



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2017 – 10:09 PM EST

PDB ID : 2UTG  
Title : STRUCTURE AND REFINEMENT OF THE OXIDIZED P21 FORM OF  
UTEROGLOBIN AT 1.64 ANGSTROMS RESOLUTION  
Authors : Bally, R.; Delettre, J.  
Deposited on : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

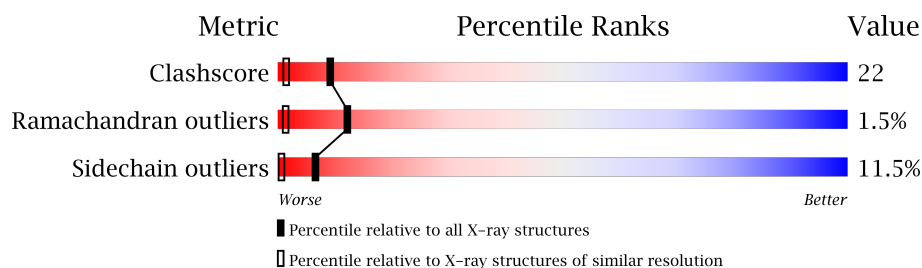
# 1 Overall quality at a glance

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	112137	2356 (1.66-1.62)
Ramachandran outliers	110173	2315 (1.66-1.62)
Sidechain outliers	110143	2315 (1.66-1.62)

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

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 and DNA 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.


Note EDS was not executed.

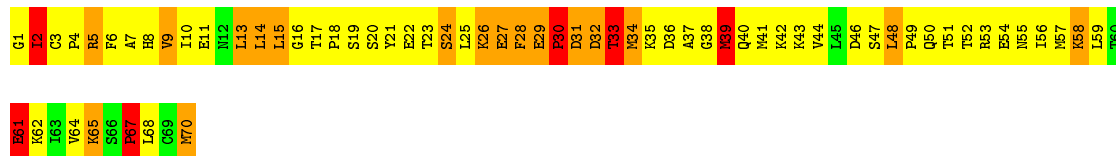
#### • Molecule 1: UTEROGLOBIN

Chain A: 



#### • Molecule 1: UTEROGLOBIN

Chain B: 



## 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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	2.92	54/556 (9.7%)	5.36	158/746 (21.2%)
1	B	2.85	44/556 (7.9%)	4.74	150/746 (20.1%)
All	All	2.89	98/1112 (8.8%)	5.06	308/1492 (20.6%)

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	2

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	18	PRO	N-CD	12.80	1.65	1.47
1	A	13	LEU	C-O	11.92	1.46	1.23
1	A	61	GLU	CD-OE2	11.90	1.38	1.25
1	A	20	SER	CB-OG	11.56	1.57	1.42
1	A	49	PRO	N-CD	11.56	1.64	1.47
1	A	22	GLU	CD-OE2	11.52	1.38	1.25
1	B	15	LEU	C-N	-11.12	1.13	1.33
1	A	45	LEU	C-O	-9.70	1.04	1.23
1	A	11	GLU	CD-OE1	-9.67	1.15	1.25
1	B	18	PRO	N-CA	-9.18	1.31	1.47
1	A	47	SER	C-O	8.93	1.40	1.23
1	A	22	GLU	CD-OE1	-8.89	1.15	1.25
1	B	29	GLU	CD-OE2	8.34	1.34	1.25
1	A	27	GLU	CD-OE1	-7.92	1.17	1.25
1	B	16	GLY	N-CA	7.76	1.57	1.46
1	A	14	LEU	N-CA	7.59	1.61	1.46
1	B	53	ARG	NE-CZ	-7.45	1.23	1.33
1	B	61	GLU	CD-OE2	7.43	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	LYS	CB-CG	7.41	1.72	1.52
1	B	46	ASP	CG-OD2	-7.31	1.08	1.25
1	B	18	PRO	C-O	-7.22	1.08	1.23
1	B	53	ARG	CZ-NH2	-7.21	1.23	1.33
1	A	21	TYR	CB-CG	7.18	1.62	1.51
1	A	22	GLU	CB-CG	-7.08	1.38	1.52
1	B	55	ASN	CG-OD1	-7.00	1.08	1.24
1	A	53	ARG	CZ-NH1	-7.00	1.24	1.33
1	B	15	LEU	C-O	7.00	1.36	1.23
1	A	13	LEU	N-CA	6.88	1.60	1.46
1	A	5	ARG	CB-CG	6.87	1.71	1.52
1	A	50	GLN	CG-CD	-6.86	1.35	1.51
1	A	42	LYS	N-CA	6.86	1.60	1.46
1	B	19	SER	C-N	-6.71	1.18	1.34
1	A	21	TYR	CE2-CZ	6.69	1.47	1.38
1	A	39	MET	N-CA	6.60	1.59	1.46
1	A	21	TYR	CG-CD2	-6.37	1.30	1.39
1	A	65	LYS	C-O	6.33	1.35	1.23
1	B	37	ALA	C-N	-6.31	1.21	1.33
1	A	42	LYS	C-O	6.26	1.35	1.23
1	A	11	GLU	CB-CG	6.23	1.64	1.52
1	B	20	SER	CA-CB	-6.07	1.43	1.52
1	A	55	ASN	C-N	-6.01	1.20	1.34
1	A	66	SER	CB-OG	-5.99	1.34	1.42
1	A	28	PHE	CG-CD2	5.97	1.47	1.38
1	A	40	GLN	CD-OE1	-5.88	1.11	1.24
1	B	36	ASP	CG-OD1	5.81	1.38	1.25
1	A	53	ARG	CZ-NH2	5.81	1.40	1.33
1	A	64	VAL	C-N	-5.79	1.20	1.34
1	B	28	PHE	CE2-CZ	5.79	1.48	1.37
1	B	27	GLU	CD-OE2	5.78	1.32	1.25
1	B	19	SER	C-O	5.76	1.34	1.23
1	A	48	LEU	C-N	-5.75	1.23	1.34
1	B	3	CYS	CB-SG	-5.75	1.72	1.81
1	A	48	LEU	N-CA	-5.73	1.34	1.46
1	A	44	VAL	CA-CB	5.73	1.66	1.54
1	B	35	LYS	CB-CG	-5.69	1.37	1.52
1	B	11	GLU	CB-CG	5.69	1.62	1.52
1	B	14	LEU	C-N	-5.66	1.21	1.34
1	A	42	LYS	CE-NZ	5.64	1.63	1.49
1	B	6	PHE	CB-CG	-5.63	1.41	1.51
1	A	5	ARG	CD-NE	5.58	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	HIS	CG-CD2	5.57	1.45	1.35
1	A	22	GLU	N-CA	5.55	1.57	1.46
1	A	19	SER	C-N	-5.54	1.21	1.34
1	A	62	LYS	CE-NZ	-5.52	1.35	1.49
1	B	47	SER	CA-CB	-5.50	1.44	1.52
1	A	36	ASP	CB-CG	-5.50	1.40	1.51
1	B	24	SER	CB-OG	-5.49	1.35	1.42
1	B	38	GLY	N-CA	5.44	1.54	1.46
1	B	19	SER	CA-CB	5.43	1.61	1.52
1	A	57	MET	CG-SD	-5.43	1.67	1.81
1	B	14	LEU	CG-CD2	-5.37	1.31	1.51
1	B	44	VAL	CA-CB	5.35	1.66	1.54
1	A	8	HIS	N-CA	5.35	1.57	1.46
1	A	47	SER	N-CA	5.35	1.57	1.46
1	A	30	PRO	C-N	-5.33	1.21	1.34
1	A	32	ASP	C-O	5.33	1.33	1.23
1	B	44	VAL	C-O	5.29	1.33	1.23
1	B	44	VAL	CB-CG1	-5.22	1.41	1.52
1	A	7	ALA	C-O	5.21	1.33	1.23
1	B	48	LEU	C-O	5.21	1.33	1.23
1	B	20	SER	CB-OG	-5.21	1.35	1.42
1	A	51	THR	CB-OG1	5.20	1.53	1.43
1	B	35	LYS	C-N	-5.17	1.22	1.34
1	A	28	PHE	CG-CD1	5.15	1.46	1.38
1	A	38	GLY	CA-C	5.13	1.60	1.51
1	B	22	GLU	CG-CD	-5.13	1.44	1.51
1	B	21	TYR	CG-CD1	-5.12	1.32	1.39
1	B	27	GLU	CG-CD	-5.12	1.44	1.51
1	A	47	SER	CB-OG	5.11	1.48	1.42
1	B	8	HIS	CB-CG	5.11	1.59	1.50
1	B	26	LYS	C-O	5.11	1.33	1.23
1	B	43	LYS	C-N	5.08	1.45	1.34
1	A	14	LEU	C-N	5.08	1.45	1.34
1	B	57	MET	C-N	-5.06	1.22	1.34
1	B	67	PRO	CA-CB	5.05	1.63	1.53
1	A	65	LYS	CD-CE	5.05	1.63	1.51
1	A	42	LYS	CA-C	-5.03	1.39	1.52
1	B	61	GLU	CD-OE1	-5.03	1.20	1.25

All (308) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ARG	NE-CZ-NH1	69.32	154.96	120.30
1	B	5	ARG	NE-CZ-NH2	45.74	143.17	120.30
1	A	53	ARG	NE-CZ-NH2	-29.86	105.37	120.30
1	B	53	ARG	NE-CZ-NH2	28.85	134.72	120.30
1	B	5	ARG	NE-CZ-NH1	-27.78	106.41	120.30
1	A	5	ARG	NE-CZ-NH2	-25.48	107.56	120.30
1	A	28	PHE	CB-CG-CD1	-21.82	105.53	120.80
1	B	36	ASP	CB-CG-OD2	21.65	137.79	118.30
1	A	46	ASP	CB-CG-OD1	-20.75	99.63	118.30
1	A	31	ASP	CB-CG-OD2	20.27	136.54	118.30
1	A	5	ARG	NE-CZ-NH1	19.50	130.05	120.30
1	B	31	ASP	CA-CB-CG	18.66	154.46	113.40
1	A	53	ARG	NH1-CZ-NH2	-17.95	99.65	119.40
1	A	57	MET	CG-SD-CE	16.34	126.35	100.20
1	B	53	ARG	NH1-CZ-NH2	-16.06	101.73	119.40
1	B	15	LEU	O-C-N	15.11	148.88	123.20
1	A	39	MET	CG-SD-CE	14.49	123.38	100.20
1	A	27	GLU	OE1-CD-OE2	13.21	139.15	123.30
1	A	40	GLN	CG-CD-OE1	-13.12	95.35	121.60
1	B	46	ASP	CB-CG-OD1	-12.88	106.70	118.30
1	B	57	MET	CG-SD-CE	12.87	120.80	100.20
1	B	29	GLU	OE1-CD-OE2	-12.43	108.38	123.30
1	A	43	LYS	O-C-N	-12.42	102.83	122.70
1	B	14	LEU	CA-CB-CG	12.39	143.79	115.30
1	B	28	PHE	CG-CD2-CE2	12.29	134.32	120.80
1	A	67	PRO	O-C-N	-12.28	103.05	122.70
1	B	33	THR	CA-CB-CG2	12.16	129.42	112.40
1	B	28	PHE	CB-CG-CD1	12.15	129.31	120.80
1	A	28	PHE	CB-CG-CD2	11.95	129.17	120.80
1	A	51	THR	CA-CB-CG2	11.92	129.09	112.40
1	A	44	VAL	O-C-N	-11.89	103.68	122.70
1	A	6	PHE	CB-CG-CD2	-11.65	112.64	120.80
1	A	55	ASN	OD1-CG-ND2	-11.58	95.26	121.90
1	B	37	ALA	C-N-CA	11.46	146.37	122.30
1	A	16	GLY	CA-C-O	11.34	141.01	120.60
1	B	26	LYS	CB-CA-C	11.33	133.05	110.40
1	B	26	LYS	CB-CG-CD	11.31	141.00	111.60
1	A	36	ASP	CB-CG-OD1	-11.14	108.27	118.30
1	A	45	LEU	O-C-N	11.00	140.30	122.70
1	A	49	PRO	O-C-N	-10.92	105.23	122.70
1	B	15	LEU	CA-C-O	-10.82	97.37	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ASP	OD1-CG-OD2	10.80	143.82	123.30
1	A	32	ASP	CB-CG-OD2	10.78	128.00	118.30
1	B	23	THR	CA-CB-OG1	-10.76	86.40	109.00
1	B	61	GLU	OE1-CD-OE2	10.73	136.18	123.30
1	A	34	MET	N-CA-CB	10.65	129.76	110.60
1	A	31	ASP	OD1-CG-OD2	-10.63	103.09	123.30
1	A	40	GLN	OE1-CD-NE2	10.53	146.12	121.90
1	A	63	ILE	O-C-N	-10.45	105.98	122.70
1	A	49	PRO	CA-C-O	10.38	145.11	120.20
1	B	29	GLU	CG-CD-OE1	10.18	138.66	118.30
1	A	32	ASP	CB-CG-OD1	-10.07	109.24	118.30
1	B	47	SER	O-C-N	-10.05	106.62	122.70
1	A	64	VAL	CA-CB-CG2	9.97	125.86	110.90
1	A	66	SER	CA-CB-OG	9.93	138.01	111.20
1	A	59	LEU	CA-CB-CG	9.75	137.73	115.30
1	B	50	GLN	CA-C-N	9.58	138.28	117.20
1	A	28	PHE	CG-CD2-CE2	-9.58	110.27	120.80
1	A	43	LYS	CA-C-O	9.57	140.19	120.10
1	B	58	LYS	N-CA-CB	9.56	127.81	110.60
1	A	68	LEU	CB-CG-CD2	9.54	127.23	111.00
1	B	50	GLN	CA-C-O	-9.50	100.14	120.10
1	A	42	LYS	CA-CB-CG	-9.48	92.53	113.40
1	B	25	LEU	CB-CG-CD2	9.48	127.12	111.00
1	B	37	ALA	O-C-N	-9.39	107.23	123.20
1	B	51	THR	O-C-N	9.37	137.69	122.70
1	A	50	GLN	CG-CD-NE2	9.33	139.08	116.70
1	A	21	TYR	CB-CG-CD2	-9.30	115.42	121.00
1	B	54	GLU	O-C-N	9.29	137.57	122.70
1	A	51	THR	OG1-CB-CG2	-9.25	88.73	110.00
1	A	61	GLU	CG-CD-OE2	9.24	136.78	118.30
1	A	35	LYS	CD-CE-NZ	9.18	132.81	111.70
1	B	37	ALA	CA-C-N	9.12	134.44	116.20
1	A	18	PRO	N-CD-CG	-9.10	89.55	103.20
1	A	27	GLU	CG-CD-OE1	-9.06	100.18	118.30
1	B	61	GLU	CG-CD-OE1	-9.04	100.21	118.30
1	A	57	MET	CB-CG-SD	9.04	139.53	112.40
1	A	36	ASP	N-CA-CB	-9.04	94.33	110.60
1	A	19	SER	CA-C-O	-9.02	101.16	120.10
1	B	61	GLU	O-C-N	8.96	137.03	122.70
1	A	50	GLN	OE1-CD-NE2	-8.95	101.31	121.90
1	B	5	ARG	NH1-CZ-NH2	-8.93	109.58	119.40
1	B	62	LYS	CB-CG-CD	8.89	134.71	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	GLU	OE1-CD-OE2	8.88	133.96	123.30
1	A	16	GLY	O-C-N	-8.84	108.56	122.70
1	A	47	SER	CA-C-O	-8.81	101.61	120.10
1	A	15	LEU	C-N-CA	-8.76	103.91	122.30
1	B	40	GLN	CG-CD-NE2	8.72	137.63	116.70
1	A	47	SER	CA-C-N	8.71	136.36	117.20
1	B	28	PHE	CD1-CE1-CZ	8.69	130.53	120.10
1	B	2	ILE	CA-C-O	-8.68	101.88	120.10
1	B	17	THR	CA-C-N	8.65	141.32	117.10
1	A	53	ARG	C-N-CA	8.57	143.13	121.70
1	A	68	LEU	O-C-N	8.49	136.28	122.70
1	B	39	MET	CG-SD-CE	8.45	113.72	100.20
1	B	3	CYS	N-CA-CB	8.39	125.70	110.60
1	A	15	LEU	O-C-N	8.38	137.46	123.20
1	B	1	GLY	CA-C-O	8.35	135.64	120.60
1	A	70	MET	CG-SD-CE	8.33	113.53	100.20
1	A	67	PRO	C-N-CA	8.32	142.50	121.70
1	B	2	ILE	CA-C-N	8.28	135.42	117.20
1	B	21	TYR	CG-CD1-CE1	8.25	127.90	121.30
1	B	21	TYR	CG-CD2-CE2	-8.24	114.71	121.30
1	B	58	LYS	CD-CE-NZ	-8.24	92.75	111.70
1	A	69	CYS	C-N-CA	8.23	142.28	121.70
1	A	22	GLU	CB-CG-CD	8.22	136.40	114.20
1	B	64	VAL	CB-CA-C	8.11	126.80	111.40
1	A	53	ARG	O-C-N	-8.10	109.74	122.70
1	B	27	GLU	CG-CD-OE2	8.10	134.50	118.30
1	A	35	LYS	O-C-N	8.02	135.53	122.70
1	A	14	LEU	N-CA-CB	-8.02	94.36	110.40
1	B	67	PRO	CA-C-O	7.99	139.38	120.20
1	A	53	ARG	CD-NE-CZ	7.94	134.72	123.60
1	B	46	ASP	OD1-CG-OD2	7.93	138.37	123.30
1	A	4	PRO	CA-N-CD	7.93	122.80	111.70
1	A	45	LEU	CB-CG-CD1	-7.91	97.55	111.00
1	B	20	SER	N-CA-CB	7.90	122.35	110.50
1	A	12	ASN	CB-CG-OD1	-7.90	105.81	121.60
1	A	56	ILE	CG1-CB-CG2	7.87	128.71	111.40
1	B	11	GLU	OE1-CD-OE2	-7.79	113.95	123.30
1	B	22	GLU	CA-CB-CG	-7.78	96.28	113.40
1	A	19	SER	CA-C-N	7.78	134.31	117.20
1	B	42	LYS	CG-CD-CE	7.77	135.20	111.90
1	B	36	ASP	CB-CG-OD1	-7.74	111.34	118.30
1	A	55	ASN	CB-CG-OD1	7.68	136.97	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	ARG	CA-CB-CG	-7.58	96.72	113.40
1	A	25	LEU	CB-CG-CD1	-7.57	98.14	111.00
1	A	50	GLN	CA-C-N	7.55	133.82	117.20
1	B	31	ASP	CB-CG-OD1	-7.55	111.50	118.30
1	A	42	LYS	CD-CE-NZ	-7.44	94.58	111.70
1	B	23	THR	CA-C-O	-7.44	104.48	120.10
1	A	23	THR	CA-CB-OG1	-7.43	93.39	109.00
1	A	28	PHE	CG-CD1-CE1	-7.42	112.64	120.80
1	A	7	ALA	N-CA-CB	-7.41	99.72	110.10
1	B	2	ILE	CB-CG1-CD1	7.35	134.49	113.90
1	A	28	PHE	CZ-CE2-CD2	7.35	128.91	120.10
1	A	35	LYS	CB-CG-CD	7.33	130.67	111.60
1	A	23	THR	O-C-N	7.33	134.43	122.70
1	B	14	LEU	O-C-N	7.26	134.32	122.70
1	B	48	LEU	CB-CA-C	-7.26	96.40	110.20
1	B	32	ASP	O-C-N	-7.26	111.09	122.70
1	A	65	LYS	CB-CA-C	7.25	124.90	110.40
1	A	28	PHE	C-N-CA	7.23	139.79	121.70
1	B	16	GLY	CA-C-O	7.22	133.59	120.60
1	B	8	HIS	CB-CA-C	7.22	124.84	110.40
1	B	68	LEU	CA-CB-CG	7.18	131.81	115.30
1	B	48	LEU	O-C-N	7.15	134.69	121.10
1	B	3	CYS	CA-CB-SG	7.15	126.87	114.00
1	A	1	GLY	O-C-N	7.15	134.13	122.70
1	A	62	LYS	CD-CE-NZ	7.12	128.09	111.70
1	B	65	LYS	CD-CE-NZ	-7.07	95.45	111.70
1	B	35	LYS	CA-CB-CG	7.05	128.92	113.40
1	B	26	LYS	CA-C-O	-7.03	105.34	120.10
1	B	28	PHE	CZ-CE2-CD2	-7.03	111.67	120.10
1	A	70	MET	CB-CA-C	-7.02	96.36	110.40
1	B	24	SER	CB-CA-C	-7.01	96.79	110.10
1	B	4	PRO	CA-C-O	-6.98	103.45	120.20
1	B	54	GLU	CA-CB-CG	6.98	128.75	113.40
1	A	68	LEU	CA-C-O	-6.97	105.46	120.10
1	B	30	PRO	N-CD-CG	-6.97	92.75	103.20
1	A	4	PRO	O-C-N	-6.96	111.56	122.70
1	A	28	PHE	CD1-CE1-CZ	6.96	128.45	120.10
1	A	4	PRO	N-CD-CG	-6.93	92.81	103.20
1	B	57	MET	CA-CB-CG	6.91	125.05	113.30
1	A	29	GLU	O-C-N	6.89	134.19	121.10
1	B	58	LYS	C-N-CA	-6.88	104.50	121.70
1	A	63	ILE	CA-C-O	6.86	134.51	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	GLU	CA-CB-CG	6.86	128.48	113.40
1	B	49	PRO	O-C-N	-6.83	111.78	122.70
1	A	11	GLU	CB-CG-CD	-6.82	95.80	114.20
1	B	9	VAL	CG1-CB-CG2	-6.81	100.00	110.90
1	B	17	THR	O-C-N	-6.80	108.19	121.10
1	B	65	LYS	CA-CB-CG	6.78	128.32	113.40
1	B	2	ILE	CB-CA-C	6.73	125.07	111.60
1	B	26	LYS	CD-CE-NZ	-6.69	96.31	111.70
1	B	40	GLN	CB-CA-C	-6.69	97.02	110.40
1	B	52	THR	OG1-CB-CG2	-6.69	94.62	110.00
1	B	18	PRO	O-C-N	6.68	133.40	122.70
1	B	54	GLU	CB-CA-C	-6.68	97.04	110.40
1	A	13	LEU	N-CA-CB	-6.68	97.04	110.40
1	A	6	PHE	CB-CG-CD1	6.67	125.47	120.80
1	A	47	SER	CB-CA-C	6.64	122.71	110.10
1	B	36	ASP	OD1-CG-OD2	-6.64	110.69	123.30
1	B	44	VAL	O-C-N	-6.62	112.11	122.70
1	A	36	ASP	C-N-CA	-6.61	105.18	121.70
1	B	70	MET	CA-C-O	-6.59	106.27	120.10
1	B	35	LYS	CA-C-N	6.53	131.57	117.20
1	B	67	PRO	O-C-N	-6.53	112.25	122.70
1	B	25	LEU	CA-CB-CG	6.53	130.32	115.30
1	B	25	LEU	CB-CG-CD1	6.49	122.03	111.00
1	B	20	SER	CA-CB-OG	6.48	128.70	111.20
1	B	25	LEU	C-N-CA	6.47	137.87	121.70
1	A	61	GLU	OE1-CD-OE2	-6.43	115.59	123.30
1	B	54	GLU	CG-CD-OE1	6.41	131.12	118.30
1	A	36	ASP	CA-CB-CG	6.39	127.45	113.40
1	B	4	PRO	O-C-N	6.36	132.88	122.70
1	B	29	GLU	CA-CB-CG	6.32	127.30	113.40
1	A	12	ASN	CB-CG-ND2	6.32	131.86	116.70
1	B	33	THR	CA-CB-OG1	-6.28	95.81	109.00
1	A	65	LYS	CA-CB-CG	6.26	127.17	113.40
1	B	3	CYS	CB-CA-C	-6.25	97.90	110.40
1	B	61	GLU	CA-CB-CG	-6.25	99.65	113.40
1	B	21	TYR	CD1-CE1-CZ	-6.25	114.18	119.80
1	B	32	ASP	CA-C-O	6.24	133.21	120.10
1	A	44	VAL	CA-C-O	6.22	133.17	120.10
1	A	8	HIS	CA-CB-CG	6.21	124.15	113.60
1	A	62	LYS	N-CA-CB	-6.20	99.44	110.60
1	B	5	ARG	O-C-N	-6.20	112.79	122.70
1	A	44	VAL	N-CA-CB	-6.19	97.88	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	THR	CA-CB-OG1	-6.19	96.00	109.00
1	B	23	THR	OG1-CB-CG2	6.18	124.22	110.00
1	B	58	LYS	O-C-N	6.18	132.59	122.70
1	B	44	VAL	CA-CB-CG1	-6.17	101.64	110.90
1	A	27	GLU	O-C-N	-6.16	112.84	122.70
1	B	19	SER	N-CA-CB	-6.15	101.27	110.50
1	B	41	MET	O-C-N	-6.15	112.86	122.70
1	A	15	LEU	CB-CG-CD1	6.14	121.43	111.00
1	B	61	GLU	CA-C-N	-6.13	103.71	117.20
1	B	49	PRO	CA-CB-CG	6.13	116.45	104.80
1	B	47	SER	CA-C-N	6.12	130.66	117.20
1	B	10	ILE	O-C-N	-6.11	112.93	122.70
1	B	59	LEU	CA-C-O	6.09	132.89	120.10
1	B	13	LEU	CB-CG-CD2	-6.09	100.65	111.00
1	B	16	GLY	O-C-N	-6.03	113.05	122.70
1	A	50	GLN	CA-C-O	-6.02	107.45	120.10
1	B	53	ARG	CA-C-N	-5.97	104.07	117.20
1	B	13	LEU	CA-CB-CG	-5.96	101.58	115.30
1	A	22	GLU	OE1-CD-OE2	5.94	130.43	123.30
1	B	54	GLU	CG-CD-OE2	-5.94	106.42	118.30
1	A	49	PRO	CB-CA-C	5.89	126.73	112.00
1	B	59	LEU	N-CA-CB	-5.87	98.66	110.40
1	B	25	LEU	CD1-CG-CD2	-5.87	92.88	110.50
1	B	15	LEU	CB-CG-CD1	5.87	120.98	111.00
1	A	29	GLU	N-CA-CB	5.86	121.14	110.60
1	A	51	THR	CA-CB-OG1	-5.85	96.71	109.00
1	A	21	TYR	CZ-CE2-CD2	-5.85	114.53	119.80
1	B	18	PRO	C-N-CA	-5.84	107.09	121.70
1	B	26	LYS	N-CA-CB	-5.84	100.08	110.60
1	B	53	ARG	CG-CD-NE	5.84	124.06	111.80
1	B	19	SER	C-N-CA	5.84	136.30	121.70
1	A	9	VAL	CG1-CB-CG2	-5.83	101.57	110.90
1	B	15	LEU	CB-CG-CD2	5.83	120.91	111.00
1	A	17	THR	O-C-N	5.82	132.16	121.10
1	A	10	ILE	CA-C-O	5.81	132.30	120.10
1	A	2	ILE	C-N-CA	5.76	136.11	121.70
1	B	48	LEU	CA-C-O	-5.76	108.00	120.10
1	B	29	GLU	CA-C-O	5.76	132.19	120.10
1	A	26	LYS	CD-CE-NZ	-5.74	98.49	111.70
1	A	44	VAL	CG1-CB-CG2	5.68	120.00	110.90
1	B	2	ILE	CA-CB-CG1	5.67	121.78	111.00
1	A	61	GLU	CB-CG-CD	-5.66	98.91	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	THR	C-N-CD	-5.66	108.14	120.60
1	A	34	MET	O-C-N	5.65	131.74	122.70
1	A	45	LEU	CA-C-N	-5.64	104.79	117.20
1	B	1	GLY	O-C-N	-5.60	113.74	122.70
1	A	7	ALA	CB-CA-C	5.57	118.46	110.10
1	A	8	HIS	N-CA-CB	5.57	120.63	110.60
1	A	39	MET	CA-CB-CG	-5.57	103.83	113.30
1	A	34	MET	CB-CG-SD	5.56	129.09	112.40
1	B	52	THR	CA-CB-OG1	5.54	120.64	109.00
1	A	23	THR	CA-CB-CG2	5.53	120.14	112.40
1	B	58	LYS	CB-CG-CD	-5.53	97.23	111.60
1	B	53	ARG	CD-NE-CZ	5.52	131.33	123.60
1	A	44	VAL	CB-CA-C	5.50	121.85	111.40
1	A	12	ASN	O-C-N	5.47	131.45	122.70
1	B	40	GLN	N-CA-CB	5.46	120.43	110.60
1	A	29	GLU	CB-CG-CD	5.46	128.95	114.20
1	B	34	MET	N-CA-CB	5.42	120.35	110.60
1	A	8	HIS	CB-CG-CD2	-5.41	114.02	130.80
1	A	49	PRO	N-CD-CG	-5.40	95.10	103.20
1	A	32	ASP	CA-CB-CG	-5.39	101.54	113.40
1	A	41	MET	CA-CB-CG	-5.38	104.14	113.30
1	B	59	LEU	O-C-N	-5.37	114.10	122.70
1	B	40	GLN	OE1-CD-NE2	-5.37	109.55	121.90
1	A	39	MET	O-C-N	-5.37	114.11	122.70
1	B	7	ALA	O-C-N	5.36	131.27	122.70
1	B	27	GLU	CG-CD-OE1	-5.34	107.61	118.30
1	A	5	ARG	CA-C-O	5.34	131.32	120.10
1	A	61	GLU	CG-CD-OE1	-5.33	107.63	118.30
1	B	22	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	A	46	ASP	CB-CA-C	5.33	121.06	110.40
1	B	50	GLN	C-N-CA	5.30	134.95	121.70
1	B	43	LYS	CG-CD-CE	5.28	127.75	111.90
1	A	28	PHE	CD1-CG-CD2	5.28	125.17	118.30
1	A	1	GLY	CA-C-O	-5.28	111.10	120.60
1	B	21	TYR	O-C-N	-5.27	114.27	122.70
1	B	4	PRO	N-CD-CG	-5.25	95.33	103.20
1	A	5	ARG	CB-CA-C	5.23	120.86	110.40
1	A	37	ALA	N-CA-CB	5.23	117.42	110.10
1	A	20	SER	CA-C-N	-5.22	105.72	117.20
1	A	58	LYS	C-N-CA	-5.21	108.68	121.70
1	A	21	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	63	ILE	CB-CG1-CD1	5.19	128.42	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	LEU	CD1-CG-CD2	-5.18	94.96	110.50
1	A	3	CYS	N-CA-CB	5.16	119.89	110.60
1	B	26	LYS	C-N-CA	-5.16	108.79	121.70
1	A	25	LEU	CA-C-O	-5.16	109.27	120.10
1	A	41	MET	CB-CA-C	5.15	120.70	110.40
1	A	8	HIS	CB-CG-ND1	5.14	136.05	123.20
1	A	26	LYS	CG-CD-CE	-5.14	96.48	111.90
1	A	54	GLU	CA-CB-CG	-5.13	102.11	113.40
1	A	60	THR	CA-C-O	5.12	130.85	120.10
1	B	5	ARG	N-CA-CB	5.11	119.79	110.60
1	B	23	THR	N-CA-CB	5.09	119.97	110.30
1	A	20	SER	O-C-N	5.06	130.80	122.70
1	A	69	CYS	CA-CB-SG	-5.02	104.96	114.00
1	B	57	MET	C-N-CA	5.02	134.25	121.70
1	A	70	MET	CB-CG-SD	5.00	127.41	112.40

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 ⓘ

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	561	33	0
1	B	548	0	557	25	0
2	A	82	0	0	3	0
2	B	83	0	0	2	0
All	All	1261	0	1118	49	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 22.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:HD3	1:A:46:ASP:OD1	1.84	0.76
1:B:67:PRO:HA	1:B:70:MET:CE	2.16	0.75
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: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:39:MET:HE3	1:B:39:MET:HA	1.80	0.63
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:A:34:MET:HE2	1:B:58:LYS:HD2	1.83	0.60
1:B:67:PRO:HA	1:B:70:MET:HE2	1.85	0.58
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: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: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: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:34:MET:HE1	1:B:58:LYS:HD2	1.94	0.48
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:A:49:PRO:O	1:A:50:GLN:C	2.54	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:B:67:PRO:HA	1:B:70:MET:HE1	1.98	0.44
1:A:59:LEU:CD1	1:B:30:PRO:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:61:GLU:O	1:B:65:LYS:HB2	2.21	0.41
1:B:29:GLU:O	1:B:30:PRO:C	2.58	0.41
1:A:21:TYR:CZ	1:A:25:LEU:HD11	2.56	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%)	5	0
All	All	136/140 (97%)	130 (96%)	4 (3%)	2 (2%)	12	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%)	59 (91%)	6 (9%)	11	1
1	B	65/65 (100%)	56 (86%)	9 (14%)	4	0
All	All	130/130 (100%)	115 (88%)	15 (12%)	6	0

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	10	ILE
1	A	44	VAL
1	A	65	LYS
1	A	66	SER
1	A	70	MET
1	B	2	ILE
1	B	14	LEU
1	B	15	LEU
1	B	32	ASP
1	B	33	THR
1	B	39	MET
1	B	48	LEU
1	B	61	GLU
1	B	67	PRO

Some 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 ⓘ

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

## 5.5 Carbohydrates ⓘ

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](#)

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.