



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:43 PM UTC

PDB ID : 1RLR / pdb_00001rlr
Title : STRUCTURE OF RIBONUCLEOTIDE REDUCTASE PROTEIN R1
Authors : Uhlin, U.; Eklund, H.
Deposited on : 1994-08-12
Resolution : 2.50 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

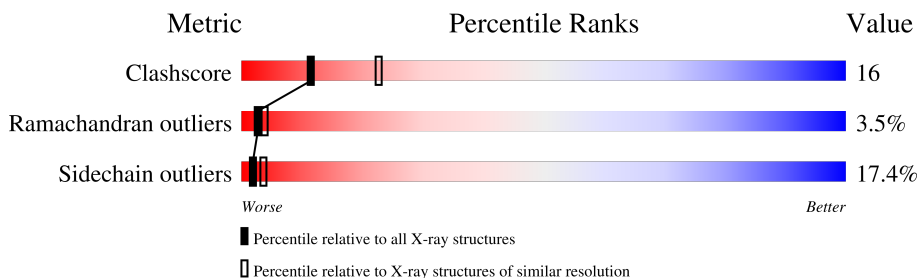
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	761	43% 36% 14% 5% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5875 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 RIBONUCLEOTIDE REDUCTASE PROTEIN R1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	0	0
			5875	3729	1007	1115	24			

There are 12 discrepancies between the modelled and reference sequences:

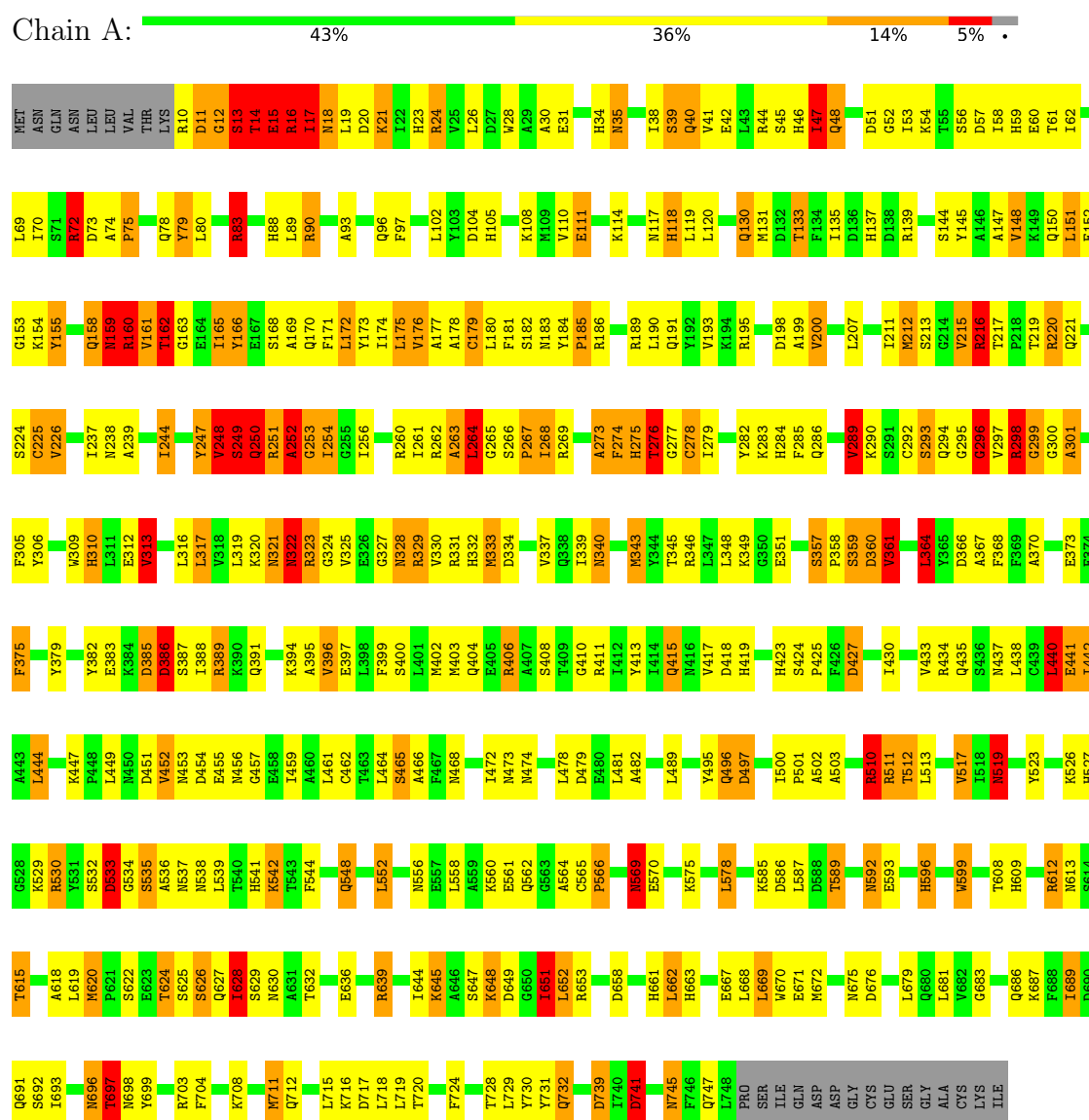
Chain	Residue	Modelled	Actual	Comment	Reference
A	479	ASP	GLU	conflict	UNP P00452
A	526	LYS	ASN	conflict	UNP P00452
A	527	HIS	ASP	conflict	UNP P00452
A	739	ASP	GLY	conflict	UNP P00452
A	740	ILE	ALA	conflict	UNP P00452
A	741	ASP	GLU	conflict	UNP P00452
A	743	LEU	ALA	conflict	UNP P00452
A	744	SER	GLN	conflict	UNP P00452
A	745	ASN	ASP	conflict	UNP P00452
A	746	PHE	ASP	conflict	UNP P00452
A	747	GLN	LEU	conflict	UNP P00452
A	748	LEU	VAL	conflict	UNP P00452

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: RIBONUCLEOTIDE REDUCTASE PROTEIN R1



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	226.00Å 226.00Å 341.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5875	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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	1.75	93/6003 (1.5%)	2.59	408/8130 (5.0%)

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	5

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	ALA	C-N	39.02	1.79	1.33
1	A	200	VAL	CA-CB	25.49	1.89	1.54
1	A	176	VAL	CA-CB	20.87	1.82	1.54
1	A	17	ILE	N-CA	16.63	1.67	1.46
1	A	274	PHE	CA-C	14.61	1.70	1.52
1	A	274	PHE	C-N	12.98	1.51	1.33
1	A	275	HIS	N-CA	12.96	1.63	1.46
1	A	18	ASN	N-CA	12.00	1.61	1.46
1	A	17	ILE	C-N	11.40	1.49	1.33
1	A	387	SER	C-N	-11.29	1.11	1.33
1	A	12	GLY	N-CA	11.25	1.61	1.45
1	A	298	ARG	N-CA	10.70	1.59	1.46
1	A	17	ILE	CA-C	10.69	1.66	1.52
1	A	17	ILE	CA-CB	10.58	1.68	1.54
1	A	263	ALA	CA-C	10.08	1.65	1.52
1	A	263	ALA	C-N	9.56	1.47	1.33
1	A	253	GLY	N-CA	9.50	1.59	1.45
1	A	296	GLY	C-N	-9.46	1.20	1.33
1	A	264	LEU	C-N	9.44	1.47	1.33
1	A	16	ARG	N-CA	-8.78	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	ILE	N-CA	8.73	1.57	1.46
1	A	13	SER	C-N	8.67	1.45	1.33
1	A	267	PRO	CA-C	8.60	1.64	1.52
1	A	16	ARG	C-N	8.40	1.45	1.33
1	A	275	HIS	CB-CG	8.32	1.61	1.50
1	A	137	HIS	CD2-NE2	-8.30	1.28	1.37
1	A	279	ILE	CA-CB	-7.90	1.50	1.54
1	A	11	ASP	CA-C	7.81	1.63	1.52
1	A	297	VAL	N-CA	-7.75	1.36	1.46
1	A	388	ILE	C-N	-7.63	1.22	1.33
1	A	275	HIS	CA-C	7.55	1.62	1.52
1	A	609	HIS	CD2-NE2	-7.45	1.29	1.37
1	A	248	VAL	N-CA	7.34	1.55	1.46
1	A	105	HIS	CD2-NE2	-7.33	1.29	1.37
1	A	59	HIS	CD2-NE2	-7.29	1.29	1.37
1	A	296	GLY	CA-C	-7.25	1.41	1.51
1	A	275	HIS	CA-CB	7.23	1.62	1.52
1	A	268	ILE	CA-C	7.12	1.61	1.52
1	A	263	ALA	N-CA	7.01	1.54	1.46
1	A	88	HIS	CD2-NE2	-6.93	1.30	1.37
1	A	13	SER	N-CA	6.91	1.54	1.46
1	A	298	ARG	CA-C	6.89	1.61	1.52
1	A	472	ILE	CA-CB	6.89	1.62	1.54
1	A	299	GLY	N-CA	6.83	1.55	1.45
1	A	155	TYR	CA-CB	-6.76	1.42	1.54
1	A	652	LEU	N-CA	6.72	1.54	1.46
1	A	360	ASP	CA-C	6.70	1.61	1.53
1	A	118	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	361	VAL	N-CA	6.60	1.54	1.46
1	A	267	PRO	N-CA	6.54	1.55	1.47
1	A	310	HIS	CD2-NE2	-6.52	1.30	1.37
1	A	12	GLY	C-O	-6.35	1.15	1.23
1	A	527	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	254	ILE	N-CA	6.29	1.53	1.46
1	A	249	SER	N-CA	-6.25	1.38	1.46
1	A	34	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	248	VAL	C-N	-6.18	1.25	1.33
1	A	297	VAL	CA-C	6.16	1.60	1.52
1	A	596	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	23	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	284	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	19	LEU	N-CA	6.05	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	SER	CA-CB	-6.03	1.44	1.53
1	A	663	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	19	LEU	CA-C	5.94	1.60	1.52
1	A	261	ILE	CA-CB	5.93	1.61	1.54
1	A	300	GLY	N-CA	5.91	1.53	1.45
1	A	359	SER	N-CA	5.89	1.54	1.46
1	A	15	GLU	CA-C	-5.87	1.45	1.52
1	A	247	TYR	CA-C	5.73	1.60	1.52
1	A	730	TYR	N-CA	-5.65	1.42	1.46
1	A	596	HIS	CG-ND1	-5.58	1.32	1.38
1	A	239	ALA	CA-CB	-5.58	1.44	1.53
1	A	18	ASN	CA-C	5.54	1.59	1.52
1	A	334	ASP	CA-CB	-5.45	1.45	1.53
1	A	618	ALA	CA-CB	-5.43	1.44	1.53
1	A	419	HIS	CD2-NE2	-5.37	1.31	1.37
1	A	252	ALA	C-N	5.33	1.41	1.33
1	A	541	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	20	ASP	N-CA	5.32	1.52	1.46
1	A	456	ASN	N-CA	5.31	1.52	1.46
1	A	269	ARG	N-CA	5.30	1.53	1.46
1	A	13	SER	CA-C	5.26	1.58	1.52
1	A	289	VAL	CA-CB	5.26	1.61	1.54
1	A	53	ILE	CA-CB	5.25	1.60	1.54
1	A	592	ASN	CA-C	5.24	1.59	1.52
1	A	299	GLY	CA-C	5.24	1.59	1.51
1	A	482	ALA	CA-CB	-5.18	1.44	1.53
1	A	661	HIS	CD2-NE2	-5.14	1.32	1.37
1	A	423	HIS	CD2-NE2	-5.11	1.32	1.37
1	A	11	ASP	N-CA	5.08	1.52	1.46
1	A	160	ARG	C-N	5.07	1.40	1.33
1	A	266	SER	CA-C	5.01	1.58	1.52

All (408) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	GLY	O-C-N	-33.93	78.59	122.70
1	A	12	GLY	CA-C-N	-29.39	81.56	123.00
1	A	12	GLY	C-N-CA	-29.39	81.56	123.00
1	A	474	ASN	CA-CB-CG	23.88	136.48	112.60
1	A	264	LEU	O-C-N	-21.17	99.09	123.22
1	A	13	SER	N-CA-C	17.89	137.56	108.41
1	A	388	ILE	O-C-N	-17.66	104.21	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	ASP	CA-CB-CG	16.75	129.35	112.60
1	A	322	ASN	OD1-CG-ND2	-15.04	107.56	122.60
1	A	275	HIS	O-C-N	14.35	142.21	122.41
1	A	14	THR	O-C-N	-14.17	103.75	122.59
1	A	248	VAL	CB-CA-C	-13.26	89.54	111.29
1	A	745	ASN	OD1-CG-ND2	-13.24	109.36	122.60
1	A	609	HIS	CA-CB-CG	-13.04	100.76	113.80
1	A	221	GLN	OE1-CD-NE2	-12.96	109.64	122.60
1	A	562	GLN	OE1-CD-NE2	-12.85	109.75	122.60
1	A	15	GLU	CA-C-N	-12.85	97.01	121.54
1	A	15	GLU	C-N-CA	-12.85	97.01	121.54
1	A	322	ASN	CB-CG-ND2	12.79	135.58	116.40
1	A	264	LEU	CA-C-O	12.76	134.96	120.54
1	A	274	PHE	N-CA-C	12.76	128.36	108.07
1	A	263	ALA	O-C-N	-12.68	106.84	122.19
1	A	741	ASP	CA-CB-CG	12.61	125.21	112.60
1	A	615	THR	N-CA-CB	12.51	133.64	111.00
1	A	275	HIS	CA-CB-CG	12.50	126.30	113.80
1	A	630	ASN	OD1-CG-ND2	-12.15	110.45	122.60
1	A	275	HIS	CA-C-N	12.08	144.61	121.54
1	A	275	HIS	C-N-CA	12.08	144.61	121.54
1	A	696	ASN	OD1-CG-ND2	-12.03	110.57	122.60
1	A	730	TYR	N-CA-CB	-12.02	100.41	111.59
1	A	387	SER	CA-C-N	11.52	139.38	122.91
1	A	387	SER	C-N-CA	11.52	139.38	122.91
1	A	16	ARG	N-CA-C	11.46	135.21	110.80
1	A	322	ASN	CA-CB-CG	11.36	123.95	112.60
1	A	279	ILE	CA-C-O	-11.33	110.10	118.71
1	A	675	ASN	OD1-CG-ND2	-11.20	111.40	122.60
1	A	473	ASN	OD1-CG-ND2	-11.18	111.42	122.60
1	A	200	VAL	N-CA-CB	11.05	129.01	110.56
1	A	496	GLN	OE1-CD-NE2	-10.83	111.77	122.60
1	A	387	SER	O-C-N	-10.82	106.63	122.43
1	A	155	TYR	CA-CB-CG	10.79	133.33	113.90
1	A	170	GLN	OE1-CD-NE2	-10.65	111.95	122.60
1	A	14	THR	CA-C-N	-10.64	101.21	121.54
1	A	14	THR	C-N-CA	-10.64	101.21	121.54
1	A	17	ILE	N-CA-CB	10.64	128.79	111.23
1	A	297	VAL	CB-CA-C	10.62	128.71	111.29
1	A	40	GLN	OE1-CD-NE2	-10.58	112.02	122.60
1	A	252	ALA	O-C-N	10.58	136.66	122.59
1	A	53	ILE	N-CA-C	10.37	122.26	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	ASN	OD1-CG-ND2	-10.33	112.27	122.60
1	A	266	SER	O-C-N	-10.20	112.97	121.44
1	A	745	ASN	CB-CG-ND2	10.12	131.58	116.40
1	A	176	VAL	CB-CA-C	-10.08	95.72	112.16
1	A	276	THR	N-CA-C	10.08	132.28	110.80
1	A	158	GLN	O-C-N	9.94	134.16	122.72
1	A	313	VAL	CB-CA-C	-9.89	98.79	112.14
1	A	730	TYR	O-C-N	-9.85	114.84	122.03
1	A	548	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	A	323	ARG	O-C-N	9.75	134.53	123.42
1	A	745	ASN	CA-CB-CG	9.59	122.19	112.60
1	A	533	ASP	N-CA-C	9.55	121.69	111.28
1	A	627	GLN	OE1-CD-NE2	-9.44	113.16	122.60
1	A	532	SER	N-CA-C	9.33	124.45	112.89
1	A	254	ILE	N-CA-C	9.32	121.16	108.11
1	A	263	ALA	N-CA-C	9.31	126.06	112.94
1	A	328	ASN	OD1-CG-ND2	-9.30	113.30	122.60
1	A	424	SER	O-C-N	-9.24	115.80	121.71
1	A	396	VAL	CB-CA-C	-9.19	99.73	112.14
1	A	698	ASN	OD1-CG-ND2	-9.07	113.53	122.60
1	A	503	ALA	N-CA-C	-8.99	101.43	111.14
1	A	118	HIS	CA-CB-CG	-8.89	104.91	113.80
1	A	618	ALA	O-C-N	-8.83	113.08	123.41
1	A	244	ILE	O-C-N	-8.82	112.43	121.96
1	A	263	ALA	CA-C-N	8.79	134.59	122.19
1	A	263	ALA	C-N-CA	8.79	134.59	122.19
1	A	13	SER	CB-CA-C	-8.78	95.58	110.16
1	A	178	ALA	O-C-N	-8.77	112.97	122.09
1	A	452	VAL	CB-CA-C	-8.70	97.02	111.29
1	A	46	HIS	CA-C-O	-8.64	111.26	120.42
1	A	273	ALA	N-CA-C	8.64	122.82	109.60
1	A	40	GLN	CG-CD-NE2	8.64	129.35	116.40
1	A	252	ALA	CA-C-N	8.64	138.34	121.41
1	A	252	ALA	C-N-CA	8.64	138.34	121.41
1	A	200	VAL	CB-CA-C	-8.60	100.72	112.24
1	A	418	ASP	CA-CB-CG	8.58	121.18	112.60
1	A	589	THR	CA-CB-OG1	-8.56	96.76	109.60
1	A	189	ARG	CB-CG-CD	-8.55	91.64	111.30
1	A	636	GLU	N-CA-C	8.46	120.42	109.93
1	A	331	ARG	N-CA-C	8.39	122.78	112.54
1	A	537	ASN	OD1-CG-ND2	-8.38	114.22	122.60
1	A	526	LYS	CB-CG-CD	-8.34	92.12	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	VAL	N-CA-CB	-8.34	97.78	111.45
1	A	273	ALA	O-C-N	-8.29	111.50	121.79
1	A	440	LEU	N-CA-C	8.28	122.83	111.90
1	A	562	GLN	CG-CD-NE2	8.27	128.81	116.40
1	A	698	ASN	CB-CG-ND2	8.24	128.77	116.40
1	A	613	ASN	OD1-CG-ND2	-8.23	114.37	122.60
1	A	696	ASN	CB-CG-ND2	8.05	128.48	116.40
1	A	274	PHE	CA-C-N	8.04	136.47	122.32
1	A	274	PHE	C-N-CA	8.04	136.47	122.32
1	A	739	ASP	CA-CB-CG	8.02	120.61	112.60
1	A	747	GLN	OE1-CD-NE2	-8.00	114.61	122.60
1	A	497	ASP	CA-CB-CG	-7.99	104.61	112.60
1	A	238	ASN	O-C-N	-7.98	113.06	122.15
1	A	321	ASN	OD1-CG-ND2	-7.98	114.62	122.60
1	A	512	THR	N-CA-C	7.97	121.44	109.25
1	A	719	LEU	O-C-N	-7.94	113.51	122.09
1	A	468	ASN	OD1-CG-ND2	-7.89	114.71	122.60
1	A	599	TRP	CG-CD2-CE3	7.85	141.75	133.90
1	A	712	GLN	OE1-CD-NE2	-7.78	114.82	122.60
1	A	13	SER	O-C-N	7.77	132.28	123.27
1	A	651	ILE	O-C-N	-7.68	114.29	122.81
1	A	411	ARG	N-CA-C	7.67	122.38	112.41
1	A	104	ASP	CA-CB-CG	7.66	120.26	112.60
1	A	48	GLN	OE1-CD-NE2	-7.60	115.00	122.60
1	A	453	ASN	OD1-CG-ND2	-7.58	115.02	122.60
1	A	671	GLU	CA-CB-CG	7.53	129.17	114.10
1	A	244	ILE	N-CA-CB	-7.48	102.76	110.62
1	A	561	GLU	N-CA-C	7.44	119.18	111.14
1	A	648	LYS	CA-C-O	7.44	128.63	119.78
1	A	627	GLN	CG-CD-NE2	7.43	127.55	116.40
1	A	732	GLN	OE1-CD-NE2	-7.43	115.17	122.60
1	A	388	ILE	CA-C-O	7.41	129.44	120.84
1	A	556	ASN	CB-CG-ND2	7.40	127.50	116.40
1	A	179	CYS	O-C-N	-7.36	114.32	122.12
1	A	530	ARG	CG-CD-NE	-7.34	95.85	112.00
1	A	578	LEU	O-C-N	-7.30	115.88	121.14
1	A	385	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	415	GLN	OE1-CD-NE2	-7.28	115.32	122.60
1	A	158	GLN	CA-C-N	7.28	135.44	121.54
1	A	158	GLN	C-N-CA	7.28	135.44	121.54
1	A	532	SER	CA-C-N	7.22	129.96	120.28
1	A	532	SER	C-N-CA	7.22	129.96	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ASN	CA-CB-CG	-7.21	105.39	112.60
1	A	323	ARG	CA-C-N	7.21	129.31	120.51
1	A	323	ARG	C-N-CA	7.21	129.31	120.51
1	A	137	HIS	CA-CB-CG	-7.20	106.60	113.80
1	A	80	LEU	CD1-CG-CD2	-7.18	95.01	110.80
1	A	544	PHE	CA-CB-CG	-7.15	106.65	113.80
1	A	687	LYS	CG-CD-CE	-7.14	94.89	111.30
1	A	191	GLN	CB-CA-C	-7.10	99.69	110.90
1	A	624	THR	N-CA-C	7.06	118.77	111.14
1	A	534	GLY	O-C-N	-7.02	113.52	122.43
1	A	262	ARG	CD-NE-CZ	6.97	134.15	124.40
1	A	417	VAL	N-CA-C	6.93	117.72	110.72
1	A	569	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	A	158	GLN	N-CA-C	6.91	117.36	108.24
1	A	386	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	183	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	A	198	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	370	ALA	N-CA-C	6.90	121.69	113.28
1	A	159	ASN	CA-CB-CG	6.80	119.40	112.60
1	A	360	ASP	N-CA-CB	-6.76	99.70	110.19
1	A	191	GLN	CA-CB-CG	6.76	127.62	114.10
1	A	564	ALA	O-C-N	-6.76	114.50	122.81
1	A	117	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	A	268	ILE	N-CA-C	6.74	123.36	109.34
1	A	28	TRP	CG-CD2-CE3	6.72	140.62	133.90
1	A	351	GLU	N-CA-C	6.70	120.25	109.86
1	A	118	HIS	CB-CG-CD2	-6.67	122.52	131.20
1	A	675	ASN	CB-CG-ND2	6.64	126.36	116.40
1	A	368	PHE	CA-CB-CG	6.63	120.43	113.80
1	A	274	PHE	CB-CA-C	-6.62	98.65	110.03
1	A	404	GLN	OE1-CD-NE2	-6.62	115.98	122.60
1	A	364	LEU	N-CA-C	6.61	118.14	111.07
1	A	321	ASN	N-CA-C	6.59	120.61	110.20
1	A	88	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	A	267	PRO	CB-CA-C	-6.57	100.72	111.56
1	A	408	SER	CB-CA-C	-6.56	99.89	110.79
1	A	511	ARG	CD-NE-CZ	-6.55	115.22	124.40
1	A	130	GLN	N-CA-C	6.53	118.48	111.36
1	A	72	ARG	N-CA-C	-6.51	104.27	111.82
1	A	513	LEU	O-C-N	-6.49	113.94	122.97
1	A	268	ILE	CB-CA-C	-6.45	100.71	111.29
1	A	195	ARG	N-CA-C	6.45	118.31	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ALA	CB-CA-C	-6.43	99.58	110.64
1	A	322	ASN	N-CA-C	6.42	124.48	110.80
1	A	388	ILE	CA-C-N	6.41	130.47	121.24
1	A	388	ILE	C-N-CA	6.41	130.47	121.24
1	A	225	CYS	CA-CB-SG	6.40	129.12	114.40
1	A	111	GLU	CA-CB-CG	6.39	126.87	114.10
1	A	473	ASN	CB-CG-ND2	6.38	125.98	116.40
1	A	671	GLU	N-CA-CB	-6.37	100.50	110.44
1	A	182	SER	N-CA-C	6.37	118.22	111.28
1	A	406	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	A	366	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	466	ALA	N-CA-C	6.34	118.95	108.99
1	A	14	THR	N-CA-C	-6.34	97.29	110.80
1	A	14	THR	CA-C-O	6.34	129.57	120.51
1	A	15	GLU	N-CA-C	-6.30	97.37	110.80
1	A	17	ILE	CA-CB-CG1	6.30	121.11	110.40
1	A	691	GLN	CG-CD-NE2	6.29	125.84	116.40
1	A	19	LEU	N-CA-C	6.29	124.20	110.80
1	A	556	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	80	LEU	O-C-N	-6.26	115.62	122.07
1	A	200	VAL	O-C-N	-6.26	113.58	121.84
1	A	548	GLN	CG-CD-NE2	6.24	125.76	116.40
1	A	627	GLN	CB-CG-CD	-6.23	102.01	112.60
1	A	391	GLN	O-C-N	-6.23	115.79	123.33
1	A	444	LEU	CA-C-O	-6.23	114.48	120.64
1	A	560	LYS	CG-CD-CE	-6.21	97.01	111.30
1	A	663	HIS	CB-CG-CD2	-6.21	123.12	131.20
1	A	189	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	A	441	GLU	CB-CG-CD	6.18	123.11	112.60
1	A	56	SER	CA-CB-OG	-6.18	98.75	111.10
1	A	609	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	A	301	ALA	N-CA-C	6.13	123.85	110.80
1	A	309	TRP	CG-CD2-CE3	6.12	140.02	133.90
1	A	396	VAL	N-CA-CB	6.11	118.84	110.54
1	A	226	VAL	O-C-N	-6.09	116.59	123.10
1	A	51	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	523	TYR	O-C-N	-6.06	115.79	122.09
1	A	313	VAL	N-CA-C	6.06	116.80	110.62
1	A	468	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	675	ASN	CA-CB-CG	-6.06	106.54	112.60
1	A	589	THR	CA-CB-CG2	6.02	120.74	110.50
1	A	346	ARG	CA-C-O	-6.02	114.50	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	A	663	HIS	N-CA-C	6.01	119.44	111.75
1	A	704	PHE	N-CA-C	6.01	119.39	110.32
1	A	248	VAL	N-CA-CB	6.00	121.14	111.23
1	A	375	PHE	CA-CB-CG	-5.99	107.81	113.80
1	A	427	ASP	CA-C-N	5.99	126.09	119.87
1	A	427	ASP	C-N-CA	5.99	126.09	119.87
1	A	137	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	A	145	TYR	N-CA-C	5.97	118.27	111.11
1	A	724	PHE	CA-C-O	5.97	126.65	119.43
1	A	170	GLN	CG-CD-NE2	5.97	125.35	116.40
1	A	608	THR	CB-CA-C	-5.96	100.28	110.24
1	A	442	ILE	O-C-N	-5.95	116.62	122.93
1	A	626	SER	CA-CB-OG	-5.95	99.19	111.10
1	A	78	GLN	CA-CB-CG	5.94	125.98	114.10
1	A	19	LEU	O-C-N	-5.94	114.69	122.59
1	A	70	ILE	N-CA-CB	5.93	117.00	110.53
1	A	267	PRO	N-CA-C	5.93	124.69	112.47
1	A	168	SER	CA-CB-OG	5.93	122.96	111.10
1	A	691	GLN	OE1-CD-NE2	-5.93	116.67	122.60
1	A	497	ASP	N-CA-C	5.92	119.73	110.32
1	A	541	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	A	333	MET	CA-C-O	-5.87	114.59	121.46
1	A	608	THR	N-CA-CB	-5.87	100.47	110.33
1	A	630	ASN	CB-CG-ND2	5.87	125.20	116.40
1	A	39	SER	CA-C-O	-5.84	112.90	119.79
1	A	332	HIS	CA-CB-CG	-5.83	107.97	113.80
1	A	83	ARG	CA-CB-CG	-5.83	102.45	114.10
1	A	589	THR	N-CA-CB	-5.82	100.94	110.14
1	A	75	PRO	CB-CA-C	-5.81	102.67	111.44
1	A	510	ARG	CB-CG-CD	5.80	124.64	111.30
1	A	12	GLY	CA-C-O	5.79	130.64	120.57
1	A	221	GLN	CG-CD-NE2	5.79	125.08	116.40
1	A	542	LYS	CB-CG-CD	-5.79	97.99	111.30
1	A	166	TYR	N-CA-C	5.78	120.49	113.38
1	A	305	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	44	ARG	N-CA-C	5.76	117.56	111.28
1	A	620	MET	CA-C-O	-5.76	114.68	120.96
1	A	343	MET	CG-SD-CE	-5.76	88.24	100.90
1	A	527	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	A	711	MET	CG-SD-CE	-5.74	88.27	100.90
1	A	454	ASP	CA-CB-CG	5.74	118.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	N-CA-CB	5.71	118.36	110.07
1	A	332	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	A	389	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	367	ALA	N-CA-C	5.71	118.23	111.33
1	A	172	LEU	CA-CB-CG	5.70	136.26	116.30
1	A	23	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	A	225	CYS	N-CA-C	5.68	117.73	108.76
1	A	404	GLN	CG-CD-NE2	5.67	124.91	116.40
1	A	331	ARG	CB-CG-CD	-5.65	98.31	111.30
1	A	313	VAL	N-CA-CB	5.64	118.22	110.54
1	A	46	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	A	237	ILE	O-C-N	-5.62	116.42	121.87
1	A	609	HIS	N-CA-C	5.62	120.14	113.28
1	A	424	SER	CA-C-O	-5.61	115.34	120.50
1	A	34	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	191	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	A	697	THR	CB-CA-C	5.58	119.81	109.70
1	A	444	LEU	CA-C-N	5.58	125.55	120.03
1	A	444	LEU	C-N-CA	5.58	125.55	120.03
1	A	130	GLN	CB-CG-CD	-5.58	103.12	112.60
1	A	720	THR	CB-CA-C	-5.58	101.48	110.74
1	A	358	PRO	O-C-N	-5.57	116.16	122.18
1	A	17	ILE	O-C-N	-5.57	115.61	122.57
1	A	267	PRO	CA-C-N	5.57	131.99	121.97
1	A	267	PRO	C-N-CA	5.57	131.99	121.97
1	A	468	ASN	CB-CG-ND2	5.56	124.73	116.40
1	A	169	ALA	N-CA-C	5.54	118.04	111.33
1	A	451	ASP	O-C-N	-5.54	117.17	123.48
1	A	42	GLU	N-CA-C	5.54	117.31	111.28
1	A	430	ILE	O-C-N	-5.52	115.67	122.57
1	A	252	ALA	N-CA-C	5.52	122.56	110.80
1	A	261	ILE	CA-C-O	5.52	127.53	121.13
1	A	689	ILE	N-CA-CB	-5.52	102.74	110.13
1	A	438	LEU	O-C-N	-5.52	116.39	122.07
1	A	15	GLU	CB-CA-C	5.51	121.38	110.42
1	A	732	GLN	N-CA-C	-5.50	99.55	108.52
1	A	212	MET	N-CA-C	5.50	118.79	111.75
1	A	78	GLN	CB-CA-C	-5.50	100.46	110.63
1	A	191	GLN	N-CA-C	-5.49	105.21	111.14
1	A	97	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	408	SER	N-CA-C	5.49	117.26	111.28
1	A	537	ASN	CB-CG-ND2	5.49	124.63	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	TYR	CB-CA-C	5.48	118.69	110.08
1	A	16	ARG	CG-CD-NE	-5.48	99.94	112.00
1	A	155	TYR	N-CA-CB	5.48	119.87	110.34
1	A	31	GLU	CA-C-O	5.47	127.16	120.92
1	A	298	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	A	88	HIS	O-C-N	-5.46	116.45	122.07
1	A	535	SER	N-CA-C	5.45	119.19	112.54
1	A	277	GLY	O-C-N	5.45	129.78	122.70
1	A	653	ARG	CB-CG-CD	-5.44	98.78	111.30
1	A	90	ARG	O-C-N	-5.44	116.36	122.12
1	A	599	TRP	CB-CG-CD1	-5.43	118.75	126.90
1	A	173	TYR	O-C-N	-5.43	115.96	122.15
1	A	221	GLN	O-C-N	-5.42	116.59	123.05
1	A	262	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	A	41	VAL	O-C-N	-5.42	116.52	121.94
1	A	148	VAL	O-C-N	-5.41	116.62	121.87
1	A	628	ILE	O-C-N	-5.41	116.40	121.87
1	A	59	HIS	N-CA-C	5.40	116.85	111.07
1	A	647	SER	O-C-N	-5.40	116.89	123.10
1	A	176	VAL	N-CA-CB	-5.39	100.76	110.95
1	A	40	GLN	CB-CG-CD	-5.38	103.45	112.60
1	A	252	ALA	CB-CA-C	-5.38	99.72	110.42
1	A	339	ILE	O-C-N	-5.37	117.39	123.03
1	A	718	LEU	CA-C-N	5.37	127.74	120.44
1	A	718	LEU	C-N-CA	5.37	127.74	120.44
1	A	296	GLY	O-C-N	5.36	129.67	122.70
1	A	592	ASN	CA-CB-CG	5.36	117.96	112.60
1	A	16	ARG	CB-CA-C	-5.35	99.77	110.42
1	A	340	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	533	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	461	LEU	N-CA-C	5.34	117.67	109.07
1	A	52	GLY	N-CA-C	5.33	121.92	115.31
1	A	199	ALA	CA-C-O	5.32	126.19	120.55
1	A	309	TRP	CE2-CD2-CG	-5.31	100.83	107.20
1	A	324	GLY	N-CA-C	-5.31	102.48	111.08
1	A	717	ASP	N-CA-C	5.30	119.00	112.54
1	A	435	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	382	TYR	O-C-N	-5.29	116.03	122.22
1	A	74	ALA	CA-C-N	5.29	125.37	119.87
1	A	74	ALA	C-N-CA	5.29	125.37	119.87
1	A	323	ARG	CA-C-O	5.28	126.58	120.14
1	A	613	ASN	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	GLU	N-CA-C	5.27	117.95	110.10
1	A	334	ASP	CA-C-O	-5.27	115.20	121.89
1	A	587	LEU	N-CA-C	5.27	117.77	111.71
1	A	474	ASN	O-C-N	-5.26	116.32	123.15
1	A	59	HIS	CB-CA-C	-5.25	102.63	110.88
1	A	406	ARG	CG-CD-NE	-5.25	100.44	112.00
1	A	456	ASN	CA-C-O	5.25	125.78	119.59
1	A	133	THR	OG1-CB-CG2	5.23	119.77	109.30
1	A	133	THR	CA-CB-OG1	-5.23	101.75	109.60
1	A	519	ASN	O-C-N	-5.23	115.41	122.41
1	A	161	VAL	O-C-N	5.23	129.10	122.57
1	A	133	THR	N-CA-CB	-5.22	101.67	110.49
1	A	360	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	211	ILE	CB-CG1-CD1	-5.20	102.88	113.80
1	A	321	ASN	CB-CG-ND2	5.20	124.20	116.40
1	A	697	THR	O-C-N	-5.17	117.26	123.31
1	A	62	ILE	O-C-N	-5.17	116.86	121.87
1	A	683	GLY	O-C-N	-5.17	117.23	122.19
1	A	649	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	145	TYR	O-C-N	-5.16	116.72	122.09
1	A	375	PHE	O-C-N	-5.15	116.66	122.12
1	A	589	THR	N-CA-C	5.15	118.35	111.75
1	A	459	ILE	N-CA-C	-5.15	100.90	108.11
1	A	667	GLU	O-C-N	-5.15	117.20	123.27
1	A	672	MET	CA-C-O	-5.14	114.66	119.80
1	A	676	ASP	N-CA-C	5.14	116.88	111.28
1	A	697	THR	N-CA-CB	-5.14	101.91	110.80
1	A	256	ILE	O-C-N	-5.13	117.76	123.20
1	A	517	VAL	CA-C-N	-5.13	116.69	122.48
1	A	517	VAL	C-N-CA	-5.13	116.69	122.48
1	A	152	GLU	O-C-N	-5.13	116.55	122.09
1	A	46	HIS	CB-CG-ND1	5.12	130.39	122.70
1	A	357	SER	CA-C-O	-5.11	115.47	119.66
1	A	731	TYR	N-CA-C	5.10	117.29	110.35
1	A	527	HIS	CB-CG-ND1	5.10	130.35	122.70
1	A	441	GLU	CB-CA-C	-5.09	101.00	109.55
1	A	53	ILE	CA-C-O	5.09	126.84	121.04
1	A	215	VAL	CA-C-N	5.09	131.25	121.54
1	A	215	VAL	C-N-CA	5.09	131.25	121.54
1	A	423	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	538	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	A	599	TRP	CE2-CD2-CG	-5.08	101.10	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	GLY	N-CA-C	-5.08	108.31	115.32
1	A	286	GLN	CB-CG-CD	-5.08	103.97	112.60
1	A	173	TYR	N-CA-C	5.07	116.88	111.36
1	A	433	VAL	N-CA-CB	-5.07	105.28	111.21
1	A	47	ILE	CB-CA-C	-5.05	100.71	111.32
1	A	238	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	177	ALA	O-C-N	-5.05	116.87	122.07
1	A	13	SER	CA-C-N	5.05	131.18	121.54
1	A	13	SER	C-N-CA	5.05	131.18	121.54
1	A	153	GLY	O-C-N	-5.05	116.35	122.71
1	A	18	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	151	LEU	CB-CA-C	-5.04	102.97	110.88
1	A	72	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	A	155	TYR	CB-CG-CD2	-5.02	113.27	120.80
1	A	670	TRP	CE2-CD2-CG	-5.02	101.17	107.20
1	A	530	ARG	O-C-N	-5.02	117.10	123.17
1	A	159	ASN	N-CA-C	5.02	121.48	110.80
1	A	612	ARG	CD-NE-CZ	-5.01	117.38	124.40
1	A	57	ASP	CA-CB-CG	-5.01	107.59	112.60
1	A	496	GLN	N-CA-CB	-5.01	102.81	110.42
1	A	406	ARG	NE-CZ-NH1	5.01	126.51	121.50
1	A	466	ALA	O-C-N	-5.01	117.67	123.33
1	A	150	GLN	O-C-N	-5.00	116.44	122.15

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	GLY	Mainchain
1	A	16	ARG	Peptide
1	A	264	LEU	Mainchain
1	A	361	VAL	Peptide
1	A	79	TYR	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	5875	0	5776	187	1
All	All	5875	0	5776	187	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 16.

All (187) 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:176:VAL:CA	1:A:176:VAL:CB	1.82	1.57
1:A:200:VAL:CA	1:A:200:VAL:CB	1.89	1.50
1:A:273:ALA:C	1:A:274:PHE:N	1.79	1.40
1:A:264:LEU:HD23	1:A:389:ARG:NH1	1.66	1.09
1:A:249:SER:HB3	1:A:292:CYS:HB2	1.31	1.08
1:A:248:VAL:HG13	1:A:254:ILE:HG13	1.38	1.06
1:A:13:SER:HB2	1:A:15:GLU:H	1.22	1.04
1:A:248:VAL:HG13	1:A:254:ILE:CG1	1.90	1.00
1:A:328:ASN:O	1:A:329:ARG:NH1	1.97	0.97
1:A:329:ARG:HH11	1:A:329:ARG:HG3	1.28	0.96
1:A:250:GLN:NE2	1:A:251:ARG:HH11	1.65	0.93
1:A:248:VAL:HG11	1:A:289:VAL:HB	1.53	0.91
1:A:249:SER:HB3	1:A:292:CYS:CB	2.00	0.90
1:A:155:TYR:HE2	1:A:628:ILE:HD13	1.36	0.90
1:A:14:THR:C	1:A:16:ARG:N	2.18	0.90
1:A:250:GLN:NE2	1:A:251:ARG:NH1	2.19	0.89
1:A:14:THR:C	1:A:16:ARG:H	1.78	0.88
1:A:14:THR:HG22	1:A:54:LYS:HA	1.55	0.87
1:A:248:VAL:HG21	1:A:289:VAL:HA	1.55	0.86
1:A:155:TYR:CE2	1:A:628:ILE:HD13	2.09	0.86
1:A:250:GLN:HE22	1:A:251:ARG:NH1	1.74	0.84
1:A:160:ARG:O	1:A:162:THR:N	2.09	0.84
1:A:159:ASN:HB2	1:A:163:GLY:H	1.41	0.84
1:A:276:THR:HG23	1:A:276:THR:O	1.77	0.83
1:A:176:VAL:CB	1:A:176:VAL:C	2.50	0.83
1:A:249:SER:O	1:A:251:ARG:N	2.14	0.81
1:A:249:SER:CB	1:A:292:CYS:HB2	2.11	0.81
1:A:264:LEU:CD2	1:A:389:ARG:NH1	2.43	0.80
1:A:329:ARG:HH11	1:A:329:ARG:CG	1.96	0.78
1:A:321:ASN:O	1:A:329:ARG:HD3	1.83	0.78
1:A:13:SER:C	1:A:15:GLU:H	1.90	0.78
1:A:329:ARG:NH1	1:A:329:ARG:HG3	1.99	0.77
1:A:118:HIS:HD2	1:A:220:ARG:HH22	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:HG11	1:A:289:VAL:CB	2.16	0.75
1:A:13:SER:C	1:A:15:GLU:N	2.44	0.73
1:A:155:TYR:CE2	1:A:628:ILE:CD1	2.72	0.72
1:A:345:THR:O	1:A:349:LYS:HG2	1.89	0.72
1:A:248:VAL:HG13	1:A:254:ILE:HG12	1.70	0.72
1:A:402:MET:HE3	1:A:403:MET:HE3	1.71	0.72
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.71	0.72
1:A:118:HIS:CD2	1:A:220:ARG:HH22	2.08	0.71
1:A:200:VAL:CB	1:A:200:VAL:C	2.64	0.71
1:A:13:SER:HB2	1:A:15:GLU:N	2.03	0.70
1:A:130:GLN:O	1:A:133:THR:HB	1.91	0.69
1:A:13:SER:CB	1:A:15:GLU:H	2.03	0.68
1:A:176:VAL:CB	1:A:176:VAL:N	2.55	0.68
1:A:425:PRO:HG2	1:A:615:THR:HG22	1.74	0.68
1:A:519:ASN:ND2	1:A:632:THR:H	1.92	0.68
1:A:402:MET:HE3	1:A:403:MET:CE	2.23	0.68
1:A:276:THR:O	1:A:276:THR:CG2	2.43	0.67
1:A:14:THR:HG21	1:A:54:LYS:HD2	1.75	0.67
1:A:30:ALA:HB2	1:A:38:ILE:HD11	1.74	0.67
1:A:251:ARG:O	1:A:252:ALA:HB2	1.94	0.67
1:A:110:VAL:HG11	1:A:120:LEU:HD12	1.76	0.66
1:A:364:LEU:HD22	1:A:375:PHE:CE1	2.30	0.66
1:A:658:ASP:HB3	1:A:662:LEU:HD22	1.78	0.65
1:A:160:ARG:C	1:A:162:THR:N	2.55	0.64
1:A:322:ASN:HD22	1:A:323:ARG:H	1.46	0.64
1:A:442:ILE:HD11	1:A:464:LEU:HD21	1.80	0.64
1:A:263:ALA:HB1	1:A:312:GLU:HG3	1.78	0.64
1:A:533:ASP:HB3	1:A:535:SER:H	1.62	0.64
1:A:244:ILE:HG22	1:A:248:VAL:CG2	2.30	0.62
1:A:176:VAL:CA	1:A:176:VAL:CG2	2.77	0.61
1:A:14:THR:CG2	1:A:54:LYS:HA	2.29	0.61
1:A:449:LEU:HD12	1:A:457:GLY:HA3	1.84	0.60
1:A:244:ILE:CG2	1:A:248:VAL:HG22	2.32	0.60
1:A:207:LEU:HB2	1:A:212:MET:HE3	1.83	0.60
1:A:249:SER:O	1:A:250:GLN:C	2.44	0.59
1:A:686:GLN:HE22	1:A:692:SER:HA	1.67	0.59
1:A:131:MET:HE2	1:A:193:VAL:HG11	1.85	0.58
1:A:159:ASN:ND2	1:A:162:THR:HG22	2.17	0.58
1:A:345:THR:CG2	1:A:349:LYS:HD3	2.34	0.58
1:A:14:THR:O	1:A:15:GLU:C	2.26	0.58
1:A:406:ARG:HH21	1:A:413:TYR:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ARG:HG3	1:A:669:LEU:HD12	1.85	0.58
1:A:24:ARG:HG3	1:A:24:ARG:NH1	2.18	0.58
1:A:249:SER:HB3	1:A:292:CYS:SG	2.43	0.57
1:A:15:GLU:C	1:A:16:ARG:CG	2.74	0.57
1:A:155:TYR:HE2	1:A:628:ILE:CD1	2.12	0.57
1:A:159:ASN:HD22	1:A:162:THR:HG22	1.69	0.57
1:A:79:TYR:O	1:A:83:ARG:HG3	2.05	0.56
1:A:317:LEU:HD11	1:A:337:VAL:HG21	1.86	0.56
1:A:14:THR:O	1:A:16:ARG:N	2.36	0.56
1:A:18:ASN:O	1:A:21:LYS:HD3	2.05	0.56
1:A:114:LYS:HE3	1:A:166:TYR:CE2	2.41	0.56
1:A:711:MET:CE	1:A:715:LEU:HG	2.37	0.55
1:A:159:ASN:HB2	1:A:163:GLY:N	2.18	0.55
1:A:179:CYS:SG	1:A:216:ARG:HA	2.47	0.55
1:A:319:LEU:O	1:A:329:ARG:HG2	2.06	0.55
1:A:322:ASN:HD22	1:A:323:ARG:N	2.05	0.54
1:A:345:THR:HG22	1:A:349:LYS:HD3	1.89	0.54
1:A:644:ILE:HG23	1:A:651:ILE:HG23	1.89	0.54
1:A:519:ASN:HD22	1:A:632:THR:H	1.56	0.53
1:A:176:VAL:CA	1:A:176:VAL:CG1	2.80	0.53
1:A:529:LYS:HB3	1:A:536:ALA:HB2	1.91	0.52
1:A:244:ILE:HG23	1:A:248:VAL:HG22	1.92	0.52
1:A:357:SER:O	1:A:360:ASP:HB3	2.08	0.52
1:A:273:ALA:HB1	1:A:274:PHE:N	2.25	0.52
1:A:403:MET:HB2	1:A:711:MET:HE1	1.92	0.52
1:A:171:PHE:O	1:A:175:LEU:HB2	2.09	0.52
1:A:510:ARG:HB2	1:A:512:THR:HG23	1.92	0.52
1:A:244:ILE:CG2	1:A:248:VAL:CG2	2.88	0.52
1:A:379:TYR:O	1:A:383:GLU:HG3	2.10	0.52
1:A:586:ASP:O	1:A:589:THR:HB	2.10	0.52
1:A:14:THR:CA	1:A:16:ARG:H	2.22	0.51
1:A:442:ILE:HG13	1:A:462:CYS:SG	2.50	0.51
1:A:310:HIS:O	1:A:313:VAL:HG22	2.10	0.51
1:A:148:VAL:HA	1:A:151:LEU:HD12	1.92	0.51
1:A:325:VAL:HG22	1:A:327:GLY:H	1.76	0.50
1:A:200:VAL:CA	1:A:200:VAL:CG1	2.84	0.50
1:A:294:GLN:HA	1:A:294:GLN:OE1	2.12	0.50
1:A:45:SER:HB2	1:A:61:THR:HG22	1.93	0.49
1:A:395:ALA:O	1:A:399:PHE:HD1	1.95	0.49
1:A:403:MET:CB	1:A:711:MET:HE1	2.42	0.49
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:THR:OG1	1:A:219:THR:HG22	2.13	0.49
1:A:15:GLU:C	1:A:16:ARG:HG3	2.37	0.49
1:A:24:ARG:HG3	1:A:24:ARG:HH11	1.78	0.48
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.95	0.48
1:A:455:GLU:HG3	1:A:501:PRO:HB2	1.96	0.48
1:A:427:ASP:OD2	1:A:575:LYS:HE2	2.14	0.48
1:A:697:THR:HG22	1:A:732:GLN:HG3	1.95	0.48
1:A:248:VAL:CG1	1:A:254:ILE:HG12	2.41	0.48
1:A:321:ASN:O	1:A:329:ARG:CD	2.58	0.48
1:A:212:MET:O	1:A:216:ARG:NH2	2.46	0.48
1:A:244:ILE:HG22	1:A:248:VAL:HG21	1.96	0.48
1:A:215:VAL:O	1:A:216:ARG:HB3	2.14	0.47
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.95	0.47
1:A:72:ARG:O	1:A:75:PRO:HD3	2.15	0.47
1:A:283:LYS:HG2	1:A:330:VAL:HG22	1.96	0.47
1:A:17:ILE:HD13	1:A:17:ILE:HG21	1.75	0.47
1:A:200:VAL:CA	1:A:200:VAL:CG2	2.84	0.47
1:A:278:CYS:HB2	1:A:312:GLU:OE2	2.15	0.47
1:A:644:ILE:HG23	1:A:651:ILE:CG2	2.45	0.47
1:A:15:GLU:O	1:A:16:ARG:CB	2.46	0.47
1:A:144:SER:O	1:A:147:ALA:HB3	2.15	0.46
1:A:668:LEU:O	1:A:669:LEU:C	2.57	0.46
1:A:578:LEU:HD13	1:A:599:TRP:HE3	1.81	0.46
1:A:220:ARG:HG2	1:A:495:TYR:O	2.16	0.46
1:A:290:LYS:HB3	1:A:296:GLY:HA2	1.98	0.46
1:A:529:LYS:N	1:A:529:LYS:HD2	2.32	0.45
1:A:15:GLU:O	1:A:15:GLU:HG3	2.16	0.45
1:A:158:GLN:HB2	1:A:159:ASN:H	1.47	0.45
1:A:273:ALA:CA	1:A:274:PHE:N	2.74	0.45
1:A:320:LYS:HE3	1:A:333:MET:O	2.16	0.45
1:A:415:GLN:HG3	1:A:728:THR:HG22	1.98	0.45
1:A:440:LEU:HD12	1:A:728:THR:HB	1.98	0.45
1:A:697:THR:HG23	1:A:699:TYR:HE1	1.81	0.45
1:A:47:ILE:H	1:A:47:ILE:HG13	1.65	0.44
1:A:155:TYR:CE2	1:A:628:ILE:HD11	2.52	0.44
1:A:181:PHE:O	1:A:184:TYR:HB2	2.18	0.44
1:A:285:PHE:O	1:A:289:VAL:HG13	2.18	0.44
1:A:293:SER:HB2	1:A:294:GLN:H	1.73	0.44
1:A:47:ILE:HD12	1:A:48:GLN:HG3	1.99	0.43
1:A:593:GLU:OE2	1:A:596:HIS:HE1	2.01	0.43
1:A:548:GLN:O	1:A:552:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLY:O	1:A:502:ALA:HB1	2.19	0.43
1:A:176:VAL:C	1:A:176:VAL:CG1	2.92	0.43
1:A:708:LYS:HA	1:A:708:LYS:HD3	1.88	0.43
1:A:248:VAL:CG2	1:A:289:VAL:HA	2.38	0.43
1:A:282:TYR:CE2	1:A:316:LEU:HD22	2.53	0.43
1:A:329:ARG:NH1	1:A:329:ARG:CG	2.65	0.43
1:A:264:LEU:HD23	1:A:389:ARG:CZ	2.42	0.43
1:A:264:LEU:HD23	1:A:389:ARG:HH11	1.73	0.42
1:A:155:TYR:OH	1:A:624:THR:HG22	2.19	0.42
1:A:159:ASN:CG	1:A:159:ASN:O	2.63	0.42
1:A:620:MET:SD	1:A:620:MET:N	2.86	0.42
1:A:500:ILE:O	1:A:501:PRO:C	2.62	0.42
1:A:226:VAL:HG21	1:A:247:TYR:CG	2.55	0.42
1:A:90:ARG:HH11	1:A:90:ARG:HD2	1.62	0.42
1:A:413:TYR:HB3	1:A:729:LEU:O	2.20	0.42
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.32	0.41
1:A:263:ALA:HB1	1:A:312:GLU:CG	2.48	0.41
1:A:569:ASN:ND2	1:A:569:ASN:H	2.17	0.41
1:A:15:GLU:HG2	1:A:16:ARG:HG2	2.02	0.41
1:A:93:ALA:HB2	1:A:165:ILE:HG22	2.02	0.41
1:A:160:ARG:HB2	1:A:166:TYR:OH	2.19	0.41
1:A:558:LEU:HD23	1:A:612:ARG:HG2	2.02	0.41
1:A:711:MET:HE3	1:A:715:LEU:HG	2.02	0.41
1:A:340:ASN:OD1	1:A:343:MET:HG2	2.21	0.41
1:A:406:ARG:O	1:A:410:GLY:N	2.51	0.41
1:A:250:GLN:CD	1:A:251:ARG:HH11	2.25	0.41
1:A:264:LEU:CD2	1:A:389:ARG:HH11	2.31	0.41
1:A:645:LYS:HB2	1:A:652:LEU:HB2	2.03	0.41
1:A:244:ILE:HD13	1:A:244:ILE:HG21	1.77	0.40
1:A:306:TYR:OH	1:A:317:LEU:HD13	2.21	0.40
1:A:565:CYS:HA	1:A:566:PRO:HD3	1.95	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:276:THR:OG1	1:A:293:SER:O[18_655]	1.19	1.01

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	733/761 (96%)	661 (90%)	46 (6%)	26 (4%)	3 4

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	216	ARG
1	A	250	GLN
1	A	267	PRO
1	A	276	THR
1	A	298	ARG
1	A	385	ASP
1	A	386	ASP
1	A	161	VAL
1	A	253	GLY
1	A	295	GLY
1	A	296	GLY
1	A	299	GLY
1	A	301	ALA
1	A	322	ASN
1	A	511	ARG
1	A	185	PRO
1	A	252	ALA
1	A	741	ASP
1	A	162	THR
1	A	361	VAL
1	A	16	ARG
1	A	268	ILE
1	A	17	ILE
1	A	248	VAL
1	A	265	GLY

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	633/654 (97%)	523 (83%)	110 (17%)	2 3

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	11	ASP
1	A	13	SER
1	A	14	THR
1	A	15	GLU
1	A	16	ARG
1	A	21	LYS
1	A	24	ARG
1	A	26	LEU
1	A	35	ASN
1	A	39	SER
1	A	40	GLN
1	A	47	ILE
1	A	58	ILE
1	A	60	GLU
1	A	69	LEU
1	A	72	ARG
1	A	73	ASP
1	A	83	ARG
1	A	89	LEU
1	A	96	GLN
1	A	102	LEU
1	A	108	LYS
1	A	111	GLU
1	A	119	LEU
1	A	139	ARG
1	A	154	LYS
1	A	159	ASN
1	A	160	ARG
1	A	162	THR

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Mol	Chain	Res	Type
1	A	165	ILE
1	A	172	LEU
1	A	175	LEU
1	A	180	LEU
1	A	185	PRO
1	A	186	ARG
1	A	190	LEU
1	A	216	ARG
1	A	220	ARG
1	A	224	SER
1	A	225	CYS
1	A	248	VAL
1	A	249	SER
1	A	250	GLN
1	A	251	ARG
1	A	260	ARG
1	A	264	LEU
1	A	275	HIS
1	A	276	THR
1	A	278	CYS
1	A	289	VAL
1	A	293	SER
1	A	298	ARG
1	A	313	VAL
1	A	317	LEU
1	A	322	ASN
1	A	329	ARG
1	A	348	LEU
1	A	359	SER
1	A	364	LEU
1	A	373	GLU
1	A	386	ASP
1	A	394	LYS
1	A	396	VAL
1	A	397	GLU
1	A	400	SER
1	A	434	ARG
1	A	440	LEU
1	A	441	GLU
1	A	447	LYS
1	A	452	VAL
1	A	465	SER

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Mol	Chain	Res	Type
1	A	478	LEU
1	A	481	LEU
1	A	496	GLN
1	A	497	ASP
1	A	510	ARG
1	A	517	VAL
1	A	519	ASN
1	A	530	ARG
1	A	533	ASP
1	A	539	LEU
1	A	542	LYS
1	A	552	LEU
1	A	566	PRO
1	A	569	ASN
1	A	570	GLU
1	A	585	LYS
1	A	592	ASN
1	A	622	SER
1	A	625	SER
1	A	626	SER
1	A	628	ILE
1	A	629	SER
1	A	639	ARG
1	A	645	LYS
1	A	648	LYS
1	A	651	ILE
1	A	662	LEU
1	A	669	LEU
1	A	679	LEU
1	A	681	LEU
1	A	689	ILE
1	A	696	ASN
1	A	697	THR
1	A	703	ARG
1	A	716	LYS
1	A	739	ASP
1	A	741	ASP
1	A	745	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	105	HIS
1	A	118	HIS
1	A	159	ASN
1	A	250	GLN
1	A	257	ASN
1	A	322	ASN
1	A	415	GLN
1	A	453	ASN
1	A	496	GLN
1	A	519	ASN
1	A	548	GLN
1	A	569	ASN
1	A	596	HIS
1	A	630	ASN
1	A	654	GLN
1	A	686	GLN
1	A	698	ASN
1	A	732	GLN
1	A	733	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	736:ASP	C	739:ASP	N	26.00
1	A	273:ALA	C	274:PHE	N	1.79
1	A	387:SER	C	388:ILE	N	1.11

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.