



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:11 AM UTC

PDB ID : 2UTG / pdb_00002utg
Title : STRUCTURE AND REFINEMENT OF THE OXIDIZED P21 FORM OF
UTEROGLOBIN AT 1.64 ANGSTROMS RESOLUTION
Authors : Bally, R.; Delettre, J.
Deposited on : 1989-05-17
Resolution : 1.64 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

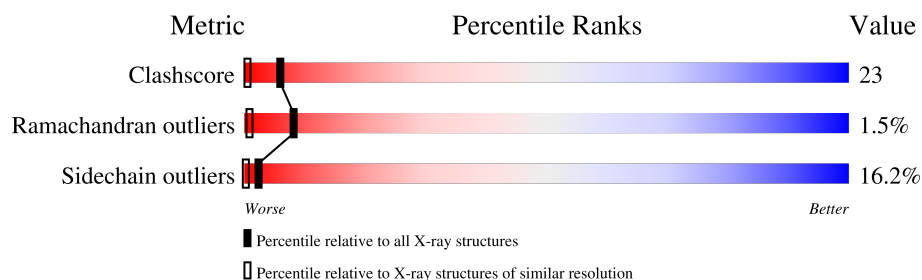
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	70	
1	B	70	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1261 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 UTEROGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	70	Total	C	N	O	S	0	0	0
			548	345	89	107	7			
1	B	70	Total	C	N	O	S	0	0	0
			548	345	89	107	7			

- Molecule 2 is water.

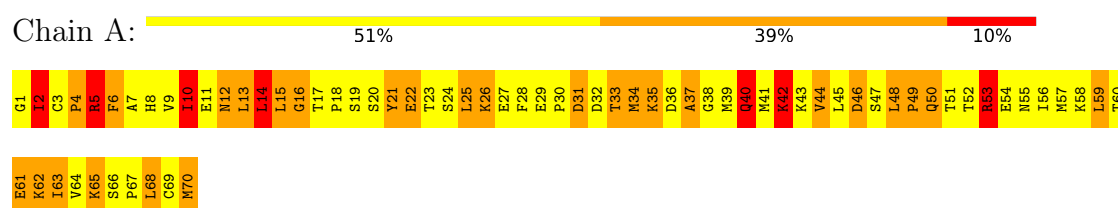
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total	O	0	0
			82	82		
2	B	83	Total	O	0	0
			83	83		

3 Residue-property plots

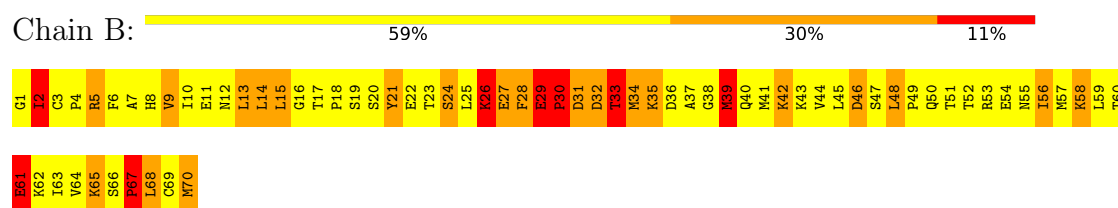
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: UTEROGLOBIN



• Molecule 1: UTEROGLOBIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.56 Å 46.06 Å 37.43 Å 90.00° 120.92° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.64	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.64)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1261	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

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	3.78	87/556 (15.6%)	5.87	237/746 (31.8%)
1	B	3.84	99/556 (17.8%)	5.80	229/746 (30.7%)
All	All	3.81	186/1112 (16.7%)	5.84	466/1492 (31.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (186) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	LEU	C-O	18.71	1.46	1.24
1	B	15	LEU	C-N	-17.90	1.13	1.33
1	A	45	LEU	C-O	-15.21	1.04	1.24
1	B	18	PRO	N-CD	12.87	1.65	1.47
1	A	47	SER	C-O	12.43	1.40	1.24
1	B	18	PRO	C-O	-12.42	1.08	1.24
1	B	18	PRO	N-CA	-12.03	1.31	1.47
1	B	19	SER	C-N	-12.02	1.18	1.33
1	A	14	LEU	N-CA	11.92	1.61	1.46
1	A	49	PRO	N-CD	11.63	1.64	1.47
1	A	13	LEU	N-CA	11.37	1.60	1.46
1	A	42	LYS	N-CA	11.33	1.60	1.46
1	A	39	MET	N-CA	10.91	1.59	1.46
1	A	55	ASN	C-N	-10.87	1.20	1.33
1	A	19	SER	C-N	-10.45	1.21	1.33
1	B	8	HIS	ND1-CE1	10.30	1.42	1.32
1	B	58	LYS	CA-C	10.22	1.65	1.52
1	A	42	LYS	CA-C	-9.93	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	ALA	C-N	-9.88	1.21	1.33
1	B	43	LYS	C-N	9.83	1.45	1.33
1	A	8	HIS	CG-ND1	9.79	1.49	1.38
1	A	29	GLU	CA-C	9.75	1.60	1.53
1	B	15	LEU	C-O	9.63	1.36	1.24
1	B	16	GLY	N-CA	9.56	1.57	1.44
1	A	42	LYS	C-O	9.51	1.35	1.24
1	A	29	GLU	CA-CB	9.50	1.59	1.52
1	A	13	LEU	CA-C	-9.43	1.40	1.52
1	B	35	LYS	C-N	-9.23	1.22	1.33
1	A	30	PRO	C-N	-9.08	1.21	1.33
1	B	57	MET	C-N	-9.04	1.22	1.33
1	B	8	HIS	CA-C	-8.98	1.41	1.52
1	B	40	GLN	C-N	-8.91	1.22	1.33
1	A	44	VAL	CA-CB	8.88	1.66	1.54
1	B	46	ASP	CG-OD2	-8.85	1.08	1.25
1	A	64	VAL	C-N	-8.81	1.20	1.33
1	B	53	ARG	NE-CZ	-8.80	1.23	1.33
1	A	22	GLU	N-CA	8.70	1.57	1.46
1	A	65	LYS	C-O	8.60	1.35	1.24
1	B	42	LYS	C-N	-8.60	1.23	1.33
1	A	8	HIS	CG-CD2	8.52	1.45	1.35
1	B	14	LEU	C-N	-8.45	1.21	1.33
1	B	54	GLU	C-N	-8.41	1.22	1.33
1	B	60	THR	C-O	-8.39	1.14	1.24
1	B	19	SER	C-O	8.38	1.34	1.24
1	A	47	SER	N-CA	8.36	1.57	1.46
1	B	9	VAL	C-N	8.34	1.44	1.33
1	A	8	HIS	N-CA	8.32	1.57	1.46
1	B	44	VAL	CA-CB	8.31	1.66	1.54
1	A	45	LEU	CA-C	8.31	1.64	1.52
1	A	51	THR	C-N	-8.25	1.23	1.33
1	B	60	THR	CA-CB	8.20	1.66	1.53
1	B	17	THR	CA-CB	8.10	1.66	1.53
1	A	48	LEU	C-N	-8.06	1.23	1.33
1	A	29	GLU	C-O	-8.04	1.20	1.23
1	A	43	LYS	C-N	8.01	1.43	1.33
1	A	32	ASP	C-O	8.00	1.33	1.24
1	B	55	ASN	CG-OD1	-7.90	1.08	1.23
1	B	45	LEU	C-N	-7.83	1.23	1.33
1	B	6	PHE	C-O	-7.77	1.14	1.24
1	A	60	THR	CA-CB	7.76	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	ILE	N-CA	7.76	1.56	1.46
1	A	59	LEU	N-CA	7.75	1.55	1.46
1	B	7	ALA	CA-C	7.71	1.63	1.52
1	A	48	LEU	N-CA	-7.66	1.34	1.46
1	A	10	ILE	CA-CB	7.60	1.62	1.54
1	A	41	MET	C-N	7.59	1.43	1.33
1	A	20	SER	CB-OG	7.57	1.57	1.42
1	A	44	VAL	C-O	-7.57	1.14	1.24
1	B	53	ARG	CZ-NH2	-7.52	1.23	1.33
1	B	50	GLN	C-N	-7.47	1.24	1.34
1	B	48	LEU	C-O	7.46	1.33	1.23
1	B	15	LEU	CA-CB	-7.45	1.43	1.54
1	A	14	LEU	C-N	7.39	1.45	1.33
1	A	44	VAL	C-N	7.38	1.44	1.34
1	B	8	HIS	N-CA	7.35	1.55	1.46
1	B	32	ASP	CA-CB	7.33	1.64	1.53
1	A	7	ALA	C-O	7.32	1.33	1.24
1	B	25	LEU	C-N	-7.17	1.24	1.34
1	B	26	LYS	C-O	7.17	1.33	1.24
1	B	8	HIS	CA-CB	7.16	1.64	1.53
1	B	44	VAL	C-O	7.16	1.33	1.24
1	A	39	MET	CA-C	-7.12	1.43	1.52
1	A	37	ALA	C-O	-7.11	1.15	1.24
1	A	40	GLN	N-CA	7.10	1.54	1.46
1	A	38	GLY	CA-C	7.08	1.60	1.51
1	A	21	TYR	C-O	7.07	1.32	1.24
1	A	61	GLU	CD-OE2	7.05	1.38	1.25
1	B	36	ASP	CG-OD1	7.03	1.38	1.25
1	B	8	HIS	C-N	7.02	1.42	1.33
1	B	59	LEU	C-O	7.01	1.32	1.24
1	B	67	PRO	CA-CB	6.96	1.63	1.53
1	B	24	SER	CA-C	-6.95	1.43	1.52
1	A	5	ARG	CD-NE	6.91	1.55	1.46
1	B	35	LYS	C-O	6.87	1.32	1.24
1	A	22	GLU	CD-OE2	6.83	1.38	1.25
1	B	47	SER	N-CA	6.82	1.55	1.46
1	A	21	TYR	C-N	-6.73	1.24	1.34
1	B	38	GLY	N-CA	6.72	1.54	1.45
1	A	50	GLN	CG-CD	-6.71	1.35	1.52
1	A	42	LYS	CB-CG	6.71	1.72	1.52
1	B	26	LYS	CA-C	-6.64	1.43	1.52
1	A	40	GLN	CD-OE1	-6.60	1.11	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	ASP	N-CA	6.56	1.54	1.46
1	A	13	LEU	CB-CG	6.55	1.66	1.53
1	B	41	MET	C-N	6.55	1.42	1.33
1	B	52	THR	C-N	-6.55	1.25	1.34
1	A	29	GLU	N-CA	-6.54	1.41	1.46
1	B	8	HIS	CB-CG	6.50	1.59	1.50
1	B	47	SER	CA-C	-6.49	1.43	1.52
1	B	8	HIS	CG-ND1	-6.39	1.31	1.38
1	B	17	THR	C-O	6.37	1.30	1.23
1	B	52	THR	N-CA	6.35	1.53	1.46
1	A	2	ILE	N-CA	6.35	1.53	1.46
1	A	34	MET	N-CA	-6.35	1.38	1.46
1	B	63	ILE	CA-CB	6.34	1.63	1.54
1	A	28	PHE	C-O	6.33	1.32	1.24
1	B	25	LEU	C-O	-6.31	1.16	1.24
1	A	53	ARG	CZ-NH1	-6.28	1.24	1.32
1	B	62	LYS	C-N	-6.24	1.25	1.33
1	B	14	LEU	CG-CD2	-6.23	1.31	1.52
1	B	9	VAL	CA-C	-6.22	1.45	1.52
1	A	5	ARG	CB-CG	6.21	1.71	1.52
1	B	45	LEU	C-O	-6.21	1.16	1.24
1	A	51	THR	CB-OG1	6.18	1.53	1.43
1	A	33	THR	N-CA	6.17	1.53	1.46
1	B	17	THR	C-N	-6.17	1.26	1.33
1	B	20	SER	CA-CB	-6.13	1.43	1.53
1	B	17	THR	CA-C	-6.13	1.43	1.52
1	A	41	MET	C-O	-6.12	1.17	1.24
1	B	42	LYS	CA-C	-6.12	1.44	1.52
1	B	2	ILE	CA-CB	6.09	1.62	1.54
1	B	39	MET	SD-CE	-6.03	1.64	1.79
1	B	4	PRO	C-N	-6.01	1.26	1.33
1	A	38	GLY	C-O	-5.97	1.16	1.23
1	A	56	ILE	N-CA	5.97	1.53	1.46
1	B	40	GLN	CA-C	5.96	1.60	1.52
1	B	6	PHE	C-N	-5.88	1.26	1.34
1	A	34	MET	CA-C	5.87	1.60	1.52
1	B	27	GLU	CA-CB	-5.85	1.43	1.53
1	A	61	GLU	CA-CB	5.84	1.62	1.53
1	B	14	LEU	C-O	5.83	1.31	1.24
1	B	33	THR	CA-C	5.77	1.60	1.52
1	A	15	LEU	C-N	5.77	1.41	1.33
1	B	55	ASN	N-CA	5.74	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	PRO	CA-CB	-5.73	1.45	1.53
1	B	58	LYS	CG-CD	5.61	1.69	1.52
1	B	65	LYS	CA-CB	-5.61	1.44	1.53
1	B	54	GLU	N-CA	5.60	1.53	1.46
1	B	41	MET	C-O	-5.54	1.17	1.24
1	A	49	PRO	CA-CB	-5.51	1.46	1.53
1	A	53	ARG	CZ-NH2	5.50	1.40	1.33
1	B	37	ALA	CA-CB	5.50	1.61	1.53
1	A	57	MET	CG-SD	-5.49	1.67	1.80
1	B	34	MET	N-CA	5.46	1.52	1.46
1	B	5	ARG	CD-NE	5.46	1.53	1.46
1	A	11	GLU	CD-OE1	-5.44	1.15	1.25
1	B	28	PHE	N-CA	5.43	1.53	1.46
1	B	18	PRO	C-N	5.41	1.41	1.33
1	B	8	HIS	CE1-NE2	5.39	1.38	1.32
1	A	53	ARG	N-CA	-5.39	1.40	1.46
1	B	12	ASN	CA-C	5.38	1.59	1.52
1	B	12	ASN	C-O	-5.37	1.17	1.24
1	B	39	MET	C-O	-5.35	1.17	1.24
1	B	13	LEU	C-O	-5.33	1.18	1.24
1	B	3	CYS	CA-C	5.29	1.59	1.52
1	A	69	CYS	C-O	-5.26	1.17	1.23
1	A	5	ARG	N-CA	5.22	1.52	1.46
1	A	36	ASP	C-N	5.21	1.41	1.34
1	A	65	LYS	C-N	5.18	1.40	1.33
1	B	13	LEU	CA-CB	5.18	1.61	1.53
1	A	61	GLU	C-N	5.15	1.40	1.33
1	A	42	LYS	CA-CB	5.15	1.61	1.53
1	B	59	LEU	N-CA	5.14	1.52	1.46
1	A	56	ILE	C-O	5.14	1.30	1.24
1	A	23	THR	CB-OG1	5.12	1.51	1.43
1	A	30	PRO	C-O	5.12	1.29	1.23
1	B	37	ALA	CA-C	-5.12	1.46	1.52
1	B	56	ILE	CA-C	-5.10	1.44	1.52
1	A	18	PRO	C-O	5.09	1.31	1.24
1	B	35	LYS	CB-CG	-5.09	1.37	1.52
1	A	36	ASP	C-O	-5.08	1.17	1.24
1	B	43	LYS	N-CA	5.07	1.52	1.46
1	A	43	LYS	C-O	-5.04	1.18	1.24
1	B	20	SER	CA-C	5.03	1.59	1.52
1	B	38	GLY	CA-C	-5.02	1.46	1.52
1	A	17	THR	CA-C	-5.02	1.46	1.53

All (466) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ASP	CA-CB-CG	41.86	154.46	112.60
1	A	53	ARG	NE-CZ-NH1	33.46	154.96	121.50
1	A	55	ASN	OD1-CG-ND2	-27.34	95.26	122.60
1	B	5	ARG	NE-CZ-NH2	26.64	143.17	119.20
1	B	15	LEU	O-C-N	24.13	148.88	122.34
1	B	37	ALA	CA-C-N	23.81	146.37	119.94
1	B	37	ALA	C-N-CA	23.81	146.37	119.94
1	A	40	GLN	OE1-CD-NE2	23.52	146.12	122.60
1	B	17	THR	CA-C-N	21.35	142.76	119.28
1	B	17	THR	C-N-CA	21.35	142.76	119.28
1	A	50	GLN	OE1-CD-NE2	-21.29	101.31	122.60
1	A	49	PRO	CA-C-O	21.01	145.11	121.36
1	B	15	LEU	CA-C-O	-19.28	97.37	118.77
1	B	50	GLN	CA-C-O	-19.25	100.14	120.55
1	A	19	SER	CA-C-O	-18.72	101.16	120.82
1	A	43	LYS	O-C-N	-17.99	102.83	122.08
1	A	43	LYS	CA-C-O	17.38	140.19	121.07
1	B	53	ARG	NE-CZ-NH2	17.25	134.72	119.20
1	A	16	GLY	CA-C-O	17.17	141.01	122.47
1	A	53	ARG	CA-C-N	16.61	143.13	120.38
1	A	53	ARG	C-N-CA	16.61	143.13	120.38
1	A	16	GLY	O-C-N	-16.57	108.56	122.81
1	A	44	VAL	O-C-N	-16.04	103.68	121.80
1	A	63	ILE	O-C-N	-15.96	105.98	121.94
1	A	28	PHE	CA-C-N	15.70	139.79	122.83
1	A	28	PHE	C-N-CA	15.70	139.79	122.83
1	B	23	THR	CA-C-O	-15.56	104.48	120.82
1	B	23	THR	CA-CB-OG1	-15.47	86.40	109.60
1	A	67	PRO	CA-C-N	15.43	142.50	120.28
1	A	67	PRO	C-N-CA	15.43	142.50	120.28
1	A	53	ARG	NE-CZ-NH2	-15.37	105.37	119.20
1	A	50	GLN	CG-CD-NE2	15.12	139.08	116.40
1	B	2	ILE	CA-C-O	-15.12	101.88	120.78
1	A	53	ARG	NH1-CZ-NH2	-15.11	99.65	119.30
1	B	5	ARG	NE-CZ-NH1	-15.09	106.41	121.50
1	A	67	PRO	O-C-N	-14.86	103.05	122.22
1	A	36	ASP	CA-CB-CG	14.85	127.45	112.60
1	A	45	LEU	O-C-N	14.66	140.30	122.27
1	B	37	ALA	O-C-N	-14.29	107.23	122.09
1	B	40	GLN	CG-CD-NE2	14.15	137.63	116.40
1	A	22	GLU	CB-CG-CD	14.00	136.40	112.60
1	A	49	PRO	O-C-N	-13.90	105.23	122.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	SER	CA-C-O	-13.68	101.61	119.11
1	A	34	MET	N-CA-CB	13.62	129.76	110.01
1	B	54	GLU	O-C-N	13.52	137.57	122.15
1	B	53	ARG	NH1-CZ-NH2	-13.52	101.73	119.30
1	B	17	THR	O-C-N	-13.48	108.19	120.99
1	A	66	SER	CA-CB-OG	13.46	138.01	111.10
1	B	51	THR	O-C-N	13.22	137.69	122.22
1	A	8	HIS	CB-CG-CD2	-13.21	114.02	131.20
1	A	15	LEU	O-C-N	13.09	137.46	122.27
1	A	15	LEU	CA-C-N	-13.08	103.91	121.96
1	A	15	LEU	C-N-CA	-13.08	103.91	121.96
1	A	35	LYS	O-C-N	13.07	135.53	122.07
1	B	26	LYS	CA-C-O	-13.06	105.34	120.10
1	B	40	GLN	OE1-CD-NE2	-13.05	109.55	122.60
1	A	68	LEU	CA-C-O	-12.96	105.46	120.10
1	A	5	ARG	NE-CZ-NH2	-12.93	107.56	119.20
1	B	26	LYS	CB-CG-CD	12.91	141.00	111.30
1	A	63	ILE	CA-C-O	12.73	134.51	121.27
1	A	40	GLN	CG-CD-OE1	-12.72	95.35	120.80
1	B	16	GLY	O-C-N	-12.39	113.05	122.71
1	A	50	GLN	CA-C-O	-12.36	107.45	120.55
1	B	58	LYS	N-CA-CB	12.28	127.81	110.01
1	B	48	LEU	CA-C-O	-12.28	108.00	120.64
1	B	25	LEU	CA-C-N	12.21	137.87	120.28
1	B	25	LEU	C-N-CA	12.21	137.87	120.28
1	B	19	SER	CA-C-N	12.20	136.30	120.44
1	B	19	SER	C-N-CA	12.20	136.30	120.44
1	B	26	LYS	CB-CA-C	12.12	133.05	110.63
1	A	68	LEU	O-C-N	12.02	136.28	122.22
1	A	53	ARG	O-C-N	-11.97	109.74	122.07
1	A	49	PRO	CB-CA-C	11.94	126.73	111.56
1	B	32	ASP	CA-C-O	11.80	133.21	120.82
1	B	58	LYS	CA-C-N	-11.77	104.50	120.28
1	B	58	LYS	C-N-CA	-11.77	104.50	120.28
1	A	44	VAL	CA-C-O	11.76	133.17	120.47
1	B	59	LEU	CA-C-O	11.64	132.89	120.55
1	A	23	THR	O-C-N	11.61	134.43	122.12
1	A	57	MET	CG-SD-CE	11.57	126.35	100.90
1	B	47	SER	O-C-N	-11.48	106.62	122.46
1	A	69	CYS	CA-C-N	11.44	142.28	121.70
1	A	69	CYS	C-N-CA	11.44	142.28	121.70
1	B	4	PRO	CA-C-O	-11.44	103.45	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	THR	CA-C-O	-11.41	110.33	120.60
1	A	48	LEU	CA-C-N	11.31	131.43	119.90
1	A	48	LEU	C-N-CA	11.31	131.43	119.90
1	B	8	HIS	CE1-NE2-CD2	-11.20	97.80	109.00
1	A	29	GLU	O-C-N	11.19	134.19	121.32
1	B	33	THR	CA-CB-CG2	11.13	129.42	110.50
1	A	25	LEU	CA-C-O	-11.10	109.27	120.70
1	B	17	THR	CA-C-O	-11.10	109.73	121.27
1	A	32	ASP	CA-CB-CG	-11.06	101.54	112.60
1	A	51	THR	CA-CB-CG2	10.94	129.09	110.50
1	B	61	GLU	O-C-N	10.86	137.03	122.59
1	A	23	THR	CA-CB-OG1	-10.80	93.39	109.60
1	A	42	LYS	CA-CB-CG	-10.78	92.53	114.10
1	B	63	ILE	N-CA-C	10.73	122.70	111.00
1	B	32	ASP	O-C-N	-10.66	111.09	122.07
1	A	14	LEU	N-CA-CB	-10.64	94.36	110.33
1	B	57	MET	CA-C-N	10.62	134.25	120.44
1	B	57	MET	C-N-CA	10.62	134.25	120.44
1	A	10	ILE	CA-C-O	10.61	132.30	121.27
1	B	42	LYS	CG-CD-CE	10.39	135.20	111.30
1	A	8	HIS	CA-CB-CG	10.35	124.15	113.80
1	B	67	PRO	CA-C-O	10.32	139.38	120.60
1	B	20	SER	N-CA-C	-10.31	100.03	111.07
1	A	12	ASN	CB-CG-ND2	10.30	131.86	116.40
1	A	36	ASP	N-CA-CB	-10.29	94.33	110.28
1	A	51	THR	OG1-CB-CG2	-10.29	88.73	109.30
1	B	48	LEU	O-C-N	10.28	134.69	121.64
1	A	39	MET	CG-SD-CE	10.22	123.38	100.90
1	B	58	LYS	O-C-N	10.21	132.59	122.07
1	B	32	ASP	CA-CB-CG	-10.19	102.41	112.60
1	B	50	GLN	CA-C-N	10.19	134.95	120.28
1	B	50	GLN	C-N-CA	10.19	134.95	120.28
1	B	62	LYS	CB-CG-CD	10.18	134.71	111.30
1	A	5	ARG	CA-C-O	10.16	131.32	120.55
1	A	36	ASP	CA-C-N	-9.95	105.18	120.31
1	A	36	ASP	C-N-CA	-9.95	105.18	120.31
1	A	37	ALA	CA-C-N	9.93	131.21	119.99
1	A	37	ALA	C-N-CA	9.93	131.21	119.99
1	A	11	GLU	CB-CG-CD	-9.88	95.80	112.60
1	B	2	ILE	CB-CG1-CD1	9.85	134.49	113.80
1	B	55	ASN	OD1-CG-ND2	-9.74	112.86	122.60
1	B	40	GLN	CA-C-N	9.73	133.09	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	GLN	C-N-CA	9.73	133.09	120.44
1	B	16	GLY	CA-C-O	9.67	133.59	122.76
1	A	29	GLU	CB-CG-CD	9.62	128.95	112.60
1	B	35	LYS	CA-C-N	9.58	132.89	120.44
1	B	35	LYS	C-N-CA	9.58	132.89	120.44
1	B	10	ILE	CA-C-N	9.55	133.86	120.29
1	B	10	ILE	C-N-CA	9.55	133.86	120.29
1	A	60	THR	CA-C-O	9.55	130.85	120.82
1	B	4	PRO	O-C-N	9.48	132.88	122.17
1	A	34	MET	O-C-N	9.38	131.74	122.07
1	A	38	GLY	N-CA-C	-9.25	101.45	112.64
1	B	53	ARG	CA-C-O	9.22	130.52	120.10
1	B	10	ILE	O-C-N	-9.21	112.93	121.87
1	B	33	THR	CA-CB-OG1	-9.19	95.81	109.60
1	B	49	PRO	CA-C-O	9.12	132.14	121.56
1	A	18	PRO	N-CD-CG	-9.10	89.55	103.20
1	A	64	VAL	CA-CB-CG2	9.09	125.86	110.40
1	A	52	THR	CA-CB-OG1	-9.07	96.00	109.60
1	B	49	PRO	O-C-N	-9.06	111.78	123.01
1	B	57	MET	CG-SD-CE	9.04	120.80	100.90
1	A	39	MET	CA-C-O	9.00	130.09	120.55
1	B	64	VAL	CB-CA-C	8.98	126.80	112.16
1	B	58	LYS	N-CA-C	-8.97	101.47	111.07
1	B	38	GLY	N-CA-C	-8.96	102.11	112.50
1	A	57	MET	CB-CG-SD	8.94	139.53	112.70
1	B	41	MET	O-C-N	-8.94	112.86	122.07
1	A	28	PHE	CB-CG-CD1	-8.92	105.53	120.70
1	B	22	GLU	CA-CB-CG	-8.91	96.28	114.10
1	A	8	HIS	CB-CG-ND1	8.90	136.05	122.70
1	A	13	LEU	N-CA-CB	-8.90	97.04	110.12
1	B	8	HIS	CB-CA-C	8.82	124.84	110.90
1	B	29	GLU	CG-CD-OE1	8.81	138.66	118.40
1	B	5	ARG	O-C-N	-8.80	112.79	122.12
1	B	20	SER	CA-CB-OG	8.80	128.70	111.10
1	B	29	GLU	CA-C-O	8.78	132.19	120.16
1	A	46	ASP	OD1-CG-OD2	8.72	143.82	122.90
1	A	5	ARG	CA-CB-CG	-8.69	96.72	114.10
1	B	66	SER	CA-C-O	-8.68	111.70	120.64
1	B	18	PRO	O-C-N	8.66	133.40	122.22
1	B	11	GLU	CB-CG-CD	8.64	127.28	112.60
1	A	29	GLU	CA-C-O	-8.62	113.85	120.48
1	A	51	THR	CA-CB-OG1	-8.60	96.71	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	VAL	O-C-N	-8.58	112.11	121.80
1	A	5	ARG	NE-CZ-NH1	8.55	130.05	121.50
1	B	60	THR	CB-CA-C	8.53	124.10	110.96
1	B	20	SER	N-CA-CB	8.51	122.35	110.01
1	B	49	PRO	CB-CA-C	8.49	122.09	111.23
1	B	48	LEU	CB-CA-C	-8.47	96.40	109.11
1	B	36	ASP	CB-CG-OD2	8.43	137.79	118.40
1	A	35	LYS	CB-CG-CD	8.42	130.67	111.30
1	B	14	LEU	O-C-N	8.42	134.32	122.36
1	B	2	ILE	CB-CA-C	8.40	125.07	111.29
1	B	8	HIS	CB-CG-CD2	-8.39	120.29	131.20
1	B	8	HIS	CG-CD2-NE2	8.37	115.57	107.20
1	B	50	GLN	OE1-CD-NE2	8.31	130.91	122.60
1	B	14	LEU	CA-C-O	-8.31	109.88	119.60
1	B	68	LEU	N-CA-C	8.28	122.80	112.87
1	A	31	ASP	OD1-CG-OD2	-8.25	103.09	122.90
1	A	21	TYR	CA-C-O	-8.24	112.17	120.82
1	A	41	MET	CA-C-N	-8.22	109.27	120.28
1	A	41	MET	C-N-CA	-8.22	109.27	120.28
1	A	41	MET	N-CA-C	-8.19	102.29	111.14
1	A	58	LYS	CA-C-N	-8.18	108.68	120.29
1	A	58	LYS	C-N-CA	-8.18	108.68	120.29
1	A	46	ASP	CB-CG-OD1	-8.16	99.63	118.40
1	A	12	ASN	O-C-N	8.15	131.45	122.15
1	A	20	SER	O-C-N	8.15	130.80	122.08
1	B	25	LEU	CD1-CG-CD2	-8.14	92.88	110.80
1	B	40	GLN	CB-CA-C	-8.13	97.02	110.85
1	B	54	GLU	CB-CA-C	-8.13	97.04	110.85
1	A	55	ASN	CB-CG-OD1	8.09	136.97	120.80
1	A	61	GLU	CB-CG-CD	-8.05	98.91	112.60
1	B	28	PHE	CG-CD2-CE2	8.01	134.32	120.70
1	A	61	GLU	CG-CD-OE2	7.99	136.78	118.40
1	B	55	ASN	CA-C-O	7.94	129.10	119.49
1	A	4	PRO	O-C-N	-7.94	111.56	122.27
1	B	19	SER	CA-C-O	-7.93	111.44	120.24
1	A	27	GLU	CG-CD-OE1	-7.92	100.18	118.40
1	B	61	GLU	CG-CD-OE1	-7.91	100.21	118.40
1	B	18	PRO	CA-C-N	-7.89	107.09	120.58
1	B	18	PRO	C-N-CA	-7.89	107.09	120.58
1	A	31	ASP	CB-CG-OD2	7.89	136.54	118.40
1	B	36	ASP	CA-CB-CG	7.87	120.47	112.60
1	B	50	GLN	CB-CG-CD	-7.86	99.24	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	LEU	CA-CB-CG	7.86	143.79	116.30
1	B	3	CYS	N-CA-CB	7.85	125.70	109.45
1	A	48	LEU	CA-C-O	-7.82	113.62	120.19
1	B	59	LEU	N-CA-CB	-7.80	98.66	110.12
1	B	15	LEU	N-CA-CB	-7.79	100.53	110.90
1	B	7	ALA	O-C-N	7.73	131.27	122.22
1	A	4	PRO	CA-N-CD	7.71	122.80	112.00
1	B	67	PRO	O-C-N	-7.70	112.25	122.64
1	B	59	LEU	O-C-N	-7.56	114.10	122.12
1	A	39	MET	O-C-N	-7.55	114.11	122.12
1	B	41	MET	CA-C-O	7.55	128.75	120.82
1	B	56	ILE	N-CA-C	-7.54	101.34	111.44
1	A	53	ARG	CA-C-O	7.53	128.73	120.82
1	A	12	ASN	CB-CG-OD1	-7.50	105.81	120.80
1	B	36	ASP	CA-C-O	7.48	128.68	120.82
1	B	5	ARG	NH1-CZ-NH2	-7.48	109.58	119.30
1	B	23	THR	OG1-CB-CG2	7.46	124.22	109.30
1	A	44	VAL	CA-C-N	7.45	131.63	120.31
1	A	44	VAL	C-N-CA	7.45	131.63	120.31
1	A	24	SER	N-CA-C	-7.42	103.28	111.36
1	B	35	LYS	CA-CB-CG	7.41	128.92	114.10
1	B	51	THR	CA-C-N	-7.41	110.56	120.63
1	B	51	THR	C-N-CA	-7.41	110.56	120.63
1	A	67	PRO	CA-C-O	7.38	130.77	119.55
1	A	53	ARG	CD-NE-CZ	7.37	134.72	124.40
1	B	24	SER	CA-C-N	7.37	130.02	120.44
1	B	24	SER	C-N-CA	7.37	130.02	120.44
1	B	52	THR	CA-CB-OG1	7.36	120.64	109.60
1	A	27	GLU	O-C-N	-7.35	112.84	122.39
1	B	52	THR	OG1-CB-CG2	-7.34	94.62	109.30
1	B	54	GLU	CA-CB-CG	7.33	128.75	114.10
1	A	62	LYS	N-CA-CB	-7.26	99.44	110.12
1	A	12	ASN	N-CA-C	-7.25	103.45	111.36
1	A	70	MET	CB-CA-C	-7.23	96.36	110.10
1	A	54	GLU	O-C-N	7.23	129.78	122.12
1	B	61	GLU	CA-CB-CG	-7.23	99.65	114.10
1	B	15	LEU	CD1-CG-CD2	-7.20	94.96	110.80
1	A	30	PRO	CA-C-O	-7.19	113.14	121.34
1	A	22	GLU	CA-CB-CG	7.19	128.48	114.10
1	B	3	CYS	CB-CA-C	-7.19	97.90	109.69
1	B	21	TYR	O-C-N	-7.19	114.27	122.03
1	A	9	VAL	CA-C-N	7.15	129.83	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	VAL	C-N-CA	7.15	129.83	120.60
1	B	43	LYS	CG-CD-CE	7.15	127.75	111.30
1	B	44	VAL	CA-C-O	7.14	128.18	120.47
1	A	65	LYS	CB-CA-C	7.13	124.90	109.99
1	B	34	MET	N-CA-CB	7.13	120.35	110.01
1	A	44	VAL	N-CA-CB	-7.12	97.88	110.77
1	B	65	LYS	CA-CB-CG	7.11	128.32	114.10
1	A	6	PHE	CA-C-O	-7.11	112.35	120.24
1	A	66	SER	N-CA-C	7.08	119.68	109.84
1	A	56	ILE	N-CA-C	-7.07	103.41	110.62
1	B	1	GLY	CA-C-O	7.07	135.64	120.80
1	A	8	HIS	CG-CD2-NE2	-7.06	100.14	107.20
1	B	24	SER	CB-CA-C	-7.05	96.79	110.46
1	A	12	ASN	CA-C-N	-7.01	110.89	120.28
1	A	12	ASN	C-N-CA	-7.01	110.89	120.28
1	B	27	GLU	CG-CD-OE2	7.00	134.50	118.40
1	B	35	LYS	CA-C-O	-6.99	113.01	120.42
1	A	21	TYR	CA-C-N	-6.98	109.69	120.31
1	A	21	TYR	C-N-CA	-6.98	109.69	120.31
1	A	58	LYS	O-C-N	6.98	130.11	122.15
1	A	19	SER	N-CA-C	-6.97	103.61	111.07
1	B	30	PRO	N-CD-CG	-6.97	92.75	103.20
1	A	63	ILE	CB-CG1-CD1	6.96	128.42	113.80
1	A	1	GLY	O-C-N	6.96	134.13	123.00
1	B	40	GLN	N-CA-CB	6.94	120.43	110.16
1	A	4	PRO	N-CD-CG	-6.93	92.81	103.20
1	B	23	THR	N-CA-CB	6.87	119.97	110.01
1	A	64	VAL	CA-C-N	6.86	133.15	121.14
1	A	64	VAL	C-N-CA	6.86	133.15	121.14
1	A	55	ASN	CB-CG-ND2	6.82	126.63	116.40
1	A	7	ALA	N-CA-CB	-6.82	99.72	110.22
1	A	10	ILE	O-C-N	-6.79	115.14	121.94
1	A	27	GLU	OE1-CD-OE2	6.77	139.15	122.90
1	A	35	LYS	CA-C-O	-6.75	113.73	120.82
1	A	29	GLU	N-CA-CB	6.74	121.14	111.51
1	A	8	HIS	N-CA-CB	6.71	120.63	110.30
1	B	2	ILE	CA-CB-CG1	6.70	121.78	110.40
1	B	8	HIS	CA-C-O	6.68	127.58	120.70
1	A	66	SER	CA-C-O	6.65	128.20	120.69
1	A	15	LEU	CA-C-O	-6.64	111.60	118.90
1	A	26	LYS	CA-C-O	-6.64	112.77	120.20
1	A	4	PRO	CA-C-O	6.63	129.09	119.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	ILE	N-CA-CB	-6.60	100.33	111.23
1	B	29	GLU	CA-CB-CG	6.60	127.30	114.10
1	B	8	HIS	ND1-CE1-NE2	6.60	115.00	108.40
1	B	26	LYS	N-CA-CB	-6.58	100.08	110.22
1	B	44	VAL	CA-C-N	6.58	129.64	120.29
1	B	44	VAL	C-N-CA	6.58	129.64	120.29
1	A	50	GLN	CB-CG-CD	6.56	123.75	112.60
1	B	26	LYS	CA-C-N	-6.56	108.79	121.58
1	B	26	LYS	C-N-CA	-6.56	108.79	121.58
1	B	58	LYS	CB-CA-C	-6.54	100.62	110.88
1	A	52	THR	CA-C-O	6.54	127.68	120.82
1	A	35	LYS	CD-CE-NZ	6.53	132.81	111.90
1	A	65	LYS	CA-CB-CG	6.53	127.17	114.10
1	B	52	THR	CA-C-O	-6.53	114.17	120.90
1	B	12	ASN	CA-C-O	-6.53	113.50	120.42
1	A	63	ILE	CB-CA-C	-6.51	103.55	111.88
1	B	5	ARG	N-CA-CB	6.49	119.79	110.06
1	B	55	ASN	CB-CG-ND2	6.46	126.09	116.40
1	A	42	LYS	O-C-N	-6.45	115.28	122.12
1	B	46	ASP	OD1-CG-OD2	6.45	138.37	122.90
1	A	26	LYS	CG-CD-CE	-6.44	96.48	111.30
1	B	42	LYS	N-CA-C	-6.44	104.27	111.28
1	B	69	CYS	CB-CA-C	6.42	120.17	109.38
1	A	47	SER	CB-CA-C	6.41	122.71	109.95
1	A	5	ARG	O-C-N	-6.41	115.33	122.12
1	A	41	MET	O-C-N	6.38	128.98	122.09
1	A	49	PRO	N-CA-C	-6.34	101.14	111.15
1	B	19	SER	O-C-N	6.33	130.45	122.23
1	A	13	LEU	O-C-N	-6.31	115.43	122.12
1	A	65	LYS	N-CA-C	-6.29	105.09	112.89
1	A	67	PRO	N-CA-C	-6.29	105.16	113.65
1	B	49	PRO	CA-CB-CG	6.29	116.45	104.50
1	A	14	LEU	CA-C-N	-6.26	112.40	122.23
1	A	14	LEU	C-N-CA	-6.26	112.40	122.23
1	B	29	GLU	O-C-N	-6.22	114.16	121.32
1	A	41	MET	CB-CA-C	6.21	120.70	110.90
1	A	47	SER	N-CA-C	-6.21	105.67	113.18
1	A	66	SER	CA-C-N	6.20	126.10	119.28
1	A	66	SER	C-N-CA	6.20	126.10	119.28
1	A	11	GLU	CA-C-O	-6.18	113.86	120.42
1	B	58	LYS	CA-C-O	-6.16	114.35	120.82
1	A	28	PHE	CG-CD2-CE2	-6.14	110.27	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	VAL	CA-C-O	6.13	126.87	120.25
1	A	59	LEU	CA-CB-CG	6.12	137.73	116.30
1	B	22	GLU	O-C-N	6.12	129.15	122.11
1	B	58	LYS	CB-CG-CD	-6.12	97.23	111.30
1	B	12	ASN	O-C-N	6.10	129.10	122.15
1	B	23	THR	O-C-N	6.10	128.35	122.07
1	A	40	GLN	O-C-N	-6.07	115.68	122.12
1	A	5	ARG	CB-CA-C	6.07	120.86	110.79
1	B	29	GLU	OE1-CD-OE2	-6.05	108.38	122.90
1	B	35	LYS	O-C-N	-6.04	115.26	122.15
1	A	69	CYS	CB-CA-C	-6.04	101.29	110.83
1	A	11	GLU	O-C-N	6.00	128.99	122.15
1	A	56	ILE	CG1-CB-CG2	6.00	128.71	110.70
1	A	54	GLU	CA-CB-CG	-6.00	102.11	114.10
1	B	19	SER	N-CA-CB	-5.99	101.27	110.20
1	B	58	LYS	CD-CE-NZ	-5.98	92.75	111.90
1	A	34	MET	CB-CA-C	-5.97	101.51	110.88
1	A	8	HIS	CE1-NE2-CD2	5.94	114.94	109.00
1	A	44	VAL	CB-CA-C	5.92	121.85	112.26
1	A	26	LYS	N-CA-C	5.89	119.30	111.75
1	A	2	ILE	CA-C-N	5.87	136.11	121.80
1	A	2	ILE	C-N-CA	5.87	136.11	121.80
1	A	19	SER	CA-C-N	5.87	128.94	120.79
1	A	19	SER	C-N-CA	5.87	128.94	120.79
1	A	53	ARG	CB-CA-C	5.86	120.07	110.88
1	B	28	PHE	CD1-CE1-CZ	5.85	130.53	120.00
1	A	36	ASP	O-C-N	5.83	129.45	122.27
1	B	39	MET	CG-SD-CE	5.83	113.72	100.90
1	A	12	ASN	CA-C-O	-5.82	114.25	120.42
1	A	54	GLU	CA-C-N	-5.81	112.04	120.29
1	A	54	GLU	C-N-CA	-5.81	112.04	120.29
1	B	44	VAL	N-CA-C	5.81	118.35	111.09
1	B	1	GLY	O-C-N	-5.79	113.74	123.00
1	B	22	GLU	CA-C-N	-5.77	112.94	120.44
1	B	22	GLU	C-N-CA	-5.77	112.94	120.44
1	A	33	THR	CA-C-N	5.76	127.92	120.44
1	A	33	THR	C-N-CA	5.76	127.92	120.44
1	A	70	MET	CG-SD-CE	5.74	113.53	100.90
1	B	22	GLU	CA-C-O	-5.74	114.49	120.92
1	B	9	VAL	N-CA-CB	-5.71	103.87	110.55
1	A	24	SER	CB-CA-C	-5.70	101.16	110.85
1	A	11	GLU	N-CA-C	5.69	117.56	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	GLU	CA-C-N	-5.68	111.51	120.60
1	B	54	GLU	C-N-CA	-5.68	111.51	120.60
1	A	24	SER	O-C-N	-5.68	115.68	122.15
1	A	23	THR	CA-CB-CG2	5.67	120.14	110.50
1	A	10	ILE	CB-CG1-CD1	5.65	125.66	113.80
1	A	38	GLY	CA-C-O	5.63	126.85	121.05
1	A	27	GLU	N-CA-C	-5.62	105.52	112.38
1	B	12	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	2	ILE	CB-CA-C	5.61	119.14	110.28
1	A	22	GLU	N-CA-C	5.59	118.30	111.82
1	A	3	CYS	CA-C-O	5.58	127.81	120.16
1	A	25	LEU	O-C-N	5.55	128.09	122.09
1	A	9	VAL	N-CA-CB	-5.53	103.49	110.57
1	B	61	GLU	OE1-CD-OE2	5.53	136.18	122.90
1	B	54	GLU	CG-CD-OE1	5.53	131.12	118.40
1	B	21	TYR	CA-C-N	5.52	129.11	120.82
1	B	21	TYR	C-N-CA	5.52	129.11	120.82
1	B	25	LEU	O-C-N	-5.51	116.39	122.07
1	B	58	LYS	CG-CD-CE	-5.51	98.62	111.30
1	A	68	LEU	CB-CG-CD2	5.51	127.23	110.70
1	B	60	THR	O-C-N	-5.49	116.33	122.03
1	B	53	ARG	CG-CD-NE	5.48	124.06	112.00
1	B	48	LEU	N-CA-CB	5.48	117.44	110.04
1	B	57	MET	CA-CB-CG	5.48	125.05	114.10
1	B	25	LEU	CB-CG-CD2	5.47	127.12	110.70
1	A	34	MET	CB-CG-SD	5.46	129.09	112.70
1	A	64	VAL	CA-C-O	-5.46	114.57	120.47
1	A	5	ARG	CD-NE-CZ	-5.46	116.76	124.40
1	A	53	ARG	CB-CG-CD	5.45	123.83	111.30
1	A	61	GLU	CA-C-O	-5.44	115.08	120.90
1	B	3	CYS	CA-CB-SG	5.42	126.87	114.40
1	A	62	LYS	CA-C-O	5.42	126.30	120.55
1	A	42	LYS	CD-CE-NZ	-5.41	94.58	111.90
1	A	49	PRO	N-CD-CG	-5.40	95.10	103.20
1	B	8	HIS	N-CA-C	-5.39	105.31	111.14
1	B	30	PRO	CA-C-N	5.36	132.91	121.45
1	B	30	PRO	C-N-CA	5.36	132.91	121.45
1	B	6	PHE	CA-C-O	-5.35	114.75	120.42
1	A	3	CYS	N-CA-CB	5.35	119.89	110.37
1	A	39	MET	N-CA-CB	-5.35	102.26	110.12
1	A	46	ASP	CB-CA-C	5.34	121.06	110.17
1	A	62	LYS	CG-CD-CE	-5.34	99.03	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	MET	CA-C-N	5.33	127.87	120.29
1	A	57	MET	C-N-CA	5.33	127.87	120.29
1	B	61	GLU	CA-C-N	-5.33	112.72	120.29
1	B	61	GLU	C-N-CA	-5.33	112.72	120.29
1	B	8	HIS	CA-CB-CG	-5.32	108.48	113.80
1	B	52	THR	CA-C-N	5.31	127.93	120.28
1	B	52	THR	C-N-CA	5.31	127.93	120.28
1	B	28	PHE	CA-CB-CG	-5.27	108.53	113.80
1	B	54	GLU	N-CA-CB	5.27	117.96	110.16
1	A	15	LEU	CD1-CG-CD2	-5.26	99.23	110.80
1	B	4	PRO	N-CD-CG	-5.25	95.33	103.20
1	B	32	ASP	N-CA-C	-5.25	105.46	111.07
1	B	59	LEU	N-CA-C	5.25	117.00	111.28
1	B	21	TYR	N-CA-C	5.23	116.83	111.03
1	A	22	GLU	N-CA-CB	-5.22	102.19	110.28
1	A	20	SER	CB-CA-C	5.21	119.20	110.92
1	A	31	ASP	O-C-N	-5.21	116.53	122.68
1	B	54	GLU	CG-CD-OE2	-5.21	106.42	118.40
1	A	3	CYS	O-C-N	-5.20	115.34	121.32
1	B	45	LEU	N-CA-CB	5.19	117.84	110.16
1	B	42	LYS	CA-C-N	5.17	127.16	120.44
1	B	42	LYS	C-N-CA	5.17	127.16	120.44
1	A	57	MET	CA-C-O	-5.16	115.08	120.55
1	A	26	LYS	CA-C-N	5.15	128.84	120.60
1	A	26	LYS	C-N-CA	5.15	128.84	120.60
1	B	44	VAL	CA-CB-CG1	-5.15	101.64	110.40
1	B	65	LYS	CD-CE-NZ	-5.14	95.45	111.90
1	B	8	HIS	CG-ND1-CE1	-5.14	100.56	109.30
1	A	20	SER	N-CA-CB	5.14	117.63	109.82
1	A	39	MET	CA-CB-CG	-5.13	103.83	114.10
1	A	40	GLN	CB-CG-CD	5.12	121.31	112.60
1	A	17	THR	O-C-N	5.09	132.16	121.77
1	B	36	ASP	OD1-CG-OD2	-5.09	110.69	122.90
1	B	70	MET	CB-CA-C	5.09	119.77	110.10
1	B	46	ASP	CB-CG-OD1	-5.08	106.70	118.40
1	B	17	THR	CA-CB-OG1	-5.08	101.98	109.60
1	B	33	THR	CB-CA-C	5.07	119.21	110.79
1	B	41	MET	CA-C-N	5.07	127.07	120.28
1	B	41	MET	C-N-CA	5.07	127.07	120.28
1	B	28	PHE	CB-CG-CD1	5.06	129.31	120.70
1	A	62	LYS	CD-CE-NZ	5.06	128.09	111.90
1	B	41	MET	N-CA-CB	5.06	117.34	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	THR	N-CA-CB	5.05	117.33	110.01
1	A	2	ILE	N-CA-CB	-5.03	103.42	111.58
1	B	54	GLU	CA-C-O	-5.03	115.08	120.42
1	B	51	THR	CA-CB-OG1	5.02	117.13	109.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	LEU	Mainchain
1	A	5	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	548	0	566	34	0
1	B	548	0	564	25	0
2	A	82	0	0	3	0
2	B	83	0	0	3	0
All	All	1261	0	1130	51	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 23.

All (51) 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:67:PRO:HA	1:B:70:MET:HE2	1.30	1.06
1:A:34:MET:HE2	1:B:58:LYS:HD2	1.50	0.94
1:B:67:PRO:CA	1:B:70:MET:HE2	2.11	0.81
1:A:42:LYS:HD3	1:A:46:ASP:OD1	1.84	0.76
1:A:4:PRO:HD2	1:A:5:ARG:HH22	1.50	0.74
1:A:31:ASP:OD1	1:A:34:MET:HG3	1.91	0.71
1:B:67:PRO:HA	1:B:70:MET:CE	2.16	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ASP:OD2	1:B:33:THR:HG23	1.93	0.68
1:A:13:LEU:HD13	1:A:21:TYR:CE1	2.32	0.65
1:B:9:VAL:HG22	1:B:24:SER:HB3	1.79	0.65
1:A:34:MET:CE	1:B:58:LYS:HD2	2.27	0.64
1:B:29:GLU:N	1:B:30:PRO:HD2	2.14	0.62
1:B:31:ASP:HB3	1:B:34:MET:HG3	1.82	0.62
1:A:4:PRO:HD2	1:A:5:ARG:NH2	2.14	0.61
1:A:6:PHE:CE1	1:A:10:ILE:HD11	2.34	0.61
1:B:39:MET:HA	1:B:39:MET:CE	2.33	0.57
1:A:59:LEU:HD13	1:B:34:MET:HB3	1.86	0.57
1:A:31:ASP:HB3	2:A:74:HOH:O	2.05	0.56
1:B:67:PRO:O	1:B:70:MET:HG2	2.07	0.55
1:A:14:LEU:O	1:A:15:LEU:HD23	2.07	0.55
1:B:29:GLU:N	1:B:30:PRO:CD	2.71	0.54
1:A:2:ILE:HD11	1:A:6:PHE:CD2	2.44	0.53
1:B:21:TYR:CD2	1:B:39:MET:HE3	2.44	0.53
1:B:5:ARG:HD3	1:B:27:GLU:OE2	2.09	0.53
1:A:59:LEU:HD13	1:B:34:MET:CB	2.39	0.53
1:A:62:LYS:HG3	2:A:101:HOH:O	2.10	0.51
1:A:6:PHE:CZ	1:A:10:ILE:HD11	2.46	0.51
1:A:49:PRO:O	1:A:50:GLN:C	2.54	0.50
1:A:63:ILE:HG23	1:B:28:PHE:CE1	2.46	0.50
1:B:13:LEU:HD23	2:B:108:HOH:O	2.11	0.50
1:A:34:MET:HE1	2:B:76:HOH:O	2.11	0.50
1:A:37:ALA:HB1	1:B:56:ILE:HG13	1.95	0.49
1:A:42:LYS:HG2	1:A:42:LYS:O	2.11	0.49
1:B:26:LYS:HE2	2:B:110:HOH:O	2.13	0.49
1:A:22:GLU:HG3	1:A:35:LYS:HE2	1.93	0.49
1:A:26:LYS:HE3	1:A:35:LYS:HE3	1.95	0.47
1:A:5:ARG:HG3	1:A:5:ARG:NH1	2.28	0.47
1:A:59:LEU:HD11	1:B:30:PRO:HB3	1.97	0.46
1:B:29:GLU:O	1:B:30:PRO:C	2.58	0.45
1:A:33:THR:HG22	2:A:83:HOH:O	2.16	0.45
1:A:40:GLN:HA	1:A:40:GLN:OE1	2.17	0.45
1:A:61:GLU:O	1:A:65:LYS:HB2	2.17	0.44
1:A:59:LEU:CD1	1:B:30:PRO:HB3	2.47	0.44
1:A:22:GLU:O	1:A:26:LYS:HG3	2.16	0.44
1:A:50:GLN:OE1	1:A:53:ARG:NH2	2.51	0.43
1:A:42:LYS:HD3	1:A:46:ASP:CG	2.41	0.43
1:A:48:LEU:HB2	1:A:53:ARG:HD3	2.02	0.42
1:A:12:ASN:O	1:A:16:GLY:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLU:O	1:B:65:LYS:HB2	2.21	0.41
1:A:21:TYR:CZ	1:A:25:LEU:HD11	2.56	0.40
1:B:42:LYS:NZ	1:B:46:ASP:OD2	2.53	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	68/70 (97%)	68 (100%)	0	0	100	100
1	B	68/70 (97%)	62 (91%)	4 (6%)	2 (3%)	3	0
All	All	136/140 (97%)	130 (96%)	4 (3%)	2 (2%)	8	1

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	PRO
1	B	2	ILE

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	65/65 (100%)	57 (88%)	8 (12%)	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	65/65 (100%)	52 (80%)	13 (20%)	1	0
All	All	130/130 (100%)	109 (84%)	21 (16%)	2	0

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	10	ILE
1	A	40	GLN
1	A	42	LYS
1	A	44	VAL
1	A	53	ARG
1	A	68	LEU
1	A	70	MET
1	B	2	ILE
1	B	14	LEU
1	B	15	LEU
1	B	26	LYS
1	B	29	GLU
1	B	32	ASP
1	B	33	THR
1	B	35	LYS
1	B	39	MET
1	B	48	LEU
1	B	61	GLU
1	B	67	PRO
1	B	68	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	12	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	55:ASN	C	56:ILE	N	1.20
1	B	19:SER	C	20:SER	N	1.18
1	B	15:LEU	C	16:GLY	N	1.13

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.