



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:49 PM BST

PDB ID : 1HOD
Title : NMR STRUCTURE OF D130I MUTANT T3-I2, A 32 RESIDUE PEPTIDE
FROM THE ALPHA 2A ADRENERGIC RECEPTOR
Authors : Chung, D.A.; Zuiderweg, E.R.; Neubig, R.R.
Deposited on : 2000-12-10

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

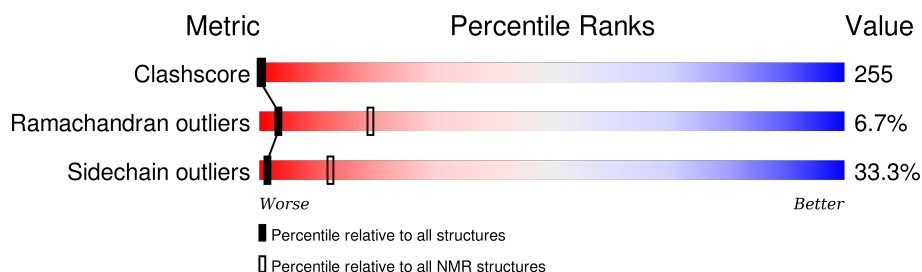
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	

2 Ensemble composition and analysis ⓘ

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 547 atoms, of which 281 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
			547	170	281	50	45	1	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ILE	ASP	CONFLICT	UNP P08913

4 Residue-property plots [i](#)

These plots are provided for all protein, RNA and DNA 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. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	26.38	181/271 (66.8%)	16.31	113/367 (30.8%)
All	All	26.38	181/271 (66.8%)	16.31	113/367 (30.8%)

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	6	0
All	All	6	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	23	GLU	CD-OE1	-101.41	0.14	1.25
1	A	14	ARG	CZ-NH1	-93.88	0.11	1.33
1	A	31	ARG	NE-CZ	-80.92	0.27	1.33
1	A	32	ARG	NE-CZ	-75.36	0.35	1.33
1	A	23	GLU	CD-OE2	-69.56	0.49	1.25
1	A	30	PRO	N-CD	-69.45	0.50	1.47
1	A	32	ARG	CZ-NH1	-68.81	0.43	1.33
1	A	31	ARG	CZ-NH1	-67.44	0.45	1.33
1	A	32	ARG	CZ-NH2	-63.56	0.50	1.33
1	A	32	ARG	C-O	-60.15	0.09	1.23
1	A	32	ARG	CA-CB	-59.65	0.22	1.53
1	A	28	ARG	CZ-NH1	-59.28	0.56	1.33
1	A	15	TYR	CE1-CZ	-59.05	0.61	1.38
1	A	15	TYR	CE2-CZ	-58.06	0.63	1.38
1	A	15	TYR	CG-CD2	-56.66	0.65	1.39
1	A	24	TYR	CE1-CZ	-56.35	0.65	1.38
1	A	30	PRO	CA-CB	-56.27	0.41	1.53
1	A	32	ARG	CG-CD	-55.83	0.12	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	TYR	CG-CD1	-55.62	0.66	1.39
1	A	31	ARG	CA-CB	-55.28	0.32	1.53
1	A	24	TYR	CE2-CZ	-54.69	0.67	1.38
1	A	24	TYR	CG-CD2	-54.64	0.68	1.39
1	A	31	ARG	CZ-NH2	-54.47	0.62	1.33
1	A	32	ARG	CD-NE	-53.83	0.55	1.46
1	A	28	ARG	CZ-NH2	-53.59	0.63	1.33
1	A	24	TYR	CG-CD1	-52.85	0.70	1.39
1	A	23	GLU	CG-CD	-51.80	0.74	1.51
1	A	2	SER	CB-OG	-51.37	0.75	1.42
1	A	28	ARG	NE-CZ	-48.78	0.69	1.33
1	A	29	THR	CB-OG1	-46.80	0.49	1.43
1	A	31	ARG	CD-NE	-46.44	0.67	1.46
1	A	27	LYS	CE-NZ	-45.94	0.34	1.49
1	A	20	GLN	CD-OE1	-45.63	0.23	1.24
1	A	31	ARG	C-O	-45.58	0.36	1.23
1	A	29	THR	C-N	-45.23	0.48	1.34
1	A	32	ARG	N-CA	-44.68	0.56	1.46
1	A	28	ARG	CD-NE	-44.26	0.71	1.46
1	A	30	PRO	C-O	-44.19	0.34	1.23
1	A	32	ARG	CA-C	-43.37	0.40	1.52
1	A	31	ARG	CG-CD	-42.24	0.46	1.51
1	A	29	THR	C-O	-41.76	0.44	1.23
1	A	14	ARG	CZ-NH2	-41.31	0.79	1.33
1	A	14	ARG	NE-CZ	-37.51	0.84	1.33
1	A	31	ARG	CA-C	-36.92	0.56	1.52
1	A	27	LYS	C-O	-36.86	0.53	1.23
1	A	23	GLU	CB-CG	-36.66	0.82	1.52
1	A	27	LYS	CD-CE	-35.47	0.62	1.51
1	A	32	ARG	CB-CG	-35.09	0.57	1.52
1	A	20	GLN	CD-NE2	-33.29	0.49	1.32
1	A	30	PRO	N-CA	-32.97	0.91	1.47
1	A	20	GLN	CG-CD	-32.73	0.75	1.51
1	A	30	PRO	CA-C	-32.68	0.87	1.52
1	A	14	ARG	CD-NE	-32.41	0.91	1.46
1	A	31	ARG	CB-CG	-32.22	0.65	1.52
1	A	31	ARG	C-N	-31.98	0.60	1.34
1	A	26	LEU	C-O	-31.69	0.63	1.23
1	A	28	ARG	CG-CD	-31.12	0.74	1.51
1	A	31	ARG	N-CA	-30.27	0.85	1.46
1	A	27	LYS	C-N	-30.06	0.65	1.34
1	A	29	THR	CA-CB	-29.88	0.75	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	ARG	CA-CB	-29.46	0.89	1.53
1	A	16	TRP	C-O	-29.32	0.67	1.23
1	A	30	PRO	C-N	-29.16	0.67	1.34
1	A	28	ARG	CB-CG	-28.77	0.74	1.52
1	A	27	LYS	CA-CB	-27.90	0.92	1.53
1	A	29	THR	N-CA	-27.34	0.91	1.46
1	A	28	ARG	C-O	-27.27	0.71	1.23
1	A	26	LEU	CG-CD2	-26.10	0.55	1.51
1	A	14	ARG	CG-CD	-25.57	0.88	1.51
1	A	6	HIS	CG-CD2	-25.43	0.92	1.35
1	A	19	THR	CB-OG1	-25.43	0.92	1.43
1	A	29	THR	CB-CG2	-25.17	0.69	1.52
1	A	30	PRO	CG-CD	-24.16	0.70	1.50
1	A	3	SER	CB-OG	-23.41	1.11	1.42
1	A	27	LYS	CB-CG	-23.04	0.90	1.52
1	A	8	CYS	CB-SG	-22.89	1.43	1.82
1	A	26	LEU	C-N	-22.80	0.81	1.34
1	A	28	ARG	CA-C	-22.61	0.94	1.52
1	A	21	ALA	C-O	-22.59	0.80	1.23
1	A	26	LEU	CG-CD1	-22.18	0.69	1.51
1	A	29	THR	CA-C	-21.88	0.96	1.52
1	A	7	LEU	CB-CG	-21.87	0.89	1.52
1	A	11	SER	CB-OG	-21.58	1.14	1.42
1	A	27	LYS	CG-CD	-21.56	0.79	1.52
1	A	6	HIS	CE1-NE2	-21.00	0.84	1.32
1	A	16	TRP	C-N	-20.92	0.85	1.34
1	A	28	ARG	C-N	-18.32	0.92	1.34
1	A	7	LEU	CG-CD2	-18.07	0.85	1.51
1	A	12	LEU	CG-CD2	-17.91	0.85	1.51
1	A	7	LEU	C-O	-17.31	0.90	1.23
1	A	26	LEU	CA-CB	-16.91	1.14	1.53
1	A	12	LEU	CG-CD1	-16.66	0.90	1.51
1	A	25	ASN	C-O	-16.20	0.92	1.23
1	A	11	SER	C-O	-16.04	0.92	1.23
1	A	27	LYS	N-CA	-15.98	1.14	1.46
1	A	26	LEU	CB-CG	-15.88	1.06	1.52
1	A	21	ALA	C-N	-15.29	0.98	1.34
1	A	28	ARG	N-CA	-15.26	1.15	1.46
1	A	6	HIS	CG-ND1	-15.02	1.05	1.38
1	A	24	TYR	CB-CG	-14.68	1.29	1.51
1	A	30	PRO	CB-CG	-14.50	0.77	1.50
1	A	7	LEU	C-N	-13.93	1.02	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	THR	CB-CG2	-13.50	1.07	1.52
1	A	24	TYR	CZ-OH	-13.27	1.15	1.37
1	A	1	THR	CB-OG1	-13.22	1.16	1.43
1	A	26	LEU	N-CA	-13.10	1.20	1.46
1	A	26	LEU	CA-C	-13.07	1.19	1.52
1	A	4	ILE	CG1-CD1	-12.91	0.61	1.50
1	A	1	THR	N-CA	-12.61	1.21	1.46
1	A	20	GLN	CB-CG	-12.48	1.18	1.52
1	A	27	LYS	CA-C	-12.17	1.21	1.52
1	A	18	ILE	CG1-CD1	-11.98	0.67	1.50
1	A	24	TYR	CD1-CE1	-11.56	1.22	1.39
1	A	25	ASN	N-CA	-11.50	1.23	1.46
1	A	24	TYR	CD2-CE2	-11.50	1.22	1.39
1	A	11	SER	C-N	-11.43	1.07	1.34
1	A	16	TRP	CD2-CE2	-11.18	1.27	1.41
1	A	23	GLU	CA-CB	-10.76	1.30	1.53
1	A	25	ASN	CA-C	-10.72	1.25	1.52
1	A	25	ASN	C-N	-10.71	1.09	1.34
1	A	1	THR	CB-CG2	-10.40	1.18	1.52
1	A	2	SER	C-O	-10.36	1.03	1.23
1	A	6	HIS	CB-CG	-10.21	1.31	1.50
1	A	14	ARG	CB-CG	-10.16	1.25	1.52
1	A	7	LEU	CG-CD1	-9.88	1.15	1.51
1	A	18	ILE	CB-CG1	-9.83	1.26	1.54
1	A	6	HIS	ND1-CE1	-9.71	1.10	1.34
1	A	6	HIS	CD2-NE2	-9.71	1.16	1.38
1	A	24	TYR	CA-CB	-9.44	1.33	1.53
1	A	25	ASN	CB-CG	-9.29	1.29	1.51
1	A	23	GLU	C-O	-9.14	1.05	1.23
1	A	16	TRP	CG-CD1	-8.99	1.24	1.36
1	A	24	TYR	CA-C	-8.95	1.29	1.52
1	A	3	SER	C-O	-8.92	1.06	1.23
1	A	1	THR	C-N	-8.84	1.13	1.34
1	A	2	SER	N-CA	-8.71	1.28	1.46
1	A	1	THR	CA-CB	-8.63	1.30	1.53
1	A	5	VAL	CB-CG2	-8.57	1.34	1.52
1	A	25	ASN	CG-OD1	-8.45	1.05	1.24
1	A	18	ILE	CB-CG2	-8.28	1.27	1.52
1	A	17	SER	CB-OG	-8.16	1.31	1.42
1	A	3	SER	C-N	-8.11	1.15	1.34
1	A	23	GLU	C-N	-8.09	1.15	1.34
1	A	2	SER	C-N	-7.87	1.16	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	ASN	CG-ND2	-7.48	1.14	1.32
1	A	23	GLU	N-CA	-7.19	1.31	1.46
1	A	5	VAL	CB-CG1	-7.08	1.38	1.52
1	A	2	SER	CA-CB	-7.05	1.42	1.52
1	A	16	TRP	CZ3-CH2	-7.02	1.28	1.40
1	A	22	ILE	CB-CG1	-6.99	1.34	1.54
1	A	16	TRP	NE1-CE2	-6.94	1.28	1.37
1	A	3	SER	N-CA	-6.91	1.32	1.46
1	A	1	THR	C-O	-6.88	1.10	1.23
1	A	16	TRP	CD2-CE3	-6.81	1.30	1.40
1	A	15	TYR	CZ-OH	-6.69	1.26	1.37
1	A	1	THR	CA-C	-6.36	1.36	1.52
1	A	22	ILE	C-O	-6.35	1.11	1.23
1	A	15	TYR	CB-CG	-6.27	1.42	1.51
1	A	22	ILE	C-N	-6.27	1.19	1.34
1	A	6	HIS	N-CA	-6.18	1.33	1.46
1	A	3	SER	CA-CB	-6.11	1.43	1.52
1	A	16	TRP	CE2-CZ2	-6.02	1.29	1.39
1	A	5	VAL	C-O	-5.96	1.12	1.23
1	A	16	TRP	CD1-NE1	-5.96	1.27	1.38
1	A	16	TRP	CG-CD2	-5.95	1.33	1.43
1	A	22	ILE	CA-CB	-5.89	1.41	1.54
1	A	24	TYR	C-O	-5.84	1.12	1.23
1	A	4	ILE	CA-CB	-5.73	1.41	1.54
1	A	22	ILE	CB-CG2	-5.72	1.35	1.52
1	A	12	LEU	C-N	-5.66	1.21	1.34
1	A	24	TYR	N-CA	-5.54	1.35	1.46
1	A	25	ASN	CA-CB	-5.43	1.39	1.53
1	A	2	SER	CA-C	-5.42	1.38	1.52
1	A	22	ILE	N-CA	-5.41	1.35	1.46
1	A	15	TYR	C-O	-5.40	1.13	1.23
1	A	22	ILE	CA-C	-5.38	1.39	1.52
1	A	16	TRP	CE3-CZ3	-5.26	1.29	1.38
1	A	24	TYR	C-N	-5.16	1.22	1.34
1	A	5	VAL	CA-CB	-5.13	1.44	1.54
1	A	6	HIS	C-O	-5.11	1.13	1.23
1	A	15	TYR	C-N	-5.09	1.22	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH1	-110.65	64.98	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	NE-CZ-NH2	106.54	173.57	120.30
1	A	15	TYR	CD1-CG-CD2	-83.40	26.16	117.90
1	A	15	TYR	CB-CG-CD1	76.77	167.06	121.00
1	A	15	TYR	CB-CG-CD2	76.30	166.78	121.00
1	A	15	TYR	CE1-CZ-CE2	-57.61	27.62	119.80
1	A	15	TYR	CG-CD1-CE1	57.17	167.04	121.30
1	A	15	TYR	CG-CD2-CE2	56.80	166.74	121.30
1	A	15	TYR	CZ-CE2-CD2	51.72	166.35	119.80
1	A	15	TYR	CD1-CE1-CZ	51.44	166.09	119.80
1	A	14	ARG	NH1-CZ-NH2	-49.53	64.92	119.40
1	A	24	TYR	CD1-CG-CD2	-48.70	64.33	117.90
1	A	32	ARG	CB-CA-C	-47.34	15.73	110.40
1	A	24	TYR	CB-CG-CD1	45.61	148.37	121.00
1	A	23	GLU	OE1-CD-OE2	-44.19	70.27	123.30
1	A	24	TYR	CB-CG-CD2	43.83	147.30	121.00
1	A	32	ARG	NE-CZ-NH1	-38.73	100.93	120.30
1	A	31	ARG	NE-CZ-NH2	36.65	138.63	120.30
1	A	14	ARG	CD-NE-CZ	36.10	174.13	123.60
1	A	24	TYR	CG-CD1-CE1	33.85	148.38	121.30
1	A	31	ARG	NH1-CZ-NH2	33.63	156.40	119.40
1	A	24	TYR	CE1-CZ-CE2	-32.69	67.49	119.80
1	A	24	TYR	CG-CD2-CE2	32.46	147.27	121.30
1	A	30	PRO	N-CD-CG	-31.04	56.64	103.20
1	A	27	LYS	O-C-N	-30.99	73.11	122.70
1	A	24	TYR	CZ-CE2-CD2	30.09	146.88	119.80
1	A	24	TYR	CD1-CE1-CZ	28.71	145.64	119.80
1	A	29	THR	O-C-N	-27.50	68.84	121.10
1	A	16	TRP	O-C-N	-25.93	81.21	122.70
1	A	23	GLU	CG-CD-OE2	24.06	166.43	118.30
1	A	28	ARG	CG-CD-NE	23.87	161.92	111.80
1	A	32	ARG	N-CA-CB	23.43	152.78	110.60
1	A	29	THR	C-N-CD	-22.73	70.58	120.60
1	A	20	GLN	OE1-CD-NE2	-22.61	69.89	121.90
1	A	30	PRO	CA-N-CD	22.19	142.76	111.70
1	A	32	ARG	CA-C-O	21.69	165.66	120.10
1	A	28	ARG	NE-CZ-NH2	20.73	130.67	120.30
1	A	29	THR	CA-CB-OG1	-20.63	65.67	109.00
1	A	26	LEU	CB-CG-CD1	19.90	144.83	111.00
1	A	15	TYR	OH-CZ-CE2	17.11	166.31	120.10
1	A	15	TYR	CE1-CZ-OH	17.02	166.07	120.10
1	A	20	GLN	CG-CD-NE2	16.54	156.40	116.70
1	A	32	ARG	NH1-CZ-NH2	15.97	136.96	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	PRO	O-C-N	-15.12	98.51	122.70
1	A	26	LEU	O-C-N	-14.19	100.00	122.70
1	A	26	LEU	CB-CG-CD2	14.19	135.12	111.00
1	A	6	HIS	ND1-CG-CD2	-14.04	86.34	106.00
1	A	30	PRO	CA-C-N	13.82	147.61	117.20
1	A	32	ARG	N-CA-C	13.74	148.11	111.00
1	A	18	ILE	CB-CG1-CD1	13.72	152.31	113.90
1	A	14	ARG	CG-CD-NE	13.63	140.41	111.80
1	A	7	LEU	CA-CB-CG	13.55	146.48	115.30
1	A	6	HIS	CG-ND1-CE1	13.13	126.58	108.20
1	A	4	ILE	CB-CG1-CD1	12.84	149.86	113.90
1	A	29	THR	CA-C-O	12.70	146.78	120.10
1	A	27	LYS	CA-C-N	12.65	145.02	117.20
1	A	31	ARG	CB-CA-C	-12.60	85.21	110.40
1	A	31	ARG	CA-C-O	-12.38	94.11	120.10
1	A	29	THR	CA-CB-CG2	12.35	129.69	112.40
1	A	26	LEU	CD1-CG-CD2	-11.90	74.81	110.50
1	A	31	ARG	CD-NE-CZ	11.78	140.09	123.60
1	A	21	ALA	O-C-N	-11.66	104.05	122.70
1	A	30	PRO	C-N-CA	11.57	150.63	121.70
1	A	16	TRP	CA-C-N	11.36	142.19	117.20
1	A	32	ARG	CA-CB-CG	11.16	137.95	113.40
1	A	12	LEU	CB-CG-CD1	10.93	129.59	111.00
1	A	30	PRO	N-CA-C	10.84	140.27	112.10
1	A	31	ARG	N-CA-C	10.78	140.10	111.00
1	A	30	PRO	CB-CG-CD	10.59	147.81	106.50
1	A	7	LEU	O-C-N	-10.52	105.87	122.70
1	A	27	LYS	CA-C-O	10.37	141.87	120.10
1	A	27	LYS	C-N-CA	10.26	147.35	121.70
1	A	14	ARG	CB-CG-CD	9.97	137.52	111.60
1	A	24	TYR	OH-CZ-CE2	9.91	146.86	120.10
1	A	30	PRO	CA-CB-CG	-9.77	85.43	104.00
1	A	29	THR	CA-C-N	9.74	144.38	117.10
1	A	20	GLN	CB-CG-CD	9.73	136.91	111.60
1	A	32	ARG	CB-CG-CD	9.70	136.83	111.60
1	A	28	ARG	NH1-CZ-NH2	-9.57	108.88	119.40
1	A	24	TYR	CE1-CZ-OH	9.46	145.64	120.10
1	A	16	TRP	C-N-CA	9.27	144.88	121.70
1	A	31	ARG	CA-C-N	8.94	136.87	117.20
1	A	28	ARG	CA-CB-CG	8.64	132.41	113.40
1	A	11	SER	O-C-N	-8.63	108.89	122.70
1	A	31	ARG	C-N-CA	8.16	142.10	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	CG-CD-NE	7.91	128.41	111.80
1	A	26	LEU	CA-C-N	7.90	134.57	117.20
1	A	16	TRP	CA-C-O	7.86	136.60	120.10
1	A	28	ARG	CD-NE-CZ	7.76	134.47	123.60
1	A	32	ARG	CG-CD-NE	7.76	128.09	111.80
1	A	12	LEU	CB-CG-CD2	7.60	123.92	111.00
1	A	7	LEU	CB-CG-CD2	7.51	123.77	111.00
1	A	23	GLU	CB-CG-CD	7.50	134.45	114.20
1	A	27	LYS	CD-CE-NZ	7.38	128.68	111.70
1	A	12	LEU	CD1-CG-CD2	-7.18	88.95	110.50
1	A	31	ARG	CB-CG-CD	6.67	128.94	111.60
1	A	26	LEU	C-N-CA	6.64	138.30	121.70
1	A	29	THR	N-CA-C	6.32	128.06	111.00
1	A	21	ALA	CA-C-N	6.31	131.09	117.20
1	A	6	HIS	ND1-CE1-NE2	-6.30	96.04	109.90
1	A	6	HIS	CG-CD2-NE2	6.19	120.96	109.20
1	A	20	GLN	CG-CD-OE1	6.06	133.71	121.60
1	A	26	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	2	SER	CA-CB-OG	5.89	127.12	111.20
1	A	29	THR	C-N-CA	5.87	146.66	122.00
1	A	19	THR	CA-CB-CG2	5.75	120.45	112.40
1	A	6	HIS	CB-CG-ND1	5.59	137.18	123.20
1	A	7	LEU	CD1-CG-CD2	-5.51	93.96	110.50
1	A	21	ALA	C-N-CA	5.34	135.04	121.70
1	A	1	THR	CA-CB-CG2	-5.29	105.00	112.40
1	A	28	ARG	CA-C-O	-5.13	109.33	120.10
1	A	7	LEU	CB-CG-CD1	5.08	119.64	111.00
1	A	27	LYS	N-CA-C	5.05	124.64	111.00

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	28	ARG	CA
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	281	263	135
All	All	266	281	263	135

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 255.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:14:ARG:CD	1:A:14:ARG:CZ	1.63	1.75
1:A:24:TYR:CD1	1:A:24:TYR:CZ	1.62	1.79
1:A:24:TYR:CG	1:A:24:TYR:CE2	1.62	1.82
1:A:24:TYR:CD2	1:A:24:TYR:CZ	1.60	1.82
1:A:24:TYR:CG	1:A:24:TYR:CE1	1.59	1.85
1:A:15:TYR:CZ	1:A:15:TYR:CD1	1.56	1.94
1:A:23:GLU:CA	1:A:23:GLU:CG	1.54	1.83
1:A:15:TYR:CZ	1:A:15:TYR:CD2	1.52	1.95
1:A:15:TYR:CE2	1:A:15:TYR:CG	1.52	1.97
1:A:24:TYR:CD2	1:A:24:TYR:CB	1.51	1.90
1:A:15:TYR:CE1	1:A:15:TYR:CG	1.49	1.99
1:A:20:GLN:CB	1:A:20:GLN:CD	1.46	1.81
1:A:14:ARG:CG	1:A:14:ARG:NE	1.46	1.68
1:A:26:LEU:CA	1:A:26:LEU:O	1.44	1.63
1:A:14:ARG:NH2	1:A:14:ARG:NE	1.44	1.62
1:A:24:TYR:CB	1:A:24:TYR:CD1	1.44	1.92
1:A:26:LEU:C	1:A:27:LYS:CA	1.44	1.83
1:A:15:TYR:CB	1:A:15:TYR:CD2	1.39	2.06
1:A:12:LEU:CB	1:A:12:LEU:CD2	1.39	2.01
1:A:14:ARG:CD	1:A:14:ARG:CB	1.38	1.98
1:A:26:LEU:CA	1:A:27:LYS:N	1.35	1.85
1:A:24:TYR:CE1	1:A:24:TYR:OH	1.29	1.72
1:A:15:TYR:CB	1:A:15:TYR:CD1	1.28	2.07
1:A:15:TYR:CE1	1:A:15:TYR:OH	1.28	1.86
1:A:12:LEU:CB	1:A:12:LEU:CD1	1.23	2.09
1:A:24:TYR:CE2	1:A:24:TYR:OH	1.18	1.75
1:A:16:TRP:C	1:A:17:SER:CA	1.12	2.18
1:A:2:SER:HB3	1:A:2:SER:OG	1.12	1.37

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:2:SER:CA	1:A:2:SER:OG	1.12	1.97
1:A:15:TYR:CE2	1:A:15:TYR:OH	1.10	1.87
1:A:26:LEU:C	1:A:27:LYS:CB	1.07	2.24
1:A:16:TRP:CA	1:A:16:TRP:O	1.05	2.03
1:A:2:SER:CB	1:A:2:SER:OG	1.04	0.75
1:A:2:SER:HB2	1:A:2:SER:OG	1.02	1.37
1:A:16:TRP:CA	1:A:17:SER:N	1.01	2.22
1:A:12:LEU:CD2	1:A:12:LEU:HG	0.99	1.62
1:A:12:LEU:CG	1:A:12:LEU:HD13	0.98	1.53
1:A:12:LEU:HD11	1:A:12:LEU:CG	0.96	1.53
1:A:12:LEU:CD1	1:A:12:LEU:HG	0.96	1.60
1:A:12:LEU:CG	1:A:12:LEU:HD12	0.95	1.53
1:A:12:LEU:CG	1:A:12:LEU:HD22	0.94	1.49
1:A:12:LEU:CG	1:A:12:LEU:HD23	0.93	1.49
1:A:12:LEU:HD21	1:A:12:LEU:CG	0.92	1.49
1:A:23:GLU:HB3	1:A:23:GLU:CG	0.92	1.45
1:A:20:GLN:HG3	1:A:20:GLN:CD	0.91	1.35
1:A:23:GLU:HB2	1:A:23:GLU:CG	0.91	1.45
1:A:14:ARG:HG3	1:A:14:ARG:CD	0.91	1.44
1:A:26:LEU:N	1:A:27:LYS:N	0.90	2.19
1:A:12:LEU:CG	1:A:12:LEU:CD1	0.90	0.90
1:A:14:ARG:CD	1:A:14:ARG:HG2	0.89	1.44
1:A:20:GLN:HG2	1:A:20:GLN:CD	0.89	1.35
1:A:14:ARG:CG	1:A:14:ARG:HD2	0.88	1.43
1:A:14:ARG:HD3	1:A:14:ARG:CG	0.88	1.43
1:A:14:ARG:CD	1:A:14:ARG:CG	0.87	0.88
1:A:26:LEU:C	1:A:27:LYS:HB2	0.87	1.89
1:A:26:LEU:O	1:A:26:LEU:CB	0.86	2.21
1:A:12:LEU:CG	1:A:12:LEU:CD2	0.85	0.85
1:A:14:ARG:HE	1:A:14:ARG:CG	0.84	1.66
1:A:14:ARG:HH21	1:A:14:ARG:NH1	0.84	1.44
1:A:20:GLN:CG	1:A:20:GLN:CD	0.84	0.75
1:A:14:ARG:HH11	1:A:14:ARG:NH2	0.84	1.47
1:A:23:GLU:CB	1:A:23:GLU:CG	0.82	0.82
1:A:23:GLU:CB	1:A:23:GLU:HG3	0.81	1.41
1:A:28:ARG:CB	1:A:28:ARG:HG3	0.81	1.38
1:A:16:TRP:C	1:A:17:SER:N	0.80	0.85
1:A:14:ARG:NH2	1:A:14:ARG:CZ	0.80	0.79
1:A:23:GLU:CB	1:A:23:GLU:HG2	0.79	1.41
1:A:28:ARG:CG	1:A:28:ARG:HB3	0.78	1.36
1:A:28:ARG:HB2	1:A:28:ARG:CG	0.78	1.36
1:A:23:GLU:CD	1:A:23:GLU:HG3	0.76	1.35

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:14:ARG:HH21	1:A:14:ARG:HH12	0.75	0.97
1:A:23:GLU:CD	1:A:23:GLU:HG2	0.74	1.35
1:A:24:TYR:CA	1:A:24:TYR:CD1	0.73	2.70
1:A:14:ARG:HH22	1:A:14:ARG:CZ	0.73	1.43
1:A:26:LEU:C	1:A:27:LYS:N	0.73	0.81
1:A:14:ARG:HH21	1:A:14:ARG:CZ	0.72	1.43
1:A:23:GLU:HA	1:A:23:GLU:CG	0.69	2.08
1:A:16:TRP:O	1:A:18:ILE:N	0.67	2.21
1:A:16:TRP:C	1:A:16:TRP:O	0.66	0.67
1:A:24:TYR:CG	1:A:24:TYR:CD1	0.65	0.70
1:A:25:ASN:C	1:A:27:LYS:N	0.65	2.49
1:A:14:ARG:HH22	1:A:14:ARG:HH12	0.64	0.66
1:A:24:TYR:CA	1:A:24:TYR:CD2	0.63	2.72
1:A:23:GLU:C	1:A:23:GLU:CG	0.62	2.65
1:A:12:LEU:HB3	1:A:12:LEU:CD2	0.61	2.20
1:A:14:ARG:NH2	1:A:14:ARG:HH12	0.60	0.20
1:A:24:TYR:CG	1:A:24:TYR:CD2	0.60	0.68
1:A:2:SER:HG	1:A:2:SER:CB	0.60	1.30
1:A:14:ARG:NH2	1:A:14:ARG:NH1	0.59	0.75
1:A:28:ARG:HG2	1:A:28:ARG:CB	0.59	1.38
1:A:14:ARG:HD2	1:A:14:ARG:CZ	0.59	2.14
1:A:24:TYR:CE1	1:A:24:TYR:CZ	0.58	0.65
1:A:24:TYR:CE2	1:A:24:TYR:CZ	0.58	0.67
1:A:28:ARG:HG2	1:A:30:PRO:HD3	0.58	1.57
1:A:20:GLN:HE22	1:A:20:GLN:CD	0.58	1.18
1:A:20:GLN:CD	1:A:20:GLN:HE21	0.57	1.18
1:A:26:LEU:C	1:A:27:LYS:HA	0.57	2.04
1:A:24:TYR:CG	1:A:24:TYR:HD1	0.55	1.31
1:A:24:TYR:HE2	1:A:24:TYR:CZ	0.53	1.29
1:A:23:GLU:O	1:A:26:LEU:N	0.53	2.41
1:A:24:TYR:CG	1:A:24:TYR:HD2	0.53	1.29
1:A:14:ARG:HE	1:A:14:ARG:CZ	0.53	1.23
1:A:20:GLN:HB3	1:A:20:GLN:CD	0.53	2.09
1:A:23:GLU:O	1:A:24:TYR:C	0.53	2.37
1:A:24:TYR:HE1	1:A:24:TYR:CZ	0.53	1.28
1:A:14:ARG:HH22	1:A:14:ARG:NH1	0.53	1.34
1:A:15:TYR:CG	1:A:15:TYR:CD1	0.53	0.66
1:A:22:ILE:HG22	1:A:23:GLU:N	0.52	2.19
1:A:19:THR:HA	1:A:22:ILE:HD12	0.52	1.82
1:A:23:GLU:C	1:A:23:GLU:HG2	0.51	2.26
1:A:15:TYR:CG	1:A:15:TYR:CD2	0.50	0.65
1:A:13:ILE:O	1:A:16:TRP:HB3	0.50	2.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:25:ASN:O	1:A:27:LYS:N	0.50	2.45
1:A:23:GLU:CD	1:A:23:GLU:CG	0.50	0.74
1:A:23:GLU:HG3	1:A:23:GLU:CA	0.49	1.94
1:A:15:TYR:CZ	1:A:15:TYR:CE2	0.49	0.63
1:A:16:TRP:CG	1:A:17:SER:N	0.48	2.81
1:A:23:GLU:CA	1:A:23:GLU:HG2	0.48	1.91
1:A:26:LEU:CB	1:A:27:LYS:N	0.47	2.57
1:A:15:TYR:CZ	1:A:15:TYR:CE1	0.47	0.61
1:A:26:LEU:C	1:A:26:LEU:O	0.45	0.63
1:A:15:TYR:CG	1:A:15:TYR:HD1	0.45	1.20
1:A:15:TYR:HD2	1:A:15:TYR:CG	0.44	1.20
1:A:20:GLN:NE2	1:A:20:GLN:CD	0.44	0.49
1:A:14:ARG:HD3	1:A:14:ARG:CZ	0.44	2.14
1:A:24:TYR:O	1:A:27:LYS:O	0.43	2.34
1:A:24:TYR:O	1:A:27:LYS:C	0.42	2.57
1:A:15:TYR:CZ	1:A:15:TYR:HE2	0.42	1.18
1:A:19:THR:O	1:A:20:GLN:C	0.42	2.54
1:A:26:LEU:HB3	1:A:26:LEU:O	0.41	2.10
1:A:15:TYR:CZ	1:A:15:TYR:HE1	0.41	1.17
1:A:13:ILE:C	1:A:15:TYR:N	0.41	2.73
1:A:4:ILE:O	1:A:5:VAL:C	0.41	2.54
1:A:28:ARG:HG2	1:A:29:THR:HA	0.40	1.57
1:A:1:THR:C	1:A:3:SER:N	0.40	2.68

6.3 Torsion angles

6.3.1 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 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%)	23 (77%)	5 (17%)	2 (7%)	3	19
All	All	30/32 (94%)	23 (77%)	5 (17%)	2 (7%)	3	19

All 2 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	17	SER
1	A	18	ILE

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%)	20 (67%)	10 (33%)	1	12
All	All	30/30 (100%)	20 (67%)	10 (33%)	1	12

All 10 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	16	TRP
1	A	4	ILE
1	A	11	SER
1	A	24	TYR
1	A	2	SER
1	A	19	THR
1	A	32	ARG
1	A	26	LEU
1	A	18	ILE
1	A	3	SER

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 carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided