



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:41 PM GMT

PDB ID : 1LKR  
Title : MONOCLINIC HEN EGG WHITE LYSOZYME IODIDE  
Authors : Steinrauf, L.K.  
Deposited on : 1998-01-20  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

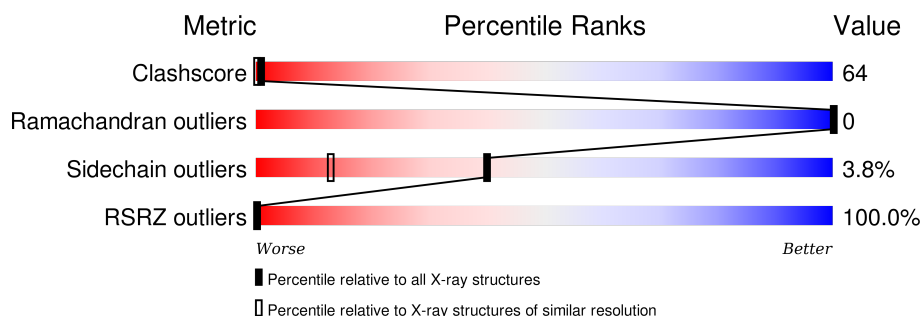
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	129	<div> <div>100%</div> <div> <div>7%</div> <div>59%</div> <div>33%</div> <div>.</div> </div> </div>
1	B	129	<div> <div>100%</div> <div> <div>6%</div> <div>69%</div> <div>22%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	142	-	-	X	X
2	IOD	B	131	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2330 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			
1	B	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	I	0	0
			6	6		
2	A	11	Total	I	0	0
			11	11		

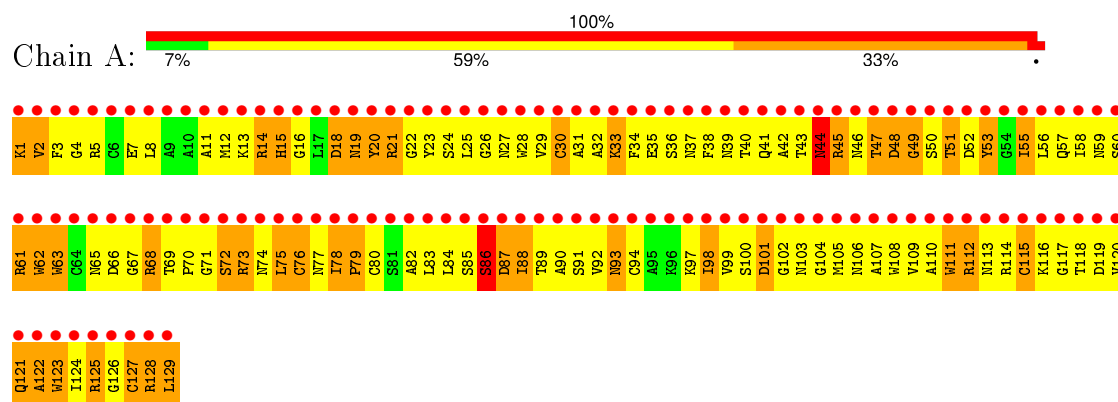
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total	O	0	0
			143	143		
3	B	168	Total	O	0	0
			168	168		

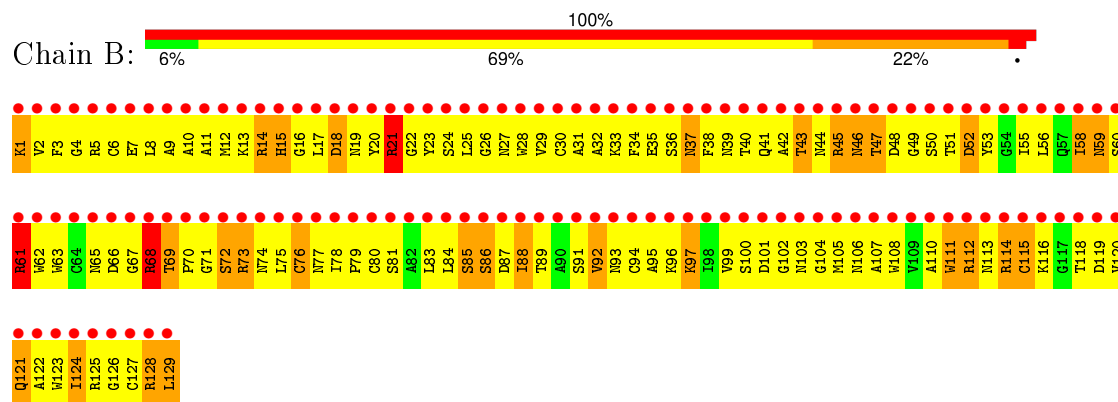
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: LYSOZYME



#### • Molecule 1: LYSOZYME



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	27.89Å 63.15Å 60.23Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	8.00 – 1.60 27.97 – 0.82	Depositor EDS
% Data completeness (in resolution range)	63.0 (8.00-1.60) 9.5 (27.97-0.82)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 0.82Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.106 , 0.140 0.496 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	0.1	Xtriage
Anisotropy	2.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 15.5	EDS
Estimated twinning fraction	0.012 for -h,-l,-k 0.000 for -h,l,k 0.065 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 19471 reflections	Xtriage
$F_o, F_c$ correlation	0.34	EDS
Total number of atoms	2330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	4.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	6.61	314/1021 (30.8%)	7.37	392/1379 (28.4%)
1	B	6.84	298/1021 (29.2%)	7.63	345/1379 (25.0%)
All	All	6.72	612/2042 (30.0%)	7.50	737/2758 (26.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (612) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	21	ARG	NE-CZ	-77.11	0.32	1.33
1	B	61	ARG	CZ-NH1	65.64	2.18	1.33
1	A	45	ARG	CZ-NH1	52.65	2.01	1.33
1	B	45	ARG	CZ-NH1	40.81	1.86	1.33
1	B	128	ARG	NE-CZ	38.80	1.83	1.33
1	B	114	ARG	NE-CZ	37.45	1.81	1.33
1	B	128	ARG	CZ-NH2	35.97	1.79	1.33
1	A	112	ARG	CZ-NH1	-33.47	0.89	1.33
1	B	73	ARG	CZ-NH1	31.80	1.74	1.33
1	A	45	ARG	NE-CZ	31.75	1.74	1.33
1	A	125	ARG	CZ-NH1	30.22	1.72	1.33
1	B	14	ARG	CD-NE	-30.19	0.95	1.46
1	A	47	THR	N-CA	30.12	2.06	1.46
1	A	87	ASP	CB-CG	29.64	2.13	1.51
1	A	112	ARG	CZ-NH2	29.45	1.71	1.33
1	A	48	ASP	C-N	29.43	1.86	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	ARG	CB-CG	29.05	2.31	1.52
1	B	61	ARG	CZ-NH2	26.69	1.67	1.33
1	A	14	ARG	CZ-NH1	-24.49	1.01	1.33
1	B	114	ARG	CZ-NH2	24.33	1.64	1.33
1	A	68	ARG	NE-CZ	-23.81	1.02	1.33
1	A	62	TRP	CG-CD2	-23.59	1.03	1.43
1	A	121	GLN	CB-CG	23.20	2.15	1.52
1	B	45	ARG	NE-CZ	-22.87	1.03	1.33
1	B	53	TYR	CE1-CZ	-22.34	1.09	1.38
1	A	14	ARG	CD-NE	22.12	1.84	1.46
1	B	47	THR	CB-OG1	21.55	1.86	1.43
1	A	21	ARG	NE-CZ	20.80	1.60	1.33
1	A	45	ARG	CG-CD	20.68	2.03	1.51
1	B	68	ARG	CD-NE	-20.53	1.11	1.46
1	A	129	LEU	CA-CB	20.04	1.99	1.53
1	A	45	ARG	CD-NE	-19.61	1.13	1.46
1	A	72	SER	CA-CB	19.61	1.82	1.52
1	A	5	ARG	CZ-NH2	19.57	1.58	1.33
1	A	87	ASP	CA-CB	19.04	1.95	1.53
1	A	114	ARG	CZ-NH1	-18.91	1.08	1.33
1	B	21	ARG	CZ-NH2	18.88	1.57	1.33
1	A	112	ARG	CD-NE	18.03	1.77	1.46
1	B	19	ASN	CB-CG	-17.85	1.09	1.51
1	B	61	ARG	CD-NE	-17.41	1.16	1.46
1	A	48	ASP	CG-OD1	-17.09	0.86	1.25
1	B	5	ARG	C-O	-17.07	0.91	1.23
1	B	15	HIS	CB-CG	17.04	1.80	1.50
1	B	112	ARG	CB-CG	-17.02	1.06	1.52
1	B	19	ASN	CG-OD1	16.84	1.61	1.24
1	A	7	GLU	CG-CD	-16.60	1.27	1.51
1	B	21	ARG	CZ-NH1	16.45	1.54	1.33
1	A	72	SER	C-O	16.11	1.53	1.23
1	B	14	ARG	NE-CZ	16.06	1.53	1.33
1	A	68	ARG	CD-NE	15.99	1.73	1.46
1	A	2	VAL	CA-CB	-15.95	1.21	1.54
1	A	62	TRP	CD1-NE1	15.93	1.65	1.38
1	A	30	CYS	CB-SG	15.87	2.09	1.82
1	B	44	ASN	C-O	-15.86	0.93	1.23
1	A	62	TRP	CZ2-CH2	15.86	1.67	1.37
1	A	108	TRP	CD2-CE2	15.74	1.60	1.41
1	A	41	GLN	CD-OE1	15.45	1.57	1.24
1	A	57	GLN	CD-OE1	15.38	1.57	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	SER	CA-CB	15.37	1.75	1.52
1	B	73	ARG	NE-CZ	-15.29	1.13	1.33
1	A	78	ILE	CA-CB	15.22	1.89	1.54
1	B	69	THR	CB-OG1	15.19	1.73	1.43
1	A	62	TRP	CA-CB	15.15	1.87	1.53
1	A	34	PHE	CG-CD2	-15.12	1.16	1.38
1	B	44	ASN	CG-ND2	-15.07	0.95	1.32
1	A	121	GLN	CD-OE1	14.93	1.56	1.24
1	A	45	ARG	CZ-NH2	-14.90	1.13	1.33
1	B	60	SER	CB-OG	-14.84	1.23	1.42
1	B	62	TRP	CG-CD1	-14.81	1.16	1.36
1	A	69	THR	C-O	-14.80	0.95	1.23
1	A	128	ARG	N-CA	14.71	1.75	1.46
1	A	63	TRP	CE3-CZ3	14.71	1.63	1.38
1	A	128	ARG	CZ-NH2	-14.59	1.14	1.33
1	B	46	ASN	N-CA	-14.52	1.17	1.46
1	A	125	ARG	CD-NE	-14.52	1.21	1.46
1	B	121	GLN	CD-NE2	14.51	1.69	1.32
1	A	48	ASP	CA-CB	14.43	1.85	1.53
1	B	128	ARG	CG-CD	14.28	1.87	1.51
1	A	86	SER	CB-OG	14.19	1.60	1.42
1	B	23	TYR	CZ-OH	14.04	1.61	1.37
1	A	61	ARG	CG-CD	14.04	1.87	1.51
1	B	63	TRP	CE2-CZ2	-13.82	1.16	1.39
1	A	101	ASP	CB-CG	13.71	1.80	1.51
1	A	33	LYS	CD-CE	13.70	1.85	1.51
1	B	123	TRP	NE1-CE2	-13.68	1.19	1.37
1	A	63	TRP	CZ3-CH2	-13.49	1.18	1.40
1	B	60	SER	CA-CB	13.46	1.73	1.52
1	A	47	THR	CA-CB	-13.41	1.18	1.53
1	A	122	ALA	CA-C	13.31	1.87	1.52
1	B	50	SER	C-O	13.12	1.48	1.23
1	A	15	HIS	CG-ND1	-13.11	1.09	1.38
1	B	50	SER	CB-OG	13.00	1.59	1.42
1	B	21	ARG	C-O	12.82	1.47	1.23
1	B	61	ARG	CG-CD	12.66	1.83	1.51
1	A	46	ASN	CG-ND2	-12.58	1.01	1.32
1	A	47	THR	C-O	-12.57	0.99	1.23
1	A	34	PHE	CG-CD1	12.52	1.57	1.38
1	A	114	ARG	CZ-NH2	12.50	1.49	1.33
1	A	125	ARG	CZ-NH2	-12.47	1.16	1.33
1	A	21	ARG	CZ-NH1	12.44	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	34	PHE	CG-CD2	-12.38	1.20	1.38
1	B	121	GLN	CG-CD	12.38	1.79	1.51
1	A	21	ARG	CZ-NH2	-12.35	1.17	1.33
1	B	67	GLY	N-CA	12.31	1.64	1.46
1	A	3	PHE	CG-CD2	-12.25	1.20	1.38
1	B	1	LYS	CD-CE	12.21	1.81	1.51
1	B	35	GLU	CG-CD	-12.14	1.33	1.51
1	B	42	ALA	C-N	-12.04	1.06	1.34
1	B	43	THR	C-O	12.02	1.46	1.23
1	A	115	CYS	N-CA	-11.93	1.22	1.46
1	A	53	TYR	CG-CD2	-11.92	1.23	1.39
1	A	66	ASP	CA-CB	-11.90	1.27	1.53
1	B	114	ARG	CD-NE	11.87	1.66	1.46
1	A	112	ARG	CG-CD	11.82	1.81	1.51
1	B	43	THR	CB-CG2	11.76	1.91	1.52
1	A	71	GLY	CA-C	11.75	1.70	1.51
1	B	20	TYR	CD2-CE2	-11.66	1.21	1.39
1	B	19	ASN	CG-ND2	11.65	1.61	1.32
1	A	123	TRP	NE1-CE2	-11.65	1.22	1.37
1	A	68	ARG	CG-CD	11.65	1.81	1.51
1	B	48	ASP	C-O	11.44	1.45	1.23
1	A	48	ASP	C-O	-11.39	1.01	1.23
1	A	53	TYR	CG-CD1	-11.34	1.24	1.39
1	A	21	ARG	N-CA	11.31	1.69	1.46
1	A	2	VAL	CA-C	11.30	1.82	1.52
1	A	87	ASP	CG-OD2	-11.14	0.99	1.25
1	A	38	PHE	CD2-CE2	-11.10	1.17	1.39
1	A	86	SER	CA-CB	11.07	1.69	1.52
1	B	112	ARG	CD-NE	-10.99	1.27	1.46
1	A	108	TRP	CG-CD2	-10.98	1.25	1.43
1	A	93	ASN	CB-CG	10.96	1.76	1.51
1	A	7	GLU	CD-OE1	10.95	1.37	1.25
1	B	21	ARG	CB-CG	10.91	1.82	1.52
1	B	93	ASN	CB-CG	-10.89	1.25	1.51
1	A	14	ARG	NE-CZ	10.89	1.47	1.33
1	A	61	ARG	CZ-NH2	-10.88	1.19	1.33
1	B	129	LEU	CB-CG	-10.83	1.21	1.52
1	A	47	THR	CB-CG2	10.78	1.88	1.52
1	A	39	ASN	CG-OD1	10.75	1.47	1.24
1	B	63	TRP	CD2-CE3	-10.75	1.24	1.40
1	A	14	ARG	CG-CD	10.71	1.78	1.51
1	A	109	VAL	CB-CG1	-10.62	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	ASN	CG-OD1	10.62	1.47	1.24
1	B	21	ARG	C-N	10.61	1.52	1.33
1	A	44	ASN	CB-CG	10.58	1.75	1.51
1	B	21	ARG	CA-CB	10.58	1.77	1.53
1	B	41	GLN	CB-CG	-10.47	1.24	1.52
1	B	49	GLY	C-N	-10.42	1.10	1.34
1	A	127	CYS	CA-C	10.41	1.80	1.52
1	B	20	TYR	CE1-CZ	10.41	1.52	1.38
1	B	21	ARG	CD-NE	-10.40	1.28	1.46
1	A	128	ARG	CA-C	10.35	1.79	1.52
1	B	67	GLY	CA-C	10.29	1.68	1.51
1	B	69	THR	C-N	10.29	1.53	1.34
1	A	118	THR	C-O	-10.27	1.03	1.23
1	A	66	ASP	C-O	10.25	1.42	1.23
1	A	102	GLY	N-CA	10.22	1.61	1.46
1	B	46	ASN	CB-CG	10.21	1.74	1.51
1	A	4	GLY	N-CA	10.17	1.61	1.46
1	B	61	ARG	NE-CZ	-10.17	1.19	1.33
1	B	18	ASP	CB-CG	10.15	1.73	1.51
1	B	86	SER	CA-CB	10.12	1.68	1.52
1	B	14	ARG	CZ-NH1	10.09	1.46	1.33
1	A	68	ARG	CZ-NH1	10.09	1.46	1.33
1	A	113	ASN	N-CA	-10.06	1.26	1.46
1	B	22	GLY	C-O	9.99	1.39	1.23
1	A	39	ASN	CB-CG	-9.96	1.28	1.51
1	A	85	SER	CA-CB	9.95	1.67	1.52
1	A	63	TRP	CG-CD1	-9.92	1.22	1.36
1	A	74	ASN	C-N	9.88	1.56	1.34
1	B	81	SER	CB-OG	9.88	1.55	1.42
1	A	35	GLU	CD-OE1	9.87	1.36	1.25
1	A	111	TRP	CZ3-CH2	-9.87	1.24	1.40
1	B	45	ARG	C-N	-9.87	1.11	1.34
1	A	72	SER	CB-OG	9.86	1.55	1.42
1	B	29	VAL	CB-CG1	9.86	1.73	1.52
1	B	71	GLY	N-CA	9.85	1.60	1.46
1	B	68	ARG	C-O	9.83	1.42	1.23
1	A	110	ALA	C-O	9.81	1.42	1.23
1	A	62	TRP	CE3-CZ3	9.81	1.55	1.38
1	B	126	GLY	CA-C	9.78	1.67	1.51
1	A	13	LYS	CA-C	-9.76	1.27	1.52
1	B	68	ARG	NE-CZ	9.73	1.45	1.33
1	A	51	THR	C-O	-9.72	1.04	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	CYS	N-CA	-9.72	1.26	1.46
1	A	123	TRP	CE3-CZ3	9.62	1.54	1.38
1	B	28	TRP	CD2-CE2	9.60	1.52	1.41
1	A	63	TRP	NE1-CE2	-9.59	1.25	1.37
1	A	46	ASN	CB-CG	-9.58	1.29	1.51
1	B	62	TRP	CB-CG	9.58	1.67	1.50
1	B	39	ASN	CG-OD1	-9.55	1.02	1.24
1	A	67	GLY	C-O	9.52	1.38	1.23
1	A	111	TRP	CD2-CE3	9.51	1.54	1.40
1	A	76	CYS	CA-CB	9.45	1.74	1.53
1	B	76	CYS	CA-CB	9.43	1.74	1.53
1	A	16	GLY	N-CA	9.39	1.60	1.46
1	B	50	SER	N-CA	-9.39	1.27	1.46
1	A	45	ARG	CA-CB	9.38	1.74	1.53
1	A	63	TRP	CE2-CZ2	-9.36	1.23	1.39
1	B	15	HIS	CG-ND1	9.36	1.59	1.38
1	A	24	SER	C-O	9.35	1.41	1.23
1	B	108	TRP	CG-CD1	9.32	1.49	1.36
1	B	17	LEU	C-O	9.29	1.41	1.23
1	B	6	CYS	CA-CB	9.28	1.74	1.53
1	B	86	SER	CB-OG	9.27	1.54	1.42
1	A	15	HIS	C-N	-9.26	1.16	1.33
1	B	20	TYR	C-O	-9.24	1.05	1.23
1	A	63	TRP	CG-CD2	9.21	1.59	1.43
1	A	115	CYS	CA-CB	9.18	1.74	1.53
1	A	62	TRP	CB-CG	9.15	1.66	1.50
1	B	110	ALA	C-O	9.11	1.40	1.23
1	A	63	TRP	CD2-CE2	9.09	1.52	1.41
1	A	78	ILE	CB-CG2	-9.09	1.24	1.52
1	B	45	ARG	CZ-NH2	9.09	1.44	1.33
1	A	124	ILE	CA-CB	-9.07	1.33	1.54
1	B	20	TYR	CG-CD1	9.07	1.50	1.39
1	B	41	GLN	CD-NE2	9.07	1.55	1.32
1	A	68	ARG	CB-CG	-9.05	1.28	1.52
1	B	85	SER	CA-C	9.04	1.76	1.52
1	A	34	PHE	CE2-CZ	-9.03	1.20	1.37
1	A	119	ASP	C-O	-9.03	1.06	1.23
1	A	97	LYS	C-O	9.02	1.40	1.23
1	A	51	THR	CB-CG2	-8.98	1.22	1.52
1	B	72	SER	N-CA	-8.95	1.28	1.46
1	B	63	TRP	CE3-CZ3	8.92	1.53	1.38
1	B	33	LYS	CD-CE	8.91	1.73	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	ARG	CD-NE	8.88	1.61	1.46
1	B	47	THR	C-O	8.85	1.40	1.23
1	B	42	ALA	N-CA	-8.81	1.28	1.46
1	A	60	SER	CA-CB	8.81	1.66	1.52
1	A	22	GLY	C-O	-8.80	1.09	1.23
1	A	115	CYS	C-O	8.80	1.40	1.23
1	B	72	SER	CB-OG	-8.78	1.30	1.42
1	B	67	GLY	C-O	8.78	1.37	1.23
1	B	116	LYS	C-O	-8.75	1.06	1.23
1	B	111	TRP	CE2-CZ2	-8.74	1.24	1.39
1	B	37	ASN	CA-C	8.73	1.75	1.52
1	A	2	VAL	N-CA	8.72	1.63	1.46
1	A	120	VAL	C-O	-8.65	1.06	1.23
1	B	68	ARG	C-N	-8.63	1.14	1.34
1	A	52	ASP	CB-CG	-8.61	1.33	1.51
1	A	62	TRP	NE1-CE2	8.59	1.48	1.37
1	A	83	LEU	C-O	8.58	1.39	1.23
1	B	129	LEU	CA-C	-8.58	1.30	1.52
1	B	45	ARG	CD-NE	8.56	1.61	1.46
1	B	5	ARG	CA-CB	8.54	1.72	1.53
1	B	80	CYS	CA-C	-8.54	1.30	1.52
1	B	121	GLN	C-O	8.53	1.39	1.23
1	B	79	PRO	N-CA	-8.50	1.32	1.47
1	B	77	ASN	CB-CG	8.49	1.70	1.51
1	B	58	ILE	N-CA	8.45	1.63	1.46
1	A	109	VAL	CA-CB	8.42	1.72	1.54
1	B	104	GLY	CA-C	8.42	1.65	1.51
1	B	14	ARG	CG-CD	-8.41	1.30	1.51
1	A	66	ASP	CA-C	-8.39	1.31	1.52
1	A	15	HIS	CG-CD2	-8.39	1.21	1.35
1	B	5	ARG	CZ-NH2	8.38	1.44	1.33
1	A	14	ARG	CZ-NH2	8.37	1.44	1.33
1	B	46	ASN	C-O	8.37	1.39	1.23
1	A	126	GLY	C-O	8.34	1.37	1.23
1	B	100	SER	CA-CB	8.34	1.65	1.52
1	A	114	ARG	NE-CZ	8.32	1.43	1.33
1	A	77	ASN	C-O	-8.32	1.07	1.23
1	A	107	ALA	C-N	-8.30	1.15	1.34
1	B	69	THR	C-O	-8.30	1.07	1.23
1	A	100	SER	C-O	8.28	1.39	1.23
1	B	129	LEU	C-OXT	8.28	1.39	1.23
1	B	2	VAL	CA-CB	-8.27	1.37	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	LEU	C-O	8.25	1.39	1.23
1	B	66	ASP	CA-CB	-8.18	1.35	1.53
1	A	121	GLN	N-CA	-8.17	1.30	1.46
1	A	57	GLN	CD-NE2	-8.13	1.12	1.32
1	A	86	SER	N-CA	8.13	1.62	1.46
1	A	128	ARG	NE-CZ	-8.13	1.22	1.33
1	B	122	ALA	C-N	8.11	1.52	1.34
1	A	73	ARG	C-O	8.10	1.38	1.23
1	B	76	CYS	N-CA	-8.10	1.30	1.46
1	B	68	ARG	N-CA	8.10	1.62	1.46
1	B	50	SER	CA-CB	8.09	1.65	1.52
1	A	23	TYR	C-O	8.07	1.38	1.23
1	A	41	GLN	CA-C	-8.07	1.31	1.52
1	B	68	ARG	CZ-NH1	8.05	1.43	1.33
1	A	104	GLY	CA-C	8.05	1.64	1.51
1	B	91	SER	N-CA	8.03	1.62	1.46
1	B	3	PHE	CA-CB	8.03	1.71	1.53
1	A	94	CYS	N-CA	8.02	1.62	1.46
1	B	108	TRP	CA-C	8.01	1.73	1.52
1	A	15	HIS	CE1-NE2	-8.01	1.14	1.32
1	B	87	ASP	C-O	8.00	1.38	1.23
1	A	16	GLY	CA-C	-8.00	1.39	1.51
1	A	124	ILE	CB-CG1	-7.96	1.31	1.54
1	B	78	ILE	C-O	7.96	1.38	1.23
1	A	67	GLY	CA-C	-7.95	1.39	1.51
1	A	23	TYR	CG-CD2	-7.93	1.28	1.39
1	B	108	TRP	CB-CG	7.93	1.64	1.50
1	A	26	GLY	C-O	7.92	1.36	1.23
1	B	63	TRP	NE1-CE2	-7.92	1.27	1.37
1	B	63	TRP	CB-CG	7.90	1.64	1.50
1	B	1	LYS	CE-NZ	-7.88	1.29	1.49
1	A	93	ASN	CG-OD1	7.86	1.41	1.24
1	A	110	ALA	N-CA	-7.84	1.30	1.46
1	B	88	ILE	CA-C	-7.84	1.32	1.52
1	B	35	GLU	CD-OE1	7.80	1.34	1.25
1	A	51	THR	CB-OG1	7.79	1.58	1.43
1	A	73	ARG	NE-CZ	-7.77	1.23	1.33
1	A	48	ASP	N-CA	7.75	1.61	1.46
1	A	2	VAL	C-N	-7.72	1.16	1.34
1	A	4	GLY	C-N	-7.69	1.16	1.34
1	A	41	GLN	C-O	7.69	1.38	1.23
1	A	129	LEU	CA-C	-7.69	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	ASN	CB-CG	7.68	1.68	1.51
1	A	122	ALA	N-CA	-7.64	1.31	1.46
1	A	20	TYR	CD1-CE1	-7.64	1.27	1.39
1	B	38	PHE	CG-CD2	-7.59	1.27	1.38
1	A	108	TRP	CD2-CE3	7.57	1.51	1.40
1	B	121	GLN	CA-CB	-7.55	1.37	1.53
1	B	45	ARG	C-O	7.54	1.37	1.23
1	A	3	PHE	N-CA	-7.52	1.31	1.46
1	A	119	ASP	CB-CG	7.51	1.67	1.51
1	B	7	GLU	CA-CB	7.48	1.70	1.53
1	A	109	VAL	CB-CG2	7.48	1.68	1.52
1	B	38	PHE	CD1-CE1	-7.48	1.24	1.39
1	B	111	TRP	CE3-CZ3	7.46	1.51	1.38
1	A	5	ARG	C-N	-7.46	1.17	1.34
1	B	1	LYS	CB-CG	-7.45	1.32	1.52
1	B	38	PHE	CE1-CZ	7.43	1.51	1.37
1	B	63	TRP	C-O	-7.43	1.09	1.23
1	B	45	ARG	N-CA	-7.43	1.31	1.46
1	A	128	ARG	C-N	-7.41	1.17	1.34
1	B	20	TYR	CB-CG	7.37	1.62	1.51
1	A	101	ASP	CA-C	-7.37	1.33	1.52
1	B	105	MET	C-N	7.35	1.50	1.34
1	B	39	ASN	CG-ND2	7.32	1.51	1.32
1	B	49	GLY	N-CA	-7.29	1.35	1.46
1	B	21	ARG	CA-C	7.29	1.72	1.52
1	A	107	ALA	CA-CB	7.28	1.67	1.52
1	A	70	PRO	N-CA	-7.26	1.34	1.47
1	A	43	THR	C-O	7.25	1.37	1.23
1	B	99	VAL	C-N	-7.23	1.17	1.34
1	A	72	SER	N-CA	7.23	1.60	1.46
1	B	3	PHE	CD2-CE2	-7.22	1.24	1.39
1	A	60	SER	N-CA	-7.21	1.31	1.46
1	B	77	ASN	CG-OD1	7.21	1.39	1.24
1	B	80	CYS	CA-CB	-7.20	1.38	1.53
1	A	63	TRP	C-N	7.20	1.50	1.34
1	B	124	ILE	N-CA	-7.20	1.31	1.46
1	A	108	TRP	NE1-CE2	7.20	1.47	1.37
1	A	121	GLN	C-O	7.19	1.37	1.23
1	A	3	PHE	CB-CG	-7.18	1.39	1.51
1	B	47	THR	CA-C	7.17	1.71	1.52
1	A	75	LEU	C-N	-7.16	1.17	1.34
1	B	42	ALA	C-O	7.13	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	TYR	N-CA	7.13	1.60	1.46
1	A	112	ARG	CA-C	-7.12	1.34	1.52
1	B	24	SER	CA-CB	7.10	1.63	1.52
1	A	123	TRP	CG-CD2	7.09	1.55	1.43
1	B	38	PHE	CG-CD1	-7.08	1.28	1.38
1	B	46	ASN	CG-ND2	7.08	1.50	1.32
1	A	97	LYS	CD-CE	7.07	1.69	1.51
1	A	123	TRP	CA-CB	7.07	1.69	1.53
1	A	103	ASN	CG-OD1	-7.06	1.08	1.24
1	B	122	ALA	C-O	-7.06	1.09	1.23
1	B	61	ARG	C-O	7.05	1.36	1.23
1	A	42	ALA	CA-C	7.05	1.71	1.52
1	B	58	ILE	CB-CG2	7.02	1.74	1.52
1	B	121	GLN	CA-C	-7.02	1.34	1.52
1	A	119	ASP	CA-C	7.02	1.71	1.52
1	B	53	TYR	N-CA	-7.01	1.32	1.46
1	B	97	LYS	CE-NZ	7.01	1.66	1.49
1	B	114	ARG	C-N	-7.01	1.18	1.34
1	A	33	LYS	CE-NZ	6.98	1.66	1.49
1	B	55	ILE	CA-C	6.97	1.71	1.52
1	B	62	TRP	CZ3-CH2	6.97	1.51	1.40
1	A	62	TRP	CD2-CE3	6.95	1.50	1.40
1	A	23	TYR	CD2-CE2	6.91	1.49	1.39
1	B	81	SER	N-CA	6.89	1.60	1.46
1	B	69	THR	N-CA	-6.88	1.32	1.46
1	A	29	VAL	N-CA	6.87	1.60	1.46
1	B	9	ALA	C-N	6.87	1.49	1.34
1	A	111	TRP	CZ2-CH2	-6.86	1.24	1.37
1	A	108	TRP	C-N	6.85	1.49	1.34
1	B	22	GLY	C-N	-6.85	1.18	1.34
1	B	96	LYS	CD-CE	-6.84	1.34	1.51
1	B	65	ASN	CB-CG	-6.84	1.35	1.51
1	B	43	THR	CA-CB	-6.83	1.35	1.53
1	B	66	ASP	CG-OD2	6.81	1.41	1.25
1	B	116	LYS	N-CA	6.78	1.59	1.46
1	A	65	ASN	C-O	6.76	1.36	1.23
1	B	88	ILE	C-N	-6.74	1.18	1.34
1	A	68	ARG	CA-C	6.74	1.70	1.52
1	B	4	GLY	C-O	-6.74	1.12	1.23
1	A	18	ASP	N-CA	6.73	1.59	1.46
1	B	87	ASP	CG-OD2	-6.71	1.09	1.25
1	A	62	TRP	CE2-CZ2	-6.66	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	PRO	CA-C	6.66	1.66	1.52
1	A	123	TRP	CD2-CE3	-6.64	1.30	1.40
1	A	3	PHE	CG-CD1	-6.63	1.28	1.38
1	B	14	ARG	C-O	6.62	1.35	1.23
1	A	40	THR	CA-C	-6.62	1.35	1.52
1	A	15	HIS	CB-CG	6.61	1.61	1.50
1	A	55	ILE	CA-CB	6.61	1.70	1.54
1	B	12	MET	C-O	6.59	1.35	1.23
1	A	112	ARG	NE-CZ	6.57	1.41	1.33
1	A	128	ARG	CZ-NH1	-6.57	1.24	1.33
1	A	1	LYS	CA-CB	-6.57	1.39	1.53
1	A	61	ARG	CB-CG	6.56	1.70	1.52
1	B	114	ARG	CZ-NH1	6.55	1.41	1.33
1	A	101	ASP	C-O	6.55	1.35	1.23
1	A	2	VAL	C-O	6.55	1.35	1.23
1	A	32	ALA	CA-CB	6.55	1.66	1.52
1	B	84	LEU	C-N	-6.54	1.19	1.34
1	B	123	TRP	C-O	6.54	1.35	1.23
1	B	87	ASP	CA-CB	6.54	1.68	1.53
1	A	73	ARG	C-N	-6.54	1.19	1.34
1	A	7	GLU	C-O	6.52	1.35	1.23
1	A	98	ILE	N-CA	-6.52	1.33	1.46
1	A	70	PRO	CA-C	6.51	1.65	1.52
1	A	75	LEU	C-O	-6.51	1.10	1.23
1	B	52	ASP	CG-OD2	6.50	1.40	1.25
1	A	48	ASP	CB-CG	6.50	1.65	1.51
1	B	20	TYR	CD1-CE1	-6.46	1.29	1.39
1	B	21	ARG	CG-CD	-6.46	1.35	1.51
1	B	46	ASN	CG-OD1	6.43	1.38	1.24
1	B	12	MET	N-CA	6.43	1.59	1.46
1	B	78	ILE	CA-CB	6.42	1.69	1.54
1	B	63	TRP	CA-CB	6.42	1.68	1.53
1	B	38	PHE	CE2-CZ	-6.41	1.25	1.37
1	B	24	SER	C-O	-6.41	1.11	1.23
1	A	105	MET	N-CA	-6.40	1.33	1.46
1	B	18	ASP	CG-OD2	6.39	1.40	1.25
1	A	5	ARG	NE-CZ	-6.39	1.24	1.33
1	A	39	ASN	C-O	-6.38	1.11	1.23
1	B	43	THR	C-N	-6.35	1.19	1.34
1	A	20	TYR	CG-CD1	-6.34	1.30	1.39
1	B	19	ASN	CA-C	-6.34	1.36	1.52
1	A	1	LYS	N-CA	6.32	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	TRP	CD2-CE2	6.28	1.48	1.41
1	B	37	ASN	C-O	6.28	1.35	1.23
1	B	66	ASP	CG-OD1	6.27	1.39	1.25
1	B	51	THR	CB-OG1	6.27	1.55	1.43
1	B	22	GLY	CA-C	6.26	1.61	1.51
1	B	40	THR	CA-C	-6.26	1.36	1.52
1	B	53	TYR	CG-CD2	6.25	1.47	1.39
1	B	23	TYR	CE2-CZ	-6.23	1.30	1.38
1	B	102	GLY	C-N	-6.23	1.19	1.34
1	B	13	LYS	CA-CB	6.22	1.67	1.53
1	A	33	LYS	CA-C	6.21	1.69	1.52
1	B	111	TRP	CD2-CE3	6.20	1.49	1.40
1	B	73	ARG	CB-CG	6.19	1.69	1.52
1	A	70	PRO	CA-CB	-6.18	1.41	1.53
1	A	71	GLY	C-N	-6.18	1.19	1.34
1	A	123	TRP	CG-CD1	6.17	1.45	1.36
1	B	3	PHE	CG-CD1	-6.15	1.29	1.38
1	A	28	TRP	CA-C	-6.15	1.36	1.52
1	B	111	TRP	CD1-NE1	6.12	1.48	1.38
1	A	117	GLY	N-CA	6.12	1.55	1.46
1	A	77	ASN	CG-ND2	-6.11	1.17	1.32
1	A	113	ASN	CG-OD1	-6.10	1.10	1.24
1	B	106	ASN	CG-OD1	-6.09	1.10	1.24
1	A	1	LYS	CB-CG	-6.08	1.36	1.52
1	A	21	ARG	C-N	-6.08	1.22	1.33
1	A	36	SER	C-N	6.08	1.48	1.34
1	A	73	ARG	CZ-NH2	6.08	1.41	1.33
1	A	24	SER	CB-OG	-6.08	1.34	1.42
1	B	15	HIS	C-O	-6.08	1.11	1.23
1	A	59	ASN	C-N	6.07	1.48	1.34
1	A	34	PHE	CA-CB	6.07	1.67	1.53
1	B	56	LEU	CG-CD2	6.07	1.74	1.51
1	B	68	ARG	CB-CG	-6.06	1.36	1.52
1	B	34	PHE	CE1-CZ	6.06	1.48	1.37
1	B	47	THR	CB-CG2	6.05	1.72	1.52
1	A	49	GLY	CA-C	6.05	1.61	1.51
1	A	109	VAL	CA-C	-6.04	1.37	1.52
1	A	14	ARG	CA-CB	6.03	1.67	1.53
1	A	79	PRO	N-CD	-6.03	1.39	1.47
1	A	20	TYR	CZ-OH	6.03	1.48	1.37
1	B	33	LYS	CA-C	-6.02	1.37	1.52
1	A	113	ASN	CG-ND2	-5.99	1.17	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	THR	CB-OG1	5.99	1.55	1.43
1	A	38	PHE	CE2-CZ	5.98	1.48	1.37
1	A	68	ARG	N-CA	-5.98	1.34	1.46
1	B	125	ARG	CA-C	5.97	1.68	1.52
1	A	50	SER	C-N	5.97	1.47	1.34
1	A	38	PHE	CB-CG	-5.95	1.41	1.51
1	B	44	ASN	CB-CG	5.95	1.64	1.51
1	A	108	TRP	CG-CD1	-5.94	1.28	1.36
1	B	70	PRO	N-CA	5.94	1.57	1.47
1	B	75	LEU	CA-CB	-5.93	1.40	1.53
1	A	50	SER	CA-CB	5.92	1.61	1.52
1	A	35	GLU	CG-CD	-5.88	1.43	1.51
1	A	108	TRP	CB-CG	5.88	1.60	1.50
1	B	66	ASP	CA-C	-5.87	1.37	1.52
1	B	119	ASP	CA-C	-5.86	1.37	1.52
1	A	42	ALA	C-O	-5.84	1.12	1.23
1	A	125	ARG	C-O	5.84	1.34	1.23
1	A	112	ARG	C-N	5.84	1.47	1.34
1	B	106	ASN	CG-ND2	5.84	1.47	1.32
1	B	55	ILE	N-CA	5.84	1.58	1.46
1	A	103	ASN	C-O	5.83	1.34	1.23
1	B	116	LYS	C-N	5.83	1.43	1.33
1	A	60	SER	C-N	-5.83	1.20	1.34
1	B	96	LYS	C-O	5.82	1.34	1.23
1	B	116	LYS	CD-CE	-5.80	1.36	1.51
1	A	124	ILE	C-O	-5.80	1.12	1.23
1	A	7	GLU	CA-CB	5.79	1.66	1.53
1	A	39	ASN	C-N	5.78	1.47	1.34
1	B	41	GLN	CG-CD	-5.77	1.37	1.51
1	A	102	GLY	CA-C	5.77	1.61	1.51
1	A	36	SER	CB-OG	5.75	1.49	1.42
1	B	124	ILE	CB-CG1	-5.75	1.38	1.54
1	A	62	TRP	CZ3-CH2	5.75	1.49	1.40
1	A	99	VAL	C-O	-5.74	1.12	1.23
1	A	50	SER	N-CA	-5.73	1.34	1.46
1	B	83	LEU	C-N	-5.71	1.21	1.34
1	B	120	VAL	CA-CB	5.71	1.66	1.54
1	B	113	ASN	CB-CG	-5.71	1.38	1.51
1	B	18	ASP	C-O	5.70	1.34	1.23
1	A	14	ARG	N-CA	5.69	1.57	1.46
1	B	16	GLY	CA-C	5.68	1.60	1.51
1	A	43	THR	CB-CG2	-5.68	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	ASN	N-CA	-5.67	1.35	1.46
1	B	42	ALA	CA-CB	-5.66	1.40	1.52
1	A	87	ASP	N-CA	5.66	1.57	1.46
1	B	23	TYR	CD2-CE2	5.64	1.47	1.39
1	B	47	THR	C-N	-5.64	1.21	1.34
1	A	129	LEU	CB-CG	-5.63	1.36	1.52
1	B	40	THR	N-CA	5.62	1.57	1.46
1	A	73	ARG	CG-CD	5.61	1.66	1.51
1	B	19	ASN	C-O	5.58	1.33	1.23
1	B	36	SER	CA-CB	5.58	1.61	1.52
1	B	23	TYR	CG-CD2	-5.57	1.31	1.39
1	B	111	TRP	CA-CB	-5.57	1.41	1.53
1	A	90	ALA	N-CA	-5.56	1.35	1.46
1	B	41	GLN	C-O	-5.55	1.12	1.23
1	A	116	LYS	N-CA	-5.54	1.35	1.46
1	A	114	ARG	C-O	5.52	1.33	1.23
1	A	128	ARG	CA-CB	-5.51	1.41	1.53
1	A	116	LYS	CD-CE	5.51	1.65	1.51
1	B	94	CYS	N-CA	-5.51	1.35	1.46
1	A	83	LEU	C-N	-5.50	1.21	1.34
1	A	66	ASP	CB-CG	-5.50	1.40	1.51
1	B	108	TRP	CE2-CZ2	-5.50	1.30	1.39
1	A	88	ILE	CA-C	-5.48	1.38	1.52
1	B	123	TRP	CD2-CE3	-5.48	1.32	1.40
1	B	26	GLY	CA-C	5.48	1.60	1.51
1	A	91	SER	CB-OG	-5.46	1.35	1.42
1	B	71	GLY	CA-C	5.45	1.60	1.51
1	B	9	ALA	N-CA	5.43	1.57	1.46
1	B	105	MET	N-CA	-5.43	1.35	1.46
1	A	90	ALA	C-N	5.41	1.46	1.34
1	B	66	ASP	C-N	-5.40	1.23	1.33
1	B	18	ASP	C-N	-5.38	1.21	1.34
1	B	34	PHE	CA-CB	5.37	1.65	1.53
1	A	93	ASN	N-CA	-5.36	1.35	1.46
1	A	80	CYS	N-CA	-5.36	1.35	1.46
1	A	13	LYS	CE-NZ	5.36	1.62	1.49
1	B	5	ARG	N-CA	5.36	1.57	1.46
1	A	25	LEU	C-O	-5.35	1.13	1.23
1	A	106	ASN	CA-CB	5.34	1.67	1.53
1	A	68	ARG	CA-CB	5.33	1.65	1.53
1	A	97	LYS	CE-NZ	-5.33	1.35	1.49
1	A	27	ASN	CB-CG	5.29	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	TYR	CB-CG	5.29	1.59	1.51
1	A	2	VAL	CB-CG2	5.27	1.64	1.52
1	B	74	ASN	CA-C	-5.27	1.39	1.52
1	A	58	ILE	CA-CB	-5.26	1.42	1.54
1	B	115	CYS	N-CA	-5.26	1.35	1.46
1	B	114	ARG	CG-CD	-5.26	1.38	1.51
1	A	90	ALA	CA-C	5.25	1.66	1.52
1	B	100	SER	CA-C	5.25	1.66	1.52
1	A	82	ALA	N-CA	5.25	1.56	1.46
1	A	112	ARG	N-CA	-5.24	1.35	1.46
1	B	30	CYS	C-N	5.24	1.46	1.34
1	A	78	ILE	C-N	5.23	1.44	1.34
1	B	92	VAL	C-O	5.22	1.33	1.23
1	B	28	TRP	NE1-CE2	-5.22	1.30	1.37
1	A	49	GLY	C-O	-5.21	1.15	1.23
1	B	10	ALA	N-CA	5.21	1.56	1.46
1	B	59	ASN	CA-CB	5.20	1.66	1.53
1	A	5	ARG	CZ-NH1	5.20	1.39	1.33
1	B	24	SER	CB-OG	5.20	1.49	1.42
1	B	93	ASN	CG-OD1	5.20	1.35	1.24
1	A	101	ASP	CG-OD2	-5.19	1.13	1.25
1	A	118	THR	CA-CB	5.19	1.66	1.53
1	B	53	TYR	CE2-CZ	-5.19	1.31	1.38
1	B	7	GLU	CD-OE1	5.18	1.31	1.25
1	B	7	GLU	CG-CD	5.18	1.59	1.51
1	B	71	GLY	C-N	-5.17	1.22	1.34
1	B	128	ARG	C-N	-5.17	1.22	1.34
1	A	93	ASN	CG-ND2	-5.17	1.20	1.32
1	A	59	ASN	C-O	-5.17	1.13	1.23
1	B	17	LEU	CB-CG	-5.17	1.37	1.52
1	B	29	VAL	CA-C	-5.16	1.39	1.52
1	A	128	ARG	C-O	5.16	1.33	1.23
1	B	108	TRP	CZ2-CH2	5.16	1.47	1.37
1	A	73	ARG	CD-NE	5.15	1.55	1.46
1	A	97	LYS	CA-C	5.15	1.66	1.52
1	B	103	ASN	CG-ND2	-5.14	1.20	1.32
1	B	38	PHE	C-N	-5.14	1.22	1.34
1	B	73	ARG	CG-CD	-5.14	1.39	1.51
1	B	51	THR	CA-CB	-5.12	1.40	1.53
1	B	111	TRP	CG-CD2	-5.11	1.34	1.43
1	A	73	ARG	CA-C	5.05	1.66	1.52
1	A	30	CYS	C-O	-5.05	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	TRP	CG-CD1	5.04	1.43	1.36
1	A	99	VAL	CB-CG2	-5.04	1.42	1.52
1	B	107	ALA	N-CA	5.04	1.56	1.46
1	B	116	LYS	CA-C	5.04	1.66	1.52
1	B	63	TRP	CG-CD2	5.03	1.52	1.43
1	A	5	ARG	CA-CB	5.02	1.65	1.53
1	B	15	HIS	N-CA	5.01	1.56	1.46
1	B	52	ASP	N-CA	5.00	1.56	1.46

All (737) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ARG	NE-CZ-NH2	-82.14	79.23	120.30
1	A	125	ARG	NE-CZ-NH1	74.34	157.47	120.30
1	A	125	ARG	NE-CZ-NH2	-72.57	84.01	120.30
1	B	114	ARG	NE-CZ-NH2	-66.11	87.25	120.30
1	B	61	ARG	NE-CZ-NH2	62.22	151.41	120.30
1	A	87	ASP	CB-CG-OD2	-58.29	65.83	118.30
1	B	45	ARG	NE-CZ-NH2	57.31	148.96	120.30
1	B	128	ARG	NE-CZ-NH1	-56.89	91.86	120.30
1	B	73	ARG	NE-CZ-NH2	53.87	147.24	120.30
1	A	112	ARG	NE-CZ-NH1	52.88	146.74	120.30
1	A	14	ARG	NE-CZ-NH2	-51.17	94.72	120.30
1	B	21	ARG	NE-CZ-NH1	49.59	145.09	120.30
1	B	128	ARG	NH1-CZ-NH2	46.76	170.84	119.40
1	A	14	ARG	NE-CZ-NH1	42.53	141.57	120.30
1	A	114	ARG	NE-CZ-NH2	-41.61	99.50	120.30
1	A	112	ARG	NE-CZ-NH2	-40.05	100.28	120.30
1	B	114	ARG	NE-CZ-NH1	39.50	140.05	120.30
1	B	21	ARG	NH1-CZ-NH2	-39.13	76.35	119.40
1	B	21	ARG	CD-NE-CZ	39.13	178.38	123.60
1	B	45	ARG	NE-CZ-NH1	-36.63	101.99	120.30
1	A	48	ASP	CB-CG-OD2	-33.66	88.01	118.30
1	A	73	ARG	NE-CZ-NH1	33.60	137.10	120.30
1	B	73	ARG	NE-CZ-NH1	-32.48	104.06	120.30
1	B	61	ARG	CD-NE-CZ	31.51	167.72	123.60
1	A	45	ARG	NE-CZ-NH2	-30.46	105.07	120.30
1	B	14	ARG	CD-NE-CZ	30.01	165.61	123.60
1	A	125	ARG	CD-NE-CZ	-29.75	81.95	123.60
1	B	112	ARG	NE-CZ-NH2	-28.75	105.93	120.30
1	A	114	ARG	NE-CZ-NH1	27.73	134.16	120.30
1	A	48	ASP	CB-CG-OD1	27.16	142.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	TYR	CB-CG-CD1	-26.75	104.95	121.00
1	B	21	ARG	NE-CZ-NH2	-26.75	106.93	120.30
1	A	62	TRP	CD1-CG-CD2	26.66	127.62	106.30
1	B	61	ARG	NH1-CZ-NH2	-26.16	90.62	119.40
1	A	21	ARG	CD-NE-CZ	-25.86	87.40	123.60
1	A	18	ASP	CB-CG-OD1	25.66	141.40	118.30
1	A	14	ARG	CD-NE-CZ	-24.74	88.97	123.60
1	B	114	ARG	CD-NE-CZ	-24.55	89.23	123.60
1	A	34	PHE	CB-CG-CD2	24.31	137.82	120.80
1	B	68	ARG	NE-CZ-NH2	-24.01	108.29	120.30
1	A	128	ARG	NE-CZ-NH1	23.92	132.26	120.30
1	A	87	ASP	OD1-CG-OD2	23.60	168.15	123.30
1	B	63	TRP	CE3-CZ3-CH2	-23.57	95.27	121.20
1	A	45	ARG	NE-CZ-NH1	23.51	132.06	120.30
1	B	52	ASP	CB-CG-OD2	-23.16	97.45	118.30
1	A	21	ARG	NE-CZ-NH1	22.78	131.69	120.30
1	A	75	LEU	O-C-N	22.62	158.89	122.70
1	B	112	ARG	NE-CZ-NH1	22.50	131.55	120.30
1	A	62	TRP	CZ3-CH2-CZ2	-22.14	95.04	121.60
1	B	108	TRP	CD1-CG-CD2	21.77	123.72	106.30
1	B	111	TRP	CE2-CD2-CG	21.64	124.61	107.30
1	A	63	TRP	CG-CD1-NE1	21.53	131.63	110.10
1	A	127	CYS	O-C-N	21.45	157.02	122.70
1	B	18	ASP	CB-CG-OD2	-21.43	99.01	118.30
1	B	61	ARG	NE-CZ-NH1	-21.36	109.62	120.30
1	B	14	ARG	NH1-CZ-NH2	-21.34	95.93	119.40
1	A	63	TRP	CD1-CG-CD2	-21.02	89.49	106.30
1	B	125	ARG	NE-CZ-NH1	-20.83	109.88	120.30
1	A	61	ARG	NE-CZ-NH1	-20.43	110.09	120.30
1	B	14	ARG	NE-CZ-NH2	20.35	130.48	120.30
1	A	23	TYR	CB-CG-CD2	-20.07	108.96	121.00
1	B	53	TYR	CB-CG-CD1	20.06	133.04	121.00
1	B	125	ARG	NE-CZ-NH2	19.77	130.19	120.30
1	B	20	TYR	CB-CG-CD1	-19.13	109.52	121.00
1	B	128	ARG	CD-NE-CZ	-18.97	97.04	123.60
1	A	123	TRP	CE2-CD2-CE3	18.83	141.30	118.70
1	A	47	THR	O-C-N	18.82	152.81	122.70
1	B	119	ASP	CB-CG-OD2	-18.76	101.41	118.30
1	B	23	TYR	CG-CD1-CE1	-18.61	106.41	121.30
1	A	62	TRP	CB-CG-CD1	-18.25	103.27	127.00
1	B	108	TRP	CG-CD1-NE1	-17.89	92.21	110.10
1	B	62	TRP	CD1-CG-CD2	17.74	120.49	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ASP	CB-CG-OD1	-17.62	102.44	118.30
1	A	123	TRP	CD1-NE1-CE2	17.60	124.84	109.00
1	A	5	ARG	NE-CZ-NH1	17.29	128.94	120.30
1	A	112	ARG	CG-CD-NE	-17.17	75.75	111.80
1	B	121	GLN	OE1-CD-NE2	17.11	161.25	121.90
1	A	129	LEU	N-CA-CB	-16.91	76.57	110.40
1	A	123	TRP	CG-CD1-NE1	-16.90	93.20	110.10
1	A	63	TRP	CH2-CZ2-CE2	16.89	134.29	117.40
1	B	15	HIS	CG-ND1-CE1	-16.69	84.00	105.70
1	A	62	TRP	CE3-CZ3-CH2	16.65	139.51	121.20
1	A	18	ASP	CB-CG-OD2	-16.54	103.42	118.30
1	B	35	GLU	OE1-CD-OE2	-16.51	103.49	123.30
1	A	53	TYR	CB-CG-CD2	-16.39	111.17	121.00
1	B	119	ASP	CB-CG-OD1	16.37	133.03	118.30
1	A	123	TRP	CZ3-CH2-CZ2	16.33	141.20	121.60
1	B	53	TYR	CZ-CE2-CD2	-16.23	105.19	119.80
1	B	129	LEU	CB-CG-CD2	16.22	138.58	111.00
1	A	44	ASN	CB-CG-OD1	-16.14	89.32	121.60
1	B	66	ASP	CB-CG-OD2	16.12	132.81	118.30
1	B	19	ASN	OD1-CG-ND2	-15.93	85.27	121.90
1	A	123	TRP	CG-CD2-CE3	-15.77	119.70	133.90
1	A	108	TRP	NE1-CE2-CD2	-15.74	91.56	107.30
1	B	18	ASP	CB-CG-OD1	15.54	132.28	118.30
1	A	47	THR	CA-CB-CG2	15.51	134.12	112.40
1	A	128	ARG	CA-C-O	-15.48	87.58	120.10
1	A	68	ARG	O-C-N	15.46	147.44	122.70
1	A	108	TRP	CD2-CE3-CZ3	15.34	138.74	118.80
1	B	68	ARG	CD-NE-CZ	-15.31	102.17	123.60
1	A	63	TRP	CB-CG-CD1	15.04	146.55	127.00
1	A	108	TRP	CE2-CD2-CE3	-14.96	100.75	118.70
1	A	72	SER	O-C-N	-14.94	98.80	122.70
1	B	68	ARG	CA-C-O	-14.85	88.91	120.10
1	A	108	TRP	CG-CD2-CE3	14.74	147.17	133.90
1	A	48	ASP	C-N-CA	-14.70	91.44	122.30
1	A	121	GLN	CB-CG-CD	-14.68	73.43	111.60
1	B	3	PHE	CB-CG-CD1	14.52	130.97	120.80
1	B	23	TYR	CD1-CG-CD2	14.48	133.83	117.90
1	A	66	ASP	CB-CG-OD2	14.46	131.31	118.30
1	A	38	PHE	CB-CG-CD2	14.44	130.91	120.80
1	A	47	THR	CA-C-O	-14.42	89.81	120.10
1	B	5	ARG	NE-CZ-NH1	14.21	127.41	120.30
1	B	5	ARG	O-C-N	14.00	145.10	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	TRP	CG-CD1-NE1	-13.95	96.15	110.10
1	A	100	SER	O-C-N	-13.94	100.39	122.70
1	A	23	TYR	CD1-CG-CD2	13.92	133.22	117.90
1	B	65	ASN	CB-CG-OD1	13.92	149.44	121.60
1	B	68	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	B	123	TRP	CG-CD2-CE3	-13.85	121.44	133.90
1	A	70	PRO	N-CA-CB	13.83	119.90	103.30
1	A	75	LEU	CA-C-O	-13.71	91.32	120.10
1	A	62	TRP	CH2-CZ2-CE2	13.65	131.05	117.40
1	A	72	SER	CA-C-N	13.53	146.96	117.20
1	B	47	THR	CA-CB-OG1	-13.52	80.61	109.00
1	B	53	TYR	CD1-CE1-CZ	13.49	131.94	119.80
1	A	3	PHE	CG-CD2-CE2	13.47	135.61	120.80
1	A	68	ARG	NE-CZ-NH1	13.35	126.98	120.30
1	A	15	HIS	O-C-N	13.33	145.86	123.20
1	A	47	THR	OG1-CB-CG2	-13.32	79.37	110.00
1	B	108	TRP	CE2-CD2-CG	-13.32	96.65	107.30
1	A	128	ARG	NH1-CZ-NH2	-13.27	104.80	119.40
1	B	69	THR	CA-C-O	13.24	147.91	120.10
1	B	111	TRP	CH2-CZ2-CE2	13.19	130.59	117.40
1	B	43	THR	OG1-CB-CG2	-13.18	79.69	110.00
1	B	20	TYR	CG-CD1-CE1	-13.13	110.79	121.30
1	A	23	TYR	CG-CD2-CE2	-13.07	110.84	121.30
1	B	28	TRP	CD1-NE1-CE2	12.95	120.66	109.00
1	B	123	TRP	CE2-CD2-CE3	12.95	134.24	118.70
1	B	3	PHE	CZ-CE2-CD2	-12.90	104.62	120.10
1	A	101	ASP	CB-CG-OD2	-12.79	106.79	118.30
1	B	63	TRP	CZ3-CH2-CZ2	12.65	136.78	121.60
1	A	20	TYR	CG-CD1-CE1	-12.64	111.18	121.30
1	B	53	TYR	CG-CD2-CE2	12.64	131.41	121.30
1	B	34	PHE	CB-CG-CD1	-12.60	111.98	120.80
1	B	123	TRP	CD2-CE2-CZ2	-12.59	107.19	122.30
1	B	3	PHE	CD1-CE1-CZ	-12.49	105.11	120.10
1	A	39	ASN	CA-C-O	12.49	146.34	120.10
1	A	72	SER	C-N-CA	12.49	152.91	121.70
1	A	107	ALA	O-C-N	12.48	142.66	122.70
1	A	28	TRP	CD1-NE1-CE2	-12.46	97.78	109.00
1	B	70	PRO	N-CA-CB	12.30	118.06	103.30
1	A	123	TRP	CH2-CZ2-CE2	-12.24	105.16	117.40
1	A	108	TRP	CE3-CZ3-CH2	-12.24	107.74	121.20
1	B	62	TRP	CD1-NE1-CE2	12.14	119.93	109.00
1	B	43	THR	CA-CB-CG2	-12.13	95.41	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	HIS	ND1-CG-CD2	12.13	125.78	108.80
1	A	43	THR	O-C-N	-12.12	103.30	122.70
1	B	114	ARG	NH1-CZ-NH2	12.09	132.69	119.40
1	B	19	ASN	CB-CG-ND2	12.06	145.65	116.70
1	B	86	SER	CA-CB-OG	-12.03	78.73	111.20
1	B	111	TRP	CD1-CG-CD2	-12.02	96.68	106.30
1	B	66	ASP	OD1-CG-OD2	-11.98	100.53	123.30
1	A	122	ALA	O-C-N	11.95	141.82	122.70
1	B	129	LEU	CB-CA-C	11.94	132.88	110.20
1	A	112	ARG	O-C-N	-11.90	103.66	122.70
1	B	39	ASN	CB-CG-OD1	11.87	145.33	121.60
1	A	61	ARG	CD-NE-CZ	-11.78	107.11	123.60
1	B	102	GLY	CA-C-O	-11.77	99.42	120.60
1	B	87	ASP	CB-CG-OD1	-11.75	107.73	118.30
1	A	1	LYS	O-C-N	-11.70	103.98	122.70
1	B	62	TRP	CG-CD1-NE1	-11.67	98.43	110.10
1	A	78	ILE	CA-CB-CG2	11.63	134.17	110.90
1	B	21	ARG	CA-CB-CG	-11.62	87.83	113.40
1	A	63	TRP	NE1-CE2-CZ2	11.59	143.15	130.40
1	A	39	ASN	OD1-CG-ND2	-11.55	95.34	121.90
1	A	62	TRP	CD1-NE1-CE2	-11.55	98.61	109.00
1	B	63	TRP	CE2-CD2-CE3	11.53	132.54	118.70
1	A	13	LYS	O-C-N	-11.51	104.28	122.70
1	A	28	TRP	CG-CD1-NE1	11.50	121.60	110.10
1	B	48	ASP	O-C-N	-11.48	103.68	123.20
1	B	50	SER	CB-CA-C	-11.46	88.33	110.10
1	A	66	ASP	CA-C-N	11.31	138.81	116.20
1	B	53	TYR	CD1-CG-CD2	-11.28	105.50	117.90
1	A	118	THR	O-C-N	11.26	140.72	122.70
1	A	3	PHE	CG-CD1-CE1	11.26	133.18	120.80
1	A	93	ASN	CB-CG-OD1	-11.25	99.10	121.60
1	A	61	ARG	NH1-CZ-NH2	11.24	131.76	119.40
1	B	28	TRP	CD1-CG-CD2	11.24	115.29	106.30
1	B	108	TRP	CG-CD2-CE3	11.16	143.94	133.90
1	B	78	ILE	O-C-N	-11.14	99.94	121.10
1	B	63	TRP	CD1-NE1-CE2	11.12	119.01	109.00
1	B	108	TRP	CD1-NE1-CE2	11.11	119.00	109.00
1	A	73	ARG	NH1-CZ-NH2	-11.11	107.18	119.40
1	A	68	ARG	CA-C-O	-11.06	96.88	120.10
1	A	123	TRP	CE3-CZ3-CH2	-11.05	109.05	121.20
1	A	45	ARG	CA-CB-CG	-11.01	89.18	113.40
1	A	51	THR	O-C-N	10.99	140.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	THR	CA-CB-CG2	10.99	127.78	112.40
1	A	12	MET	O-C-N	10.95	140.22	122.70
1	B	125	ARG	O-C-N	10.95	141.81	123.20
1	B	22	GLY	CA-C-O	-10.93	100.92	120.60
1	A	35	GLU	OE1-CD-OE2	-10.88	110.24	123.30
1	B	68	ARG	CA-C-N	10.84	141.05	117.20
1	A	3	PHE	CB-CG-CD1	10.84	128.38	120.80
1	B	70	PRO	CA-C-N	-10.84	94.53	116.20
1	B	50	SER	CA-C-N	10.67	140.67	117.20
1	A	108	TRP	NE1-CE2-CZ2	10.64	142.11	130.40
1	A	87	ASP	CB-CA-C	-10.63	89.14	110.40
1	B	28	TRP	CG-CD1-NE1	-10.62	99.48	110.10
1	A	122	ALA	CB-CA-C	-10.58	94.23	110.10
1	B	68	ARG	CA-CB-CG	10.57	136.66	113.40
1	A	111	TRP	CE2-CD2-CG	10.57	115.75	107.30
1	A	3	PHE	CD1-CG-CD2	-10.56	104.57	118.30
1	A	127	CYS	C-N-CA	-10.52	95.39	121.70
1	A	65	ASN	CB-CG-OD1	10.48	142.56	121.60
1	A	128	ARG	CA-C-N	10.48	140.25	117.20
1	A	66	ASP	O-C-N	-10.45	105.44	123.20
1	B	62	TRP	CZ3-CH2-CZ2	10.42	134.10	121.60
1	B	93	ASN	OD1-CG-ND2	-10.40	97.97	121.90
1	A	123	TRP	CE2-CD2-CG	-10.39	98.99	107.30
1	B	15	HIS	ND1-CG-CD2	10.36	123.31	108.80
1	B	71	GLY	O-C-N	10.33	139.22	122.70
1	B	20	TYR	CA-C-O	10.23	141.59	120.10
1	B	62	TRP	CE3-CZ3-CH2	-10.17	110.01	121.20
1	B	69	THR	OG1-CB-CG2	-10.13	86.70	110.00
1	B	101	ASP	CB-CG-OD2	10.11	127.40	118.30
1	A	44	ASN	CB-CG-ND2	10.02	140.76	116.70
1	A	20	TYR	CZ-CE2-CD2	-10.01	110.79	119.80
1	A	73	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	B	14	ARG	CG-CD-NE	10.00	132.80	111.80
1	B	63	TRP	CG-CD2-CE3	-9.99	124.91	133.90
1	B	14	ARG	N-CA-CB	9.99	128.57	110.60
1	B	23	TYR	CG-CD2-CE2	-9.97	113.32	121.30
1	A	15	HIS	CG-CD2-NE2	-9.97	90.26	109.20
1	B	34	PHE	CG-CD1-CE1	9.94	131.74	120.80
1	B	73	ARG	NH1-CZ-NH2	-9.93	108.48	119.40
1	B	121	GLN	CG-CD-NE2	-9.90	92.93	116.70
1	B	20	TYR	CB-CG-CD2	9.89	126.93	121.00
1	A	66	ASP	C-N-CA	9.89	143.07	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ASN	O-C-N	9.88	138.50	122.70
1	A	78	ILE	CA-CB-CG1	-9.88	92.24	111.00
1	A	72	SER	N-CA-CB	-9.86	95.71	110.50
1	B	63	TRP	CG-CD1-NE1	-9.86	100.25	110.10
1	A	68	ARG	NH1-CZ-NH2	-9.84	108.58	119.40
1	A	78	ILE	CB-CA-C	-9.81	91.97	111.60
1	A	39	ASN	O-C-N	-9.80	107.03	122.70
1	A	15	HIS	CA-C-O	-9.79	99.54	120.10
1	A	127	CYS	CA-C-O	-9.76	99.61	120.10
1	B	88	ILE	CA-CB-CG2	9.74	130.38	110.90
1	B	43	THR	N-CA-CB	9.73	128.79	110.30
1	B	3	PHE	CG-CD2-CE2	9.72	131.50	120.80
1	B	111	TRP	CG-CD2-CE3	-9.72	125.15	133.90
1	B	17	LEU	CA-C-N	9.68	138.50	117.20
1	B	69	THR	CA-C-N	-9.64	90.10	117.10
1	B	80	CYS	CA-CB-SG	9.64	131.34	114.00
1	B	3	PHE	CE1-CZ-CE2	9.63	137.33	120.00
1	A	5	ARG	NH1-CZ-NH2	-9.61	108.83	119.40
1	A	67	GLY	CA-C-N	9.59	138.30	117.20
1	B	68	ARG	N-CA-CB	-9.58	93.36	110.60
1	B	61	ARG	CG-CD-NE	-9.57	91.70	111.80
1	B	62	TRP	NE1-CE2-CD2	-9.57	97.73	107.30
1	A	43	THR	C-N-CA	9.54	145.54	121.70
1	A	41	GLN	CG-CD-NE2	9.49	139.48	116.70
1	B	123	TRP	NE1-CE2-CD2	9.49	116.79	107.30
1	A	47	THR	CA-CB-OG1	9.48	128.90	109.00
1	B	34	PHE	CD1-CE1-CZ	-9.47	108.74	120.10
1	B	29	VAL	CG1-CB-CG2	-9.43	95.82	110.90
1	A	7	GLU	OE1-CD-OE2	-9.42	111.99	123.30
1	A	74	ASN	O-C-N	-9.41	107.64	122.70
1	B	45	ARG	NH1-CZ-NH2	-9.41	109.05	119.40
1	B	125	ARG	CD-NE-CZ	9.41	136.77	123.60
1	A	125	ARG	CA-CB-CG	9.39	134.05	113.40
1	A	52	ASP	CB-CG-OD2	9.34	126.71	118.30
1	A	114	ARG	CA-C-O	-9.33	100.50	120.10
1	B	69	THR	CB-CA-C	-9.29	86.52	111.60
1	B	86	SER	O-C-N	-9.28	107.85	122.70
1	B	59	ASN	OD1-CG-ND2	9.27	143.21	121.90
1	B	66	ASP	CB-CG-OD1	9.25	126.62	118.30
1	A	13	LYS	CA-C-O	9.24	139.50	120.10
1	B	111	TRP	NE1-CE2-CD2	-9.19	98.11	107.30
1	B	21	ARG	CB-CA-C	-9.18	92.04	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	GLY	CA-C-O	-9.16	104.11	120.60
1	A	128	ARG	CB-CA-C	9.16	128.72	110.40
1	A	40	THR	CA-CB-CG2	9.15	125.21	112.40
1	A	111	TRP	CD1-CG-CD2	-9.14	98.99	106.30
1	A	108	TRP	CD1-CG-CD2	9.14	113.61	106.30
1	A	122	ALA	N-CA-CB	9.13	122.88	110.10
1	B	67	GLY	CA-C-N	9.11	137.24	117.20
1	B	43	THR	O-C-N	-9.06	108.20	122.70
1	A	107	ALA	CA-C-O	-9.05	101.10	120.10
1	A	38	PHE	CG-CD1-CE1	9.05	130.75	120.80
1	A	21	ARG	CA-C-N	9.04	134.28	116.20
1	A	41	GLN	O-C-N	-9.04	108.24	122.70
1	A	53	TYR	O-C-N	9.02	138.54	123.20
1	A	123	TRP	CD1-CG-CD2	9.01	113.51	106.30
1	A	61	ARG	C-N-CA	-8.97	99.27	121.70
1	B	46	ASN	N-CA-CB	8.96	126.72	110.60
1	A	3	PHE	CB-CG-CD2	8.90	127.03	120.80
1	A	34	PHE	CD1-CG-CD2	-8.89	106.74	118.30
1	A	74	ASN	CA-C-O	8.89	138.76	120.10
1	B	105	MET	CA-C-O	8.87	138.73	120.10
1	B	23	TYR	CD1-CE1-CZ	8.85	127.76	119.80
1	B	60	SER	N-CA-CB	-8.82	97.27	110.50
1	A	118	THR	N-CA-CB	8.82	127.05	110.30
1	A	34	PHE	CZ-CE2-CD2	8.81	130.67	120.10
1	B	63	TRP	NE1-CE2-CZ2	8.81	140.09	130.40
1	A	21	ARG	CB-CA-C	8.78	127.97	110.40
1	A	86	SER	CA-CB-OG	-8.76	87.54	111.20
1	A	112	ARG	CD-NE-CZ	-8.76	111.34	123.60
1	B	18	ASP	CA-C-O	-8.75	101.72	120.10
1	B	108	TRP	CB-CG-CD1	-8.72	115.66	127.00
1	A	83	LEU	CA-C-O	-8.72	101.80	120.10
1	A	45	ARG	CB-CG-CD	-8.71	88.96	111.60
1	A	124	ILE	CB-CG1-CD1	8.71	138.28	113.90
1	B	63	TRP	CD2-CE2-CZ2	-8.70	111.86	122.30
1	A	101	ASP	OD1-CG-OD2	8.69	139.80	123.30
1	B	123	TRP	CH2-CZ2-CE2	8.68	126.08	117.40
1	A	20	TYR	CD1-CE1-CZ	8.68	127.61	119.80
1	A	84	LEU	O-C-N	-8.64	108.87	122.70
1	B	21	ARG	CG-CD-NE	8.63	129.93	111.80
1	B	5	ARG	N-CA-CB	-8.61	95.10	110.60
1	B	125	ARG	C-N-CA	-8.55	104.33	122.30
1	B	29	VAL	O-C-N	-8.55	109.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ASN	O-C-N	8.54	136.36	122.70
1	B	44	ASN	C-N-CA	-8.54	100.35	121.70
1	A	87	ASP	CA-CB-CG	-8.54	94.62	113.40
1	B	34	PHE	CG-CD2-CE2	-8.52	111.43	120.80
1	A	18	ASP	CA-CB-CG	-8.48	94.74	113.40
1	B	97	LYS	CD-CE-NZ	-8.47	92.21	111.70
1	A	84	LEU	CB-CG-CD1	-8.47	96.60	111.00
1	A	91	SER	N-CA-CB	-8.46	97.81	110.50
1	A	83	LEU	CB-CG-CD1	-8.46	96.62	111.00
1	A	123	TRP	CD2-CE3-CZ3	-8.45	107.81	118.80
1	A	53	TYR	CZ-CE2-CD2	-8.45	112.19	119.80
1	B	15	HIS	ND1-CE1-NE2	8.43	128.45	109.90
1	A	34	PHE	CB-CG-CD1	-8.42	114.91	120.80
1	B	48	ASP	CA-C-N	8.41	133.01	116.20
1	A	100	SER	CA-C-N	8.39	135.66	117.20
1	B	52	ASP	OD1-CG-OD2	8.39	139.24	123.30
1	B	110	ALA	CA-C-N	8.39	135.65	117.20
1	B	62	TRP	NE1-CE2-CZ2	8.37	139.60	130.40
1	A	34	PHE	CG-CD2-CE2	8.35	129.99	120.80
1	B	5	ARG	CA-C-N	-8.32	98.89	117.20
1	A	57	GLN	CG-CD-OE1	-8.31	104.97	121.60
1	B	28	TRP	NE1-CE2-CZ2	8.30	139.53	130.40
1	B	42	ALA	CA-C-O	-8.29	102.69	120.10
1	A	78	ILE	N-CA-CB	-8.26	91.81	110.80
1	A	39	ASN	CB-CG-ND2	8.25	136.51	116.70
1	B	5	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	2	VAL	CA-C-O	-8.24	102.80	120.10
1	A	53	TYR	CD1-CE1-CZ	-8.24	112.38	119.80
1	B	73	ARG	CD-NE-CZ	8.23	135.13	123.60
1	A	21	ARG	CB-CG-CD	8.21	132.96	111.60
1	A	68	ARG	NE-CZ-NH2	8.19	124.39	120.30
1	B	66	ASP	C-N-CA	8.18	139.48	122.30
1	A	111	TRP	NE1-CE2-CZ2	8.17	139.39	130.40
1	B	43	THR	CA-C-N	8.17	135.18	117.20
1	A	63	TRP	CD2-CE2-CZ2	-8.15	112.52	122.30
1	A	43	THR	CA-CB-CG2	-8.15	100.99	112.40
1	B	3	PHE	CB-CA-C	-8.14	94.11	110.40
1	B	7	GLU	CG-CD-OE1	8.12	134.54	118.30
1	B	3	PHE	CG-CD1-CE1	8.11	129.72	120.80
1	B	3	PHE	CA-C-O	8.10	137.10	120.10
1	A	86	SER	CA-C-N	8.09	135.00	117.20
1	A	48	ASP	CA-CB-CG	-8.07	95.64	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	TRP	N-CA-CB	-8.07	96.07	110.60
1	B	46	ASN	CA-C-N	8.07	134.95	117.20
1	B	95	ALA	O-C-N	8.02	135.53	122.70
1	A	46	ASN	OD1-CG-ND2	-8.01	103.47	121.90
1	A	59	ASN	CA-C-O	8.01	136.92	120.10
1	B	104	GLY	CA-C-O	-8.00	106.21	120.60
1	B	12	MET	O-C-N	7.99	135.49	122.70
1	B	65	ASN	OD1-CG-ND2	-7.96	103.59	121.90
1	A	52	ASP	OD1-CG-OD2	-7.96	108.18	123.30
1	B	50	SER	CA-C-O	-7.94	103.42	120.10
1	A	72	SER	CA-CB-OG	-7.94	89.77	111.20
1	B	121	GLN	CG-CD-OE1	-7.94	105.73	121.60
1	A	78	ILE	O-C-N	-7.93	106.03	121.10
1	B	55	ILE	O-C-N	7.91	135.35	122.70
1	B	39	ASN	CA-CB-CG	-7.89	96.03	113.40
1	A	1	LYS	CA-C-O	7.89	136.67	120.10
1	B	68	ARG	CB-CG-CD	7.87	132.06	111.60
1	B	45	ARG	C-N-CA	7.87	141.37	121.70
1	B	21	ARG	CB-CG-CD	7.86	132.04	111.60
1	B	34	PHE	CZ-CE2-CD2	7.86	129.53	120.10
1	B	39	ASN	CB-CG-ND2	-7.82	97.93	116.70
1	B	128	ARG	CG-CD-NE	-7.81	95.39	111.80
1	B	119	ASP	CA-CB-CG	-7.75	96.34	113.40
1	A	93	ASN	CA-CB-CG	-7.75	96.36	113.40
1	B	111	TRP	CB-CG-CD2	7.74	136.66	126.60
1	B	69	THR	C-N-CD	7.73	144.63	128.40
1	B	27	ASN	CA-C-N	-7.67	100.33	117.20
1	A	28	TRP	CD1-CG-CD2	-7.64	100.19	106.30
1	B	62	TRP	CH2-CZ2-CE2	-7.63	109.77	117.40
1	A	46	ASN	CA-C-N	-7.62	100.43	117.20
1	B	3	PHE	O-C-N	-7.61	110.27	123.20
1	A	38	PHE	CD1-CG-CD2	-7.60	108.42	118.30
1	B	86	SER	N-CA-CB	-7.60	99.10	110.50
1	A	30	CYS	CA-CB-SG	-7.59	100.33	114.00
1	A	86	SER	CA-C-O	-7.59	104.15	120.10
1	A	53	TYR	CA-C-O	-7.58	104.19	120.10
1	B	67	GLY	CA-C-O	-7.56	106.98	120.60
1	A	41	GLN	CA-C-N	7.55	133.81	117.20
1	A	75	LEU	C-N-CA	-7.55	102.83	121.70
1	A	84	LEU	CA-C-N	7.54	133.80	117.20
1	A	118	THR	CA-CB-CG2	-7.54	101.84	112.40
1	A	52	ASP	CB-CG-OD1	7.54	125.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	111	TRP	CH2-CZ2-CE2	7.52	124.92	117.40
1	A	38	PHE	CA-C-O	-7.51	104.33	120.10
1	B	28	TRP	NE1-CE2-CD2	-7.50	99.80	107.30
1	A	43	THR	CA-C-N	7.50	133.71	117.20
1	A	34	PHE	CE1-CZ-CE2	-7.50	106.51	120.00
1	B	108	TRP	CZ3-CH2-CZ2	-7.47	112.64	121.60
1	B	23	TYR	CA-C-N	-7.46	100.78	117.20
1	A	97	LYS	CG-CD-CE	-7.40	89.69	111.90
1	B	88	ILE	CB-CA-C	7.39	126.38	111.60
1	A	63	TRP	CA-C-O	7.38	135.60	120.10
1	B	8	LEU	CA-C-N	-7.36	101.01	117.20
1	A	53	TYR	CG-CD1-CE1	7.35	127.18	121.30
1	B	106	ASN	CB-CG-ND2	-7.35	99.05	116.70
1	B	23	TYR	N-CA-CB	-7.34	97.39	110.60
1	B	121	GLN	O-C-N	-7.34	110.95	122.70
1	A	125	ARG	O-C-N	-7.33	110.75	123.20
1	A	129	LEU	CD1-CG-CD2	-7.32	88.55	110.50
1	A	33	LYS	CG-CD-CE	-7.31	89.96	111.90
1	A	47	THR	C-N-CA	-7.31	103.42	121.70
1	A	44	ASN	CB-CA-C	7.30	124.99	110.40
1	B	99	VAL	CA-C-O	-7.28	104.81	120.10
1	A	57	GLN	CG-CD-NE2	7.27	134.15	116.70
1	B	129	LEU	CA-CB-CG	7.27	132.02	115.30
1	B	99	VAL	O-C-N	7.26	134.32	122.70
1	A	35	GLU	O-C-N	-7.25	111.11	122.70
1	B	43	THR	CB-CA-C	-7.22	92.11	111.60
1	A	83	LEU	CA-C-N	7.21	133.07	117.20
1	B	62	TRP	C-N-CA	-7.19	103.72	121.70
1	A	112	ARG	CA-C-O	7.17	135.15	120.10
1	B	37	ASN	OD1-CG-ND2	-7.14	105.47	121.90
1	A	46	ASN	CA-C-O	7.10	135.02	120.10
1	B	46	ASN	CA-C-O	-7.10	105.19	120.10
1	B	69	THR	N-CA-CB	7.10	123.79	110.30
1	A	71	GLY	CA-C-O	-7.09	107.83	120.60
1	A	124	ILE	CA-CB-CG1	7.09	124.48	111.00
1	B	24	SER	N-CA-CB	-7.09	99.87	110.50
1	B	111	TRP	CE2-CD2-CE3	-7.07	110.22	118.70
1	B	111	TRP	CZ3-CH2-CZ2	-7.06	113.12	121.60
1	A	31	ALA	O-C-N	7.05	133.97	122.70
1	A	109	VAL	O-C-N	-7.04	111.44	122.70
1	B	33	LYS	CD-CE-NZ	-7.04	95.51	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LEU	CB-CG-CD2	-7.03	99.05	111.00
1	A	69	THR	CA-CB-CG2	-7.03	102.56	112.40
1	B	123	TRP	CE3-CZ3-CH2	-7.01	113.49	121.20
1	A	108	TRP	O-C-N	-7.01	111.49	122.70
1	A	63	TRP	N-CA-C	7.00	129.89	111.00
1	B	93	ASN	CB-CG-ND2	6.99	133.48	116.70
1	A	33	LYS	CD-CE-NZ	-6.99	95.63	111.70
1	A	21	ARG	CA-C-O	-6.97	105.47	120.10
1	B	95	ALA	C-N-CA	-6.95	104.33	121.70
1	A	21	ARG	NH1-CZ-NH2	-6.94	111.77	119.40
1	B	62	TRP	O-C-N	6.93	133.79	122.70
1	B	70	PRO	CA-C-O	6.92	136.82	120.20
1	A	65	ASN	CB-CG-ND2	-6.91	100.11	116.70
1	A	62	TRP	CD2-CE3-CZ3	-6.91	109.81	118.80
1	B	36	SER	N-CA-CB	-6.90	100.15	110.50
1	A	122	ALA	C-N-CA	-6.90	104.45	121.70
1	A	70	PRO	CA-N-CD	-6.89	101.85	111.50
1	A	23	TYR	CG-CD1-CE1	-6.89	115.79	121.30
1	A	119	ASP	CB-CG-OD1	-6.87	112.12	118.30
1	A	77	ASN	O-C-N	6.86	133.67	122.70
1	B	8	LEU	CB-CG-CD2	-6.83	99.39	111.00
1	B	46	ASN	CB-CA-C	-6.80	96.80	110.40
1	A	113	ASN	CB-CG-OD1	-6.80	108.01	121.60
1	B	12	MET	CA-C-O	-6.79	105.83	120.10
1	B	75	LEU	N-CA-CB	6.79	123.99	110.40
1	B	17	LEU	CA-C-O	-6.78	105.87	120.10
1	A	19	ASN	CA-CB-CG	-6.77	98.50	113.40
1	B	123	TRP	CB-CG-CD2	6.73	135.35	126.60
1	A	125	ARG	CA-C-O	6.71	134.18	120.10
1	A	86	SER	CB-CA-C	-6.70	97.37	110.10
1	A	15	HIS	CE1-NE2-CD2	6.70	123.34	106.60
1	A	124	ILE	C-N-CA	-6.69	104.97	121.70
1	A	37	ASN	CB-CG-OD1	6.68	134.96	121.60
1	A	108	TRP	CD1-NE1-CE2	6.65	114.99	109.00
1	A	24	SER	N-CA-CB	-6.65	100.53	110.50
1	A	51	THR	CA-C-N	-6.64	102.58	117.20
1	B	35	GLU	CG-CD-OE1	6.64	131.59	118.30
1	A	20	TYR	CB-CG-CD1	-6.63	117.02	121.00
1	A	38	PHE	CG-CD2-CE2	6.62	128.09	120.80
1	A	53	TYR	CD1-CG-CD2	6.61	125.17	117.90
1	B	31	ALA	O-C-N	-6.59	112.15	122.70
1	B	70	PRO	CA-N-CD	-6.59	102.27	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ARG	CB-CA-C	6.59	123.58	110.40
1	A	100	SER	C-N-CA	6.57	138.12	121.70
1	A	15	HIS	ND1-CE1-NE2	-6.56	95.47	109.90
1	B	20	TYR	C-N-CA	6.55	138.09	121.70
1	A	120	VAL	CA-CB-CG2	-6.55	101.08	110.90
1	B	102	GLY	O-C-N	6.54	133.17	122.70
1	A	11	ALA	O-C-N	6.53	133.16	122.70
1	A	69	THR	C-N-CD	6.53	142.11	128.40
1	B	48	ASP	CB-CG-OD2	6.53	124.17	118.30
1	B	116	LYS	C-N-CA	-6.52	108.60	122.30
1	A	66	ASP	OD1-CG-OD2	-6.51	110.92	123.30
1	B	38	PHE	CE1-CZ-CE2	-6.50	108.30	120.00
1	B	44	ASN	CA-C-N	-6.49	102.91	117.20
1	B	80	CYS	N-CA-CB	-6.49	98.91	110.60
1	B	72	SER	CB-CA-C	-6.49	97.77	110.10
1	A	115	CYS	CA-C-O	-6.49	106.48	120.10
1	B	47	THR	C-N-CA	-6.48	105.50	121.70
1	B	13	LYS	N-CA-CB	-6.47	98.94	110.60
1	A	30	CYS	N-CA-CB	-6.47	98.95	110.60
1	A	73	ARG	CG-CD-NE	-6.47	98.21	111.80
1	B	10	ALA	CA-C-O	-6.47	106.52	120.10
1	A	111	TRP	CE2-CD2-CE3	-6.46	110.95	118.70
1	A	99	VAL	O-C-N	6.46	133.03	122.70
1	A	28	TRP	NE1-CE2-CZ2	-6.46	123.30	130.40
1	A	63	TRP	CA-C-N	-6.44	103.02	117.20
1	A	13	LYS	CD-CE-NZ	6.43	126.50	111.70
1	B	96	LYS	CA-C-O	-6.42	106.62	120.10
1	A	69	THR	CA-C-N	-6.41	99.16	117.10
1	A	14	ARG	CG-CD-NE	-6.41	98.35	111.80
1	B	49	GLY	CA-C-O	-6.39	109.09	120.60
1	A	76	CYS	CA-CB-SG	-6.39	102.50	114.00
1	A	128	ARG	CD-NE-CZ	-6.38	114.66	123.60
1	B	63	TRP	N-CA-C	6.38	128.23	111.00
1	B	22	GLY	CA-C-N	6.36	131.19	117.20
1	B	119	ASP	O-C-N	-6.35	112.54	122.70
1	A	86	SER	N-CA-C	-6.34	93.89	111.00
1	B	80	CYS	O-C-N	-6.33	112.57	122.70
1	A	123	TRP	O-C-N	6.33	132.82	122.70
1	A	63	TRP	C-N-CA	-6.32	105.90	121.70
1	A	127	CYS	CA-C-N	-6.31	103.33	117.20
1	B	89	THR	OG1-CB-CG2	-6.31	95.50	110.00
1	A	49	GLY	CA-C-O	6.30	131.95	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	SER	CA-C-N	-6.30	103.33	117.20
1	A	114	ARG	NH1-CZ-NH2	6.29	126.32	119.40
1	B	7	GLU	CG-CD-OE2	-6.29	105.72	118.30
1	B	66	ASP	CB-CA-C	6.29	122.98	110.40
1	A	111	TRP	NE1-CE2-CD2	-6.28	101.02	107.30
1	A	86	SER	N-CA-CB	-6.27	101.10	110.50
1	B	41	GLN	OE1-CD-NE2	-6.24	107.55	121.90
1	B	50	SER	N-CA-CB	6.22	119.84	110.50
1	B	41	GLN	CA-C-O	6.20	133.12	120.10
1	B	7	GLU	O-C-N	-6.19	112.80	122.70
1	A	116	LYS	CA-C-N	-6.18	103.83	116.20
1	A	39	ASN	CB-CA-C	-6.17	98.06	110.40
1	B	20	TYR	O-C-N	-6.16	112.84	122.70
1	A	128	ARG	CG-CD-NE	6.15	124.72	111.80
1	B	15	HIS	CG-CD2-NE2	-6.12	97.57	109.20
1	A	15	HIS	CB-CG-CD2	-6.11	111.87	130.80
1	A	97	LYS	CB-CG-CD	-6.10	95.75	111.60
1	A	51	THR	CA-CB-OG1	-6.09	96.22	109.00
1	B	106	ASN	CB-CG-OD1	6.08	133.77	121.60
1	A	108	TRP	CB-CG-CD1	-6.08	119.10	127.00
1	A	11	ALA	N-CA-CB	6.08	118.61	110.10
1	A	33	LYS	O-C-N	6.07	132.41	122.70
1	A	38	PHE	CA-CB-CG	6.06	128.45	113.90
1	A	38	PHE	CB-CA-C	6.06	122.52	110.40
1	A	44	ASN	O-C-N	-6.05	113.01	122.70
1	B	62	TRP	CB-CG-CD1	-6.05	119.13	127.00
1	A	12	MET	C-N-CA	-6.05	106.58	121.70
1	A	109	VAL	CA-CB-CG1	-6.05	101.83	110.90
1	A	65	ASN	CA-C-N	6.05	130.51	117.20
1	A	25	LEU	CA-C-N	-6.03	104.14	116.20
1	A	93	ASN	N-CA-CB	6.00	121.40	110.60
1	A	4	GLY	CA-C-O	-5.99	109.82	120.60
1	A	36	SER	N-CA-C	5.99	127.17	111.00
1	A	85	SER	CA-C-O	-5.99	107.52	120.10
1	A	108	TRP	CE2-CD2-CG	5.98	112.08	107.30
1	B	63	TRP	CE2-CD2-CG	-5.98	102.51	107.30
1	A	73	ARG	CA-C-N	5.96	130.32	117.20
1	A	116	LYS	N-CA-CB	-5.95	99.89	110.60
1	A	69	THR	CA-C-O	5.95	132.59	120.10
1	A	109	VAL	CA-CB-CG2	-5.94	101.99	110.90
1	B	41	GLN	CA-CB-CG	5.92	126.42	113.40
1	A	128	ARG	O-C-N	5.92	132.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ILE	CB-CA-C	-5.91	99.78	111.60
1	A	61	ARG	O-C-N	5.90	132.13	122.70
1	A	112	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	B	112	ARG	CA-CB-CG	5.88	126.34	113.40
1	B	5	ARG	C-N-CA	-5.88	107.01	121.70
1	B	14	ARG	O-C-N	-5.87	113.31	122.70
1	B	53	TYR	OH-CZ-CE2	-5.86	104.27	120.10
1	A	37	ASN	CA-CB-CG	-5.85	100.54	113.40
1	A	47	THR	N-CA-C	-5.84	95.22	111.00
1	A	121	GLN	CG-CD-NE2	-5.84	102.68	116.70
1	B	45	ARG	CA-C-N	5.82	130.00	117.20
1	A	63	TRP	N-CA-CB	-5.81	100.13	110.60
1	A	77	ASN	C-N-CA	-5.81	107.19	121.70
1	B	116	LYS	CA-C-N	-5.81	104.59	116.20
1	A	89	THR	CA-CB-CG2	5.80	120.52	112.40
1	B	24	SER	O-C-N	5.79	131.97	122.70
1	B	8	LEU	C-N-CA	-5.79	107.23	121.70
1	A	41	GLN	N-CA-CB	5.78	121.01	110.60
1	A	59	ASN	OD1-CG-ND2	-5.78	108.61	121.90
1	A	65	ASN	C-N-CA	5.78	136.14	121.70
1	B	12	MET	N-CA-CB	-5.77	100.21	110.60
1	B	113	ASN	CB-CG-OD1	5.76	133.13	121.60
1	A	108	TRP	CZ3-CH2-CZ2	5.76	128.51	121.60
1	B	41	GLN	N-CA-C	5.75	126.54	111.00
1	B	68	ARG	N-CA-C	-5.75	95.47	111.00
1	B	110	ALA	O-C-N	-5.75	113.50	122.70
1	A	66	ASP	CB-CA-C	5.74	121.88	110.40
1	B	122	ALA	CA-C-N	-5.72	104.61	117.20
1	A	114	ARG	CD-NE-CZ	-5.72	115.60	123.60
1	A	125	ARG	CB-CG-CD	5.71	126.44	111.60
1	B	74	ASN	C-N-CA	5.71	135.97	121.70
1	A	90	ALA	CB-CA-C	-5.71	101.54	110.10
1	A	22	GLY	N-CA-C	5.70	127.35	113.10
1	B	118	THR	CA-C-O	-5.70	108.13	120.10
1	B	128	ARG	CA-C-O	-5.70	108.14	120.10
1	B	61	ARG	O-C-N	5.69	131.81	122.70
1	B	40	THR	CA-CB-CG2	5.69	120.37	112.40
1	A	123	TRP	CD2-CE2-CZ2	-5.69	115.47	122.30
1	B	5	ARG	N-CA-C	5.69	126.36	111.00
1	B	5	ARG	CG-CD-NE	5.68	123.73	111.80
1	B	56	LEU	CB-CG-CD2	-5.67	101.37	111.00
1	B	12	MET	C-N-CA	-5.62	107.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	GLN	OE1-CD-NE2	-5.62	108.98	121.90
1	A	43	THR	N-CA-CB	5.61	120.96	110.30
1	A	60	SER	O-C-N	-5.61	113.72	122.70
1	A	75	LEU	CB-CG-CD2	5.61	120.53	111.00
1	A	65	ASN	CA-CB-CG	-5.60	101.09	113.40
1	A	73	ARG	CD-NE-CZ	-5.59	115.77	123.60
1	B	67	GLY	N-CA-C	-5.59	99.13	113.10
1	A	43	THR	CA-CB-OG1	-5.58	97.28	109.00
1	A	84	LEU	CB-CG-CD2	5.58	120.48	111.00
1	A	14	ARG	CA-C-O	5.57	131.79	120.10
1	A	70	PRO	CA-C-O	5.56	133.55	120.20
1	A	109	VAL	CG1-CB-CG2	-5.56	102.01	110.90
1	B	56	LEU	O-C-N	-5.55	113.82	122.70
1	A	14	ARG	CB-CG-CD	-5.54	97.19	111.60
1	A	103	ASN	CA-C-N	5.54	127.28	116.20
1	B	65	ASN	O-C-N	5.54	131.56	122.70
1	A	39	ASN	N-CA-CB	-5.53	100.64	110.60
1	A	103	ASN	OD1-CG-ND2	5.53	134.62	121.90
1	A	97	LYS	CA-C-N	5.53	129.36	117.20
1	B	113	ASN	OD1-CG-ND2	-5.52	109.20	121.90
1	B	45	ARG	CB-CA-C	-5.51	99.37	110.40
1	A	109	VAL	CA-C-N	5.51	129.31	117.20
1	A	84	LEU	CA-CB-CG	-5.50	102.66	115.30
1	A	15	HIS	C-N-CA	-5.49	110.77	122.30
1	A	69	THR	N-CA-CB	-5.49	99.86	110.30
1	A	74	ASN	CB-CG-ND2	-5.49	103.53	116.70
1	A	78	ILE	CA-C-O	5.48	131.61	120.10
1	A	1	LYS	C-N-CA	5.48	135.40	121.70
1	B	51	THR	OG1-CB-CG2	-5.47	97.42	110.00
1	B	52	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	20	TYR	CA-C-N	-5.46	105.18	117.20
1	B	122	ALA	N-CA-CB	-5.46	102.46	110.10
1	B	38	PHE	CG-CD2-CE2	5.45	126.80	120.80
1	A	92	VAL	CA-CB-CG2	-5.43	102.75	110.90
1	A	101	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	B	11	ALA	O-C-N	5.43	131.39	122.70
1	A	100	SER	N-CA-CB	-5.43	102.35	110.50
1	A	34	PHE	N-CA-CB	-5.43	100.83	110.60
1	A	118	THR	CA-CB-OG1	-5.43	97.60	109.00
1	A	2	VAL	N-CA-CB	5.42	123.43	111.50
1	B	59	ASN	CB-CG-ND2	-5.42	103.69	116.70
1	B	28	TRP	CG-CD2-CE3	5.42	138.78	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	PRO	N-CA-C	-5.42	98.01	112.10
1	B	106	ASN	N-CA-CB	5.42	120.35	110.60
1	A	23	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	A	18	ASP	N-CA-CB	-5.41	100.86	110.60
1	B	55	ILE	CA-C-O	-5.41	108.74	120.10
1	B	32	ALA	N-CA-CB	-5.40	102.54	110.10
1	A	114	ARG	O-C-N	5.40	131.33	122.70
1	B	100	SER	CB-CA-C	-5.39	99.86	110.10
1	A	61	ARG	CB-CG-CD	-5.39	97.60	111.60
1	B	120	VAL	CG1-CB-CG2	5.39	119.52	110.90
1	A	23	TYR	O-C-N	-5.38	114.09	122.70
1	B	15	HIS	CA-CB-CG	-5.37	104.47	113.60
1	A	115	CYS	CA-CB-SG	-5.37	104.34	114.00
1	A	20	TYR	CD1-CG-CD2	5.36	123.80	117.90
1	A	121	GLN	CA-C-O	5.36	131.35	120.10
1	A	42	ALA	CB-CA-C	-5.35	102.07	110.10
1	A	25	LEU	C-N-CA	-5.35	111.06	122.30
1	B	34	PHE	CD1-CG-CD2	5.35	125.25	118.30
1	A	48	ASP	CB-CA-C	-5.34	99.72	110.40
1	B	89	THR	CA-C-O	5.34	131.31	120.10
1	A	7	GLU	O-C-N	-5.33	114.18	122.70
1	A	87	ASP	N-CA-CB	-5.32	101.02	110.60
1	A	71	GLY	O-C-N	5.31	131.20	122.70
1	B	111	TRP	NE1-CE2-CZ2	5.31	136.25	130.40
1	A	34	PHE	CD1-CE1-CZ	5.31	126.47	120.10
1	B	46	ASN	N-CA-C	5.30	125.30	111.00
1	B	87	ASP	CA-CB-CG	5.30	125.05	113.40
1	A	99	VAL	CG1-CB-CG2	5.29	119.36	110.90
1	B	88	ILE	CB-CG1-CD1	5.27	128.67	113.90
1	B	44	ASN	CB-CG-OD1	-5.26	111.07	121.60
1	B	78	ILE	CA-C-N	5.26	131.84	117.10
1	B	62	TRP	CE2-CD2-CE3	5.26	125.01	118.70
1	B	129	LEU	CD1-CG-CD2	-5.26	94.72	110.50
1	A	123	TRP	N-CA-CB	-5.26	101.13	110.60
1	B	25	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	B	43	THR	C-N-CA	5.25	134.83	121.70
1	A	32	ALA	O-C-N	5.21	131.04	122.70
1	B	72	SER	N-CA-CB	-5.21	102.68	110.50
1	B	105	MET	O-C-N	-5.21	114.36	122.70
1	A	35	GLU	CA-C-O	5.21	131.03	120.10
1	A	14	ARG	CA-C-N	-5.20	105.75	117.20
1	B	65	ASN	CA-CB-CG	-5.20	101.95	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	CYS	CB-CA-C	5.20	120.81	110.40
1	A	92	VAL	CA-C-O	5.20	131.02	120.10
1	B	7	GLU	N-CA-CB	-5.19	101.26	110.60
1	B	21	ARG	C-N-CA	-5.19	111.40	122.30
1	A	107	ALA	CB-CA-C	-5.18	102.33	110.10
1	B	3	PHE	CD1-CG-CD2	-5.17	111.58	118.30
1	A	2	VAL	O-C-N	5.16	130.95	122.70
1	B	23	TYR	CA-C-O	5.16	130.93	120.10
1	B	123	TRP	CA-CB-CG	-5.16	103.90	113.70
1	A	128	ARG	C-N-CA	-5.15	108.83	121.70
1	B	105	MET	CG-SD-CE	-5.14	91.97	100.20
1	A	53	TYR	N-CA-C	5.14	124.88	111.00
1	A	129	LEU	CB-CG-CD2	5.13	119.72	111.00
1	B	15	HIS	O-C-N	-5.12	114.50	123.20
1	A	33	LYS	C-N-CA	-5.12	108.91	121.70
1	B	42	ALA	CA-C-N	5.11	128.45	117.20
1	A	41	GLN	CG-CD-OE1	-5.11	111.38	121.60
1	B	73	ARG	CA-CB-CG	-5.11	102.16	113.40
1	B	108	TRP	CE3-CZ3-CH2	5.11	126.82	121.20
1	B	123	TRP	NE1-CE2-CZ2	5.10	136.01	130.40
1	A	38	PHE	O-C-N	5.09	130.85	122.70
1	A	35	GLU	CG-CD-OE2	5.09	128.48	118.30
1	B	25	LEU	N-CA-C	5.09	124.73	111.00
1	A	38	PHE	CD1-CE1-CZ	-5.08	114.01	120.10
1	B	85	SER	CA-C-O	-5.08	109.44	120.10
1	B	100	SER	N-CA-CB	-5.07	102.89	110.50
1	B	87	ASP	CA-C-N	5.07	128.35	117.20
1	A	23	TYR	N-CA-CB	-5.05	101.51	110.60
1	B	20	TYR	CD1-CG-CD2	5.05	123.45	117.90
1	A	3	PHE	CA-C-O	5.04	130.68	120.10
1	A	129	LEU	CA-C-O	-5.03	109.53	120.10
1	A	12	MET	CA-C-O	-5.03	109.54	120.10
1	B	77	ASN	O-C-N	5.02	130.74	122.70
1	A	61	ARG	CG-CD-NE	-5.02	101.27	111.80
1	B	125	ARG	CA-C-O	-5.02	109.56	120.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	ARG	Sidechain
1	B	21	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	61	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1001	0	947	151	0
1	B	1001	0	941	98	0
2	A	11	0	0	5	0
2	B	6	0	0	2	0
3	A	143	0	0	5	0
3	B	168	0	0	8	0
All	All	2330	0	1888	250	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:CD	1:A:14:ARG:CG	1.78	1.61
1:B:21:ARG:CB	1:B:21:ARG:CA	1.77	1.60
1:B:15:HIS:CB	1:B:15:HIS:CG	1.80	1.60
1:A:45:ARG:CB	1:A:45:ARG:CA	1.74	1.59
1:B:76:CYS:CA	1:B:76:CYS:CB	1.74	1.59
1:A:76:CYS:CA	1:A:76:CYS:CB	1.74	1.59
1:A:68:ARG:CG	1:A:68:ARG:CD	1.81	1.58
1:B:21:ARG:CB	1:B:21:ARG:CG	1.82	1.58
1:B:72:SER:CA	1:B:72:SER:CB	1.76	1.58
1:B:124:ILE:CD1	1:B:124:ILE:CG1	1.75	1.57
1:B:58:ILE:CG2	1:B:58:ILE:CB	1.74	1.57
1:B:1:LYS:CD	1:B:1:LYS:CE	1.81	1.56
1:A:112:ARG:CD	1:A:112:ARG:CG	1.81	1.55
1:B:61:ARG:CG	1:B:61:ARG:CD	1.83	1.54
1:A:121:GLN:HG2	2:A:142:IOD:I	1.76	1.54
1:A:112:ARG:NH2	1:A:112:ARG:CZ	1.71	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASN:CB	1:A:44:ASN:CG	1.75	1.54
1:A:21:ARG:CA	1:A:21:ARG:N	1.69	1.53
1:B:46:ASN:CB	1:B:46:ASN:CG	1.74	1.53
1:A:33:LYS:CD	1:A:33:LYS:CE	1.85	1.53
1:B:37:ASN:C	1:B:37:ASN:CA	1.75	1.52
1:A:72:SER:CA	1:A:72:SER:CB	1.82	1.52
1:A:61:ARG:CD	1:A:61:ARG:CG	1.87	1.51
1:A:62:TRP:CA	1:A:62:TRP:CB	1.87	1.51
1:A:93:ASN:CB	1:A:93:ASN:CG	1.76	1.51
1:A:68:ARG:NE	1:A:68:ARG:CD	1.73	1.50
1:B:121:GLN:CG	1:B:121:GLN:CD	1.79	1.50
1:B:85:SER:CA	1:B:85:SER:C	1.76	1.50
1:B:61:ARG:NH2	1:B:61:ARG:CZ	1.67	1.50
1:A:127:CYS:CA	1:A:127:CYS:C	1.80	1.50
1:A:45:ARG:CZ	1:A:45:ARG:NE	1.74	1.50
1:A:125:ARG:CZ	1:A:125:ARG:NH1	1.72	1.49
1:A:78:ILE:CB	1:A:78:ILE:CA	1.89	1.49
1:A:48:ASP:CA	1:A:48:ASP:CB	1.85	1.49
1:A:128:ARG:CA	1:A:128:ARG:C	1.79	1.49
1:B:128:ARG:CD	1:B:128:ARG:CG	1.87	1.49
1:A:112:ARG:CD	1:A:112:ARG:NE	1.77	1.48
1:B:73:ARG:CZ	1:B:73:ARG:NH1	1.74	1.48
1:A:47:THR:CG2	1:A:47:THR:CB	1.87	1.47
1:A:101:ASP:CB	1:A:101:ASP:CG	1.80	1.47
1:A:128:ARG:N	1:A:128:ARG:CA	1.75	1.46
1:A:2:VAL:CA	1:A:2:VAL:C	1.82	1.46
1:B:43:THR:CG2	1:B:43:THR:CB	1.91	1.45
1:B:121:GLN:NE2	1:B:121:GLN:CD	1.69	1.44
1:B:128:ARG:CZ	1:B:128:ARG:NH2	1.79	1.43
1:B:114:ARG:CZ	1:B:114:ARG:NE	1.81	1.42
1:B:128:ARG:CZ	1:B:128:ARG:NE	1.83	1.41
1:A:122:ALA:CA	1:A:122:ALA:C	1.87	1.40
1:A:129:LEU:CA	1:A:129:LEU:CB	1.99	1.40
1:A:30:CYS:CB	1:A:30:CYS:SG	2.09	1.40
1:A:87:ASP:CA	1:A:87:ASP:CB	1.95	1.40
1:A:14:ARG:CD	1:A:14:ARG:NE	1.84	1.39
1:B:45:ARG:CZ	1:B:45:ARG:NH1	1.86	1.38
1:B:69:THR:CB	1:B:69:THR:OG1	1.73	1.37
1:A:45:ARG:CD	1:A:45:ARG:CG	2.03	1.36
1:B:128:ARG:CD	1:B:128:ARG:HH11	1.38	1.34
1:A:48:ASP:C	1:A:49:GLY:N	1.86	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLN:CB	1:A:121:GLN:CG	2.15	1.24
1:A:45:ARG:NH1	1:A:45:ARG:CZ	2.01	1.23
1:B:47:THR:CB	1:B:47:THR:OG1	1.86	1.23
1:B:128:ARG:CD	1:B:128:ARG:NH1	2.05	1.19
1:B:128:ARG:HH11	1:B:128:ARG:HD3	1.07	1.19
1:A:47:THR:CA	1:A:47:THR:N	2.06	1.18
1:A:87:ASP:CG	1:A:87:ASP:CB	2.14	1.16
1:A:87:ASP:OD2	1:A:87:ASP:CB	1.95	1.15
1:A:121:GLN:CG	2:A:142:IOD:I	2.66	1.13
1:A:45:ARG:CB	1:A:45:ARG:CG	2.31	1.08
1:A:14:ARG:CD	1:A:14:ARG:CZ	2.33	1.07
1:B:61:ARG:CZ	1:B:61:ARG:NH1	2.18	1.06
1:B:61:ARG:CG	1:B:61:ARG:NE	2.20	1.05
1:A:112:ARG:NE	1:A:112:ARG:CG	2.20	1.04
1:A:112:ARG:HD3	3:A:350:HOH:O	1.58	1.02
1:A:129:LEU:N	1:A:129:LEU:CB	2.21	1.02
1:A:121:GLN:CB	1:A:121:GLN:CD	2.27	1.01
1:A:68:ARG:CZ	1:A:68:ARG:CD	2.37	1.00
1:A:127:CYS:C	1:A:128:ARG:CA	2.29	1.00
1:A:14:ARG:CD	1:A:14:ARG:CB	2.41	0.99
1:A:78:ILE:CG1	1:A:78:ILE:CA	2.41	0.98
1:A:73:ARG:HD3	3:A:302:HOH:O	1.64	0.97
1:B:43:THR:CG2	1:B:43:THR:CA	2.44	0.96
1:B:128:ARG:NH1	1:B:128:ARG:HD3	1.75	0.95
1:B:18:ASP:OD1	3:B:334:HOH:O	1.85	0.95
1:B:114:ARG:CD	1:B:114:ARG:CZ	2.44	0.94
1:A:44:ASN:OD1	1:A:44:ASN:CB	2.14	0.94
1:A:33:LYS:CG	1:A:33:LYS:CE	2.44	0.94
1:A:47:THR:OG1	1:A:47:THR:CG2	2.15	0.93
1:B:124:ILE:CD1	1:B:124:ILE:CB	2.47	0.93
1:B:128:ARG:CZ	1:B:128:ARG:CD	2.46	0.92
1:A:48:ASP:C	1:A:49:GLY:CA	2.38	0.91
1:B:21:ARG:CG	1:B:21:ARG:CA	2.49	0.90
1:B:43:THR:CG2	1:B:43:THR:OG1	2.19	0.90
1:A:128:ARG:O	1:A:128:ARG:CA	2.19	0.89
1:A:78:ILE:C	1:A:78:ILE:CB	2.40	0.88
1:B:128:ARG:HH11	1:B:128:ARG:HD2	1.38	0.87
1:A:121:GLN:NE2	2:A:142:IOD:I	2.77	0.86
1:B:72:SER:CB	1:B:72:SER:N	2.39	0.85
1:B:47:THR:OG1	1:B:47:THR:CA	2.24	0.85
1:B:15:HIS:CA	1:B:15:HIS:CG	2.60	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:CA	1:B:58:ILE:CG2	2.54	0.85
1:A:14:ARG:HH11	1:A:14:ARG:HD3	1.41	0.83
1:B:45:ARG:NH1	1:B:45:ARG:CD	2.42	0.83
1:B:76:CYS:CB	1:B:76:CYS:C	2.49	0.80
1:B:21:ARG:CB	1:B:21:ARG:C	2.51	0.80
1:A:87:ASP:C	1:A:87:ASP:CB	2.51	0.80
1:A:78:ILE:CB	1:A:78:ILE:N	2.45	0.79
1:A:127:CYS:CA	1:A:128:ARG:N	2.46	0.79
1:B:73:ARG:NH1	1:B:73:ARG:NE	2.29	0.78
1:A:68:ARG:CB	1:A:68:ARG:CD	2.56	0.78
1:B:128:ARG:NH2	1:B:128:ARG:NE	2.31	0.78
1:B:45:ARG:NH1	1:B:45:ARG:NE	2.30	0.78
1:B:69:THR:CG2	1:B:69:THR:OG1	2.32	0.78
1:B:128:ARG:NE	1:B:128:ARG:CG	2.46	0.77
1:A:127:CYS:CA	1:A:127:CYS:O	2.33	0.77
1:B:61:ARG:CD	1:B:61:ARG:CB	2.62	0.77
1:A:93:ASN:CA	1:A:93:ASN:CG	2.52	0.77
1:B:72:SER:C	1:B:72:SER:CB	2.53	0.76
1:A:62:TRP:N	1:A:62:TRP:CB	2.48	0.76
1:A:112:ARG:NH2	1:A:112:ARG:NH1	2.21	0.76
1:A:112:ARG:NE	1:A:112:ARG:HG2	1.99	0.76
1:A:112:ARG:CD	1:A:112:ARG:CZ	2.63	0.75
1:A:45:ARG:NH2	1:A:45:ARG:NE	2.31	0.74
1:A:48:ASP:O	1:A:49:GLY:HA3	1.86	0.74
1:A:48:ASP:C	1:A:49:GLY:HA3	2.06	0.74
1:A:122:ALA:C	1:A:122:ALA:CB	2.56	0.74
1:B:58:ILE:CG2	1:B:58:ILE:CG1	2.65	0.74
1:B:121:GLN:NE2	1:B:121:GLN:CG	2.52	0.72
1:B:72:SER:OG	1:B:72:SER:CA	2.34	0.72
1:A:14:ARG:CD	1:A:14:ARG:NH1	2.53	0.72
1:B:46:ASN:CA	1:B:46:ASN:CG	2.59	0.71
1:A:61:ARG:CB	1:A:61:ARG:CD	2.68	0.71
1:A:76:CYS:CA	1:A:76:CYS:SG	2.79	0.71
1:A:72:SER:CA	1:A:72:SER:OG	2.38	0.71
1:B:37:ASN:CB	1:B:37:ASN:C	2.56	0.70
1:A:76:CYS:C	1:A:76:CYS:CB	2.60	0.70
1:B:85:SER:CB	1:B:85:SER:C	2.60	0.70
1:B:114:ARG:NE	1:B:114:ARG:NH2	2.39	0.70
1:A:48:ASP:CA	1:A:48:ASP:CG	2.60	0.70
1:A:72:SER:N	1:A:72:SER:CB	2.54	0.70
1:B:114:ARG:CZ	1:B:114:ARG:HD3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HD3	1:A:14:ARG:NH1	2.06	0.69
1:A:76:CYS:N	1:A:76:CYS:CB	2.55	0.69
1:A:101:ASP:OD2	1:A:101:ASP:CB	2.39	0.69
1:A:112:ARG:NH2	1:A:112:ARG:NE	2.40	0.69
1:B:37:ASN:N	1:B:37:ASN:C	2.43	0.69
1:A:48:ASP:C	1:A:48:ASP:CB	2.60	0.69
1:A:20:TYR:C	1:A:21:ARG:CA	2.56	0.69
1:A:2:VAL:CB	1:A:2:VAL:C	2.54	0.69
1:B:21:ARG:CZ	3:B:388:HOH:O	2.40	0.68
1:B:45:ARG:HH11	1:B:45:ARG:CD	2.04	0.68
1:A:62:TRP:C	1:A:62:TRP:CB	2.62	0.68
1:B:46:ASN:CB	1:B:46:ASN:ND2	2.58	0.67
1:A:93:ASN:CB	1:A:93:ASN:OD1	2.42	0.67
1:B:21:ARG:CB	1:B:21:ARG:N	2.57	0.66
1:A:122:ALA:CA	1:A:123:TRP:N	2.55	0.66
1:A:112:ARG:CD	1:A:112:ARG:CB	2.67	0.65
1:A:30:CYS:SG	1:A:30:CYS:CA	2.84	0.65
1:A:45:ARG:CZ	1:A:45:ARG:CD	2.61	0.65
2:A:134:IOD:I	3:B:198:HOH:O	2.84	0.64
1:B:15:HIS:HB3	1:B:92:VAL:HG11	1.78	0.64
1:A:72:SER:C	1:A:72:SER:CB	2.64	0.64
1:A:78:ILE:HG13	1:A:78:ILE:CA	2.26	0.64
1:A:33:LYS:NZ	1:A:33:LYS:CD	2.60	0.64
1:A:21:ARG:C	1:A:21:ARG:N	2.48	0.64
1:A:47:THR:N	1:A:47:THR:CB	2.58	0.64
1:B:61:ARG:HG3	1:B:61:ARG:NH1	2.12	0.64
1:A:125:ARG:HD3	1:A:125:ARG:NH1	2.12	0.64
1:A:129:LEU:N	1:A:129:LEU:HG	2.13	0.63
1:A:63:TRP:O	1:A:76:CYS:HB2	1.99	0.63
1:A:121:GLN:HB3	1:A:121:GLN:CD	2.20	0.62
1:B:76:CYS:CA	1:B:76:CYS:SG	2.87	0.62
1:B:1:LYS:NZ	1:B:1:LYS:CD	2.56	0.62
1:A:93:ASN:HD22	1:A:93:ASN:HA	1.65	0.62
1:A:21:ARG:CB	1:A:21:ARG:N	2.63	0.61
1:B:121:GLN:CG	1:B:121:GLN:OE1	2.41	0.61
1:A:129:LEU:CB	1:A:129:LEU:C	2.65	0.61
1:A:14:ARG:CD	1:A:14:ARG:HB2	2.31	0.60
1:A:45:ARG:CG	1:A:45:ARG:NE	2.56	0.60
1:A:129:LEU:CB	1:A:129:LEU:H	2.09	0.59
1:A:44:ASN:CG	1:A:44:ASN:CA	2.69	0.56
1:B:45:ARG:HD3	1:B:45:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:TRP:CD1	1:A:115:CYS:HB2	2.40	0.56
1:B:85:SER:O	1:B:85:SER:CA	2.46	0.56
1:A:75:LEU:HA	3:A:313:HOH:O	2.05	0.55
1:A:88:ILE:HG12	2:A:133:IOD:I	2.77	0.55
1:A:2:VAL:CA	1:A:2:VAL:O	2.50	0.55
1:A:93:ASN:HA	1:A:93:ASN:ND2	2.22	0.55
1:B:45:ARG:HD3	1:B:45:ARG:NH1	2.22	0.55
1:A:14:ARG:HD3	1:A:14:ARG:CZ	2.27	0.55
1:B:73:ARG:NH1	1:B:73:ARG:CD	2.69	0.55
1:A:68:ARG:NH1	1:A:68:ARG:CD	2.70	0.55
1:A:129:LEU:H	1:A:129:LEU:HB2	1.73	0.54
1:A:101:ASP:CA	1:A:101:ASP:CG	2.69	0.54
1:A:45:ARG:CA	1:A:45:ARG:CG	2.87	0.53
1:A:62:TRP:CG	1:A:62:TRP:CA	2.88	0.53
1:B:97:LYS:HE2	3:B:428:HOH:O	2.09	0.53
1:A:45:ARG:CB	1:A:45:ARG:N	2.62	0.52
1:B:69:THR:O	1:B:72:SER:HB3	2.10	0.51
1:A:48:ASP:CG	1:A:48:ASP:C	2.70	0.51
1:A:15:HIS:HD2	3:A:444:HOH:O	1.93	0.51
1:B:76:CYS:CB	1:B:76:CYS:N	2.58	0.51
1:A:14:ARG:CG	1:A:14:ARG:NE	2.74	0.50
1:B:61:ARG:CG	1:B:61:ARG:CZ	2.86	0.50
1:A:45:ARG:CB	1:A:45:ARG:C	2.72	0.50
1:A:61:ARG:NE	1:A:61:ARG:CG	2.69	0.50
1:A:128:ARG:N	1:A:128:ARG:CB	2.66	0.49
1:A:47:THR:N	1:A:48:ASP:N	2.59	0.49
1:A:87:ASP:N	1:A:87:ASP:CB	2.73	0.48
1:A:127:CYS:C	1:A:127:CYS:CB	2.74	0.48
1:A:68:ARG:NE	1:A:68:ARG:CG	2.74	0.48
1:A:78:ILE:CD1	1:A:78:ILE:CA	2.92	0.48
1:B:21:ARG:HD3	1:B:21:ARG:HA	1.96	0.47
1:A:63:TRP:CE2	1:A:98:ILE:HG12	2.49	0.47
1:B:128:ARG:HD2	1:B:128:ARG:NH1	2.07	0.47
1:B:1:LYS:HE3	3:B:342:HOH:O	2.15	0.47
1:A:78:ILE:HG13	1:A:79:PRO:HD2	1.96	0.47
1:B:43:THR:N	1:B:43:THR:CG2	2.78	0.47
1:A:129:LEU:CA	1:A:129:LEU:CG	2.81	0.46
1:B:61:ARG:CG	1:B:61:ARG:NH1	2.78	0.46
1:A:45:ARG:CB	1:A:45:ARG:HA	2.19	0.46
1:A:93:ASN:ND2	1:A:93:ASN:CA	2.77	0.46
1:A:93:ASN:HA	1:A:93:ASN:CG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:HH11	1:B:68:ARG:HD2	1.60	0.45
1:B:37:ASN:O	1:B:37:ASN:CA	2.56	0.45
1:A:121:GLN:CA	1:A:121:GLN:CG	2.94	0.45
1:B:68:ARG:NH2	3:B:267:HOH:O	2.48	0.44
1:B:121:GLN:HG2	2:B:131:IOD:I	2.87	0.44
1:A:18:ASP:O	1:A:19:ASN:HB2	2.18	0.44
1:A:14:ARG:HD3	1:A:14:ARG:HB2	1.98	0.44
1:B:97:LYS:CE	3:B:428:HOH:O	2.66	0.44
1:B:128:ARG:CB	1:B:128:ARG:CD	2.84	0.44
1:B:114:ARG:HD3	1:B:114:ARG:NH1	2.33	0.44
1:A:51:THR:HB	1:A:53:TYR:CE1	2.52	0.44
1:A:47:THR:C	1:A:47:THR:N	2.71	0.43
1:A:48:ASP:CB	1:A:48:ASP:N	2.73	0.43
1:B:61:ARG:HB2	1:B:61:ARG:NH1	2.33	0.43
1:A:78:ILE:HD12	1:A:78:ILE:CA	2.49	0.43
1:A:128:ARG:N	1:A:128:ARG:C	2.71	0.43
1:A:14:ARG:HH11	1:A:14:ARG:CD	2.13	0.42
1:A:1:LYS:NZ	3:A:333:HOH:O	2.49	0.42
1:B:88:ILE:HG12	2:B:138:IOD:I	2.90	0.41
1:B:124:ILE:CD1	1:B:124:ILE:HB	2.42	0.41
1:B:121:GLN:NE2	1:B:121:GLN:HG3	2.34	0.41
1:A:61:ARG:HH11	1:A:61:ARG:HD2	1.14	0.41
1:B:46:ASN:HB3	3:B:356:HOH:O	2.20	0.41
1:A:47:THR:N	1:A:48:ASP:H	2.19	0.41
1:A:1:LYS:HB2	1:A:86:SER:OG	2.21	0.41
1:B:52:ASP:OD1	1:B:59:ASN:HB2	2.21	0.40
1:B:73:ARG:NH1	1:B:73:ARG:NH2	2.54	0.40
1:B:111:TRP:CD1	1:B:115:CYS:HB2	2.56	0.40
1:A:8:LEU:HD12	1:A:8:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	B	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
All	All	254/258 (98%)	250 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	105/105 (100%)	102 (97%)	3 (3%)	50	21
1	B	105/105 (100%)	100 (95%)	5 (5%)	31	8
All	All	210/210 (100%)	202 (96%)	8 (4%)	40	13

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	55	ILE
1	A	86	SER
1	B	61	ARG
1	B	68	ARG
1	B	86	SER
1	B	112	ARG
1	B	129	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	57	GLN
1	A	77	ASN
1	A	93	ASN
1	B	44	ASN

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Mol	Chain	Res	Type
1	B	77	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 17 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	129/129 (100%)	6.84	129 (100%) <b>0</b> <b>0</b>	1, 5, 7, 8	21 (16%)
1	B	129/129 (100%)	6.80	129 (100%) <b>0</b> <b>0</b>	1, 5, 8, 9	17 (13%)
All	All	258/258 (100%)	6.82	258 (100%) <b>0</b> <b>0</b>	1, 5, 8, 9	38 (14%)

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	LEU	38.4
1	B	112	ARG	20.6
1	B	71	GLY	17.1
1	A	62	TRP	15.3
1	A	129	LEU	15.3
1	A	111	TRP	15.1
1	A	23	TYR	14.6
1	B	126	GLY	14.1
1	A	108	TRP	13.8
1	A	83	LEU	13.2
1	B	45	ARG	13.2
1	A	128	ARG	13.1
1	A	112	ARG	13.0
1	B	99	VAL	12.8
1	B	83	LEU	11.8
1	B	25	LEU	11.7
1	B	62	TRP	11.5
1	A	22	GLY	11.4
1	A	107	ALA	11.4
1	B	78	ILE	11.2
1	A	48	ASP	11.1
1	B	76	CYS	11.1
1	A	119	ASP	11.0
1	B	72	SER	11.0

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Mol	Chain	Res	Type	RSRZ
1	B	23	TYR	11.0
1	A	30	CYS	10.9
1	B	10	ALA	10.9
1	A	47	THR	10.9
1	B	80	CYS	10.7
1	B	92	VAL	10.6
1	A	84	LEU	10.6
1	A	123	TRP	10.5
1	A	120	VAL	10.5
1	A	126	GLY	10.5
1	A	78	ILE	10.4
1	A	28	TRP	10.4
1	B	88	ILE	10.4
1	B	128	ARG	10.2
1	B	3	PHE	10.0
1	A	114	ARG	9.8
1	A	34	PHE	9.7
1	B	44	ASN	9.7
1	B	85	SER	9.7
1	B	70	PRO	9.6
1	B	14	ARG	9.6
1	B	21	ARG	9.6
1	B	20	TYR	9.4
1	B	2	VAL	9.3
1	A	53	TYR	8.9
1	A	40	THR	8.9
1	A	57	GLN	8.9
1	B	58	ILE	8.9
1	A	49	GLY	8.9
1	A	92	VAL	8.8
1	B	104	GLY	8.7
1	A	75	LEU	8.7
1	A	115	CYS	8.7
1	B	34	PHE	8.7
1	A	58	ILE	8.6
1	B	28	TRP	8.6
1	A	109	VAL	8.6
1	A	3	PHE	8.6
1	A	29	VAL	8.5
1	B	11	ALA	8.5
1	B	124	ILE	8.5
1	B	36	SER	8.4

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Mol	Chain	Res	Type	RSRZ
1	A	11	ALA	8.4
1	A	90	ALA	8.4
1	A	89	THR	8.3
1	B	111	TRP	8.3
1	A	32	ALA	8.2
1	A	21	ARG	8.1
1	A	39	ASN	8.1
1	B	113	ASN	8.0
1	A	44	ASN	8.0
1	A	113	ASN	7.9
1	A	43	THR	7.9
1	B	108	TRP	7.9
1	B	75	LEU	7.7
1	B	114	ARG	7.6
1	A	8	LEU	7.5
1	A	25	LEU	7.5
1	A	4	GLY	7.5
1	A	1	LYS	7.4
1	A	100	SER	7.4
1	B	59	ASN	7.4
1	A	127	CYS	7.3
1	A	56	LEU	7.3
1	A	6	CYS	7.3
1	A	122	ALA	7.3
1	A	45	ARG	7.3
1	A	15	HIS	7.3
1	A	94	CYS	7.2
1	B	98	ILE	7.2
1	B	90	ALA	7.1
1	B	53	TYR	7.1
1	B	48	ASP	7.1
1	B	120	VAL	7.0
1	B	109	VAL	7.0
1	A	54	GLY	7.0
1	B	68	ARG	6.9
1	B	93	ASN	6.9
1	B	30	CYS	6.8
1	B	38	PHE	6.8
1	A	118	THR	6.8
1	A	87	ASP	6.8
1	B	22	GLY	6.7
1	A	98	ILE	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	43	THR	6.7
1	A	55	ILE	6.7
1	B	121	GLN	6.7
1	B	94	CYS	6.6
1	B	29	VAL	6.6
1	A	85	SER	6.6
1	A	99	VAL	6.6
1	A	61	ARG	6.6
1	B	6	CYS	6.6
1	A	2	VAL	6.5
1	A	46	ASN	6.5
1	B	39	ASN	6.5
1	A	9	ALA	6.5
1	A	88	ILE	6.4
1	B	123	TRP	6.4
1	B	31	ALA	6.4
1	B	17	LEU	6.3
1	A	77	ASN	6.3
1	A	64	CYS	6.3
1	B	8	LEU	6.3
1	B	81	SER	6.2
1	A	80	CYS	6.2
1	A	38	PHE	6.2
1	B	55	ILE	6.2
1	A	91	SER	6.2
1	B	118	THR	6.2
1	B	54	GLY	6.2
1	A	66	ASP	6.2
1	B	122	ALA	6.1
1	A	103	ASN	6.1
1	B	5	ARG	6.1
1	A	116	LYS	6.1
1	B	47	THR	6.0
1	A	20	TYR	6.0
1	B	115	CYS	6.0
1	B	37	ASN	5.9
1	A	125	ARG	5.9
1	A	63	TRP	5.9
1	B	15	HIS	5.9
1	B	127	CYS	5.9
1	A	67	GLY	5.8
1	B	16	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	9	ALA	5.7
1	B	89	THR	5.7
1	A	76	CYS	5.7
1	A	17	LEU	5.7
1	B	32	ALA	5.7
1	B	91	SER	5.6
1	B	77	ASN	5.6
1	B	66	ASP	5.4
1	B	125	ARG	5.4
1	A	93	ASN	5.4
1	A	60	SER	5.4
1	B	82	ALA	5.3
1	B	57	GLN	5.3
1	A	95	ALA	5.3
1	B	56	LEU	5.2
1	B	95	ALA	5.2
1	B	35	GLU	5.1
1	B	41	GLN	5.0
1	B	51	THR	5.0
1	A	19	ASN	5.0
1	B	84	LEU	5.0
1	A	24	SER	5.0
1	A	41	GLN	5.0
1	B	19	ASN	4.9
1	B	1	LYS	4.9
1	A	51	THR	4.9
1	A	117	GLY	4.9
1	B	119	ASP	4.8
1	A	72	SER	4.8
1	A	79	PRO	4.8
1	B	63	TRP	4.8
1	A	31	ALA	4.8
1	A	124	ILE	4.8
1	A	73	ARG	4.7
1	B	96	LYS	4.7
1	A	104	GLY	4.7
1	A	14	ARG	4.6
1	A	110	ALA	4.6
1	A	96	LYS	4.6
1	A	36	SER	4.5
1	A	102	GLY	4.5
1	B	100	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	16	GLY	4.5
1	A	74	ASN	4.5
1	B	103	ASN	4.4
1	B	46	ASN	4.4
1	B	69	THR	4.4
1	A	27	ASN	4.4
1	A	86	SER	4.3
1	A	82	ALA	4.3
1	A	10	ALA	4.3
1	A	68	ARG	4.2
1	A	42	ALA	4.1
1	A	37	ASN	4.1
1	B	67	GLY	4.1
1	B	42	ALA	4.1
1	B	87	ASP	4.1
1	A	71	GLY	4.0
1	B	12	MET	4.0
1	B	97	LYS	3.9
1	A	106	ASN	3.9
1	B	27	ASN	3.9
1	A	50	SER	3.9
1	B	49	GLY	3.8
1	B	64	CYS	3.8
1	B	65	ASN	3.8
1	B	60	SER	3.8
1	A	33	LYS	3.7
1	B	33	LYS	3.7
1	A	52	ASP	3.7
1	B	61	ARG	3.7
1	B	110	ALA	3.7
1	B	105	MET	3.6
1	A	97	LYS	3.6
1	B	117	GLY	3.6
1	A	59	ASN	3.5
1	A	81	SER	3.4
1	B	40	THR	3.4
1	A	69	THR	3.4
1	B	18	ASP	3.3
1	B	102	GLY	3.3
1	B	79	PRO	3.3
1	A	12	MET	3.3
1	B	116	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	101	ASP	3.2
1	A	18	ASP	3.2
1	A	5	ARG	3.1
1	B	24	SER	3.0
1	B	50	SER	3.0
1	A	121	GLN	3.0
1	B	26	GLY	2.9
1	B	52	ASP	2.9
1	A	65	ASN	2.9
1	B	106	ASN	2.8
1	A	26	GLY	2.8
1	B	13	LYS	2.7
1	B	74	ASN	2.7
1	A	35	GLU	2.7
1	A	13	LYS	2.6
1	B	107	ALA	2.6
1	A	105	MET	2.6
1	A	70	PRO	2.5
1	B	73	ARG	2.5
1	B	7	GLU	2.4
1	B	101	ASP	2.4
1	A	7	GLU	2.3
1	B	86	SER	2.2
1	B	4	GLY	2.2

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IOD	A	142	1/1	0.62	0.48	1.53	4,4,4,4	1
2	IOD	B	131	1/1	0.85	0.49	0.92	0,0,0,0	1
2	IOD	A	133	1/1	0.67	0.36	-0.73	1,1,1,1	1
2	IOD	A	144	1/1	0.93	0.07	-1.25	5,5,5,5	1
2	IOD	A	145	1/1	0.97	0.12	-1.58	5,5,5,5	0
2	IOD	A	134	1/1	0.82	0.21	-1.61	6,6,6,6	1
2	IOD	A	135	1/1	0.86	0.14	-2.08	0,0,0,0	1
2	IOD	B	138	1/1	0.90	0.19	-2.17	5,5,5,5	1
2	IOD	A	130	1/1	0.97	0.13	-2.18	3,3,3,3	1
2	IOD	B	137	1/1	0.96	0.12	-2.20	8,8,8,8	1
2	IOD	A	140	1/1	0.95	0.14	-2.26	9,9,9,9	1
2	IOD	B	139	1/1	0.94	0.07	-2.84	8,8,8,8	1
2	IOD	A	132	1/1	0.94	0.16	-3.66	6,6,6,6	1
2	IOD	A	143	1/1	0.82	0.32	-	6,6,6,6	1
2	IOD	B	136	1/1	0.73	0.09	-	5,5,5,5	1
2	IOD	B	146	1/1	0.89	0.12	-	3,3,3,3	1
2	IOD	A	141	1/1	0.76	0.18	-	9,9,9,9	1

## 6.5 Other polymers

There are no such residues in this entry.