



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:47 PM UTC

PDB ID : 1B04 / pdb_00001b04
Title : STRUCTURE OF THE ADENYLATION DOMAIN OF AN NAD⁺ DEPENDENT LIGASE
Authors : Singleton, M.R.; Hakansson, K.; Timson, D.J.; Wigley, D.B.
Deposited on : 1998-11-16
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

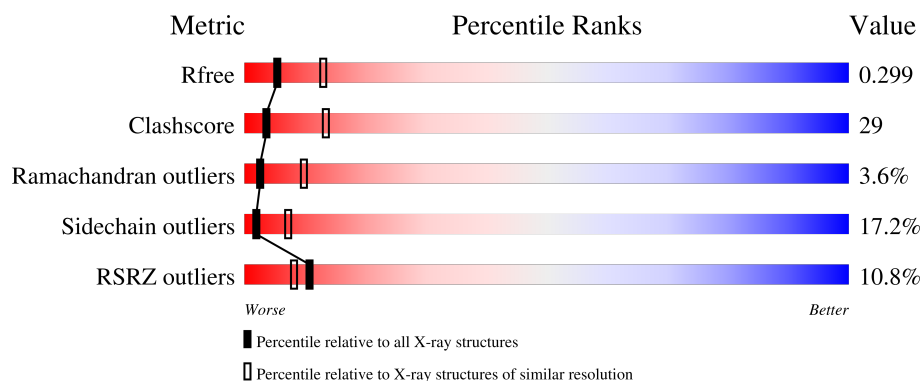
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	318	9% 35% 36% 19% 8% .
1	B	318	12% 29% 40% 20% 8% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5126 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 (DNA LIGASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2464	1547	444	467	6			
1	B	311	Total	C	N	O	S	0	0	0
			2472	1552	445	468	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	ALA	LYS	engineered mutation	UNP O87703
B	114	ALA	LYS	engineered mutation	UNP O87703

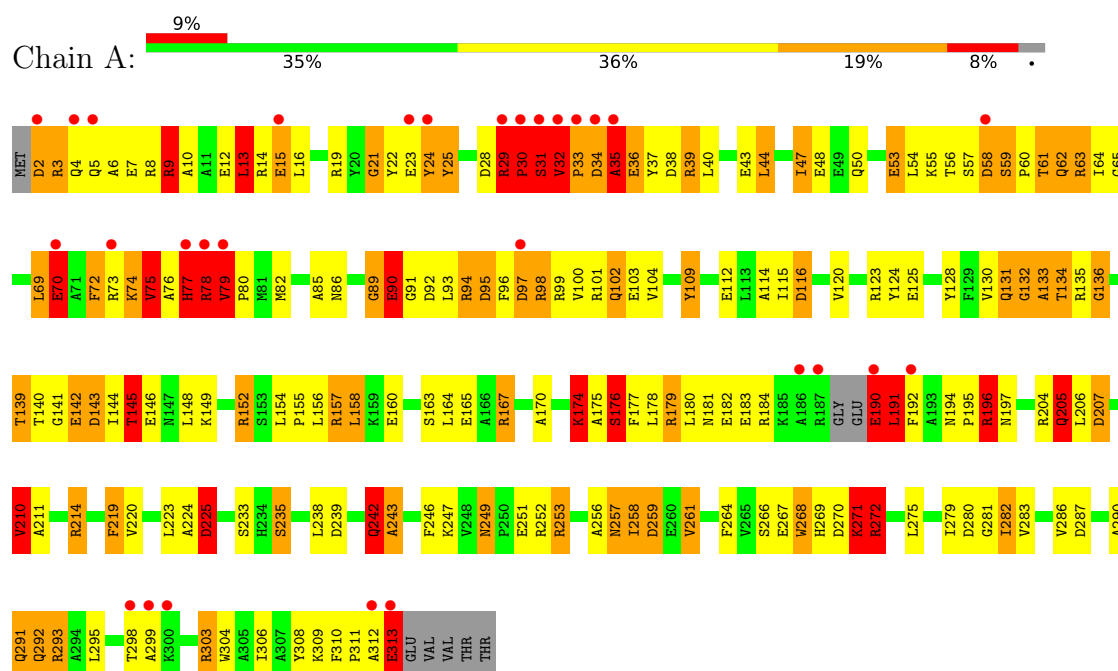
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	112	Total	O	0	0
			112	112		

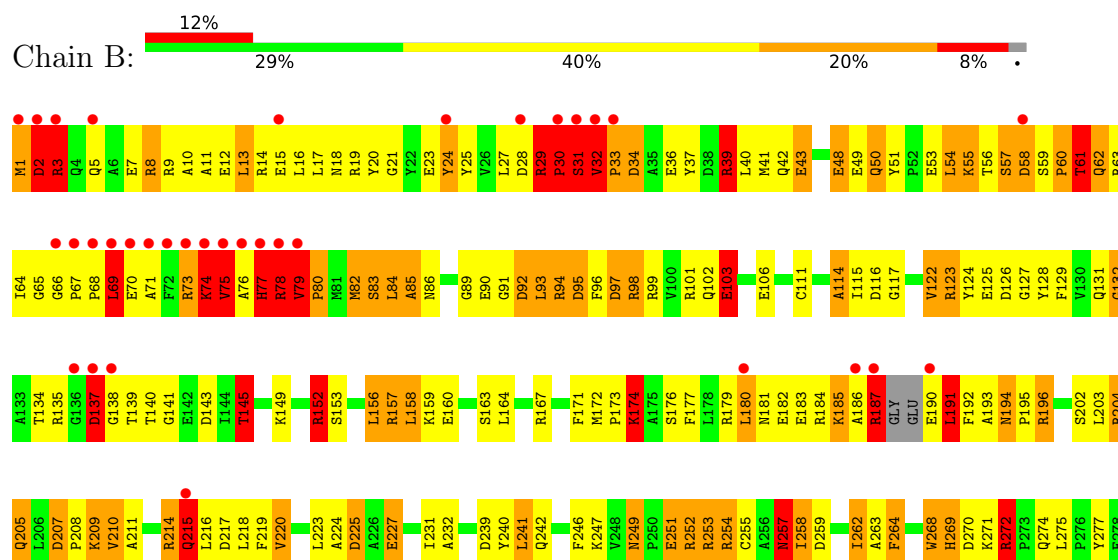
3 Residue-property plots

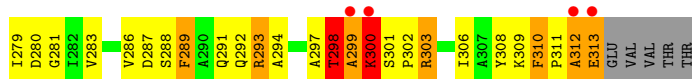
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: PROTEIN (DNA LIGASE)



• Molecule 1: PROTEIN (DNA LIGASE)





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.72Å 95.72Å 225.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.80) 97.2 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.310 0.226 , 0.299	Depositor DCC
R_{free} test set	1301 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 80.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5126	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.01	2/2511 (0.1%)	2.89	238/3393 (7.0%)
1	B	1.13	6/2519 (0.2%)	3.18	308/3403 (9.1%)
All	All	1.07	8/5030 (0.2%)	3.04	546/6796 (8.0%)

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
1	B	0	2
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	GLU	CD-OE1	8.35	1.41	1.25
1	B	32	VAL	N-CA	-7.20	1.37	1.46
1	B	78	ARG	NE-CZ	6.95	1.40	1.33
1	A	313	GLU	CG-CD	6.16	1.67	1.52
1	B	32	VAL	CA-C	-5.45	1.47	1.52
1	B	252	ARG	CD-NE	-5.10	1.39	1.46
1	B	1	MET	SD-CE	5.00	1.92	1.79
1	B	294	ALA	N-CA	-5.00	1.40	1.46

All (546) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ARG	CD-NE-CZ	33.31	171.03	124.40
1	A	19	ARG	CD-NE-CZ	33.01	170.61	124.40
1	A	179	ARG	CD-NE-CZ	32.40	169.76	124.40
1	B	252	ARG	CD-NE-CZ	26.75	161.85	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	SER	CA-C-N	23.81	166.18	122.13
1	B	31	SER	C-N-CA	23.81	166.18	122.13
1	B	77	HIS	CA-CB-CG	22.96	136.76	113.80
1	B	187	ARG	CD-NE-CZ	21.68	154.75	124.40
1	A	8	ARG	CD-NE-CZ	17.95	149.53	124.40
1	A	90	GLU	CA-C-O	-17.56	104.38	120.88
1	A	72	PHE	CA-CB-CG	15.44	129.24	113.80
1	A	34	ASP	CA-CB-CG	15.33	127.93	112.60
1	B	78	ARG	CA-C-N	15.23	150.32	122.13
1	B	78	ARG	C-N-CA	15.23	150.32	122.13
1	A	225	ASP	CA-CB-CG	-14.72	97.88	112.60
1	A	253	ARG	CD-NE-CZ	14.61	144.85	124.40
1	B	73	ARG	CD-NE-CZ	14.24	144.34	124.40
1	B	214	ARG	CD-NE-CZ	14.16	144.22	124.40
1	B	219	PHE	CA-CB-CG	14.05	127.85	113.80
1	A	196	ARG	CD-NE-CZ	13.85	143.79	124.40
1	B	225	ASP	CA-CB-CG	-13.73	98.86	112.60
1	B	8	ARG	CD-NE-CZ	13.57	143.39	124.40
1	B	98	ARG	CD-NE-CZ	13.56	143.38	124.40
1	B	32	VAL	N-CA-C	13.33	137.67	108.88
1	B	67	PRO	O-C-N	-13.19	115.24	121.31
1	B	137	ASP	CA-CB-CG	13.19	125.78	112.60
1	B	293	ARG	CA-C-N	12.74	138.38	120.29
1	B	293	ARG	C-N-CA	12.74	138.38	120.29
1	A	311	PRO	CA-C-N	12.66	145.73	121.54
1	A	311	PRO	C-N-CA	12.66	145.73	121.54
1	B	31	SER	CA-C-O	12.50	138.38	120.51
1	A	4	GLN	OE1-CD-NE2	12.44	135.04	122.60
1	A	3	ARG	CD-NE-CZ	12.29	141.61	124.40
1	A	98	ARG	CD-NE-CZ	12.24	141.54	124.40
1	A	92	ASP	N-CA-C	-12.16	96.90	112.23
1	B	31	SER	O-C-N	-12.15	106.43	122.59
1	B	293	ARG	CD-NE-CZ	11.95	141.13	124.40
1	B	101	ARG	CD-NE-CZ	11.93	141.10	124.40
1	B	32	VAL	CA-CB-CG1	11.76	130.40	110.40
1	A	30	PRO	CB-CA-C	11.76	130.96	111.56
1	A	44	LEU	N-CA-CB	11.62	126.87	109.91
1	A	76	ALA	CA-C-N	11.55	143.60	121.54
1	A	76	ALA	C-N-CA	11.55	143.60	121.54
1	A	279	ILE	CA-C-N	11.44	141.15	121.14
1	A	279	ILE	C-N-CA	11.44	141.15	121.14
1	B	98	ARG	CA-C-O	-11.38	108.49	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ARG	CA-CB-CG	11.37	136.83	114.10
1	B	272	ARG	CD-NE-CZ	11.31	140.23	124.40
1	B	280	ASP	N-CA-CB	-11.23	95.38	110.88
1	B	76	ALA	CA-C-O	-11.22	108.48	121.16
1	A	313	GLU	CB-CG-CD	-11.03	93.85	112.60
1	A	256	ALA	CA-C-O	-11.01	108.88	120.55
1	B	33	PRO	N-CA-C	-10.72	94.53	111.03
1	B	310	PHE	CA-CB-CG	10.67	124.47	113.80
1	A	143	ASP	CA-CB-CG	-10.57	102.03	112.60
1	B	78	ARG	NE-CZ-NH2	-10.57	109.69	119.20
1	B	157	ARG	NE-CZ-NH1	-10.51	110.99	121.50
1	A	299	ALA	CA-C-N	10.51	141.61	121.54
1	A	299	ALA	C-N-CA	10.51	141.61	121.54
1	B	174	LYS	CA-CB-CG	10.48	135.06	114.10
1	B	152	ARG	CD-NE-CZ	10.45	139.04	124.40
1	B	33	PRO	O-C-N	-10.30	111.17	123.01
1	B	34	ASP	CA-C-O	10.29	131.94	119.49
1	A	157	ARG	CD-NE-CZ	10.20	138.68	124.40
1	B	3	ARG	CD-NE-CZ	10.18	138.66	124.40
1	A	89	GLY	CA-C-O	-10.17	111.91	121.06
1	B	280	ASP	CA-CB-CG	-10.14	102.46	112.60
1	A	2	ASP	CA-CB-CG	10.12	122.72	112.60
1	B	312	ALA	N-CA-C	10.08	123.52	111.33
1	A	58	ASP	CA-CB-CG	10.05	122.65	112.60
1	B	49	GLU	CA-C-O	-10.04	109.78	120.42
1	B	34	ASP	CA-C-N	10.03	133.72	120.28
1	B	34	ASP	C-N-CA	10.03	133.72	120.28
1	B	99	ARG	NE-CZ-NH1	-9.96	111.54	121.50
1	A	23	GLU	CA-C-O	-9.91	109.91	120.42
1	A	44	LEU	CA-C-O	-9.90	110.61	121.00
1	A	179	ARG	NE-CZ-NH2	9.79	128.01	119.20
1	B	163	SER	CA-C-O	-9.67	110.48	120.54
1	B	99	ARG	NH1-CZ-NH2	9.57	131.74	119.30
1	B	33	PRO	CB-CA-C	9.57	123.70	111.64
1	A	313	GLU	CB-CA-C	9.56	128.27	110.10
1	B	73	ARG	CA-C-O	9.56	132.22	121.51
1	A	280	ASP	N-CA-CB	-9.42	95.04	110.40
1	B	191	LEU	N-CA-C	9.40	123.36	109.07
1	B	2	ASP	CA-C-O	-9.38	107.10	120.51
1	A	311	PRO	CA-C-O	9.22	137.38	120.60
1	B	32	VAL	N-CA-CB	-9.18	98.36	111.21
1	B	92	ASP	CA-C-O	9.18	130.28	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ARG	CD-NE-CZ	-9.09	111.67	124.40
1	A	299	ALA	CA-C-O	9.05	133.45	120.51
1	A	8	ARG	NE-CZ-NH2	8.98	127.28	119.20
1	B	60	PRO	O-C-N	-8.95	111.95	122.24
1	B	138	GLY	N-CA-C	8.92	123.49	112.79
1	A	12	GLU	CA-C-O	8.88	130.14	120.82
1	A	280	ASP	CA-CB-CG	-8.75	103.85	112.60
1	B	232	ALA	CA-C-N	8.74	136.34	122.36
1	B	232	ALA	C-N-CA	8.74	136.34	122.36
1	A	303	ARG	N-CA-C	-8.66	102.72	113.28
1	A	30	PRO	CA-C-N	8.66	138.07	121.54
1	A	30	PRO	C-N-CA	8.66	138.07	121.54
1	B	32	VAL	CA-C-N	-8.62	110.52	119.83
1	B	32	VAL	C-N-CA	-8.62	110.52	119.83
1	B	80	PRO	N-CA-C	8.62	124.70	111.34
1	A	74	LYS	N-CA-CB	8.61	123.38	110.29
1	A	21	GLY	CA-C-O	8.60	129.76	120.30
1	A	43	GLU	CA-C-O	-8.59	111.85	120.70
1	B	300	LYS	CA-CB-CG	8.52	131.13	114.10
1	B	204	ARG	NE-CZ-NH2	8.50	126.85	119.20
1	B	39	ARG	CD-NE-CZ	8.44	136.22	124.40
1	A	167	ARG	CD-NE-CZ	8.39	136.15	124.40
1	B	56	THR	N-CA-CB	-8.34	96.40	110.49
1	A	130	VAL	CB-CA-C	-8.29	102.02	111.55
1	B	41	MET	CA-C-O	8.28	129.20	120.42
1	B	94	ARG	NE-CZ-NH2	8.26	126.64	119.20
1	A	63	ARG	CD-NE-CZ	-8.24	112.87	124.40
1	A	313	GLU	OE1-CD-OE2	8.23	142.66	122.90
1	B	126	ASP	CA-CB-CG	8.12	120.72	112.60
1	B	241	LEU	CA-C-O	8.11	129.02	120.42
1	B	73	ARG	O-C-N	-8.07	112.79	122.96
1	A	35	ALA	O-C-N	-8.03	111.91	122.59
1	A	196	ARG	NE-CZ-NH1	-8.03	113.47	121.50
1	B	270	ASP	CB-CA-C	8.03	123.74	110.17
1	A	29	ARG	CG-CD-NE	8.01	129.63	112.00
1	A	30	PRO	CA-N-CD	-8.01	100.78	112.00
1	B	96	PHE	N-CA-C	-8.01	102.50	111.07
1	A	77	HIS	N-CA-C	7.99	127.83	110.80
1	B	74	LYS	CA-C-N	7.99	136.35	121.97
1	B	74	LYS	C-N-CA	7.99	136.35	121.97
1	B	291	GLN	OE1-CD-NE2	-7.98	114.62	122.60
1	B	11	ALA	CA-C-O	-7.97	112.37	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ARG	NH1-CZ-NH2	-7.95	108.97	119.30
1	B	98	ARG	NE-CZ-NH1	7.92	129.42	121.50
1	B	50	GLN	N-CA-CB	7.90	122.77	110.44
1	A	78	ARG	CD-NE-CZ	7.88	135.44	124.40
1	A	176	SER	N-CA-C	-7.86	94.05	110.80
1	B	135	ARG	NE-CZ-NH2	7.86	126.27	119.20
1	B	30	PRO	N-CA-C	7.83	128.60	112.47
1	A	98	ARG	NE-CZ-NH1	-7.80	113.70	121.50
1	A	73	ARG	NE-CZ-NH1	7.79	129.29	121.50
1	A	256	ALA	N-CA-CB	7.79	121.57	110.12
1	B	254	ARG	CD-NE-CZ	7.79	135.30	124.40
1	A	268	TRP	CA-CB-CG	-7.76	98.85	113.60
1	A	9	ARG	CD-NE-CZ	7.75	135.26	124.40
1	B	254	ARG	CA-C-O	-7.75	111.79	120.54
1	B	218	LEU	CA-C-N	-7.71	112.37	123.00
1	B	218	LEU	C-N-CA	-7.71	112.37	123.00
1	A	97	ASP	N-CA-CB	7.70	121.55	110.16
1	B	291	GLN	CG-CD-NE2	7.69	127.94	116.40
1	B	232	ALA	N-CA-C	7.69	125.14	113.61
1	A	259	ASP	CA-C-O	-7.68	112.75	120.82
1	B	313	GLU	CB-CG-CD	7.66	125.63	112.60
1	B	53	GLU	CA-CB-CG	7.66	129.41	114.10
1	A	157	ARG	O-C-N	-7.63	114.39	123.31
1	B	32	VAL	CA-CB-CG2	-7.62	97.44	110.40
1	B	207	ASP	CA-CB-CG	7.62	120.22	112.60
1	A	44	LEU	CB-CA-C	-7.57	99.30	110.96
1	A	158	LEU	N-CA-CB	-7.54	98.95	110.42
1	B	123	ARG	NE-CZ-NH2	-7.53	112.42	119.20
1	B	293	ARG	CG-CD-NE	7.52	128.55	112.00
1	B	24	TYR	N-CA-CB	7.50	121.22	110.13
1	A	219	PHE	CA-CB-CG	7.47	121.27	113.80
1	A	204	ARG	CD-NE-CZ	7.45	134.82	124.40
1	B	58	ASP	CB-CA-C	7.44	125.23	110.42
1	A	25	TYR	N-CA-C	7.43	120.26	111.71
1	A	292	GLN	OE1-CD-NE2	-7.41	115.19	122.60
1	A	86	ASN	OD1-CG-ND2	-7.40	115.20	122.60
1	A	24	TYR	N-CA-CB	7.38	122.96	110.49
1	A	39	ARG	CA-C-O	7.35	128.54	120.82
1	B	303	ARG	N-CA-C	-7.35	103.46	113.30
1	A	192	PHE	N-CA-CB	7.34	121.15	110.06
1	B	99	ARG	CG-CD-NE	7.31	128.09	112.00
1	B	159	LYS	N-CA-C	7.31	120.30	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	PRO	O-C-N	-7.30	112.78	122.64
1	A	211	ALA	CA-C-O	7.30	128.49	120.82
1	A	29	ARG	CA-C-N	7.30	128.96	119.84
1	A	29	ARG	C-N-CA	7.30	128.96	119.84
1	B	293	ARG	O-C-N	-7.29	114.51	122.09
1	A	130	VAL	CA-C-O	-7.29	112.30	120.32
1	B	84	LEU	CA-CB-CG	7.20	141.51	116.30
1	B	249	ASN	CB-CA-C	7.17	120.88	109.62
1	B	289	PHE	O-C-N	-7.17	113.45	122.27
1	B	61	THR	CA-C-O	-7.17	112.89	120.63
1	B	292	GLN	CA-CB-CG	7.17	128.44	114.10
1	B	24	TYR	CB-CA-C	-7.16	98.75	110.79
1	A	253	ARG	CB-CG-CD	7.13	127.70	111.30
1	B	173	PRO	CB-CA-C	7.13	120.51	111.39
1	B	91	GLY	O-C-N	-7.12	115.35	122.19
1	B	78	ARG	NH1-CZ-NH2	7.12	128.55	119.30
1	B	55	LYS	CG-CD-CE	7.12	127.67	111.30
1	A	31	SER	CA-C-N	7.11	135.28	122.13
1	A	31	SER	C-N-CA	7.11	135.28	122.13
1	A	131	GLN	CA-C-N	7.10	127.08	121.61
1	A	131	GLN	C-N-CA	7.10	127.08	121.61
1	B	29	ARG	CA-C-N	7.10	128.71	119.84
1	B	29	ARG	C-N-CA	7.10	128.71	119.84
1	A	190	GLU	CA-C-O	-7.08	108.76	120.80
1	B	303	ARG	NE-CZ-NH1	-7.08	114.42	121.50
1	B	56	THR	CA-CB-OG1	-7.06	99.01	109.60
1	B	117	GLY	CA-C-N	-7.06	112.35	122.94
1	B	117	GLY	C-N-CA	-7.06	112.35	122.94
1	B	98	ARG	NH1-CZ-NH2	-7.03	110.16	119.30
1	A	97	ASP	CA-CB-CG	-7.02	105.58	112.60
1	B	30	PRO	CA-C-N	7.01	134.93	121.54
1	B	30	PRO	C-N-CA	7.01	134.93	121.54
1	B	303	ARG	CD-NE-CZ	-7.00	114.59	124.40
1	B	139	THR	CA-C-O	6.99	127.53	119.35
1	A	39	ARG	CD-NE-CZ	6.98	134.17	124.40
1	A	135	ARG	N-CA-CB	6.96	120.47	110.16
1	A	58	ASP	CB-CA-C	6.95	124.25	110.42
1	B	209	LYS	CA-C-O	-6.93	110.24	119.11
1	A	9	ARG	CA-C-O	-6.90	113.23	120.55
1	B	141	GLY	CA-C-O	6.88	128.61	121.38
1	B	311	PRO	CA-C-N	6.87	129.80	120.38
1	B	311	PRO	C-N-CA	6.87	129.80	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	GLY	CA-C-O	-6.85	114.07	120.57
1	B	18	ASN	OD1-CG-ND2	-6.84	115.76	122.60
1	A	55	LYS	CA-C-N	6.82	130.39	120.71
1	A	55	LYS	C-N-CA	6.82	130.39	120.71
1	A	39	ARG	NE-CZ-NH2	-6.81	113.07	119.20
1	B	215	GLN	CB-CG-CD	6.76	124.10	112.60
1	B	215	GLN	OE1-CD-NE2	-6.75	115.84	122.60
1	B	60	PRO	CA-C-N	6.75	129.63	120.38
1	B	60	PRO	C-N-CA	6.75	129.63	120.38
1	A	34	ASP	N-CA-C	-6.75	103.64	112.41
1	B	269	HIS	CA-C-N	-6.74	112.05	122.49
1	B	269	HIS	C-N-CA	-6.74	112.05	122.49
1	A	132	GLY	CA-C-O	-6.73	115.72	121.57
1	B	246	PHE	CA-C-O	-6.72	113.79	121.72
1	B	28	ASP	CB-CA-C	6.71	120.86	111.86
1	A	207	ASP	CB-CA-C	6.71	116.81	110.17
1	B	89	GLY	O-C-N	-6.70	115.58	123.55
1	A	272	ARG	NE-CZ-NH2	6.70	125.23	119.20
1	B	32	VAL	O-C-N	-6.68	113.48	121.10
1	B	106	GLU	CB-CG-CD	6.68	123.96	112.60
1	B	60	PRO	CA-C-O	6.68	131.12	119.84
1	B	30	PRO	N-CA-CB	-6.62	96.30	103.25
1	A	145	THR	N-CA-CB	6.62	119.58	109.98
1	A	61	THR	N-CA-CB	-6.61	99.69	110.14
1	A	135	ARG	CD-NE-CZ	6.60	133.65	124.40
1	A	303	ARG	N-CA-CB	6.60	120.82	110.46
1	A	69	LEU	N-CA-C	-6.59	99.43	109.85
1	A	133	ALA	CA-C-O	-6.59	114.21	121.33
1	A	207	ASP	CA-C-O	6.59	124.89	119.36
1	B	29	ARG	CA-CB-CG	6.58	127.27	114.10
1	A	14	ARG	CD-NE-CZ	6.58	133.61	124.40
1	A	59	SER	N-CA-CB	6.57	119.16	110.29
1	B	145	THR	CA-C-O	-6.56	113.60	120.55
1	A	44	LEU	N-CA-C	-6.54	103.84	110.97
1	B	157	ARG	CG-CD-NE	-6.50	97.69	112.00
1	B	114	ALA	CA-C-O	6.50	127.53	120.58
1	A	12	GLU	CA-C-N	6.50	129.31	120.54
1	A	12	GLU	C-N-CA	6.50	129.31	120.54
1	B	95	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	96	PHE	N-CA-C	-6.49	104.29	111.36
1	B	2	ASP	O-C-N	-6.49	113.96	122.59
1	A	100	VAL	CA-C-N	6.48	129.49	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	VAL	C-N-CA	6.48	129.49	120.29
1	B	85	ALA	CA-C-O	6.48	129.78	120.51
1	A	69	LEU	CA-C-N	-6.48	112.49	122.60
1	A	69	LEU	C-N-CA	-6.48	112.49	122.60
1	A	256	ALA	O-C-N	6.46	128.97	122.12
1	B	137	ASP	CA-C-O	-6.45	111.69	119.49
1	B	242	GLN	CA-C-N	6.45	130.11	120.31
1	B	242	GLN	C-N-CA	6.45	130.11	120.31
1	A	40	LEU	CA-C-O	-6.43	113.74	120.55
1	B	277	TYR	N-CA-C	-6.42	99.55	109.24
1	B	279	ILE	CA-C-N	6.42	132.30	122.23
1	B	279	ILE	C-N-CA	6.42	132.30	122.23
1	B	297	ALA	CA-C-N	6.39	132.78	123.13
1	B	297	ALA	C-N-CA	6.39	132.78	123.13
1	B	103	GLU	CB-CG-CD	-6.38	101.75	112.60
1	B	82	MET	CA-CB-CG	6.37	126.84	114.10
1	A	34	ASP	N-CA-CB	-6.36	100.71	111.20
1	A	290	ALA	CA-C-N	-6.35	110.65	120.31
1	A	290	ALA	C-N-CA	-6.35	110.65	120.31
1	B	103	GLU	O-C-N	-6.35	114.79	122.48
1	B	255	CYS	CA-C-O	6.35	127.37	120.32
1	A	291	GLN	CB-CA-C	6.34	122.84	110.67
1	B	257	ASN	O-C-N	-6.34	116.61	123.26
1	B	73	ARG	CA-C-N	6.33	133.64	121.54
1	B	73	ARG	C-N-CA	6.33	133.64	121.54
1	B	268	TRP	CA-CB-CG	-6.33	101.56	113.60
1	B	152	ARG	CA-C-O	-6.33	113.11	120.20
1	B	37	TYR	N-CA-C	-6.33	104.30	111.07
1	B	2	ASP	CA-CB-CG	6.33	118.92	112.60
1	B	179	ARG	NE-CZ-NH1	-6.32	115.18	121.50
1	A	13	LEU	O-C-N	6.30	128.64	122.09
1	A	116	ASP	CA-CB-CG	-6.30	106.30	112.60
1	A	205	GLN	O-C-N	-6.29	115.89	122.94
1	A	77	HIS	CA-C-N	6.28	133.54	121.54
1	A	77	HIS	C-N-CA	6.28	133.54	121.54
1	B	62	GLN	CG-CD-NE2	6.28	125.81	116.40
1	B	70	GLU	CA-CB-CG	6.25	126.60	114.10
1	B	79	VAL	N-CA-CB	6.24	119.95	111.21
1	B	287	ASP	CA-CB-CG	-6.24	106.36	112.60
1	B	292	GLN	CA-C-O	-6.24	113.81	120.42
1	B	75	VAL	CA-C-O	-6.24	112.99	120.78
1	A	62	GLN	O-C-N	-6.23	114.14	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ASP	CA-C-N	6.20	128.59	120.28
1	B	225	ASP	C-N-CA	6.20	128.59	120.28
1	A	63	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	A	70	GLU	N-CA-C	-6.18	104.91	112.88
1	A	247	LYS	CA-C-N	-6.17	115.54	123.19
1	A	247	LYS	C-N-CA	-6.17	115.54	123.19
1	B	116	ASP	CA-C-O	-6.17	114.32	120.98
1	B	194	ASN	CB-CG-ND2	-6.16	107.16	116.40
1	B	262	ILE	O-C-N	-6.16	115.31	121.96
1	A	102	GLN	CG-CD-NE2	6.14	125.61	116.40
1	A	38	ASP	CA-CB-CG	-6.14	106.46	112.60
1	A	65	GLY	O-C-N	6.13	130.68	122.70
1	B	280	ASP	CA-C-O	6.13	125.65	118.90
1	B	73	ARG	N-CA-C	6.12	118.26	109.14
1	B	92	ASP	CA-C-N	6.12	128.76	120.38
1	B	92	ASP	C-N-CA	6.12	128.76	120.38
1	A	5	GLN	CB-CG-CD	6.10	122.97	112.60
1	A	282	ILE	CA-C-O	-6.10	114.11	120.64
1	B	99	ARG	CA-CB-CG	6.10	126.29	114.10
1	B	152	ARG	O-C-N	-6.09	115.26	122.20
1	B	126	ASP	N-CA-CB	6.08	121.26	111.65
1	B	8	ARG	N-CA-CB	6.07	119.05	109.82
1	B	30	PRO	O-C-N	-6.05	114.47	122.64
1	B	145	THR	CA-CB-CG2	6.04	120.78	110.50
1	A	44	LEU	O-C-N	6.04	128.31	122.03
1	B	58	ASP	O-C-N	-6.04	114.56	122.59
1	A	78	ARG	CA-C-N	6.04	133.30	122.13
1	A	78	ARG	C-N-CA	6.04	133.30	122.13
1	B	289	PHE	CA-C-O	6.04	126.91	119.97
1	A	134	THR	CA-C-O	-6.03	115.01	121.94
1	A	75	VAL	CA-C-O	6.02	126.99	120.43
1	B	2	ASP	CB-CA-C	6.02	122.40	110.42
1	A	29	ARG	N-CA-C	-6.00	96.54	109.81
1	A	32	VAL	N-CA-CB	-5.99	102.82	111.21
1	A	174	LYS	CA-C-N	5.99	131.22	122.41
1	A	174	LYS	C-N-CA	5.99	131.22	122.41
1	B	231	ILE	O-C-N	-5.99	115.88	122.83
1	B	191	LEU	N-CA-CB	-5.99	101.67	111.66
1	A	259	ASP	CA-CB-CG	-5.98	106.62	112.60
1	B	303	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	B	78	ARG	CD-NE-CZ	-5.98	116.03	124.40
1	B	252	ARG	NE-CZ-NH2	-5.98	113.82	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	MET	CG-SD-CE	-5.96	87.78	100.90
1	A	152	ARG	CD-NE-CZ	5.95	132.73	124.40
1	A	280	ASP	N-CA-C	5.95	120.26	112.89
1	B	193	ALA	O-C-N	-5.94	115.73	122.08
1	B	202	SER	CB-CA-C	-5.93	101.31	110.81
1	A	279	ILE	N-CA-CB	5.93	119.31	111.25
1	A	82	MET	CA-C-N	5.92	133.51	122.74
1	A	82	MET	C-N-CA	5.92	133.51	122.74
1	B	28	ASP	O-C-N	-5.89	115.51	122.58
1	A	290	ALA	CA-C-O	-5.87	114.20	120.42
1	A	103	GLU	CA-C-O	-5.87	112.74	119.60
1	B	303	ARG	CA-CB-CG	5.87	125.83	114.10
1	B	101	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	A	271	LYS	CA-C-O	5.86	126.36	119.28
1	A	116	ASP	CA-C-O	-5.85	115.03	121.58
1	B	303	ARG	N-CA-CB	5.85	119.44	110.61
1	B	78	ARG	O-C-N	-5.84	114.83	122.59
1	B	264	PHE	CA-CB-CG	5.83	119.63	113.80
1	B	134	THR	CA-C-O	5.82	128.62	121.99
1	A	182	GLU	CB-CG-CD	-5.82	102.71	112.60
1	B	157	ARG	CA-CB-CG	-5.81	102.47	114.10
1	B	79	VAL	CA-C-N	5.81	126.14	119.92
1	B	79	VAL	C-N-CA	5.81	126.14	119.92
1	B	137	ASP	CB-CA-C	-5.81	98.06	110.32
1	B	71	ALA	CB-CA-C	5.80	122.54	111.17
1	A	141	GLY	O-C-N	-5.79	117.16	123.29
1	A	177	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	72	PHE	CB-CG-CD1	5.77	130.51	120.70
1	A	225	ASP	N-CA-C	5.76	123.07	110.80
1	A	89	GLY	O-C-N	5.75	127.64	123.27
1	B	214	ARG	NH1-CZ-NH2	-5.75	111.83	119.30
1	A	72	PHE	CB-CG-CD2	-5.74	110.94	120.70
1	B	159	LYS	CA-CB-CG	-5.74	102.62	114.10
1	B	157	ARG	NH1-CZ-NH2	5.73	126.75	119.30
1	B	252	ARG	NE-CZ-NH1	5.72	127.22	121.50
1	B	242	GLN	CB-CG-CD	-5.71	102.89	112.60
1	A	223	LEU	N-CA-CB	-5.71	101.64	110.65
1	B	137	ASP	N-CA-CB	5.71	120.02	110.32
1	A	21	GLY	O-C-N	-5.70	116.07	122.28
1	B	8	ARG	N-CA-C	-5.68	104.09	111.02
1	B	270	ASP	N-CA-CB	-5.68	102.03	110.61
1	B	10	ALA	CA-C-O	5.68	126.78	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	LEU	CA-C-O	-5.67	112.42	119.28
1	B	50	GLN	CG-CD-NE2	-5.67	107.90	116.40
1	B	122	VAL	O-C-N	-5.67	117.22	122.71
1	B	211	ALA	N-CA-C	-5.67	105.01	111.07
1	B	270	ASP	OD1-CG-OD2	5.66	136.49	122.90
1	B	92	ASP	N-CA-CB	-5.66	101.80	110.12
1	A	258	ILE	CA-CB-CG1	-5.66	100.78	110.40
1	A	73	ARG	NH1-CZ-NH2	-5.65	111.95	119.30
1	A	120	VAL	O-C-N	-5.65	116.64	123.02
1	B	94	ARG	O-C-N	5.64	129.88	122.33
1	A	79	VAL	CA-C-N	5.62	125.63	119.90
1	A	79	VAL	C-N-CA	5.62	125.63	119.90
1	B	49	GLU	N-CA-C	-5.62	105.24	111.36
1	B	287	ASP	N-CA-C	5.60	117.19	111.14
1	B	298	THR	CB-CA-C	-5.60	101.83	111.23
1	B	122	VAL	CA-C-O	5.59	126.38	120.51
1	B	24	TYR	N-CA-C	-5.58	104.59	111.40
1	A	243	ALA	CA-C-O	-5.58	113.95	120.20
1	B	14	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	B	224	ALA	N-CA-C	-5.57	102.28	110.52
1	A	253	ARG	CG-CD-NE	5.56	124.23	112.00
1	A	78	ARG	N-CA-C	5.54	122.60	110.80
1	B	77	HIS	CB-CG-ND1	5.54	131.01	122.70
1	A	39	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	A	135	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	A	146	GLU	CA-C-O	-5.53	114.66	120.63
1	A	253	ARG	N-CA-CB	-5.53	101.24	111.13
1	B	55	LYS	CA-C-N	5.53	132.09	121.54
1	B	55	LYS	C-N-CA	5.53	132.09	121.54
1	A	69	LEU	N-CA-CB	5.52	120.15	111.20
1	A	131	GLN	O-C-N	-5.52	117.09	123.33
1	A	70	GLU	N-CA-CB	5.52	119.28	110.73
1	A	225	ASP	CB-CG-OD2	-5.51	105.72	118.40
1	B	174	LYS	CA-C-O	5.51	126.40	120.55
1	A	205	GLN	CB-CA-C	5.51	119.48	109.83
1	B	24	TYR	O-C-N	5.51	128.84	122.17
1	B	184	ARG	CD-NE-CZ	5.51	132.11	124.40
1	B	70	GLU	CA-C-O	5.50	126.71	120.00
1	A	139	THR	N-CA-C	-5.50	107.22	114.31
1	A	197	ASN	CB-CG-OD1	5.49	131.79	120.80
1	B	293	ARG	CB-CG-CD	5.49	123.92	111.30
1	A	242	GLN	O-C-N	-5.49	116.16	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	TYR	CA-CB-CG	5.48	123.77	113.90
1	B	286	VAL	CA-C-O	-5.47	114.78	121.13
1	B	97	ASP	CB-CG-OD1	5.45	130.94	118.40
1	B	99	ARG	N-CA-C	-5.45	105.50	111.82
1	B	54	LEU	CA-C-N	-5.45	112.73	122.32
1	B	54	LEU	C-N-CA	-5.45	112.73	122.32
1	A	30	PRO	O-C-N	-5.44	115.30	122.64
1	A	78	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	A	253	ARG	O-C-N	-5.43	116.76	123.33
1	A	309	LYS	O-C-N	-5.43	116.42	122.93
1	B	92	ASP	N-CA-C	-5.42	105.37	111.28
1	A	109	TYR	CA-C-N	5.42	130.24	123.14
1	A	109	TYR	C-N-CA	5.42	130.24	123.14
1	B	53	GLU	N-CA-C	-5.42	105.77	112.38
1	B	69	LEU	CA-C-O	5.41	126.44	120.71
1	B	71	ALA	N-CA-CB	-5.41	103.13	111.46
1	A	72	PHE	CA-C-O	-5.40	115.00	121.11
1	A	261	VAL	CA-C-N	5.40	128.15	120.53
1	A	261	VAL	C-N-CA	5.40	128.15	120.53
1	A	36	GLU	N-CA-CB	5.39	119.60	110.49
1	A	298	THR	CA-C-N	5.39	131.84	121.54
1	A	298	THR	C-N-CA	5.39	131.84	121.54
1	B	48	GLU	O-C-N	-5.39	115.64	122.27
1	A	280	ASP	OD1-CG-OD2	5.39	135.83	122.90
1	A	259	ASP	O-C-N	5.38	127.62	122.07
1	B	249	ASN	O-C-N	-5.38	116.52	121.30
1	B	56	THR	CA-CB-CG2	5.36	119.62	110.50
1	B	254	ARG	NH1-CZ-NH2	5.36	126.27	119.30
1	B	127	GLY	CA-C-N	5.35	130.10	122.72
1	B	127	GLY	C-N-CA	5.35	130.10	122.72
1	B	204	ARG	CA-C-O	5.35	125.53	119.27
1	B	43	GLU	CB-CG-CD	5.35	121.69	112.60
1	B	223	LEU	CA-C-O	-5.34	114.60	120.36
1	A	116	ASP	CB-CA-C	-5.33	102.72	111.68
1	B	187	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	B	48	GLU	CG-CD-OE2	5.32	130.65	118.40
1	B	73	ARG	CB-CG-CD	5.32	123.53	111.30
1	B	83	SER	CA-C-N	-5.32	115.27	123.14
1	B	83	SER	C-N-CA	-5.32	115.27	123.14
1	B	209	LYS	N-CA-CB	5.32	119.34	110.41
1	A	299	ALA	O-C-N	-5.30	115.53	122.59
1	B	27	LEU	CB-CA-C	-5.30	100.48	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ARG	N-CA-CB	5.30	118.50	110.28
1	A	35	ALA	CA-C-N	5.29	131.65	121.54
1	A	35	ALA	C-N-CA	5.29	131.65	121.54
1	B	64	ILE	CB-CG1-CD1	-5.28	102.72	113.80
1	B	56	THR	CA-C-O	5.28	128.05	120.51
1	B	214	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	A	133	ALA	O-C-N	5.27	129.26	123.25
1	A	8	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	204	ARG	O-C-N	-5.27	116.02	122.34
1	B	77	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	B	79	VAL	N-CA-C	5.25	120.22	108.88
1	B	176	SER	N-CA-C	-5.25	105.56	111.28
1	B	227	GLU	CA-C-O	-5.24	114.86	120.42
1	A	85	ALA	CA-C-N	-5.24	114.44	122.87
1	A	85	ALA	C-N-CA	-5.24	114.44	122.87
1	A	170	ALA	CB-CA-C	-5.24	101.21	109.80
1	A	30	PRO	N-CA-CB	-5.24	97.75	103.25
1	A	157	ARG	N-CA-CB	-5.23	101.75	110.80
1	A	47	ILE	CB-CA-C	-5.23	105.00	112.22
1	B	292	GLN	N-CA-C	-5.23	105.66	111.36
1	A	90	GLU	CA-C-N	-5.23	111.16	121.41
1	A	90	GLU	C-N-CA	-5.23	111.16	121.41
1	A	94	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	B	249	ASN	CA-C-O	5.22	124.66	119.75
1	B	68	PRO	CA-C-O	5.22	130.10	120.60
1	B	196	ARG	CD-NE-CZ	5.22	131.71	124.40
1	A	10	ALA	CA-C-N	5.21	127.69	120.29
1	A	10	ALA	C-N-CA	5.21	127.69	120.29
1	A	210	VAL	CA-CB-CG2	5.21	119.26	110.40
1	B	73	ARG	CB-CA-C	-5.21	99.05	110.67
1	A	136	GLY	CA-C-O	-5.21	115.21	121.67
1	B	167	ARG	NE-CZ-NH1	-5.21	116.30	121.50
1	A	32	VAL	CA-C-O	-5.20	112.98	119.95
1	B	194	ASN	CB-CG-OD1	5.20	131.20	120.80
1	A	270	ASP	CB-CA-C	5.19	118.68	109.65
1	A	53	GLU	CA-CB-CG	-5.19	103.72	114.10
1	B	270	ASP	CA-C-N	5.18	131.09	122.54
1	B	270	ASP	C-N-CA	5.18	131.09	122.54
1	B	254	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	A	96	PHE	CA-C-O	-5.18	114.93	120.42
1	B	312	ALA	CA-C-O	-5.18	115.04	120.63
1	A	142	GLU	CA-C-O	5.17	126.19	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ASN	CA-C-N	5.17	124.79	119.56
1	B	249	ASN	C-N-CA	5.17	124.79	119.56
1	B	9	ARG	N-CA-C	5.17	116.60	111.07
1	B	153	SER	CA-CB-OG	-5.16	100.77	111.10
1	B	258	ILE	CB-CG1-CD1	5.15	124.62	113.80
1	B	239	ASP	OD1-CG-OD2	-5.15	110.54	122.90
1	B	12	GLU	CA-C-N	5.15	127.60	120.29
1	B	12	GLU	C-N-CA	5.15	127.60	120.29
1	A	286	VAL	CA-C-O	-5.14	114.73	120.95
1	A	313	GLU	CG-CD-OE1	-5.13	106.60	118.40
1	B	280	ASP	OD1-CG-OD2	5.12	135.20	122.90
1	A	157	ARG	CG-CD-NE	-5.12	100.74	112.00
1	A	22	TYR	CA-CB-CG	-5.11	104.71	113.90
1	B	76	ALA	CB-CA-C	5.11	118.71	109.37
1	A	80	PRO	CA-C-O	-5.09	115.61	121.36
1	A	149	LYS	N-CA-CB	5.08	118.82	110.39
1	A	311	PRO	N-CA-C	5.08	122.92	112.47
1	B	54	LEU	N-CA-C	-5.07	106.88	113.16
1	B	101	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	B	24	TYR	CA-C-O	-5.06	115.14	120.55
1	A	25	TYR	CA-CB-CG	-5.05	104.81	113.90
1	A	135	ARG	CA-C-O	-5.05	115.07	120.42
1	A	286	VAL	N-CA-C	-5.05	102.17	108.84
1	B	49	GLU	N-CA-CB	5.05	117.63	110.16
1	B	129	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	204	ARG	CB-CA-C	5.04	119.07	110.56
1	A	211	ALA	CB-CA-C	-5.04	102.97	110.88
1	A	264	PHE	CA-CB-CG	5.03	118.83	113.80
1	B	288	SER	N-CA-CB	-5.02	102.36	109.85
1	A	79	VAL	N-CA-C	5.02	119.72	108.88
1	B	48	GLU	CA-C-O	5.02	125.74	119.97
1	B	67	PRO	CB-CA-C	5.01	116.10	111.39
1	A	63	ARG	CG-CD-NE	5.01	123.03	112.00
1	B	65	GLY	CA-C-N	-5.01	114.00	121.87
1	B	65	GLY	C-N-CA	-5.01	114.00	121.87
1	B	80	PRO	CA-C-O	5.00	128.21	121.95
1	B	249	ASN	N-CA-CB	-5.00	100.77	109.73
1	B	280	ASP	CB-CA-C	-5.00	100.97	109.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	GLN	Mainchain
1	A	29	ARG	Mainchain
1	B	32	VAL	Mainchain
1	B	69	LEU	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	2464	0	2429	147	1
1	B	2472	0	2440	153	1
2	A	78	0	0	5	0
2	B	112	0	0	5	0
All	All	5126	0	4869	287	1

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 29.

All (287) 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:32:VAL:HB	1:A:33:PRO:HD2	1.36	1.06
1:A:205:GLN:NE2	1:A:207:ASP:H	1.59	1.01
1:A:205:GLN:HE22	1:A:207:ASP:H	1.05	0.95
1:A:58:ASP:HB3	1:A:156:LEU:HB3	1.48	0.95
1:B:77:HIS:O	1:B:78:ARG:HB2	1.67	0.95
1:B:1:MET:SD	1:B:5:GLN:HB2	2.06	0.94
1:B:66:GLY:H	1:B:208:PRO:HB2	1.35	0.92
1:A:24:TYR:HB3	1:A:31:SER:HB3	1.54	0.87
1:A:91:GLY:O	1:A:95:ASP:OD1	1.93	0.86
1:B:257:ASN:HD22	1:B:259:ASP:H	1.22	0.85
1:B:58:ASP:HB3	1:B:156:LEU:HB3	1.56	0.85
1:A:205:GLN:HE22	1:A:207:ASP:N	1.75	0.84
1:A:3:ARG:HH21	1:A:53:GLU:HG3	1.44	0.81
1:B:257:ASN:HD21	1:B:259:ASP:HB2	1.45	0.81
1:B:180:LEU:HD23	1:B:181:ASN:N	1.96	0.80
1:A:32:VAL:HB	1:A:33:PRO:CD	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:HIS:NE2	1:B:86:ASN:N	2.30	0.78
1:A:75:VAL:HG23	1:A:77:HIS:HB2	1.66	0.78
1:A:312:ALA:O	1:A:313:GLU:C	2.27	0.77
1:B:182:GLU:HA	1:B:185:LYS:HD3	1.68	0.76
1:A:175:ALA:O	1:A:176:SER:HB2	1.84	0.76
1:A:257:ASN:HD22	1:A:259:ASP:N	1.83	0.76
1:A:257:ASN:HD22	1:A:259:ASP:H	1.31	0.75
1:B:24:TYR:OH	1:B:32:VAL:HG22	1.86	0.75
1:A:3:ARG:NH2	1:A:53:GLU:HG3	2.01	0.74
1:A:9:ARG:HG3	1:A:13:LEU:HD22	1.68	0.74
1:B:203:LEU:HD21	1:B:216:LEU:HD13	1.69	0.73
1:B:257:ASN:ND2	1:B:259:ASP:HB2	2.04	0.73
1:A:32:VAL:CB	1:A:33:PRO:HD2	2.17	0.71
1:B:132:GLY:H	1:B:145:THR:HG22	1.55	0.71
1:B:32:VAL:O	1:B:33:PRO:C	2.29	0.71
1:B:143:ASP:OD1	1:B:145:THR:HG23	1.89	0.71
1:B:32:VAL:O	1:B:32:VAL:HG12	1.91	0.70
1:B:207:ASP:HB3	1:B:210:VAL:HG13	1.74	0.70
1:B:103:GLU:HG3	2:B:595:HOH:O	1.91	0.70
1:A:77:HIS:CD2	1:B:86:ASN:H	2.10	0.69
1:A:132:GLY:H	1:A:145:THR:HG22	1.58	0.68
1:A:165:GLU:OE2	1:A:167:ARG:NH1	2.26	0.68
1:B:172:MET:HE1	1:B:180:LEU:HD13	1.75	0.68
1:B:257:ASN:HD22	1:B:259:ASP:N	1.92	0.68
1:A:97:ASP:OD1	1:A:97:ASP:O	2.11	0.68
1:B:69:LEU:HD23	1:B:208:PRO:HD3	1.76	0.67
1:B:90:GLU:OE2	1:B:94:ARG:NH1	2.26	0.67
1:B:298:THR:O	1:B:299:ALA:HB3	1.95	0.67
1:B:298:THR:HG23	1:B:303:ARG:NH1	2.09	0.67
1:A:131:GLN:HE22	1:B:86:ASN:ND2	1.93	0.67
1:B:123:ARG:NH2	1:B:125:GLU:OE2	2.24	0.67
1:A:7:GLU:HG2	1:A:54:LEU:CD2	2.25	0.67
1:A:238:LEU:HD13	1:A:252:ARG:HD2	1.77	0.66
1:A:98:ARG:HD3	2:A:630:HOH:O	1.95	0.66
1:B:180:LEU:HD11	1:B:192:PHE:CE2	2.30	0.66
1:B:185:LYS:HG2	1:B:186:ALA:N	2.10	0.66
1:A:181:ASN:HA	1:A:184:ARG:HG3	1.78	0.66
1:B:77:HIS:O	1:B:78:ARG:CB	2.42	0.65
1:B:90:GLU:HG3	1:B:262:ILE:HD13	1.78	0.65
1:B:93:LEU:HD23	1:B:262:ILE:HG12	1.77	0.65
1:A:7:GLU:HG2	1:A:54:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASN:HD22	1:A:251:GLU:H	1.45	0.64
1:B:123:ARG:HD3	2:B:447:HOH:O	1.98	0.63
1:B:180:LEU:HD21	1:B:192:PHE:HD2	1.62	0.63
1:B:33:PRO:HB2	1:B:36:GLU:HG2	1.80	0.63
1:A:136:GLY:HA3	1:A:140:THR:O	1.98	0.63
1:A:190:GLU:O	1:A:191:LEU:HB2	1.99	0.63
1:A:257:ASN:ND2	1:A:259:ASP:H	1.96	0.63
1:A:194:ASN:HD21	1:A:196:ARG:HB3	1.64	0.63
1:A:249:ASN:ND2	1:A:251:GLU:H	1.95	0.62
1:B:31:SER:N	1:B:32:VAL:HG23	2.13	0.62
1:B:180:LEU:HD12	1:B:214:ARG:HD2	1.80	0.62
1:A:184:ARG:NH2	1:A:190:GLU:HB2	2.14	0.62
1:A:32:VAL:O	1:A:33:PRO:C	2.43	0.62
1:A:257:ASN:HD21	1:A:259:ASP:HB2	1.65	0.62
1:B:227:GLU:CD	1:B:293:ARG:HH11	2.08	0.62
1:A:2:ASP:OD2	1:A:50:GLN:NE2	2.33	0.61
1:A:114:ALA:HB2	1:A:283:VAL:HG23	1.83	0.61
1:B:59:SER:OG	1:B:61:THR:HB	2.00	0.61
1:A:132:GLY:H	1:A:145:THR:CG2	2.13	0.61
1:B:48:GLU:OE1	1:B:61:THR:HG21	2.00	0.61
1:B:132:GLY:H	1:B:145:THR:CG2	2.13	0.61
1:B:73:ARG:O	1:B:74:LYS:HB2	2.00	0.61
1:B:251:GLU:HG3	1:B:268:TRP:CZ2	2.36	0.60
1:A:70:GLU:HB2	1:B:204:ARG:HH21	1.64	0.60
1:B:7:GLU:HG2	1:B:54:LEU:HD22	1.84	0.60
1:A:268:TRP:O	1:A:272:ARG:HB3	2.02	0.60
1:B:143:ASP:OD1	1:B:145:THR:CG2	2.50	0.60
1:A:132:GLY:HA3	1:A:148:LEU:HD12	1.83	0.59
1:B:220:VAL:CG1	1:B:241:LEU:HD13	2.32	0.59
1:B:32:VAL:O	1:B:32:VAL:CG1	2.45	0.59
1:A:131:GLN:HE22	1:B:86:ASN:HD22	1.49	0.59
1:B:24:TYR:CE1	1:B:32:VAL:HG21	2.37	0.59
1:A:74:LYS:HG2	1:B:137:ASP:HB3	1.84	0.58
1:A:154:LEU:HD12	1:A:155:PRO:HD2	1.85	0.58
1:B:299:ALA:O	1:B:300:LYS:HD3	2.04	0.58
1:B:30:PRO:HB3	1:B:32:VAL:CB	2.34	0.58
1:A:267:GLU:O	1:A:271:LYS:HB2	2.04	0.58
1:A:125:GLU:OE2	1:B:92:ASP:OD2	2.22	0.57
1:A:60:PRO:O	1:A:63:ARG:HG2	2.04	0.57
1:B:131:GLN:HA	1:B:145:THR:HG21	1.85	0.57
1:B:114:ALA:HB2	1:B:283:VAL:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASP:OD2	1:B:247:LYS:NZ	2.37	0.57
1:A:257:ASN:ND2	1:A:259:ASP:N	2.51	0.56
1:B:180:LEU:HD12	1:B:214:ARG:CD	2.35	0.56
1:A:184:ARG:HB2	1:A:191:LEU:HD12	1.86	0.56
1:A:235:SER:OG	1:A:287:ASP:OD2	2.19	0.56
1:A:58:ASP:HB3	1:A:156:LEU:CB	2.30	0.56
1:A:207:ASP:HB3	1:A:210:VAL:HG13	1.88	0.56
1:A:78:ARG:HD2	1:A:123:ARG:CZ	2.36	0.56
1:B:50:GLN:HG3	1:B:51:TYR:CE1	2.41	0.55
1:B:69:LEU:CD2	1:B:208:PRO:HD3	2.35	0.55
1:B:171:PHE:CZ	1:B:217:ASP:HB3	2.41	0.55
1:A:258:ILE:HD12	1:A:261:VAL:HB	1.88	0.55
1:A:134:THR:HG23	1:A:144:ILE:HD13	1.87	0.55
1:B:271:LYS:O	1:B:274:GLN:HG2	2.06	0.55
1:B:5:GLN:HG2	2:B:495:HOH:O	2.07	0.54
1:B:215:GLN:HE21	1:B:215:GLN:N	2.05	0.54
1:A:95:ASP:OD1	1:A:95:ASP:N	2.41	0.54
1:B:55:LYS:HE3	1:B:61:THR:CG2	2.38	0.54
1:A:91:GLY:O	1:A:95:ASP:CG	2.51	0.54
1:B:55:LYS:O	1:B:55:LYS:HG2	2.08	0.54
1:A:74:LYS:NZ	1:B:137:ASP:HB2	2.23	0.54
1:B:174:LYS:O	1:B:177:PHE:HB3	2.07	0.54
1:A:176:SER:HA	1:A:179:ARG:HH11	1.73	0.53
1:B:1:MET:O	1:B:2:ASP:C	2.51	0.53
1:B:257:ASN:ND2	1:B:259:ASP:H	1.99	0.53
1:A:164:LEU:C	1:A:164:LEU:HD12	2.35	0.52
1:A:194:ASN:HD21	1:A:196:ARG:CB	2.22	0.52
1:B:298:THR:HG23	1:B:303:ARG:CZ	2.39	0.52
1:A:131:GLN:NE2	1:B:86:ASN:HD22	2.07	0.52
1:A:34:ASP:O	1:A:37:TYR:HB3	2.10	0.52
1:B:63:ARG:NH1	1:B:156:LEU:HD13	2.23	0.52
1:B:30:PRO:O	1:B:31:SER:HB2	2.08	0.52
1:B:66:GLY:N	1:B:208:PRO:HB2	2.17	0.52
1:A:143:ASP:HB3	2:A:576:HOH:O	2.08	0.52
1:B:128:TYR:CE2	1:B:157:ARG:HD2	2.45	0.52
1:B:160:GLU:HA	1:B:160:GLU:OE1	2.09	0.51
1:B:180:LEU:HD23	1:B:181:ASN:H	1.72	0.51
1:A:44:LEU:HD22	1:A:48:GLU:OE2	2.09	0.51
1:A:32:VAL:O	1:A:34:ASP:N	2.43	0.51
1:B:24:TYR:HE1	1:B:32:VAL:CG1	2.23	0.51
1:A:69:LEU:O	1:A:206:LEU:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HB3	1:B:20:TYR:CE2	2.46	0.51
1:A:257:ASN:ND2	1:A:259:ASP:HB2	2.26	0.51
1:B:181:ASN:OD1	1:B:191:LEU:HG	2.10	0.51
1:A:97:ASP:OD1	1:A:101:ARG:HG3	2.11	0.50
1:B:182:GLU:O	1:B:183:GLU:C	2.54	0.50
1:B:13:LEU:HD12	1:B:40:LEU:HD22	1.92	0.50
1:A:30:PRO:HB3	1:A:32:VAL:CG1	2.42	0.49
1:B:98:ARG:O	1:B:102:GLN:HG3	2.11	0.49
1:B:111:CYS:HB3	1:B:264:PHE:CE1	2.47	0.49
1:B:298:THR:O	1:B:299:ALA:CB	2.57	0.49
1:A:15:GLU:HG2	1:A:16:LEU:N	2.26	0.49
1:A:144:ILE:HG13	1:A:148:LEU:HG	1.94	0.49
1:A:128:TYR:OH	1:A:157:ARG:NH1	2.45	0.49
1:A:142:GLU:OE2	1:B:137:ASP:OD2	2.30	0.49
1:A:194:ASN:ND2	1:A:196:ARG:N	2.61	0.49
1:B:24:TYR:HE1	1:B:32:VAL:HG11	1.76	0.49
1:A:195:PRO:O	1:A:196:ARG:C	2.55	0.49
1:A:56:THR:HG22	1:A:58:ASP:H	1.77	0.49
1:B:90:GLU:HG3	1:B:262:ILE:CD1	2.43	0.49
1:B:185:LYS:HG2	1:B:186:ALA:H	1.78	0.49
1:B:21:GLY:O	1:B:25:TYR:HB2	2.13	0.48
1:B:23:GLU:HB3	1:B:29:ARG:O	2.12	0.48
1:A:70:GLU:HB2	1:B:204:ARG:NH2	2.27	0.48
1:B:143:ASP:OD1	1:B:143:ASP:C	2.55	0.48
1:A:133:ALA:HA	1:A:142:GLU:O	2.13	0.48
1:B:182:GLU:CA	1:B:185:LYS:HD3	2.42	0.48
1:A:190:GLU:O	1:A:191:LEU:CB	2.61	0.48
1:B:203:LEU:CD2	1:B:216:LEU:HD13	2.41	0.48
1:B:269:HIS:HB2	1:B:310:PHE:CE1	2.48	0.48
1:A:143:ASP:OD1	1:A:143:ASP:C	2.55	0.48
1:B:31:SER:H	1:B:32:VAL:HG23	1.79	0.48
1:A:58:ASP:CB	1:A:156:LEU:HB3	2.32	0.48
1:A:115:ILE:HD13	1:A:219:PHE:HD2	1.78	0.48
1:A:295:LEU:O	1:A:303:ARG:HD2	2.14	0.48
1:A:48:GLU:OE1	1:A:61:THR:HG21	2.13	0.48
1:A:112:GLU:O	1:A:282:ILE:HG23	2.13	0.48
1:B:30:PRO:HB3	1:B:32:VAL:CG2	2.44	0.48
1:A:98:ARG:O	1:A:102:GLN:HG3	2.14	0.47
1:B:182:GLU:O	1:B:185:LYS:N	2.46	0.47
1:A:30:PRO:HB3	1:A:32:VAL:HG13	1.95	0.47
1:B:281:GLY:HA3	1:B:308:TYR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:O	1:A:34:ASP:HB2	2.14	0.47
1:B:2:ASP:O	1:B:3:ARG:C	2.57	0.47
1:A:143:ASP:OD1	1:A:145:THR:HG23	2.14	0.47
1:A:30:PRO:HB2	2:A:640:HOH:O	2.14	0.47
1:A:77:HIS:O	1:A:78:ARG:HB2	2.15	0.47
1:A:249:ASN:HD22	1:A:249:ASN:C	2.21	0.47
1:A:293:ARG:HG3	1:A:293:ARG:HH11	1.79	0.47
1:B:17:LEU:HD21	1:B:40:LEU:HB2	1.96	0.47
1:A:89:GLY:O	1:A:90:GLU:C	2.57	0.47
1:A:131:GLN:HA	1:A:145:THR:HG21	1.96	0.47
1:A:178:LEU:O	1:A:179:ARG:C	2.57	0.47
1:A:9:ARG:HG3	1:A:13:LEU:CD2	2.41	0.47
1:A:35:ALA:O	1:A:36:GLU:C	2.56	0.47
1:A:194:ASN:ND2	1:A:196:ARG:H	2.13	0.47
1:B:124:TYR:CE2	1:B:158:LEU:HD13	2.50	0.47
1:A:292:GLN:HG2	1:A:304:TRP:CD2	2.50	0.47
1:A:24:TYR:O	1:A:28:ASP:HA	2.15	0.47
1:B:55:LYS:HE3	1:B:61:THR:HG22	1.97	0.47
1:B:145:THR:O	1:B:149:LYS:HG3	2.16	0.47
1:B:227:GLU:CD	1:B:293:ARG:NH1	2.73	0.47
1:A:257:ASN:HD22	1:A:257:ASN:C	2.23	0.46
1:A:292:GLN:HG2	1:A:304:TRP:CG	2.49	0.46
1:A:9:ARG:O	1:A:13:LEU:HB2	2.15	0.46
1:A:97:ASP:CG	1:A:109:TYR:OH	2.59	0.46
1:B:262:ILE:O	1:B:263:ALA:C	2.56	0.46
1:A:205:GLN:HE22	1:A:207:ASP:CA	2.28	0.46
1:A:104:VAL:HG21	1:A:291:GLN:HB3	1.96	0.46
1:B:152:ARG:HD2	2:B:524:HOH:O	2.15	0.46
1:A:293:ARG:HA	1:A:293:ARG:HD3	1.81	0.46
1:B:251:GLU:HG3	1:B:268:TRP:CH2	2.50	0.46
1:B:29:ARG:O	1:B:29:ARG:HD2	2.16	0.46
1:B:268:TRP:O	1:B:272:ARG:HB3	2.15	0.46
1:A:242:GLN:O	1:A:243:ALA:C	2.58	0.45
1:B:39:ARG:O	1:B:43:GLU:HG3	2.15	0.45
1:B:73:ARG:HH21	1:B:74:LYS:HD3	1.81	0.45
1:B:194:ASN:HD21	1:B:196:ARG:HB3	1.81	0.45
1:B:1:MET:CG	1:B:5:GLN:HB2	2.46	0.45
1:B:7:GLU:HG2	1:B:54:LEU:CD2	2.45	0.45
1:B:195:PRO:HB2	2:B:637:HOH:O	2.15	0.45
1:A:239:ASP:OD1	1:A:252:ARG:NH2	2.50	0.45
1:B:74:LYS:HD2	1:B:74:LYS:HA	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLN:NE2	1:B:207:ASP:H	2.15	0.45
1:B:205:GLN:HE22	1:B:207:ASP:H	1.65	0.45
1:B:215:GLN:HE21	1:B:215:GLN:CA	2.29	0.45
1:B:24:TYR:CZ	1:B:32:VAL:CG2	3.00	0.44
1:A:56:THR:HG22	1:A:58:ASP:N	2.31	0.44
1:B:3:ARG:HG2	1:B:3:ARG:HH11	1.82	0.44
1:B:30:PRO:HB3	1:B:32:VAL:HB	1.99	0.44
1:B:32:VAL:O	1:B:34:ASP:N	2.50	0.44
1:B:95:ASP:OD1	1:B:98:ARG:NH1	2.50	0.44
1:B:180:LEU:HD11	1:B:192:PHE:HE2	1.79	0.44
1:A:7:GLU:HG2	1:A:54:LEU:HD22	2.00	0.44
1:A:59:SER:OG	1:A:61:THR:HB	2.18	0.44
1:A:238:LEU:CD1	1:A:252:ARG:HD2	2.47	0.44
1:B:252:ARG:O	1:B:252:ARG:HG3	2.16	0.44
1:A:2:ASP:O	1:A:6:ALA:N	2.45	0.44
1:A:98:ARG:HE	1:A:98:ARG:HB3	1.51	0.44
1:B:57:SER:O	1:B:62:GLN:HG3	2.17	0.44
1:B:164:LEU:HD12	1:B:164:LEU:C	2.42	0.43
1:A:132:GLY:HA3	1:A:148:LEU:CD1	2.47	0.43
1:B:214:ARG:O	1:B:215:GLN:HB2	2.17	0.43
1:B:215:GLN:HE21	1:B:215:GLN:H	1.65	0.43
1:A:258:ILE:HD12	1:A:258:ILE:HA	1.78	0.43
1:B:59:SER:O	1:B:60:PRO:C	2.61	0.43
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.18	0.43
1:B:122:VAL:HG23	1:B:122:VAL:O	2.18	0.43
1:B:187:ARG:HD2	1:B:190:GLU:OE2	2.19	0.43
1:B:303:ARG:HH11	1:B:303:ARG:HD3	1.41	0.43
1:A:143:ASP:OD1	1:A:145:THR:CG2	2.66	0.43
1:A:124:TYR:O	1:A:163:SER:HA	2.18	0.43
1:A:233:SER:HB2	2:A:482:HOH:O	2.18	0.43
1:A:268:TRP:O	1:A:269:HIS:C	2.60	0.43
1:A:32:VAL:CB	1:A:33:PRO:CD	2.82	0.43
1:A:74:LYS:HZ1	1:B:137:ASP:HB2	1.83	0.42
1:B:24:TYR:OH	1:B:32:VAL:CG2	2.62	0.42
1:B:289:PHE:HB3	1:B:293:ARG:NH1	2.33	0.42
1:A:24:TYR:HD1	1:A:29:ARG:O	2.01	0.42
1:A:63:ARG:CZ	1:A:156:LEU:HG	2.50	0.42
1:B:79:VAL:HA	1:B:80:PRO:HD2	1.85	0.42
1:B:63:ARG:CZ	1:B:156:LEU:HD13	2.49	0.42
1:A:57:SER:HA	1:A:62:GLN:NE2	2.35	0.42
1:A:214:ARG:HH11	1:A:214:ARG:HD3	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:HG21	1:A:246:PHE:CD1	2.54	0.42
1:B:24:TYR:CZ	1:B:32:VAL:HG22	2.54	0.42
1:A:174:LYS:HB2	2:A:610:HOH:O	2.20	0.42
1:B:31:SER:H	1:B:32:VAL:CG2	2.33	0.42
1:A:101:ARG:O	1:A:102:GLN:C	2.61	0.42
1:A:257:ASN:ND2	1:A:257:ASN:C	2.78	0.42
1:B:257:ASN:ND2	1:B:259:ASP:N	2.61	0.42
1:B:301:SER:O	1:B:302:PRO:C	2.63	0.41
1:A:224:ALA:O	1:A:225:ASP:C	2.63	0.41
1:B:39:ARG:HA	1:B:42:GLN:NE2	2.35	0.41
1:B:180:LEU:CD1	1:B:214:ARG:HD2	2.49	0.41
1:A:154:LEU:HD12	1:A:155:PRO:CD	2.50	0.41
1:A:269:HIS:HB2	1:A:310:PHE:CE1	2.54	0.41
1:B:24:TYR:CD1	1:B:30:PRO:HG3	2.55	0.41
1:A:268:TRP:HB2	1:A:282:ILE:HD11	2.03	0.41
1:A:281:GLY:HA3	1:A:308:TYR:O	2.21	0.41
1:B:253:ARG:HH11	1:B:253:ARG:HD2	1.55	0.41
1:A:13:LEU:HD12	1:A:13:LEU:HA	1.91	0.40
1:A:21:GLY:O	1:A:25:TYR:HB2	2.20	0.40
1:A:72:PHE:O	1:B:137:ASP:OD1	2.38	0.40
1:A:308:TYR:HE1	1:A:310:PHE:CD1	2.39	0.40
1:B:94:ARG:HH11	1:B:94:ARG:HD2	1.71	0.40
1:A:53:GLU:CD	1:A:53:GLU:H	2.27	0.40
1:A:79:VAL:HG12	1:A:167:ARG:HH22	1.85	0.40
1:B:312:ALA:O	1:B:313:GLU:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:N	1:B:31:SER:OG[7_455]	2.05	0.15

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	306/318 (96%)	270 (88%)	24 (8%)	12 (4%)	2	8
1	B	307/318 (96%)	282 (92%)	15 (5%)	10 (3%)	3	11
All	All	613/636 (96%)	552 (90%)	39 (6%)	22 (4%)	2	10

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	31	SER
1	A	32	VAL
1	A	77	HIS
1	A	78	ARG
1	A	176	SER
1	B	2	ASP
1	B	30	PRO
1	B	31	SER
1	B	75	VAL
1	B	78	ARG
1	A	35	ALA
1	A	191	LEU
1	B	74	LYS
1	B	299	ALA
1	B	32	VAL
1	A	33	PRO
1	A	79	VAL
1	A	174	LYS
1	A	180	LEU
1	B	85	ALA
1	B	300	LYS

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/259 (97%)	213 (84%)	39 (16%)	2	9
1	B	253/259 (98%)	205 (81%)	48 (19%)	1	5
All	All	505/518 (98%)	418 (83%)	87 (17%)	2	7

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	13	LEU
1	A	15	GLU
1	A	30	PRO
1	A	39	ARG
1	A	47	ILE
1	A	64	ILE
1	A	70	GLU
1	A	75	VAL
1	A	77	HIS
1	A	90	GLU
1	A	93	LEU
1	A	94	ARG
1	A	95	ASP
1	A	99	ARG
1	A	116	ASP
1	A	139	THR
1	A	145	THR
1	A	152	ARG
1	A	158	LEU
1	A	183	GLU
1	A	190	GLU
1	A	191	LEU
1	A	196	ARG
1	A	205	GLN
1	A	210	VAL
1	A	214	ARG
1	A	225	ASP
1	A	235	SER
1	A	249	ASN
1	A	253	ARG
1	A	257	ASN
1	A	266	SER
1	A	271	LYS
1	A	272	ARG

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Mol	Chain	Res	Type
1	A	275	LEU
1	A	293	ARG
1	A	306	ILE
1	A	313	GLU
1	B	2	ASP
1	B	3	ARG
1	B	8	ARG
1	B	13	LEU
1	B	15	GLU
1	B	29	ARG
1	B	30	PRO
1	B	39	ARG
1	B	57	SER
1	B	61	THR
1	B	74	LYS
1	B	75	VAL
1	B	77	HIS
1	B	79	VAL
1	B	82	MET
1	B	83	SER
1	B	84	LEU
1	B	93	LEU
1	B	97	ASP
1	B	103	GLU
1	B	115	ILE
1	B	137	ASP
1	B	140	THR
1	B	145	THR
1	B	152	ARG
1	B	156	LEU
1	B	158	LEU
1	B	174	LYS
1	B	180	LEU
1	B	185	LYS
1	B	187	ARG
1	B	191	LEU
1	B	205	GLN
1	B	209	LYS
1	B	210	VAL
1	B	215	GLN
1	B	220	VAL
1	B	225	ASP

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Mol	Chain	Res	Type
1	B	249	ASN
1	B	251	GLU
1	B	254	ARG
1	B	257	ASN
1	B	258	ILE
1	B	272	ARG
1	B	275	LEU
1	B	298	THR
1	B	306	ILE
1	B	309	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	42	GLN
1	A	194	ASN
1	A	205	GLN
1	A	249	ASN
1	A	257	ASN
1	A	291	GLN
1	B	5	GLN
1	B	42	GLN
1	B	50	GLN
1	B	86	ASN
1	B	194	ASN
1	B	205	GLN
1	B	215	GLN
1	B	249	ASN
1	B	257	ASN
1	B	291	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	310/318 (97%)	0.41	29 (9%) 14 10	6, 49, 85, 97	0
1	B	311/318 (97%)	0.33	38 (12%) 8 6	22, 39, 80, 90	0
All	All	621/636 (97%)	0.37	67 (10%) 11 8	6, 43, 82, 97	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	SER	9.0
1	B	190	GLU	8.7
1	A	313	GLU	8.2
1	B	1	MET	7.8
1	B	33	PRO	7.4
1	B	187	ARG	7.3
1	A	32	VAL	6.6
1	B	24	TYR	6.3
1	B	76	ALA	6.1
1	A	30	PRO	6.0
1	B	78	ARG	5.4
1	A	4	GLN	5.2
1	A	33	PRO	4.9
1	B	75	VAL	4.9
1	B	32	VAL	4.7
1	A	29	ARG	4.5
1	B	69	LEU	4.5
1	B	73	ARG	4.5
1	A	77	HIS	4.2
1	B	72	PHE	4.2
1	B	71	ALA	4.2
1	B	77	HIS	4.1
1	A	2	ASP	4.0
1	B	28	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	2	ASP	3.9
1	B	67	PRO	3.8
1	A	190	GLU	3.8
1	B	74	LYS	3.7
1	A	78	ARG	3.7
1	A	5	GLN	3.6
1	B	30	PRO	3.5
1	A	312	ALA	3.5
1	B	136	GLY	3.3
1	A	97	ASP	3.3
1	B	312	ALA	3.3
1	B	5	GLN	3.3
1	B	186	ALA	3.2
1	B	68	PRO	3.2
1	A	34	ASP	3.1
1	A	300	LYS	3.1
1	A	70	GLU	3.1
1	A	187	ARG	3.0
1	A	35	ALA	2.8
1	B	3	ARG	2.8
1	B	31	SER	2.8
1	B	300	LYS	2.8
1	B	215	GLN	2.8
1	B	70	GLU	2.8
1	A	24	TYR	2.8
1	A	186	ALA	2.8
1	B	79	VAL	2.7
1	B	137	ASP	2.7
1	A	298	THR	2.7
1	B	66	GLY	2.6
1	A	58	ASP	2.6
1	B	299	ALA	2.6
1	A	73	ARG	2.6
1	A	15	GLU	2.5
1	B	58	ASP	2.4
1	A	299	ALA	2.4
1	B	15	GLU	2.4
1	A	192	PHE	2.4
1	B	138	GLY	2.4
1	A	23	GLU	2.2
1	B	313	GLU	2.2
1	A	79	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	180	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.