



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 06:05 AM UTC

PDB ID : 1L3E / pdb_00001l3e
Title : NMR Structures of the HIF-1alpha CTAD/p300 CH1 Complex
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Eck, M.J.
Deposited on : 2002-02-26

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 ⓘ 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

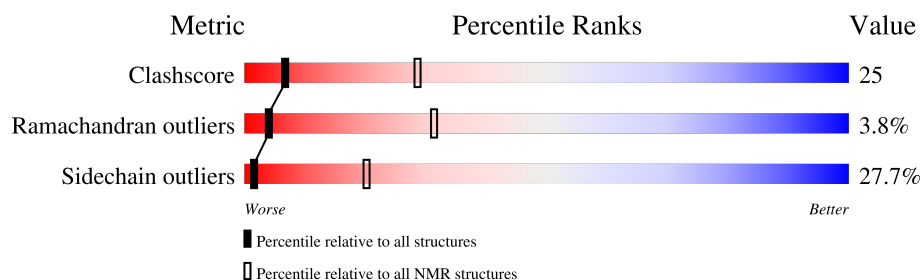
1 Overall quality at a glance

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	42	
2	B	101	

2 Ensemble composition and analysis

This entry contains 17 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:8-A:41, B:108-B:196 (123)	0.91	8

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 7, 8, 9, 10, 11, 12, 13, 15, 16, 17
2	3, 6, 14

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2207 atoms, of which 1096 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypoxia inducible factor-1 alpha subunit.

Mol	Chain	Residues	Atoms						Trace
1	A	42	Total	C	H	N	O	S	0
			624	191	306	55	70	2	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	GLN	cloning artifact	UNP Q16665

- Molecule 2 is a protein called p300 protein.

Mol	Chain	Residues	Atoms						Trace
2	B	101	Total	C	H	N	O	S	0
			1580	475	790	164	139	12	

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

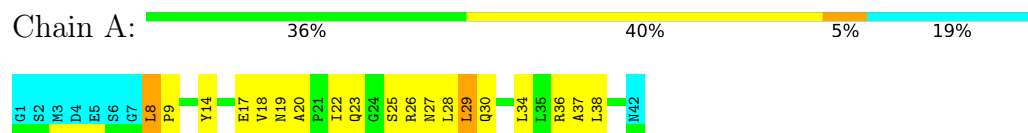
Mol	Chain	Residues	Atoms	
3	B	3	Total	Zn
			3	3

4 Residue-property plots

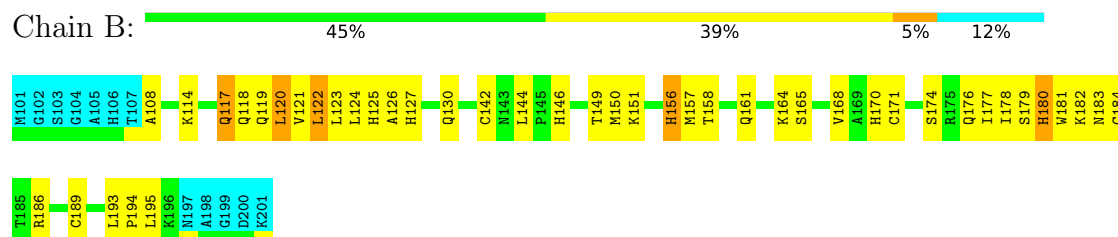
4.1 Average score per residue in the NMR ensemble

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: hypoxia inducible factor-1 alpha subunit



- Molecule 2: p300 protein

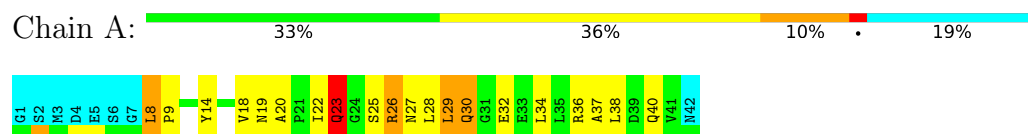


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

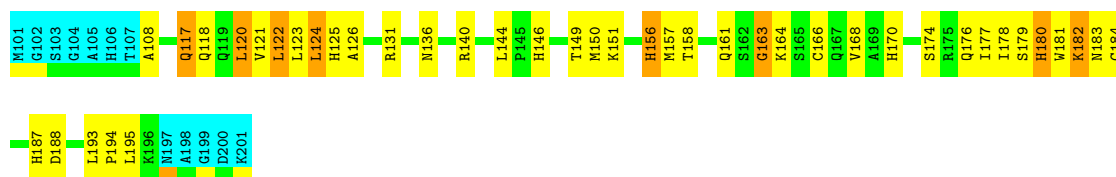
4.2.1 Score per residue for model 1

- Molecule 1: hypoxia inducible factor-1 alpha subunit



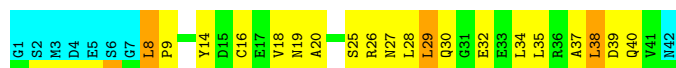
- Molecule 2: p300 protein



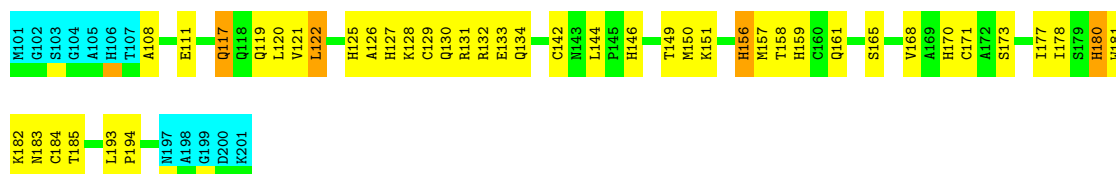


4.2.2 Score per residue for model 2

- Molecule 1: hypoxia inducible factor-1 alpha subunit



- Molecule 2: p300 protein

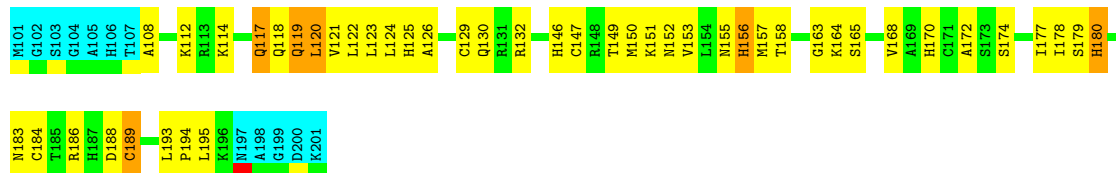


4.2.3 Score per residue for model 3

- Molecule 1: hypoxia inducible factor-1 alpha subunit

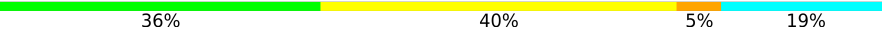


- Molecule 2: p300 protein



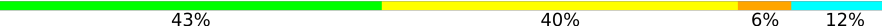
4.2.4 Score per residue for model 4

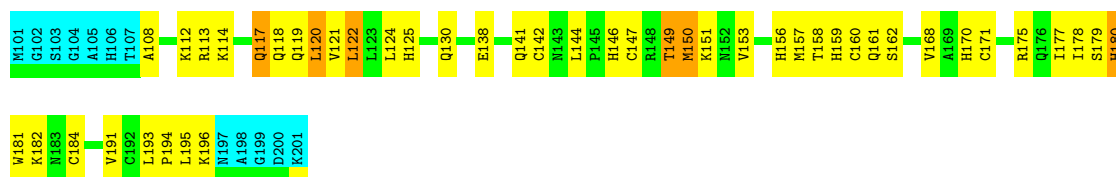
- Molecule 1: hypoxia inducible factor-1 alpha subunit

Chain A: 



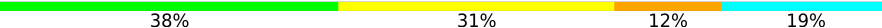
- Molecule 2: p300 protein

Chain B: 



4.2.5 Score per residue for model 5

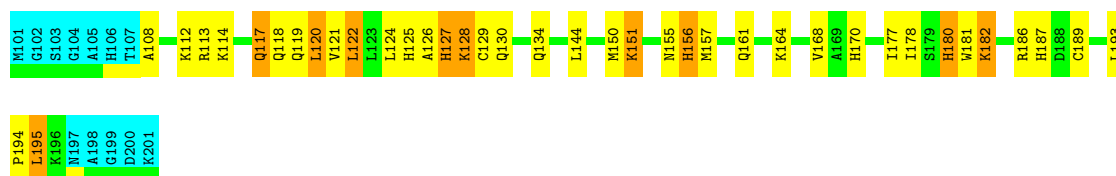
- Molecule 1: hypoxia inducible factor-1 alpha subunit

Chain A: 



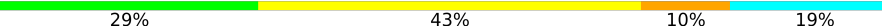
- Molecule 2: p300 protein

Chain B: 



4.2.6 Score per residue for model 6

- Molecule 1: hypoxia inducible factor-1 alpha subunit

Chain A: 



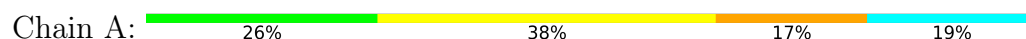
- Molecule 2: p300 protein

Chain B: 

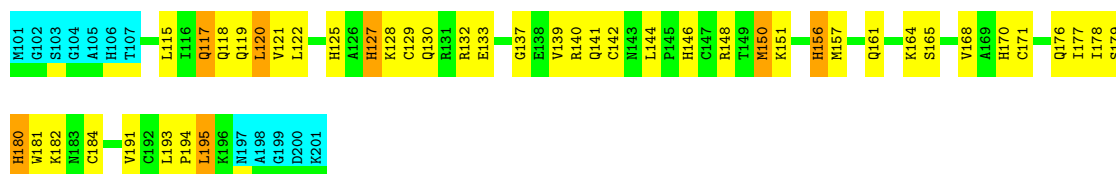


4.2.7 Score per residue for model 7

- Molecule 1: hypoxia inducible factor-1 alpha subunit

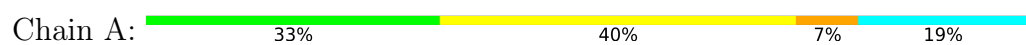


- Molecule 2: p300 protein

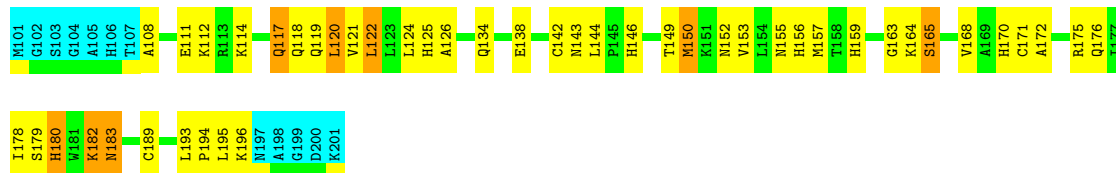


4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: hypoxia inducible factor-1 alpha subunit

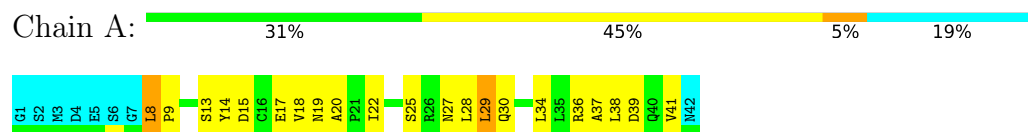


- Molecule 2: p300 protein

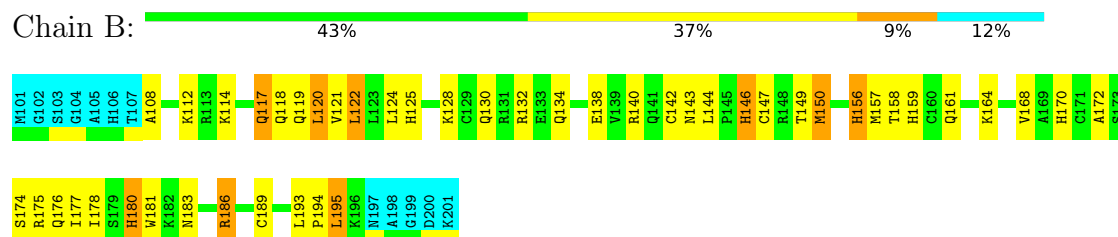


4.2.9 Score per residue for model 9

- Molecule 1: hypoxia inducible factor-1 alpha subunit

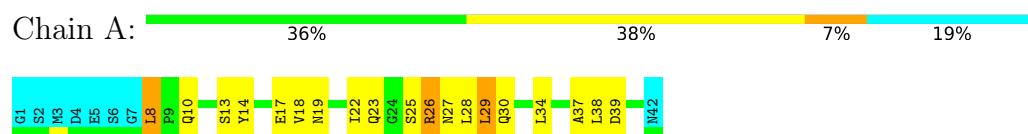


- Molecule 2: p300 protein

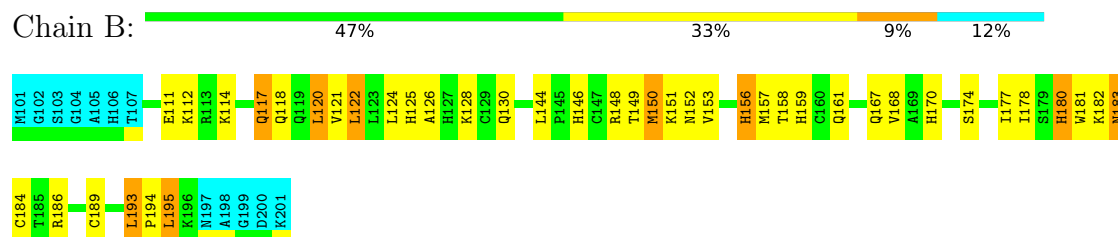


4.2.10 Score per residue for model 10

- Molecule 1: hypoxia inducible factor-1 alpha subunit

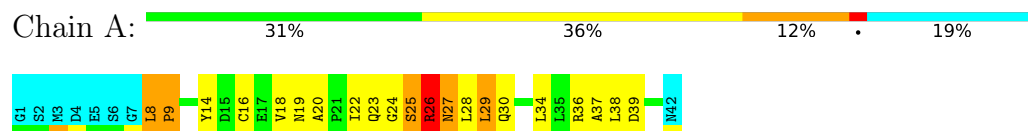


- Molecule 2: p300 protein



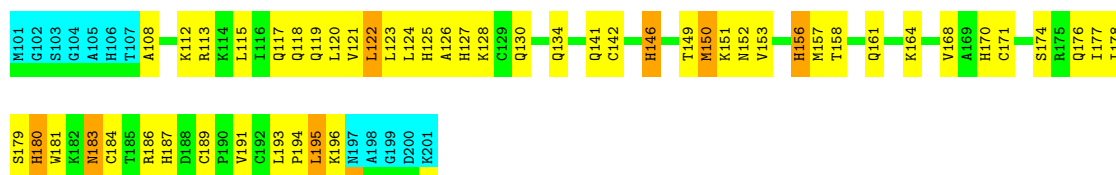
4.2.11 Score per residue for model 11

- Molecule 1: hypoxia inducible factor-1 alpha subunit



- Molecule 2: p300 protein





4.2.12 Score per residue for model 12

- Molecule 1: hypoxia inducible factor-1 alpha subunit

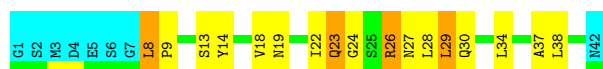


- Molecule 2: p300 protein

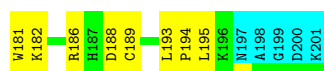


4.2.13 Score per residue for model 13

- Molecule 1: hypoxia inducible factor-1 alpha subunit

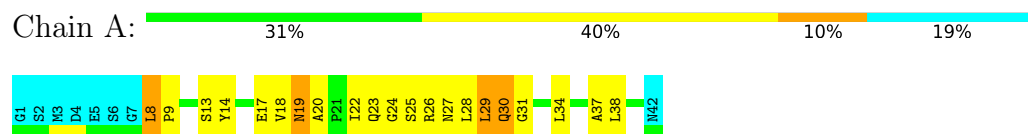


- Molecule 2: p300 protein

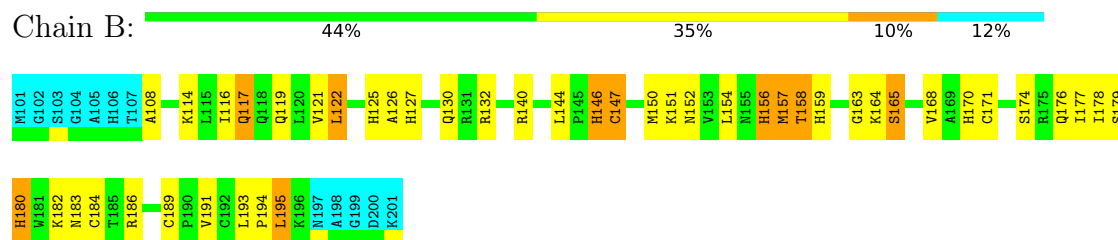


4.2.14 Score per residue for model 14

- Molecule 1: hypoxia inducible factor-1 alpha subunit

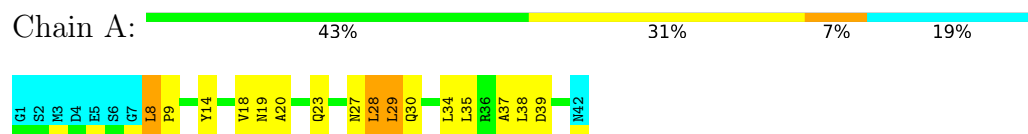


- Molecule 2: p300 protein

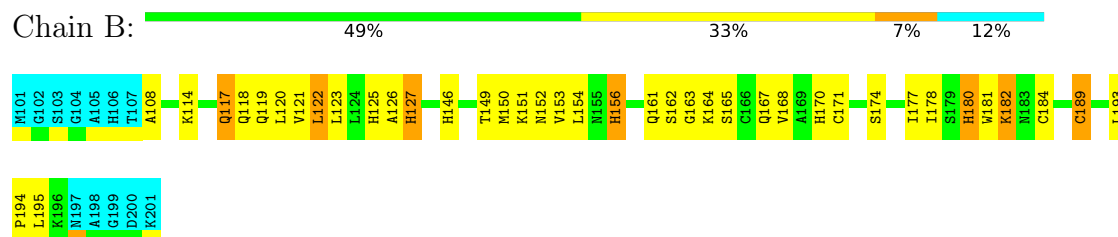


4.2.15 Score per residue for model 15

- Molecule 1: hypoxia inducible factor-1 alpha subunit

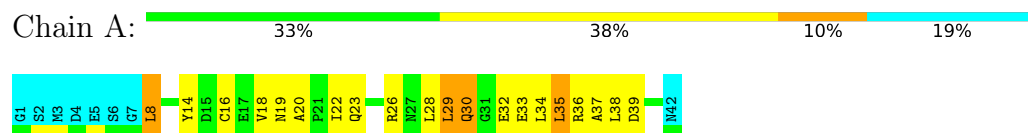


- Molecule 2: p300 protein



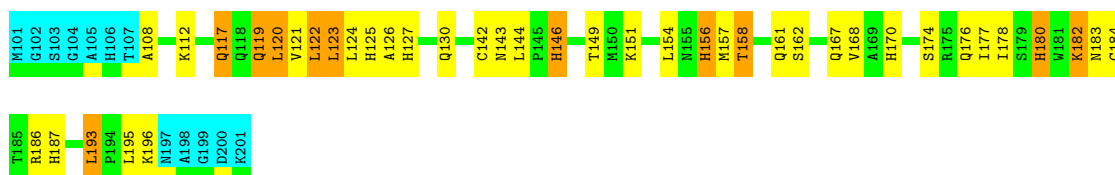
4.2.16 Score per residue for model 16

- Molecule 1: hypoxia inducible factor-1 alpha subunit



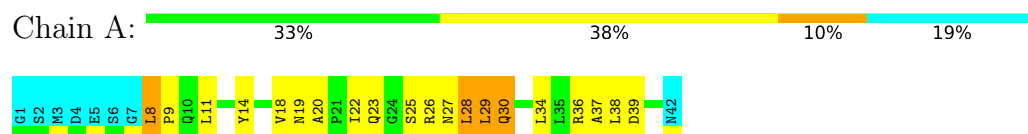
- Molecule 2: p300 protein



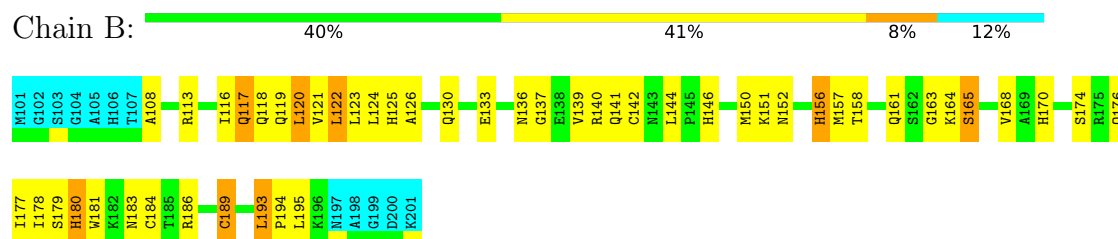


4.2.17 Score per residue for model 17

- Molecule 1: hypoxia inducible factor-1 alpha subunit



- Molecule 2: p300 protein



5 Refinement protocol and experimental data overview ⓘ

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

Of the 25 calculated structures, 17 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

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

Software name	Classification	Version
DYANA	structure solution	1.4
X-PLOR	refinement	3.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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	264	263	263	25±4
2	B	711	717	712	36±5
All	All	16626	16660	16575	819

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:121:VAL:HG22	2:B:195:LEU:HD21	0.94	1.33	3	15
1:A:38:LEU:HD11	2:B:178:ILE:HD13	0.94	1.39	15	12
1:A:8:LEU:HD12	2:B:170:HIS:CE1	0.92	1.99	4	5
2:B:121:VAL:CG2	2:B:195:LEU:HD21	0.84	2.02	13	14
1:A:38:LEU:HD21	2:B:178:ILE:HG23	0.83	1.48	13	10
1:A:35:LEU:HD22	2:B:154:LEU:HD22	0.80	1.53	16	2
1:A:20:ALA:HB1	2:B:180:HIS:CE1	0.80	2.10	16	9
2:B:117:GLN:O	2:B:121:VAL:HG23	0.80	1.76	17	17
1:A:30:GLN:O	1:A:34:LEU:HD12	0.79	1.77	7	17
1:A:29:LEU:HD13	1:A:34:LEU:CD2	0.79	2.07	11	1
1:A:29:LEU:HD22	1:A:37:ALA:CB	0.79	2.08	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:HD13	2:B:157:MET:HE3	0.77	1.56	7	11
1:A:35:LEU:CD2	2:B:154:LEU:HD22	0.75	2.11	6	3
1:A:29:LEU:HD23	1:A:37:ALA:HB3	0.74	1.59	13	2
2:B:123:LEU:CD2	2:B:178:ILE:HD11	0.74	2.12	16	1
2:B:123:LEU:HD22	2:B:178:ILE:HD11	0.73	1.60	1	6
2:B:122:LEU:HD11	2:B:150:MET:HB2	0.73	1.58	13	8
1:A:14:TYR:O	1:A:18:VAL:HG23	0.72	1.85	6	16
1:A:34:LEU:HD13	2:B:157:MET:CE	0.71	2.15	5	8
2:B:122:LEU:O	2:B:122:LEU:HD12	0.71	1.85	14	13
1:A:29:LEU:HD13	1:A:37:ALA:HB3	0.71	1.63	9	10
2:B:174:SER:HA	2:B:177:ILE:HD12	0.71	1.63	3	9
1:A:32:GLU:HG3	2:B:158:THR:HG22	0.70	1.61	16	1
2:B:122:LEU:HD13	2:B:150:MET:SD	0.70	2.27	7	2
2:B:189:CYS:O	2:B:193:LEU:HD12	0.70	1.87	10	1
1:A:22:ILE:HG23	2:B:183:ASN:HB3	0.69	1.61	10	8
1:A:29:LEU:HD21	2:B:182:LYS:CB	0.69	2.18	5	1
1:A:29:LEU:HD13	1:A:34:LEU:HD21	0.68	1.65	11	1
1:A:27:ASN:OD1	1:A:29:LEU:HD22	0.68	1.89	15	2
2:B:122:LEU:HD12	2:B:122:LEU:C	0.68	2.14	14	13
2:B:149:THR:O	2:B:153:VAL:HG23	0.68	1.88	6	7
1:A:29:LEU:H	1:A:29:LEU:HD13	0.67	1.49	15	4
2:B:122:LEU:HD22	2:B:146:HIS:HB3	0.67	1.66	10	12
1:A:29:LEU:HD13	1:A:37:ALA:CB	0.67	2.19	16	10
2:B:133:GLU:CB	2:B:139:VAL:HG13	0.66	2.20	12	1
2:B:120:LEU:HD21	2:B:181:TRP:CE3	0.66	2.25	11	6
2:B:120:LEU:HD22	2:B:177:ILE:CG2	0.66	2.20	5	4
1:A:34:LEU:CD1	2:B:157:MET:HE3	0.66	2.21	13	9
1:A:38:LEU:HD21	2:B:178:ILE:CG2	0.65	2.21	9	9
1:A:20:ALA:HB1	2:B:180:HIS:CD2	0.65	2.26	6	2
2:B:122:LEU:HD11	2:B:146:HIS:HB3	0.65	1.66	7	3
1:A:22:ILE:HG23	2:B:183:ASN:CB	0.65	2.21	9	8
1:A:29:LEU:HD22	1:A:37:ALA:HB1	0.65	1.69	4	9
1:A:29:LEU:HD23	1:A:37:ALA:CB	0.65	2.21	13	3
1:A:38:LEU:HD11	2:B:127:HIS:CD2	0.65	2.26	7	3
2:B:122:LEU:HD11	2:B:150:MET:CG	0.64	2.22	11	7
1:A:18:VAL:HG11	2:B:108:ALA:HB2	0.64	1.70	6	1
1:A:29:LEU:HD13	1:A:29:LEU:N	0.64	2.07	15	4
2:B:123:LEU:HD11	2:B:174:SER:OG	0.63	1.93	12	4
2:B:157:MET:HE1	2:B:178:ILE:HD12	0.63	1.69	16	3
2:B:189:CYS:O	2:B:193:LEU:HD13	0.62	1.94	3	4
2:B:156:HIS:CD2	2:B:168:VAL:HG21	0.62	2.28	6	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:120:LEU:HD13	2:B:177:ILE:HG22	0.62	1.69	15	1
2:B:122:LEU:HD11	2:B:150:MET:CB	0.62	2.25	13	3
2:B:122:LEU:HD21	2:B:150:MET:SD	0.62	2.34	9	4
2:B:122:LEU:HD22	2:B:146:HIS:CG	0.62	2.29	9	2
2:B:133:GLU:HA	2:B:139:VAL:HG21	0.61	1.72	13	2
1:A:34:LEU:HD22	2:B:178:ILE:CG2	0.61	2.25	16	2
1:A:18:VAL:CG1	2:B:108:ALA:HB2	0.61	2.24	6	1
1:A:27:ASN:ND2	1:A:29:LEU:HD11	0.61	2.10	13	1
1:A:38:LEU:C	1:A:38:LEU:HD12	0.61	2.20	16	2
1:A:32:GLU:HA	2:B:158:THR:HG23	0.60	1.73	6	1
1:A:8:LEU:HD23	2:B:170:HIS:CE1	0.60	2.31	16	12
1:A:29:LEU:HD22	1:A:37:ALA:HB2	0.60	1.73	16	8
1:A:29:LEU:HD12	1:A:34:LEU:HD23	0.60	1.73	9	2
1:A:22:ILE:HD11	2:B:179:SER:OG	0.60	1.96	3	3
2:B:120:LEU:HD22	2:B:195:LEU:HD13	0.60	1.72	12	1
2:B:133:GLU:CG	2:B:139:VAL:HG13	0.60	2.26	12	1
1:A:34:LEU:HD13	2:B:157:MET:HE1	0.60	1.73	14	1
1:A:34:LEU:HD22	2:B:178:ILE:HG21	0.59	1.73	16	12
2:B:164:LYS:HA	2:B:172:ALA:HB1	0.59	1.74	3	2
2:B:120:LEU:O	2:B:124:LEU:HD13	0.58	1.97	9	7
1:A:22:ILE:HG23	2:B:183:ASN:CG	0.58	2.23	3	1
1:A:29:LEU:HD22	1:A:29:LEU:N	0.58	2.14	8	2
1:A:29:LEU:HD21	2:B:182:LYS:HG2	0.57	1.75	4	3
2:B:120:LEU:HB3	2:B:195:LEU:HD11	0.57	1.76	10	3
1:A:19:ASN:HB3	2:B:116:ILE:HD13	0.57	1.75	14	1
1:A:29:LEU:H	1:A:29:LEU:HD22	0.57	1.59	17	3
2:B:113:ARG:HA	2:B:116:ILE:HD12	0.57	1.75	17	1
1:A:8:LEU:HD13	1:A:9:PRO:CD	0.56	2.30	6	5
1:A:29:LEU:HD12	1:A:37:ALA:CB	0.56	2.31	17	3
2:B:120:LEU:HD22	2:B:195:LEU:CD1	0.56	2.29	12	1
1:A:29:LEU:N	1:A:29:LEU:HD22	0.56	2.16	5	2
1:A:29:LEU:HD12	1:A:37:ALA:HB2	0.56	1.78	17	2
1:A:20:ALA:HB1	2:B:180:HIS:CG	0.56	2.36	5	4
1:A:8:LEU:HD13	1:A:9:PRO:HD2	0.55	1.78	6	5
2:B:121:VAL:HG22	2:B:195:LEU:CD2	0.55	2.24	12	7
2:B:122:LEU:HD22	2:B:146:HIS:CB	0.55	2.31	9	5
1:A:8:LEU:CD2	2:B:150:MET:HE1	0.55	2.32	7	1
1:A:34:LEU:CD1	2:B:157:MET:HE1	0.55	2.32	14	1
1:A:38:LEU:CD2	2:B:178:ILE:HG23	0.54	2.32	12	2
2:B:153:VAL:HG11	2:B:170:HIS:HB3	0.54	1.79	13	1
1:A:38:LEU:HD11	2:B:178:ILE:CD1	0.54	2.25	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:133:GLU:HB3	2:B:139:VAL:HG13	0.54	1.78	12	1
1:A:29:LEU:HB2	1:A:34:LEU:HD23	0.54	1.79	16	10
1:A:8:LEU:HD12	2:B:170:HIS:ND1	0.54	2.17	15	3
2:B:157:MET:HE1	2:B:178:ILE:CD1	0.54	2.32	16	1
2:B:119:GLN:O	2:B:123:LEU:HD12	0.54	2.03	16	2
1:A:29:LEU:HD22	1:A:34:LEU:HD23	0.54	1.80	12	2
1:A:29:LEU:HD12	1:A:29:LEU:N	0.54	2.17	13	2
1:A:8:LEU:HD13	2:B:149:THR:HG21	0.54	1.80	1	2
2:B:189:CYS:O	2:B:193:LEU:HD22	0.53	2.04	3	2
2:B:120:LEU:HD21	2:B:181:TRP:HE3	0.53	1.61	11	1
1:A:8:LEU:HD12	2:B:146:HIS:ND1	0.53	2.18	14	1
1:A:35:LEU:HD21	2:B:154:LEU:HD22	0.53	1.78	15	2
1:A:29:LEU:HD23	1:A:29:LEU:N	0.53	2.18	9	3
1:A:22:ILE:HG21	1:A:27:ASN:HB2	0.53	1.79	17	1
1:A:35:LEU:HD11	2:B:158:THR:OG1	0.53	2.04	6	1
1:A:32:GLU:CA	2:B:158:THR:HG23	0.52	2.34	6	1
1:A:35:LEU:HD22	2:B:127:HIS:CE1	0.52	2.39	5	1
2:B:156:HIS:NE2	2:B:168:VAL:HG21	0.52	2.20	2	6
1:A:38:LEU:HD12	1:A:38:LEU:O	0.52	2.04	5	3
2:B:125:HIS:O	2:B:129:CYS:N	0.51	2.39	5	4
1:A:41:VAL:O	1:A:41:VAL:HG13	0.51	2.05	9	1
1:A:14:TYR:CE2	1:A:18:VAL:HG21	0.51	2.40	7	3
1:A:8:LEU:CD2	2:B:170:HIS:CE1	0.51	2.94	8	12
1:A:29:LEU:HD21	2:B:182:LYS:HB3	0.51	1.82	5	1
1:A:29:LEU:HD13	1:A:34:LEU:HD23	0.51	1.82	11	1
2:B:117:GLN:CD	2:B:191:VAL:HG13	0.51	2.31	6	1
1:A:38:LEU:HD12	1:A:38:LEU:C	0.51	2.30	5	2
1:A:27:ASN:CG	1:A:28:LEU:N	0.51	2.69	11	12
1:A:19:ASN:CB	2:B:116:ILE:HD13	0.51	2.35	14	1
1:A:22:ILE:HD11	2:B:179:SER:HB3	0.50	1.82	6	2
2:B:193:LEU:CB	2:B:194:PRO:HD3	0.50	2.35	15	5
1:A:28:LEU:HB3	1:A:29:LEU:HD13	0.50	1.83	15	3
1:A:14:TYR:CZ	1:A:18:VAL:HG21	0.50	2.42	13	1
1:A:29:LEU:H	1:A:29:LEU:CD1	0.50	2.16	5	4
1:A:38:LEU:HD12	1:A:39:ASP:N	0.50	2.22	16	1
2:B:156:HIS:NE2	2:B:168:VAL:CG2	0.50	2.75	5	17
1:A:35:LEU:N	1:A:35:LEU:HD23	0.49	2.21	16	2
2:B:120:LEU:O	2:B:120:LEU:HD13	0.49	2.08	16	2
1:A:38:LEU:HD13	2:B:127:HIS:HB2	0.49	1.84	15	1
1:A:29:LEU:HD11	2:B:182:LYS:CB	0.49	2.37	16	1
2:B:120:LEU:HD22	2:B:177:ILE:HG22	0.49	1.85	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LEU:HD13	2:B:149:THR:CG2	0.49	2.38	8	1
1:A:29:LEU:HD22	1:A:29:LEU:H	0.48	1.67	15	1
2:B:180:HIS:O	2:B:184:CYS:N	0.48	2.47	6	13
2:B:125:HIS:CD2	2:B:147:CYS:SG	0.48	3.06	14	4
1:A:20:ALA:HB1	2:B:180:HIS:NE2	0.48	2.24	6	2
1:A:29:LEU:HD23	1:A:37:ALA:HB1	0.48	1.85	11	1
1:A:20:ALA:HB2	2:B:191:VAL:HG21	0.48	1.86	11	3
1:A:29:LEU:H	1:A:29:LEU:CD2	0.48	2.20	17	4
1:A:34:LEU:HD12	2:B:157:MET:HE3	0.48	1.85	8	1
1:A:30:GLN:C	1:A:34:LEU:HD12	0.48	2.34	7	1
2:B:126:ALA:HB1	2:B:151:LYS:HD2	0.47	1.86	5	1
2:B:125:HIS:CD2	2:B:126:ALA:N	0.47	2.82	15	11
2:B:156:HIS:CD2	2:B:168:VAL:HG11	0.47	2.43	2	1
2:B:117:GLN:OE1	2:B:191:VAL:HG13	0.47	2.10	4	2
2:B:122:LEU:HD22	2:B:146:HIS:CD2	0.47	2.44	9	1
2:B:144:LEU:HD23	2:B:147:CYS:HB2	0.47	1.85	12	1
1:A:38:LEU:C	1:A:38:LEU:CD1	0.47	2.88	16	1
2:B:156:HIS:CD2	2:B:168:VAL:CG2	0.47	2.98	11	4
1:A:38:LEU:CD1	2:B:127:HIS:CD2	0.46	2.97	7	2
2:B:125:HIS:O	2:B:128:LYS:N	0.46	2.49	5	3
1:A:29:LEU:HD21	2:B:182:LYS:CG	0.46	2.40	5	1
2:B:120:LEU:HD12	2:B:124:LEU:HD22	0.46	1.88	3	2
2:B:122:LEU:C	2:B:122:LEU:CD1	0.46	2.87	8	8
1:A:22:ILE:HD13	2:B:179:SER:HB3	0.46	1.87	11	4
1:A:29:LEU:HG	1:A:37:ALA:CB	0.46	2.41	8	2
1:A:34:LEU:CD2	2:B:178:ILE:HG21	0.45	2.40	3	3
1:A:14:TYR:CZ	1:A:18:VAL:CG2	0.45	3.00	13	1
2:B:120:LEU:HD11	2:B:181:TRP:CE3	0.45	2.46	6	1
1:A:29:LEU:HD21	2:B:182:LYS:HD2	0.45	1.87	8	2
2:B:180:HIS:CD2	2:B:180:HIS:C	0.45	2.94	8	12
2:B:168:VAL:HB	2:B:171:CYS:HB2	0.45	1.89	15	6
1:A:34:LEU:O	1:A:38:LEU:HG	0.45	2.11	16	1
2:B:193:LEU:CB	2:B:194:PRO:CD	0.45	2.95	5	15
1:A:29:LEU:HD11	2:B:182:LYS:CD	0.45	2.42	15	1
1:A:22:ILE:HD11	2:B:179:SER:CB	0.44	2.41	3	1
1:A:16:CYS:SG	2:B:177:ILE:HD13	0.44	2.52	7	2
2:B:122:LEU:CD2	2:B:146:HIS:CD2	0.44	3.00	9	1
1:A:14:TYR:CE1	1:A:18:VAL:CG2	0.44	3.00	13	1
2:B:180:HIS:CD2	2:B:181:TRP:N	0.44	2.85	9	13
1:A:22:ILE:O	1:A:23:GLN:CB	0.44	2.66	13	4
1:A:38:LEU:HD11	2:B:127:HIS:CG	0.44	2.47	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:137:GLY:O	2:B:139:VAL:HG23	0.44	2.12	7	2
1:A:38:LEU:CB	2:B:127:HIS:CE1	0.44	3.01	12	2
2:B:133:GLU:HG3	2:B:139:VAL:HG13	0.44	1.89	12	1
1:A:27:ASN:OD1	1:A:29:LEU:CD2	0.44	2.66	5	2
2:B:122:LEU:HD21	2:B:146:HIS:ND1	0.44	2.28	6	1
1:A:32:GLU:CG	2:B:158:THR:HG22	0.44	2.40	16	1
1:A:20:ALA:HB2	2:B:191:VAL:CG2	0.44	2.42	7	1
1:A:29:LEU:CD2	1:A:37:ALA:CB	0.44	2.92	14	1
1:A:26:ARG:CD	1:A:26:ARG:N	0.44	2.81	11	1
1:A:27:ASN:OD1	1:A:29:LEU:HD11	0.43	2.13	12	1
2:B:150:MET:O	2:B:154:LEU:N	0.43	2.48	14	2
1:A:30:GLN:O	1:A:34:LEU:CD1	0.43	2.64	16	2
2:B:189:CYS:HB3	2:B:193:LEU:HD13	0.43	1.90	15	1
1:A:29:LEU:HD11	2:B:182:LYS:HD2	0.43	1.90	15	1
1:A:27:ASN:ND2	1:A:29:LEU:O	0.43	2.51	8	1
2:B:160:CYS:C	2:B:162:SER:N	0.42	2.76	4	1
1:A:34:LEU:CD2	2:B:178:ILE:CG2	0.42	2.96	7	2
2:B:156:HIS:HD2	2:B:168:VAL:HG11	0.42	1.74	2	1
1:A:22:ILE:CG2	2:B:183:ASN:ND2	0.42	2.82	6	3
1:A:22:ILE:HG23	2:B:183:ASN:ND2	0.42	2.30	6	1
2:B:120:LEU:CD1	2:B:181:TRP:CE3	0.42	3.02	6	1
2:B:164:LYS:O	2:B:172:ALA:HB1	0.42	2.15	9	1
1:A:16:CYS:O	1:A:20:ALA:N	0.42	2.52	11	3
2:B:156:HIS:CD2	2:B:171:CYS:HB2	0.42	2.50	4	5
2:B:163:GLY:O	2:B:164:LYS:CB	0.42	2.67	1	1
2:B:124:LEU:O	2:B:127:HIS:HB3	0.42	2.15	6	1
1:A:29:LEU:N	1:A:29:LEU:CD1	0.42	2.82	8	2
1:A:29:LEU:HB2	1:A:34:LEU:HA	0.42	1.91	11	1
1:A:8:LEU:HD13	1:A:9:PRO:N	0.42	2.30	11	1
2:B:120:LEU:HD23	2:B:195:LEU:HD12	0.42	1.91	11	1
1:A:20:ALA:HB1	2:B:180:HIS:ND1	0.41	2.28	17	2
1:A:11:LEU:HD12	2:B:177:ILE:HD11	0.41	1.92	6	1
2:B:122:LEU:HD11	2:B:150:MET:HG3	0.41	1.92	1	2
2:B:127:HIS:CD2	2:B:127:HIS:C	0.41	2.98	15	1
1:A:22:ILE:CG2	2:B:183:ASN:CB	0.41	2.99	11	1
2:B:156:HIS:NE2	2:B:168:VAL:HB	0.41	2.31	15	1
2:B:186:ARG:CG	2:B:187:HIS:N	0.41	2.83	12	1
1:A:38:LEU:HD23	2:B:178:ILE:HD13	0.41	1.90	16	1
2:B:121:VAL:O	2:B:125:HIS:N	0.41	2.47	7	2
2:B:120:LEU:CD2	2:B:181:TRP:CE3	0.41	3.04	1	1
2:B:120:LEU:HD12	2:B:177:ILE:HG23	0.41	1.92	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ASN:ND2	1:A:29:LEU:CD2	0.41	2.84	17	1
1:A:20:ALA:C	2:B:180:HIS:ND1	0.41	2.79	6	1
1:A:29:LEU:N	1:A:29:LEU:CD2	0.41	2.83	17	1
2:B:118:GLN:O	2:B:122:LEU:HD23	0.41	2.16	6	1
1:A:27:ASN:HB3	2:B:179:SER:HB2	0.41	1.93	8	1
2:B:125:HIS:CE1	2:B:144:LEU:HD13	0.41	2.51	9	1
2:B:113:ARG:O	2:B:117:GLN:CG	0.41	2.69	11	1
2:B:164:LYS:O	2:B:165:SER:CB	0.41	2.68	15	1
1:A:22:ILE:HG22	2:B:183:ASN:ND2	0.41	2.31	17	1
1:A:27:ASN:ND2	1:A:29:LEU:CD1	0.41	2.84	13	1
2:B:125:HIS:O	2:B:126:ALA:C	0.40	2.64	2	2
2:B:120:LEU:HD13	2:B:124:LEU:HD13	0.40	1.92	16	1
1:A:31:GLY:C	2:B:158:THR:HG23	0.40	2.41	14	1
2:B:157:MET:CG	2:B:175:ARG:NH2	0.40	2.84	4	1
2:B:128:LYS:O	2:B:132:ARG:N	0.40	2.55	2	1

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	34/42 (81%)	23±1 (69±4%)	8±2 (24±5%)	2±2 (7±5%)	2	16
2	B	89/101 (88%)	71±2 (80±2%)	15±2 (17±3%)	2±1 (3±1%)	6	42
All	All	2091/2431 (86%)	1610 (77%)	402 (19%)	79 (4%)	4	31

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	108	ALA	14
1	A	9	PRO	10
1	A	25	SER	8
1	A	26	ARG	8
2	B	163	GLY	7
2	B	165	SER	6

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Mol	Chain	Res	Type	Models (Total)
2	B	142	CYS	5
1	A	28	LEU	5
1	A	24	GLY	5
1	A	23	GLN	4
2	B	186	ARG	4
2	B	188	ASP	3

6.3.2 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 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	30/36 (83%)	21±2 (71±6%)	9±2 (29±6%)	1	19
2	B	82/89 (92%)	60±4 (73±4%)	22±4 (27±4%)	1	21
All	All	1904/2125 (90%)	1377 (72%)	527 (28%)	1	20

All 79 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	8	LEU	17
1	A	19	ASN	17
1	A	29	LEU	17
2	B	180	HIS	17
2	B	117	GLN	16
2	B	122	LEU	15
2	B	151	LYS	15
2	B	156	HIS	15
2	B	119	GLN	15
2	B	161	GLN	14
2	B	118	GLN	13
2	B	130	GLN	13
1	A	26	ARG	12
2	B	120	LEU	12
2	B	144	LEU	12
2	B	158	THR	11
2	B	150	MET	11
1	A	23	GLN	10

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Mol	Chain	Res	Type	Models (Total)
2	B	176	GLN	10
1	A	17	GLU	10
1	A	36	ARG	9
2	B	182	LYS	9
1	A	25	SER	9
2	B	114	LYS	9
2	B	186	ARG	9
2	B	189	CYS	9
1	A	30	GLN	8
2	B	159	HIS	8
2	B	112	LYS	8
2	B	152	ASN	8
1	A	13	SER	8
2	B	140	ARG	7
1	A	39	ASP	7
2	B	195	LEU	7
1	A	32	GLU	5
2	B	187	HIS	5
2	B	134	GLN	5
2	B	132	ARG	5
2	B	127	HIS	5
2	B	128	LYS	5
2	B	164	LYS	5
2	B	167	GLN	5
2	B	193	LEU	5
2	B	165	SER	5
2	B	142	CYS	5
2	B	146	HIS	5
2	B	183	ASN	4
2	B	141	GLN	4
2	B	196	LYS	4
2	B	143	ASN	4
2	B	115	LEU	4
2	B	162	SER	4
1	A	40	GLN	3
2	B	124	LEU	3
1	A	35	LEU	3
1	A	38	LEU	3
2	B	111	GLU	3
2	B	133	GLU	3
2	B	149	THR	3
2	B	155	ASN	3

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Mol	Chain	Res	Type	Models (Total)
2	B	113	ARG	3
2	B	138	GLU	3
2	B	148	ARG	3
1	A	27	ASN	3
2	B	131	ARG	2
2	B	136	ASN	2
2	B	123	LEU	2
1	A	10	GLN	2
2	B	175	ARG	2
2	B	166	CYS	1
2	B	188	ASP	1
2	B	173	SER	1
2	B	185	THR	1
1	A	15	ASP	1
2	B	147	CYS	1
2	B	157	MET	1
1	A	28	LEU	1
1	A	33	GLU	1
1	A	11	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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