



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 05:09 PM UTC

PDB ID : 1HLL / pdb_00001hll
Title : NMR STRUCTURE OF T3-I2, A 32 RESIDUE PEPTIDE FROM THE
ALPHA-2A ADRENERGIC RECEPTOR
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Deposited on : 2000-12-01

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A user guide is available at

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

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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

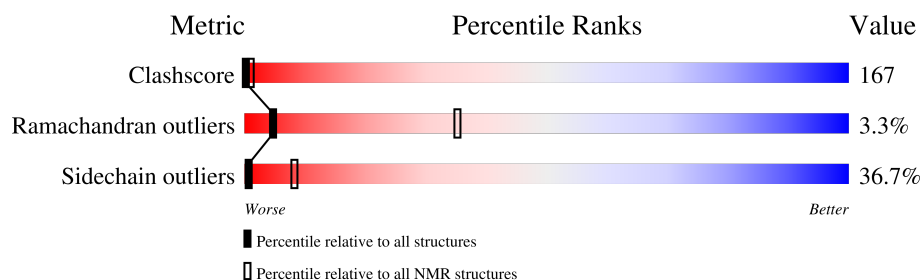
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	32	19% 66% 16%

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 540 atoms, of which 274 are hydrogens and 0 are deuteriums.

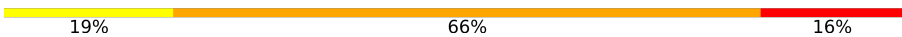
- Molecule 1 is a protein called ALPHA-2A ADRENERGIC RECEPTOR.

Mol	Chain	Residues	Atoms						Trace
1	A	32	Total	C	H	N	O	S	0
			540	168	274	50	47	1	

4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: ALPHA-2A ADRENERGIC RECEPTOR

Chain A: 



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing in torsion angle space*.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
DYANA	structure solution	
DYANA	refinement	

No chemical shift data was provided.

6 Model quality

6.1 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 (average) 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	28.48	178/271 (65.7%)	11.81	122/367 (33.2%)
All	All	28.48	178/271 (65.7%)	11.81	122/367 (33.2%)

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

Mol	Chain	Chirality	Planarity
1	A	5	0
All	All	5	0

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	THR	CA-C	-93.87	0.34	1.52
1	A	30	PRO	N-CA	-90.84	0.31	1.47
1	A	31	ARG	NE-CZ	-90.16	0.33	1.33
1	A	31	ARG	CA-C	-89.80	0.38	1.52
1	A	32	ARG	NE-CZ	-89.74	0.34	1.33
1	A	31	ARG	CZ-NH1	-88.03	0.09	1.32
1	A	31	ARG	CD-NE	-81.41	0.32	1.46
1	A	31	ARG	CZ-NH2	-81.28	0.27	1.33
1	A	32	ARG	CD-NE	-80.67	0.33	1.46
1	A	30	PRO	N-CD	-79.96	0.35	1.47
1	A	32	ARG	CZ-NH2	-79.95	0.29	1.33
1	A	32	ARG	CZ-NH1	-75.93	0.26	1.32
1	A	28	ARG	CZ-NH1	-73.75	0.29	1.32
1	A	28	ARG	NE-CZ	-73.53	0.52	1.33
1	A	29	THR	C-O	-73.23	0.30	1.24
1	A	30	PRO	C-N	-71.94	0.38	1.33
1	A	30	PRO	CA-CB	-70.60	0.53	1.53
1	A	32	ARG	CA-CB	-63.63	0.26	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	THR	CA-CB	-63.17	0.53	1.53
1	A	31	ARG	CA-CB	-62.34	0.43	1.53
1	A	32	ARG	N-CA	-56.50	0.39	1.46
1	A	29	THR	CB-OG1	-56.05	0.54	1.43
1	A	14	ARG	CZ-NH1	-54.95	0.55	1.32
1	A	28	ARG	CZ-NH2	-53.75	0.63	1.33
1	A	28	ARG	CD-NE	-53.49	0.71	1.46
1	A	23	GLU	CD-OE2	-53.44	0.23	1.25
1	A	32	ARG	C-O	-52.76	0.18	1.23
1	A	29	THR	C-N	-49.23	0.18	1.33
1	A	14	ARG	NE-CZ	-48.74	0.79	1.33
1	A	31	ARG	C-O	-48.39	0.61	1.23
1	A	23	GLU	CD-OE1	-48.28	0.33	1.25
1	A	20	GLN	CD-OE1	-48.12	0.32	1.23
1	A	24	TYR	CG-CD2	-45.69	0.43	1.39
1	A	31	ARG	C-N	-42.76	0.73	1.33
1	A	31	ARG	CG-CD	-42.56	0.24	1.52
1	A	13	ASP	CG-OD1	-41.73	0.46	1.25
1	A	32	ARG	CG-CD	-41.56	0.27	1.52
1	A	24	TYR	CE1-CZ	-40.51	0.41	1.38
1	A	30	PRO	CG-CD	-37.77	0.22	1.50
1	A	11	SER	C-O	-36.81	0.77	1.24
1	A	32	ARG	CB-CG	-35.63	0.45	1.52
1	A	6	HIS	CG-ND1	-34.68	1.00	1.38
1	A	13	ASP	CG-OD2	-33.48	0.61	1.25
1	A	15	TYR	CG-CD2	-32.56	0.70	1.39
1	A	6	HIS	CE1-NE2	-32.51	1.00	1.32
1	A	14	ARG	CZ-NH2	-32.27	0.91	1.33
1	A	15	TYR	CG-CD1	-31.36	0.73	1.39
1	A	14	ARG	CD-NE	-31.33	1.02	1.46
1	A	20	GLN	C-O	-31.26	0.84	1.24
1	A	23	GLU	CG-CD	-30.45	0.76	1.52
1	A	30	PRO	C-O	-30.15	0.84	1.24
1	A	15	TYR	CE1-CZ	-29.57	0.67	1.38
1	A	1	THR	CB-OG1	-29.43	0.96	1.43
1	A	25	ASN	CG-OD1	-28.91	0.68	1.23
1	A	15	TYR	CE2-CZ	-28.54	0.69	1.38
1	A	29	THR	CB-CG2	-28.35	0.59	1.52
1	A	11	SER	CB-OG	-27.81	0.86	1.42
1	A	28	ARG	CA-C	-27.53	1.20	1.52
1	A	11	SER	C-N	-27.50	0.96	1.33
1	A	24	TYR	CG-CD1	-27.37	0.81	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	ARG	CB-CG	-27.25	0.70	1.52
1	A	20	GLN	CG-CD	-26.77	0.85	1.52
1	A	20	GLN	CD-NE2	-26.65	0.77	1.33
1	A	2	SER	CB-OG	-26.24	0.89	1.42
1	A	21	ALA	C-O	-25.69	0.88	1.23
1	A	32	ARG	CA-C	-25.08	1.00	1.52
1	A	30	PRO	CB-CG	-25.03	0.24	1.49
1	A	12	LEU	CB-CG	-24.89	1.03	1.53
1	A	24	TYR	CE2-CZ	-24.74	0.78	1.38
1	A	28	ARG	C-O	-24.50	0.92	1.23
1	A	31	ARG	N-CA	-24.30	1.13	1.45
1	A	28	ARG	CB-CG	-23.52	0.81	1.52
1	A	27	LYS	CD-CE	-21.82	0.86	1.52
1	A	29	THR	N-CA	-21.71	1.15	1.46
1	A	15	TYR	C-N	-21.51	1.06	1.33
1	A	6	HIS	CD2-NE2	-21.35	1.14	1.37
1	A	28	ARG	N-CA	-21.32	1.20	1.45
1	A	4	ILE	CG1-CD1	-21.09	0.69	1.51
1	A	25	ASN	CG-ND2	-20.97	0.89	1.33
1	A	27	LYS	CE-NZ	-20.81	0.86	1.49
1	A	12	LEU	CG-CD2	-20.50	0.84	1.52
1	A	19	THR	CB-OG1	-20.36	1.11	1.43
1	A	7	LEU	CG-CD2	-19.87	0.86	1.52
1	A	26	LEU	CG-CD2	-19.77	0.87	1.52
1	A	15	TYR	C-O	-19.68	0.97	1.24
1	A	30	PRO	CA-C	-19.57	1.24	1.52
1	A	27	LYS	CA-C	-19.34	1.26	1.52
1	A	23	GLU	C-O	-19.01	0.99	1.24
1	A	20	GLN	C-N	-18.69	1.06	1.33
1	A	12	LEU	CG-CD1	-18.54	0.91	1.52
1	A	21	ALA	C-N	-18.44	1.08	1.33
1	A	27	LYS	C-O	-18.41	1.00	1.24
1	A	10	ILE	CG1-CD1	-18.08	0.81	1.51
1	A	24	TYR	N-CA	-17.93	1.24	1.46
1	A	27	LYS	C-N	-17.69	1.09	1.33
1	A	17	SER	C-O	-17.57	1.03	1.24
1	A	26	LEU	C-O	-17.52	1.01	1.24
1	A	26	LEU	CA-CB	-17.50	1.23	1.53
1	A	22	ILE	C-N	-17.14	1.11	1.33
1	A	26	LEU	C-N	-17.04	1.09	1.33
1	A	24	TYR	CA-C	-16.75	1.31	1.52
1	A	1	THR	N-CA	-16.43	1.15	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	LYS	CB-CG	-16.38	1.03	1.52
1	A	26	LEU	CG-CD1	-16.19	0.99	1.52
1	A	7	LEU	CG-CD1	-15.98	0.99	1.52
1	A	23	GLU	C-N	-15.89	1.12	1.33
1	A	27	LYS	CG-CD	-15.77	1.05	1.52
1	A	9	ALA	C-O	-15.75	1.00	1.24
1	A	25	ASN	C-O	-15.70	1.02	1.23
1	A	23	GLU	CA-C	-15.69	1.30	1.52
1	A	17	SER	C-N	-15.51	1.15	1.33
1	A	24	TYR	CZ-OH	-15.22	1.06	1.38
1	A	25	ASN	N-CA	-15.20	1.24	1.47
1	A	23	GLU	CA-CB	-15.14	1.25	1.53
1	A	18	ILE	CG1-CD1	-15.04	0.93	1.51
1	A	28	ARG	CG-CD	-14.99	1.07	1.52
1	A	24	TYR	CB-CG	-14.69	1.19	1.51
1	A	24	TYR	C-O	-14.21	1.07	1.24
1	A	3	SER	C-O	-14.16	1.05	1.24
1	A	27	LYS	CA-CB	-14.00	1.29	1.53
1	A	25	ASN	CB-CG	-13.89	1.17	1.52
1	A	6	HIS	CG-CD2	-13.71	1.20	1.35
1	A	26	LEU	N-CA	-13.49	1.28	1.46
1	A	1	THR	CB-CG2	-13.32	1.08	1.52
1	A	26	LEU	CB-CG	-13.15	1.27	1.53
1	A	3	SER	C-N	-13.12	1.15	1.33
1	A	22	ILE	C-O	-12.46	1.09	1.24
1	A	24	TYR	C-N	-12.16	1.11	1.34
1	A	3	SER	CB-OG	-12.04	1.18	1.42
1	A	25	ASN	C-N	-11.82	1.17	1.33
1	A	23	GLU	CB-CG	-11.73	1.17	1.52
1	A	28	ARG	CA-CB	-11.69	1.35	1.53
1	A	22	ILE	CG1-CD1	-11.64	1.06	1.51
1	A	25	ASN	CA-C	-11.62	1.34	1.53
1	A	22	ILE	CA-CB	-11.38	1.39	1.54
1	A	22	ILE	CB-CG1	-11.27	1.30	1.53
1	A	28	ARG	C-N	-11.27	1.10	1.33
1	A	7	LEU	CB-CG	-11.23	1.30	1.53
1	A	1	THR	CA-CB	-11.08	1.24	1.54
1	A	20	GLN	CB-CG	-10.53	1.20	1.52
1	A	23	GLU	N-CA	-10.53	1.31	1.46
1	A	22	ILE	CA-C	-10.22	1.39	1.52
1	A	27	LYS	N-CA	-10.21	1.33	1.46
1	A	19	THR	CB-CG2	-10.17	1.19	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	LEU	CA-C	-9.47	1.40	1.52
1	A	9	ALA	C-N	-9.38	1.19	1.33
1	A	14	ARG	CG-CD	-9.37	1.24	1.52
1	A	12	LEU	C-N	-9.11	1.22	1.33
1	A	24	TYR	CD2-CE2	-8.80	1.12	1.38
1	A	24	TYR	CD1-CE1	-8.78	1.12	1.38
1	A	17	SER	CB-OG	-8.71	1.24	1.42
1	A	4	ILE	CA-CB	-8.17	1.47	1.55
1	A	24	TYR	CA-CB	-7.99	1.40	1.53
1	A	10	ILE	CA-CB	-7.94	1.46	1.55
1	A	12	LEU	C-O	-7.75	1.14	1.23
1	A	1	THR	C-N	-7.50	1.22	1.33
1	A	25	ASN	CA-CB	-7.16	1.31	1.53
1	A	9	ALA	CA-CB	-6.96	1.42	1.53
1	A	8	CYS	CB-SG	-6.51	1.59	1.81
1	A	6	HIS	CB-CG	-6.45	1.41	1.50
1	A	6	HIS	C-N	-6.44	1.26	1.33
1	A	6	HIS	ND1-CE1	-6.37	1.26	1.32
1	A	2	SER	C-N	-6.34	1.24	1.33
1	A	22	ILE	N-CA	-6.12	1.38	1.46
1	A	5	VAL	C-N	-6.08	1.26	1.33
1	A	16	TRP	C-N	-5.96	1.26	1.33
1	A	22	ILE	CB-CG2	-5.92	1.33	1.52
1	A	21	ALA	CA-C	-5.88	1.44	1.52
1	A	4	ILE	C-N	-5.85	1.25	1.33
1	A	5	VAL	CA-CB	-5.63	1.46	1.54
1	A	13	ASP	CB-CG	-5.59	1.38	1.52
1	A	20	GLN	CA-C	-5.45	1.45	1.52
1	A	4	ILE	N-CA	-5.40	1.39	1.46
1	A	3	SER	N-CA	-5.30	1.39	1.46
1	A	8	CYS	N-CA	-5.24	1.39	1.46
1	A	18	ILE	CA-CB	-5.12	1.48	1.54
1	A	5	VAL	N-CA	-5.10	1.40	1.46
1	A	21	ALA	N-CA	-5.02	1.39	1.46

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	PRO	N-CA-CB	-56.17	44.27	103.25
1	A	31	ARG	NE-CZ-NH2	53.72	167.54	119.20
1	A	31	ARG	NH1-CZ-NH2	-51.19	52.75	119.30
1	A	15	TYR	CD1-CG-CD2	-49.98	43.14	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	GLU	OE1-CD-OE2	-43.57	18.34	122.90
1	A	28	ARG	NE-CZ-NH1	-40.67	80.83	121.50
1	A	28	ARG	NE-CZ-NH2	37.65	153.08	119.20
1	A	15	TYR	CE1-CZ-CE2	-37.35	45.59	120.30
1	A	13	ASP	OD1-CG-OD2	-36.68	34.87	122.90
1	A	24	TYR	CD1-CG-CD2	-35.90	64.26	118.10
1	A	31	ARG	CD-NE-CZ	31.66	168.73	124.40
1	A	29	THR	CB-CA-C	-30.97	49.16	110.17
1	A	30	PRO	CB-CA-C	29.98	161.02	111.56
1	A	32	ARG	CB-CG-CD	-27.86	47.21	111.30
1	A	31	ARG	CB-CG-CD	26.53	172.31	111.30
1	A	14	ARG	NE-CZ-NH2	26.27	142.84	119.20
1	A	31	ARG	CG-CD-NE	26.19	169.61	112.00
1	A	24	TYR	CE1-CZ-CE2	-26.03	68.24	120.30
1	A	15	TYR	CB-CG-CD1	25.36	158.83	120.80
1	A	24	TYR	CB-CG-CD1	25.34	158.81	120.80
1	A	15	TYR	CG-CD1-CE1	25.10	158.84	121.20
1	A	24	TYR	CG-CD1-CE1	25.09	158.83	121.20
1	A	31	ARG	O-C-N	24.92	154.35	122.96
1	A	14	ARG	NE-CZ-NH1	-24.86	96.64	121.50
1	A	15	TYR	CB-CG-CD2	24.82	158.03	120.80
1	A	15	TYR	CG-CD2-CE2	24.54	158.01	121.20
1	A	30	PRO	O-C-N	-24.44	89.65	122.64
1	A	29	THR	N-CA-CB	24.13	153.32	110.37
1	A	23	GLU	CG-CD-OE1	23.48	172.41	118.40
1	A	20	GLN	CG-CD-NE2	23.23	151.24	116.40
1	A	31	ARG	CA-C-O	-23.04	95.71	121.51
1	A	29	THR	OG1-CB-CG2	-22.91	63.49	109.30
1	A	30	PRO	CA-N-CD	22.66	143.72	112.00
1	A	12	LEU	CD1-CG-CD2	-22.60	61.08	110.80
1	A	29	THR	CA-C-N	-22.60	91.59	119.84
1	A	29	THR	C-N-CA	-22.60	91.59	119.84
1	A	23	GLU	CG-CD-OE2	22.11	169.25	118.40
1	A	28	ARG	CD-NE-CZ	21.69	154.77	124.40
1	A	24	TYR	CZ-CE2-CD2	21.32	157.97	119.60
1	A	15	TYR	CZ-CE2-CD2	21.11	157.60	119.60
1	A	29	THR	CA-C-O	20.90	148.80	120.16
1	A	30	PRO	CA-C-O	20.90	158.64	120.60
1	A	4	ILE	CB-CG1-CD1	20.81	157.50	113.80
1	A	15	TYR	CD1-CE1-CZ	20.68	156.82	119.60
1	A	13	ASP	CB-CG-OD2	20.35	165.20	118.40
1	A	29	THR	N-CA-C	20.28	154.63	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	SER	O-C-N	-20.16	96.18	122.39
1	A	30	PRO	CA-CB-CG	19.35	141.27	104.50
1	A	20	GLN	CB-CG-CD	19.32	145.45	112.60
1	A	29	THR	CA-CB-CG2	18.48	141.92	110.50
1	A	31	ARG	NE-CZ-NH1	18.21	139.71	121.50
1	A	30	PRO	N-CA-C	18.17	149.91	112.47
1	A	13	ASP	CB-CG-OD1	18.06	159.93	118.40
1	A	6	HIS	CG-CD2-NE2	16.96	124.17	107.20
1	A	30	PRO	N-CD-CG	15.63	126.65	103.20
1	A	14	ARG	CD-NE-CZ	14.90	145.26	124.40
1	A	6	HIS	CE1-NE2-CD2	-14.82	94.18	109.00
1	A	32	ARG	CG-CD-NE	-14.77	79.50	112.00
1	A	10	ILE	CB-CG1-CD1	14.60	144.47	113.80
1	A	25	ASN	OD1-CG-ND2	-14.49	108.11	122.60
1	A	23	GLU	CB-CG-CD	14.48	137.21	112.60
1	A	28	ARG	CG-CD-NE	14.01	142.82	112.00
1	A	32	ARG	NE-CZ-NH2	14.00	131.80	119.20
1	A	24	TYR	OH-CZ-CE2	12.70	157.99	119.90
1	A	6	HIS	ND1-CG-CD2	-12.60	93.50	106.10
1	A	15	TYR	OH-CZ-CE2	12.56	157.58	119.90
1	A	15	TYR	CE1-CZ-OH	12.31	156.82	119.90
1	A	20	GLN	CG-CD-OE1	-12.05	96.70	120.80
1	A	31	ARG	N-CA-CB	12.03	131.10	111.62
1	A	27	LYS	CB-CG-CD	11.93	138.74	111.30
1	A	20	GLN	O-C-N	-11.69	107.19	122.39
1	A	32	ARG	NH1-CZ-NH2	-11.65	104.15	119.30
1	A	2	SER	CA-CB-OG	11.13	133.35	111.10
1	A	32	ARG	CB-CA-C	-11.12	88.97	110.10
1	A	12	LEU	CB-CG-CD1	10.97	143.60	110.70
1	A	24	TYR	CB-CG-CD2	10.76	136.93	120.80
1	A	20	GLN	OE1-CD-NE2	-10.54	112.06	122.60
1	A	7	LEU	CD1-CG-CD2	-10.54	87.61	110.80
1	A	24	TYR	CG-CD2-CE2	10.47	136.91	121.20
1	A	1	THR	OG1-CB-CG2	-10.14	89.01	109.30
1	A	12	LEU	CB-CG-CD2	9.82	140.17	110.70
1	A	21	ALA	O-C-N	-9.69	110.23	122.34
1	A	30	PRO	CB-CG-CD	-9.34	76.23	106.10
1	A	31	ARG	CA-CB-CG	9.06	132.22	114.10
1	A	25	ASN	CB-CG-ND2	9.02	129.92	116.40
1	A	1	THR	CA-CB-CG2	8.76	125.39	110.50
1	A	27	LYS	CA-CB-CG	8.76	131.62	114.10
1	A	6	HIS	CB-CG-CD2	8.70	142.51	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ARG	N-CA-CB	8.60	125.13	110.50
1	A	18	ILE	CB-CG1-CD1	8.55	131.76	113.80
1	A	32	ARG	CD-NE-CZ	8.17	135.84	124.40
1	A	24	TYR	CD1-CE1-CZ	7.89	133.80	119.60
1	A	11	SER	CA-C-N	7.74	138.52	121.80
1	A	11	SER	C-N-CA	7.74	138.52	121.80
1	A	15	TYR	O-C-N	-7.71	110.99	122.39
1	A	11	SER	CA-C-O	7.69	128.79	119.49
1	A	20	GLN	CA-C-N	7.63	135.13	122.54
1	A	20	GLN	C-N-CA	7.63	135.13	122.54
1	A	27	LYS	CG-CD-CE	7.52	128.59	111.30
1	A	11	SER	CA-CB-OG	7.48	126.06	111.10
1	A	7	LEU	CB-CG-CD1	6.94	131.51	110.70
1	A	6	HIS	ND1-CE1-NE2	6.51	114.91	108.40
1	A	32	ARG	CA-C-O	6.39	131.66	120.80
1	A	27	LYS	CD-CE-NZ	6.18	131.67	111.90
1	A	22	ILE	CB-CG1-CD1	6.07	126.55	113.80
1	A	21	ALA	CA-C-N	5.93	132.64	121.97
1	A	21	ALA	C-N-CA	5.93	132.64	121.97
1	A	32	ARG	CA-CB-CG	-5.89	102.31	114.10
1	A	28	ARG	CB-CG-CD	5.82	124.69	111.30
1	A	28	ARG	CA-C-O	-5.70	114.67	121.56
1	A	9	ALA	CA-C-N	5.58	128.71	123.08
1	A	9	ALA	C-N-CA	5.58	128.71	123.08
1	A	17	SER	O-C-N	-5.54	116.24	122.12
1	A	19	THR	OG1-CB-CG2	-5.39	98.53	109.30
1	A	12	LEU	CA-CB-CG	5.33	134.97	116.30
1	A	30	PRO	CA-C-N	-5.23	113.99	122.36
1	A	30	PRO	C-N-CA	-5.23	113.99	122.36
1	A	28	ARG	NH1-CZ-NH2	5.22	126.08	119.30
1	A	15	TYR	CA-C-O	5.20	125.93	119.12
1	A	26	LEU	CD1-CG-CD2	-5.18	99.41	110.80
1	A	15	TYR	CA-C-N	5.17	127.66	120.63
1	A	15	TYR	C-N-CA	5.17	127.66	120.63

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	29	THR	CB,CA
1	A	30	PRO	CA
1	A	31	ARG	CA
1	A	32	ARG	CA

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	266	274	255	87
All	All	266	274	255	87

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 167.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:12:LEU:CD2	1:A:12:LEU:CB	1.59	1.77
1:A:12:LEU:CB	1:A:12:LEU:CD1	1.54	1.84
1:A:23:GLU:CD	1:A:23:GLU:CB	1.52	1.80
1:A:15:TYR:CZ	1:A:15:TYR:CD1	1.46	2.02
1:A:15:TYR:CG	1:A:15:TYR:CE2	1.42	2.06
1:A:15:TYR:CZ	1:A:15:TYR:CD2	1.41	2.05
1:A:15:TYR:CG	1:A:15:TYR:CE1	1.37	2.09
1:A:20:GLN:CD	1:A:20:GLN:CB	1.37	1.96
1:A:15:TYR:CD2	1:A:15:TYR:CB	1.29	2.15
1:A:13:ASP:OD1	1:A:13:ASP:CB	1.28	1.81
1:A:15:TYR:CD1	1:A:15:TYR:CB	1.23	2.18
1:A:10:ILE:CD1	1:A:10:ILE:CB	1.22	2.17
1:A:15:TYR:CE1	1:A:15:TYR:OH	1.18	1.95
1:A:18:ILE:CD1	1:A:18:ILE:CB	1.18	2.21
1:A:13:ASP:CB	1:A:13:ASP:OD2	1.11	1.98
1:A:15:TYR:CE2	1:A:15:TYR:OH	1.09	1.97
1:A:12:LEU:CD1	1:A:12:LEU:HG	1.08	1.76
1:A:12:LEU:CD2	1:A:12:LEU:HG	1.04	1.72
1:A:12:LEU:CD2	1:A:12:LEU:HD12	1.03	1.83
1:A:12:LEU:CD1	1:A:12:LEU:HD23	1.02	1.83
1:A:12:LEU:HD12	1:A:12:LEU:CG	1.00	1.53
1:A:18:ILE:CG1	1:A:18:ILE:HD13	0.99	1.55
1:A:12:LEU:CG	1:A:12:LEU:HD11	0.99	1.54
1:A:18:ILE:CG1	1:A:18:ILE:HD12	0.99	1.55
1:A:18:ILE:CG1	1:A:18:ILE:HD11	0.98	1.55

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:12:LEU:CG	1:A:12:LEU:HD13	0.97	1.53
1:A:18:ILE:CD1	1:A:18:ILE:HG12	0.96	1.50
1:A:12:LEU:CG	1:A:12:LEU:HD22	0.95	1.48
1:A:18:ILE:CD1	1:A:18:ILE:HG13	0.95	1.50
1:A:18:ILE:CD1	1:A:18:ILE:CG1	0.93	0.93
1:A:12:LEU:HD23	1:A:12:LEU:CG	0.92	1.48
1:A:10:ILE:CG1	1:A:10:ILE:HD11	0.91	1.45
1:A:20:GLN:CD	1:A:20:GLN:HG3	0.91	1.40
1:A:12:LEU:CD1	1:A:12:LEU:CG	0.91	0.91
1:A:10:ILE:CG1	1:A:10:ILE:HD13	0.90	1.45
1:A:10:ILE:CG1	1:A:10:ILE:HD12	0.90	1.46
1:A:20:GLN:CD	1:A:20:GLN:CG	0.89	0.85
1:A:12:LEU:CD2	1:A:12:LEU:CD1	0.89	0.89
1:A:20:GLN:CD	1:A:20:GLN:HG2	0.88	1.40
1:A:23:GLU:CD	1:A:23:GLU:HG2	0.86	1.35
1:A:23:GLU:CD	1:A:23:GLU:HG3	0.85	1.35
1:A:12:LEU:CD2	1:A:12:LEU:CG	0.84	0.84
1:A:12:LEU:CG	1:A:12:LEU:HD21	0.84	1.48
1:A:10:ILE:CD1	1:A:10:ILE:HG12	0.82	1.37
1:A:10:ILE:CD1	1:A:10:ILE:HG13	0.82	1.37
1:A:13:ASP:OD2	1:A:13:ASP:CG	0.81	0.61
1:A:10:ILE:CD1	1:A:10:ILE:CG1	0.80	0.81
1:A:23:GLU:CD	1:A:23:GLU:CG	0.80	0.75
1:A:12:LEU:CD1	1:A:12:LEU:HD22	0.80	1.33
1:A:12:LEU:CD2	1:A:12:LEU:HD13	0.79	1.32
1:A:12:LEU:CD1	1:A:12:LEU:HD21	0.77	0.94
1:A:12:LEU:HD13	1:A:12:LEU:HD22	0.76	0.92
1:A:20:GLN:CD	1:A:20:GLN:HE22	0.76	1.41
1:A:12:LEU:CD2	1:A:12:LEU:HB3	0.75	2.06
1:A:20:GLN:CD	1:A:20:GLN:HE21	0.75	1.41
1:A:12:LEU:CD2	1:A:12:LEU:HB2	0.69	2.05
1:A:20:GLN:CD	1:A:20:GLN:NE2	0.67	0.77
1:A:15:TYR:CD1	1:A:15:TYR:CG	0.66	0.73
1:A:13:ASP:OD1	1:A:13:ASP:CG	0.65	0.46
1:A:6:HIS:O	1:A:9:ALA:HB3	0.64	1.92
1:A:15:TYR:CZ	1:A:15:TYR:CE2	0.63	0.69
1:A:15:TYR:CG	1:A:15:TYR:CD2	0.63	0.71
1:A:15:TYR:CZ	1:A:15:TYR:CE1	0.61	0.67
1:A:12:LEU:CD1	1:A:12:LEU:HB2	0.60	2.13
1:A:12:LEU:CD2	1:A:12:LEU:HD11	0.60	1.04
1:A:13:ASP:O	1:A:16:TRP:HB3	0.56	2.00
1:A:24:TYR:CG	1:A:24:TYR:HD1	0.56	1.34

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:22:ILE:C	1:A:24:TYR:N	0.55	2.51
1:A:4:ILE:O	1:A:5:VAL:C	0.53	2.49
1:A:15:TYR:CG	1:A:15:TYR:HD1	0.53	1.28
1:A:5:VAL:O	1:A:6:HIS:C	0.52	2.51
1:A:15:TYR:CG	1:A:15:TYR:HD2	0.52	1.27
1:A:24:TYR:CZ	1:A:24:TYR:HE2	0.51	1.33
1:A:15:TYR:CZ	1:A:15:TYR:HE2	0.50	1.26
1:A:27:LYS:O	1:A:27:LYS:HG2	0.50	2.01
1:A:15:TYR:CZ	1:A:15:TYR:HE1	0.50	1.25
1:A:22:ILE:HG22	1:A:23:GLU:N	0.47	2.15
1:A:7:LEU:C	1:A:9:ALA:N	0.47	2.69
1:A:28:ARG:HG2	1:A:29:THR:N	0.47	2.23
1:A:23:GLU:CD	1:A:23:GLU:HB2	0.46	2.11
1:A:26:LEU:HD23	1:A:26:LEU:C	0.46	2.36
1:A:22:ILE:O	1:A:24:TYR:N	0.44	2.50
1:A:13:ASP:O	1:A:14:ARG:C	0.43	2.60
1:A:10:ILE:CD1	1:A:10:ILE:CG2	0.42	2.90
1:A:26:LEU:HD23	1:A:27:LYS:N	0.41	2.30
1:A:12:LEU:O	1:A:13:ASP:C	0.41	2.58
1:A:22:ILE:O	1:A:23:GLU:C	0.41	2.50

6.3 Torsion angles [i](#)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	5	35
All	All	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	5	35

All 1 Ramachandran outliers are listed below.

Mol	Chain	Res	Type
1	A	29	THR

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	30/30 (100%)	19 (63%)	11 (37%)	1	8
All	All	30/30 (100%)	19 (63%)	11 (37%)	1	8

All 11 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	2	SER
1	A	7	LEU
1	A	8	CYS
1	A	11	SER
1	A	13	ASP
1	A	17	SER
1	A	20	GLN
1	A	24	TYR
1	A	25	ASN
1	A	29	THR
1	A	31	ARG

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	17

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	9:ALA	C	10:ILE	N	1.19
1	A	25:ASN	C	26:LEU	N	1.17
1	A	3:SER	C	4:ILE	N	1.14
1	A	17:SER	C	18:ILE	N	1.14
1	A	23:GLU	C	24:TYR	N	1.12
1	A	22:ILE	C	23:GLU	N	1.11
1	A	24:TYR	C	25:ASN	N	1.11
1	A	28:ARG	C	29:THR	N	1.10
1	A	26:LEU	C	27:LYS	N	1.09
1	A	27:LYS	C	28:ARG	N	1.09
1	A	21:ALA	C	22:ILE	N	1.08
1	A	15:TYR	C	16:TRP	N	1.06
1	A	20:GLN	C	21:ALA	N	1.06
1	A	11:SER	C	12:LEU	N	0.96
1	A	31:ARG	C	32:ARG	N	0.73
1	A	30:PRO	C	31:ARG	N	0.37
1	A	29:THR	C	30:PRO	N	0.18

7 Chemical shift validation

No chemical shift data were provided