Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 08:36 PM BST

PDB ID	:	2HQ3
Title	:	Solution NMR structure of the apo-NosL protein from Achromobacter cycloclastes
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Deposited on	:	2006-07-18

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

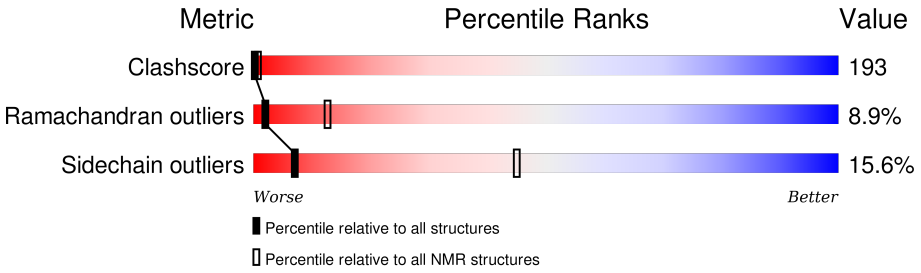
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	175	19% 17% 27% 9% 28%

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

There is only 1 type of molecule in this entry. The entry contains 1818 atoms, of which 891 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NosL protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	126	1818	587	891	155	182	3	0

There are 2 discrepancies between the modelled and reference sequences:

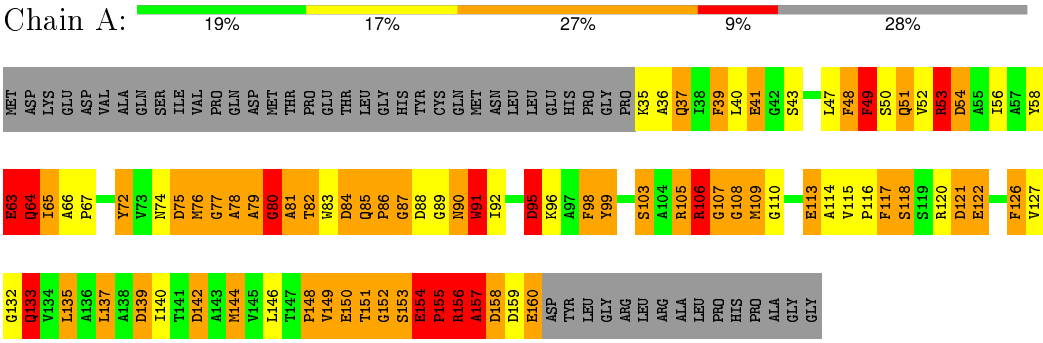
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP O68481
A	2	ASP	-	CLONING ARTIFACT	UNP O68481

4 Residue-property plots (i)

These plots are provided for all protein, RNA and DNA 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: NosL protein

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Ambiguous Restraints for Iterative Assignments (ARIA 1.2), torsion angle dynamics, simulated annealing.*.

Of the ? calculated structures, 1 were deposited, based on the following criterion: *minimized average structure*.

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

Software name	Classification	Version
ARIA	structure solution	1.2
CNS	refinement	1.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (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	19.23	350/948 (36.9%)	18.33	287/1293 (22.2%)
All	All	19.23	350/948 (36.9%)	18.33	287/1293 (22.2%)

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	3	0
All	All	3	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)
1	A	113	GLU	CD-OE1	-94.54	0.21	1.25
1	A	160	GLU	CD-OE1	-92.89	0.23	1.25
1	A	154	GLU	CD-OE2	-91.72	0.24	1.25
1	A	91	TRP	NE1-CE2	-90.83	0.19	1.37
1	A	106	ARG	CZ-NH2	-83.61	0.24	1.33
1	A	150	GLU	CD-OE1	-81.57	0.35	1.25
1	A	160	GLU	CD-OE2	-79.89	0.37	1.25
1	A	63	GLU	CD-OE1	-79.76	0.38	1.25
1	A	91	TRP	CD2-CE3	-74.03	0.29	1.40
1	A	83	TRP	NE1-CE2	-72.67	0.43	1.37
1	A	153	SER	CB-OG	-70.75	0.50	1.42
1	A	106	ARG	CD-NE	-67.95	0.30	1.46
1	A	154	GLU	CD-OE1	-66.85	0.52	1.25
1	A	58	TYR	CE2-CZ	-66.79	0.51	1.38
1	A	130	GLU	CD-OE2	-66.23	0.52	1.25
1	A	60	ARG	CZ-NH2	-66.03	0.47	1.33
1	A	58	TYR	CG-CD1	-65.42	0.54	1.39
1	A	83	TRP	CD2-CE3	-64.61	0.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	GLU	CD-OE1	-64.42	0.54	1.25
1	A	63	GLU	CD-OE2	-62.53	0.56	1.25
1	A	113	GLU	CD-OE2	-61.02	0.58	1.25
1	A	88	ASP	CB-CG	-60.94	0.23	1.51
1	A	130	GLU	CD-OE1	-59.70	0.59	1.25
1	A	48	PHE	CG-CD2	-59.49	0.49	1.38
1	A	150	GLU	CD-OE2	-57.35	0.62	1.25
1	A	58	TYR	CE1-CZ	-56.78	0.64	1.38
1	A	91	TRP	CZ2-CH2	-56.25	0.30	1.37
1	A	72	TYR	CE1-CZ	-56.19	0.65	1.38
1	A	117	PHE	CG-CD1	-56.11	0.54	1.38
1	A	41	GLU	CD-OE2	-55.66	0.64	1.25
1	A	58	TYR	CG-CD2	-55.47	0.67	1.39
1	A	160	GLU	CG-CD	-55.13	0.69	1.51
1	A	49	PHE	CG-CD2	-54.90	0.56	1.38
1	A	72	TYR	CG-CD2	-54.53	0.68	1.39
1	A	60	ARG	CZ-NH1	-54.19	0.62	1.33
1	A	106	ARG	CZ-NH1	-53.26	0.63	1.33
1	A	99	TYR	CE1-CZ	-52.98	0.69	1.38
1	A	99	TYR	CG-CD2	-51.65	0.72	1.39
1	A	60	ARG	CD-NE	-51.35	0.59	1.46
1	A	72	TYR	CE2-CZ	-50.15	0.73	1.38
1	A	63	GLU	C-O	-49.75	0.28	1.23
1	A	83	TRP	CZ2-CH2	-49.59	0.43	1.37
1	A	103	SER	CB-OG	-49.51	0.77	1.42
1	A	154	GLU	CG-CD	-49.08	0.78	1.51
1	A	160	GLU	CB-CG	-48.58	0.59	1.52
1	A	72	TYR	CG-CD1	-48.51	0.76	1.39
1	A	126	PHE	CG-CD2	-47.64	0.67	1.38
1	A	48	PHE	CG-CD1	-47.64	0.67	1.38
1	A	99	TYR	CE2-CZ	-47.25	0.77	1.38
1	A	48	PHE	CE1-CZ	-46.89	0.48	1.37
1	A	91	TRP	CG-CD1	-46.55	0.71	1.36
1	A	99	TYR	CG-CD1	-45.92	0.79	1.39
1	A	83	TRP	CG-CD1	-45.63	0.72	1.36
1	A	88	ASP	CG-OD2	-45.14	0.21	1.25
1	A	158	ASP	CG-OD1	-44.84	0.22	1.25
1	A	105	ARG	CZ-NH2	-44.67	0.74	1.33
1	A	122	GLU	CD-OE1	-44.58	0.76	1.25
1	A	117	PHE	CE2-CZ	-44.10	0.53	1.37
1	A	91	TRP	CG-CD2	-43.46	0.69	1.43
1	A	49	PHE	CG-CD1	-43.44	0.73	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	PHE	CE1-CZ	-43.24	0.55	1.37
1	A	76	MET	CG-SD	-42.72	0.70	1.81
1	A	160	GLU	C-O	-42.07	0.43	1.23
1	A	64	GLN	CG-CD	-41.59	0.55	1.51
1	A	156	ARG	CZ-NH1	-41.36	0.79	1.33
1	A	159	ASP	C-O	-41.26	0.45	1.23
1	A	122	GLU	CD-OE2	-41.24	0.80	1.25
1	A	39	PHE	CG-CD2	-40.77	0.77	1.38
1	A	98	PHE	CG-CD1	-40.52	0.78	1.38
1	A	64	GLN	CD-OE1	-39.65	0.36	1.24
1	A	64	GLN	CA-CB	-39.56	0.67	1.53
1	A	106	ARG	NE-CZ	-38.81	0.82	1.33
1	A	77	GLY	C-N	-38.80	0.44	1.34
1	A	98	PHE	CG-CD2	-38.72	0.80	1.38
1	A	88	ASP	CG-OD1	-38.70	0.36	1.25
1	A	126	PHE	CG-CD1	-38.20	0.81	1.38
1	A	126	PHE	CE1-CZ	-37.57	0.66	1.37
1	A	48	PHE	CE2-CZ	-37.45	0.66	1.37
1	A	39	PHE	CG-CD1	-37.01	0.83	1.38
1	A	85	GLN	CD-NE2	-36.69	0.41	1.32
1	A	105	ARG	CD-NE	-36.64	0.84	1.46
1	A	156	ARG	NE-CZ	-36.61	0.85	1.33
1	A	64	GLN	CB-CG	-36.49	0.54	1.52
1	A	109	MET	CG-SD	-36.24	0.86	1.81
1	A	113	GLU	CG-CD	-36.15	0.97	1.51
1	A	64	GLN	CD-NE2	-35.90	0.43	1.32
1	A	117	PHE	CG-CD2	-35.84	0.84	1.38
1	A	76	MET	C-N	-35.40	0.69	1.33
1	A	49	PHE	CE2-CZ	-34.25	0.72	1.37
1	A	160	GLU	CA-C	-33.81	0.65	1.52
1	A	95	ASP	CG-OD1	-33.50	0.48	1.25
1	A	83	TRP	CG-CD2	-33.11	0.87	1.43
1	A	74	ASN	CG-OD1	-32.98	0.51	1.24
1	A	105	ARG	CZ-NH1	-32.87	0.90	1.33
1	A	159	ASP	CG-OD1	-32.42	0.50	1.25
1	A	90	ASN	CG-ND2	-32.36	0.52	1.32
1	A	105	ARG	C-O	-32.02	0.62	1.23
1	A	39	PHE	CE1-CZ	-31.97	0.76	1.37
1	A	98	PHE	CE2-CZ	-31.84	0.76	1.37
1	A	95	ASP	CG-OD2	-31.76	0.52	1.25
1	A	35	LYS	CD-CE	-31.57	0.72	1.51
1	A	88	ASP	C-O	-31.43	0.63	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLU	CG-CD	-31.42	1.04	1.51
1	A	106	ARG	C-O	-31.17	0.64	1.23
1	A	84	ASP	CG-OD1	-31.08	0.53	1.25
1	A	78	ALA	C-N	-30.84	0.63	1.34
1	A	98	PHE	CE1-CZ	-30.47	0.79	1.37
1	A	142	ASP	CG-OD2	-30.42	0.55	1.25
1	A	139	ASP	CG-OD2	-30.21	0.55	1.25
1	A	126	PHE	CE2-CZ	-30.10	0.80	1.37
1	A	91	TRP	CE2-CZ2	-30.04	0.88	1.39
1	A	158	ASP	CG-OD2	-29.69	0.57	1.25
1	A	91	TRP	CE3-CZ3	-29.59	0.88	1.38
1	A	84	ASP	CG-OD2	-29.56	0.57	1.25
1	A	87	GLY	C-O	-29.31	0.76	1.23
1	A	77	GLY	CA-C	-29.18	1.05	1.51
1	A	39	PHE	CE2-CZ	-29.04	0.82	1.37
1	A	139	ASP	CG-OD1	-28.77	0.59	1.25
1	A	121	ASP	CG-OD2	-28.68	0.59	1.25
1	A	117	PHE	CE1-CZ	-28.10	0.83	1.37
1	A	64	GLN	C-O	-28.00	0.70	1.23
1	A	90	ASN	CG-OD1	-27.93	0.62	1.24
1	A	89	GLY	N-CA	-27.89	1.04	1.46
1	A	159	ASP	CG-OD2	-27.88	0.61	1.25
1	A	37	GLN	CD-OE1	-27.71	0.62	1.24
1	A	50	SER	CB-OG	-27.66	1.06	1.42
1	A	121	ASP	CG-OD1	-27.54	0.62	1.25
1	A	133	GLN	CD-OE1	-27.50	0.63	1.24
1	A	88	ASP	CA-CB	-27.38	0.93	1.53
1	A	106	ARG	CG-CD	-27.29	0.83	1.51
1	A	109	MET	CB-CG	-27.28	0.64	1.51
1	A	37	GLN	CD-NE2	-26.85	0.65	1.32
1	A	160	GLU	CA-CB	-26.76	0.95	1.53
1	A	85	GLN	CD-OE1	-26.75	0.65	1.24
1	A	76	MET	C-O	-26.60	0.72	1.23
1	A	78	ALA	N-CA	-26.43	0.93	1.46
1	A	107	GLY	C-O	-26.26	0.81	1.23
1	A	91	TRP	CD2-CE2	-26.15	1.09	1.41
1	A	142	ASP	CG-OD1	-26.02	0.65	1.25
1	A	54	ASP	CG-OD1	-25.86	0.65	1.25
1	A	158	ASP	CB-CG	-25.53	0.98	1.51
1	A	150	GLU	C-O	-25.48	0.74	1.23
1	A	109	MET	SD-CE	-25.30	0.36	1.77
1	A	75	ASP	CG-OD1	-24.89	0.68	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	ALA	CA-CB	-24.58	1.00	1.52
1	A	78	ALA	C-O	-24.55	0.76	1.23
1	A	157	ALA	C-O	-24.50	0.76	1.23
1	A	133	GLN	CD-NE2	-24.27	0.72	1.32
1	A	90	ASN	CB-CG	-24.08	0.95	1.51
1	A	80	GLY	N-CA	-23.93	1.10	1.46
1	A	156	ARG	CZ-NH2	-23.89	1.01	1.33
1	A	83	TRP	CD2-CE2	-23.87	1.12	1.41
1	A	75	ASP	CG-OD2	-23.59	0.71	1.25
1	A	35	LYS	CE-NZ	-23.35	0.90	1.49
1	A	107	GLY	C-N	-23.34	0.91	1.33
1	A	158	ASP	C-O	-23.33	0.79	1.23
1	A	79	ALA	CA-CB	-23.18	1.03	1.52
1	A	51	GLN	CD-OE1	-22.93	0.73	1.24
1	A	150	GLU	CG-CD	-22.72	1.17	1.51
1	A	83	TRP	CE2-CZ2	-21.97	1.02	1.39
1	A	79	ALA	C-N	-21.89	0.93	1.33
1	A	106	ARG	C-N	-21.74	0.94	1.33
1	A	83	TRP	CE3-CZ3	-21.58	1.01	1.38
1	A	128	LEU	CG-CD2	-21.54	0.72	1.51
1	A	157	ALA	C-N	-21.50	0.84	1.34
1	A	63	GLU	CB-CG	-21.40	1.11	1.52
1	A	60	ARG	NE-CZ	-21.27	1.05	1.33
1	A	64	GLN	C-N	-21.27	0.85	1.34
1	A	159	ASP	CB-CG	-21.10	1.07	1.51
1	A	51	GLN	CD-NE2	-20.79	0.80	1.32
1	A	113	GLU	CB-CG	-20.49	1.13	1.52
1	A	76	MET	SD-CE	-20.38	0.63	1.77
1	A	153	SER	CA-CB	-20.33	1.22	1.52
1	A	74	ASN	CG-ND2	-20.31	0.82	1.32
1	A	54	ASP	CG-OD2	-20.25	0.78	1.25
1	A	159	ASP	C-N	-19.83	0.88	1.34
1	A	63	GLU	C-N	-19.77	0.88	1.34
1	A	91	TRP	CZ3-CH2	-19.62	1.08	1.40
1	A	77	GLY	C-O	-19.62	0.92	1.23
1	A	156	ARG	CD-NE	-19.54	1.13	1.46
1	A	76	MET	CB-CG	-19.25	0.89	1.51
1	A	86	PRO	N-CD	-19.11	1.21	1.47
1	A	85	GLN	CG-CD	-18.43	1.08	1.51
1	A	150	GLU	C-N	-18.36	0.91	1.34
1	A	48	PHE	CB-CG	-18.36	1.20	1.51
1	A	91	TRP	CD1-NE1	-18.30	1.06	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	TRP	CZ3-CH2	-18.09	1.11	1.40
1	A	159	ASP	CA-CB	-17.81	1.14	1.53
1	A	155	PRO	C-O	-17.56	0.88	1.23
1	A	87	GLY	C-N	-17.28	0.94	1.34
1	A	80	GLY	CA-C	-17.10	1.24	1.51
1	A	108	GLY	N-CA	-17.03	1.20	1.46
1	A	160	GLU	N-CA	-16.70	1.12	1.46
1	A	88	ASP	CA-C	-16.69	1.09	1.52
1	A	105	ARG	C-N	-16.68	0.95	1.34
1	A	81	ALA	CA-CB	-16.52	1.17	1.52
1	A	115	VAL	CB-CG2	-16.48	1.18	1.52
1	A	58	TYR	CB-CG	-16.45	1.26	1.51
1	A	85	GLN	CA-CB	-16.40	1.17	1.53
1	A	88	ASP	C-N	-16.39	1.03	1.33
1	A	152	GLY	CA-C	-16.32	1.25	1.51
1	A	107	GLY	CA-C	-16.26	1.25	1.51
1	A	115	VAL	CB-CG1	-15.52	1.20	1.52
1	A	58	TYR	CD1-CE1	-15.40	1.16	1.39
1	A	80	GLY	C-O	-15.37	0.99	1.23
1	A	58	TYR	CD2-CE2	-15.34	1.16	1.39
1	A	91	TRP	CB-CG	-15.12	1.23	1.50
1	A	155	PRO	C-N	-15.05	0.99	1.34
1	A	120	ARG	CZ-NH1	-15.01	1.13	1.33
1	A	74	ASN	CB-CG	-14.96	1.16	1.51
1	A	48	PHE	CD2-CE2	-14.39	1.10	1.39
1	A	128	LEU	CG-CD1	-14.38	0.98	1.51
1	A	48	PHE	CD1-CE1	-14.33	1.10	1.39
1	A	149	VAL	C-O	-14.29	0.96	1.23
1	A	151	THR	C-O	-14.03	0.96	1.23
1	A	79	ALA	CA-C	-13.97	1.16	1.52
1	A	159	ASP	CA-C	-13.97	1.16	1.52
1	A	144	MET	SD-CE	-13.91	0.99	1.77
1	A	95	ASP	CB-CG	-13.90	1.22	1.51
1	A	86	PRO	CA-CB	-13.53	1.26	1.53
1	A	62	PRO	C-O	-13.20	0.96	1.23
1	A	153	SER	N-CA	-13.18	1.20	1.46
1	A	64	GLN	N-CA	-13.18	1.20	1.46
1	A	158	ASP	C-N	-13.11	1.03	1.34
1	A	43	SER	CB-OG	-13.10	1.25	1.42
1	A	83	TRP	CD1-NE1	-12.97	1.16	1.38
1	A	58	TYR	CZ-OH	-12.92	1.15	1.37
1	A	77	GLY	N-CA	-12.72	1.26	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	GLY	N-CA	-12.70	1.27	1.46
1	A	83	TRP	N-CA	-12.61	1.21	1.46
1	A	108	GLY	C-O	-12.52	1.03	1.23
1	A	131	GLY	C-O	-12.44	1.03	1.23
1	A	155	PRO	N-CD	-12.43	1.30	1.47
1	A	80	GLY	C-N	-12.40	1.05	1.34
1	A	120	ARG	NE-CZ	-12.34	1.17	1.33
1	A	109	MET	C-N	-12.34	1.10	1.33
1	A	81	ALA	N-CA	-12.30	1.21	1.46
1	A	105	ARG	NE-CZ	-12.13	1.17	1.33
1	A	84	ASP	CA-CB	-12.13	1.27	1.53
1	A	151	THR	CB-OG1	-11.82	1.19	1.43
1	A	110	GLY	N-CA	-11.80	1.28	1.46
1	A	156	ARG	CG-CD	-11.80	1.22	1.51
1	A	117	PHE	CB-CG	-11.59	1.31	1.51
1	A	83	TRP	CB-CG	-11.59	1.29	1.50
1	A	85	GLN	C-O	-11.58	1.01	1.23
1	A	63	GLU	CA-C	-11.30	1.23	1.52
1	A	109	MET	CA-CB	-11.02	1.29	1.53
1	A	53	ARG	CZ-NH1	-10.68	1.19	1.33
1	A	65	ILE	N-CA	-10.66	1.25	1.46
1	A	83	TRP	C-O	-10.59	1.03	1.23
1	A	82	THR	CA-C	-10.42	1.25	1.52
1	A	152	GLY	C-O	-10.38	1.07	1.23
1	A	84	ASP	C-N	-10.34	1.10	1.34
1	A	64	GLN	CA-C	-9.84	1.27	1.52
1	A	82	THR	CA-CB	-9.79	1.27	1.53
1	A	85	GLN	CB-CG	-9.74	1.26	1.52
1	A	63	GLU	CA-CB	-9.71	1.32	1.53
1	A	120	ARG	CZ-NH2	-9.62	1.20	1.33
1	A	76	MET	CA-CB	-9.58	1.32	1.53
1	A	152	GLY	C-N	-9.53	1.12	1.34
1	A	83	TRP	C-N	-9.35	1.12	1.34
1	A	139	ASP	CB-CG	-9.31	1.32	1.51
1	A	156	ARG	CB-CG	-9.30	1.27	1.52
1	A	151	THR	CB-CG2	-9.09	1.22	1.52
1	A	62	PRO	C-N	-8.93	1.13	1.34
1	A	117	PHE	CD1-CE1	-8.92	1.21	1.39
1	A	117	PHE	CD2-CE2	-8.84	1.21	1.39
1	A	86	PRO	C-N	-8.80	1.17	1.33
1	A	133	GLN	CG-CD	-8.79	1.30	1.51
1	A	151	THR	C-N	-8.66	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	ASP	N-CA	-8.63	1.29	1.46
1	A	65	ILE	CB-CG1	-8.57	1.30	1.54
1	A	86	PRO	N-CA	-8.55	1.32	1.47
1	A	82	THR	N-CA	-8.50	1.29	1.46
1	A	65	ILE	CA-CB	-8.45	1.35	1.54
1	A	86	PRO	C-O	-8.43	1.06	1.23
1	A	49	PHE	CB-CG	-8.39	1.37	1.51
1	A	82	THR	CB-CG2	-8.34	1.24	1.52
1	A	149	VAL	C-N	-8.29	1.15	1.34
1	A	81	ALA	C-N	-8.20	1.15	1.34
1	A	149	VAL	CB-CG2	-8.20	1.35	1.52
1	A	137	LEU	CG-CD2	-8.11	1.21	1.51
1	A	148	PRO	C-N	-8.09	1.15	1.34
1	A	158	ASP	N-CA	-8.01	1.30	1.46
1	A	154	GLU	C-O	-7.97	1.08	1.23
1	A	87	GLY	CA-C	-7.96	1.39	1.51
1	A	153	SER	C-N	-7.75	1.16	1.34
1	A	76	MET	CA-C	-7.73	1.32	1.52
1	A	128	LEU	CB-CG	-7.72	1.30	1.52
1	A	158	ASP	CA-C	-7.67	1.33	1.52
1	A	151	THR	CA-CB	-7.65	1.33	1.53
1	A	84	ASP	CB-CG	-7.53	1.35	1.51
1	A	108	GLY	C-N	-7.49	1.16	1.34
1	A	39	PHE	CB-CG	-7.49	1.38	1.51
1	A	85	GLN	C-N	-7.40	1.20	1.34
1	A	154	GLU	CA-CB	-7.35	1.37	1.53
1	A	47	LEU	CG-CD1	-7.30	1.24	1.51
1	A	120	ARG	CD-NE	-7.29	1.34	1.46
1	A	156	ARG	C-O	-7.28	1.09	1.23
1	A	47	LEU	CG-CD2	-7.24	1.25	1.51
1	A	151	THR	CA-C	-7.09	1.34	1.52
1	A	158	ASP	CA-CB	-7.07	1.38	1.53
1	A	130	GLU	CG-CD	-6.97	1.41	1.51
1	A	149	VAL	CB-CG1	-6.96	1.38	1.52
1	A	149	VAL	CA-CB	-6.92	1.40	1.54
1	A	86	PRO	CG-CD	-6.85	1.28	1.50
1	A	87	GLY	N-CA	-6.75	1.35	1.46
1	A	79	ALA	N-CA	-6.72	1.32	1.46
1	A	148	PRO	C-O	-6.66	1.09	1.23
1	A	156	ARG	N-CA	-6.64	1.33	1.46
1	A	65	ILE	CB-CG2	-6.63	1.32	1.52
1	A	79	ALA	C-O	-6.58	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	PRO	CA-CB	-6.57	1.40	1.53
1	A	65	ILE	C-O	-6.55	1.10	1.23
1	A	130	GLU	C-O	-6.51	1.10	1.23
1	A	49	PHE	CD1-CE1	-6.49	1.26	1.39
1	A	49	PHE	CD2-CE2	-6.43	1.26	1.39
1	A	154	GLU	N-CA	-6.36	1.33	1.46
1	A	106	ARG	CB-CG	-6.34	1.35	1.52
1	A	155	PRO	CA-C	-6.34	1.40	1.52
1	A	150	GLU	CA-CB	-6.32	1.40	1.53
1	A	109	MET	CA-C	-6.31	1.36	1.52
1	A	118	SER	CB-OG	-6.30	1.34	1.42
1	A	81	ALA	CA-C	-6.29	1.36	1.52
1	A	96	LYS	CE-NZ	-6.27	1.33	1.49
1	A	86	PRO	CB-CG	-6.25	1.18	1.50
1	A	106	ARG	CA-CB	-6.25	1.40	1.53
1	A	153	SER	C-O	-6.25	1.11	1.23
1	A	84	ASP	N-CA	-6.22	1.33	1.46
1	A	130	GLU	C-N	-6.12	1.22	1.33
1	A	156	ARG	C-N	-6.11	1.20	1.34
1	A	65	ILE	CG1-CD1	-5.93	1.09	1.50
1	A	157	ALA	CA-C	-5.92	1.37	1.52
1	A	39	PHE	CD1-CE1	-5.88	1.27	1.39
1	A	39	PHE	CD2-CE2	-5.86	1.27	1.39
1	A	110	GLY	C-O	-5.85	1.14	1.23
1	A	85	GLN	N-CA	-5.73	1.34	1.46
1	A	149	VAL	N-CA	-5.71	1.34	1.46
1	A	82	THR	C-O	-5.67	1.12	1.23
1	A	85	GLN	CA-C	-5.63	1.38	1.52
1	A	149	VAL	CA-C	-5.63	1.38	1.52
1	A	108	GLY	CA-C	-5.53	1.43	1.51
1	A	88	ASP	N-CA	-5.48	1.35	1.46
1	A	146	LEU	CG-CD2	-5.41	1.31	1.51
1	A	83	TRP	CA-C	-5.36	1.39	1.52
1	A	150	GLU	CB-CG	-5.28	1.42	1.52
1	A	131	GLY	C-N	-5.18	1.23	1.33
1	A	82	THR	C-N	-5.12	1.22	1.34
1	A	84	ASP	C-O	-5.06	1.13	1.23
1	A	150	GLU	N-CA	-5.04	1.36	1.46

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	TRP	CD1-CG-CD2	-101.14	25.39	106.30
1	A	58	TYR	CD1-CG-CD2	-98.80	9.22	117.90
1	A	106	ARG	NE-CZ-NH1	96.29	168.45	120.30
1	A	130	GLU	OE1-CD-OE2	-93.23	11.42	123.30
1	A	60	ARG	NE-CZ-NH1	92.14	166.37	120.30
1	A	58	TYR	CB-CG-CD2	90.76	175.46	121.00
1	A	58	TYR	CB-CG-CD1	90.48	175.29	121.00
1	A	72	TYR	CD1-CG-CD2	-89.64	19.30	117.90
1	A	91	TRP	CG-CD2-CE3	-87.42	55.23	133.90
1	A	41	GLU	OE1-CD-OE2	-85.22	21.03	123.30
1	A	49	PHE	CD1-CG-CD2	-83.48	9.77	118.30
1	A	72	TYR	CB-CG-CD1	83.03	170.82	121.00
1	A	72	TYR	CB-CG-CD2	81.43	169.86	121.00
1	A	60	ARG	NE-CZ-NH2	80.81	160.71	120.30
1	A	60	ARG	NH1-CZ-NH2	-78.62	32.92	119.40
1	A	49	PHE	CB-CG-CD1	78.36	175.65	120.80
1	A	113	GLU	OE1-CD-OE2	-76.94	30.97	123.30
1	A	49	PHE	CB-CG-CD2	76.82	174.58	120.80
1	A	150	GLU	OE1-CD-OE2	-73.20	35.46	123.30
1	A	88	ASP	CB-CG-OD2	-72.22	53.31	118.30
1	A	91	TRP	CH2-CZ2-CE2	-70.95	46.45	117.40
1	A	83	TRP	CD1-CG-CD2	-70.34	50.02	106.30
1	A	91	TRP	CE2-CD2-CG	69.66	163.03	107.30
1	A	48	PHE	CD1-CG-CD2	-69.52	27.93	118.30
1	A	58	TYR	CE1-CZ-CE2	-68.92	9.53	119.80
1	A	48	PHE	CB-CG-CD1	68.42	168.69	120.80
1	A	58	TYR	CG-CD2-CE2	68.10	175.78	121.30
1	A	106	ARG	NH1-CZ-NH2	-67.95	44.66	119.40
1	A	58	TYR	CG-CD1-CE1	67.06	174.95	121.30
1	A	99	TYR	CD1-CG-CD2	-62.51	49.14	117.90
1	A	58	TYR	CD1-CE1-CZ	62.26	175.84	119.80
1	A	72	TYR	CE1-CZ-CE2	-62.25	20.19	119.80
1	A	72	TYR	CG-CD1-CE1	62.01	170.91	121.30
1	A	49	PHE	CE1-CZ-CE2	-61.10	10.02	120.00
1	A	58	TYR	CZ-CE2-CD2	60.98	174.69	119.80
1	A	158	ASP	CB-CG-OD2	60.89	173.10	118.30
1	A	48	PHE	CB-CG-CD2	60.83	163.38	120.80
1	A	72	TYR	CG-CD2-CE2	60.69	169.85	121.30
1	A	99	TYR	CB-CG-CD1	59.62	156.77	121.00
1	A	121	ASP	CB-CG-OD1	57.62	170.15	118.30
1	A	142	ASP	CB-CG-OD1	57.44	169.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	GLU	OE1-CD-OE2	-56.75	55.20	123.30
1	A	126	PHE	CD1-CG-CD2	-56.46	44.90	118.30
1	A	72	TYR	CZ-CE2-CD2	56.20	170.38	119.80
1	A	142	ASP	CB-CG-OD2	56.11	168.79	118.30
1	A	121	ASP	CB-CG-OD2	56.04	168.74	118.30
1	A	126	PHE	CB-CG-CD1	55.62	159.73	120.80
1	A	63	GLU	OE1-CD-OE2	-55.56	56.63	123.30
1	A	91	TRP	CG-CD1-NE1	55.21	165.31	110.10
1	A	99	TYR	CB-CG-CD2	55.09	154.06	121.00
1	A	72	TYR	CD1-CE1-CZ	55.07	169.36	119.80
1	A	117	PHE	CB-CG-CD2	54.62	159.03	120.80
1	A	121	ASP	OD1-CG-OD2	-53.79	21.10	123.30
1	A	142	ASP	OD1-CG-OD2	-53.76	21.16	123.30
1	A	95	ASP	CB-CG-OD2	53.65	166.58	118.30
1	A	158	ASP	OD1-CG-OD2	-53.55	21.56	123.30
1	A	84	ASP	CB-CG-OD1	53.43	166.38	118.30
1	A	91	TRP	CD2-CE3-CZ3	-53.33	49.47	118.80
1	A	106	ARG	NE-CZ-NH2	53.12	146.86	120.30
1	A	95	ASP	CB-CG-OD1	52.82	165.83	118.30
1	A	83	TRP	CE2-CD2-CG	52.70	149.46	107.30
1	A	84	ASP	CB-CG-OD2	52.38	165.45	118.30
1	A	158	ASP	CB-CG-OD1	52.26	165.33	118.30
1	A	48	PHE	CE1-CZ-CE2	-50.86	28.44	120.00
1	A	95	ASP	OD1-CG-OD2	-50.41	27.52	123.30
1	A	84	ASP	OD1-CG-OD2	-50.09	28.13	123.30
1	A	49	PHE	CG-CD1-CE1	50.02	175.82	120.80
1	A	98	PHE	CD1-CG-CD2	-49.65	53.76	118.30
1	A	126	PHE	CB-CG-CD2	49.38	155.37	120.80
1	A	49	PHE	CG-CD2-CE2	48.77	174.44	120.80
1	A	117	PHE	CD1-CG-CD2	-48.31	55.49	118.30
1	A	98	PHE	CB-CG-CD2	46.95	153.67	120.80
1	A	49	PHE	CZ-CE2-CD2	46.30	175.66	120.10
1	A	98	PHE	CB-CG-CD1	45.38	152.57	120.80
1	A	49	PHE	CD1-CE1-CZ	45.16	174.29	120.10
1	A	99	TYR	CG-CD1-CE1	44.24	156.69	121.30
1	A	48	PHE	CG-CD1-CE1	43.25	168.37	120.80
1	A	91	TRP	CE3-CZ3-CH2	43.03	168.53	121.20
1	A	99	TYR	CE1-CZ-CE2	-42.97	51.05	119.80
1	A	139	ASP	CB-CG-OD1	42.73	156.76	118.30
1	A	139	ASP	CB-CG-OD2	41.35	155.52	118.30
1	A	99	TYR	CG-CD2-CE2	41.22	154.28	121.30
1	A	126	PHE	CE1-CZ-CE2	-41.22	45.81	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	83	TRP	CG-CD2-CE3	-40.64	97.32	133.90
1	A	99	TYR	CZ-CE2-CD2	40.03	155.82	119.80
1	A	48	PHE	CZ-CE2-CD2	40.02	168.12	120.10
1	A	139	ASP	OD1-CG-OD2	-39.81	47.65	123.30
1	A	154	GLU	OE1-CD-OE2	-39.72	75.64	123.30
1	A	105	ARG	NE-CZ-NH1	39.34	139.97	120.30
1	A	48	PHE	CG-CD2-CE2	38.97	163.67	120.80
1	A	91	TRP	CD2-CE2-CZ2	38.75	168.80	122.30
1	A	88	ASP	CB-CG-OD1	37.39	151.96	118.30
1	A	83	TRP	CG-CD1-NE1	37.31	147.41	110.10
1	A	99	TYR	CD1-CE1-CZ	36.92	153.03	119.80
1	A	109	MET	CG-SD-CE	36.67	158.88	100.20
1	A	98	PHE	CE1-CZ-CE2	-36.20	54.84	120.00
1	A	48	PHE	CD1-CE1-CZ	36.14	163.47	120.10
1	A	39	PHE	CD1-CG-CD2	-35.97	71.54	118.30
1	A	126	PHE	CG-CD1-CE1	35.48	159.83	120.80
1	A	39	PHE	CB-CG-CD1	35.31	145.52	120.80
1	A	117	PHE	CB-CG-CD1	35.24	145.47	120.80
1	A	122	GLU	OE1-CD-OE2	-35.22	81.04	123.30
1	A	117	PHE	CE1-CZ-CE2	-35.21	56.62	120.00
1	A	117	PHE	CG-CD2-CE2	34.67	158.93	120.80
1	A	63	GLU	O-C-N	-34.63	67.28	122.70
1	A	75	ASP	CB-CG-OD2	33.17	148.16	118.30
1	A	83	TRP	CE3-CZ3-CH2	33.09	157.60	121.20
1	A	126	PHE	CZ-CE2-CD2	32.78	159.44	120.10
1	A	83	TRP	CH2-CZ2-CE2	-32.21	85.19	117.40
1	A	75	ASP	CB-CG-OD1	32.20	147.28	118.30
1	A	54	ASP	CB-CG-OD2	32.19	147.27	118.30
1	A	117	PHE	CD1-CE1-CZ	32.05	158.57	120.10
1	A	156	ARG	NE-CZ-NH1	-32.01	104.30	120.30
1	A	91	TRP	CB-CG-CD1	31.79	168.32	127.00
1	A	39	PHE	CB-CG-CD2	31.62	142.94	120.80
1	A	37	GLN	OE1-CD-NE2	-31.44	49.59	121.90
1	A	126	PHE	CG-CD2-CE2	31.35	155.28	120.80
1	A	75	ASP	OD1-CG-OD2	-30.94	64.52	123.30
1	A	91	TRP	CB-CG-CD2	30.53	166.29	126.60
1	A	78	ALA	O-C-N	-30.16	74.45	122.70
1	A	83	TRP	CD2-CE2-CZ2	29.87	158.15	122.30
1	A	98	PHE	CG-CD2-CE2	29.79	153.57	120.80
1	A	98	PHE	CG-CD1-CE1	29.07	152.77	120.80
1	A	35	LYS	CD-CE-NZ	29.06	178.55	111.70
1	A	126	PHE	CD1-CE1-CZ	28.87	154.74	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	ARG	CD-NE-CZ	28.49	163.48	123.60
1	A	159	ASP	CB-CG-OD2	28.41	143.87	118.30
1	A	130	GLU	CG-CD-OE1	28.13	174.56	118.30
1	A	130	GLU	CG-CD-OE2	27.86	174.01	118.30
1	A	98	PHE	CD1-CE1-CZ	27.37	152.94	120.10
1	A	91	TRP	NE1-CE2-CZ2	-27.32	100.34	130.40
1	A	98	PHE	CZ-CE2-CD2	26.67	152.11	120.10
1	A	105	ARG	NH1-CZ-NH2	-26.50	90.25	119.40
1	A	113	GLU	CG-CD-OE2	26.39	171.07	118.30
1	A	39	PHE	CE1-CZ-CE2	-26.24	72.76	120.00
1	A	41	GLU	CG-CD-OE2	26.07	170.44	118.30
1	A	83	TRP	NE1-CE2-CD2	-25.94	81.36	107.30
1	A	54	ASP	OD1-CG-OD2	-25.84	74.21	123.30
1	A	41	GLU	CG-CD-OE1	25.10	168.51	118.30
1	A	150	GLU	CG-CD-OE2	24.41	167.12	118.30
1	A	105	ARG	O-C-N	-23.91	84.44	122.70
1	A	76	MET	O-C-N	-23.35	83.50	123.20
1	A	83	TRP	CD2-CE3-CZ3	-23.22	88.61	118.80
1	A	83	TRP	CB-CG-CD2	23.07	156.60	126.60
1	A	128	LEU	CB-CG-CD1	22.72	149.62	111.00
1	A	39	PHE	CG-CD1-CE1	22.64	145.71	120.80
1	A	117	PHE	CG-CD1-CE1	22.57	145.63	120.80
1	A	54	ASP	CB-CG-OD1	22.44	138.49	118.30
1	A	159	ASP	OD1-CG-OD2	-21.82	81.85	123.30
1	A	106	ARG	CD-NE-CZ	21.77	154.08	123.60
1	A	106	ARG	O-C-N	-21.42	86.79	123.20
1	A	85	GLN	OE1-CD-NE2	-21.32	72.85	121.90
1	A	63	GLU	CA-C-N	20.86	163.09	117.20
1	A	39	PHE	CZ-CE2-CD2	20.81	145.07	120.10
1	A	58	TYR	CE1-CZ-OH	20.65	175.85	120.10
1	A	117	PHE	CZ-CE2-CD2	20.55	144.76	120.10
1	A	35	LYS	CG-CD-CE	20.44	173.22	111.90
1	A	83	TRP	CB-CG-CD1	20.29	153.38	127.00
1	A	58	TYR	OH-CZ-CE2	20.19	174.62	120.10
1	A	154	GLU	CG-CD-OE1	20.09	158.47	118.30
1	A	156	ARG	NE-CZ-NH2	20.02	130.31	120.30
1	A	160	GLU	CG-CD-OE2	20.02	158.33	118.30
1	A	39	PHE	CG-CD2-CE2	20.02	142.82	120.80
1	A	133	GLN	OE1-CD-NE2	-19.87	76.20	121.90
1	A	113	GLU	CG-CD-OE1	19.83	157.95	118.30
1	A	51	GLN	OE1-CD-NE2	-19.79	76.38	121.90
1	A	77	GLY	CA-C-O	19.61	155.90	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	GLU	CG-CD-OE1	19.56	157.42	118.30
1	A	91	TRP	CZ3-CH2-CZ2	19.50	145.00	121.60
1	A	63	GLU	CG-CD-OE2	19.46	157.23	118.30
1	A	91	TRP	CE2-CD2-CE3	19.21	141.75	118.70
1	A	105	ARG	NE-CZ-NH2	18.93	129.76	120.30
1	A	78	ALA	N-CA-CB	-18.71	83.91	110.10
1	A	72	TYR	OH-CZ-CE2	18.64	170.43	120.10
1	A	128	LEU	CB-CG-CD2	18.56	142.56	111.00
1	A	109	MET	CA-CB-CG	18.38	144.55	113.30
1	A	39	PHE	CD1-CE1-CZ	18.33	142.09	120.10
1	A	72	TYR	CE1-CZ-OH	18.25	169.38	120.10
1	A	150	GLU	O-C-N	-18.19	93.59	122.70
1	A	128	LEU	CD1-CG-CD2	-18.14	56.08	110.50
1	A	157	ALA	O-C-N	-17.92	94.03	122.70
1	A	159	ASP	O-C-N	-17.78	94.25	122.70
1	A	159	ASP	CB-CG-OD1	17.72	134.25	118.30
1	A	63	GLU	C-N-CA	17.69	165.92	121.70
1	A	76	MET	CA-CB-CG	17.41	142.89	113.30
1	A	37	GLN	CG-CD-OE1	17.30	156.20	121.60
1	A	85	GLN	CG-CD-OE1	16.96	155.52	121.60
1	A	160	GLU	N-CA-CB	16.87	140.97	110.60
1	A	153	SER	CA-CB-OG	16.74	156.39	111.20
1	A	88	ASP	OD1-CG-OD2	16.54	154.73	123.30
1	A	91	TRP	NE1-CE2-CD2	-16.44	90.86	107.30
1	A	64	GLN	O-C-N	-15.81	97.40	122.70
1	A	37	GLN	CG-CD-NE2	15.63	154.21	116.70
1	A	87	GLY	O-C-N	-15.43	98.01	122.70
1	A	77	GLY	CA-C-N	-15.20	83.75	117.20
1	A	91	TRP	CD1-NE1-CE2	-15.09	95.42	109.00
1	A	160	GLU	CA-CB-CG	-15.02	80.36	113.40
1	A	160	GLU	CA-C-O	14.88	151.34	120.10
1	A	77	GLY	C-N-CA	-14.65	85.07	121.70
1	A	78	ALA	CB-CA-C	14.60	132.00	110.10
1	A	159	ASP	CA-C-N	14.58	149.28	117.20
1	A	78	ALA	CA-C-O	14.43	150.40	120.10
1	A	106	ARG	CG-CD-NE	14.30	141.84	111.80
1	A	160	GLU	CG-CD-OE1	14.08	146.47	118.30
1	A	74	ASN	OD1-CG-ND2	-14.04	89.62	121.90
1	A	105	ARG	CG-CD-NE	13.93	141.05	111.80
1	A	63	GLU	CG-CD-OE1	13.92	146.13	118.30
1	A	106	ARG	CA-C-N	13.79	143.78	116.20
1	A	99	TYR	OH-CZ-CE2	13.24	155.86	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	GLN	N-CA-C	13.19	146.62	111.00
1	A	77	GLY	N-CA-C	13.02	145.66	113.10
1	A	105	ARG	CA-C-N	13.01	145.82	117.20
1	A	159	ASP	C-N-CA	12.82	153.76	121.70
1	A	99	TYR	CE1-CZ-OH	12.22	153.09	120.10
1	A	154	GLU	CB-CG-CD	12.08	146.82	114.20
1	A	74	ASN	CB-CG-ND2	11.98	145.45	116.70
1	A	106	ARG	C-N-CA	11.51	146.47	122.30
1	A	90	ASN	OD1-CG-ND2	-11.30	95.91	121.90
1	A	122	GLU	CG-CD-OE2	11.27	140.83	118.30
1	A	88	ASP	CB-CA-C	-11.18	88.04	110.40
1	A	64	GLN	CB-CA-C	-11.11	88.19	110.40
1	A	88	ASP	CA-C-N	10.98	138.16	116.20
1	A	76	MET	CG-SD-CE	-10.93	82.71	100.20
1	A	76	MET	CA-C-O	10.68	142.53	120.10
1	A	105	ARG	C-N-CA	10.63	148.27	121.70
1	A	133	GLN	CG-CD-NE2	10.54	141.99	116.70
1	A	155	PRO	O-C-N	-10.40	106.06	122.70
1	A	51	GLN	CG-CD-OE1	10.35	142.30	121.60
1	A	51	GLN	CG-CD-NE2	10.26	141.32	116.70
1	A	90	ASN	CB-CG-OD1	10.12	141.83	121.60
1	A	133	GLN	CG-CD-OE1	10.10	141.80	121.60
1	A	89	GLY	N-CA-C	9.97	138.02	113.10
1	A	122	GLU	CG-CD-OE1	9.91	138.13	118.30
1	A	109	MET	CB-CG-SD	9.79	141.77	112.40
1	A	152	GLY	N-CA-C	9.67	137.27	113.10
1	A	83	TRP	NE1-CE2-CZ2	-9.01	120.49	130.40
1	A	107	GLY	O-C-N	-8.90	108.07	123.20
1	A	76	MET	CA-C-N	8.88	133.96	116.20
1	A	160	GLU	CB-CA-C	-8.87	92.67	110.40
1	A	88	ASP	C-N-CA	8.85	140.88	122.30
1	A	158	ASP	O-C-N	-8.62	108.90	122.70
1	A	105	ARG	CD-NE-CZ	8.58	135.62	123.60
1	A	88	ASP	N-CA-C	8.57	134.14	111.00
1	A	113	GLU	CB-CG-CD	8.49	137.12	114.20
1	A	79	ALA	CA-C-N	-8.40	99.41	116.20
1	A	88	ASP	CA-C-O	-8.31	102.64	120.10
1	A	79	ALA	C-N-CA	-8.17	105.14	122.30
1	A	78	ALA	CA-C-N	8.16	135.14	117.20
1	A	150	GLU	CA-C-N	8.09	134.99	117.20
1	A	65	ILE	CB-CG1-CD1	8.07	136.49	113.90
1	A	87	GLY	CA-C-N	7.95	134.68	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	GLN	CA-CB-CG	7.76	130.48	113.40
1	A	60	ARG	CG-CD-NE	7.71	127.99	111.80
1	A	64	GLN	CA-C-N	7.62	133.97	117.20
1	A	64	GLN	CB-CG-CD	7.59	131.33	111.60
1	A	150	GLU	C-N-CA	7.46	140.36	121.70
1	A	62	PRO	O-C-N	-7.02	111.46	122.70
1	A	144	MET	CG-SD-CE	6.92	111.27	100.20
1	A	157	ALA	CA-C-O	6.82	134.42	120.10
1	A	48	PHE	CA-CB-CG	6.75	130.11	113.90
1	A	158	ASP	C-N-CA	6.71	138.48	121.70
1	A	115	VAL	CG1-CB-CG2	-6.59	100.36	110.90
1	A	53	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	157	ALA	CA-C-N	6.52	131.55	117.20
1	A	87	GLY	C-N-CA	6.51	137.98	121.70
1	A	64	GLN	C-N-CA	6.39	137.67	121.70
1	A	120	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	A	137	LEU	CB-CG-CD1	6.24	121.60	111.00
1	A	156	ARG	CD-NE-CZ	6.22	132.31	123.60
1	A	85	GLN	CG-CD-NE2	6.22	131.63	116.70
1	A	78	ALA	N-CA-C	6.13	127.55	111.00
1	A	115	VAL	CA-CB-CG1	6.03	119.94	110.90
1	A	158	ASP	CA-C-N	5.89	130.16	117.20
1	A	157	ALA	C-N-CA	5.87	136.39	121.70
1	A	90	ASN	CA-CB-CG	5.84	126.25	113.40
1	A	103	SER	CA-CB-OG	5.82	126.91	111.20
1	A	79	ALA	CA-C-O	5.75	132.17	120.10
1	A	88	ASP	N-CA-CB	5.67	120.81	110.60
1	A	76	MET	C-N-CA	5.67	134.20	122.30
1	A	91	TRP	CA-CB-CG	5.58	124.30	113.70
1	A	78	ALA	C-N-CA	5.58	135.64	121.70
1	A	95	ASP	CA-CB-CG	5.45	125.39	113.40
1	A	156	ARG	NH1-CZ-NH2	5.45	125.39	119.40
1	A	150	GLU	CA-C-O	5.38	131.39	120.10
1	A	80	GLY	N-CA-C	5.37	126.51	113.10
1	A	63	GLU	N-CA-CB	5.34	120.22	110.60
1	A	85	GLN	N-CA-C	5.17	124.95	111.00

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	64	GLN	CA
1	A	78	ALA	CA
1	A	160	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	927	891	858	345
All	All	927	891	858	345

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 193.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:49:PHE:CE2	1:A:49:PHE:CG	1.63	1.82
1:A:49:PHE:CD1	1:A:49:PHE:CZ	1.63	1.80
1:A:39:PHE:CZ	1:A:39:PHE:CD1	1.57	1.93
1:A:156:ARG:CZ	1:A:156:ARG:CD	1.56	1.81
1:A:109:MET:CG	1:A:109:MET:CA	1.52	1.85
1:A:126:PHE:CD1	1:A:126:PHE:CZ	1.52	1.95
1:A:39:PHE:CE2	1:A:39:PHE:CG	1.52	1.94
1:A:99:TYR:CD1	1:A:99:TYR:CZ	1.52	1.97
1:A:126:PHE:CG	1:A:126:PHE:CE2	1.51	1.96
1:A:105:ARG:CZ	1:A:105:ARG:CD	1.50	1.86
1:A:49:PHE:CD2	1:A:49:PHE:CB	1.50	1.92
1:A:78:ALA:C	1:A:79:ALA:CA	1.47	1.83
1:A:99:TYR:CE2	1:A:99:TYR:CG	1.46	2.00
1:A:39:PHE:CD2	1:A:39:PHE:CZ	1.46	2.00
1:A:128:LEU:CB	1:A:128:LEU:CD2	1.45	1.92
1:A:39:PHE:CE1	1:A:39:PHE:CG	1.45	2.01
1:A:99:TYR:CD2	1:A:99:TYR:CZ	1.44	2.05
1:A:72:TYR:CE2	1:A:72:TYR:CG	1.44	2.04
1:A:72:TYR:CZ	1:A:72:TYR:CD1	1.44	2.01
1:A:76:MET:C	1:A:77:GLY:CA	1.44	1.81
1:A:99:TYR:CE1	1:A:99:TYR:CG	1.41	2.08
1:A:95:ASP:OD1	1:A:95:ASP:CB	1.40	1.69
1:A:98:PHE:CZ	1:A:98:PHE:CD2	1.40	2.08
1:A:39:PHE:CD2	1:A:39:PHE:CB	1.40	2.05
1:A:85:GLN:OE1	1:A:85:GLN:CG	1.40	1.69

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:60:ARG:NE	1:A:60:ARG:NH1	1.39	1.66
1:A:153:SER:OG	1:A:153:SER:CA	1.39	1.69
1:A:156:ARG:NH2	1:A:156:ARG:NH1	1.39	1.61
1:A:126:PHE:CE1	1:A:126:PHE:CG	1.37	2.12
1:A:98:PHE:CE1	1:A:98:PHE:CG	1.37	2.10
1:A:98:PHE:CZ	1:A:98:PHE:CD1	1.36	2.11
1:A:126:PHE:CD2	1:A:126:PHE:CZ	1.36	2.10
1:A:76:MET:CA	1:A:77:GLY:N	1.36	1.87
1:A:72:TYR:CG	1:A:72:TYR:CE1	1.36	2.12
1:A:156:ARG:NH2	1:A:156:ARG:NE	1.35	1.69
1:A:126:PHE:CD2	1:A:126:PHE:CB	1.35	2.08
1:A:95:ASP:OD2	1:A:95:ASP:CB	1.35	1.73
1:A:98:PHE:CE2	1:A:98:PHE:CG	1.35	2.12
1:A:78:ALA:CA	1:A:79:ALA:N	1.34	1.90
1:A:72:TYR:CZ	1:A:72:TYR:CD2	1.33	2.09
1:A:64:GLN:C	1:A:65:ILE:CA	1.32	1.96
1:A:99:TYR:CD2	1:A:99:TYR:CB	1.32	2.12
1:A:39:PHE:CB	1:A:39:PHE:CD1	1.31	2.12
1:A:133:GLN:NE2	1:A:133:GLN:CG	1.30	1.92
1:A:64:GLN:CA	1:A:64:GLN:O	1.30	1.79
1:A:157:ALA:C	1:A:158:ASP:CA	1.29	1.99
1:A:49:PHE:CZ	1:A:49:PHE:CD2	1.28	1.98
1:A:150:GLU:CG	1:A:150:GLU:OE2	1.28	1.79
1:A:76:MET:CG	1:A:76:MET:CA	1.27	2.11
1:A:64:GLN:CA	1:A:65:ILE:N	1.27	1.95
1:A:49:PHE:CG	1:A:49:PHE:CE1	1.26	1.99
1:A:72:TYR:CD2	1:A:72:TYR:CB	1.24	2.17
1:A:139:ASP:OD2	1:A:139:ASP:CB	1.24	1.84
1:A:64:GLN:O	1:A:64:GLN:CB	1.22	1.87
1:A:98:PHE:CD1	1:A:98:PHE:CB	1.22	2.21
1:A:157:ALA:CA	1:A:158:ASP:N	1.21	2.03
1:A:139:ASP:CB	1:A:139:ASP:OD1	1.20	1.87
1:A:84:ASP:OD1	1:A:84:ASP:CB	1.20	1.88
1:A:133:GLN:OE1	1:A:133:GLN:CG	1.19	1.84
1:A:84:ASP:CB	1:A:84:ASP:OD2	1.19	1.91
1:A:37:GLN:CG	1:A:37:GLN:NE2	1.19	2.04
1:A:64:GLN:CB	1:A:65:ILE:N	1.18	2.07
1:A:98:PHE:CB	1:A:98:PHE:CD2	1.18	2.25
1:A:103:SER:OG	1:A:103:SER:HB3	1.16	1.39
1:A:130:GLU:CG	1:A:130:GLU:OE2	1.15	1.93
1:A:99:TYR:OH	1:A:99:TYR:CE1	1.14	1.96
1:A:78:ALA:C	1:A:79:ALA:CB	1.14	2.15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:154:GLU:CD	1:A:154:GLU:CB	1.13	2.14
1:A:99:TYR:CD1	1:A:99:TYR:CB	1.13	2.20
1:A:72:TYR:CE1	1:A:72:TYR:OH	1.12	2.01
1:A:157:ALA:O	1:A:157:ALA:CA	1.12	1.98
1:A:76:MET:HE1	1:A:76:MET:CG	1.11	1.74
1:A:105:ARG:CG	1:A:105:ARG:NE	1.09	2.15
1:A:144:MET:SD	1:A:144:MET:CE	1.09	0.99
1:A:54:ASP:OD1	1:A:54:ASP:CB	1.09	1.99
1:A:144:MET:CE	1:A:144:MET:CG	1.08	2.30
1:A:78:ALA:HA	1:A:79:ALA:N	1.08	1.59
1:A:130:GLU:CG	1:A:130:GLU:OE1	1.07	2.00
1:A:103:SER:CB	1:A:103:SER:OG	1.07	0.77
1:A:51:GLN:NE2	1:A:51:GLN:CG	1.07	2.18
1:A:41:GLU:OE1	1:A:41:GLU:CG	1.07	2.01
1:A:76:MET:CA	1:A:76:MET:O	1.06	1.95
1:A:37:GLN:CG	1:A:37:GLN:OE1	1.06	2.02
1:A:142:ASP:CB	1:A:142:ASP:OD2	1.05	2.03
1:A:128:LEU:HG	1:A:128:LEU:CD2	1.04	1.63
1:A:103:SER:CA	1:A:103:SER:OG	1.02	2.07
1:A:128:LEU:HD12	1:A:128:LEU:CD2	1.02	1.74
1:A:103:SER:HB2	1:A:103:SER:OG	1.02	1.39
1:A:121:ASP:CB	1:A:121:ASP:OD2	1.01	2.08
1:A:64:GLN:HB2	1:A:65:ILE:N	1.01	1.51
1:A:105:ARG:HD2	1:A:105:ARG:NE	1.00	1.40
1:A:75:ASP:OD1	1:A:75:ASP:CB	1.00	2.09
1:A:41:GLU:CG	1:A:41:GLU:OE2	0.99	2.11
1:A:105:ARG:CD	1:A:105:ARG:NE	0.99	0.84
1:A:121:ASP:CB	1:A:121:ASP:OD1	0.98	2.11
1:A:105:ARG:HD3	1:A:105:ARG:NE	0.98	1.40
1:A:76:MET:CG	1:A:76:MET:HE2	0.98	1.51
1:A:75:ASP:OD2	1:A:75:ASP:CB	0.97	2.12
1:A:51:GLN:OE1	1:A:51:GLN:CG	0.97	2.11
1:A:144:MET:SD	1:A:144:MET:HE3	0.97	1.60
1:A:142:ASP:OD1	1:A:142:ASP:CB	0.95	2.14
1:A:122:GLU:OE1	1:A:122:GLU:CG	0.95	2.13
1:A:76:MET:CE	1:A:87:GLY:O	0.95	2.14
1:A:144:MET:SD	1:A:144:MET:HE1	0.95	1.60
1:A:64:GLN:HB3	1:A:64:GLN:O	0.95	1.58
1:A:99:TYR:CE2	1:A:99:TYR:OH	0.94	2.05
1:A:144:MET:SD	1:A:144:MET:HE2	0.94	1.60
1:A:84:ASP:C	1:A:85:GLN:HG3	0.94	1.79
1:A:128:LEU:HD12	1:A:128:LEU:HD21	0.92	1.33

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:122:GLU:CG	1:A:122:GLU:OE2	0.92	2.18
1:A:77:GLY:O	1:A:79:ALA:N	0.91	2.03
1:A:153:SER:OG	1:A:153:SER:HB2	0.91	1.14
1:A:76:MET:CG	1:A:76:MET:HB2	0.90	1.44
1:A:153:SER:OG	1:A:153:SER:HB3	0.90	1.14
1:A:76:MET:HE2	1:A:87:GLY:O	0.90	1.66
1:A:150:GLU:O	1:A:152:GLY:N	0.90	1.86
1:A:126:PHE:CD1	1:A:126:PHE:CB	0.90	2.23
1:A:76:MET:CG	1:A:76:MET:CB	0.89	0.89
1:A:72:TYR:CB	1:A:72:TYR:CD1	0.88	2.25
1:A:76:MET:CG	1:A:76:MET:CE	0.88	0.88
1:A:154:GLU:CD	1:A:154:GLU:HG3	0.88	1.34
1:A:106:ARG:CZ	1:A:113:GLU:O	0.88	2.22
1:A:76:MET:HB3	1:A:76:MET:CG	0.87	1.44
1:A:154:GLU:CD	1:A:154:GLU:HG2	0.87	1.34
1:A:154:GLU:CD	1:A:154:GLU:CG	0.87	0.78
1:A:98:PHE:CE2	1:A:98:PHE:HZ	0.86	1.65
1:A:78:ALA:C	1:A:80:GLY:N	0.86	2.29
1:A:39:PHE:CE1	1:A:39:PHE:HZ	0.86	1.61
1:A:128:LEU:CG	1:A:128:LEU:HD23	0.84	1.39
1:A:54:ASP:OD2	1:A:54:ASP:CB	0.84	2.15
1:A:51:GLN:HE21	1:A:51:GLN:CD	0.83	1.44
1:A:142:ASP:OD1	1:A:142:ASP:CG	0.83	0.65
1:A:128:LEU:CD2	1:A:128:LEU:CD1	0.83	0.83
1:A:122:GLU:CD	1:A:122:GLU:OE1	0.83	0.76
1:A:107:GLY:O	1:A:109:MET:N	0.83	2.12
1:A:51:GLN:CD	1:A:51:GLN:HE22	0.82	1.44
1:A:41:GLU:CD	1:A:41:GLU:OE2	0.82	0.64
1:A:37:GLN:OE1	1:A:37:GLN:CD	0.81	0.63
1:A:39:PHE:CE2	1:A:39:PHE:CZ	0.81	0.82
1:A:39:PHE:HZ	1:A:39:PHE:CE2	0.80	1.66
1:A:85:GLN:OE1	1:A:85:GLN:NE2	0.80	0.65
1:A:122:GLU:CD	1:A:122:GLU:OE2	0.80	0.80
1:A:39:PHE:CD1	1:A:39:PHE:CG	0.80	0.83
1:A:76:MET:CG	1:A:76:MET:SD	0.80	0.70
1:A:85:GLN:OE1	1:A:85:GLN:CB	0.80	2.28
1:A:64:GLN:C	1:A:65:ILE:N	0.79	0.85
1:A:157:ALA:C	1:A:158:ASP:N	0.78	0.84
1:A:128:LEU:CD2	1:A:128:LEU:HD13	0.78	1.34
1:A:54:ASP:OD2	1:A:54:ASP:CG	0.78	0.78
1:A:121:ASP:CG	1:A:121:ASP:OD1	0.78	0.62
1:A:128:LEU:HD21	1:A:128:LEU:CD1	0.78	0.71

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:98:PHE:CD2	1:A:98:PHE:CG	0.77	0.80
1:A:75:ASP:CG	1:A:75:ASP:OD2	0.77	0.71
1:A:133:GLN:CD	1:A:133:GLN:HE21	0.77	1.37
1:A:126:PHE:CE1	1:A:126:PHE:HZ	0.76	1.55
1:A:98:PHE:CZ	1:A:98:PHE:CE1	0.76	0.79
1:A:121:ASP:CG	1:A:121:ASP:OD2	0.76	0.59
1:A:98:PHE:HZ	1:A:98:PHE:CE1	0.76	1.67
1:A:126:PHE:CG	1:A:126:PHE:CD1	0.75	0.81
1:A:98:PHE:CD1	1:A:98:PHE:CG	0.75	0.78
1:A:51:GLN:NE2	1:A:51:GLN:CD	0.75	0.80
1:A:39:PHE:CD2	1:A:39:PHE:CG	0.74	0.77
1:A:39:PHE:CE1	1:A:39:PHE:CZ	0.74	0.76
1:A:153:SER:OG	1:A:153:SER:CB	0.74	0.50
1:A:99:TYR:CD1	1:A:99:TYR:CG	0.73	0.79
1:A:98:PHE:CZ	1:A:98:PHE:CE2	0.73	0.76
1:A:139:ASP:CG	1:A:139:ASP:OD1	0.73	0.59
1:A:85:GLN:OE1	1:A:85:GLN:CD	0.73	0.65
1:A:76:MET:HG3	1:A:76:MET:SD	0.73	1.38
1:A:78:ALA:CA	1:A:78:ALA:O	0.73	2.10
1:A:128:LEU:HD22	1:A:128:LEU:CD1	0.72	1.28
1:A:133:GLN:HE22	1:A:133:GLN:CD	0.72	1.37
1:A:128:LEU:CG	1:A:128:LEU:HD22	0.72	1.39
1:A:106:ARG:NH2	1:A:113:GLU:O	0.72	2.14
1:A:109:MET:HB2	1:A:109:MET:CG	0.72	1.25
1:A:130:GLU:CD	1:A:130:GLU:OE1	0.72	0.60
1:A:139:ASP:CG	1:A:139:ASP:OD2	0.71	0.55
1:A:150:GLU:CD	1:A:150:GLU:OE2	0.71	0.62
1:A:128:LEU:HD22	1:A:128:LEU:HD13	0.71	0.93
1:A:82:THR:O	1:A:85:GLN:HG2	0.71	1.85
1:A:156:ARG:HH11	1:A:156:ARG:CZ	0.71	1.43
1:A:109:MET:CG	1:A:109:MET:HB3	0.71	1.25
1:A:126:PHE:CZ	1:A:126:PHE:CE2	0.71	0.80
1:A:95:ASP:HA	1:A:137:LEU:HD13	0.71	1.62
1:A:49:PHE:CE1	1:A:49:PHE:HZ	0.71	1.48
1:A:156:ARG:HE	1:A:156:ARG:CZ	0.71	1.43
1:A:78:ALA:C	1:A:79:ALA:HB3	0.71	2.05
1:A:128:LEU:CG	1:A:128:LEU:CD2	0.71	0.72
1:A:84:ASP:CG	1:A:84:ASP:OD2	0.70	0.57
1:A:51:GLN:CD	1:A:51:GLN:OE1	0.70	0.73
1:A:99:TYR:CE2	1:A:99:TYR:CZ	0.70	0.77
1:A:142:ASP:OD2	1:A:142:ASP:CG	0.69	0.55
1:A:41:GLU:CD	1:A:41:GLU:OE1	0.69	0.54

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:156:ARG:HH12	1:A:156:ARG:CZ	0.69	1.43
1:A:37:GLN:CD	1:A:37:GLN:HE21	0.69	1.31
1:A:37:GLN:CD	1:A:37:GLN:HE22	0.69	1.31
1:A:105:ARG:HE	1:A:105:ARG:CD	0.69	1.41
1:A:157:ALA:C	1:A:158:ASP:C	0.69	2.51
1:A:60:ARG:NH1	1:A:60:ARG:CZ	0.69	0.62
1:A:76:MET:HE1	1:A:87:GLY:O	0.69	1.87
1:A:54:ASP:OD1	1:A:54:ASP:CG	0.69	0.65
1:A:106:ARG:NH1	1:A:113:GLU:O	0.68	2.23
1:A:135:LEU:HD13	1:A:140:ILE:HD13	0.68	1.64
1:A:130:GLU:O	1:A:131:GLY:O	0.68	2.11
1:A:75:ASP:OD1	1:A:75:ASP:CG	0.67	0.68
1:A:76:MET:HG3	1:A:76:MET:HE3	0.67	1.11
1:A:156:ARG:CZ	1:A:156:ARG:NE	0.67	0.85
1:A:109:MET:CB	1:A:109:MET:HG3	0.67	1.26
1:A:37:GLN:NE2	1:A:37:GLN:CD	0.67	0.65
1:A:133:GLN:NE2	1:A:133:GLN:CD	0.66	0.72
1:A:76:MET:HG2	1:A:76:MET:CE	0.66	1.04
1:A:37:GLN:OE1	1:A:37:GLN:NE2	0.66	0.54
1:A:109:MET:CB	1:A:109:MET:HG2	0.66	1.26
1:A:109:MET:HG2	1:A:109:MET:SD	0.66	1.42
1:A:76:MET:C	1:A:77:GLY:HA2	0.66	2.03
1:A:39:PHE:HD1	1:A:39:PHE:CG	0.65	1.42
1:A:126:PHE:CE1	1:A:126:PHE:CZ	0.65	0.66
1:A:84:ASP:CG	1:A:84:ASP:OD1	0.65	0.53
1:A:39:PHE:CZ	1:A:39:PHE:HE2	0.65	1.41
1:A:82:THR:HG1	1:A:85:GLN:N	0.65	1.90
1:A:156:ARG:HD2	1:A:156:ARG:CZ	0.65	2.12
1:A:109:MET:HG3	1:A:109:MET:SD	0.65	1.42
1:A:85:GLN:HB3	1:A:86:PRO:HD2	0.65	1.66
1:A:76:MET:CB	1:A:76:MET:O	0.65	2.45
1:A:99:TYR:CD2	1:A:99:TYR:CG	0.64	0.72
1:A:92:ILE:HG21	1:A:118:SER:HB2	0.64	1.69
1:A:156:ARG:CZ	1:A:156:ARG:NH1	0.64	0.79
1:A:77:GLY:HA2	1:A:86:PRO:HG3	0.63	1.71
1:A:105:ARG:HD3	1:A:130:GLU:OE1	0.63	1.94
1:A:130:GLU:CD	1:A:130:GLU:OE2	0.63	0.52
1:A:99:TYR:CZ	1:A:99:TYR:CE1	0.62	0.69
1:A:105:ARG:CZ	1:A:105:ARG:HD3	0.62	1.88
1:A:72:TYR:CG	1:A:72:TYR:CD1	0.62	0.76
1:A:72:TYR:CE2	1:A:72:TYR:OH	0.62	2.09
1:A:39:PHE:HD2	1:A:39:PHE:CG	0.62	1.38

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:153:SER:N	1:A:153:SER:OG	0.62	2.27
1:A:76:MET:HG3	1:A:76:MET:CB	0.62	1.53
1:A:39:PHE:CZ	1:A:39:PHE:HE1	0.61	1.38
1:A:76:MET:C	1:A:77:GLY:N	0.61	0.69
1:A:103:SER:CB	1:A:103:SER:HG	0.61	1.32
1:A:109:MET:CB	1:A:109:MET:CG	0.59	0.64
1:A:126:PHE:CD2	1:A:126:PHE:CG	0.59	0.67
1:A:72:TYR:CZ	1:A:72:TYR:CE1	0.59	0.65
1:A:106:ARG:CZ	1:A:106:ARG:HH11	0.59	1.30
1:A:98:PHE:CG	1:A:98:PHE:HD2	0.59	1.36
1:A:109:MET:CG	1:A:109:MET:N	0.59	2.58
1:A:72:TYR:CZ	1:A:72:TYR:CE2	0.59	0.73
1:A:98:PHE:CZ	1:A:98:PHE:HE1	0.59	1.35
1:A:99:TYR:HD1	1:A:99:TYR:CG	0.58	1.34
1:A:126:PHE:CG	1:A:126:PHE:HD1	0.58	1.34
1:A:60:ARG:NH1	1:A:60:ARG:HH21	0.58	1.15
1:A:98:PHE:CZ	1:A:98:PHE:HE2	0.58	1.34
1:A:95:ASP:OD2	1:A:95:ASP:CG	0.58	0.52
1:A:98:PHE:HD1	1:A:98:PHE:CG	0.58	1.34
1:A:85:GLN:HB3	1:A:86:PRO:CD	0.58	2.25
1:A:95:ASP:OD1	1:A:95:ASP:CG	0.57	0.48
1:A:126:PHE:HE2	1:A:126:PHE:CZ	0.57	1.33
1:A:149:VAL:O	1:A:149:VAL:HG12	0.57	1.99
1:A:128:LEU:HD11	1:A:128:LEU:CD2	0.57	1.10
1:A:144:MET:HE2	1:A:144:MET:CG	0.57	2.12
1:A:99:TYR:CZ	1:A:99:TYR:HE2	0.57	1.32
1:A:77:GLY:HA2	1:A:86:PRO:CG	0.57	2.30
1:A:76:MET:HG2	1:A:76:MET:HE2	0.56	1.22
1:A:157:ALA:N	1:A:158:ASP:N	0.56	2.52
1:A:157:ALA:O	1:A:157:ALA:C	0.56	0.76
1:A:133:GLN:NE2	1:A:144:MET:SD	0.56	2.78
1:A:78:ALA:C	1:A:78:ALA:O	0.55	0.76
1:A:78:ALA:C	1:A:79:ALA:N	0.55	0.63
1:A:133:GLN:NE2	1:A:133:GLN:CB	0.55	2.67
1:A:60:ARG:HH11	1:A:60:ARG:HH22	0.55	0.62
1:A:130:GLU:O	1:A:131:GLY:C	0.55	2.43
1:A:60:ARG:HH12	1:A:60:ARG:HH21	0.55	0.79
1:A:99:TYR:HD2	1:A:99:TYR:CG	0.54	1.29
1:A:60:ARG:HH11	1:A:60:ARG:CZ	0.54	1.29
1:A:158:ASP:O	1:A:158:ASP:CG	0.54	2.43
1:A:91:TRP:HZ3	1:A:91:TRP:CE2	0.54	1.39
1:A:49:PHE:CZ	1:A:49:PHE:CE1	0.53	0.55

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:105:ARG:NH1	1:A:105:ARG:HD3	0.53	2.12
1:A:128:LEU:HB3	1:A:128:LEU:CD2	0.53	2.20
1:A:99:TYR:CZ	1:A:99:TYR:HE1	0.53	1.28
1:A:139:ASP:OD2	1:A:156:ARG:NH2	0.53	2.41
1:A:80:GLY:O	1:A:81:ALA:C	0.53	2.33
1:A:72:TYR:CG	1:A:72:TYR:CD2	0.53	0.68
1:A:133:GLN:OE1	1:A:133:GLN:CD	0.52	0.63
1:A:76:MET:C	1:A:76:MET:O	0.52	0.72
1:A:60:ARG:HE	1:A:60:ARG:CB	0.52	1.83
1:A:76:MET:C	1:A:77:GLY:HA3	0.52	2.11
1:A:144:MET:HE2	1:A:155:PRO:CB	0.52	2.35
1:A:92:ILE:HD13	1:A:118:SER:HB2	0.52	1.80
1:A:80:GLY:O	1:A:81:ALA:HB3	0.52	2.04
1:A:84:ASP:O	1:A:85:GLN:CB	0.52	2.47
1:A:41:GLU:HB3	1:A:67:PRO:HG2	0.51	1.80
1:A:76:MET:SD	1:A:87:GLY:O	0.51	2.52
1:A:109:MET:HE3	1:A:109:MET:SD	0.51	1.14
1:A:109:MET:HE2	1:A:109:MET:SD	0.51	1.14
1:A:109:MET:SD	1:A:109:MET:HE1	0.51	1.14
1:A:105:ARG:HD3	1:A:130:GLU:OE2	0.51	2.06
1:A:109:MET:HG2	1:A:109:MET:CA	0.51	1.94
1:A:95:ASP:CA	1:A:137:LEU:HD13	0.51	2.35
1:A:53:ARG:HD3	1:A:54:ASP:N	0.50	2.22
1:A:49:PHE:CD1	1:A:49:PHE:CG	0.50	0.73
1:A:126:PHE:HE1	1:A:126:PHE:CZ	0.50	1.25
1:A:49:PHE:CZ	1:A:49:PHE:CE2	0.50	0.72
1:A:126:PHE:CG	1:A:126:PHE:HD2	0.50	1.26
1:A:84:ASP:O	1:A:85:GLN:HG3	0.49	2.06
1:A:64:GLN:C	1:A:64:GLN:O	0.49	0.70
1:A:72:TYR:CG	1:A:72:TYR:HD1	0.48	1.24
1:A:157:ALA:O	1:A:157:ALA:CB	0.48	2.56
1:A:106:ARG:HE	1:A:113:GLU:H	0.48	1.50
1:A:91:TRP:CG	1:A:91:TRP:HD1	0.48	1.24
1:A:40:LEU:HD23	1:A:66:ALA:HB3	0.47	1.84
1:A:95:ASP:HA	1:A:137:LEU:CD1	0.47	2.38
1:A:127:VAL:HA	1:A:131:GLY:HA3	0.47	1.85
1:A:144:MET:CE	1:A:155:PRO:CB	0.47	2.92
1:A:36:ALA:HB2	1:A:52:VAL:HA	0.47	1.87
1:A:56:ILE:CD1	1:A:114:ALA:HB3	0.47	2.39
1:A:72:TYR:CZ	1:A:72:TYR:HE2	0.47	1.23
1:A:144:MET:HE2	1:A:155:PRO:HB2	0.46	1.85
1:A:139:ASP:OD2	1:A:139:ASP:OD1	0.46	0.46

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:65:ILE:HG23	1:A:66:ALA:N	0.46	2.26
1:A:76:MET:HG2	1:A:76:MET:CB	0.46	1.53
1:A:82:THR:C	1:A:84:ASP:N	0.45	2.58
1:A:49:PHE:HD1	1:A:49:PHE:CG	0.45	1.20
1:A:75:ASP:N	1:A:90:ASN:O	0.45	2.49
1:A:76:MET:HG2	1:A:76:MET:HE3	0.45	0.65
1:A:72:TYR:CG	1:A:72:TYR:HD2	0.44	1.20
1:A:56:ILE:HD12	1:A:114:ALA:HB3	0.44	1.88
1:A:49:PHE:CZ	1:A:49:PHE:HE2	0.44	1.20
1:A:137:LEU:HD23	1:A:137:LEU:O	0.44	2.12
1:A:106:ARG:HG3	1:A:113:GLU:H	0.44	1.73
1:A:72:TYR:CZ	1:A:72:TYR:HE1	0.43	1.18
1:A:133:GLN:CD	1:A:144:MET:SD	0.43	2.97
1:A:156:ARG:HG3	1:A:157:ALA:N	0.42	2.29
1:A:158:ASP:O	1:A:158:ASP:CB	0.42	2.34
1:A:157:ALA:C	1:A:158:ASP:CB	0.42	2.77
1:A:149:VAL:O	1:A:150:GLU:HB2	0.42	2.14
1:A:156:ARG:NH1	1:A:156:ARG:HH22	0.42	1.90
1:A:130:GLU:HG3	1:A:131:GLY:N	0.42	2.30
1:A:114:ALA:O	1:A:116:PRO:HD3	0.41	2.16
1:A:137:LEU:HD23	1:A:137:LEU:C	0.41	2.35
1:A:153:SER:HG	1:A:153:SER:CB	0.41	1.11
1:A:84:ASP:O	1:A:85:GLN:CG	0.40	2.66
1:A:84:ASP:O	1:A:85:GLN:HB2	0.40	2.13
1:A:36:ALA:CB	1:A:52:VAL:HA	0.40	2.46
1:A:76:MET:CG	1:A:76:MET:HE3	0.40	0.94

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	124/175 (71%)	101 (81%)	12 (10%)	11 (9%)	2 13
All	All	124/175 (71%)	101 (81%)	12 (10%)	11 (9%)	2 13

All 11 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	157	ALA
1	A	61	GLY
1	A	131	GLY
1	A	151	THR
1	A	80	GLY
1	A	148	PRO
1	A	106	ARG
1	A	132	GLY
1	A	155	PRO
1	A	63	GLU
1	A	108	GLY

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	90/131 (69%)	76 (84%)	14 (16%)	7 45
All	All	90/131 (69%)	76 (84%)	14 (16%)	7 45

All 14 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	135	LEU
1	A	49	PHE
1	A	117	PHE
1	A	91	TRP
1	A	64	GLN
1	A	154	GLU
1	A	53	ARG
1	A	160	GLU
1	A	48	PHE
1	A	156	ARG
1	A	128	LEU
1	A	133	GLN
1	A	63	GLU
1	A	95	ASP

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided