Full wwPDB NMR Structure Validation Report (i)

Jun 16, 2024 – 06:39 AM EDT

PDB ID	:	2IXQ
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 (i) 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 (i)) were used in the production of this report:

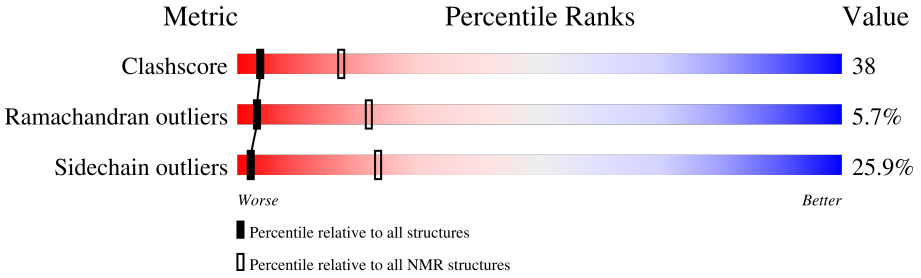
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	142	17% 45% 30% 8%
2	B	143	31% 45% 21% •

2 Ensemble composition and analysis (i)

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

3 Entry composition (i)

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
			Total	C	H	N	O	S	
1	A	142	2061	653	986	205	213	4	0

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
			Total	C	H	N	O	S	
2	B	143	2118	677	1030	188	220	3	0

There are 20 discrepancies between the modelled and reference sequences:

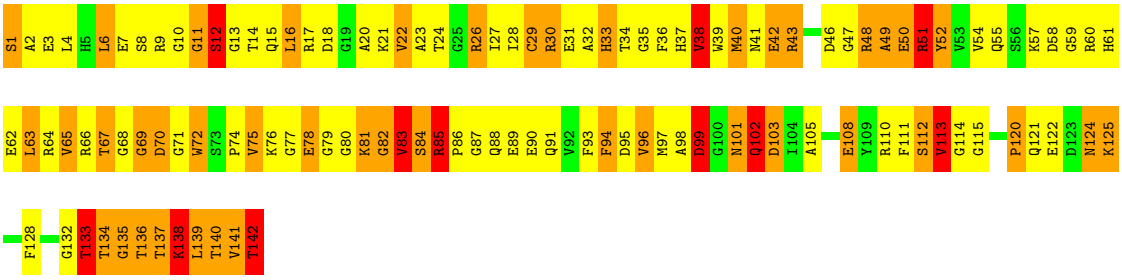
Chain	Residue	Modelled	Actual	Comment	Reference
B	124	ASP	-	expression tag	UNP Q57254
B	125	ASN	-	expression tag	UNP Q57254
B	126	LYS	-	expression tag	UNP Q57254
B	127	GLN	-	expression tag	UNP Q57254
B	128	GLY	-	expression tag	UNP Q57254
B	129	PHE	-	expression tag	UNP Q57254
B	130	THR	-	expression tag	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 (i)

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.

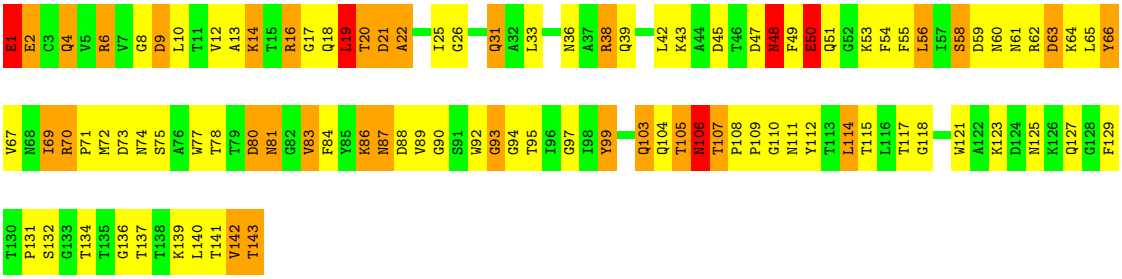
- Molecule 1: Protein AfaD

Chain A: 17% 45% 30% 8%



- Molecule 2: Afimbrial adhesin AFA-III

Chain B: 31% 45% 21% •



5 Refinement protocol and experimental data overview (i)

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	8.04	320/1094 (29.3%)	3.63	119/1471 (8.1%)
2	B	8.41	220/1109 (19.8%)	4.31	113/1510 (7.5%)
All	All	8.23	540/2203 (24.5%)	3.99	232/2981 (7.8%)

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	CG-CD	-77.45	0.35	1.51
2	B	2	GLU	CD-OE2	-68.63	0.50	1.25
2	B	50	GLU	CD-OE2	-60.67	0.58	1.25
2	B	1	GLU	CB-CG	-59.42	0.39	1.52
2	B	50	GLU	CD-OE1	-58.85	0.60	1.25
2	B	1	GLU	CA-CB	-57.52	0.27	1.53
1	A	142	THR	C-O	-54.06	0.20	1.23
2	B	2	GLU	CD-OE1	-50.95	0.69	1.25
2	B	2	GLU	CB-CG	-50.30	0.56	1.52
2	B	1	GLU	CD-OE2	-49.87	0.70	1.25
2	B	2	GLU	CG-CD	-42.88	0.87	1.51
1	A	108	GLU	CD-OE1	-42.70	0.78	1.25
2	B	58	SER	CB-OG	-40.56	0.89	1.42
1	A	142	THR	CA-CB	-40.29	0.48	1.53
1	A	142	THR	CB-OG1	-39.37	0.64	1.43
2	B	1	GLU	CD-OE1	-38.11	0.83	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	66	TYR	CE1-CZ	-37.00	0.90	1.38
2	B	66	TYR	CE2-CZ	-36.87	0.90	1.38
1	A	138	LYS	CE-NZ	-36.15	0.58	1.49
2	B	66	TYR	CG-CD2	-35.92	0.92	1.39
2	B	66	TYR	CG-CD1	-35.83	0.92	1.39
2	B	1	GLU	C-O	-35.52	0.55	1.23
1	A	13	GLY	C-O	-35.20	0.67	1.23
1	A	67	THR	CB-OG1	-34.87	0.73	1.43
1	A	142	THR	C-OXT	-34.06	0.58	1.23
1	A	12	SER	CB-OG	-33.38	0.98	1.42
1	A	58	ASP	C-O	-33.23	0.60	1.23
2	B	4	GLN	CD-NE2	-33.08	0.50	1.32
1	A	141	VAL	CB-CG1	-32.86	0.83	1.52
1	A	96	VAL	CB-CG2	-32.12	0.85	1.52
1	A	141	VAL	CB-CG2	-31.54	0.86	1.52
2	B	16	ARG	CZ-NH1	-31.26	0.92	1.33
1	A	140	THR	CB-OG1	-30.80	0.81	1.43
1	A	50	GLU	CG-CD	-30.78	1.05	1.51
2	B	75	SER	CB-OG	-30.76	1.02	1.42
2	B	63	ASP	CG-OD2	-30.38	0.55	1.25
1	A	99	ASP	CG-OD2	-30.12	0.56	1.25
1	A	108	GLU	CD-OE2	-30.02	0.92	1.25
1	A	30	ARG	CZ-NH1	-29.09	0.95	1.33
2	B	4	GLN	CD-OE1	-29.06	0.60	1.24
1	A	96	VAL	CB-CG1	-28.43	0.93	1.52
1	A	141	VAL	C-O	-28.42	0.69	1.23
1	A	99	ASP	CB-CG	-28.28	0.92	1.51
1	A	50	GLU	CD-OE1	-27.84	0.95	1.25
2	B	2	GLU	CA-CB	-27.54	0.93	1.53
1	A	141	VAL	C-N	-27.34	0.71	1.34
1	A	42	GLU	CD-OE1	-27.11	0.95	1.25
1	A	26	ARG	CZ-NH1	-27.04	0.97	1.33
1	A	85	ARG	CZ-NH1	-26.95	0.98	1.33
1	A	50	GLU	CB-CG	-26.92	1.01	1.52
1	A	12	SER	CA-CB	-26.36	1.13	1.52
1	A	122	GLU	CD-OE2	-26.22	0.96	1.25
2	B	1	GLU	N-CA	-26.02	0.94	1.46
1	A	142	THR	CA-C	-25.89	0.85	1.52
1	A	70	ASP	C-O	-25.81	0.74	1.23
1	A	50	GLU	CD-OE2	-25.76	0.97	1.25
1	A	78	GLU	CD-OE1	-24.88	0.98	1.25
2	B	2	GLU	N-CA	-24.45	0.97	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	GLY	C-O	-24.27	0.84	1.23
2	B	16	ARG	CZ-NH2	-24.02	1.01	1.33
1	A	78	GLU	CD-OE2	-23.97	0.99	1.25
1	A	68	GLY	CA-C	-23.00	1.15	1.51
2	B	63	ASP	CG-OD1	-22.73	0.73	1.25
1	A	114	GLY	C-O	-22.22	0.88	1.23
2	B	1	GLU	C-N	-22.12	0.83	1.34
2	B	48	ASN	CG-ND2	-22.03	0.77	1.32
1	A	69	GLY	N-CA	-21.99	1.13	1.46
1	A	49	ALA	C-O	-21.27	0.82	1.23
1	A	64	ARG	CZ-NH1	-20.84	1.05	1.33
2	B	1	GLU	CA-C	-20.65	0.99	1.52
1	A	94	PHE	C-O	-20.63	0.84	1.23
1	A	42	GLU	CD-OE2	-20.52	1.03	1.25
2	B	19	LEU	CG-CD1	-20.40	0.76	1.51
2	B	48	ASN	CG-OD1	-20.25	0.79	1.24
1	A	58	ASP	C-N	-20.23	0.96	1.33
1	A	11	GLY	C-O	-20.18	0.91	1.23
1	A	70	ASP	C-N	-20.01	0.97	1.33
1	A	49	ALA	C-N	-20.00	0.88	1.34
1	A	142	THR	CB-CG2	-19.86	0.86	1.52
2	B	74	ASN	C-O	-19.77	0.85	1.23
1	A	90	GLU	CD-OE2	-19.73	1.03	1.25
1	A	77	GLY	C-O	-19.26	0.92	1.23
2	B	87	ASN	CG-OD1	-19.12	0.81	1.24
1	A	108	GLU	CG-CD	-19.12	1.23	1.51
2	B	19	LEU	CG-CD2	-18.98	0.81	1.51
2	B	50	GLU	CB-CG	-18.90	1.16	1.52
2	B	87	ASN	CB-CG	-18.80	1.07	1.51
2	B	6	ARG	CZ-NH1	-18.69	1.08	1.33
1	A	140	THR	CB-CG2	-18.62	0.91	1.52
1	A	122	GLU	CD-OE1	-18.37	1.05	1.25
1	A	22	VAL	CB-CG1	-18.36	1.14	1.52
2	B	51	GLN	C-O	-18.31	0.88	1.23
1	A	115	GLY	C-O	-18.19	0.94	1.23
1	A	89	GLU	CD-OE2	-18.12	1.05	1.25
2	B	38	ARG	CZ-NH1	-18.10	1.09	1.33
2	B	16	ARG	CD-NE	-18.08	1.15	1.46
1	A	67	THR	CB-CG2	-18.00	0.93	1.52
2	B	70	ARG	CZ-NH1	-17.56	1.10	1.33
1	A	89	GLU	CD-OE1	-17.52	1.06	1.25
1	A	14	THR	C-O	-17.34	0.90	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	SER	CB-OG	-17.31	1.19	1.42
2	B	38	ARG	CZ-NH2	-17.26	1.10	1.33
2	B	92	TRP	C-O	-17.20	0.90	1.23
2	B	106	ASN	CG-OD1	-17.16	0.86	1.24
2	B	2	GLU	C-O	-17.12	0.90	1.23
1	A	43	ARG	CZ-NH1	-17.04	1.10	1.33
2	B	36	ASN	CG-ND2	-16.98	0.90	1.32
2	B	56	LEU	CG-CD2	-16.82	0.89	1.51
2	B	48	ASN	CB-CG	-16.64	1.12	1.51
1	A	17	ARG	CZ-NH1	-16.40	1.11	1.33
1	A	41	ASN	CG-ND2	-16.34	0.92	1.32
2	B	36	ASN	CG-OD1	-16.12	0.88	1.24
2	B	94	GLY	C-O	-16.02	0.98	1.23
2	B	105	THR	C-O	-15.92	0.93	1.23
1	A	13	GLY	C-N	-15.90	0.97	1.34
1	A	69	GLY	CA-C	-15.90	1.26	1.51
2	B	112	TYR	CE1-CZ	-15.76	1.18	1.38
2	B	81	ASN	CG-OD1	-15.71	0.89	1.24
2	B	142	VAL	CB-CG1	-15.66	1.20	1.52
2	B	31	GLN	CD-NE2	-15.56	0.94	1.32
1	A	102	GLN	C-O	-15.54	0.93	1.23
2	B	64	LYS	CD-CE	-15.52	1.12	1.51
1	A	132	GLY	C-O	-15.48	0.98	1.23
1	A	30	ARG	CZ-NH2	-15.45	1.12	1.33
1	A	82	GLY	C-O	-15.40	0.99	1.23
1	A	79	GLY	C-O	-15.36	0.99	1.23
2	B	18	GLN	CB-CG	-15.33	1.11	1.52
1	A	22	VAL	CB-CG2	-15.27	1.20	1.52
1	A	99	ASP	CG-OD1	-15.22	0.90	1.25
1	A	90	GLU	CD-OE1	-15.21	1.08	1.25
2	B	112	TYR	CG-CD2	-15.21	1.19	1.39
2	B	87	ASN	CG-ND2	-15.18	0.94	1.32
1	A	93	PHE	C-O	-15.15	0.94	1.23
1	A	38	VAL	CB-CG2	-15.04	1.21	1.52
1	A	7	GLU	CD-OE2	-14.98	1.09	1.25
1	A	12	SER	C-O	-14.78	0.95	1.23
1	A	101	ASN	C-O	-14.60	0.95	1.23
2	B	84	PHE	CG-CD1	-14.38	1.17	1.38
2	B	106	ASN	CG-ND2	-14.29	0.97	1.32
1	A	138	LYS	CG-CD	-14.26	1.03	1.52
2	B	106	ASN	CB-CG	-14.25	1.18	1.51
2	B	83	VAL	C-O	-14.19	0.96	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	142	VAL	CB-CG2	-14.18	1.23	1.52
2	B	103	GLN	CD-OE1	-14.18	0.92	1.24
1	A	83	VAL	C-O	-14.07	0.96	1.23
2	B	86	LYS	CD-CE	-13.96	1.16	1.51
2	B	4	GLN	CB-CG	-13.96	1.14	1.52
1	A	38	VAL	CB-CG1	-13.95	1.23	1.52
1	A	52	TYR	C-O	-13.90	0.96	1.23
1	A	103	ASP	CG-OD1	-13.85	0.93	1.25
1	A	67	THR	C-O	-13.81	0.97	1.23
2	B	38	ARG	CD-NE	-13.68	1.23	1.46
1	A	50	GLU	C-O	-13.62	0.97	1.23
2	B	62	ARG	CZ-NH1	-13.59	1.15	1.33
1	A	23	ALA	C-O	-13.59	0.97	1.23
1	A	75	VAL	CB-CG1	-13.46	1.24	1.52
2	B	2	GLU	C-N	-13.43	1.03	1.34
1	A	94	PHE	CB-CG	-13.34	1.28	1.51
2	B	9	ASP	CG-OD1	-13.27	0.94	1.25
2	B	53	LYS	C-O	-13.21	0.98	1.23
1	A	101	ASN	CG-OD1	-13.20	0.94	1.24
1	A	101	ASN	C-N	-13.20	1.03	1.34
1	A	16	LEU	CB-CG	-13.18	1.14	1.52
1	A	69	GLY	C-O	-13.17	1.02	1.23
1	A	84	SER	CB-OG	-13.16	1.25	1.42
2	B	51	GLN	C-N	-13.09	1.09	1.33
1	A	28	ILE	CB-CG1	-13.07	1.17	1.54
2	B	84	PHE	CG-CD2	-13.00	1.19	1.38
1	A	77	GLY	C-N	-12.96	1.04	1.34
2	B	43	LYS	CE-NZ	-12.92	1.16	1.49
1	A	17	ARG	NE-CZ	-12.91	1.16	1.33
2	B	47	ASP	CB-CG	-12.83	1.24	1.51
1	A	70	ASP	CB-CG	-12.77	1.25	1.51
1	A	122	GLU	CB-CG	-12.76	1.27	1.52
1	A	94	PHE	C-N	-12.70	1.04	1.34
1	A	81	LYS	CE-NZ	-12.70	1.17	1.49
1	A	52	TYR	CE2-CZ	-12.69	1.22	1.38
2	B	43	LYS	CB-CG	-12.69	1.18	1.52
1	A	16	LEU	CG-CD1	-12.63	1.05	1.51
2	B	45	ASP	CG-OD1	-12.57	0.96	1.25
1	A	78	GLU	CG-CD	-12.57	1.33	1.51
1	A	120	PRO	C-O	-12.56	0.98	1.23
1	A	70	ASP	CA-CB	-12.53	1.26	1.53
2	B	81	ASN	CG-ND2	-12.48	1.01	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	GLY	C-N	-12.40	1.10	1.33
1	A	64	ARG	CZ-NH2	-12.33	1.17	1.33
1	A	17	ARG	CZ-NH2	-12.21	1.17	1.33
2	B	103	GLN	CD-NE2	-12.21	1.02	1.32
1	A	52	TYR	CG-CD1	-12.18	1.23	1.39
1	A	85	ARG	NE-CZ	-12.14	1.17	1.33
2	B	31	GLN	CB-CG	-12.14	1.19	1.52
2	B	105	THR	C-N	-12.12	1.06	1.34
2	B	47	ASP	CG-OD1	-12.09	0.97	1.25
1	A	30	ARG	CB-CG	-12.01	1.20	1.52
1	A	83	VAL	CA-CB	-11.99	1.29	1.54
2	B	6	ARG	NE-CZ	-11.97	1.17	1.33
2	B	73	ASP	CG-OD2	-11.89	0.98	1.25
1	A	47	GLY	C-O	-11.89	1.04	1.23
2	B	56	LEU	CB-CG	-11.81	1.18	1.52
1	A	70	ASP	N-CA	-11.77	1.22	1.46
1	A	43	ARG	CZ-NH2	-11.67	1.17	1.33
2	B	4	GLN	CG-CD	-11.66	1.24	1.51
1	A	51	ARG	CZ-NH2	-11.60	1.18	1.33
1	A	102	GLN	C-N	-11.57	1.07	1.34
2	B	54	PHE	CG-CD2	-11.56	1.21	1.38
1	A	30	ARG	CD-NE	-11.55	1.26	1.46
1	A	21	LYS	CE-NZ	-11.49	1.20	1.49
2	B	31	GLN	CD-OE1	-11.41	0.98	1.24
2	B	103	GLN	CB-CG	-11.40	1.21	1.52
2	B	74	ASN	C-N	-11.38	1.07	1.34
1	A	83	VAL	CB-CG2	-11.35	1.29	1.52
1	A	24	THR	C-O	-11.23	1.02	1.23
1	A	50	GLU	C-N	-11.20	1.08	1.34
1	A	67	THR	C-N	-11.11	1.13	1.33
1	A	40	MET	CG-SD	-10.99	1.52	1.81
1	A	57	LYS	C-O	-10.88	1.02	1.23
1	A	16	LEU	CG-CD2	-10.85	1.11	1.51
2	B	18	GLN	C-O	-10.82	1.02	1.23
1	A	75	VAL	CB-CG2	-10.81	1.30	1.52
1	A	94	PHE	CG-CD2	-10.80	1.22	1.38
1	A	103	ASP	CG-OD2	-10.80	1.00	1.25
2	B	13	ALA	C-O	-10.74	1.02	1.23
1	A	51	ARG	C-O	-10.74	1.02	1.23
1	A	11	GLY	CA-C	-10.73	1.34	1.51
1	A	110	ARG	CB-CG	-10.72	1.23	1.52
1	A	134	THR	C-O	-10.65	1.03	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	88	ASP	CG-OD2	-10.60	1.00	1.25
1	A	70	ASP	CG-OD2	-10.56	1.01	1.25
2	B	49	PHE	CG-CD2	-10.53	1.23	1.38
2	B	6	ARG	CZ-NH2	-10.50	1.19	1.33
1	A	94	PHE	CD1-CE1	-10.50	1.18	1.39
2	B	111	ASN	C-O	-10.50	1.03	1.23
1	A	94	PHE	CD2-CE2	-10.48	1.18	1.39
1	A	26	ARG	NE-CZ	-10.47	1.19	1.33
2	B	112	TYR	CE2-CZ	-10.45	1.25	1.38
1	A	64	ARG	NE-CZ	-10.44	1.19	1.33
2	B	88	ASP	CG-OD1	-10.41	1.01	1.25
1	A	51	ARG	CD-NE	-10.40	1.28	1.46
2	B	14	LYS	C-O	-10.37	1.03	1.23
2	B	81	ASN	CB-CG	-10.24	1.27	1.51
1	A	76	LYS	CD-CE	-10.24	1.25	1.51
2	B	50	GLU	CG-CD	-10.21	1.36	1.51
2	B	9	ASP	CG-OD2	-10.16	1.01	1.25
1	A	64	ARG	CB-CG	-10.14	1.25	1.52
1	A	76	LYS	CB-CG	-10.14	1.25	1.52
2	B	92	TRP	C-N	-10.02	1.15	1.33
1	A	85	ARG	CZ-NH2	-10.00	1.20	1.33
2	B	70	ARG	CZ-NH2	-10.00	1.20	1.33
2	B	62	ARG	CG-CD	-9.98	1.26	1.51
1	A	12	SER	C-N	-9.95	1.15	1.33
2	B	140	LEU	CG-CD1	-9.95	1.15	1.51
2	B	9	ASP	CB-CG	-9.94	1.30	1.51
1	A	72	TRP	NE1-CE2	-9.94	1.24	1.37
1	A	138	LYS	CD-CE	-9.91	1.26	1.51
1	A	81	LYS	CD-CE	-9.89	1.26	1.51
2	B	112	TYR	CG-CD1	-9.89	1.26	1.39
1	A	7	GLU	CD-OE1	-9.86	1.14	1.25
2	B	43	LYS	CD-CE	-9.78	1.26	1.51
1	A	17	ARG	CD-NE	-9.78	1.29	1.46
1	A	41	ASN	CB-CG	-9.77	1.28	1.51
1	A	10	GLY	C-O	-9.76	1.08	1.23
1	A	93	PHE	C-N	-9.74	1.11	1.34
1	A	93	PHE	CG-CD1	-9.74	1.24	1.38
1	A	140	THR	C-O	-9.74	1.04	1.23
2	B	49	PHE	CG-CD1	-9.73	1.24	1.38
2	B	99	TYR	C-O	-9.71	1.04	1.23
1	A	14	THR	C-N	-9.67	1.11	1.34
2	B	83	VAL	C-N	-9.64	1.11	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ARG	CD-NE	-9.64	1.30	1.46
2	B	73	ASP	CG-OD1	-9.62	1.03	1.25
1	A	101	ASN	CG-ND2	-9.54	1.09	1.32
1	A	94	PHE	CG-CD1	-9.51	1.24	1.38
1	A	48	ARG	CZ-NH1	-9.46	1.20	1.33
1	A	13	GLY	N-CA	-9.45	1.31	1.46
1	A	83	VAL	CB-CG1	-9.40	1.33	1.52
2	B	62	ARG	NE-CZ	-9.37	1.20	1.33
2	B	125	ASN	C-O	-9.37	1.05	1.23
2	B	45	ASP	CG-OD2	-9.29	1.03	1.25
2	B	94	GLY	C-N	-9.22	1.12	1.34
1	A	10	GLY	C-N	-9.21	1.16	1.33
1	A	52	TYR	C-N	-9.21	1.12	1.34
1	A	30	ARG	NE-CZ	-9.20	1.21	1.33
2	B	140	LEU	CB-CG	-9.15	1.26	1.52
2	B	107	THR	CB-OG1	-9.06	1.25	1.43
1	A	28	ILE	CB-CG2	-9.05	1.24	1.52
1	A	48	ARG	CZ-NH2	-9.02	1.21	1.33
2	B	109	PRO	C-O	-9.01	1.05	1.23
2	B	21	ASP	C-O	-8.97	1.06	1.23
1	A	43	ARG	CD-NE	-8.97	1.31	1.46
1	A	17	ARG	CB-CG	-8.96	1.28	1.52
1	A	97	MET	C-O	-8.95	1.06	1.23
1	A	15	GLN	CB-CG	-8.95	1.28	1.52
2	B	18	GLN	CG-CD	-8.86	1.30	1.51
1	A	15	GLN	CG-CD	-8.83	1.30	1.51
2	B	84	PHE	CD1-CE1	-8.80	1.21	1.39
1	A	137	THR	CB-OG1	-8.79	1.25	1.43
1	A	80	GLY	N-CA	-8.78	1.32	1.46
1	A	49	ALA	CA-CB	-8.77	1.34	1.52
2	B	139	LYS	CD-CE	-8.74	1.29	1.51
2	B	90	GLY	C-O	-8.74	1.09	1.23
1	A	78	GLU	C-N	-8.73	1.17	1.33
2	B	84	PHE	CD2-CE2	-8.73	1.21	1.39
2	B	54	PHE	CE1-CZ	-8.71	1.20	1.37
1	A	66	ARG	NE-CZ	-8.64	1.21	1.33
1	A	79	GLY	CA-C	-8.64	1.38	1.51
2	B	54	PHE	CG-CD1	-8.62	1.25	1.38
1	A	41	ASN	CG-OD1	-8.53	1.05	1.24
1	A	72	TRP	CD2-CE3	-8.52	1.27	1.40
2	B	86	LYS	CE-NZ	-8.52	1.27	1.49
1	A	71	GLY	N-CA	-8.48	1.33	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	GLN	CD-NE2	-8.45	1.11	1.32
2	B	6	ARG	CD-NE	-8.40	1.32	1.46
1	A	24	THR	CB-OG1	-8.36	1.26	1.43
1	A	46	ASP	CG-OD1	-8.36	1.06	1.25
2	B	129	PHE	C-O	-8.31	1.07	1.23
1	A	69	GLY	C-N	-8.30	1.15	1.34
1	A	110	ARG	CZ-NH1	-8.29	1.22	1.33
1	A	51	ARG	NE-CZ	-8.20	1.22	1.33
1	A	114	GLY	CA-C	-8.19	1.38	1.51
2	B	93	GLY	C-O	-8.14	1.10	1.23
1	A	103	ASP	CB-CG	-8.09	1.34	1.51
1	A	80	GLY	C-O	-8.04	1.10	1.23
1	A	66	ARG	CZ-NH1	-8.04	1.22	1.33
2	B	110	GLY	C-O	-8.03	1.10	1.23
1	A	111	PHE	CG-CD2	-8.01	1.26	1.38
1	A	94	PHE	CE1-CZ	-7.98	1.22	1.37
2	B	59	ASP	CG-OD2	-7.97	1.07	1.25
2	B	70	ARG	NE-CZ	-7.97	1.22	1.33
1	A	46	ASP	CG-OD2	-7.94	1.07	1.25
1	A	48	ARG	NE-CZ	-7.93	1.22	1.33
1	A	15	GLN	CD-NE2	-7.90	1.13	1.32
2	B	49	PHE	CE1-CZ	-7.89	1.22	1.37
1	A	85	ARG	CD-NE	-7.88	1.33	1.46
1	A	114	GLY	C-N	-7.87	1.18	1.33
2	B	97	GLY	C-O	-7.87	1.11	1.23
1	A	72	TRP	C-O	-7.86	1.08	1.23
1	A	115	GLY	N-CA	-7.85	1.34	1.46
1	A	102	GLN	CD-OE1	-7.84	1.06	1.24
1	A	71	GLY	C-O	-7.84	1.11	1.23
1	A	78	GLU	C-O	-7.81	1.08	1.23
2	B	19	LEU	CB-CG	-7.80	1.29	1.52
1	A	95	ASP	CG-OD1	-7.75	1.07	1.25
2	B	88	ASP	CB-CG	-7.75	1.35	1.51
1	A	26	ARG	CZ-NH2	-7.74	1.23	1.33
1	A	141	VAL	CA-CB	-7.73	1.38	1.54
1	A	68	GLY	N-CA	-7.71	1.34	1.46
1	A	70	ASP	CG-OD1	-7.69	1.07	1.25
1	A	140	THR	C-N	-7.68	1.16	1.34
2	B	70	ARG	CD-NE	-7.67	1.33	1.46
2	B	47	ASP	CG-OD2	-7.67	1.07	1.25
2	B	53	LYS	C-N	-7.65	1.16	1.34
2	B	59	ASP	CB-CG	-7.63	1.35	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	18	GLN	C-N	-7.63	1.16	1.34
2	B	104	GLN	CD-NE2	-7.59	1.13	1.32
1	A	112	SER	CB-OG	-7.57	1.32	1.42
1	A	88	GLN	C-O	-7.56	1.08	1.23
2	B	104	GLN	CD-OE1	-7.56	1.07	1.24
1	A	133	THR	C-O	-7.55	1.08	1.23
2	B	25	ILE	C-O	-7.55	1.08	1.23
1	A	24	THR	C-N	-7.54	1.19	1.33
1	A	120	PRO	C-N	-7.47	1.16	1.34
1	A	57	LYS	CE-NZ	-7.47	1.30	1.49
2	B	67	VAL	C-O	-7.45	1.09	1.23
2	B	80	ASP	C-O	-7.45	1.09	1.23
2	B	4	GLN	C-O	-7.44	1.09	1.23
2	B	14	LYS	C-N	-7.44	1.17	1.34
1	A	90	GLU	CG-CD	-7.39	1.40	1.51
1	A	134	THR	C-N	-7.39	1.19	1.33
1	A	128	PHE	CG-CD1	-7.35	1.27	1.38
2	B	109	PRO	C-N	-7.30	1.20	1.33
2	B	12	VAL	C-O	-7.28	1.09	1.23
1	A	111	PHE	CG-CD1	-7.27	1.27	1.38
1	A	1	SER	CB-OG	-7.26	1.32	1.42
1	A	48	ARG	CD-NE	-7.24	1.34	1.46
1	A	40	MET	SD-CE	-7.22	1.37	1.77
2	B	63	ASP	CB-CG	-7.22	1.36	1.51
2	B	48	ASN	C-O	-7.22	1.09	1.23
1	A	93	PHE	CE2-CZ	-7.20	1.23	1.37
2	B	69	ILE	CB-CG2	-7.18	1.30	1.52
2	B	36	ASN	CB-CG	-7.17	1.34	1.51
2	B	49	PHE	CE2-CZ	-7.17	1.23	1.37
1	A	93	PHE	CG-CD2	-7.12	1.28	1.38
1	A	132	GLY	C-N	-7.10	1.17	1.34
2	B	140	LEU	C-O	-7.09	1.09	1.23
1	A	59	GLY	C-O	-7.09	1.12	1.23
1	A	66	ARG	CG-CD	-7.09	1.34	1.51
1	A	31	GLU	CB-CG	-7.07	1.38	1.52
1	A	94	PHE	CE2-CZ	-7.07	1.24	1.37
1	A	108	GLU	CB-CG	-7.06	1.38	1.52
2	B	89	VAL	C-O	-7.02	1.10	1.23
1	A	134	THR	CB-OG1	-7.00	1.29	1.43
2	B	118	GLY	C-O	-6.98	1.12	1.23
1	A	28	ILE	C-O	-6.96	1.10	1.23
2	B	18	GLN	CD-OE1	-6.96	1.08	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	LYS	CE-NZ	-6.96	1.31	1.49
2	B	43	LYS	CG-CD	-6.95	1.28	1.52
1	A	65	VAL	C-O	-6.94	1.10	1.23
1	A	24	THR	CB-CG2	-6.88	1.29	1.52
2	B	59	ASP	CG-OD1	-6.88	1.09	1.25
1	A	79	GLY	C-N	-6.83	1.20	1.33
1	A	51	ARG	C-N	-6.82	1.18	1.34
2	B	60	ASN	CG-OD1	-6.79	1.09	1.24
2	B	69	ILE	CB-CG1	-6.79	1.35	1.54
1	A	47	GLY	C-N	-6.76	1.18	1.34
1	A	115	GLY	C-N	-6.75	1.18	1.34
1	A	15	GLN	CD-OE1	-6.73	1.09	1.24
2	B	136	GLY	C-O	-6.71	1.12	1.23
1	A	12	SER	N-CA	-6.68	1.32	1.46
1	A	58	ASP	CG-OD1	-6.68	1.09	1.25
1	A	113	VAL	CB-CG1	-6.63	1.39	1.52
2	B	42	LEU	CG-CD2	-6.62	1.27	1.51
1	A	82	GLY	CA-C	-6.62	1.41	1.51
1	A	64	ARG	C-O	-6.59	1.10	1.23
1	A	62	GLU	CD-OE2	-6.56	1.18	1.25
1	A	72	TRP	CZ2-CH2	-6.55	1.24	1.37
2	B	125	ASN	CG-OD1	-6.55	1.09	1.24
1	A	138	LYS	C-O	-6.54	1.10	1.23
1	A	31	GLU	CD-OE1	-6.50	1.18	1.25
1	A	136	THR	CB-OG1	-6.44	1.30	1.43
1	A	46	ASP	C-O	-6.42	1.11	1.23
2	B	33	LEU	CG-CD2	-6.33	1.28	1.51
2	B	54	PHE	CE2-CZ	-6.33	1.25	1.37
1	A	20	ALA	C-O	-6.32	1.11	1.23
1	A	83	VAL	C-N	-6.31	1.19	1.34
1	A	110	ARG	CZ-NH2	-6.28	1.24	1.33
1	A	133	THR	CB-OG1	-6.28	1.30	1.43
2	B	104	GLN	C-O	-6.28	1.11	1.23
1	A	23	ALA	CA-CB	-6.28	1.39	1.52
2	B	56	LEU	CG-CD1	-6.28	1.28	1.51
2	B	4	GLN	C-N	-6.27	1.19	1.34
1	A	3	GLU	CD-OE1	-6.25	1.18	1.25
2	B	25	ILE	C-N	-6.25	1.21	1.33
2	B	60	ASN	CG-ND2	-6.24	1.17	1.32
1	A	110	ARG	CG-CD	-6.21	1.36	1.51
2	B	139	LYS	CE-NZ	-6.21	1.33	1.49
2	B	143	THR	CB-OG1	-6.20	1.30	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	LEU	CG-CD1	-6.16	1.29	1.51
1	A	88	GLN	C-N	-6.14	1.20	1.34
2	B	87	ASN	C-O	-6.12	1.11	1.23
2	B	64	LYS	CE-NZ	-6.09	1.33	1.49
1	A	72	TRP	CG-CD1	-6.06	1.28	1.36
1	A	31	GLU	CD-OE2	-6.05	1.19	1.25
1	A	30	ARG	CG-CD	-6.05	1.36	1.51
1	A	142	THR	N-CA	-6.01	1.34	1.46
1	A	51	ARG	CZ-NH1	-5.98	1.25	1.33
2	B	106	ASN	C-O	-5.95	1.12	1.23
1	A	7	GLU	CG-CD	-5.93	1.43	1.51
1	A	97	MET	C-N	-5.93	1.20	1.34
1	A	89	GLU	CG-CD	-5.92	1.43	1.51
1	A	121	GLN	CD-NE2	-5.92	1.18	1.32
1	A	3	GLU	CD-OE2	-5.92	1.19	1.25
1	A	84	SER	CA-CB	-5.89	1.44	1.52
2	B	33	LEU	CG-CD1	-5.89	1.30	1.51
1	A	13	GLY	CA-C	-5.87	1.42	1.51
1	A	111	PHE	CE1-CZ	-5.83	1.26	1.37
2	B	111	ASN	C-N	-5.83	1.20	1.34
1	A	139	LEU	CB-CG	-5.83	1.35	1.52
1	A	12	SER	CA-C	-5.82	1.37	1.52
1	A	50	GLU	CA-CB	-5.78	1.41	1.53
1	A	66	ARG	CZ-NH2	-5.78	1.25	1.33
1	A	121	GLN	CD-OE1	-5.78	1.11	1.24
2	B	8	GLY	C-O	-5.78	1.14	1.23
2	B	141	THR	C-O	-5.76	1.12	1.23
2	B	112	TYR	C-O	-5.76	1.12	1.23
1	A	62	GLU	CD-OE1	-5.75	1.19	1.25
2	B	20	THR	CB-OG1	-5.74	1.31	1.43
1	A	18	ASP	C-O	-5.73	1.12	1.23
1	A	52	TYR	CE1-CZ	-5.73	1.31	1.38
2	B	18	GLN	CD-NE2	-5.70	1.18	1.32
1	A	23	ALA	C-N	-5.69	1.21	1.34
1	A	21	LYS	C-O	-5.69	1.12	1.23
1	A	48	ARG	C-O	-5.68	1.12	1.23
2	B	139	LYS	CB-CG	-5.64	1.37	1.52
2	B	84	PHE	CE2-CZ	-5.62	1.26	1.37
1	A	135	GLY	C-O	-5.61	1.14	1.23
2	B	47	ASP	C-O	-5.59	1.12	1.23
2	B	13	ALA	C-N	-5.57	1.21	1.34
1	A	57	LYS	C-N	-5.57	1.21	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	99	TYR	C-N	-5.55	1.21	1.34
1	A	66	ARG	C-O	-5.53	1.12	1.23
2	B	53	LYS	CG-CD	-5.51	1.33	1.52
1	A	110	ARG	NE-CZ	-5.51	1.25	1.33
1	A	96	VAL	C-O	-5.51	1.12	1.23
1	A	33	HIS	CG-CD2	-5.47	1.26	1.35
2	B	131	PRO	C-O	-5.46	1.12	1.23
1	A	82	GLY	C-N	-5.45	1.21	1.34
1	A	26	ARG	CD-NE	-5.45	1.37	1.46
1	A	83	VAL	N-CA	-5.43	1.35	1.46
1	A	139	LEU	CG-CD1	-5.43	1.31	1.51
2	B	106	ASN	CA-CB	-5.43	1.39	1.53
1	A	128	PHE	CE2-CZ	-5.42	1.27	1.37
2	B	111	ASN	CG-ND2	-5.41	1.19	1.32
1	A	88	GLN	CD-OE1	-5.39	1.12	1.24
2	B	80	ASP	C-N	-5.39	1.21	1.34
2	B	93	GLY	C-N	-5.39	1.23	1.33
1	A	103	ASP	C-O	-5.39	1.13	1.23
2	B	140	LEU	CG-CD2	-5.39	1.31	1.51
2	B	39	GLN	CD-NE2	-5.38	1.19	1.32
2	B	109	PRO	N-CD	-5.38	1.40	1.47
2	B	67	VAL	C-N	-5.37	1.21	1.34
2	B	125	ASN	CG-ND2	-5.36	1.19	1.32
2	B	84	PHE	CB-CG	-5.36	1.42	1.51
1	A	55	GLN	C-O	-5.33	1.13	1.23
1	A	37	HIS	CG-ND1	-5.32	1.27	1.38
2	B	17	GLY	C-O	-5.32	1.15	1.23
1	A	125	LYS	CE-NZ	-5.31	1.35	1.49
1	A	111	PHE	CE2-CZ	-5.31	1.27	1.37
2	B	97	GLY	C-N	-5.30	1.21	1.34
1	A	72	TRP	CG-CD2	-5.29	1.34	1.43
1	A	66	ARG	CB-CG	-5.29	1.38	1.52
1	A	46	ASP	CB-CG	-5.28	1.40	1.51
1	A	29	CYS	C-O	-5.26	1.13	1.23
1	A	52	TYR	CG-CD2	-5.26	1.32	1.39
1	A	113	VAL	CB-CG2	-5.26	1.41	1.52
2	B	59	ASP	CA-CB	-5.23	1.42	1.53
1	A	137	THR	CB-CG2	-5.21	1.35	1.52
2	B	51	GLN	CD-OE1	-5.20	1.12	1.24
1	A	43	ARG	NE-CZ	-5.20	1.26	1.33
1	A	46	ASP	C-N	-5.19	1.23	1.33
1	A	93	PHE	CE1-CZ	-5.18	1.27	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	107	THR	CB-CG2	-5.17	1.35	1.52
1	A	122	GLU	CG-CD	-5.16	1.44	1.51
1	A	6	LEU	CG-CD2	-5.14	1.32	1.51
2	B	143	THR	CB-CG2	-5.13	1.35	1.52
2	B	12	VAL	CB-CG1	-5.13	1.42	1.52
1	A	17	ARG	CG-CD	-5.12	1.39	1.51
1	A	128	PHE	CG-CD2	-5.12	1.31	1.38
1	A	72	TRP	C-N	-5.11	1.22	1.34
2	B	140	LEU	C-N	-5.11	1.22	1.34
1	A	32	ALA	C-O	-5.11	1.13	1.23
2	B	125	ASN	C-N	-5.10	1.22	1.34
1	A	18	ASP	C-N	-5.09	1.23	1.33
2	B	114	LEU	CB-CG	-5.08	1.37	1.52
2	B	104	GLN	C-N	-5.07	1.22	1.34
1	A	136	THR	CB-CG2	-5.06	1.35	1.52
1	A	48	ARG	C-N	-5.06	1.22	1.34
1	A	59	GLY	C-N	-5.03	1.22	1.34
1	A	133	THR	C-N	-5.03	1.22	1.34
1	A	79	GLY	N-CA	-5.02	1.38	1.46
2	B	132	SER	CB-OG	-5.01	1.35	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	50	GLU	OE1-CD-OE2	-61.96	48.95	123.30
2	B	63	ASP	CB-CG-OD1	38.10	152.59	118.30
2	B	66	TYR	CD1-CG-CD2	-34.97	79.44	117.90
2	B	66	TYR	CB-CG-CD2	32.18	140.31	121.00
2	B	66	TYR	CB-CG-CD1	32.09	140.25	121.00
2	B	4	GLN	OE1-CD-NE2	-31.94	48.44	121.90
2	B	1	GLU	OE1-CD-OE2	31.64	161.26	123.30
1	A	141	VAL	O-C-N	-31.42	72.42	122.70
2	B	63	ASP	OD1-CG-OD2	-30.41	65.53	123.30
2	B	16	ARG	NE-CZ-NH2	29.60	135.10	120.30
1	A	99	ASP	CB-CG-OD2	-26.71	94.26	118.30
2	B	63	ASP	CB-CG-OD2	26.20	141.88	118.30
1	A	99	ASP	CB-CG-OD1	25.86	141.58	118.30
2	B	2	GLU	CA-CB-CG	24.75	167.85	113.40
1	A	58	ASP	O-C-N	-24.07	82.28	123.20
2	B	66	TYR	CG-CD1-CE1	23.93	140.44	121.30
1	A	26	ARG	NE-CZ-NH2	23.81	132.21	120.30
2	B	66	TYR	CG-CD2-CE2	23.75	140.30	121.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	66	TYR	CE1-CZ-CE2	-23.69	81.90	119.80
1	A	30	ARG	NE-CZ-NH2	23.58	132.09	120.30
2	B	1	GLU	CG-CD-OE2	-22.88	72.55	118.30
1	A	85	ARG	NE-CZ-NH2	22.50	131.55	120.30
1	A	138	LYS	CD-CE-NZ	21.71	161.62	111.70
2	B	16	ARG	NH1-CZ-NH2	-21.51	95.74	119.40
1	A	50	GLU	CB-CG-CD	21.35	171.85	114.20
2	B	66	TYR	CZ-CE2-CD2	21.29	138.97	119.80
2	B	66	TYR	CD1-CE1-CZ	21.29	138.96	119.80
2	B	1	GLU	CB-CA-C	-21.25	67.89	110.40
1	A	69	GLY	N-CA-C	20.63	164.66	113.10
1	A	142	THR	CA-CB-OG1	-20.40	66.15	109.00
1	A	96	VAL	CG1-CB-CG2	-19.82	79.18	110.90
1	A	13	GLY	O-C-N	-19.19	92.00	122.70
2	B	50	GLU	CG-CD-OE1	18.96	156.23	118.30
2	B	4	GLN	CG-CD-OE1	18.87	159.34	121.60
1	A	142	THR	CA-CB-CG2	18.62	138.47	112.40
2	B	50	GLU	CG-CD-OE2	18.26	154.82	118.30
1	A	49	ALA	O-C-N	-17.75	94.31	122.70
2	B	16	ARG	NE-CZ-NH1	17.71	129.16	120.30
1	A	67	THR	CA-CB-CG2	17.57	137.00	112.40
2	B	1	GLU	N-CA-C	17.52	158.31	111.00
1	A	99	ASP	CA-CB-CG	16.80	150.35	113.40
1	A	142	THR	OG1-CB-CG2	16.64	148.26	110.00
1	A	26	ARG	NE-CZ-NH1	-16.37	112.11	120.30
2	B	19	LEU	CB-CG-CD2	16.13	138.42	111.00
1	A	96	VAL	CA-CB-CG1	16.12	135.08	110.90
1	A	142	THR	N-CA-C	15.60	153.12	111.00
2	B	1	GLU	CB-CG-CD	15.40	155.78	114.20
1	A	58	ASP	CA-C-N	15.28	146.76	116.20
1	A	85	ARG	NE-CZ-NH1	-15.21	112.69	120.30
1	A	142	THR	CB-CA-C	-14.88	71.42	111.60
2	B	4	GLN	CG-CD-NE2	14.80	152.22	116.70
1	A	70	ASP	O-C-N	-14.77	98.09	123.20
2	B	86	LYS	CD-CE-NZ	13.96	143.80	111.70
1	A	140	THR	CA-CB-CG2	13.79	131.71	112.40
1	A	96	VAL	CA-CB-CG2	13.69	131.43	110.90
1	A	94	PHE	O-C-N	-13.12	101.71	122.70
2	B	62	ARG	NE-CZ-NH1	-12.93	113.84	120.30
1	A	64	ARG	NE-CZ-NH2	12.83	126.72	120.30
1	A	58	ASP	C-N-CA	12.83	149.25	122.30
2	B	38	ARG	NE-CZ-NH2	12.67	126.64	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	141	VAL	CG1-CB-CG2	-12.43	91.02	110.90
2	B	74	ASN	O-C-N	-12.27	103.07	122.70
1	A	141	VAL	CA-C-O	12.20	145.71	120.10
2	B	2	GLU	O-C-N	-11.90	103.66	122.70
2	B	1	GLU	N-CA-CB	11.59	131.46	110.60
1	A	77	GLY	O-C-N	-11.51	104.29	122.70
1	A	13	GLY	CA-C-N	11.50	142.50	117.20
1	A	43	ARG	NE-CZ-NH2	11.32	125.96	120.30
1	A	141	VAL	CA-C-N	11.20	141.84	117.20
2	B	70	ARG	NE-CZ-NH2	11.14	125.87	120.30
2	B	45	ASP	CB-CG-OD2	11.14	128.32	118.30
2	B	16	ARG	CD-NE-CZ	10.85	138.79	123.60
2	B	73	ASP	CB-CG-OD1	10.83	128.05	118.30
1	A	101	ASN	O-C-N	-10.78	105.46	122.70
2	B	38	ARG	NE-CZ-NH1	10.57	125.59	120.30
2	B	38	ARG	NH1-CZ-NH2	-10.57	107.77	119.40
1	A	67	THR	OG1-CB-CG2	-10.55	85.73	110.00
2	B	51	GLN	O-C-N	-10.52	105.31	123.20
1	A	108	GLU	OE1-CD-OE2	-10.50	110.70	123.30
1	A	138	LYS	CB-CG-CD	10.47	138.83	111.60
2	B	48	ASN	CA-CB-CG	10.42	136.32	113.40
2	B	56	LEU	CB-CG-CD1	10.42	128.71	111.00
1	A	102	GLN	O-C-N	-10.35	106.13	122.70
1	A	140	THR	OG1-CB-CG2	-10.24	86.44	110.00
1	A	70	ASP	CA-C-N	10.11	136.41	116.20
2	B	2	GLU	OE1-CD-OE2	-10.05	111.24	123.30
1	A	122	GLU	OE1-CD-OE2	-10.04	111.25	123.30
1	A	42	GLU	OE1-CD-OE2	-10.04	111.25	123.30
2	B	6	ARG	NE-CZ-NH2	9.88	125.24	120.30
2	B	2	GLU	CG-CD-OE1	9.74	137.77	118.30
1	A	13	GLY	C-N-CA	9.62	145.76	121.70
2	B	87	ASN	CA-CB-CG	9.56	134.43	113.40
2	B	50	GLU	CA-CB-CG	9.50	134.30	113.40
1	A	103	ASP	CB-CG-OD2	9.47	126.83	118.30
2	B	112	TYR	CB-CG-CD1	9.47	126.68	121.00
2	B	105	THR	O-C-N	-9.30	107.82	122.70
2	B	62	ARG	NE-CZ-NH2	9.27	124.93	120.30
1	A	30	ARG	CB-CG-CD	9.26	135.66	111.60
2	B	1	GLU	CA-CB-CG	-9.19	93.19	113.40
1	A	81	LYS	CD-CE-NZ	9.17	132.78	111.70
1	A	30	ARG	NH1-CZ-NH2	-9.13	109.35	119.40
2	B	84	PHE	CE1-CZ-CE2	-9.06	103.69	120.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	16	LEU	CA-CB-CG	8.99	135.98	115.30
1	A	141	VAL	C-N-CA	8.99	144.18	121.70
2	B	18	GLN	CB-CG-CD	8.97	134.92	111.60
1	A	14	THR	O-C-N	-8.92	108.43	122.70
1	A	30	ARG	CD-NE-CZ	8.80	135.92	123.60
2	B	64	LYS	CD-CE-NZ	8.77	131.87	111.70
1	A	108	GLU	CB-CG-CD	8.64	137.53	114.20
1	A	50	GLU	O-C-N	-8.62	108.90	122.70
2	B	1	GLU	CA-C-N	8.62	136.15	117.20
1	A	26	ARG	CD-NE-CZ	8.61	135.65	123.60
1	A	141	VAL	CA-CB-CG1	8.57	123.75	110.90
1	A	110	ARG	CB-CG-CD	8.49	133.67	111.60
1	A	22	VAL	CA-CB-CG2	8.39	123.48	110.90
2	B	83	VAL	O-C-N	-8.34	109.36	122.70
1	A	142	THR	N-CA-CB	8.33	126.12	110.30
2	B	31	GLN	CA-CB-CG	8.23	131.50	113.40
1	A	70	ASP	C-N-CA	8.21	139.54	122.30
1	A	22	VAL	CG1-CB-CG2	-8.14	97.88	110.90
2	B	92	TRP	O-C-N	-8.11	109.41	123.20
2	B	56	LEU	CA-CB-CG	8.09	133.90	115.30
2	B	2	GLU	N-CA-CB	-8.01	96.19	110.60
1	A	50	GLU	CA-CB-CG	7.89	130.77	113.40
2	B	9	ASP	CB-CG-OD2	7.86	125.37	118.30
2	B	43	LYS	CA-CB-CG	7.84	130.65	113.40
1	A	141	VAL	CA-CB-CG2	7.79	122.59	110.90
1	A	85	ARG	CD-NE-CZ	7.74	134.44	123.60
1	A	68	GLY	N-CA-C	7.69	132.32	113.10
1	A	114	GLY	CA-C-N	7.63	131.45	116.20
2	B	16	ARG	CG-CD-NE	7.61	127.78	111.80
1	A	93	PHE	O-C-N	-7.60	110.53	122.70
2	B	6	ARG	NE-CZ-NH1	-7.60	116.50	120.30
2	B	56	LEU	CB-CG-CD2	-7.59	98.10	111.00
1	A	140	THR	CA-CB-OG1	7.58	124.93	109.00
1	A	94	PHE	CA-C-N	7.55	133.81	117.20
2	B	94	GLY	O-C-N	-7.54	110.64	122.70
2	B	51	GLN	CA-C-N	7.49	131.19	116.20
2	B	73	ASP	OD1-CG-OD2	-7.49	109.08	123.30
2	B	36	ASN	OD1-CG-ND2	-7.43	104.82	121.90
2	B	103	GLN	OE1-CD-NE2	-7.41	104.86	121.90
1	A	120	PRO	O-C-N	-7.39	110.87	122.70
1	A	138	LYS	CG-CD-CE	7.32	133.87	111.90
2	B	1	GLU	C-N-CA	7.30	139.96	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	GLU	O-C-N	-7.29	111.03	122.70
2	B	112	TYR	CG-CD1-CE1	7.27	127.11	121.30
1	A	52	TYR	O-C-N	-7.18	111.21	122.70
2	B	84	PHE	CD1-CE1-CZ	7.16	128.69	120.10
2	B	45	ASP	OD1-CG-OD2	-7.11	109.79	123.30
2	B	92	TRP	CA-C-N	7.11	130.42	116.20
2	B	66	TYR	CE1-CZ-OH	7.02	139.06	120.10
2	B	66	TYR	OH-CZ-CE2	7.02	139.05	120.10
2	B	74	ASN	CA-C-N	7.00	132.59	117.20
2	B	139	LYS	CD-CE-NZ	6.97	127.72	111.70
2	B	31	GLN	OE1-CD-NE2	-6.96	105.89	121.90
1	A	49	ALA	CA-C-O	6.91	134.62	120.10
1	A	95	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	52	TYR	CB-CG-CD2	6.89	125.14	121.00
2	B	54	PHE	CB-CG-CD1	6.87	125.61	120.80
1	A	83	VAL	CG1-CB-CG2	-6.76	100.08	110.90
2	B	19	LEU	CD1-CG-CD2	-6.74	90.28	110.50
1	A	16	LEU	CD1-CG-CD2	-6.69	90.44	110.50
1	A	51	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	78	GLU	OE1-CD-OE2	-6.64	115.34	123.30
1	A	67	THR	CA-CB-OG1	6.63	122.92	109.00
2	B	18	GLN	CA-CB-CG	6.57	127.85	113.40
2	B	50	GLU	CB-CG-CD	6.50	131.74	114.20
1	A	89	GLU	OE1-CD-OE2	-6.49	115.51	123.30
2	B	112	TYR	CZ-CE2-CD2	6.49	125.64	119.80
2	B	31	GLN	CB-CG-CD	6.48	128.45	111.60
2	B	53	LYS	O-C-N	-6.47	112.34	122.70
1	A	94	PHE	C-N-CA	6.45	137.81	121.70
1	A	108	GLU	CG-CD-OE2	6.41	131.12	118.30
2	B	112	TYR	CD1-CG-CD2	-6.39	110.87	117.90
1	A	101	ASN	OD1-CG-ND2	-6.33	107.34	121.90
1	A	17	ARG	CB-CG-CD	6.30	127.98	111.60
1	A	49	ALA	CA-C-N	6.30	131.05	117.20
1	A	51	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	B	58	SER	CA-CB-OG	6.28	128.16	111.20
1	A	15	GLN	CB-CG-CD	6.24	127.81	111.60
2	B	59	ASP	CA-CB-CG	6.23	127.10	113.40
2	B	140	LEU	CB-CG-CD2	6.11	121.39	111.00
2	B	84	PHE	CZ-CE2-CD2	6.05	127.36	120.10
2	B	47	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	14	THR	CA-C-N	6.00	130.41	117.20
2	B	4	GLN	CB-CG-CD	5.95	127.07	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	48	ASN	OD1-CG-ND2	-5.91	108.31	121.90
1	A	72	TRP	CD1-CG-CD2	-5.89	101.58	106.30
2	B	31	GLN	CG-CD-OE1	5.86	133.31	121.60
1	A	43	ARG	NH1-CZ-NH2	-5.82	113.00	119.40
2	B	92	TRP	C-N-CA	5.80	134.48	122.30
1	A	68	GLY	CA-C-O	-5.78	110.19	120.60
1	A	52	TYR	CG-CD2-CE2	5.76	125.90	121.30
2	B	38	ARG	CD-NE-CZ	5.76	131.66	123.60
1	A	41	ASN	CB-CG-OD1	5.74	133.09	121.60
2	B	74	ASN	C-N-CA	5.72	135.99	121.70
2	B	51	GLN	C-N-CA	5.71	134.29	122.30
2	B	9	ASP	CA-CB-CG	5.70	125.93	113.40
2	B	106	ASN	CA-CB-CG	5.68	125.90	113.40
1	A	114	GLY	C-N-CA	5.66	134.19	122.30
2	B	2	GLU	N-CA-C	5.61	126.14	111.00
1	A	115	GLY	O-C-N	-5.56	113.80	122.70
1	A	75	VAL	CA-CB-CG2	5.56	119.24	110.90
2	B	14	LYS	O-C-N	-5.53	113.86	122.70
1	A	15	GLN	CA-CB-CG	5.48	125.45	113.40
1	A	11	GLY	CA-C-O	-5.46	110.76	120.60
2	B	2	GLU	CB-CG-CD	5.42	128.82	114.20
1	A	132	GLY	O-C-N	-5.41	114.05	122.70
1	A	90	GLU	OE1-CD-OE2	-5.40	116.82	123.30
2	B	19	LEU	CA-CB-CG	5.35	127.59	115.30
1	A	11	GLY	CA-C-N	5.32	128.90	117.20
1	A	77	GLY	CA-C-N	5.31	128.89	117.20
2	B	47	ASP	CB-CG-OD1	-5.31	113.52	118.30
2	B	2	GLU	CA-C-N	5.29	128.83	117.20
1	A	103	ASP	OD1-CG-OD2	-5.28	113.26	123.30
2	B	19	LEU	CB-CG-CD1	5.25	119.92	111.00
1	A	134	THR	O-C-N	-5.23	114.31	123.20
1	A	28	ILE	CA-CB-CG2	5.23	121.36	110.90
1	A	14	THR	C-N-CA	5.21	134.73	121.70
1	A	11	GLY	C-N-CA	5.19	134.68	121.70
1	A	58	ASP	CA-C-O	5.17	130.96	120.10
1	A	75	VAL	CG1-CB-CG2	-5.16	102.64	110.90
1	A	52	TYR	CD1-CE1-CZ	5.16	124.44	119.80
1	A	24	THR	O-C-N	-5.12	114.50	123.20
1	A	16	LEU	CB-CG-CD2	5.09	119.65	111.00
1	A	38	VAL	CA-CB-CG1	5.08	118.53	110.90
1	A	83	VAL	O-C-N	-5.08	114.58	122.70
2	B	73	ASP	CB-CG-OD2	5.07	122.87	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	53	LYS	CD-CE-NZ	5.07	123.35	111.70
2	B	140	LEU	CA-CB-CG	5.05	126.93	115.30
1	A	58	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	115	GLY	CA-C-N	5.00	128.20	117.20

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 (i)

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	989	97
2	B	1088	1030	1023	68
All	All	2163	2016	2012	160

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 38.

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
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
1:A:141:VAL:C	1:A:142:THR:CA	1.34	1.96
2:B:66:TYR:CG	2:B:66:TYR:CE1	1.33	2.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
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: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
1:A:141:VAL:C	1:A:142:THR:OG1	1.17	1.80
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
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
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:C	1:A:142:THR:HA	0.95	1.39
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:63:ASP:OD1	2:B:63:ASP:CG	0.93	0.73
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
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
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
1:A:141:VAL:CG1	1:A:141:VAL:CB	0.83	0.83
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
1:A:138:LYS:NZ	1:A:138:LYS:HE3	0.80	1.18
2:B:50:GLU:OE1	2:B:50:GLU:CD	0.79	0.60
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:141:VAL:CG1	1:A:141:VAL:C	0.77	2.51
1:A:67:THR:OG1	1:A:67:THR:CB	0.77	0.73
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:50:GLU:OE2	2:B:50:GLU:CD	0.76	0.58
2:B:66:TYR:CG	2:B:66:TYR:HD1	0.75	1.51
2:B:63:ASP:OD2	2:B:63:ASP:CG	0.74	0.55
2:B:66:TYR:CZ	2:B:66:TYR:HE1	0.74	1.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:4:GLN:OE1	2:B:4:GLN:CD	0.74	0.60
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
2:B:2:GLU:CD	2:B:2:GLU:HG2	0.65	1.46
1:A:36:PHE:CE2	1:A:87:GLY:HA2	0.64	2.28
1:A:141:VAL:C	1:A:142:THR:N	0.63	0.71
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
2:B:4:GLN:NE2	2:B:4:GLN:OE1	0.60	0.46
1:A:141:VAL:C	1:A:141:VAL:HG12	0.60	2.12
1:A:141:VAL:C	1:A:141:VAL:O	0.59	0.69
1:A:69:GLY:O	1:A:70:ASP:HB3	0.59	1.95
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
2:B:4:GLN:CD	2:B:4:GLN:HE21	0.57	1.19
2:B:4:GLN:CD	2:B:4:GLN:HE22	0.57	1.19
1:A:67:THR:CB	1:A:67:THR:HG1	0.57	1.28
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
2:B:2:GLU:CD	2:B:2:GLU:HG3	0.54	1.46
1:A:54:VAL:HG22	1:A:63:LEU:O	0.53	2.04
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: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
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:50:GLU:OE2	2:B:50:GLU:OE1	0.49	0.49
2:B:2:GLU:CD	2:B:2:GLU:OE1	0.49	0.69
2:B:4:GLN:NE2	2:B:4:GLN:CD	0.48	0.50
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
2:B:105:THR:O	2:B:106:ASN:CB	0.47	2.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:19:LEU:HD13	2:B:19:LEU:HB3	0.47	1.76
1:A:35:GLY:C	1:A:84:SER:HB3	0.47	2.29
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:96:VAL:CG2	1:A:96:VAL:C	0.46	2.80
2:B:106:ASN:O	2:B:106:ASN:CG	0.46	2.49
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:21:ASP:O	2:B:22:ALA:C	0.45	2.53
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
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
2:B:2:GLU:CD	2:B:2:GLU:CG	0.43	0.87
1:A:67:THR:CG2	1:A:67:THR:C	0.43	2.83
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
1:A:67:THR:CA	1:A:67:THR:HG1	0.41	2.01
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%)	3 22
2	B	141/143 (99%)	112 (79%)	21 (15%)	8 (6%)	3 22
All	All	281/285 (99%)	210 (75%)	55 (20%)	16 (6%)	3 22

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 (i)

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%)	80 (72%)	31 (28%)	2 19
2	B	117/117 (100%)	89 (76%)	28 (24%)	2 27
All	All	228/228 (100%)	169 (74%)	59 (26%)	2 23

All 59 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	26	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	29	CYS
1	A	30	ARG
1	A	33	HIS
1	A	34	THR
1	A	38	VAL
1	A	42	GLU
1	A	43	ARG
1	A	51	ARG
1	A	52	TYR
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
1	A	138	LYS
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	14	LYS
2	B	20	THR
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides 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
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

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1:GLU	C	2:GLU	N	0.83
1	A	141:VAL	C	142:THR	N	0.71

7 Chemical shift validation (i)

No chemical shift data were provided