



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:35 AM UTC

PDB ID : 3NXA / pdb_00003nxa
Title : X-ray structure of the apo form of human S100A16
Authors : Calderone, V.
Deposited on : 2010-07-13
Resolution : 2.10 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

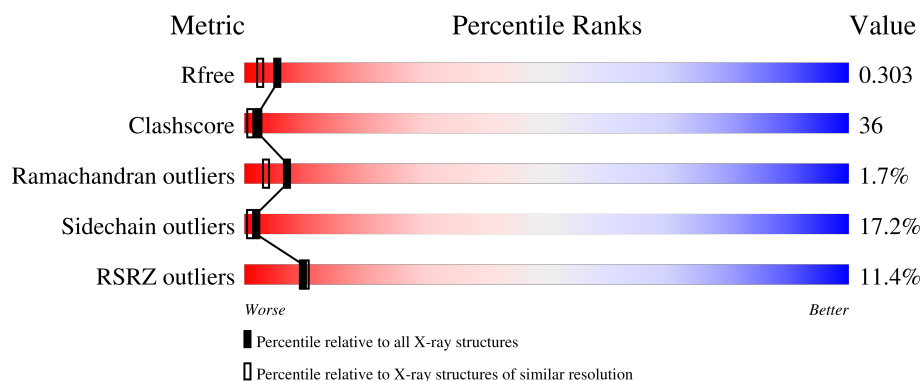
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	100	12% 8% 42% 36% 14%
1	B	100	7% 6% 46% 36% 9%
1	C	100	13% • 49% 35% 9%
1	D	100	10% • 37% 29% • 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3074 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 Protein S100-A16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	0	0
			808	511	137	157	3			
1	B	97	Total	C	N	O	S	0	0	0
			788	501	134	150	3			
1	C	97	Total	C	N	O	S	0	0	0
			788	501	134	151	2			
1	D	74	Total	C	N	O	S	0	0	0
			610	398	98	111	3			

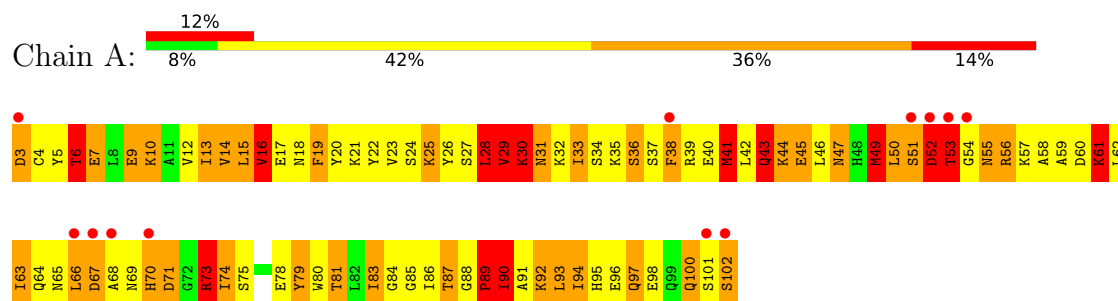
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	25	Total	O	0	0
			25	25		
2	C	22	Total	O	0	0
			22	22		
2	D	18	Total	O	0	0
			18	18		

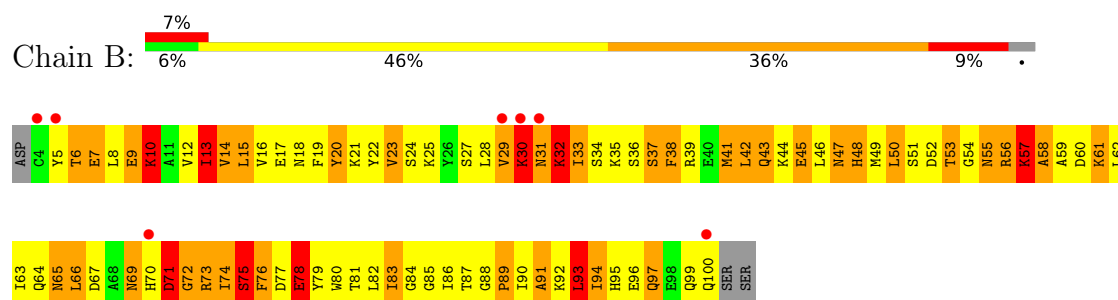
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 ($RSRZ > 2$). 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.

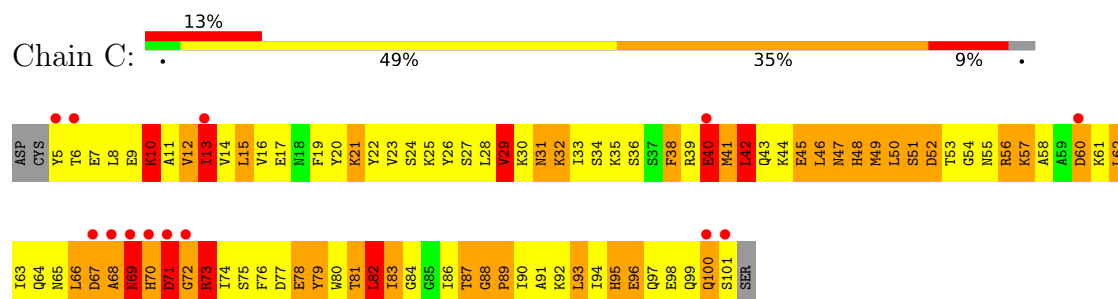
• Molecule 1: Protein S100-A16



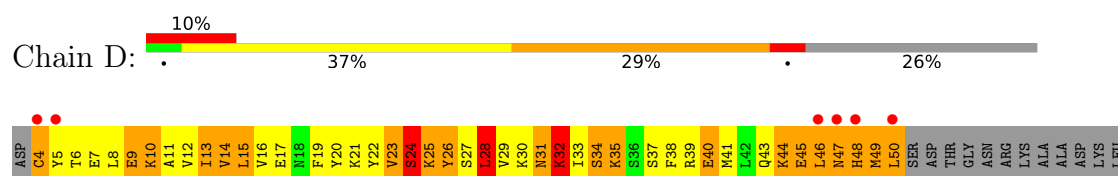
• Molecule 1: Protein S100-A16



• Molecule 1: Protein S100-A16



• Molecule 1: Protein S100-A16



ILE	GLN	ASN	LEU	ASP	ALA	ASN	HIS	ASP	G72	R73	I74	S75	F76	D77	E78	Y79	W80	T81	L82	I83	G84	G85	I86	T87	G88	P89	I90	A91	K92	L93	I94	H95	E96	Q97	E98	GLN	GLN	SER	SER		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	156.57Å 156.57Å 38.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.15 – 2.10 39.15 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.8 (39.15-2.10) 91.9 (39.15-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.248 , 0.298 0.260 , 0.303	Depositor DCC
R_{free} test set	2650 reflections (9.07%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	1.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3074	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 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 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	4.00	154/821 (18.8%)	2.77	65/1103 (5.9%)
1	B	4.25	160/801 (20.0%)	2.94	93/1076 (8.6%)
1	C	4.16	170/801 (21.2%)	2.74	68/1076 (6.3%)
1	D	4.06	106/621 (17.1%)	2.74	54/832 (6.5%)
All	All	4.12	590/3044 (19.4%)	2.80	280/4087 (6.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	6
1	C	0	4
1	D	0	4
All	All	0	18

All (590) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	13	ILE	CA-CB	20.66	1.83	1.54
1	D	90	ILE	CA-C	-19.43	1.33	1.52
1	B	13	ILE	CA-CB	19.20	1.77	1.54
1	A	13	ILE	CA-CB	19.20	1.75	1.54
1	B	91	ALA	CA-CB	18.41	1.81	1.53
1	B	29	VAL	C-O	18.26	1.44	1.24
1	B	72	GLY	CA-C	17.70	1.75	1.51
1	A	91	ALA	N-CA	-17.52	1.25	1.46
1	B	97	GLN	N-CA	16.81	1.66	1.46
1	D	29	VAL	N-CA	16.53	1.66	1.46
1	C	87	THR	N-CA	-15.12	1.27	1.46
1	D	10	LYS	C-O	15.00	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	67	ASP	CA-C	14.88	1.72	1.52
1	B	12	VAL	CA-CB	-14.19	1.37	1.54
1	B	29	VAL	C-N	14.04	1.53	1.33
1	C	67	ASP	C-O	14.00	1.40	1.23
1	A	90	ILE	CA-CB	-13.99	1.39	1.54
1	B	14	VAL	N-CA	13.83	1.65	1.46
1	D	17	GLU	CA-C	-13.57	1.35	1.52
1	A	9	GLU	C-O	13.51	1.40	1.24
1	D	16	VAL	CA-C	13.50	1.70	1.52
1	A	94	ILE	CA-C	13.38	1.70	1.52
1	C	87	THR	CA-C	13.34	1.70	1.52
1	C	32	LYS	C-O	13.31	1.39	1.23
1	A	12	VAL	CA-CB	13.28	1.70	1.54
1	D	24	SER	N-CA	13.13	1.62	1.46
1	A	24	SER	N-CA	13.05	1.61	1.46
1	B	75	SER	N-CA	13.03	1.63	1.45
1	B	58	ALA	CA-CB	12.94	1.74	1.53
1	D	16	VAL	CA-CB	-12.88	1.37	1.54
1	A	90	ILE	N-CA	-12.75	1.32	1.46
1	B	64	GLN	C-O	-12.66	1.08	1.24
1	B	51	SER	C-O	-12.31	1.09	1.24
1	C	40	GLU	CG-CD	12.01	1.82	1.52
1	D	16	VAL	C-O	-11.99	1.09	1.24
1	D	35	LYS	N-CA	11.99	1.60	1.46
1	C	60	ASP	CB-CG	11.94	1.81	1.52
1	B	97	GLN	C-O	-11.89	1.10	1.24
1	D	15	LEU	C-O	-11.89	1.09	1.24
1	B	78	GLU	C-O	-11.65	1.10	1.24
1	B	81	THR	N-CA	11.54	1.61	1.46
1	C	99	GLN	CA-C	11.51	1.68	1.52
1	D	86	ILE	CA-CB	11.46	1.68	1.54
1	A	15	LEU	CG-CD2	-11.45	1.14	1.52
1	A	19	PHE	CB-CG	11.44	1.76	1.50
1	B	87	THR	CA-CB	11.40	1.71	1.53
1	D	83	ILE	CA-CB	-11.34	1.40	1.54
1	B	33	ILE	C-O	11.30	1.35	1.24
1	C	49	MET	C-O	-11.30	1.10	1.24
1	C	60	ASP	CA-C	11.27	1.67	1.52
1	D	73	ARG	N-CA	11.24	1.60	1.45
1	D	91	ALA	CA-CB	-11.16	1.34	1.53
1	D	15	LEU	CA-CB	11.02	1.71	1.53
1	B	30	LYS	C-N	10.86	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	81	THR	C-O	-10.83	1.11	1.24
1	A	58	ALA	CA-CB	10.76	1.70	1.53
1	A	40	GLU	C-O	10.70	1.36	1.24
1	B	41	MET	C-O	10.69	1.36	1.24
1	C	83	ILE	CA-C	10.68	1.66	1.52
1	B	91	ALA	C-O	10.67	1.36	1.24
1	B	58	ALA	N-CA	10.66	1.60	1.46
1	A	86	ILE	CA-C	-10.65	1.39	1.52
1	A	29	VAL	N-CA	10.62	1.60	1.46
1	C	53	THR	C-O	10.61	1.36	1.24
1	C	76	PHE	CA-C	10.59	1.66	1.52
1	B	19	PHE	C-O	10.58	1.36	1.24
1	C	86	ILE	C-O	10.56	1.35	1.24
1	C	71	ASP	CB-CG	10.48	1.78	1.52
1	D	28	LEU	CG-CD2	10.47	1.87	1.52
1	D	26	TYR	CA-CB	10.45	1.67	1.54
1	A	33	ILE	CA-CB	-10.44	1.39	1.55
1	A	93	LEU	CG-CD1	10.39	1.86	1.52
1	D	26	TYR	N-CA	10.37	1.64	1.46
1	A	28	LEU	N-CA	10.28	1.59	1.46
1	A	70	HIS	N-CA	10.27	1.59	1.46
1	A	89	PRO	CA-C	10.26	1.68	1.52
1	C	79	TYR	N-CA	10.24	1.59	1.46
1	C	93	LEU	N-CA	-10.24	1.32	1.46
1	A	31	ASN	CB-CG	10.16	1.77	1.52
1	B	34	SER	C-O	10.15	1.37	1.23
1	C	32	LYS	CG-CD	-10.14	1.22	1.52
1	C	71	ASP	CA-CB	10.04	1.68	1.54
1	D	33	ILE	C-O	9.99	1.36	1.23
1	A	10	LYS	N-CA	9.94	1.58	1.46
1	C	79	TYR	C-O	-9.93	1.11	1.24
1	A	95	HIS	ND1-CE1	9.92	1.42	1.32
1	A	36	SER	C-O	9.89	1.36	1.24
1	D	4	CYS	C-O	9.89	1.43	1.23
1	C	87	THR	CA-CB	9.84	1.69	1.53
1	D	80	TRP	C-O	9.82	1.35	1.24
1	B	95	HIS	CA-C	9.75	1.65	1.52
1	A	5	TYR	CA-C	-9.71	1.40	1.52
1	D	13	ILE	N-CA	-9.68	1.33	1.46
1	B	59	ALA	CA-C	9.66	1.65	1.52
1	B	17	GLU	C-O	9.65	1.35	1.24
1	C	97	GLN	CA-C	-9.61	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	ALA	C-O	9.59	1.35	1.24
1	B	34	SER	CA-C	-9.55	1.40	1.53
1	B	74	ILE	CA-CB	9.51	1.65	1.54
1	D	50	LEU	CA-C	9.51	1.73	1.52
1	B	61	LYS	CG-CD	9.47	1.80	1.52
1	B	74	ILE	CA-C	-9.47	1.40	1.52
1	C	86	ILE	CA-CB	9.45	1.66	1.54
1	C	63	ILE	CA-C	-9.45	1.39	1.52
1	C	24	SER	C-O	-9.43	1.10	1.23
1	A	19	PHE	N-CA	-9.42	1.35	1.46
1	D	26	TYR	CA-C	-9.40	1.38	1.52
1	A	23	VAL	C-O	9.38	1.35	1.24
1	D	21	LYS	CA-C	-9.30	1.39	1.52
1	C	88	GLY	N-CA	-9.26	1.36	1.44
1	D	79	TYR	C-O	9.24	1.34	1.24
1	D	40	GLU	C-O	9.20	1.34	1.24
1	B	56	ARG	N-CA	-9.17	1.35	1.46
1	A	70	HIS	CA-CB	9.16	1.69	1.53
1	C	82	LEU	N-CA	-9.07	1.35	1.46
1	C	27	SER	CA-C	-9.03	1.41	1.52
1	D	28	LEU	N-CA	9.02	1.58	1.46
1	C	86	ILE	N-CA	-8.98	1.35	1.46
1	C	35	LYS	N-CA	8.95	1.57	1.46
1	B	45	GLU	CG-CD	8.92	1.74	1.52
1	B	41	MET	CA-CB	8.90	1.67	1.53
1	B	22	TYR	C-O	8.87	1.35	1.24
1	B	14	VAL	CA-CB	-8.84	1.41	1.54
1	C	96	GLU	CB-CG	8.82	1.78	1.52
1	C	29	VAL	CA-CB	-8.82	1.42	1.54
1	B	64	GLN	N-CA	8.81	1.57	1.46
1	C	30	LYS	CA-C	8.78	1.67	1.52
1	B	6	THR	CA-C	-8.78	1.41	1.53
1	B	53	THR	CA-C	8.77	1.64	1.52
1	C	77	ASP	C-O	-8.77	1.13	1.24
1	A	67	ASP	N-CA	8.72	1.56	1.46
1	C	91	ALA	C-O	8.72	1.34	1.24
1	A	101	SER	CA-C	8.72	1.64	1.52
1	B	99	GLN	CA-C	8.65	1.64	1.52
1	B	90	ILE	CB-CG1	-8.64	1.36	1.53
1	B	17	GLU	CA-C	-8.64	1.41	1.52
1	B	47	ASN	C-O	8.63	1.35	1.24
1	C	38	PHE	C-O	8.63	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	45	GLU	N-CA	-8.63	1.34	1.45
1	B	84	GLY	CA-C	-8.62	1.41	1.51
1	D	86	ILE	CG1-CD1	-8.59	1.18	1.51
1	B	83	ILE	CB-CG1	8.53	1.70	1.53
1	A	73	ARG	C-O	8.52	1.34	1.23
1	C	68	ALA	C-O	8.47	1.33	1.24
1	A	50	LEU	CA-C	8.46	1.63	1.53
1	D	90	ILE	CA-CB	8.43	1.65	1.54
1	C	62	LEU	CG-CD2	8.43	1.80	1.52
1	D	92	LYS	N-CA	8.36	1.56	1.46
1	B	47	ASN	N-CA	-8.33	1.35	1.46
1	C	36	SER	CA-CB	8.32	1.67	1.53
1	B	44	LYS	C-O	-8.31	1.13	1.24
1	C	12	VAL	CA-CB	-8.31	1.44	1.54
1	A	79	TYR	CA-C	8.29	1.63	1.52
1	D	29	VAL	CA-CB	8.29	1.63	1.53
1	B	15	LEU	N-CA	8.28	1.57	1.46
1	A	86	ILE	C-O	-8.25	1.14	1.24
1	D	93	LEU	CA-C	-8.25	1.42	1.52
1	B	25	LYS	CA-C	8.22	1.63	1.52
1	B	77	ASP	C-O	8.21	1.33	1.24
1	B	36	SER	CA-C	8.20	1.63	1.52
1	C	93	LEU	C-O	8.20	1.34	1.24
1	C	9	GLU	CA-C	-8.15	1.42	1.52
1	D	90	ILE	CG1-CD1	8.12	1.83	1.51
1	C	11	ALA	C-O	-8.12	1.14	1.24
1	C	92	LYS	CA-C	8.11	1.63	1.52
1	A	13	ILE	C-O	8.06	1.33	1.24
1	A	95	HIS	CA-CB	-8.04	1.40	1.53
1	B	39	ARG	C-O	-8.04	1.14	1.24
1	D	78	GLU	N-CA	-8.00	1.36	1.46
1	A	12	VAL	CA-C	-7.99	1.43	1.52
1	A	31	ASN	CA-CB	7.98	1.66	1.53
1	A	17	GLU	CA-CB	7.95	1.66	1.53
1	C	24	SER	CA-C	7.93	1.63	1.53
1	C	94	ILE	C-O	7.93	1.34	1.24
1	B	38	PHE	CA-C	7.92	1.63	1.52
1	A	93	LEU	C-N	7.92	1.43	1.33
1	A	26	TYR	CA-CB	7.91	1.64	1.53
1	B	65	ASN	CA-CB	-7.90	1.40	1.53
1	B	52	ASP	N-CA	-7.90	1.36	1.46
1	A	17	GLU	N-CA	7.89	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	56	ARG	C-O	-7.86	1.14	1.24
1	C	39	ARG	CZ-NH1	7.86	1.43	1.32
1	C	70	HIS	C-O	7.85	1.34	1.24
1	C	15	LEU	CA-C	7.85	1.63	1.52
1	C	97	GLN	CA-CB	-7.84	1.40	1.53
1	C	60	ASP	CG-OD2	7.82	1.40	1.25
1	A	100	GLN	N-CA	7.81	1.56	1.46
1	C	80	TRP	C-O	-7.78	1.14	1.24
1	C	68	ALA	CA-CB	7.78	1.64	1.53
1	D	86	ILE	C-O	7.78	1.31	1.23
1	C	10	LYS	C-O	7.77	1.34	1.24
1	D	35	LYS	CB-CG	7.77	1.75	1.52
1	A	70	HIS	CA-C	7.77	1.63	1.52
1	B	15	LEU	C-O	7.76	1.34	1.24
1	B	76	PHE	C-N	7.76	1.43	1.33
1	B	57	LYS	CD-CE	7.75	1.75	1.52
1	B	75	SER	CA-CB	7.73	1.65	1.53
1	C	26	TYR	CG-CD1	7.72	1.55	1.39
1	A	6	THR	CB-CG2	-7.72	1.27	1.52
1	B	76	PHE	N-CA	-7.72	1.37	1.46
1	C	23	VAL	CA-CB	-7.72	1.42	1.53
1	C	24	SER	N-CA	7.68	1.55	1.45
1	A	36	SER	CA-C	7.67	1.63	1.52
1	C	71	ASP	CA-C	7.66	1.63	1.52
1	D	6	THR	CA-C	-7.65	1.42	1.53
1	C	70	HIS	CA-C	7.65	1.63	1.52
1	B	83	ILE	CA-C	7.65	1.62	1.52
1	B	55	ASN	N-CA	7.62	1.55	1.46
1	C	98	GLU	CA-C	7.62	1.63	1.52
1	C	92	LYS	C-O	7.60	1.32	1.24
1	B	94	ILE	CG1-CD1	7.56	1.81	1.51
1	A	71	ASP	C-O	7.51	1.33	1.24
1	D	80	TRP	CD1-NE1	-7.50	1.22	1.37
1	A	23	VAL	CA-C	7.49	1.61	1.52
1	A	78	GLU	N-CA	-7.48	1.37	1.46
1	B	62	LEU	CA-C	-7.48	1.42	1.52
1	C	65	ASN	CG-ND2	7.48	1.49	1.33
1	A	79	TYR	CD2-CE2	7.47	1.61	1.38
1	C	5	TYR	CG-CD2	7.45	1.54	1.39
1	C	28	LEU	CA-C	-7.45	1.42	1.52
1	B	84	GLY	N-CA	-7.44	1.36	1.45
1	C	54	GLY	CA-C	7.38	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	15	LEU	CA-C	7.35	1.62	1.52
1	D	79	TYR	CE1-CZ	-7.33	1.20	1.38
1	A	74	ILE	CG1-CD1	7.31	1.80	1.51
1	B	13	ILE	C-N	-7.28	1.26	1.34
1	A	102	SER	N-CA	7.26	1.60	1.46
1	B	93	LEU	CG-CD1	7.26	1.76	1.52
1	C	25	LYS	N-CA	7.26	1.54	1.46
1	C	74	ILE	N-CA	7.24	1.54	1.46
1	C	23	VAL	C-O	7.22	1.31	1.24
1	B	90	ILE	CA-C	-7.22	1.43	1.52
1	B	12	VAL	CA-C	-7.19	1.44	1.52
1	C	68	ALA	N-CA	7.18	1.55	1.46
1	B	63	ILE	CA-CB	7.18	1.63	1.54
1	C	83	ILE	C-O	-7.15	1.15	1.24
1	B	39	ARG	NE-CZ	7.14	1.40	1.33
1	B	90	ILE	C-N	7.14	1.43	1.33
1	C	51	SER	CA-C	7.13	1.62	1.52
1	D	78	GLU	CA-CB	-7.13	1.42	1.53
1	C	52	ASP	CA-C	-7.12	1.43	1.52
1	A	87	THR	CB-CG2	-7.10	1.29	1.52
1	A	80	TRP	CE3-CZ3	7.07	1.59	1.38
1	A	35	LYS	CB-CG	7.04	1.73	1.52
1	A	14	VAL	CA-C	7.03	1.61	1.52
1	C	86	ILE	CB-CG1	-7.03	1.39	1.53
1	C	46	LEU	N-CA	6.99	1.54	1.46
1	B	82	LEU	CA-C	6.99	1.61	1.52
1	D	73	ARG	CG-CD	6.99	1.73	1.52
1	D	31	ASN	N-CA	6.98	1.54	1.46
1	B	74	ILE	C-O	6.97	1.31	1.24
1	C	87	THR	CB-OG1	6.95	1.54	1.43
1	B	50	LEU	CA-CB	-6.95	1.43	1.53
1	C	38	PHE	CG-CD1	-6.95	1.24	1.38
1	D	31	ASN	C-O	-6.94	1.14	1.24
1	B	47	ASN	CB-CG	6.93	1.69	1.52
1	B	60	ASP	CG-OD1	6.91	1.38	1.25
1	B	43	GLN	C-O	-6.91	1.15	1.24
1	C	43	GLN	CD-OE1	6.89	1.36	1.23
1	C	72	GLY	CA-C	6.89	1.61	1.51
1	C	40	GLU	C-O	-6.89	1.16	1.24
1	B	82	LEU	C-N	6.89	1.42	1.33
1	A	87	THR	N-CA	-6.88	1.37	1.46
1	A	97	GLN	N-CA	-6.88	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	ARG	CA-C	6.86	1.62	1.53
1	C	10	LYS	CE-NZ	6.86	1.70	1.49
1	C	5	TYR	CA-CB	6.86	1.67	1.53
1	D	82	LEU	C-N	-6.84	1.25	1.34
1	A	63	ILE	CA-C	6.83	1.60	1.52
1	C	11	ALA	CA-C	6.83	1.61	1.52
1	C	45	GLU	CA-CB	-6.83	1.43	1.54
1	D	35	LYS	CA-CB	-6.82	1.42	1.53
1	A	88	GLY	CA-C	6.80	1.61	1.51
1	A	95	HIS	CA-C	6.79	1.61	1.52
1	C	88	GLY	C-O	-6.76	1.17	1.24
1	B	27	SER	CA-C	-6.76	1.44	1.52
1	C	53	THR	N-CA	-6.75	1.38	1.46
1	A	12	VAL	N-CA	6.74	1.54	1.46
1	D	46	LEU	C-O	6.73	1.31	1.24
1	A	39	ARG	CZ-NH1	6.73	1.42	1.32
1	A	30	LYS	CG-CD	6.71	1.72	1.52
1	D	48	HIS	C-O	6.70	1.31	1.24
1	A	58	ALA	CA-C	6.69	1.61	1.52
1	C	44	LYS	C-N	6.68	1.43	1.33
1	B	74	ILE	C-N	6.68	1.42	1.33
1	B	63	ILE	CA-C	6.66	1.61	1.52
1	B	52	ASP	CG-OD1	6.66	1.38	1.25
1	A	81	THR	CB-CG2	6.65	1.74	1.52
1	A	18	ASN	N-CA	-6.64	1.37	1.46
1	B	76	PHE	CE2-CZ	6.63	1.58	1.38
1	C	68	ALA	CA-C	6.63	1.61	1.52
1	B	5	TYR	N-CA	6.63	1.54	1.45
1	C	50	LEU	CA-C	6.61	1.61	1.53
1	D	37	SER	N-CA	6.60	1.54	1.46
1	B	13	ILE	CA-C	-6.60	1.44	1.52
1	B	51	SER	C-N	-6.60	1.24	1.33
1	D	20	TYR	C-O	6.59	1.32	1.24
1	B	54	GLY	CA-C	6.58	1.61	1.51
1	A	27	SER	CA-CB	6.57	1.63	1.53
1	B	33	ILE	CB-CG1	6.57	1.66	1.53
1	B	20	TYR	N-CA	6.56	1.54	1.46
1	B	83	ILE	C-O	-6.55	1.16	1.24
1	A	59	ALA	CA-C	6.54	1.61	1.52
1	A	16	VAL	C-O	6.53	1.30	1.23
1	C	64	GLN	N-CA	6.53	1.54	1.46
1	A	80	TRP	CA-C	6.51	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	86	ILE	CA-CB	-6.50	1.45	1.54
1	D	25	LYS	CA-C	6.50	1.61	1.52
1	B	67	ASP	N-CA	6.49	1.54	1.46
1	D	32	LYS	C-O	6.49	1.31	1.23
1	C	73	ARG	C-O	6.47	1.31	1.23
1	B	77	ASP	CA-CB	-6.46	1.43	1.53
1	D	41	MET	C-O	6.45	1.31	1.24
1	C	80	TRP	CZ3-CH2	6.44	1.56	1.40
1	B	52	ASP	C-O	6.42	1.31	1.24
1	A	78	GLU	CA-C	6.41	1.61	1.52
1	B	49	MET	CA-C	6.41	1.61	1.52
1	C	12	VAL	CA-C	6.38	1.60	1.52
1	D	11	ALA	C-O	-6.37	1.16	1.24
1	A	20	TYR	N-CA	6.37	1.54	1.46
1	B	91	ALA	CA-C	6.36	1.60	1.52
1	C	64	GLN	C-N	-6.36	1.24	1.33
1	B	9	GLU	CA-CB	6.34	1.63	1.53
1	B	78	GLU	CA-CB	6.33	1.63	1.53
1	A	79	TYR	CB-CG	6.31	1.65	1.51
1	A	44	LYS	CD-CE	6.30	1.71	1.52
1	B	38	PHE	CD1-CE1	6.30	1.57	1.38
1	A	75	SER	C-N	-6.29	1.25	1.34
1	A	34	SER	C-O	6.29	1.32	1.23
1	B	76	PHE	C-O	-6.28	1.16	1.24
1	C	84	GLY	N-CA	6.28	1.53	1.45
1	B	51	SER	CB-OG	6.27	1.54	1.42
1	C	34	SER	CB-OG	6.27	1.54	1.42
1	B	71	ASP	CA-C	6.27	1.61	1.52
1	A	7	GLU	CA-CB	6.27	1.63	1.53
1	B	85	GLY	N-CA	6.26	1.54	1.45
1	D	31	ASN	CG-ND2	6.26	1.46	1.33
1	C	95	HIS	CA-CB	-6.24	1.43	1.53
1	C	70	HIS	N-CA	6.24	1.54	1.46
1	C	26	TYR	CD2-CE2	6.23	1.57	1.38
1	B	37	SER	N-CA	6.23	1.54	1.46
1	B	62	LEU	CG-CD1	6.22	1.73	1.52
1	C	100	GLN	CG-CD	6.22	1.67	1.52
1	D	28	LEU	CA-CB	-6.22	1.42	1.53
1	D	87	THR	N-CA	-6.22	1.37	1.46
1	C	67	ASP	N-CA	6.21	1.54	1.46
1	D	76	PHE	CG-CD1	6.21	1.51	1.38
1	C	87	THR	C-N	-6.20	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	ALA	N-CA	6.20	1.54	1.46
1	A	39	ARG	C-O	-6.19	1.16	1.24
1	B	70	HIS	CB-CG	6.19	1.58	1.50
1	A	68	ALA	CA-CB	6.19	1.63	1.53
1	B	10	LYS	CA-C	6.19	1.61	1.52
1	C	74	ILE	CA-CB	-6.18	1.46	1.54
1	A	18	ASN	CG-OD1	6.17	1.35	1.23
1	D	27	SER	C-O	-6.17	1.16	1.23
1	C	61	LYS	CA-C	6.16	1.61	1.52
1	B	53	THR	CA-CB	6.15	1.63	1.53
1	C	33	ILE	CA-C	6.14	1.60	1.52
1	C	29	VAL	N-CA	6.14	1.54	1.46
1	A	18	ASN	CA-CB	-6.13	1.43	1.53
1	D	74	ILE	CA-CB	6.13	1.61	1.54
1	B	35	LYS	CA-CB	6.13	1.63	1.53
1	C	89	PRO	C-O	-6.12	1.16	1.24
1	C	95	HIS	CA-C	6.12	1.60	1.52
1	A	62	LEU	CA-C	6.11	1.60	1.52
1	A	84	GLY	CA-C	6.11	1.59	1.51
1	D	13	ILE	CG1-CD1	-6.11	1.27	1.51
1	C	75	SER	CB-OG	6.10	1.54	1.42
1	A	23	VAL	CA-CB	6.10	1.61	1.54
1	A	41	MET	N-CA	6.10	1.53	1.46
1	D	72	GLY	C-N	6.08	1.41	1.33
1	B	56	ARG	CD-NE	-6.07	1.37	1.46
1	C	82	LEU	C-O	-6.07	1.16	1.24
1	B	9	GLU	CA-C	-6.06	1.44	1.52
1	D	79	TYR	CG-CD2	-6.06	1.26	1.39
1	A	16	VAL	CA-CB	6.05	1.63	1.54
1	D	39	ARG	NE-CZ	6.05	1.39	1.33
1	B	7	GLU	C-O	-6.05	1.16	1.24
1	D	78	GLU	C-N	-6.05	1.26	1.33
1	C	90	ILE	N-CA	6.04	1.52	1.46
1	A	45	GLU	CA-CB	6.03	1.63	1.53
1	A	83	ILE	CB-CG1	6.03	1.65	1.53
1	B	82	LEU	CG-CD2	-6.03	1.32	1.52
1	B	92	LYS	CE-NZ	6.03	1.67	1.49
1	C	10	LYS	CG-CD	6.02	1.70	1.52
1	C	23	VAL	CA-C	6.01	1.59	1.52
1	A	70	HIS	CB-CG	6.00	1.58	1.50
1	B	5	TYR	CE1-CZ	5.99	1.52	1.38
1	A	89	PRO	N-CA	5.98	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	76	PHE	CA-C	5.98	1.60	1.52
1	D	76	PHE	CG-CD2	-5.98	1.26	1.38
1	C	26	TYR	CE2-CZ	5.97	1.52	1.38
1	D	23	VAL	CA-CB	-5.94	1.46	1.54
1	C	64	GLN	CA-C	-5.92	1.45	1.52
1	B	80	TRP	CG-CD1	5.92	1.51	1.36
1	B	42	LEU	CA-CB	5.92	1.62	1.53
1	A	29	VAL	CB-CG2	-5.91	1.33	1.52
1	B	18	ASN	CA-C	5.89	1.60	1.52
1	A	30	LYS	CD-CE	-5.88	1.34	1.52
1	A	98	GLU	CD-OE1	5.88	1.36	1.25
1	C	45	GLU	CA-C	5.86	1.60	1.52
1	C	74	ILE	C-O	5.86	1.30	1.24
1	C	9	GLU	CG-CD	5.85	1.66	1.52
1	A	17	GLU	CA-C	5.85	1.60	1.52
1	C	91	ALA	CA-C	5.84	1.60	1.52
1	D	39	ARG	N-CA	5.82	1.53	1.46
1	C	29	VAL	C-O	5.81	1.30	1.24
1	B	69	ASN	N-CA	-5.81	1.39	1.46
1	B	65	ASN	CG-ND2	5.79	1.45	1.33
1	D	78	GLU	CG-CD	5.79	1.66	1.52
1	C	15	LEU	C-O	5.79	1.30	1.24
1	A	38	PHE	N-CA	5.78	1.53	1.46
1	D	82	LEU	CG-CD1	5.76	1.71	1.52
1	A	45	GLU	N-CA	5.76	1.53	1.46
1	A	29	VAL	C-O	5.76	1.30	1.24
1	C	39	ARG	N-CA	5.76	1.53	1.46
1	C	43	GLN	CD-NE2	5.75	1.45	1.33
1	B	93	LEU	CB-CG	5.74	1.65	1.53
1	B	42	LEU	CB-CG	5.74	1.65	1.53
1	B	70	HIS	CA-C	5.74	1.60	1.52
1	C	67	ASP	C-N	5.73	1.41	1.33
1	D	88	GLY	CA-C	5.72	1.60	1.51
1	B	41	MET	CA-C	-5.71	1.45	1.52
1	D	75	SER	CA-C	5.70	1.61	1.53
1	A	21	LYS	N-CA	5.69	1.53	1.46
1	C	35	LYS	CG-CD	5.69	1.69	1.52
1	A	50	LEU	CG-CD2	-5.69	1.33	1.52
1	A	87	THR	C-O	-5.68	1.16	1.24
1	C	13	ILE	CA-C	-5.68	1.46	1.52
1	D	39	ARG	C-O	5.67	1.30	1.24
1	B	88	GLY	N-CA	5.67	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	GLN	CA-C	-5.67	1.45	1.52
1	C	89	PRO	N-CA	-5.66	1.40	1.47
1	C	14	VAL	CA-C	5.65	1.59	1.52
1	C	52	ASP	CA-CB	-5.65	1.44	1.53
1	A	69	ASN	N-CA	5.64	1.53	1.45
1	A	32	LYS	N-CA	-5.64	1.38	1.45
1	C	38	PHE	N-CA	5.64	1.53	1.46
1	D	73	ARG	C-O	5.64	1.31	1.23
1	A	73	ARG	NE-CZ	5.64	1.39	1.33
1	C	46	LEU	C-O	5.64	1.32	1.23
1	A	14	VAL	CA-CB	5.63	1.60	1.54
1	C	26	TYR	CG-CD2	-5.63	1.27	1.39
1	D	82	LEU	C-O	5.63	1.30	1.24
1	C	55	ASN	CB-CG	5.62	1.66	1.52
1	D	12	VAL	CA-CB	5.61	1.62	1.54
1	B	23	VAL	CB-CG2	5.60	1.71	1.52
1	B	23	VAL	N-CA	5.58	1.53	1.46
1	C	36	SER	C-O	-5.58	1.16	1.24
1	D	93	LEU	C-O	-5.58	1.17	1.24
1	A	22	TYR	N-CA	5.57	1.53	1.46
1	A	62	LEU	CG-CD1	5.57	1.71	1.52
1	A	87	THR	CA-CB	5.57	1.62	1.53
1	C	60	ASP	CA-CB	5.56	1.62	1.53
1	A	47	ASN	CB-CG	-5.55	1.38	1.52
1	C	30	LYS	CD-CE	5.54	1.69	1.52
1	A	3	ASP	CB-CG	5.54	1.65	1.52
1	C	65	ASN	CG-OD1	5.54	1.34	1.23
1	C	65	ASN	CB-CG	5.53	1.65	1.52
1	A	80	TRP	CZ2-CH2	5.53	1.47	1.37
1	D	7	GLU	C-O	-5.53	1.17	1.24
1	A	64	GLN	CG-CD	5.53	1.65	1.52
1	C	17	GLU	CB-CG	5.52	1.69	1.52
1	B	65	ASN	C-O	-5.52	1.16	1.24
1	D	10	LYS	CG-CD	5.52	1.69	1.52
1	D	78	GLU	CB-CG	5.52	1.69	1.52
1	A	85	GLY	CA-C	5.52	1.59	1.51
1	C	69	ASN	C-O	5.52	1.30	1.24
1	B	51	SER	CA-CB	5.51	1.61	1.53
1	B	85	GLY	C-O	-5.51	1.16	1.23
1	B	21	LYS	CA-C	5.51	1.60	1.52
1	D	4	CYS	CA-C	5.51	1.64	1.52
1	B	78	GLU	CD-OE1	5.50	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	LYS	C-O	5.49	1.30	1.23
1	A	57	LYS	CB-CG	5.48	1.68	1.52
1	D	13	ILE	C-O	5.48	1.31	1.24
1	A	36	SER	CA-CB	5.47	1.62	1.53
1	C	65	ASN	N-CA	-5.47	1.38	1.46
1	C	31	ASN	C-O	-5.47	1.16	1.23
1	C	5	TYR	N-CA	5.46	1.56	1.46
1	A	56	ARG	CA-C	-5.46	1.45	1.52
1	C	41	MET	CA-C	5.45	1.60	1.52
1	C	42	LEU	CA-CB	5.45	1.61	1.53
1	D	76	PHE	N-CA	-5.44	1.39	1.46
1	B	50	LEU	CB-CG	5.43	1.64	1.53
1	D	31	ASN	CB-CG	5.43	1.65	1.52
1	B	28	LEU	C-N	-5.42	1.26	1.33
1	C	77	ASP	CA-C	-5.40	1.45	1.52
1	B	23	VAL	CA-CB	-5.40	1.47	1.54
1	D	28	LEU	CG-CD1	-5.40	1.34	1.52
1	A	30	LYS	CE-NZ	-5.40	1.33	1.49
1	D	39	ARG	CA-CB	5.40	1.62	1.53
1	A	7	GLU	CD-OE1	5.40	1.35	1.25
1	B	45	GLU	CD-OE1	5.39	1.35	1.25
1	A	86	ILE	N-CA	-5.39	1.40	1.46
1	B	39	ARG	CA-C	5.38	1.59	1.52
1	C	76	PHE	C-O	-5.38	1.17	1.24
1	A	33	ILE	CB-CG2	5.38	1.70	1.52
1	B	69	ASN	CB-CG	-5.38	1.38	1.52
1	B	33	ILE	CA-C	5.38	1.59	1.52
1	C	58	ALA	N-CA	-5.37	1.39	1.46
1	A	17	GLU	C-N	-5.37	1.26	1.33
1	C	16	VAL	C-O	5.37	1.30	1.24
1	A	9	GLU	CA-C	5.37	1.59	1.52
1	A	39	ARG	NE-CZ	5.37	1.39	1.33
1	D	43	GLN	CG-CD	-5.36	1.38	1.52
1	D	40	GLU	CG-CD	5.35	1.65	1.52
1	A	93	LEU	C-O	5.35	1.30	1.24
1	A	15	LEU	CA-CB	-5.34	1.44	1.53
1	A	17	GLU	C-O	-5.33	1.17	1.24
1	D	81	THR	N-CA	5.33	1.52	1.46
1	A	78	GLU	CG-CD	5.33	1.65	1.52
1	A	45	GLU	C-O	5.32	1.31	1.24
1	A	50	LEU	CA-CB	5.31	1.60	1.53
1	A	92	LYS	CA-C	5.30	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	72	GLY	N-CA	5.30	1.54	1.45
1	C	13	ILE	CA-CB	5.30	1.60	1.54
1	C	60	ASP	CG-OD1	5.29	1.35	1.25
1	B	66	LEU	CG-CD1	5.28	1.70	1.52
1	B	75	SER	CA-C	5.28	1.60	1.53
1	C	47	ASN	CB-CG	5.28	1.65	1.52
1	A	29	VAL	CA-CB	5.28	1.60	1.53
1	A	7	GLU	C-O	5.28	1.30	1.24
1	B	7	GLU	CG-CD	5.28	1.65	1.52
1	A	96	GLU	CB-CG	5.27	1.68	1.52
1	A	22	TYR	CD1-CE1	5.26	1.54	1.38
1	D	47	ASN	CB-CG	5.26	1.65	1.52
1	D	17	GLU	N-CA	5.26	1.52	1.46
1	A	21	LYS	CG-CD	5.26	1.68	1.52
1	A	59	ALA	CA-CB	5.25	1.62	1.53
1	A	39	ARG	CA-CB	-5.24	1.45	1.53
1	B	73	ARG	CA-C	5.24	1.60	1.53
1	C	19	PHE	CA-CB	-5.24	1.45	1.53
1	B	72	GLY	C-O	-5.24	1.16	1.24
1	D	35	LYS	CG-CD	5.23	1.68	1.52
1	B	5	TYR	CG-CD2	5.23	1.50	1.39
1	C	57	LYS	CG-CD	5.22	1.68	1.52
1	C	80	TRP	CA-C	5.21	1.59	1.52
1	D	16	VAL	CB-CG1	5.20	1.69	1.52
1	C	21	LYS	CE-NZ	5.19	1.65	1.49
1	A	98	GLU	N-CA	-5.19	1.40	1.46
1	C	80	TRP	CE2-CZ2	5.19	1.50	1.39
1	D	32	LYS	CA-CB	-5.19	1.43	1.54
1	C	5	TYR	CD1-CE1	5.19	1.54	1.38
1	B	76	PHE	CA-CB	5.18	1.61	1.53
1	A	83	ILE	CA-C	5.18	1.59	1.52
1	B	59	ALA	N-CA	-5.17	1.39	1.46
1	A	89	PRO	CB-CG	5.17	1.75	1.49
1	B	44	LYS	C-N	-5.16	1.25	1.33
1	A	61	LYS	CE-NZ	5.16	1.64	1.49
1	B	57	LYS	N-CA	5.16	1.52	1.46
1	C	97	GLN	CD-OE1	5.16	1.33	1.23
1	A	29	VAL	CA-C	-5.15	1.47	1.52
1	D	38	PHE	N-CA	5.14	1.52	1.46
1	B	91	ALA	N-CA	-5.14	1.40	1.46
1	C	39	ARG	CA-C	-5.13	1.45	1.52
1	C	70	HIS	C-N	5.13	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	VAL	N-CA	5.13	1.52	1.46
1	A	3	ASP	CA-C	5.13	1.63	1.52
1	D	77	ASP	CA-C	-5.12	1.46	1.52
1	B	67	ASP	C-O	5.12	1.30	1.23
1	A	25	LYS	C-N	-5.11	1.26	1.33
1	D	39	ARG	CD-NE	5.11	1.53	1.46
1	A	43	GLN	CA-C	5.10	1.59	1.52
1	B	24	SER	CA-C	-5.10	1.46	1.53
1	A	34	SER	CA-C	5.10	1.60	1.53
1	A	37	SER	CA-C	5.09	1.59	1.52
1	C	78	GLU	CA-C	-5.09	1.45	1.52
1	B	41	MET	SD-CE	-5.08	1.66	1.79
1	B	19	PHE	C-N	-5.08	1.26	1.34
1	B	80	TRP	NE1-CE2	5.08	1.43	1.37
1	D	25	LYS	C-N	-5.08	1.26	1.33
1	D	15	LEU	N-CA	-5.08	1.40	1.46
1	C	23	VAL	N-CA	5.07	1.52	1.46
1	A	78	GLU	CD-OE1	5.07	1.34	1.25
1	A	40	GLU	CA-CB	5.07	1.61	1.53
1	D	84	GLY	CA-C	5.07	1.57	1.52
1	A	28	LEU	CG-CD2	5.07	1.69	1.52
1	B	20	TYR	CA-CB	5.06	1.61	1.53
1	C	10	LYS	CA-C	5.06	1.59	1.52
1	C	44	LYS	CE-NZ	5.05	1.64	1.49
1	B	72	GLY	N-CA	5.05	1.52	1.45
1	A	67	ASP	C-O	5.04	1.29	1.23
1	C	39	ARG	CB-CG	5.04	1.67	1.52
1	C	50	LEU	N-CA	5.04	1.52	1.46
1	D	23	VAL	N-CA	5.03	1.52	1.46
1	B	89	PRO	CB-CG	5.02	1.74	1.49
1	A	4	CYS	N-CA	5.02	1.52	1.46
1	C	76	PHE	CA-CB	5.01	1.61	1.53

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	LYS	O-C-N	-18.12	101.40	123.33
1	A	55	ASN	CA-C-O	16.32	137.96	120.82
1	A	55	ASN	O-C-N	-15.12	106.50	122.07
1	D	25	LYS	CA-C-N	-14.39	99.04	125.66
1	D	25	LYS	C-N-CA	-14.39	99.04	125.66
1	B	30	LYS	CA-C-O	14.26	137.71	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ILE	N-CA-C	-13.54	99.98	112.43
1	D	96	GLU	N-CA-C	-13.30	97.92	113.21
1	C	67	ASP	N-CA-C	12.96	129.41	110.10
1	A	94	ILE	N-CA-C	-12.37	98.22	110.72
1	A	79	TYR	N-CA-C	-12.04	98.24	111.36
1	B	56	ARG	NE-CZ-NH1	-12.01	109.49	121.50
1	C	53	THR	N-CA-C	11.66	123.74	111.14
1	A	52	ASP	CA-CB-CG	11.64	124.24	112.60
1	C	16	VAL	N-CA-C	11.64	122.34	110.23
1	C	93	LEU	N-CA-C	-11.43	97.83	112.23
1	C	5	TYR	CA-C-N	10.92	141.36	121.70
1	C	5	TYR	C-N-CA	10.92	141.36	121.70
1	C	88	GLY	O-C-N	10.69	124.92	121.07
1	B	32	LYS	N-CA-C	10.64	127.53	108.69
1	A	29	VAL	CA-C-N	-10.62	105.66	122.65
1	A	29	VAL	C-N-CA	-10.62	105.66	122.65
1	A	52	ASP	CA-C-O	-10.36	105.69	120.51
1	B	29	VAL	N-CA-CB	-10.34	98.20	111.64
1	D	90	ILE	N-CA-C	-10.26	103.35	113.20
1	A	55	ASN	CA-CB-CG	10.15	122.75	112.60
1	B	29	VAL	CA-C-N	-10.15	104.92	122.37
1	B	29	VAL	C-N-CA	-10.15	104.92	122.37
1	C	42	LEU	N-CA-C	-10.01	100.45	111.36
1	B	42	LEU	N-CA-C	-9.56	100.93	111.36
1	A	51	SER	N-CA-C	9.28	121.40	111.28
1	B	97	GLN	N-CA-CB	9.27	123.76	109.94
1	A	53	THR	CB-CA-C	9.27	123.59	109.13
1	B	31	ASN	CA-CB-CG	9.22	121.83	112.60
1	D	25	LYS	O-C-N	-9.08	112.16	123.06
1	B	51	SER	CA-CB-OG	-8.99	93.11	111.10
1	C	58	ALA	N-CA-C	-8.82	101.12	112.23
1	A	13	ILE	N-CA-C	8.70	119.50	110.36
1	A	90	ILE	CA-CB-CG2	8.64	125.19	110.50
1	A	17	GLU	CA-CB-CG	-8.45	97.20	114.10
1	C	40	GLU	N-CA-CB	8.38	122.14	109.91
1	D	16	VAL	N-CA-C	-8.34	102.30	110.72
1	B	94	ILE	CA-CB-CG1	-8.31	96.27	110.40
1	A	16	VAL	N-CA-C	-8.25	103.78	111.45
1	B	99	GLN	N-CA-C	8.24	121.08	111.02
1	B	53	THR	OG1-CB-CG2	-8.24	92.83	109.30
1	B	81	THR	CA-CB-OG1	-8.18	97.32	109.60
1	D	29	VAL	N-CA-CB	-8.16	101.21	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	SER	CB-CA-C	-8.12	92.49	110.19
1	A	53	THR	CA-C-O	8.08	127.76	118.55
1	C	92	LYS	CB-CA-C	8.08	123.73	110.81
1	C	63	ILE	N-CA-CB	7.96	123.85	110.56
1	B	69	ASN	CA-CB-CG	-7.89	104.71	112.60
1	A	86	ILE	N-CA-C	-7.83	103.17	110.53
1	C	98	GLU	N-CA-C	7.81	120.69	111.71
1	B	76	PHE	CA-CB-CG	-7.78	106.03	113.80
1	A	78	GLU	N-CA-CB	-7.66	98.83	110.16
1	D	86	ILE	N-CA-C	-7.59	105.28	111.81
1	D	15	LEU	CD1-CG-CD2	-7.53	94.24	110.80
1	B	56	ARG	NE-CZ-NH2	7.40	125.86	119.20
1	B	29	VAL	CA-C-O	-7.37	112.73	120.39
1	C	20	TYR	N-CA-C	7.35	121.35	112.38
1	C	23	VAL	O-C-N	-7.35	114.80	122.66
1	C	5	TYR	N-CA-C	-7.33	90.47	111.00
1	B	97	GLN	CA-C-N	7.32	130.08	120.28
1	B	97	GLN	C-N-CA	7.32	130.08	120.28
1	D	40	GLU	CA-C-O	7.31	128.72	120.90
1	C	87	THR	CA-CB-OG1	-7.31	98.64	109.60
1	B	59	ALA	N-CA-C	-7.31	102.70	111.69
1	C	51	SER	N-CA-C	-7.28	104.40	113.28
1	D	43	GLN	N-CA-C	7.26	126.27	110.80
1	C	97	GLN	CB-CA-C	-7.25	95.58	110.38
1	B	35	LYS	CB-CG-CD	-7.25	94.63	111.30
1	C	75	SER	CA-CB-OG	-7.18	96.74	111.10
1	C	42	LEU	N-CA-CB	-7.17	99.55	110.16
1	B	65	ASN	N-CA-C	7.13	121.57	113.02
1	D	76	PHE	N-CA-C	7.10	119.92	111.33
1	A	54	GLY	O-C-N	-7.09	115.31	122.19
1	A	62	LEU	N-CA-C	-7.05	103.01	111.69
1	B	45	GLU	CB-CG-CD	-7.04	100.63	112.60
1	D	85	GLY	N-CA-C	-7.04	104.98	113.99
1	B	94	ILE	O-C-N	6.88	128.66	121.91
1	D	7	GLU	CA-CB-CG	-6.88	100.33	114.10
1	D	28	LEU	CA-C-N	-6.87	113.94	122.93
1	D	28	LEU	C-N-CA	-6.87	113.94	122.93
1	C	41	MET	CG-SD-CE	-6.86	85.80	100.90
1	A	88	GLY	N-CA-C	6.85	126.32	112.34
1	D	73	ARG	N-CA-C	6.84	119.36	110.53
1	D	16	VAL	CB-CA-C	-6.83	102.79	112.22
1	B	20	TYR	CA-C-N	-6.82	109.69	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	TYR	C-N-CA	-6.82	109.69	120.60
1	D	45	GLU	N-CA-C	-6.82	105.90	114.56
1	B	65	ASN	CB-CA-C	-6.81	98.25	110.37
1	C	21	LYS	CA-C-N	-6.81	111.98	122.60
1	C	21	LYS	C-N-CA	-6.81	111.98	122.60
1	D	84	GLY	N-CA-C	-6.80	104.06	112.77
1	B	39	ARG	N-CA-C	-6.80	103.95	111.36
1	D	73	ARG	CD-NE-CZ	6.79	133.91	124.40
1	B	61	LYS	N-CA-CB	-6.79	99.85	110.30
1	A	52	ASP	N-CA-CB	6.76	121.91	110.49
1	C	83	ILE	CA-CB-CG1	-6.75	98.93	110.40
1	A	98	GLU	N-CA-C	6.75	118.29	111.07
1	D	89	PRO	CA-C-N	-6.73	114.55	122.36
1	D	89	PRO	C-N-CA	-6.73	114.55	122.36
1	C	24	SER	N-CA-C	6.73	119.24	110.43
1	B	97	GLN	N-CA-C	6.71	119.16	111.11
1	C	84	GLY	N-CA-C	-6.70	104.72	112.50
1	A	20	TYR	CA-C-N	-6.70	110.60	120.38
1	A	20	TYR	C-N-CA	-6.70	110.60	120.38
1	D	35	LYS	N-CA-C	6.69	119.14	111.11
1	A	91	ALA	N-CA-C	6.68	118.22	111.07
1	C	52	ASP	N-CA-C	-6.68	101.08	110.50
1	C	73	ARG	NE-CZ-NH2	6.63	125.17	119.20
1	D	29	VAL	CA-CB-CG1	6.57	121.58	110.40
1	B	63	ILE	CB-CA-C	-6.56	103.43	112.02
1	C	90	ILE	CG1-CB-CG2	-6.54	91.06	110.70
1	D	24	SER	N-CA-CB	6.53	119.58	109.85
1	B	84	GLY	N-CA-C	6.53	122.12	113.37
1	D	28	LEU	N-CA-CB	-6.50	99.59	110.39
1	A	49	MET	CA-C-N	-6.47	112.96	122.86
1	A	49	MET	C-N-CA	-6.47	112.96	122.86
1	B	31	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	C	63	ILE	CA-C-O	-6.42	113.84	120.71
1	A	86	ILE	CA-C-O	-6.39	113.96	121.05
1	B	19	PHE	N-CA-CB	-6.38	100.71	110.16
1	A	6	THR	N-CA-CB	-6.35	100.30	110.46
1	B	8	LEU	CD1-CG-CD2	-6.33	96.87	110.80
1	A	46	LEU	CA-C-N	-6.33	109.24	121.58
1	A	46	LEU	C-N-CA	-6.33	109.24	121.58
1	D	30	LYS	CA-C-O	-6.32	111.66	119.18
1	B	89	PRO	CB-CA-C	-6.32	102.89	112.11
1	D	23	VAL	CB-CA-C	-6.30	102.40	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	THR	O-C-N	-6.29	115.43	122.10
1	A	54	GLY	N-CA-C	-6.26	104.76	112.77
1	A	17	GLU	CA-C-O	6.25	127.16	120.10
1	B	33	ILE	N-CA-C	-6.25	99.23	108.85
1	D	87	THR	OG1-CB-CG2	-6.25	96.81	109.30
1	B	37	SER	CB-CA-C	-6.24	97.66	110.38
1	B	16	VAL	CA-C-N	-6.21	111.47	120.29
1	B	16	VAL	C-N-CA	-6.21	111.47	120.29
1	B	78	GLU	CA-C-O	-6.21	113.97	120.55
1	A	5	TYR	N-CA-C	6.15	118.23	110.24
1	C	13	ILE	N-CA-C	-6.13	104.54	110.42
1	C	100	GLN	CA-C-O	-6.12	111.76	120.51
1	B	99	GLN	CA-CB-CG	-6.11	101.89	114.10
1	D	50	LEU	CB-CA-C	6.09	121.68	110.10
1	B	96	GLU	N-CA-C	-6.08	104.73	111.36
1	B	23	VAL	N-CA-C	-6.07	99.85	108.58
1	D	34	SER	CA-CB-OG	-6.05	99.01	111.10
1	B	15	LEU	CD1-CG-CD2	-6.03	97.53	110.80
1	D	19	PHE	CB-CA-C	-6.02	100.79	110.79
1	C	61	LYS	N-CA-CB	-6.01	101.05	110.30
1	C	45	GLU	CA-C-O	6.00	125.65	119.05
1	C	15	LEU	N-CA-C	5.95	118.25	111.11
1	C	92	LYS	N-CA-C	5.95	118.25	111.11
1	B	7	GLU	CA-C-O	-5.94	113.39	120.10
1	A	66	LEU	CB-CG-CD1	5.92	128.44	110.70
1	D	7	GLU	CB-CA-C	-5.91	99.69	110.63
1	B	56	ARG	CA-CB-CG	-5.91	102.29	114.10
1	B	78	GLU	N-CA-CB	5.90	118.79	110.12
1	C	93	LEU	CA-C-N	-5.90	110.63	120.30
1	C	93	LEU	C-N-CA	-5.90	110.63	120.30
1	B	60	ASP	CA-C-N	-5.89	110.66	120.68
1	B	60	ASP	C-N-CA	-5.89	110.66	120.68
1	C	17	GLU	CA-C-N	-5.89	111.36	120.31
1	C	17	GLU	C-N-CA	-5.89	111.36	120.31
1	A	26	TYR	N-CA-C	-5.89	104.75	113.40
1	B	74	ILE	N-CA-CB	-5.87	104.34	111.21
1	B	82	LEU	CA-C-N	-5.86	112.43	120.46
1	B	82	LEU	C-N-CA	-5.86	112.43	120.46
1	A	39	ARG	N-CA-C	-5.83	104.92	111.28
1	A	98	GLU	CA-CB-CG	-5.83	102.43	114.10
1	B	53	THR	CA-CB-OG1	-5.82	100.87	109.60
1	D	93	LEU	CB-CG-CD1	-5.80	93.30	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	THR	CB-CA-C	-5.79	100.85	110.68
1	A	43	GLN	CB-CG-CD	-5.78	102.77	112.60
1	D	26	TYR	N-CA-C	5.78	124.84	113.29
1	B	32	LYS	CA-CB-CG	5.76	125.61	114.10
1	B	60	ASP	N-CA-CB	5.76	118.52	109.94
1	C	31	ASN	CB-CA-C	-5.76	101.86	111.13
1	B	30	LYS	CB-CA-C	5.72	121.00	109.38
1	B	45	GLU	OE1-CD-OE2	-5.71	109.19	122.90
1	D	90	ILE	CA-C-O	5.70	123.91	119.46
1	C	74	ILE	N-CA-CB	-5.68	104.53	111.00
1	B	36	SER	CA-CB-OG	-5.66	99.78	111.10
1	A	19	PHE	CB-CA-C	-5.66	101.96	110.90
1	B	36	SER	N-CA-C	-5.66	105.11	111.28
1	B	36	SER	N-CA-CB	-5.66	101.80	110.12
1	B	51	SER	CA-C-N	-5.65	113.53	121.72
1	B	51	SER	C-N-CA	-5.65	113.53	121.72
1	B	64	GLN	CB-CA-C	-5.64	99.51	110.46
1	C	43	GLN	N-CA-C	5.62	117.41	111.28
1	C	25	LYS	CA-C-O	-5.62	115.00	121.19
1	A	17	GLU	O-C-N	-5.61	115.66	122.22
1	B	17	GLU	CB-CG-CD	-5.60	103.08	112.60
1	D	96	GLU	CA-CB-CG	5.60	125.30	114.10
1	C	56	ARG	N-CA-C	-5.60	105.26	111.36
1	D	31	ASN	N-CA-CB	5.60	119.41	110.73
1	B	45	GLU	CB-CA-C	5.57	120.86	109.55
1	A	36	SER	N-CA-C	-5.57	105.36	111.82
1	B	51	SER	CA-C-O	5.57	126.45	120.55
1	C	9	GLU	N-CA-CB	5.56	118.48	110.20
1	C	52	ASP	CA-C-O	-5.56	115.50	121.56
1	B	12	VAL	N-CA-CB	-5.54	104.07	110.55
1	C	94	ILE	N-CA-C	-5.54	104.16	111.09
1	A	46	LEU	CB-CA-C	-5.54	102.05	111.02
1	C	48	HIS	N-CA-C	-5.54	104.64	111.40
1	B	29	VAL	N-CA-C	-5.54	99.67	107.75
1	C	86	ILE	CA-CB-CG2	-5.52	101.12	110.50
1	A	80	TRP	N-CA-C	-5.51	104.91	111.03
1	B	47	ASN	CA-C-O	-5.51	112.06	119.11
1	A	54	GLY	CA-C-O	5.49	126.48	120.66
1	C	35	LYS	O-C-N	-5.49	115.80	122.22
1	C	68	ALA	N-CA-CB	5.48	118.15	109.71
1	A	81	THR	CA-CB-OG1	-5.48	101.38	109.60
1	C	16	VAL	O-C-N	-5.48	116.05	121.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	32	LYS	CA-C-O	5.46	127.15	120.60
1	A	28	LEU	N-CA-C	-5.43	105.91	112.54
1	B	13	ILE	O-C-N	-5.43	116.57	121.89
1	C	11	ALA	N-CA-C	-5.43	105.28	111.14
1	C	56	ARG	CA-C-O	-5.42	114.68	120.42
1	A	89	PRO	N-CA-C	-5.41	107.70	114.20
1	D	49	MET	CG-SD-CE	-5.40	89.03	100.90
1	B	94	ILE	CB-CA-C	-5.38	105.08	111.97
1	C	91	ALA	N-CA-C	5.38	117.14	111.28
1	C	40	GLU	CA-C-O	-5.38	115.36	121.00
1	B	60	ASP	CB-CG-OD1	5.37	130.75	118.40
1	C	67	ASP	CA-CB-CG	-5.37	107.23	112.60
1	B	78	GLU	CA-CB-CG	-5.34	103.41	114.10
1	B	91	ALA	O-C-N	5.34	127.57	122.07
1	C	17	GLU	CB-CA-C	-5.34	100.75	110.63
1	D	28	LEU	O-C-N	-5.33	115.28	122.43
1	D	78	GLU	N-CA-C	-5.32	105.56	111.36
1	B	22	TYR	N-CA-C	-5.31	106.67	112.72
1	A	84	GLY	CA-C-N	-5.30	111.35	120.79
1	A	84	GLY	C-N-CA	-5.30	111.35	120.79
1	B	25	LYS	CD-CE-NZ	-5.30	94.94	111.90
1	A	61	LYS	N-CA-CB	5.30	119.18	110.39
1	A	51	SER	CA-C-N	-5.29	111.44	121.54
1	A	51	SER	C-N-CA	-5.29	111.44	121.54
1	C	21	LYS	CB-CG-CD	-5.27	99.17	111.30
1	D	19	PHE	N-CA-C	-5.27	105.54	111.28
1	D	9	GLU	N-CA-CB	5.26	117.77	109.94
1	C	32	LYS	CA-C-N	-5.25	114.89	122.45
1	C	32	LYS	C-N-CA	-5.25	114.89	122.45
1	D	7	GLU	CB-CG-CD	-5.24	103.70	112.60
1	C	87	THR	CA-CB-CG2	-5.23	101.60	110.50
1	B	12	VAL	CA-CB-CG2	-5.21	101.54	110.40
1	D	74	ILE	CB-CG1-CD1	-5.19	102.90	113.80
1	B	39	ARG	CG-CD-NE	-5.18	100.60	112.00
1	B	48	HIS	N-CA-C	-5.16	106.14	112.90
1	A	41	MET	CG-SD-CE	5.16	112.25	100.90
1	B	56	ARG	CD-NE-CZ	-5.14	117.20	124.40
1	A	87	THR	CA-C-N	-5.13	113.82	121.87
1	A	87	THR	C-N-CA	-5.13	113.82	121.87
1	D	90	ILE	CA-C-N	-5.13	112.52	120.31
1	D	90	ILE	C-N-CA	-5.13	112.52	120.31
1	B	7	GLU	CA-C-N	5.12	127.57	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	GLU	C-N-CA	5.12	127.57	120.29
1	B	37	SER	N-CA-C	-5.12	105.78	112.23
1	B	92	LYS	O-C-N	5.11	127.40	122.09
1	B	83	ILE	CB-CA-C	-5.10	105.25	112.14
1	B	97	GLN	CA-C-O	-5.09	115.45	120.90
1	A	60	ASP	CA-C-N	-5.08	112.23	120.72
1	A	60	ASP	C-N-CA	-5.08	112.23	120.72
1	D	90	ILE	CB-CA-C	5.07	115.72	110.70
1	B	20	TYR	N-CA-CB	5.07	118.13	110.28
1	C	82	LEU	CB-CA-C	-5.05	102.30	110.79
1	D	39	ARG	O-C-N	5.05	127.49	122.08
1	A	78	GLU	CA-C-O	5.05	125.77	120.42
1	B	66	LEU	CD1-CG-CD2	5.05	121.90	110.80
1	A	62	LEU	N-CA-CB	5.04	117.71	110.20
1	D	30	LYS	O-C-N	5.04	129.56	122.41
1	B	28	LEU	CA-C-O	5.04	125.72	119.12
1	C	63	ILE	CG1-CB-CG2	-5.03	95.60	110.70
1	A	22	TYR	N-CA-C	5.03	119.40	113.16
1	A	78	GLU	N-CA-C	5.03	116.84	111.36
1	D	77	ASP	N-CA-CB	5.03	117.51	110.12
1	D	80	TRP	N-CA-CB	5.02	117.42	109.94
1	D	8	LEU	CA-C-O	-5.01	115.24	120.55

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	ASP	Mainchain
1	A	53	THR	Mainchain
1	A	89	PRO	Mainchain
1	A	90	ILE	Mainchain
1	B	14	VAL	Mainchain
1	B	29	VAL	Peptide
1	B	30	LYS	Mainchain
1	B	57	LYS	Mainchain
1	B	76	PHE	Sidechain
1	B	78	GLU	Sidechain
1	C	69	ASN	Peptide
1	C	73	ARG	Mainchain
1	C	81	THR	Mainchain
1	C	82	LEU	Mainchain
1	D	14	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	D	15	LEU	Mainchain
1	D	24	SER	Mainchain
1	D	76	PHE	Mainchain

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	808	0	805	63	0
1	B	788	0	791	69	0
1	C	788	0	791	54	0
1	D	610	0	623	42	0
2	A	15	0	0	6	0
2	B	25	0	0	2	0
2	C	22	0	0	8	0
2	D	18	0	0	3	0
All	All	3074	0	3010	217	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 36.

All (217) 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:B:58:ALA:CA	1:B:58:ALA:CB	1.74	1.65
1:D:35:LYS:CG	1:D:35:LYS:CB	1.75	1.63
1:A:13:ILE:CA	1:A:13:ILE:CB	1.75	1.62
1:A:19:PHE:CG	1:A:19:PHE:CB	1.77	1.62
1:B:57:LYS:CD	1:B:57:LYS:CE	1.75	1.62
1:C:62:LEU:CG	1:C:62:LEU:CD2	1.80	1.60
1:B:13:ILE:CB	1:B:13:ILE:CA	1.77	1.59
1:B:61:LYS:CD	1:B:61:LYS:CG	1.80	1.59
1:B:93:LEU:CG	1:B:93:LEU:CD1	1.76	1.59
1:A:81:THR:CB	1:A:81:THR:CG2	1.74	1.59
1:B:72:GLY:CA	1:B:72:GLY:C	1.75	1.57
1:D:13:ILE:CA	1:D:13:ILE:CB	1.83	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ILE:CD1	1:D:90:ILE:CG1	1.83	1.57
1:A:31:ASN:CB	1:A:31:ASN:CG	1.77	1.56
1:C:96:GLU:CG	1:C:96:GLU:CB	1.78	1.56
1:A:74:ILE:CG1	1:A:74:ILE:CD1	1.80	1.54
1:C:10:LYS:CE	1:C:10:LYS:NZ	1.69	1.53
1:C:71:ASP:CB	1:C:71:ASP:CG	1.78	1.53
1:C:60:ASP:CB	1:C:60:ASP:CG	1.81	1.53
1:D:28:LEU:CG	1:D:28:LEU:CD2	1.87	1.53
1:B:94:ILE:CD1	1:B:94:ILE:CG1	1.81	1.53
1:B:89:PRO:CB	1:B:89:PRO:CG	1.74	1.52
1:B:91:ALA:CA	1:B:91:ALA:CB	1.81	1.52
1:A:93:LEU:CG	1:A:93:LEU:CD1	1.86	1.50
1:C:40:GLU:CD	1:C:40:GLU:CG	1.82	1.49
1:A:89:PRO:CB	1:A:89:PRO:CG	1.75	1.48
1:A:51:SER:O	1:A:52:ASP:O	1.62	1.16
1:C:38:PHE:CE1	1:C:41:MET:HE1	1.84	1.13
1:C:38:PHE:CE2	1:C:82:LEU:HD13	1.85	1.11
1:B:69:ASN:HB3	1:B:72:GLY:H	1.15	1.08
1:C:38:PHE:HE2	1:C:82:LEU:HD13	0.99	1.07
1:C:38:PHE:HE1	1:C:41:MET:HE1	1.08	1.07
1:D:47:ASN:HB3	2:D:116:HOH:O	1.53	1.06
1:C:29:VAL:O	1:C:29:VAL:HG12	1.55	1.04
1:A:51:SER:C	1:A:52:ASP:O	1.94	1.03
1:A:93:LEU:H	1:A:93:LEU:HD12	1.27	1.00
1:A:89:PRO:HD3	2:A:111:HOH:O	1.67	0.93
1:B:38:PHE:CE1	1:B:41:MET:HE1	2.04	0.93
1:A:6:THR:HG22	1:A:9:GLU:H	1.35	0.92
1:B:69:ASN:HB3	1:B:72:GLY:N	1.86	0.90
1:D:13:ILE:HG22	2:D:104:HOH:O	1.73	0.88
1:B:61:LYS:CD	1:B:61:LYS:CB	2.52	0.86
1:A:43:GLN:O	1:A:47:ASN:HB3	1.76	0.86
1:A:93:LEU:HD12	1:A:93:LEU:N	1.91	0.85
1:B:30:LYS:HB3	1:B:30:LYS:NZ	1.91	0.85
1:A:13:ILE:CA	1:A:13:ILE:CG1	2.54	0.85
1:C:78:GLU:O	1:C:82:LEU:HD12	1.77	0.83
1:A:92:LYS:HE3	2:A:115:HOH:O	1.79	0.82
1:D:35:LYS:CG	1:D:35:LYS:CA	2.59	0.80
1:C:96:GLU:CG	1:C:96:GLU:CA	2.60	0.79
1:B:23:VAL:HG11	1:B:30:LYS:HD3	1.65	0.78
1:A:90:ILE:HA	1:A:93:LEU:HD13	1.67	0.76
1:B:13:ILE:CB	1:B:13:ILE:C	2.57	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TYR:HD1	1:B:30:LYS:HD2	1.49	0.75
1:A:6:THR:HG21	1:B:45:GLU:O	1.87	0.75
1:C:62:LEU:CD2	1:C:62:LEU:CD1	2.65	0.74
1:A:13:ILE:CA	1:A:13:ILE:CG2	2.64	0.73
1:B:7:GLU:OE1	1:B:10:LYS:NZ	2.21	0.73
1:D:13:ILE:CB	1:D:13:ILE:C	2.62	0.73
1:D:25:LYS:O	1:D:26:TYR:CB	2.29	0.73
1:B:58:ALA:CB	1:B:58:ALA:C	2.60	0.72
1:A:81:THR:CG2	1:A:81:THR:CA	2.65	0.72
1:A:93:LEU:CD1	1:A:93:LEU:H	2.02	0.72
1:B:33:ILE:O	1:B:74:ILE:N	2.22	0.72
1:B:13:ILE:CA	1:B:13:ILE:CD1	2.67	0.71
1:A:30:LYS:HB3	2:A:112:HOH:O	1.90	0.70
1:C:38:PHE:HE2	1:C:82:LEU:CD1	1.91	0.70
1:C:93:LEU:HD11	2:C:115:HOH:O	1.91	0.70
1:A:38:PHE:CD1	1:A:41:MET:CE	2.75	0.70
1:C:93:LEU:HD13	2:C:104:HOH:O	1.93	0.69
1:C:48:HIS:HD2	1:D:9:GLU:OE1	1.75	0.68
1:B:23:VAL:HG11	1:B:30:LYS:HB2	1.76	0.68
1:D:25:LYS:O	1:D:26:TYR:HB2	1.92	0.68
1:D:28:LEU:CD2	1:D:28:LEU:CB	2.72	0.68
1:B:23:VAL:CB	1:B:30:LYS:HD3	2.25	0.67
1:B:30:LYS:HB3	1:B:30:LYS:HZ3	1.58	0.66
1:C:38:PHE:CE1	1:C:41:MET:CE	2.70	0.66
1:D:40:GLU:HG3	1:D:44:LYS:HE2	1.77	0.66
1:D:13:ILE:CB	1:D:13:ILE:N	2.57	0.66
1:A:93:LEU:CD1	1:A:93:LEU:CB	2.72	0.66
1:B:23:VAL:CG1	1:B:30:LYS:HD3	2.25	0.66
1:A:13:ILE:CB	1:A:13:ILE:C	2.67	0.65
1:B:13:ILE:CA	1:B:13:ILE:CG1	2.73	0.65
1:B:61:LYS:CG	1:B:61:LYS:CE	2.73	0.65
1:D:83:ILE:O	1:D:87:THR:HG23	1.95	0.65
1:D:47:ASN:CB	2:D:116:HOH:O	2.26	0.65
1:B:57:LYS:CE	1:B:57:LYS:CG	2.75	0.64
1:D:5:TYR:O	1:D:10:LYS:NZ	2.29	0.64
1:B:93:LEU:CD1	1:B:93:LEU:CD2	2.75	0.64
1:C:71:ASP:HB2	2:C:120:HOH:O	1.98	0.62
1:A:29:VAL:O	1:A:29:VAL:HG23	2.01	0.61
1:A:49:MET:HG3	1:B:9:GLU:HG2	1.81	0.61
1:B:30:LYS:NZ	1:B:30:LYS:CB	2.63	0.61
1:C:71:ASP:CB	2:C:120:HOH:O	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:HIS:C	1:D:97:GLN:H	2.07	0.60
1:C:47:ASN:O	1:C:51:SER:HB3	2.01	0.59
1:D:35:LYS:CB	1:D:35:LYS:CD	2.80	0.59
1:B:13:ILE:N	1:B:13:ILE:HD13	2.17	0.59
1:B:55:ASN:ND2	2:B:105:HOH:O	2.33	0.59
1:C:41:MET:HE3	1:C:42:LEU:HD23	1.84	0.59
1:C:68:ALA:HA	1:C:72:GLY:HA2	1.85	0.59
1:A:93:LEU:CD1	1:A:93:LEU:N	2.61	0.59
1:B:71:ASP:HB3	1:B:73:ARG:H	1.68	0.59
1:A:19:PHE:CG	1:A:19:PHE:CA	2.83	0.58
1:D:13:ILE:CA	1:D:13:ILE:CG2	2.78	0.58
1:C:69:ASN:N	1:C:72:GLY:H	2.02	0.57
1:C:6:THR:O	1:C:10:LYS:HG2	2.04	0.57
1:C:66:LEU:HD12	1:C:67:ASP:N	2.20	0.57
1:B:50:LEU:O	1:B:56:ARG:NH1	2.38	0.56
1:B:91:ALA:CB	1:B:91:ALA:C	2.77	0.56
1:D:22:TYR:OH	1:D:45:GLU:OE2	2.15	0.56
1:B:20:TYR:CD1	1:B:30:LYS:HD2	2.37	0.56
1:C:38:PHE:CD1	1:C:41:MET:CE	2.89	0.56
1:A:19:PHE:CB	1:A:19:PHE:CD2	2.72	0.55
1:B:13:ILE:HD12	1:B:13:ILE:HA	1.88	0.55
1:C:38:PHE:CD1	1:C:41:MET:HE1	2.39	0.55
1:A:38:PHE:CD1	1:A:41:MET:HE1	2.41	0.54
1:C:93:LEU:CD1	2:C:115:HOH:O	2.53	0.54
1:D:34:SER:HB3	1:D:73:ARG:NH2	2.22	0.54
1:B:13:ILE:CA	1:B:13:ILE:CG2	2.77	0.54
1:B:93:LEU:CD1	1:B:93:LEU:HG	2.17	0.54
1:B:91:ALA:CB	1:B:91:ALA:N	2.65	0.53
1:B:78:GLU:CD	2:B:115:HOH:O	2.52	0.53
1:B:32:LYS:HD3	1:B:73:ARG:HB2	1.90	0.53
1:B:94:ILE:CD1	1:B:94:ILE:CB	2.81	0.53
1:A:93:LEU:CD1	1:A:93:LEU:CD2	2.75	0.52
1:A:6:THR:HG22	1:A:9:GLU:HB2	1.92	0.52
1:B:13:ILE:HD13	1:B:13:ILE:H	1.72	0.52
1:B:23:VAL:HG11	1:B:30:LYS:CD	2.39	0.52
1:A:38:PHE:CE1	1:A:41:MET:HE1	2.45	0.51
1:D:76:PHE:CD2	1:D:76:PHE:C	2.88	0.51
1:A:31:ASN:CG	1:A:31:ASN:CA	2.78	0.51
1:B:30:LYS:HB3	1:B:30:LYS:HZ2	1.70	0.50
1:C:42:LEU:HD22	1:C:46:LEU:HD12	1.92	0.50
1:C:62:LEU:CD2	1:C:62:LEU:CB	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ARG:HH11	1:C:56:ARG:HG2	1.77	0.50
1:B:13:ILE:CA	1:B:13:ILE:HD12	2.42	0.50
1:A:90:ILE:HG23	1:A:94:ILE:CD1	2.42	0.49
1:A:6:THR:HG23	1:A:7:GLU:N	2.25	0.49
1:A:55:ASN:O	1:A:56:ARG:C	2.52	0.49
1:D:48:HIS:C	1:D:50:LEU:N	2.70	0.49
1:C:66:LEU:HD22	1:C:82:LEU:HD11	1.94	0.49
1:A:28:LEU:HB2	2:A:107:HOH:O	2.12	0.49
1:A:61:LYS:O	1:A:65:ASN:HB3	2.13	0.49
1:A:51:SER:O	1:A:52:ASP:C	2.47	0.49
1:D:14:VAL:O	1:D:14:VAL:CG1	2.61	0.49
1:D:95:HIS:C	1:D:97:GLN:N	2.70	0.48
1:D:46:LEU:O	1:D:50:LEU:HD13	2.12	0.48
1:A:13:ILE:CG2	1:A:13:ILE:C	2.86	0.48
1:C:88:GLY:N	1:C:89:PRO:CD	2.76	0.48
1:A:19:PHE:CB	1:A:19:PHE:CD1	2.75	0.48
1:A:73:ARG:CZ	2:A:116:HOH:O	2.61	0.48
1:B:30:LYS:CB	1:B:30:LYS:HZ2	2.23	0.48
1:C:8:LEU:HD23	1:D:45:GLU:HB3	1.95	0.48
1:B:50:LEU:O	1:B:56:ARG:HD3	2.13	0.48
1:B:56:ARG:HD3	1:B:56:ARG:HH11	1.17	0.48
1:A:45:GLU:O	1:B:6:THR:OG1	2.25	0.47
1:A:16:VAL:HG11	1:B:94:ILE:HB	1.96	0.47
1:D:13:ILE:C	1:D:13:ILE:CG2	2.88	0.47
1:C:31:ASN:O	1:C:32:LYS:HG3	2.14	0.47
1:D:76:PHE:O	1:D:77:ASP:C	2.55	0.47
1:A:50:LEU:O	1:A:56:ARG:HG3	2.15	0.47
1:B:13:ILE:CD1	1:B:13:ILE:N	2.78	0.46
1:B:75:SER:OG	1:B:78:GLU:HG3	2.15	0.46
1:D:79:TYR:O	1:D:83:ILE:HG12	2.15	0.46
1:A:9:GLU:HG3	1:B:46:LEU:HD12	1.98	0.46
1:D:74:ILE:HD13	1:D:74:ILE:HG21	1.74	0.46
1:D:96:GLU:HA	1:D:96:GLU:OE1	2.15	0.46
1:A:81:THR:CG2	1:A:81:THR:OG1	2.55	0.46
1:B:97:GLN:HG3	1:D:25:LYS:HE2	1.98	0.46
1:C:32:LYS:HB3	1:C:73:ARG:HB3	1.98	0.46
1:D:23:VAL:HG22	1:D:32:LYS:O	2.15	0.46
1:B:23:VAL:HB	1:B:30:LYS:HD3	1.99	0.45
1:A:13:ILE:CB	1:A:13:ILE:N	2.67	0.45
1:C:22:TYR:OH	1:C:45:GLU:OE2	2.29	0.45
1:D:31:ASN:C	1:D:32:LYS:HG3	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PHE:CE1	1:A:41:MET:CE	3.00	0.45
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.67	0.45
1:D:13:ILE:CA	1:D:13:ILE:HD13	2.47	0.45
1:A:38:PHE:CD1	1:A:41:MET:HE3	2.50	0.45
1:B:32:LYS:HD3	1:B:73:ARG:CB	2.47	0.45
1:C:49:MET:HE3	1:C:49:MET:HB2	1.80	0.45
1:B:50:LEU:HD23	1:B:50:LEU:HA	1.76	0.45
1:A:29:VAL:O	1:A:29:VAL:CG2	2.64	0.44
1:B:23:VAL:HG21	1:B:30:LYS:CD	2.48	0.44
1:A:9:GLU:OE1	1:B:48:HIS:HD2	2.00	0.44
1:A:97:GLN:O	1:A:100:GLN:HB2	2.17	0.44
1:A:31:ASN:HB3	2:A:103:HOH:O	2.17	0.44
1:A:30:LYS:H	1:A:30:LYS:HG2	1.63	0.44
1:C:96:GLU:CB	1:C:96:GLU:CD	2.80	0.44
1:D:13:ILE:CA	1:D:13:ILE:CD1	2.95	0.44
1:C:48:HIS:O	1:C:49:MET:C	2.61	0.43
1:D:90:ILE:HG23	1:D:94:ILE:CD1	2.48	0.43
1:A:9:GLU:OE2	1:B:48:HIS:N	2.46	0.43
1:C:52:ASP:HB3	2:C:103:HOH:O	2.18	0.43
1:B:20:TYR:HA	1:B:23:VAL:HG23	1.99	0.43
1:C:6:THR:HG22	1:C:7:GLU:N	2.33	0.43
1:C:69:ASN:H	1:C:72:GLY:H	1.66	0.42
1:B:43:GLN:O	1:B:47:ASN:HB3	2.19	0.42
1:A:83:ILE:HA	1:A:83:ILE:HD13	1.74	0.42
2:C:116:HOH:O	1:D:14:VAL:HG21	2.18	0.42
1:A:63:ILE:O	1:A:66:LEU:HB2	2.19	0.42
1:B:61:LYS:CD	1:B:61:LYS:HB2	2.44	0.42
1:C:31:ASN:HD21	1:D:92:LYS:NZ	2.18	0.41
1:A:13:ILE:CA	1:A:13:ILE:HG13	2.47	0.41
1:A:14:VAL:O	1:A:15:LEU:C	2.62	0.41
1:C:83:ILE:HD13	1:C:83:ILE:HA	1.83	0.41
1:C:95:HIS:O	1:C:96:GLU:C	2.64	0.41
1:C:12:VAL:O	1:C:13:ILE:C	2.62	0.41
1:C:38:PHE:HD1	1:C:41:MET:HE2	1.86	0.41
1:C:56:ARG:NH2	2:C:121:HOH:O	2.40	0.41
1:B:83:ILE:HD13	1:B:83:ILE:HA	1.83	0.40
1:D:49:MET:C	1:D:50:LEU:HD12	2.46	0.40
1:C:10:LYS:NZ	1:C:10:LYS:CD	2.72	0.40
1:C:50:LEU:O	1:C:56:ARG:HB2	2.22	0.40
1:C:87:THR:O	1:C:88:GLY:C	2.62	0.40
1:A:6:THR:CG2	1:A:9:GLU:H	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 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	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	6	2
1	B	95/100 (95%)	91 (96%)	3 (3%)	1 (1%)	11	8
1	C	95/100 (95%)	86 (90%)	6 (6%)	3 (3%)	3	1
1	D	70/100 (70%)	63 (90%)	7 (10%)	0	100	100
All	All	358/400 (90%)	327 (91%)	25 (7%)	6 (2%)	7	3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	B	31	ASN
1	A	52	ASP
1	C	69	ASN
1	C	100	GLN
1	C	29	VAL

5.3.2 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 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	90/90 (100%)	66 (73%)	24 (27%)	0	0
1	B	87/90 (97%)	73 (84%)	14 (16%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	87/90 (97%)	73 (84%)	14 (16%)	2	1
1	D	68/90 (76%)	63 (93%)	5 (7%)	13	10
All	All	332/360 (92%)	275 (83%)	57 (17%)	2	1

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	6	THR
1	A	10	LYS
1	A	16	VAL
1	A	25	LYS
1	A	28	LEU
1	A	29	VAL
1	A	30	LYS
1	A	33	ILE
1	A	36	SER
1	A	41	MET
1	A	42	LEU
1	A	43	GLN
1	A	44	LYS
1	A	49	MET
1	A	53	THR
1	A	61	LYS
1	A	67	ASP
1	A	71	ASP
1	A	73	ARG
1	A	79	TYR
1	A	87	THR
1	A	90	ILE
1	A	102	SER
1	B	10	LYS
1	B	13	ILE
1	B	15	LEU
1	B	30	LYS
1	B	32	LYS
1	B	37	SER
1	B	53	THR
1	B	65	ASN
1	B	66	LEU
1	B	71	ASP

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Mol	Chain	Res	Type
1	B	75	SER
1	B	79	TYR
1	B	93	LEU
1	B	100	GLN
1	C	10	LYS
1	C	13	ILE
1	C	15	LEU
1	C	21	LYS
1	C	29	VAL
1	C	40	GLU
1	C	42	LEU
1	C	57	LYS
1	C	66	LEU
1	C	70	HIS
1	C	71	ASP
1	C	79	TYR
1	C	82	LEU
1	C	101	SER
1	D	4	CYS
1	D	24	SER
1	D	28	LEU
1	D	32	LYS
1	D	44	LYS

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

Mol	Chain	Res	Type
1	B	48	HIS
1	B	100	GLN
1	C	31	ASN
1	C	48	HIS
1	C	99	GLN
1	C	100	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 95th 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 ²)	Q<0.9
1	A	100/100 (100%)	0.98	12 (12%) 9 9	23, 54, 91, 98	0
1	B	97/100 (97%)	0.68	7 (7%) 21 23	20, 43, 66, 89	0
1	C	97/100 (97%)	0.88	13 (13%) 7 7	33, 50, 83, 101	0
1	D	74/100 (74%)	0.88	10 (13%) 7 7	18, 50, 79, 89	0
All	All	368/400 (92%)	0.85	42 (11%) 10 10	18, 49, 84, 101	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	TYR	7.0
1	B	30	LYS	5.6
1	A	53	THR	5.2
1	B	31	ASN	4.7
1	C	71	ASP	4.5
1	B	5	TYR	4.4
1	A	68	ALA	4.4
1	D	50	LEU	4.2
1	C	68	ALA	4.2
1	A	66	LEU	4.1
1	D	96	GLU	4.0
1	D	47	ASN	3.7
1	C	72	GLY	3.6
1	B	70	HIS	3.3
1	A	102	SER	3.3
1	C	100	GLN	3.3
1	B	29	VAL	3.2
1	D	4	CYS	3.1
1	D	48	HIS	3.0
1	D	73	ARG	2.8
1	D	90	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	70	HIS	2.7
1	A	52	ASP	2.7
1	B	100	GLN	2.7
1	C	60	ASP	2.6
1	C	6	THR	2.6
1	A	3	ASP	2.6
1	A	67	ASP	2.6
1	C	69	ASN	2.5
1	A	101	SER	2.5
1	A	38	PHE	2.5
1	A	54	GLY	2.5
1	D	94	ILE	2.4
1	C	67	ASP	2.3
1	A	51	SER	2.2
1	D	46	LEU	2.2
1	D	5	TYR	2.2
1	A	70	HIS	2.2
1	C	101	SER	2.2
1	C	40	GLU	2.1
1	B	4	CYS	2.1
1	C	13	ILE	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.