Full wwPDB NMR Structure Validation Report (i)

Oct 31, 2021 – 12:35 PM EDT

PDB ID	:	1Z60
Title	:	Solution structure of the carboxy-terminal domain of human TFIIH P44 subunit
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Deposited on	:	2005-03-21

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

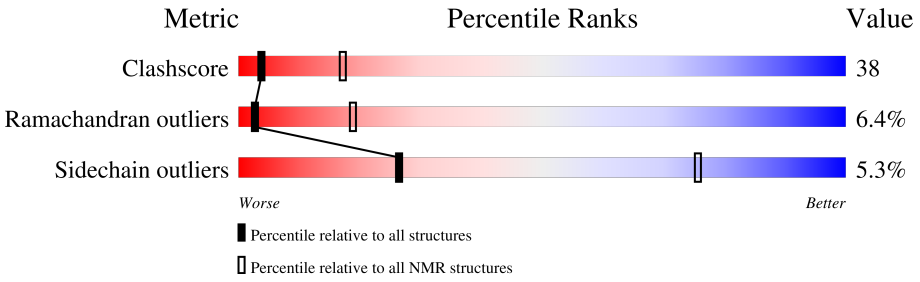
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	59	46% 37% 10% • 5%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *the best geometry*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:331-A:386 (56)	0.66	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 10
2	4, 6, 7
3	8, 9
Single-model clusters	5

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 878 atoms, of which 412 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TFIIH basal transcription factor complex p44 subunit.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	59	876	291	412	75	90	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	SER	CYS	engineered mutation	UNP Q13888

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

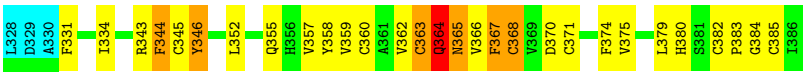
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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: TFIIH basal transcription factor complex p44 subunit

Chain A: 46% 37% 10% • 5%



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

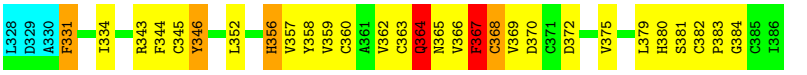
• Molecule 1: TFIIH basal transcription factor complex p44 subunit

Chain A: 51% 31% 10% • 5%

4.2.2 Score per residue for model 2

• Molecule 1: TFIIH basal transcription factor complex p44 subunit

Chain A: 46% 39% 7% • 5%



4.2.3 Score per residue for model 3 (medoid)

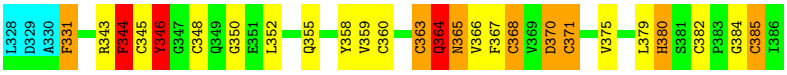
• Molecule 1: TFIIH basal transcription factor complex p44 subunit

Chain A: 42% 44% 5% • 5%

4.2.4 Score per residue for model 4

• Molecule 1: TFIIH basal transcription factor complex p44 subunit

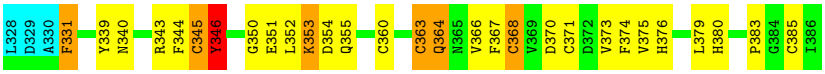
Chain A: 51% 25% 14% 5% 5%



4.2.5 Score per residue for model 5

• Molecule 1: TFIIH basal transcription factor complex p44 subunit

Chain A: 46% 37% 10% • 5%



4.2.6 Score per residue for model 6

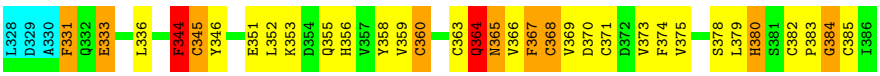
• Molecule 1: TFIIH basal transcription factor complex p44 subunit

Chain A: 41% 41% 12% • 5%

4.2.7 Score per residue for model 7

• Molecule 1: TFIIH basal transcription factor complex p44 subunit

Chain A: 39% 37% 15% • 5%



4.2.8 Score per residue for model 8

- Molecule 1: TFIIH basal transcription factor complex p44 subunit

Chain A: 42% 37% 12% • 5%

4.2.9 Score per residue for model 9

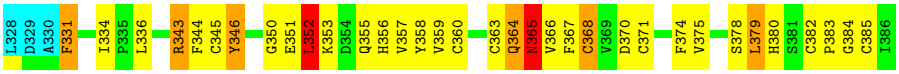
- Molecule 1: TFIIH basal transcription factor complex p44 subunit

Chain A: 42% 37% 14% • 5%

4.2.10 Score per residue for model 10

- Molecule 1: TFIIH basal transcription factor complex p44 subunit

Chain A: 37% 44% 10% • 5%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA / CNS	structure solution	1.2.
XPLOR-NIH	refinement	2.0.6

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.51±0.06	5±1/454 (1.0± 0.3%)	1.45±0.10	5±2/615 (0.9± 0.4%)
All	All	1.51	47/4540 (1.0%)	1.46	54/6150 (0.9%)

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	0.1±0.3	0.1±0.3
All	All	1	1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	368	CYS	CB-SG	-9.65	1.65	1.82	1	5
1	A	346	TYR	CD2-CE2	-8.87	1.26	1.39	10	2
1	A	364	GLN	N-CA	8.22	1.62	1.46	9	5
1	A	364	GLN	C-N	-7.92	1.15	1.34	1	9
1	A	365	ASN	N-CA	-7.43	1.31	1.46	10	7
1	A	367	PHE	CB-CG	-7.25	1.39	1.51	6	4
1	A	363	CYS	C-O	-6.60	1.10	1.23	5	1
1	A	364	GLN	CB-CG	-6.59	1.34	1.52	5	1
1	A	344	PHE	CA-CB	-6.55	1.39	1.53	2	5
1	A	363	CYS	CB-SG	-5.56	1.72	1.81	6	2
1	A	384	GLY	N-CA	-5.54	1.37	1.46	7	1
1	A	383	PRO	C-N	-5.53	1.23	1.33	8	1
1	A	360	CYS	CB-SG	5.51	1.91	1.82	6	1
1	A	365	ASN	C-O	-5.41	1.13	1.23	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	360	CYS	N-CA	5.32	1.56	1.46	6	1
1	A	350	GLY	N-CA	-5.08	1.38	1.46	10	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	346	TYR	CB-CG-CD2	-11.48	114.11	121.00	10	2
1	A	370	ASP	CB-CA-C	-10.86	88.69	110.40	4	2
1	A	346	TYR	CB-CG-CD1	9.52	126.71	121.00	10	2
1	A	339	TYR	CB-CG-CD2	-8.95	115.63	121.00	5	2
1	A	367	PHE	CB-CG-CD2	-8.10	115.13	120.80	2	1
1	A	346	TYR	N-CA-CB	-8.03	96.15	110.60	5	2
1	A	364	GLN	N-CA-CB	7.40	123.92	110.60	5	2
1	A	339	TYR	CB-CG-CD1	7.16	125.30	121.00	5	2
1	A	368	CYS	CB-CA-C	-6.88	96.63	110.40	2	4
1	A	363	CYS	CB-CA-C	6.69	123.77	110.40	5	1
1	A	367	PHE	CB-CG-CD1	-6.64	116.16	120.80	7	3
1	A	346	TYR	CA-CB-CG	6.47	125.70	113.40	5	1
1	A	331	PHE	CB-CG-CD2	-6.29	116.39	120.80	7	5
1	A	344	PHE	CB-CG-CD1	-6.28	116.41	120.80	10	1
1	A	370	ASP	CB-CG-OD1	6.23	123.90	118.30	2	1
1	A	367	PHE	N-CA-CB	6.20	121.76	110.60	7	1
1	A	370	ASP	CB-CG-OD2	-6.19	112.73	118.30	4	2
1	A	331	PHE	CB-CG-CD1	5.96	124.97	120.80	7	1
1	A	364	GLN	C-N-CA	5.96	136.59	121.70	9	3
1	A	360	CYS	N-CA-CB	5.75	120.95	110.60	6	4
1	A	343	ARG	N-CA-C	5.57	126.05	111.00	1	1
1	A	371	CYS	CB-CA-C	5.46	121.31	110.40	1	2
1	A	339	TYR	N-CA-CB	-5.34	100.99	110.60	6	2
1	A	352	LEU	CB-CA-C	5.24	120.15	110.20	10	1
1	A	380	HIS	CB-CA-C	-5.23	99.94	110.40	8	1
1	A	333	GLU	N-CA-C	-5.20	96.95	111.00	3	1
1	A	370	ASP	CA-CB-CG	5.20	124.83	113.40	4	1
1	A	363	CYS	C-N-CA	5.18	134.66	121.70	8	1
1	A	385	CYS	N-CA-C	5.10	124.78	111.00	4	1
1	A	344	PHE	CB-CG-CD2	5.06	124.34	120.80	10	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	367	PHE	CA	1

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	346	TYR	Sidechain	1

6.2 Too-close contacts (i)

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	443	392	391	32±6
All	All	4450	3920	3903	320

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 38.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:380:HIS:NE2	1:A:385:CYS:HB3	1.33	1.35	4	1
1:A:380:HIS:NE2	1:A:385:CYS:CB	1.20	2.03	4	1
1:A:345:CYS:SG	1:A:368:CYS:SG	1.08	2.51	10	1
1:A:380:HIS:CD2	1:A:385:CYS:HB3	1.06	1.84	4	1
1:A:368:CYS:SG	1:A:371:CYS:HB2	1.00	1.95	6	1
1:A:380:HIS:NE2	1:A:385:CYS:SG	0.99	2.35	4	1
1:A:345:CYS:HB3	1:A:368:CYS:SG	0.98	1.97	7	10
1:A:345:CYS:CB	1:A:368:CYS:SG	0.96	2.53	10	5
1:A:363:CYS:SG	1:A:385:CYS:HA	0.88	2.08	7	4
1:A:360:CYS:HB3	1:A:363:CYS:O	0.82	1.74	5	4
1:A:360:CYS:HB2	1:A:364:GLN:HB2	0.78	1.53	5	1
1:A:363:CYS:SG	1:A:385:CYS:HB3	0.74	2.21	5	1
1:A:368:CYS:SG	1:A:371:CYS:CB	0.73	2.68	6	1
1:A:346:TYR:HB3	1:A:367:PHE:CE1	0.73	2.19	5	2
1:A:360:CYS:CB	1:A:364:GLN:HB2	0.73	2.13	5	1
1:A:382:CYS:CB	1:A:385:CYS:SG	0.73	2.77	10	1
1:A:374:PHE:O	1:A:379:LEU:HD13	0.71	1.86	5	1
1:A:346:TYR:H	1:A:364:GLN:NE2	0.70	1.84	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:346:TYR:CE2	1:A:364:GLN:HA	0.70	2.21	5	1
1:A:363:CYS:CB	1:A:385:CYS:SG	0.69	2.81	5	1
1:A:375:VAL:HG11	1:A:382:CYS:HA	0.69	1.63	4	1
1:A:371:CYS:HA	1:A:374:PHE:HB2	0.68	1.66	10	1
1:A:382:CYS:SG	1:A:383:PRO:HD2	0.67	2.29	7	2
1:A:375:VAL:HB	1:A:380:HIS:O	0.67	1.89	1	2
1:A:382:CYS:HB3	1:A:385:CYS:SG	0.67	2.29	10	1
1:A:362:VAL:HG23	1:A:363:CYS:SG	0.67	2.30	8	1
1:A:339:TYR:CE1	1:A:352:LEU:HD12	0.67	2.25	6	1
1:A:363:CYS:HB2	1:A:385:CYS:SG	0.66	2.30	5	1
1:A:346:TYR:CD2	1:A:364:GLN:HG2	0.66	2.25	2	5
1:A:367:PHE:CE1	1:A:383:PRO:HG2	0.65	2.26	6	5
1:A:364:GLN:HG3	1:A:385:CYS:SG	0.63	2.32	5	1
1:A:334:ILE:HB	1:A:357:VAL:HG22	0.63	1.69	9	1
1:A:364:GLN:HG3	1:A:365:ASN:N	0.62	2.09	9	1
1:A:360:CYS:SG	1:A:362:VAL:HB	0.62	2.35	1	3
1:A:331:PHE:CE2	1:A:360:CYS:HA	0.62	2.29	9	6
1:A:380:HIS:CD2	1:A:385:CYS:CB	0.62	2.70	4	1
1:A:360:CYS:O	1:A:365:ASN:HA	0.61	1.93	2	5
1:A:346:TYR:CE2	1:A:384:GLY:HA2	0.61	2.30	10	1
1:A:343:ARG:O	1:A:352:LEU:HG	0.61	1.95	1	2
1:A:370:ASP:O	1:A:373:VAL:HG12	0.61	1.96	6	4
1:A:358:TYR:HB2	1:A:367:PHE:HB2	0.61	1.73	8	5
1:A:363:CYS:SG	1:A:385:CYS:CB	0.61	2.87	5	1
1:A:345:CYS:CB	1:A:368:CYS:HG	0.60	2.04	10	1
1:A:380:HIS:HD2	1:A:382:CYS:O	0.60	1.79	4	6
1:A:344:PHE:N	1:A:352:LEU:HG	0.59	2.12	7	1
1:A:346:TYR:HD2	1:A:364:GLN:NE2	0.59	1.95	3	3
1:A:345:CYS:N	1:A:352:LEU:HD21	0.59	2.11	8	1
1:A:379:LEU:CD2	1:A:383:PRO:HA	0.59	2.27	6	2
1:A:343:ARG:HB2	1:A:352:LEU:HD12	0.59	1.74	2	1
1:A:352:LEU:HD22	1:A:367:PHE:O	0.58	1.98	5	4
1:A:346:TYR:HA	1:A:364:GLN:HE21	0.58	1.57	4	1
1:A:344:PHE:O	1:A:352:LEU:HD21	0.58	1.98	4	1
1:A:363:CYS:SG	1:A:384:GLY:HA3	0.57	2.39	1	4
1:A:364:GLN:NE2	1:A:366:VAL:H	0.57	1.95	10	2
1:A:375:VAL:HG22	1:A:380:HIS:O	0.57	1.99	4	1
1:A:370:ASP:HB2	1:A:371:CYS:SG	0.57	2.39	4	2
1:A:358:TYR:CE2	1:A:369:VAL:HA	0.57	2.35	6	2
1:A:344:PHE:HB3	1:A:350:GLY:O	0.57	2.00	5	3
1:A:346:TYR:HE2	1:A:384:GLY:CA	0.57	2.13	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:359:VAL:HA	1:A:365:ASN:O	0.57	1.99	9	5
1:A:354:ASP:OD2	1:A:368:CYS:HB3	0.57	2.00	5	1
1:A:380:HIS:CE1	1:A:385:CYS:SG	0.56	2.97	4	1
1:A:345:CYS:SG	1:A:348:CYS:HB2	0.56	2.39	6	1
1:A:359:VAL:HG23	1:A:365:ASN:O	0.56	2.00	4	2
1:A:345:CYS:HB2	1:A:368:CYS:SG	0.56	2.27	6	1
1:A:363:CYS:HB2	1:A:384:GLY:O	0.56	2.00	8	1
1:A:345:CYS:HA	1:A:366:VAL:O	0.55	2.02	9	3
1:A:352:LEU:HD22	1:A:368:CYS:HA	0.55	1.78	9	2
1:A:375:VAL:HG12	1:A:379:LEU:HB2	0.55	1.77	9	1
1:A:375:VAL:HG11	1:A:382:CYS:C	0.55	2.22	9	1
1:A:346:TYR:CE2	1:A:384:GLY:HA3	0.55	2.37	2	2
1:A:345:CYS:HA	1:A:364:GLN:HE22	0.55	1.62	6	1
1:A:343:ARG:HD3	1:A:366:VAL:HG12	0.55	1.78	4	1
1:A:346:TYR:CD2	1:A:364:GLN:HA	0.54	2.37	5	1
1:A:359:VAL:HA	1:A:366:VAL:HA	0.54	1.77	6	1
1:A:351:GLU:OE2	1:A:353:LYS:HD3	0.54	2.02	5	1
1:A:346:TYR:HB3	1:A:364:GLN:CD	0.54	2.23	8	2
1:A:346:TYR:CA	1:A:364:GLN:HE21	0.53	2.16	4	1
1:A:359:VAL:HG13	1:A:365:ASN:O	0.53	2.04	7	1
1:A:360:CYS:HB2	1:A:367:PHE:CE2	0.53	2.39	6	1
1:A:360:CYS:H	1:A:365:ASN:HA	0.53	1.63	8	1
1:A:346:TYR:HB3	1:A:364:GLN:NE2	0.52	2.19	2	1
1:A:343:ARG:HB2	1:A:366:VAL:HG11	0.52	1.82	4	1
1:A:344:PHE:O	1:A:366:VAL:HB	0.52	2.04	4	1
1:A:339:TYR:CG	1:A:357:VAL:HG21	0.52	2.40	6	1
1:A:364:GLN:HG3	1:A:366:VAL:N	0.52	2.19	6	1
1:A:346:TYR:N	1:A:364:GLN:NE2	0.52	2.58	7	1
1:A:346:TYR:CZ	1:A:363:CYS:HB3	0.51	2.41	6	2
1:A:352:LEU:HD21	1:A:366:VAL:HG12	0.51	1.82	1	2
1:A:356:HIS:HB3	1:A:358:TYR:CE1	0.51	2.40	2	1
1:A:375:VAL:HG21	1:A:382:CYS:N	0.51	2.20	2	1
1:A:374:PHE:CD1	1:A:383:PRO:HB3	0.51	2.40	5	3
1:A:375:VAL:HB	1:A:383:PRO:HD3	0.51	1.81	2	1
1:A:374:PHE:CD2	1:A:379:LEU:HD21	0.51	2.40	6	1
1:A:346:TYR:HA	1:A:364:GLN:NE2	0.51	2.21	4	1
1:A:352:LEU:HD11	1:A:366:VAL:CG1	0.51	2.36	2	3
1:A:345:CYS:HB3	1:A:368:CYS:CB	0.51	2.36	6	1
1:A:380:HIS:NE2	1:A:385:CYS:HB2	0.51	2.20	6	1
1:A:346:TYR:HD2	1:A:364:GLN:HG2	0.51	1.64	2	1
1:A:380:HIS:CD2	1:A:382:CYS:H	0.50	2.24	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:346:TYR:CE1	1:A:383:PRO:HG2	0.50	2.40	2	1
1:A:375:VAL:HG21	1:A:382:CYS:C	0.50	2.26	4	1
1:A:360:CYS:SG	1:A:362:VAL:HG12	0.50	2.46	9	1
1:A:336:LEU:HD23	1:A:357:VAL:CG2	0.50	2.37	10	1
1:A:346:TYR:CD2	1:A:364:GLN:CG	0.50	2.95	8	2
1:A:363:CYS:O	1:A:364:GLN:HG3	0.50	2.07	10	1
1:A:358:TYR:O	1:A:366:VAL:HA	0.50	2.07	9	1
1:A:358:TYR:CE1	1:A:369:VAL:HB	0.50	2.41	2	1
1:A:334:ILE:O	1:A:357:VAL:HB	0.49	2.07	8	3
1:A:352:LEU:HD22	1:A:367:PHE:C	0.49	2.29	2	4
1:A:331:PHE:CZ	1:A:360:CYS:SG	0.48	3.06	3	3
1:A:346:TYR:CD2	1:A:364:GLN:NE2	0.48	2.82	10	1
1:A:334:ILE:HB	1:A:357:VAL:HB	0.48	1.86	3	1
1:A:363:CYS:C	1:A:365:ASN:N	0.48	2.67	6	3
1:A:343:ARG:C	1:A:352:LEU:HG	0.48	2.28	1	5
1:A:375:VAL:HG11	1:A:383:PRO:N	0.48	2.23	9	1
1:A:346:TYR:OH	1:A:383:PRO:HB2	0.48	2.08	3	1
1:A:333:GLU:HA	1:A:357:VAL:O	0.48	2.08	1	1
1:A:331:PHE:CE2	1:A:360:CYS:SG	0.48	3.07	2	2
1:A:375:VAL:HG21	1:A:382:CYS:CA	0.48	2.38	4	2
1:A:344:PHE:C	1:A:352:LEU:HD21	0.48	2.28	8	2
1:A:371:CYS:O	1:A:374:PHE:HB2	0.47	2.09	5	3
1:A:346:TYR:CE2	1:A:363:CYS:SG	0.47	3.07	2	1
1:A:364:GLN:HG3	1:A:366:VAL:H	0.47	1.68	6	3
1:A:375:VAL:HG12	1:A:379:LEU:CB	0.47	2.39	9	2
1:A:339:TYR:CD1	1:A:357:VAL:HG11	0.47	2.44	6	1
1:A:372:ASP:O	1:A:375:VAL:HG12	0.47	2.09	2	1
1:A:374:PHE:CE2	1:A:379:LEU:HD21	0.47	2.45	6	1
1:A:352:LEU:CD1	1:A:366:VAL:HG12	0.47	2.40	9	1
1:A:346:TYR:CE2	1:A:384:GLY:CA	0.47	2.95	10	1
1:A:346:TYR:OH	1:A:384:GLY:HA2	0.46	2.10	10	1
1:A:331:PHE:HE2	1:A:360:CYS:SG	0.46	2.34	7	3
1:A:382:CYS:SG	1:A:383:PRO:CD	0.46	3.04	1	1
1:A:375:VAL:HA	1:A:379:LEU:HB3	0.46	1.84	10	1
1:A:358:TYR:HB2	1:A:367:PHE:O	0.46	2.10	6	3
1:A:333:GLU:HB2	1:A:356:HIS:CE1	0.46	2.45	7	1
1:A:345:CYS:HB2	1:A:367:PHE:CB	0.46	2.41	7	1
1:A:367:PHE:HZ	1:A:382:CYS:SG	0.46	2.33	6	1
1:A:363:CYS:O	1:A:365:ASN:N	0.45	2.49	2	1
1:A:339:TYR:CD2	1:A:357:VAL:HG21	0.45	2.47	6	1
1:A:346:TYR:CE2	1:A:364:GLN:CA	0.45	2.98	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:375:VAL:CG2	1:A:383:PRO:HD3	0.45	2.41	7	1
1:A:363:CYS:O	1:A:364:GLN:HG2	0.45	2.12	6	1
1:A:374:PHE:CD1	1:A:379:LEU:HD11	0.45	2.47	3	1
1:A:379:LEU:O	1:A:380:HIS:HB2	0.45	2.12	4	1
1:A:345:CYS:SG	1:A:348:CYS:CB	0.45	3.05	6	1
1:A:333:GLU:HB3	1:A:358:TYR:CE2	0.45	2.47	8	1
1:A:336:LEU:HD21	1:A:353:LYS:HA	0.45	1.89	10	1
1:A:352:LEU:O	1:A:369:VAL:HG23	0.44	2.12	6	1
1:A:382:CYS:HB3	1:A:385:CYS:HB2	0.44	1.88	4	1
1:A:343:ARG:HB2	1:A:366:VAL:CG1	0.44	2.42	4	1
1:A:370:ASP:O	1:A:373:VAL:HB	0.44	2.12	5	1
1:A:375:VAL:C	1:A:377:ASP:H	0.44	2.15	6	1
1:A:346:TYR:OH	1:A:360:CYS:HB2	0.44	2.13	2	1
1:A:363:CYS:SG	1:A:384:GLY:C	0.44	2.96	2	1
1:A:360:CYS:HB3	1:A:363:CYS:C	0.43	2.29	5	1
1:A:367:PHE:CZ	1:A:382:CYS:SG	0.43	3.11	6	1
1:A:363:CYS:SG	1:A:384:GLY:CA	0.43	3.06	1	2
1:A:368:CYS:HB2	1:A:371:CYS:H	0.43	1.74	7	2
1:A:352:LEU:HD11	1:A:357:VAL:HA	0.43	1.91	10	1
1:A:358:TYR:HE2	1:A:369:VAL:HG12	0.43	1.72	3	1
1:A:360:CYS:HB3	1:A:363:CYS:H	0.43	1.73	6	1
1:A:362:VAL:O	1:A:365:ASN:ND2	0.43	2.49	6	1
1:A:368:CYS:SG	1:A:371:CYS:SG	0.43	3.16	10	1
1:A:345:CYS:O	1:A:349:GLN:HA	0.43	2.14	9	1
1:A:358:TYR:CB	1:A:367:PHE:HB2	0.43	2.42	8	3
1:A:346:TYR:CE1	1:A:367:PHE:CD2	0.43	3.07	2	1
1:A:346:TYR:CB	1:A:364:GLN:HE21	0.43	2.26	4	1
1:A:344:PHE:CA	1:A:352:LEU:HG	0.42	2.43	9	1
1:A:375:VAL:HG23	1:A:379:LEU:HB2	0.42	1.90	2	1
1:A:364:GLN:NE2	1:A:367:PHE:CD1	0.42	2.84	5	1
1:A:358:TYR:HB2	1:A:367:PHE:CB	0.42	2.42	8	1
1:A:356:HIS:HB2	1:A:358:TYR:CZ	0.42	2.48	9	1
1:A:352:LEU:HD11	1:A:366:VAL:HG11	0.42	1.91	5	1
1:A:355:GLN:HG3	1:A:369:VAL:HG11	0.42	1.90	8	1
1:A:358:TYR:HE1	1:A:369:VAL:HG12	0.42	1.73	8	1
1:A:332:GLN:NE2	1:A:334:ILE:HD11	0.42	2.30	3	1
1:A:336:LEU:HD11	1:A:353:LYS:O	0.42	2.15	8	2
1:A:336:LEU:HD23	1:A:357:VAL:HG23	0.42	1.92	10	1
1:A:358:TYR:CE2	1:A:369:VAL:HG12	0.42	2.49	3	1
1:A:343:ARG:HE	1:A:366:VAL:HG21	0.42	1.74	5	1
1:A:367:PHE:CZ	1:A:383:PRO:HG2	0.42	2.50	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:346:TYR:CB	1:A:367:PHE:CE1	0.42	3.00	5	1
1:A:346:TYR:H	1:A:364:GLN:HE22	0.42	1.56	6	1
1:A:374:PHE:CD2	1:A:379:LEU:HD22	0.42	2.50	7	1
1:A:379:LEU:HD22	1:A:380:HIS:H	0.41	1.74	3	1
1:A:379:LEU:CD2	1:A:380:HIS:H	0.41	2.27	3	1
1:A:343:ARG:C	1:A:352:LEU:HD23	0.41	2.35	10	1
1:A:352:LEU:CG	1:A:353:LYS:H	0.41	2.28	10	1
1:A:346:TYR:OH	1:A:382:CYS:SG	0.41	2.79	7	1
1:A:352:LEU:HG	1:A:353:LYS:N	0.41	2.31	10	1
1:A:344:PHE:HA	1:A:351:GLU:HA	0.41	1.91	7	1
1:A:346:TYR:HE2	1:A:363:CYS:O	0.41	1.99	2	1
1:A:375:VAL:HG23	1:A:379:LEU:CB	0.41	2.46	2	1
1:A:375:VAL:CG2	1:A:379:LEU:HB2	0.41	2.46	2	1
1:A:348:CYS:SG	1:A:350:GLY:HA3	0.41	2.55	4	1
1:A:370:ASP:OD1	1:A:371:CYS:SG	0.41	2.78	7	1
1:A:380:HIS:CD2	1:A:382:CYS:O	0.41	2.74	1	1
1:A:346:TYR:CD2	1:A:384:GLY:HA3	0.40	2.50	2	1
1:A:346:TYR:CD1	1:A:346:TYR:C	0.40	2.95	4	1
1:A:346:TYR:CG	1:A:364:GLN:NE2	0.40	2.89	4	1
1:A:334:ILE:HG13	1:A:338:GLU:HB3	0.40	1.94	8	1
1:A:360:CYS:N	1:A:365:ASN:HA	0.40	2.29	8	1

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	55/59 (93%)	48±2 (87±3%)	4±2 (7±3%)	4±1 (6±2%)	3 19
All	All	550/590 (93%)	476 (87%)	39 (7%)	35 (6%)	3 19

All 15 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	364	GLN	7

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Mol	Chain	Res	Type	Models (Total)
1	A	355	GLN	7
1	A	380	HIS	5
1	A	344	PHE	2
1	A	384	GLY	2
1	A	378	SER	2
1	A	351	GLU	2
1	A	383	PRO	1
1	A	381	SER	1
1	A	352	LEU	1
1	A	353	LYS	1
1	A	376	HIS	1
1	A	361	ALA	1
1	A	362	VAL	1
1	A	343	ARG	1

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	51/53 (96%)	48±1 (95±3%)	3±1 (5±3%)	26 75
All	All	510/530 (96%)	483 (95%)	27 (5%)	26 75

All 17 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	365	ASN	3
1	A	379	LEU	3
1	A	345	CYS	3
1	A	346	TYR	2
1	A	356	HIS	2
1	A	363	CYS	2
1	A	368	CYS	2
1	A	334	ILE	1
1	A	367	PHE	1
1	A	380	HIS	1
1	A	340	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	331	PHE	1
1	A	375	VAL	1
1	A	333	GLU	1
1	A	364	GLN	1
1	A	352	LEU	1
1	A	370	ASP	1

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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	2-A	1
1	9-A	1
1	8-A	1
1	3-A	1
1	10-A	1
1	1-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
2	A	364:GLN	C	365:ASN	N	1.20
9	A	364:GLN	C	365:ASN	N	1.20
8	A	364:GLN	C	365:ASN	N	1.19
3	A	364:GLN	C	365:ASN	N	1.17
10	A	364:GLN	C	365:ASN	N	1.16
1	A	364:GLN	C	365:ASN	N	1.15

7 Chemical shift validation (i)

No chemical shift data were provided