LEU:CG	2:B:19:LEU:HD13	0.88	1.42
2:B:19:LEU:CD1	2:B:19:LEU:HG	0.86	1.60
1:A:141:VAL:CG2	1:A:141:VAL:CB	0.86	0.86
2:B:19:LEU:CG	2:B:19:LEU:HD12	0.85	1.42

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:96:VAL:CG2	1:A:96:VAL:CB	0.85	0.85
2:B:19:LEU:CD1	2:B:19:LEU:HB3	0.84	2.02
2:B:50:GLU:OE1	2:B:50:GLU:CD	0.83	0.60
1:A:141:VAL:CG1	1:A:141:VAL:CB	0.83	0.83
1:A:141:VAL:CG1	1:A:141:VAL:C	0.82	2.51
2:B:50:GLU:OE2	2:B:50:GLU:CD	0.82	0.58
1:A:140:THR:OG1	1:A:140:THR:CB	0.81	0.81
2:B:19:LEU:CD2	2:B:19:LEU:CG	0.81	0.81
2:B:4:GLN:OE1	2:B:4:GLN:CD	0.80	0.60
1:A:138:LYS:NZ	1:A:138:LYS:HE3	0.80	1.18
2:B:63:ASP:OD2	2:B:63:ASP:CG	0.79	0.55
1:A:138:LYS:NZ	1:A:138:LYS:HE2	0.78	1.18
1:A:101:ASN:O	1:A:102:GLN:CB	0.78	2.14
1:A:67:THR:OG1	1:A:67:THR:CB	0.77	0.73
1:A:40:MET:HE3	1:A:67:THR:HG21	0.77	1.56
1:A:67:THR:OG1	1:A:67:THR:HB	0.76	1.56
2:B:19:LEU:CD1	2:B:19:LEU:CG	0.76	0.76
2:B:66:TYR:CG	2:B:66:TYR:HD1	0.75	1.51
2:B:66:TYR:CZ	2:B:66:TYR:HE1	0.74	1.50
2:B:66:TYR:CG	2:B:66:TYR:HD2	0.74	1.51
2:B:66:TYR:CZ	2:B:66:TYR:HE2	0.73	1.50
1:A:142:THR:CG2	2:B:1:GLU:N	0.71	2.47
2:B:63:ASP:OD2	2:B:63:ASP:OD1	0.70	0.71
2:B:105:THR:O	2:B:106:ASN:HB3	0.69	1.86
1:A:94:PHE:CD1	1:A:94:PHE:O	0.67	2.48
1:A:138:LYS:NZ	1:A:138:LYS:CE	0.66	0.58
1:A:50:GLU:O	1:A:51:ARG:CB	0.65	2.30
1:A:141:VAL:C	1:A:141:VAL:HG12	0.65	2.12
2:B:2:GLU:CD	2:B:2:GLU:HG2	0.65	1.46
1:A:141:VAL:C	1:A:141:VAL:O	0.64	0.69
1:A:36:PHE:CE2	1:A:87:GLY:HA2	0.64	2.28
1:A:140:THR:CB	1:A:140:THR:HG1	0.63	1.35
1:A:49:ALA:HB1	1:A:83:VAL:HG13	0.60	1.71
1:A:141:VAL:C	1:A:142:THR:N	0.60	0.71
2:B:4:GLN:NE2	2:B:4:GLN:OE1	0.60	0.46
1:A:69:GLY:O	1:A:70:ASP:HB3	0.59	1.95
1:A:67:THR:CB	1:A:67:THR:HG1	0.58	1.28
1:A:2:ALA:HB1	1:A:133:THR:OG1	0.58	1.98
1:A:142:THR:CG2	2:B:1:GLU:OE1	0.57	2.47
1:A:39:TRP:O	1:A:113:VAL:HA	0.56	2.00
1:A:141:VAL:CG2	1:A:141:VAL:N	0.56	2.66
1:A:61:HIS:CE1	1:A:105:ALA:HB3	0.54	2.37

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:96:VAL:CG2	1:A:96:VAL:C	0.54	2.80
2:B:4:GLN:CD	2:B:4:GLN:HE22	0.54	1.19
1:A:54:VAL:HG22	1:A:63:LEU:O	0.53	2.04
2:B:4:GLN:NE2	2:B:4:GLN:CD	0.53	0.50
2:B:4:GLN:CD	2:B:4:GLN:HE21	0.53	1.19
1:A:69:GLY:HA3	1:A:72:TRP:CD1	0.53	2.38
1:A:36:PHE:CD2	1:A:87:GLY:HA2	0.52	2.39
1:A:11:GLY:O	1:A:12:SER:HB2	0.52	2.03
1:A:35:GLY:C	1:A:84:SER:HB3	0.52	2.29
2:B:2:GLU:CD	2:B:2:GLU:HG3	0.51	1.46
1:A:138:LYS:CE	1:A:138:LYS:HZ2	0.51	1.22
1:A:138:LYS:CE	1:A:138:LYS:HZ3	0.51	1.22
2:B:106:ASN:O	2:B:106:ASN:CG	0.50	2.49
1:A:40:MET:SD	1:A:113:VAL:HB	0.50	2.46
1:A:138:LYS:CE	1:A:138:LYS:HZ1	0.50	1.21
2:B:21:ASP:O	2:B:22:ALA:C	0.49	2.53
1:A:67:THR:OG1	1:A:67:THR:C	0.49	2.53
2:B:50:GLU:OE2	2:B:50:GLU:OE1	0.49	0.49
2:B:16:ARG:HG2	2:B:65:LEU:HD22	0.48	1.86
1:A:49:ALA:HB1	1:A:83:VAL:CG1	0.48	2.37
1:A:51:ARG:NH1	1:A:99:ASP:OD1	0.47	2.47
1:A:67:THR:CG2	1:A:67:THR:C	0.47	2.83
2:B:19:LEU:HD13	2:B:19:LEU:HB3	0.47	1.76
2:B:4:GLN:NE2	2:B:4:GLN:CB	0.47	2.51
2:B:83:VAL:HG11	2:B:121:TRP:CZ3	0.47	2.45
1:A:65:VAL:HA	1:A:98:ALA:HA	0.45	1.89
1:A:112:SER:HA	1:A:135:GLY:O	0.45	2.11
1:A:6:LEU:HD13	1:A:137:THR:OG1	0.45	2.12
2:B:80:ASP:HB3	2:B:83:VAL:O	0.45	2.12
2:B:70:ARG:HG3	2:B:71:PRO:HD2	0.45	1.88
2:B:77:TRP:CE2	2:B:86:LYS:HB3	0.44	2.47
2:B:2:GLU:CD	2:B:2:GLU:OE1	0.44	0.69
1:A:39:TRP:HB3	1:A:81:LYS:O	0.44	2.12
1:A:48:ARG:NE	1:A:48:ARG:HA	0.44	2.27
1:A:94:PHE:CD1	1:A:94:PHE:C	0.43	2.92
1:A:67:THR:CA	1:A:67:THR:HG1	0.42	1.99
2:B:106:ASN:ND2	2:B:106:ASN:C	0.42	2.70
2:B:2:GLU:CD	2:B:2:GLU:CG	0.41	0.87
2:B:22:ALA:HB1	2:B:99:TYR:HD2	0.41	1.75
1:A:72:TRP:CD2	1:A:85:ARG:HB3	0.41	2.50
2:B:48:ASN:HB3	2:B:55:PHE:O	0.41	2.15
1:A:94:PHE:CD2	1:A:94:PHE:N	0.41	2.87

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:74:PRO:HA	1:A:83:VAL:HG12	0.40	1.93
1:A:38:VAL:O	1:A:82:GLY:HA3	0.40	2.16
1:A:27:ILE:O	1:A:91:GLN:HA	0.40	2.16

6.3 Torsion angles [i](#)

6.3.1 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 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	140/142 (99%)	98 (70%)	34 (24%)	8 (6%)	2	21
2	B	141/143 (99%)	112 (79%)	21 (15%)	8 (6%)	2	21
All	All	281/285 (99%)	210 (75%)	55 (20%)	16 (6%)	2	21

All 16 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	12	SER
1	A	51	ARG
1	A	60	ARG
1	A	86	PRO
1	A	102	GLN
1	A	120	PRO
1	A	124	ASN
1	A	125	LYS
2	B	19	LEU
2	B	22	ALA
2	B	26	GLY
2	B	61	ASN
2	B	72	MET
2	B	93	GLY
2	B	103	GLN
2	B	108	PRO

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	111/111 (100%)	81 (73%)	30 (27%)	2	21
2	B	117/117 (100%)	89 (76%)	28 (24%)	2	26
All	All	228/228 (100%)	170 (75%)	58 (25%)	2	24

All 58 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	1	SER
1	A	4	LEU
1	A	9	ARG
1	A	12	SER
1	A	16	LEU
1	A	22	VAL
1	A	28	ILE
1	A	33	HIS
1	A	34	THR
1	A	38	VAL
1	A	42	GLU
1	A	43	ARG
1	A	50	GLU
1	A	51	ARG
1	A	52	TYR
1	A	54	VAL
1	A	75	VAL
1	A	78	GLU
1	A	83	VAL
1	A	85	ARG
1	A	99	ASP
1	A	103	ASP
1	A	108	GLU
1	A	113	VAL
1	A	124	ASN
1	A	133	THR
1	A	134	THR
1	A	136	THR

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Mol	Chain	Res	Type
1	A	139	LEU
1	A	142	THR
2	B	1	GLU
2	B	6	ARG
2	B	9	ASP
2	B	10	LEU
2	B	20	THR
2	B	25	ILE
2	B	31	GLN
2	B	38	ARG
2	B	48	ASN
2	B	50	GLU
2	B	56	LEU
2	B	58	SER
2	B	69	ILE
2	B	78	THR
2	B	81	ASN
2	B	87	ASN
2	B	95	THR
2	B	106	ASN
2	B	107	THR
2	B	114	LEU
2	B	115	THR
2	B	117	THR
2	B	123	LYS
2	B	127	GLN
2	B	134	THR
2	B	137	THR
2	B	142	VAL
2	B	143	THR

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 [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	31
2	B	13

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	97:MET	C	98:ALA	N	1.20
1	A	24:THR	C	25:GLY	N	1.19
1	A	83:VAL	C	84:SER	N	1.19
1	A	88:GLN	C	89:GLU	N	1.19
1	A	134:THR	C	135:GLY	N	1.19
1	B	4:GLN	C	5:VAL	N	1.19
1	B	109:PRO	C	110:GLY	N	1.19
1	A	47:GLY	C	48:ARG	N	1.18
1	A	51:ARG	C	52:TYR	N	1.18
1	A	114:GLY	C	115:GLY	N	1.18
1	A	115:GLY	C	116:ALA	N	1.18
1	A	78:GLU	C	79:GLY	N	1.17
1	A	132:GLY	C	133:THR	N	1.17
1	A	10:GLY	C	11:GLY	N	1.16
1	A	120:PRO	C	121:GLN	N	1.16
1	A	140:THR	C	141:VAL	N	1.16
1	B	14:LYS	C	15:THR	N	1.16
1	B	18:GLN	C	19:LEU	N	1.16
1	B	53:LYS	C	54:PHE	N	1.16

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	12:SER	C	13:GLY	N	1.15
1	A	69:GLY	C	70:ASP	N	1.15
1	B	92:TRP	C	93:GLY	N	1.15
1	A	67:THR	C	68:GLY	N	1.13
1	A	52:TYR	C	53:VAL	N	1.12
1	B	94:GLY	C	95:THR	N	1.12
1	A	14:THR	C	15:GLN	N	1.11
1	A	93:PHE	C	94:PHE	N	1.11
1	B	83:VAL	C	84:PHE	N	1.11
1	A	68:GLY	C	69:GLY	N	1.10
1	B	51:GLN	C	52:GLY	N	1.09
1	A	50:GLU	C	51:ARG	N	1.08
1	A	102:GLN	C	103:ASP	N	1.07
1	B	74:ASN	C	75:SER	N	1.07
1	B	105:THR	C	106:ASN	N	1.06
1	A	77:GLY	C	78:GLU	N	1.04
1	A	94:PHE	C	95:ASP	N	1.04
1	A	101:ASN	C	102:GLN	N	1.03
1	B	2:GLU	C	3:CYS	N	1.03
1	A	13:GLY	C	14:THR	N	0.97
1	A	70:ASP	C	71:GLY	N	0.97
1	A	58:ASP	C	59:GLY	N	0.96
1	A	49:ALA	C	50:GLU	N	0.88
1	B	1:GLU	C	2:GLU	N	0.83
1	A	141:VAL	C	142:THR	N	0.71

7 Chemical shift validation

No chemical shift data were provided