



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:03 AM GMT

PDB ID : 3NXA
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

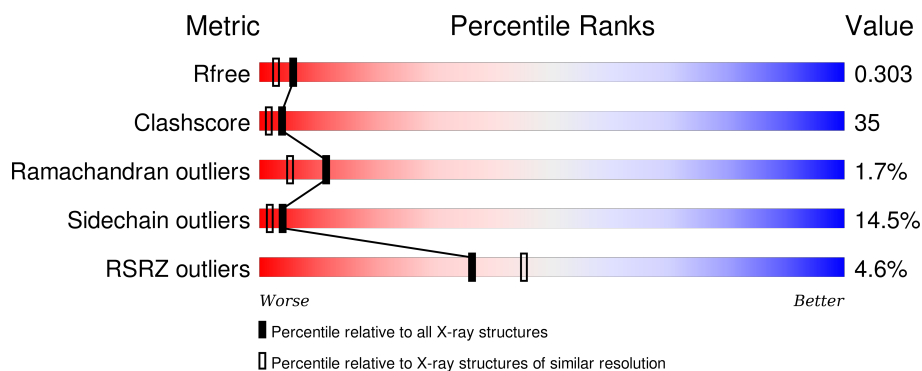
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	100	 3% 17% 45% 29% 9%
1	B	100	 3% 16% 44% 30% 7% •
1	C	100	 7% 16% 51% 20% 10% •
1	D	100	 4% 14% 29% 28% • 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			

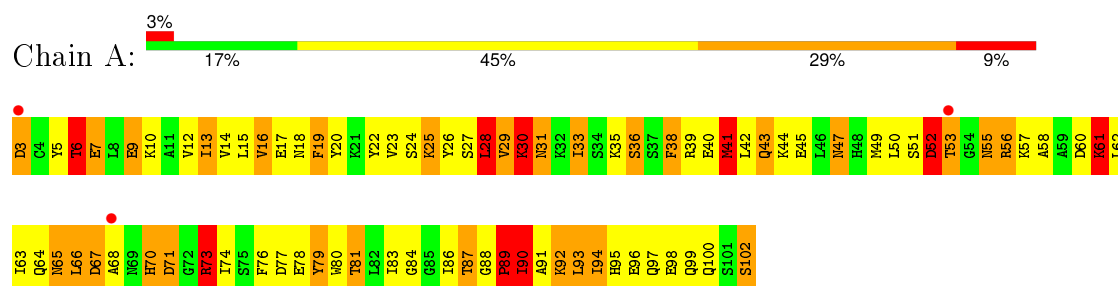
- Molecule 2 is water.

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		

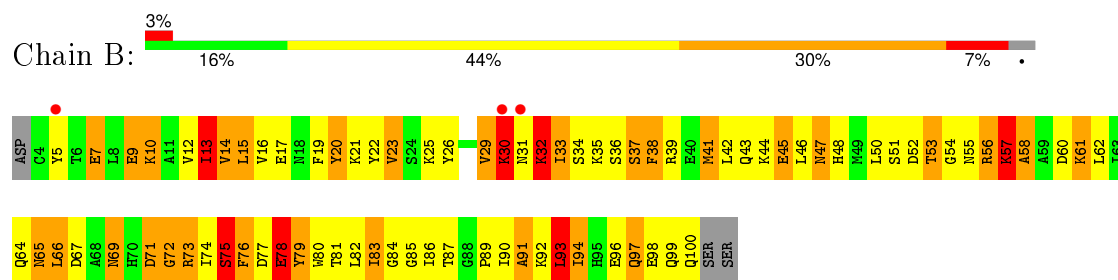
3 Residue-property plots

These plots are drawn for all protein, RNA 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 ($RSRZ > 2$). 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.

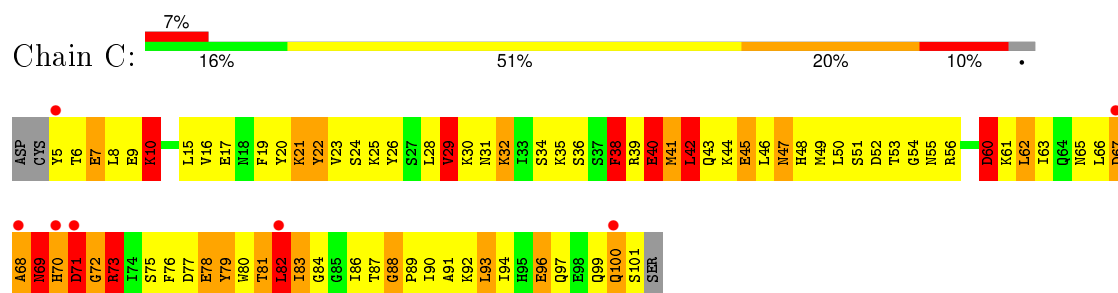
• Molecule 1: Protein S100-A16



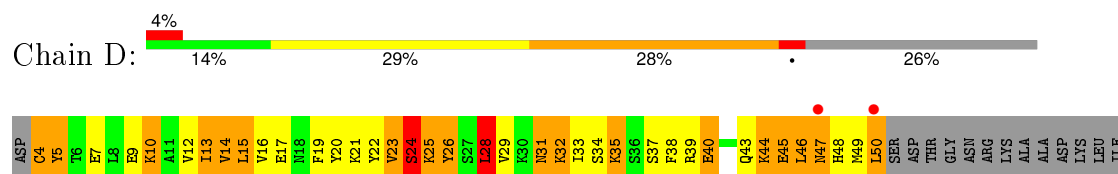
• Molecule 1: Protein S100-A16

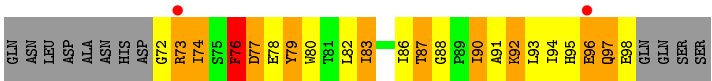


• Molecule 1: Protein S100-A16



• Molecule 1: Protein S100-A16





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 39.14 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.8 (39.15-2.10) 91.9 (39.14-2.10)	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 (9.98%)	DCC
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 , 50.4	EDS
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 29212 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	3.29	93/821 (11.3%)	2.18	33/1103 (3.0%)
1	B	3.39	102/801 (12.7%)	2.52	51/1076 (4.7%)
1	C	3.55	121/801 (15.1%)	2.19	31/1076 (2.9%)
1	D	3.28	79/621 (12.7%)	2.30	31/832 (3.7%)
All	All	3.39	395/3044 (13.0%)	2.30	146/4087 (3.6%)

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 (395) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	GLU	CG-CD	20.09	1.82	1.51
1	A	19	PHE	CB-CG	15.07	1.76	1.51
1	B	45	GLU	CG-CD	14.94	1.74	1.51
1	B	72	GLY	CA-C	14.78	1.75	1.51
1	A	79	TYR	CD2-CE2	14.48	1.61	1.39
1	C	60	ASP	CB-CG	14.36	1.81	1.51
1	C	96	GLU	CB-CG	14.09	1.78	1.52
1	B	91	ALA	CA-CB	14.02	1.81	1.52
1	D	79	TYR	CE1-CZ	-13.76	1.20	1.38
1	C	26	TYR	CG-CD1	12.62	1.55	1.39
1	C	71	ASP	CB-CG	12.62	1.78	1.51
1	A	80	TRP	CE3-CZ3	12.59	1.59	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	13	ILE	CA-CB	12.31	1.83	1.54
1	C	5	TYR	CG-CD2	12.19	1.54	1.39
1	C	26	TYR	CD2-CE2	12.00	1.57	1.39
1	A	31	ASN	CB-CG	11.47	1.77	1.51
1	B	76	PHE	CE2-CZ	11.16	1.58	1.37
1	B	29	VAL	C-O	11.03	1.44	1.23
1	B	5	TYR	CE1-CZ	10.82	1.52	1.38
1	C	26	TYR	CE2-CZ	10.79	1.52	1.38
1	B	80	TRP	CG-CD1	10.71	1.51	1.36
1	D	4	CYS	C-O	10.51	1.43	1.23
1	B	58	ALA	CA-CB	10.49	1.74	1.52
1	A	91	ALA	N-CA	-10.41	1.25	1.46
1	C	80	TRP	CZ3-CH2	10.31	1.56	1.40
1	B	97	GLN	N-CA	10.09	1.66	1.46
1	A	22	TYR	CD1-CE1	10.06	1.54	1.39
1	A	15	LEU	CG-CD2	-10.02	1.14	1.51
1	B	13	ILE	CA-CB	9.96	1.77	1.54
1	C	5	TYR	CD1-CE1	9.91	1.54	1.39
1	A	98	GLU	CD-OE1	9.88	1.36	1.25
1	C	9	GLU	CG-CD	9.82	1.66	1.51
1	D	29	VAL	N-CA	9.81	1.66	1.46
1	B	57	LYS	CD-CE	9.78	1.75	1.51
1	D	78	GLU	CG-CD	9.71	1.66	1.51
1	B	14	VAL	N-CA	9.68	1.65	1.46
1	C	38	PHE	CG-CD1	-9.66	1.24	1.38
1	D	10	LYS	C-O	9.64	1.41	1.23
1	D	79	TYR	CG-CD2	-9.63	1.26	1.39
1	B	51	SER	CB-OG	9.57	1.54	1.42
1	C	34	SER	CB-OG	9.57	1.54	1.42
1	D	28	LEU	CG-CD2	9.53	1.87	1.51
1	A	93	LEU	CG-CD1	9.46	1.86	1.51
1	A	29	VAL	CB-CG2	-9.44	1.33	1.52
1	C	36	SER	CA-CB	9.32	1.67	1.52
1	D	80	TRP	CD1-NE1	-9.32	1.22	1.38
1	C	75	SER	CB-OG	9.31	1.54	1.42
1	C	87	THR	N-CA	-9.29	1.27	1.46
1	A	79	TYR	CB-CG	9.26	1.65	1.51
1	B	78	GLU	CD-OE1	9.23	1.35	1.25
1	B	38	PHE	CD1-CE1	9.15	1.57	1.39
1	D	26	TYR	N-CA	9.14	1.64	1.46
1	C	67	ASP	C-O	9.13	1.40	1.23
1	A	13	ILE	CA-CB	9.07	1.75	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	GLU	CD-OE1	9.05	1.35	1.25
1	B	45	GLU	CD-OE1	9.04	1.35	1.25
1	D	40	GLU	CG-CD	8.99	1.65	1.51
1	A	78	GLU	CG-CD	8.94	1.65	1.51
1	C	32	LYS	CG-CD	-8.95	1.22	1.52
1	C	26	TYR	CG-CD2	-8.94	1.27	1.39
1	C	17	GLU	CB-CG	8.88	1.69	1.52
1	D	78	GLU	CB-CG	8.88	1.69	1.52
1	B	7	GLU	CG-CD	8.86	1.65	1.51
1	B	79	TYR	CE1-CZ	-8.86	1.27	1.38
1	D	76	PHE	CG-CD1	8.77	1.51	1.38
1	A	9	GLU	C-O	8.72	1.40	1.23
1	B	23	VAL	CB-CG2	8.65	1.71	1.52
1	B	75	SER	N-CA	8.63	1.63	1.46
1	B	5	TYR	CG-CD2	8.60	1.50	1.39
1	D	35	LYS	CB-CG	8.60	1.75	1.52
1	D	73	ARG	CG-CD	8.58	1.73	1.51
1	C	32	LYS	C-O	8.54	1.39	1.23
1	B	29	VAL	C-N	8.53	1.53	1.34
1	A	78	GLU	CD-OE1	8.48	1.34	1.25
1	A	96	GLU	CB-CG	8.48	1.68	1.52
1	D	91	ALA	CA-CB	-8.42	1.34	1.52
1	A	58	ALA	CA-CB	8.40	1.70	1.52
1	B	61	LYS	CG-CD	8.35	1.80	1.52
1	C	10	LYS	CE-NZ	8.35	1.70	1.49
1	D	40	GLU	CD-OE1	8.35	1.34	1.25
1	C	20	TYR	CD1-CE1	8.33	1.51	1.39
1	A	40	GLU	CG-CD	8.32	1.64	1.51
1	D	76	PHE	CG-CD2	-8.31	1.26	1.38
1	B	5	TYR	CD1-CE1	8.29	1.51	1.39
1	C	39	ARG	CZ-NH1	8.23	1.43	1.33
1	B	75	SER	CA-CB	8.16	1.65	1.52
1	C	78	GLU	CD-OE1	8.08	1.34	1.25
1	D	16	VAL	CA-CB	-8.07	1.37	1.54
1	B	12	VAL	CA-CB	-8.07	1.37	1.54
1	D	20	TYR	CG-CD1	8.06	1.49	1.39
1	A	44	LYS	CD-CE	8.04	1.71	1.51
1	D	16	VAL	CB-CG1	8.03	1.69	1.52
1	D	45	GLU	CD-OE2	7.98	1.34	1.25
1	C	5	TYR	CE2-CZ	7.98	1.49	1.38
1	B	47	ASN	CB-CG	7.97	1.69	1.51
1	C	26	TYR	CD1-CE1	7.96	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	TYR	CE2-CZ	7.94	1.48	1.38
1	D	24	SER	N-CA	7.88	1.62	1.46
1	B	64	GLN	C-O	-7.87	1.08	1.23
1	C	79	TYR	CG-CD2	-7.86	1.28	1.39
1	A	24	SER	N-CA	7.80	1.61	1.46
1	A	35	LYS	CB-CG	7.78	1.73	1.52
1	B	78	GLU	CD-OE2	7.78	1.34	1.25
1	C	40	GLU	CD-OE1	7.71	1.34	1.25
1	C	62	LEU	CG-CD2	7.71	1.80	1.51
1	A	89	PRO	CA-C	7.68	1.68	1.52
1	D	50	LEU	CA-C	7.68	1.73	1.52
1	D	90	ILE	CA-C	-7.67	1.33	1.52
1	A	6	THR	CB-CG2	-7.66	1.27	1.52
1	A	19	PHE	CE2-CZ	7.61	1.51	1.37
1	C	5	TYR	CE1-CZ	7.59	1.48	1.38
1	D	15	LEU	CA-CB	7.58	1.71	1.53
1	B	34	SER	C-O	7.55	1.37	1.23
1	B	22	TYR	CD2-CE2	7.51	1.50	1.39
1	C	67	ASP	CA-C	7.49	1.72	1.52
1	C	26	TYR	CE1-CZ	-7.46	1.28	1.38
1	B	81	THR	N-CA	7.44	1.61	1.46
1	C	5	TYR	CG-CD1	7.44	1.48	1.39
1	C	79	TYR	CG-CD1	7.41	1.48	1.39
1	A	96	GLU	CD-OE1	7.40	1.33	1.25
1	B	98	GLU	CD-OE1	7.40	1.33	1.25
1	B	92	LYS	CE-NZ	7.35	1.67	1.49
1	D	15	LEU	C-O	-7.26	1.09	1.23
1	B	7	GLU	CB-CG	-7.25	1.38	1.52
1	A	12	VAL	CA-CB	7.23	1.70	1.54
1	C	36	SER	CB-OG	7.22	1.51	1.42
1	C	100	GLN	CG-CD	7.20	1.67	1.51
1	D	35	LYS	N-CA	7.20	1.60	1.46
1	B	51	SER	C-O	-7.17	1.09	1.23
1	D	5	TYR	CG-CD2	7.17	1.48	1.39
1	C	30	LYS	CD-CE	7.13	1.69	1.51
1	A	27	SER	CA-CB	7.12	1.63	1.52
1	D	33	ILE	C-O	7.11	1.36	1.23
1	C	45	GLU	CB-CG	7.11	1.65	1.52
1	B	41	MET	C-O	7.10	1.36	1.23
1	D	16	VAL	C-O	-7.09	1.09	1.23
1	C	40	GLU	CD-OE2	7.08	1.33	1.25
1	D	73	ARG	N-CA	7.05	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	THR	CB-CG2	-7.04	1.29	1.52
1	B	87	THR	CA-CB	7.04	1.71	1.53
1	B	19	PHE	C-O	7.03	1.36	1.23
1	A	39	ARG	CZ-NH1	7.01	1.42	1.33
1	D	20	TYR	CE1-CZ	-7.01	1.29	1.38
1	D	26	TYR	CE2-CZ	-7.00	1.29	1.38
1	A	40	GLU	C-O	6.99	1.36	1.23
1	C	49	MET	C-O	-6.98	1.10	1.23
1	A	36	SER	C-O	6.95	1.36	1.23
1	A	90	ILE	N-CA	-6.94	1.32	1.46
1	B	45	GLU	CB-CG	6.92	1.65	1.52
1	B	22	TYR	CG-CD1	6.91	1.48	1.39
1	A	29	VAL	N-CA	6.89	1.60	1.46
1	B	26	TYR	CE1-CZ	6.88	1.47	1.38
1	C	53	THR	C-O	6.88	1.36	1.23
1	B	58	ALA	N-CA	6.88	1.60	1.46
1	C	16	VAL	CB-CG2	6.87	1.67	1.52
1	B	91	ALA	C-O	6.85	1.36	1.23
1	A	102	SER	N-CA	6.84	1.60	1.46
1	A	76	PHE	CD2-CE2	6.83	1.52	1.39
1	A	70	HIS	CA-CB	6.82	1.69	1.53
1	B	97	GLN	C-O	-6.82	1.10	1.23
1	A	33	ILE	CA-CB	-6.80	1.39	1.54
1	C	16	VAL	CB-CG1	6.80	1.67	1.52
1	D	80	TRP	CD2-CE2	-6.80	1.33	1.41
1	D	17	GLU	CA-C	-6.79	1.35	1.52
1	B	78	GLU	C-O	-6.77	1.10	1.23
1	A	28	LEU	N-CA	6.76	1.59	1.46
1	A	3	ASP	CB-CG	6.74	1.65	1.51
1	C	79	TYR	CB-CG	6.72	1.61	1.51
1	B	5	TYR	CD2-CE2	6.71	1.49	1.39
1	C	71	ASP	CA-CB	6.71	1.68	1.53
1	C	93	LEU	N-CA	-6.71	1.32	1.46
1	A	81	THR	CB-CG2	6.71	1.74	1.52
1	D	16	VAL	CA-C	6.70	1.70	1.52
1	B	84	GLY	CA-C	-6.69	1.41	1.51
1	C	24	SER	C-O	-6.68	1.10	1.23
1	B	93	LEU	CG-CD1	6.66	1.76	1.51
1	A	94	ILE	CA-C	6.64	1.70	1.52
1	A	90	ILE	CA-CB	-6.63	1.39	1.54
1	D	19	PHE	CG-CD1	-6.62	1.28	1.38
1	C	29	VAL	CB-CG1	-6.59	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	17	GLU	CG-CD	6.59	1.61	1.51
1	B	33	ILE	C-O	6.58	1.35	1.23
1	A	30	LYS	CD-CE	-6.57	1.34	1.51
1	A	20	TYR	CG-CD1	6.57	1.47	1.39
1	C	87	THR	CA-C	6.56	1.70	1.52
1	C	55	ASN	CB-CG	6.55	1.66	1.51
1	A	70	HIS	N-CA	6.54	1.59	1.46
1	B	84	GLY	N-CA	-6.51	1.36	1.46
1	C	86	ILE	C-O	6.50	1.35	1.23
1	C	80	TRP	CE2-CZ2	6.47	1.50	1.39
1	C	60	ASP	CG-OD2	6.46	1.40	1.25
1	B	30	LYS	C-N	6.45	1.48	1.34
1	C	65	ASN	CB-CG	6.45	1.65	1.51
1	B	17	GLU	C-O	6.45	1.35	1.23
1	C	80	TRP	CG-CD1	6.45	1.45	1.36
1	A	64	GLN	CG-CD	6.44	1.65	1.51
1	C	65	ASN	CG-ND2	6.44	1.49	1.32
1	A	38	PHE	CE2-CZ	6.44	1.49	1.37
1	B	9	GLU	CB-CG	-6.44	1.40	1.52
1	B	92	LYS	CD-CE	6.43	1.67	1.51
1	C	79	TYR	N-CA	6.43	1.59	1.46
1	A	7	GLU	CD-OE2	6.42	1.32	1.25
1	B	90	ILE	CB-CG1	-6.39	1.36	1.54
1	A	27	SER	CB-OG	6.37	1.50	1.42
1	A	30	LYS	CE-NZ	-6.36	1.33	1.49
1	C	21	LYS	CE-NZ	6.35	1.65	1.49
1	A	23	VAL	C-O	6.34	1.35	1.23
1	D	31	ASN	CB-CG	6.33	1.65	1.51
1	B	22	TYR	C-O	6.33	1.35	1.23
1	A	25	LYS	CD-CE	6.33	1.67	1.51
1	D	80	TRP	C-O	6.32	1.35	1.23
1	B	47	ASN	C-O	6.31	1.35	1.23
1	D	17	GLU	CB-CG	-6.31	1.40	1.52
1	A	61	LYS	CE-NZ	6.31	1.64	1.49
1	D	26	TYR	CA-CB	6.30	1.67	1.53
1	A	36	SER	CA-CB	6.29	1.62	1.52
1	A	10	LYS	N-CA	6.28	1.58	1.46
1	A	7	GLU	CB-CG	-6.28	1.40	1.52
1	D	13	ILE	N-CA	-6.28	1.33	1.46
1	C	81	THR	C-O	-6.26	1.11	1.23
1	C	88	GLY	N-CA	-6.25	1.36	1.46
1	B	14	VAL	CA-CB	-6.24	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	HIS	CA-CB	-6.20	1.40	1.53
1	A	91	ALA	C-O	6.20	1.35	1.23
1	C	44	LYS	CE-NZ	6.19	1.64	1.49
1	C	47	ASN	CB-CG	6.18	1.65	1.51
1	D	47	ASN	CB-CG	6.16	1.65	1.51
1	A	35	LYS	CD-CE	6.14	1.66	1.51
1	C	45	GLU	N-CA	-6.13	1.34	1.46
1	B	41	MET	CA-CB	6.12	1.67	1.53
1	A	88	GLY	CA-C	6.11	1.61	1.51
1	D	83	ILE	CA-CB	-6.11	1.40	1.54
1	A	5	TYR	CD2-CE2	6.10	1.48	1.39
1	D	79	TYR	C-O	6.09	1.34	1.23
1	C	97	GLN	CA-CB	-6.07	1.40	1.53
1	C	20	TYR	CE2-CZ	6.07	1.46	1.38
1	A	57	LYS	CB-CG	6.05	1.68	1.52
1	B	39	ARG	NE-CZ	6.04	1.40	1.33
1	B	7	GLU	CD-OE2	6.02	1.32	1.25
1	C	5	TYR	CA-CB	6.01	1.67	1.53
1	C	79	TYR	C-O	-6.00	1.11	1.23
1	C	87	THR	CA-CB	5.99	1.69	1.53
1	C	96	GLU	CG-CD	5.99	1.60	1.51
1	A	73	ARG	C-O	5.97	1.34	1.23
1	B	51	SER	CA-CB	5.97	1.61	1.52
1	D	40	GLU	C-O	5.95	1.34	1.23
1	A	26	TYR	CE2-CZ	-5.94	1.30	1.38
1	C	93	LEU	C-O	5.94	1.34	1.23
1	A	30	LYS	CG-CD	5.92	1.72	1.52
1	D	28	LEU	N-CA	5.92	1.58	1.46
1	D	78	GLU	CD-OE2	-5.92	1.19	1.25
1	C	23	VAL	CA-CB	-5.92	1.42	1.54
1	C	39	ARG	CG-CD	5.91	1.66	1.51
1	B	75	SER	CB-OG	-5.90	1.34	1.42
1	D	23	VAL	CB-CG1	5.88	1.65	1.52
1	B	83	ILE	CB-CG1	5.88	1.70	1.54
1	A	25	LYS	CE-NZ	5.87	1.63	1.49
1	C	99	GLN	CA-C	5.86	1.68	1.52
1	C	29	VAL	CA-CB	-5.85	1.42	1.54
1	D	86	ILE	CA-CB	5.83	1.68	1.54
1	B	54	GLY	CA-C	5.82	1.61	1.51
1	D	96	GLU	CG-CD	5.82	1.60	1.51
1	D	21	LYS	CE-NZ	5.82	1.63	1.49
1	C	94	ILE	C-O	5.82	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	THR	CB-OG1	5.81	1.54	1.43
1	D	80	TRP	CE3-CZ3	-5.79	1.28	1.38
1	B	21	LYS	CD-CE	5.78	1.65	1.51
1	D	38	PHE	CG-CD2	5.78	1.47	1.38
1	D	96	GLU	CD-OE2	5.78	1.32	1.25
1	C	91	ALA	C-O	5.77	1.34	1.23
1	C	43	GLN	CD-OE1	5.77	1.36	1.24
1	C	72	GLY	CA-C	5.76	1.61	1.51
1	B	61	LYS	CD-CE	5.74	1.65	1.51
1	B	62	LEU	CG-CD1	5.74	1.73	1.51
1	C	60	ASP	CA-C	5.74	1.67	1.52
1	D	25	LYS	CD-CE	5.74	1.65	1.51
1	B	76	PHE	CD2-CE2	5.72	1.50	1.39
1	D	20	TYR	CE2-CZ	5.72	1.46	1.38
1	D	45	GLU	CB-CG	5.71	1.63	1.52
1	B	60	ASP	CG-OD1	5.71	1.38	1.25
1	D	38	PHE	CD2-CE2	-5.70	1.27	1.39
1	B	26	TYR	CD2-CE2	5.68	1.47	1.39
1	A	96	GLU	CD-OE2	5.68	1.31	1.25
1	C	30	LYS	CA-C	5.68	1.67	1.52
1	A	39	ARG	CG-CD	5.68	1.66	1.51
1	C	70	HIS	C-O	5.67	1.34	1.23
1	D	38	PHE	CE1-CZ	5.67	1.48	1.37
1	C	68	ALA	CA-CB	5.65	1.64	1.52
1	B	15	LEU	C-O	5.64	1.34	1.23
1	C	82	LEU	N-CA	-5.64	1.35	1.46
1	A	17	GLU	CA-CB	5.64	1.66	1.53
1	A	19	PHE	N-CA	-5.64	1.35	1.46
1	D	12	VAL	CB-CG1	-5.63	1.41	1.52
1	A	33	ILE	CB-CG2	5.63	1.70	1.52
1	C	10	LYS	C-O	5.62	1.34	1.23
1	C	19	PHE	CD1-CE1	-5.62	1.28	1.39
1	A	65	ASN	CB-CG	5.61	1.64	1.51
1	C	38	PHE	C-O	5.60	1.33	1.23
1	A	47	ASN	CB-CG	-5.60	1.38	1.51
1	B	47	ASN	N-CA	-5.58	1.35	1.46
1	C	35	LYS	N-CA	5.58	1.57	1.46
1	B	64	GLN	N-CA	5.57	1.57	1.46
1	C	68	ALA	C-O	5.57	1.33	1.23
1	C	39	ARG	CB-CG	5.56	1.67	1.52
1	A	99	GLN	CG-CD	5.55	1.63	1.51
1	C	92	LYS	CE-NZ	5.55	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	77	ASP	CB-CG	5.54	1.63	1.51
1	A	57	LYS	CD-CE	5.53	1.65	1.51
1	B	76	PHE	CG-CD1	5.53	1.47	1.38
1	C	54	GLY	CA-C	5.51	1.60	1.51
1	B	52	ASP	CG-OD1	5.50	1.38	1.25
1	B	73	ARG	CG-CD	-5.50	1.38	1.51
1	C	73	ARG	CG-CD	-5.50	1.38	1.51
1	C	20	TYR	CE1-CZ	-5.49	1.31	1.38
1	A	80	TRP	CZ2-CH2	5.47	1.47	1.37
1	D	80	TRP	CB-CG	5.47	1.60	1.50
1	A	5	TYR	CG-CD2	5.47	1.46	1.39
1	A	96	GLU	CG-CD	5.47	1.60	1.51
1	B	96	GLU	CD-OE1	5.46	1.31	1.25
1	D	78	GLU	CA-CB	-5.45	1.42	1.53
1	B	10	LYS	CB-CG	-5.45	1.37	1.52
1	B	77	ASP	C-O	5.45	1.33	1.23
1	D	26	TYR	CA-C	-5.45	1.38	1.52
1	B	56	ARG	N-CA	-5.44	1.35	1.46
1	B	79	TYR	CG-CD1	-5.44	1.32	1.39
1	C	77	ASP	C-O	-5.43	1.13	1.23
1	C	5	TYR	CD2-CE2	5.43	1.47	1.39
1	B	69	ASN	CB-CG	-5.42	1.38	1.51
1	D	31	ASN	CG-ND2	5.42	1.46	1.32
1	C	86	ILE	N-CA	-5.41	1.35	1.46
1	C	25	LYS	CD-CE	5.40	1.64	1.51
1	A	14	VAL	CB-CG2	-5.40	1.41	1.52
1	D	43	GLN	CG-CD	-5.39	1.38	1.51
1	C	7	GLU	CB-CG	5.39	1.62	1.52
1	C	35	LYS	CE-NZ	5.38	1.62	1.49
1	D	37	SER	CB-OG	-5.38	1.35	1.42
1	B	76	PHE	CE1-CZ	-5.36	1.27	1.37
1	B	85	GLY	N-CA	5.36	1.54	1.46
1	A	92	LYS	CE-NZ	5.35	1.62	1.49
1	C	79	TYR	CZ-OH	5.34	1.47	1.37
1	C	76	PHE	CB-CG	-5.34	1.42	1.51
1	C	76	PHE	CA-C	5.33	1.66	1.52
1	B	19	PHE	CD2-CE2	5.33	1.50	1.39
1	D	82	LEU	CG-CD1	5.33	1.71	1.51
1	B	15	LEU	N-CA	5.33	1.57	1.46
1	D	72	GLY	N-CA	5.32	1.54	1.46
1	D	98	GLU	CG-CD	5.32	1.59	1.51
1	A	71	ASP	C-O	5.31	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	10	LYS	CG-CD	5.31	1.70	1.52
1	D	96	GLU	CD-OE1	5.30	1.31	1.25
1	A	16	VAL	CB-CG2	-5.30	1.41	1.52
1	A	68	ALA	CA-CB	5.29	1.63	1.52
1	C	92	LYS	CD-CE	5.28	1.64	1.51
1	B	5	TYR	CZ-OH	5.27	1.46	1.37
1	B	96	GLU	CD-OE2	5.27	1.31	1.25
1	C	99	GLN	CB-CG	-5.27	1.38	1.52
1	A	13	ILE	C-O	5.25	1.33	1.23
1	A	79	TYR	CZ-OH	-5.25	1.28	1.37
1	B	44	LYS	C-O	-5.24	1.13	1.23
1	B	78	GLU	CB-CG	5.24	1.62	1.52
1	C	86	ILE	CB-CG1	-5.24	1.39	1.54
1	C	78	GLU	CG-CD	5.20	1.59	1.51
1	B	45	GLU	CD-OE2	5.19	1.31	1.25
1	A	67	ASP	N-CA	5.19	1.56	1.46
1	B	82	LEU	CG-CD2	-5.18	1.32	1.51
1	C	86	ILE	CA-CB	5.18	1.66	1.54
1	A	45	GLU	CD-OE2	5.17	1.31	1.25
1	B	37	SER	CA-CB	5.17	1.60	1.52
1	C	83	ILE	CA-C	5.17	1.66	1.52
1	A	62	LEU	CG-CD1	5.16	1.71	1.51
1	C	73	ARG	CB-CG	5.16	1.66	1.52
1	A	18	ASN	CG-OD1	5.15	1.35	1.24
1	C	97	GLN	CA-C	-5.15	1.39	1.52
1	D	88	GLY	CA-C	5.15	1.60	1.51
1	B	35	LYS	CE-NZ	-5.15	1.36	1.49
1	C	5	TYR	N-CA	5.14	1.56	1.46
1	A	31	ASN	CA-CB	5.14	1.66	1.53
1	D	39	ARG	NE-CZ	5.12	1.39	1.33
1	C	19	PHE	CB-CG	5.12	1.60	1.51
1	B	56	ARG	CD-NE	-5.12	1.37	1.46
1	A	89	PRO	CB-CG	5.11	1.75	1.50
1	C	63	ILE	CA-C	-5.11	1.39	1.52
1	C	23	VAL	CB-CG1	5.10	1.63	1.52
1	D	35	LYS	CA-CB	-5.08	1.42	1.53
1	B	9	GLU	CG-CD	5.07	1.59	1.51
1	C	84	GLY	N-CA	5.07	1.53	1.46
1	A	86	ILE	CA-C	-5.07	1.39	1.52
1	B	19	PHE	CB-CG	5.05	1.59	1.51
1	D	21	LYS	CA-C	-5.04	1.39	1.52
1	B	20	TYR	CZ-OH	-5.04	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	TYR	CB-CG	5.04	1.59	1.51
1	B	65	ASN	CG-ND2	5.03	1.45	1.32
1	C	35	LYS	CG-CD	5.02	1.69	1.52
1	D	92	LYS	N-CA	5.02	1.56	1.46
1	D	97	GLN	CB-CG	-5.01	1.39	1.52

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	ARG	NE-CZ-NH1	-21.62	109.49	120.30
1	B	60	ASP	CB-CG-OD1	13.84	130.75	118.30
1	B	30	LYS	O-C-N	-13.31	101.40	122.70
1	D	77	ASP	CB-CG-OD1	12.77	129.79	118.30
1	B	45	GLU	OE1-CD-OE2	-11.76	109.19	123.30
1	B	56	ARG	NE-CZ-NH2	11.13	125.86	120.30
1	C	39	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	60	ASP	CB-CG-OD1	10.49	127.74	118.30
1	D	93	LEU	CB-CG-CD1	-10.41	93.30	111.00
1	A	66	LEU	CB-CG-CD1	10.26	128.44	111.00
1	B	77	ASP	CB-CG-OD1	10.21	127.49	118.30
1	A	55	ASN	O-C-N	-10.13	106.50	122.70
1	B	60	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	C	73	ARG	NE-CZ-NH2	9.74	125.17	120.30
1	A	67	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	C	67	ASP	CB-CG-OD1	-9.58	109.68	118.30
1	D	78	GLU	OE1-CD-OE2	-9.55	111.84	123.30
1	B	30	LYS	CA-C-N	-9.40	96.51	117.20
1	B	75	SER	CB-CA-C	-9.27	92.49	110.10
1	C	90	ILE	CG1-CB-CG2	-9.24	91.06	111.40
1	D	25	LYS	C-N-CA	-9.06	99.04	121.70
1	C	41	MET	CG-SD-CE	-9.00	85.80	100.20
1	A	55	ASN	CA-C-O	8.50	137.96	120.10
1	A	77	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	B	30	LYS	CA-C-O	8.38	137.71	120.10
1	A	28	LEU	CA-CB-CG	8.02	133.75	115.30
1	B	66	LEU	CB-CG-CD2	-7.98	97.43	111.00
1	C	5	TYR	C-N-CA	7.86	141.36	121.70
1	B	94	ILE	CA-CB-CG1	-7.75	96.27	111.00
1	C	87	THR	CA-CB-CG2	-7.71	101.60	112.40
1	A	17	GLU	OE1-CD-OE2	-7.62	114.16	123.30
1	C	5	TYR	N-CA-C	-7.61	90.47	111.00
1	A	66	LEU	CB-CG-CD2	-7.60	98.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	MET	CG-SD-CE	7.53	112.25	100.20
1	B	53	THR	OG1-CB-CG2	-7.47	92.83	110.00
1	B	77	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	C	97	GLN	CB-CA-C	-7.41	95.58	110.40
1	D	15	LEU	CB-CG-CD1	-7.40	98.42	111.00
1	A	17	GLU	CA-CB-CG	-7.36	97.20	113.40
1	D	73	ARG	CD-NE-CZ	7.36	133.91	123.60
1	A	19	PHE	CG-CD2-CE2	7.32	128.86	120.80
1	B	97	GLN	N-CA-CB	7.31	123.76	110.60
1	B	25	LYS	CD-CE-NZ	-7.29	94.94	111.70
1	C	60	ASP	CB-CG-OD2	7.22	124.80	118.30
1	C	63	ILE	CG1-CB-CG2	-7.18	95.60	111.40
1	D	46	LEU	CB-CG-CD2	-7.16	98.82	111.00
1	A	90	ILE	CA-CB-CG2	7.14	125.19	110.90
1	D	29	VAL	CA-CB-CG1	7.12	121.58	110.90
1	A	60	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	C	28	LEU	CB-CG-CD2	6.99	122.88	111.00
1	D	49	MET	CG-SD-CE	-6.98	89.03	100.20
1	C	40	GLU	OE1-CD-OE2	-6.97	114.93	123.30
1	B	15	LEU	CA-CB-CG	-6.93	99.36	115.30
1	D	79	TYR	CG-CD1-CE1	-6.92	115.76	121.30
1	C	93	LEU	CB-CG-CD2	-6.91	99.26	111.00
1	A	52	ASP	CA-C-O	-6.86	105.69	120.10
1	B	66	LEU	CB-CG-CD1	6.85	122.65	111.00
1	A	92	LYS	CD-CE-NZ	6.83	127.42	111.70
1	C	67	ASP	N-CA-C	6.82	129.41	111.00
1	B	39	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	B	29	VAL	C-N-CA	-6.71	104.92	121.70
1	B	51	SER	CA-CB-OG	-6.70	93.11	111.20
1	D	79	TYR	CZ-CE2-CD2	-6.67	113.79	119.80
1	B	52	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	C	92	LYS	CB-CA-C	6.67	123.73	110.40
1	C	73	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	D	26	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	D	25	LYS	O-C-N	-6.59	112.16	122.70
1	B	37	SER	CB-CA-C	-6.55	97.66	110.10
1	A	78	GLU	N-CA-CB	-6.54	98.83	110.60
1	B	35	LYS	CB-CG-CD	-6.53	94.63	111.60
1	D	73	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	D	79	TYR	CD1-CE1-CZ	6.51	125.66	119.80
1	C	96	GLU	OE1-CD-OE2	-6.51	115.49	123.30
1	A	73	ARG	NE-CZ-NH2	6.50	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	5	TYR	CZ-CE2-CD2	-6.44	114.01	119.80
1	A	29	VAL	C-N-CA	-6.42	105.66	121.70
1	C	40	GLU	N-CA-CB	6.41	122.14	110.60
1	D	28	LEU	CB-CG-CD1	-6.39	100.13	111.00
1	C	83	ILE	CA-CB-CG1	-6.35	98.93	111.00
1	B	67	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	39	ARG	NE-CZ-NH2	6.31	123.46	120.30
1	A	52	ASP	N-CA-CB	6.29	121.91	110.60
1	C	23	VAL	CG1-CB-CG2	-6.26	100.89	110.90
1	B	7	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	B	93	LEU	CB-CG-CD1	6.25	121.63	111.00
1	A	62	LEU	CA-CB-CG	6.25	129.67	115.30
1	B	12	VAL	CA-CB-CG2	-6.24	101.54	110.90
1	C	42	LEU	CB-CG-CD1	-6.18	100.50	111.00
1	C	21	LYS	CD-CE-NZ	-6.16	97.54	111.70
1	B	32	LYS	N-CA-C	6.12	127.53	111.00
1	D	80	TRP	CD1-NE1-CE2	6.10	114.49	109.00
1	A	93	LEU	CB-CG-CD2	-6.10	100.64	111.00
1	B	65	ASN	CB-CA-C	-6.07	98.25	110.40
1	D	24	SER	N-CA-CB	6.06	119.58	110.50
1	A	79	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	B	29	VAL	N-CA-CB	-6.05	98.20	111.50
1	D	50	LEU	CB-CA-C	6.04	121.68	110.20
1	B	61	LYS	N-CA-CB	-5.97	99.85	110.60
1	D	7	GLU	CA-CB-CG	-5.94	100.33	113.40
1	A	19	PHE	CZ-CE2-CD2	-5.87	113.05	120.10
1	B	36	SER	N-CA-CB	-5.80	101.80	110.50
1	C	68	ALA	N-CA-CB	5.75	118.15	110.10
1	D	87	THR	OG1-CB-CG2	-5.74	96.81	110.00
1	C	82	LEU	CB-CG-CD1	-5.73	101.27	111.00
1	D	32	LYS	CD-CE-NZ	-5.71	98.57	111.70
1	C	63	ILE	N-CA-CB	5.67	123.85	110.80
1	B	76	PHE	CD1-CE1-CZ	5.67	126.90	120.10
1	D	43	GLN	N-CA-C	5.66	126.27	111.00
1	B	16	VAL	CG1-CB-CG2	-5.65	101.85	110.90
1	B	81	THR	CA-CB-OG1	-5.56	97.32	109.00
1	B	32	LYS	CA-CB-CG	5.55	125.61	113.40
1	B	38	PHE	CZ-CE2-CD2	5.52	126.73	120.10
1	B	62	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	B	19	PHE	N-CA-CB	-5.49	100.71	110.60
1	B	64	GLN	CB-CA-C	-5.44	99.51	110.40
1	C	42	LEU	N-CA-CB	-5.42	99.55	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	15	LEU	CD1-CG-CD2	-5.42	94.24	110.50
1	D	96	GLU	CA-CB-CG	5.41	125.30	113.40
1	D	28	LEU	N-CA-CB	-5.40	99.59	110.40
1	A	67	ASP	CB-CG-OD1	5.37	123.14	118.30
1	C	75	SER	CA-CB-OG	-5.36	96.74	111.20
1	D	7	GLU	CB-CA-C	-5.35	99.69	110.40
1	B	39	ARG	CG-CD-NE	-5.33	100.60	111.80
1	B	86	ILE	CG1-CB-CG2	-5.33	99.68	111.40
1	C	61	LYS	N-CA-CB	-5.31	101.05	110.60
1	B	30	LYS	CB-CA-C	5.30	121.00	110.40
1	D	74	ILE	CG1-CB-CG2	-5.30	99.74	111.40
1	A	88	GLY	N-CA-C	5.29	126.32	113.10
1	A	79	TYR	CZ-CE2-CD2	-5.26	115.06	119.80
1	A	6	THR	N-CA-CB	-5.26	100.30	110.30
1	B	41	MET	CG-SD-CE	-5.24	91.82	100.20
1	B	99	GLN	CA-CB-CG	-5.23	101.89	113.40
1	B	45	GLU	CB-CA-C	5.23	120.86	110.40
1	A	10	LYS	CD-CE-NZ	-5.23	99.67	111.70
1	B	10	LYS	CB-CA-C	-5.22	99.95	110.40
1	D	19	PHE	CD1-CE1-CZ	-5.22	113.83	120.10
1	A	84	GLY	C-N-CA	-5.22	111.35	122.30
1	C	39	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	A	94	ILE	CG1-CB-CG2	5.18	122.81	111.40
1	A	45	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	D	26	TYR	N-CA-C	5.13	124.84	111.00
1	C	22	TYR	CG-CD2-CE2	-5.09	117.22	121.30
1	A	52	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	56	ARG	CA-CB-CG	-5.05	102.29	113.40
1	B	45	GLU	CB-CG-CD	-5.03	100.63	114.20

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

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Mol	Chain	Res	Type	Group
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
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	60	0
1	B	788	0	791	69	0
1	C	788	0	791	49	0
1	D	610	0	623	41	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	209	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 35.

All (209) 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:CB	1:B:58:ALA:CA	1.74	1.65
1:D:35:LYS:CB	1:D:35:LYS:CG	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:CE	1:B:57:LYS:CD	1.75	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LEU:CD2	1:C:62:LEU:CG	1.80	1.60
1:B:13:ILE:CB	1:B:13:ILE:CA	1.77	1.59
1:B:61:LYS:CG	1:B:61:LYS:CD	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:D:13:ILE:CB	1:D:13:ILE:CA	1.83	1.57
1:D:90:ILE:CD1	1:D:90:ILE:CG1	1.83	1.57
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:D:28:LEU:CG	1:D:28:LEU:CD2	1.87	1.53
1:B:72:GLY:C	1:B:72:GLY:CA	1.75	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:31:ASN:CG	1:A:31:ASN:CB	1.77	1.52
1:A:93:LEU:CG	1:A:93:LEU:CD1	1.86	1.50
1:C:71:ASP:CG	1:C:71:ASP:CB	1.78	1.49
1:C:60:ASP:CB	1:C:60:ASP:CG	1.81	1.49
1:C:40:GLU:CD	1:C:40:GLU:CG	1.82	1.48
1:A:89:PRO:CG	1:A:89:PRO:CB	1.75	1.48
1:A:51:SER:O	1:A:52:ASP:O	1.62	1.16
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:D:47:ASN:HB3	2:D:116:HOH:O	1.53	1.06
1:C:29:VAL:HG12	1:C:29:VAL:O	1.55	1.04
1:A:93:LEU:H	1:A:93:LEU:HD12	1.27	1.00
1:A:51:SER:C	1:A:52:ASP:O	1.94	0.99
1:A:89:PRO:HD3	2:A:111:HOH:O	1.67	0.93
1:A:6:THR:HG22	1:A:9:GLU:H	1.35	0.92
1:C:38:PHE:HE1	1:C:41:MET:HE1	1.31	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:CB	1:B:61:LYS:CD	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:CG1	1:A:13:ILE:CA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LYS:CA	1:D:35:LYS:CG	2.59	0.80
1:C:38:PHE:CE1	1:C:41:MET:HE1	2.16	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:C:38:PHE:CD1	1:C:41:MET:HE2	2.20	0.77
1:A:90:ILE:HA	1:A:93:LEU:HD13	1.67	0.76
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:CG2	1:A:13:ILE:CA	2.64	0.73
1:C:38:PHE:CE1	1:C:41:MET:CE	2.70	0.73
1:B:7:GLU:OE1	1:B:10:LYS:NZ	2.21	0.73
1:D:25:LYS:O	1:D:26:TYR:CB	2.29	0.73
1:A:81:THR:CG2	1:A:81:THR:CA	2.65	0.72
1:A:93:LEU:H	1:A:93:LEU:CD1	2.02	0.72
1:B:33:ILE:O	1:B:74:ILE:N	2.22	0.72
1:B:13:ILE:CB	1:B:13:ILE:C	2.57	0.71
1:C:38:PHE:HD1	1:C:41:MET:HE2	1.53	0.71
1:B:13:ILE:CA	1:B:13:ILE:CD1	2.67	0.71
1:C:38:PHE:HE1	1:C:41:MET:CE	2.04	0.70
1:C:38:PHE:HE2	1:C:82:LEU:CD1	1.91	0.70
1:A:30:LYS:HB3	2:A:112:HOH:O	1.90	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:58:ALA:CB	1:B:58:ALA:C	2.60	0.68
1:B:23:VAL:CB	1:B:30:LYS:HD3	2.25	0.67
1:B:30:LYS:HZ3	1:B:30:LYS:HB3	1.58	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:CB	1:A:93:LEU:CD1	2.72	0.66
1:B:23:VAL:CG1	1:B:30:LYS:HD3	2.25	0.66
1:B:38:PHE:CE1	1:B:41:MET:HE1	2.31	0.66
1:B:13:ILE:CG1	1:B:13:ILE:CA	2.73	0.65
1:B:61:LYS:CE	1:B:61:LYS:CG	2.73	0.65
1:D:13:ILE:C	1:D:13:ILE:CB	2.62	0.65
1:D:83:ILE:O	1:D:87:THR:HG23	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ASN:CB	2:D:116:HOH:O	2.26	0.65
1:B:57:LYS:CG	1:B:57:LYS:CE	2.75	0.64
1:D:5:TYR:O	1:D:10:LYS:NZ	2.29	0.64
1:B:93:LEU:CD2	1:B:93:LEU:CD1	2.75	0.64
1:C:71:ASP:HB2	2:C:120:HOH:O	1.98	0.62
1:B:30:LYS:CB	1:B:30:LYS:NZ	2.63	0.61
1:A:49:MET:HG3	1:B:9:GLU:HG2	1.81	0.61
1:A:29:VAL:HG23	1:A:29:VAL:O	2.01	0.61
1:A:13:ILE:C	1:A:13:ILE:CB	2.67	0.60
1:C:71:ASP:CB	2:C:120:HOH:O	2.49	0.60
1:C:47:ASN:O	1:C:51:SER:HB3	2.01	0.59
1:D:35:LYS:CD	1:D:35:LYS:CB	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:68:ALA:HA	1:C:72:GLY:HA2	1.85	0.59
1:A:93:LEU:N	1:A:93:LEU:CD1	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:CG2	1:D:13:ILE:CA	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:A:38:PHE:CD1	1:A:41:MET:HE1	2.39	0.56
1:B:50:LEU:O	1:B:56:ARG:NH1	2.38	0.56
1:D:22:TYR:OH	1:D:45:GLU:OE2	2.15	0.56
1:C:38:PHE:CD1	1:C:41:MET:CE	2.89	0.56
1:B:20:TYR:CD1	1:B:30:LYS:HD2	2.37	0.56
1:C:41:MET:HE3	1:C:42:LEU:HD23	1.86	0.56
1:D:95:HIS:C	1:D:97:GLN:H	2.07	0.55
1:A:19:PHE:CB	1:A:19:PHE:CD2	2.72	0.55
1:B:13:ILE:HA	1:B:13:ILE:HD12	1.88	0.55
1:A:38:PHE:CE1	1:A:41:MET:HE1	2.42	0.55
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:CG2	1:B:13:ILE:CA	2.77	0.54
1:B:93:LEU:HG	1:B:93:LEU:CD1	2.17	0.54
1:B:91:ALA:CB	1:B:91:ALA:N	2.65	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:CD2	1:A:93:LEU:CD1	2.75	0.52
1:B:13:ILE:HD13	1:B:13:ILE:H	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:THR:HG22	1:A:9:GLU:HB2	1.92	0.52
1:B:23:VAL:HG11	1:B:30:LYS:CD	2.39	0.52
1:B:38:PHE:CE1	1:B:41:MET:CE	2.94	0.51
1:C:62:LEU:CD2	1:C:62:LEU:CB	2.79	0.50
1:C:42:LEU:HD22	1:C:46:LEU:HD12	1.92	0.50
1:B:30:LYS:HZ2	1:B:30:LYS:HB3	1.70	0.50
1:C:56:ARG:HG2	1:C:56:ARG:HH11	1.77	0.50
1:B:13:ILE:CA	1:B:13:ILE:HD12	2.42	0.50
1:A:6:THR:HG23	1:A:7:GLU:N	2.25	0.49
1:A:90:ILE:HG23	1:A:94:ILE:CD1	2.42	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:D:14:VAL:CG1	1:D:14:VAL:O	2.61	0.49
1:D:46:LEU:O	1:D:50:LEU:HD13	2.12	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:B:30:LYS:CB	1:B:30:LYS:HZ2	2.23	0.48
1:A:73:ARG:CZ	2:A:116:HOH:O	2.61	0.48
1:C:8:LEU:HD23	1:D:45:GLU:HB3	1.95	0.48
1:B:78:GLU:CD	2:B:115:HOH:O	2.52	0.48
1:B:50:LEU:O	1:B:56:ARG:HD3	2.13	0.48
1:B:56:ARG:HH11	1:B:56:ARG:HD3	1.17	0.48
1:A:55:ASN:O	1:A:56:ARG:C	2.52	0.48
1:A:16:VAL:HG11	1:B:94:ILE:HB	1.96	0.47
1:C:31:ASN:O	1:C:32:LYS:HG3	2.14	0.47
1:A:50:LEU:O	1:A:56:ARG:HG3	2.15	0.47
1:B:13:ILE:N	1:B:13:ILE:CD1	2.78	0.46
1:A:31:ASN:CG	1:A:31:ASN:CA	2.78	0.46
1:D:76:PHE:C	1:D:76:PHE:CD2	2.88	0.46
1:D:79:TYR:O	1:D:83:ILE:HG12	2.15	0.46
1:B:75:SER:OG	1:B:78:GLU:HG3	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:OE1	1:D:96:GLU:HA	2.15	0.46
1:A:81:THR:OG1	1:A:81:THR:CG2	2.55	0.46
1:B:91:ALA:CB	1:B:91:ALA:C	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:N	1:A:13:ILE:CB	2.67	0.45
1:C:22:TYR:OH	1:C:45:GLU:OE2	2.29	0.45
1:D:13:ILE:CA	1:D:13:ILE:HD13	2.47	0.45
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:B:32:LYS:HD3	1:B:73:ARG:CB	2.47	0.45
1:B:50:LEU:HA	1:B:50:LEU:HD23	1.76	0.45
1:D:48:HIS:C	1:D:50:LEU:N	2.70	0.45
1:A:29:VAL:CG2	1:A:29:VAL:O	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:D:95:HIS:C	1:D:97:GLN:N	2.70	0.44
1:A:13:ILE:C	1:A:13:ILE:CG2	2.86	0.44
1:D:13:ILE:CD1	1:D:13:ILE:CA	2.95	0.44
1:A:30:LYS:H	1:A:30:LYS:HG2	1.63	0.44
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:D:13:ILE:C	1:D:13:ILE:CG2	2.88	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
2:C:116:HOH:O	1:D:14:VAL:HG21	2.18	0.42
1:A:83:ILE:HA	1:A:83:ILE:HD13	1.74	0.42
1:A:38:PHE:CD1	1:A:41:MET:HE3	2.52	0.42
1:D:76:PHE:O	1:D:77:ASP:C	2.55	0.42
1:A:63:ILE:O	1:A:66:LEU:HB2	2.19	0.42
1:B:61:LYS:HB2	1:B:61:LYS:CD	2.44	0.42
1:C:31:ASN:HD21	1:D:92:LYS:NZ	2.18	0.41
1:A:13:ILE:HG13	1:A:13:ILE:CA	2.47	0.41
1:C:83:ILE:HD13	1:C:83:ILE:HA	1.83	0.41
1:D:31:ASN:C	1:D:32:LYS:HG3	2.40	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:C:10:LYS:CD	1:C:10:LYS:NZ	2.72	0.40
1:C:50:LEU:O	1:C:56:ARG:HB2	2.22	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%)	9	4
1	B	95/100 (95%)	91 (96%)	3 (3%)	1 (1%)	17	11
1	C	95/100 (95%)	86 (90%)	6 (6%)	3 (3%)	5	1
1	D	70/100 (70%)	63 (90%)	7 (10%)	0	100	100
All	All	358/400 (90%)	327 (91%)	25 (7%)	6 (2%)	11	5

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%)	70 (78%)	20 (22%)	1	0
1	B	87/90 (97%)	75 (86%)	12 (14%)	4	2
1	C	87/90 (97%)	75 (86%)	12 (14%)	4	2
1	D	68/90 (76%)	64 (94%)	4 (6%)	24	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	332/360 (92%)	284 (86%)	48 (14%)	4 2

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	6	THR
1	A	25	LYS
1	A	28	LEU
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	53	THR
1	A	56	ARG
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	13	ILE
1	B	15	LEU
1	B	32	LYS
1	B	37	SER
1	B	53	THR
1	B	65	ASN
1	B	66	LEU
1	B	71	ASP
1	B	75	SER
1	B	79	TYR
1	B	93	LEU
1	B	100	GLN
1	C	10	LYS
1	C	15	LEU
1	C	21	LYS
1	C	38	PHE
1	C	40	GLU

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Mol	Chain	Res	Type
1	C	42	LEU
1	C	60	ASP
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	44	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	HIS
1	B	55	ASN
1	C	31	ASN
1	C	48	HIS
1	C	99	GLN

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](#)

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%)	0.30	3 (3%)	54	62	23, 54, 91, 98	0
1	B	97/100 (97%)	0.26	3 (3%)	52	61	20, 43, 66, 89	0
1	C	97/100 (97%)	0.38	7 (7%)	18	25	33, 50, 83, 101	0
1	D	74/100 (74%)	0.31	4 (5%)	29	38	18, 50, 79, 89	0
All	All	368/400 (92%)	0.32	17 (4%)	36	45	18, 49, 84, 101	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	TYR	4.9
1	C	71	ASP	3.9
1	D	47	ASN	3.7
1	B	31	ASN	3.6
1	A	3	ASP	3.6
1	C	68	ALA	3.5
1	C	5	TYR	3.2
1	D	50	LEU	3.0
1	B	30	LYS	2.9
1	A	53	THR	2.7
1	C	100	GLN	2.5
1	A	68	ALA	2.5
1	D	96	GLU	2.4
1	C	82	LEU	2.3
1	D	73	ARG	2.2
1	C	70	HIS	2.1
1	C	67	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.