



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 08:17 PM BST

PDB ID : 2A24
Title : HADDOCK Structure of HIF-2a/ARNT PAS-B Heterodimer
Authors : Card, P.B.; Erbel, P.J.; Gardner, K.H.
Deposited on : 2005-06-21

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
<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

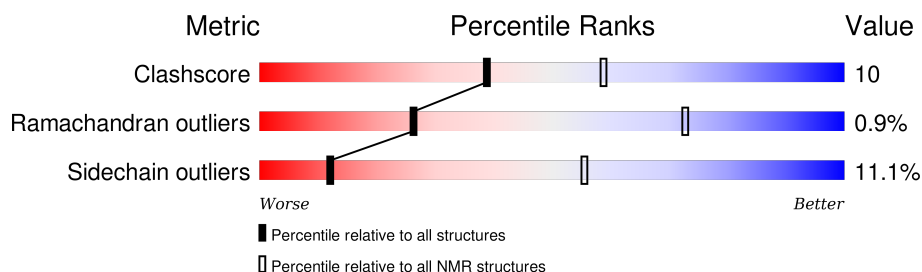
1 Overall quality at a glance

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	107	 66% 33% •
2	B	108	 75% 24% •

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 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:6-A:112, B:7-B:114 (215)	0.60	5

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 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 19, 20
2	8, 11, 15, 17
3	14, 16, 18
Single-model clusters	9; 10; 12; 13

3 Entry composition [i](#)


There are 2 unique types of molecules in this entry. The entry contains 3502 atoms, of which 1727 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Endothelial PAS domain protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1721	550	848	149	165	9	

- Molecule 2 is a protein called Aryl hydrocarbon receptor nuclear translocator.

Mol	Chain	Residues	Atoms						Trace
2	B	108	Total	C	H	N	O	S	0
			1781	575	879	155	166	6	

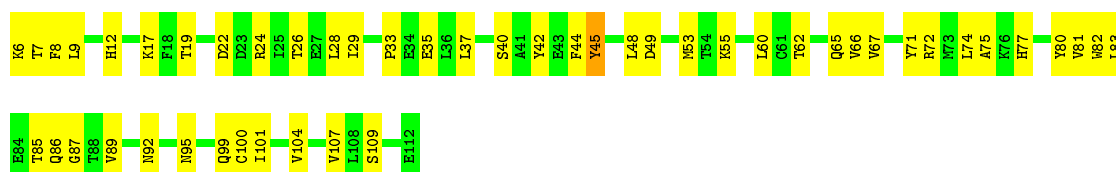
Chain B: 



4.2.2 Score per residue for model 2

- Molecule 1: Endothelial PAS domain protein 1

Chain A: 



- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

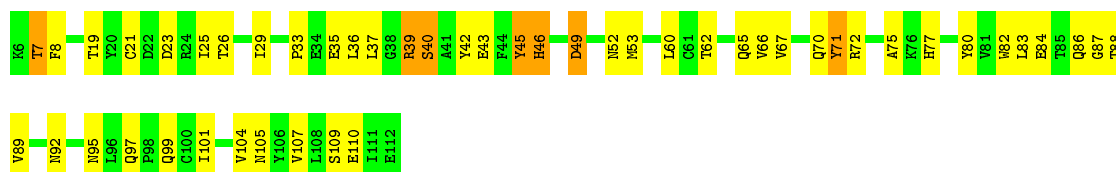
Chain B: 



4.2.3 Score per residue for model 3

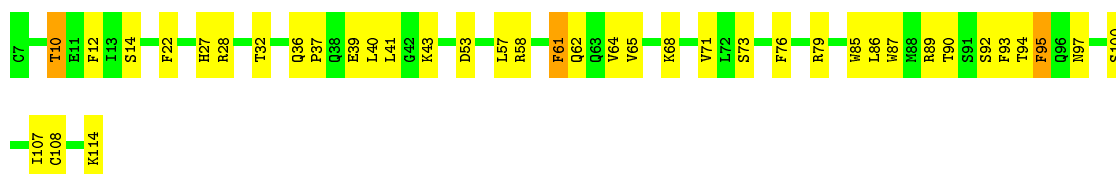
- Molecule 1: Endothelial PAS domain protein 1

Chain A: 



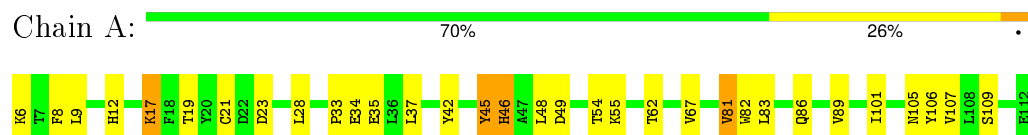
- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

Chain B: 

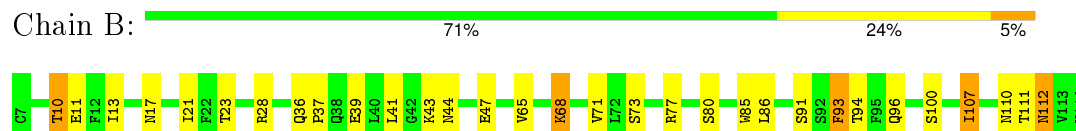


4.2.4 Score per residue for model 4

- Molecule 1: Endothelial PAS domain protein 1

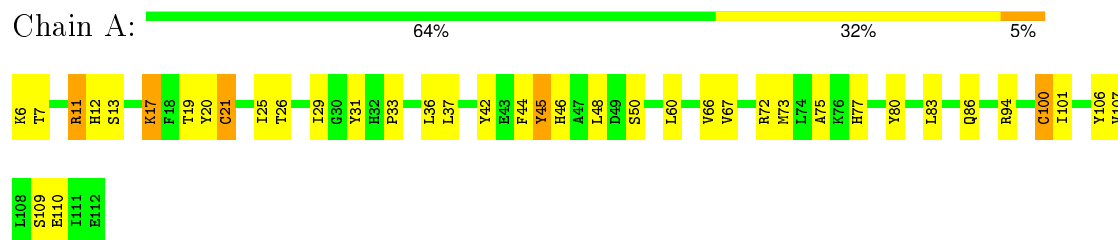


- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

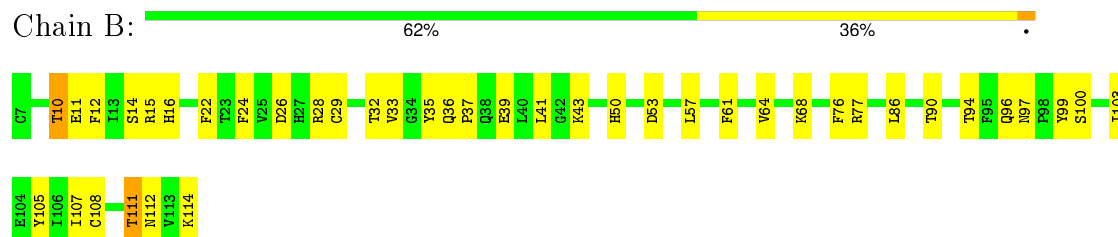


4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Endothelial PAS domain protein 1

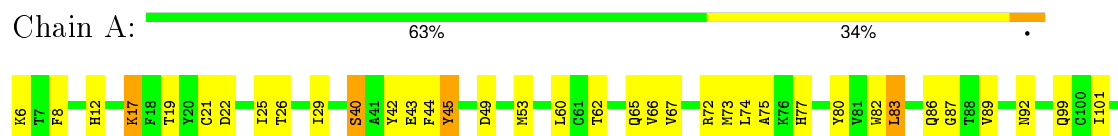


- Molecule 2: Aryl hydrocarbon receptor nuclear translocator



4.2.6 Score per residue for model 6

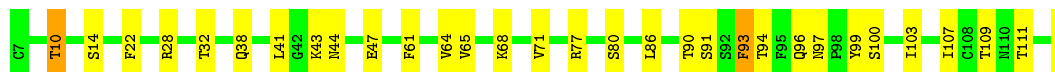
- Molecule 1: Endothelial PAS domain protein 1





- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

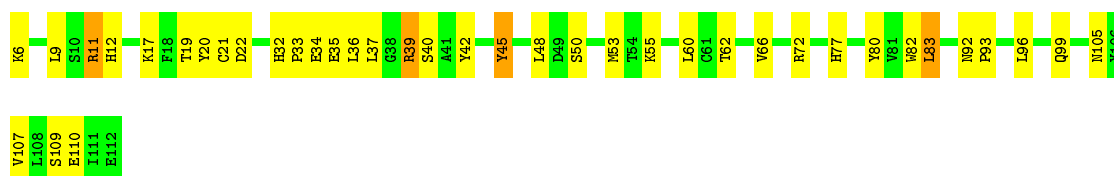
Chain B: 71% 27%



4.2.7 Score per residue for model 7

- Molecule 1: Endothelial PAS domain protein 1

Chain A: 64% 33%



- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

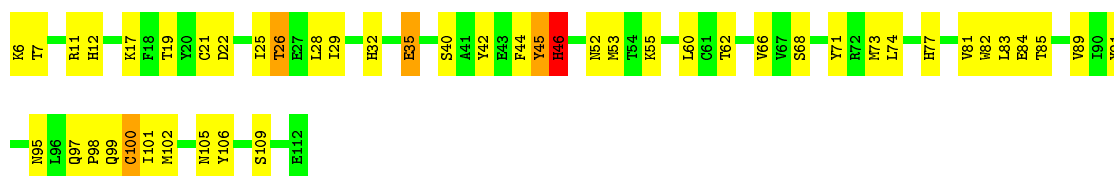
Chain B: 75% 22%



4.2.8 Score per residue for model 8

- Molecule 1: Endothelial PAS domain protein 1

Chain A: 56% 39%



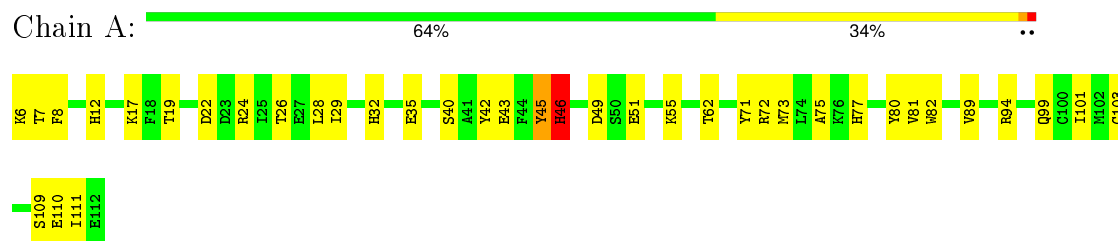
- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

Chain B: 72% 27%

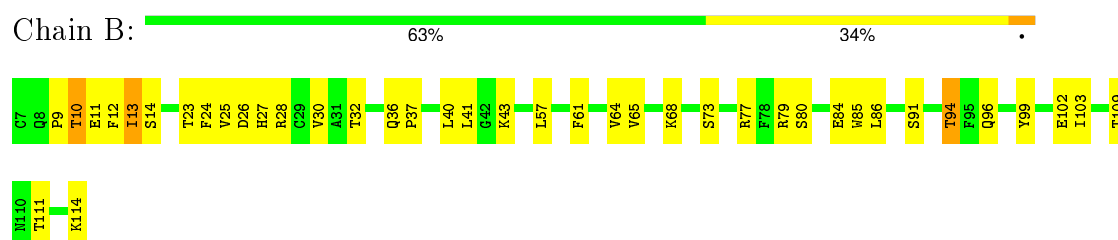


4.2.9 Score per residue for model 9

- Molecule 1: Endothelial PAS domain protein 1

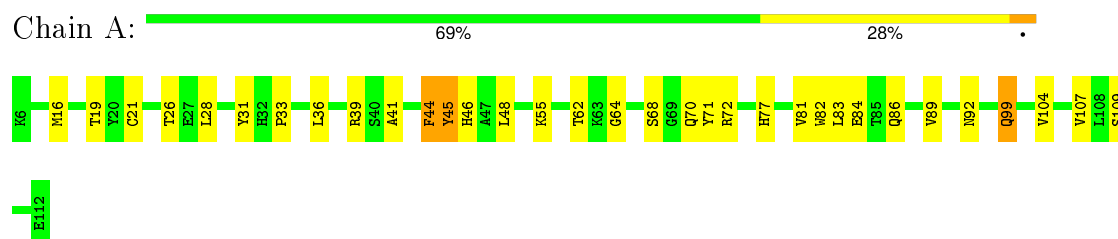


- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

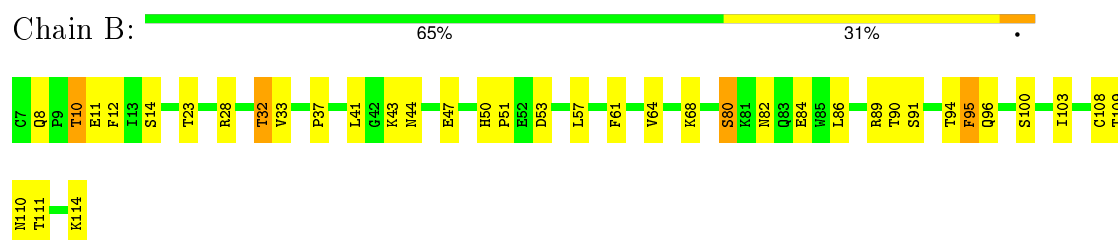


4.2.10 Score per residue for model 10

- Molecule 1: Endothelial PAS domain protein 1

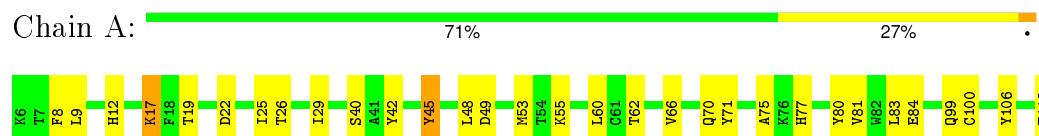


- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

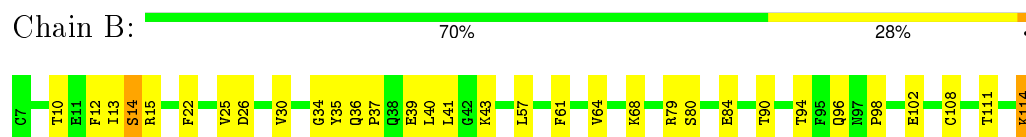


4.2.11 Score per residue for model 11

- Molecule 1: Endothelial PAS domain protein 1

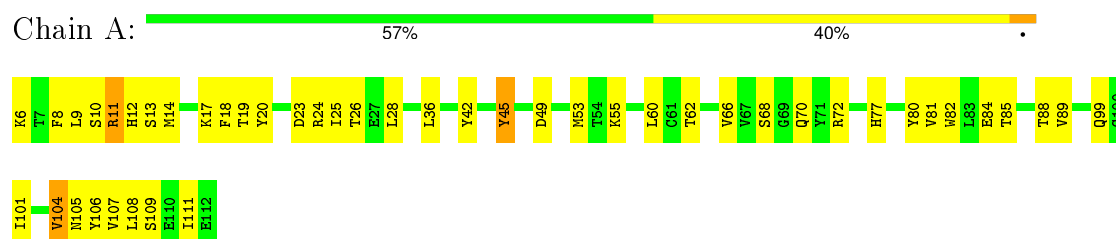


- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

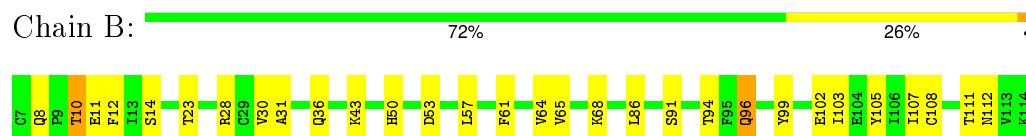


4.2.12 Score per residue for model 12

- Molecule 1: Endothelial PAS domain protein 1

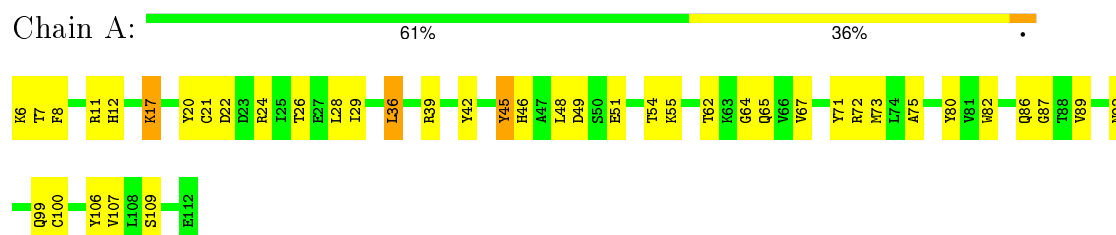


- Molecule 2: Aryl hydrocarbon receptor nuclear translocator



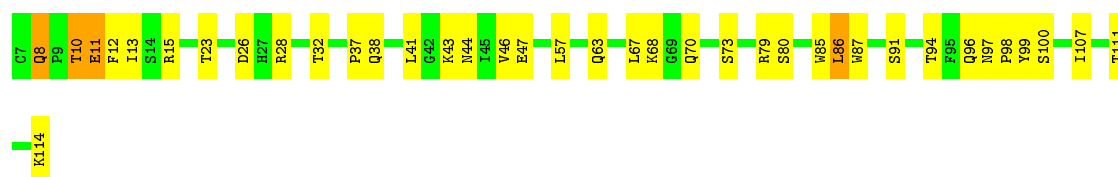
4.2.13 Score per residue for model 13

- Molecule 1: Endothelial PAS domain protein 1



- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

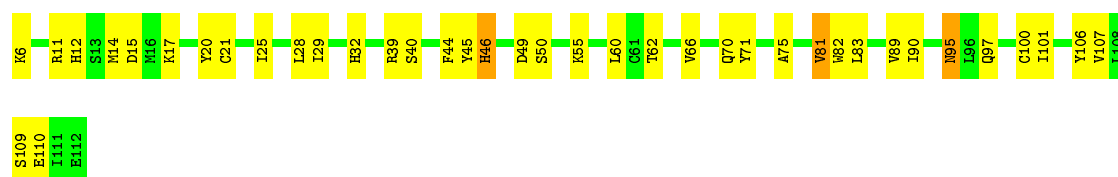




4.2.14 Score per residue for model 14

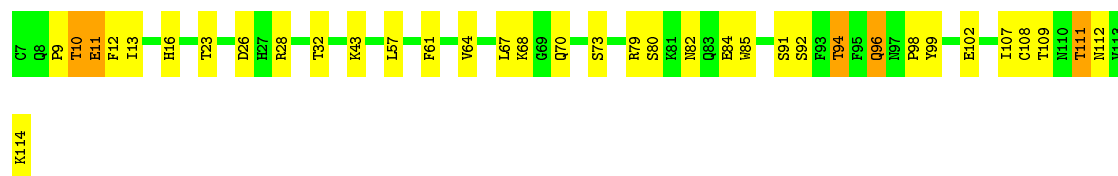
- Molecule 1: Endothelial PAS domain protein 1

Chain A: 64% 34%



- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

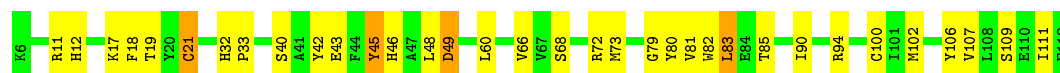
Chain B: 67% 29% 5%



4.2.15 Score per residue for model 15

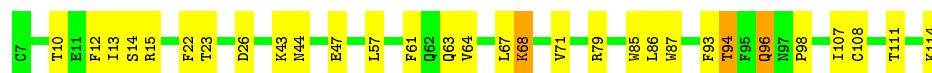
- Molecule 1: Endothelial PAS domain protein 1

Chain A: 68% 28%



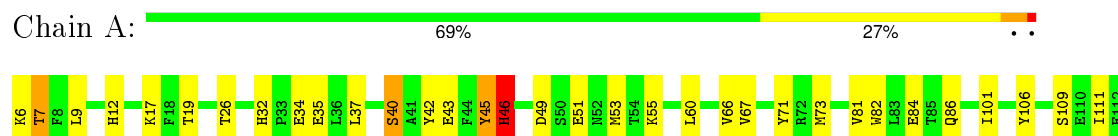
- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

Chain B: 72% 25%

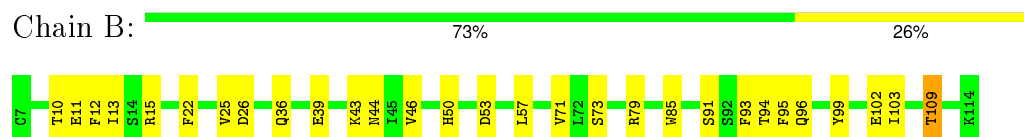


4.2.16 Score per residue for model 16

- Molecule 1: Endothelial PAS domain protein 1

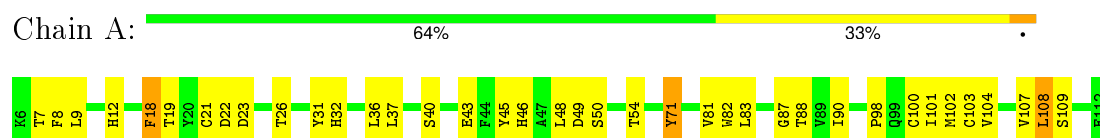


- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

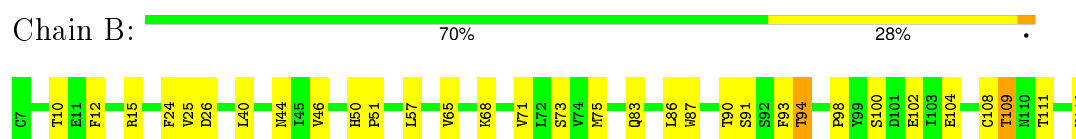


4.2.17 Score per residue for model 17

- Molecule 1: Endothelial PAS domain protein 1

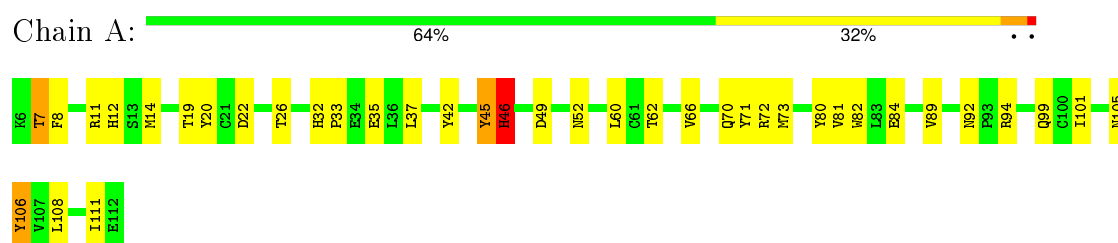


- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

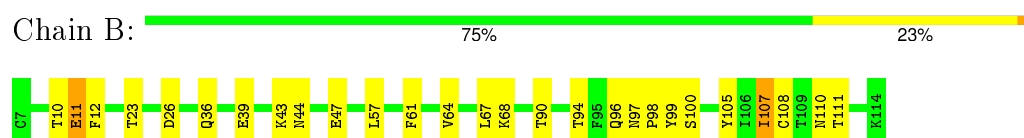


4.2.18 Score per residue for model 18

- Molecule 1: Endothelial PAS domain protein 1

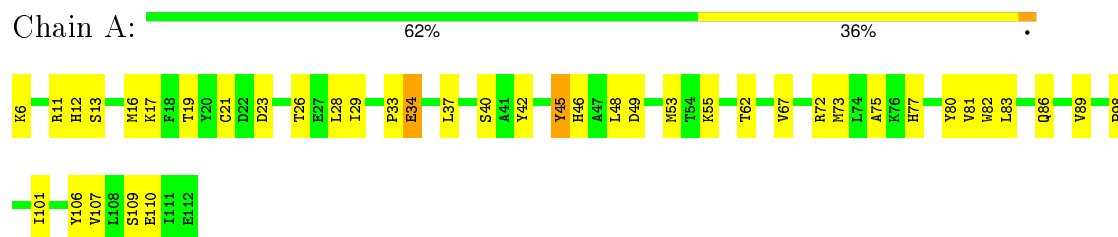


- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

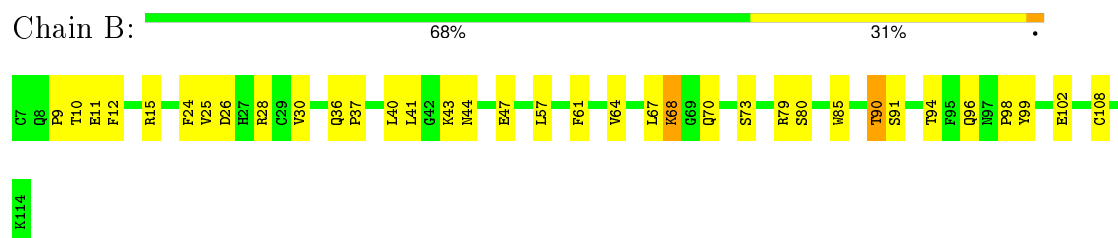


4.2.19 Score per residue for model 19

- Molecule 1: Endothelial PAS domain protein 1

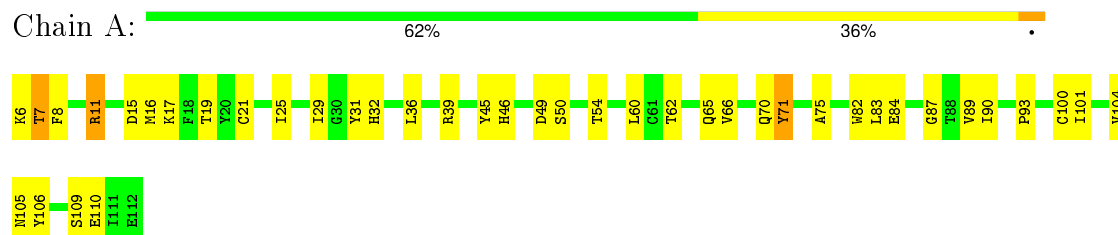


- Molecule 2: Aryl hydrocarbon receptor nuclear translocator

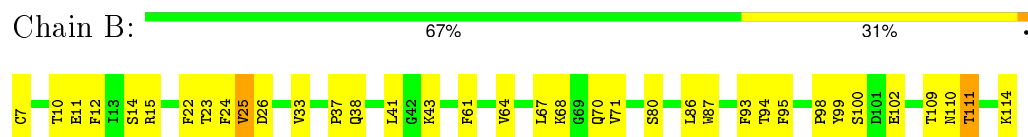


4.2.20 Score per residue for model 20

- Molecule 1: Endothelial PAS domain protein 1



- Molecule 2: Aryl hydrocarbon receptor nuclear translocator



5 Refinement protocol and experimental data overview ⓘ

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
HADDOCK	structure solution	1.2
CNS	structure solution	1.1
CNS	refinement	1.1

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

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	873	848	840	18±3
2	B	902	879	873	17±3
All	All	35500	34540	34260	666

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ARG:HB3	1:A:80:TYR:HB3	0.91	1.41	12	11
1:A:7:THR:HG22	1:A:106:TYR:HA	0.84	1.48	5	1
1:A:82:TRP:HB2	1:A:109:SER:HB2	0.80	1.51	17	16
1:A:42:TYR:HA	1:A:45:TYR:HB2	0.79	1.54	3	15
1:A:34:GLU:HA	1:A:37:LEU:HG	0.78	1.55	4	3
1:A:106:TYR:HB3	2:B:98:PRO:HG3	0.76	1.58	14	7
2:B:12:PHE:HB2	2:B:26:ASP:HB3	0.76	1.55	13	12
1:A:60:LEU:HD21	1:A:101:ILE:HG21	0.76	1.57	8	3
1:A:90:ILE:HB	1:A:100:CYS:HB2	0.76	1.57	17	3
1:A:70:GLN:HG2	1:A:84:GLU:HG2	0.75	1.57	20	3
1:A:29:ILE:HG23	1:A:75:ALA:HA	0.75	1.59	2	11
1:A:11:ARG:HB3	1:A:20:TYR:HB3	0.74	1.57	18	4
1:A:6:LYS:N	2:B:99:TYR:HH	0.72	1.83	9	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:14:SER:HB3	2:B:22:PHE:HE2	0.71	1.45	8	3
1:A:80:TYR:HB2	1:A:112:GLU:HB3	0.70	1.63	11	2
1:A:60:LEU:HD13	1:A:66:VAL:HG12	0.70	1.63	12	14
1:A:7:THR:HG23	1:A:106:TYR:HB3	0.70	1.63	18	1
2:B:90:THR:HG22	2:B:108:CYS:HB3	0.70	1.64	17	4
2:B:91:SER:HB2	2:B:109:THR:HB	0.69	1.64	9	5
1:A:67:VAL:HG22	1:A:86:GLN:HG3	0.69	1.61	2	7
2:B:82:ASN:HB2	2:B:84:GLU:HG2	0.68	1.65	14	2
2:B:43:LYS:HA	2:B:43:LYS:HE2	0.68	1.63	15	7
2:B:12:PHE:HB3	2:B:28:ARG:HB2	0.68	1.65	13	5
1:A:44:PHE:HB2	1:A:74:LEU:HD23	0.68	1.64	2	3
1:A:46:HIS:HB2	1:A:49:ASP:HB2	0.67	1.64	18	2
2:B:36:GLN:HB2	2:B:39:GLU:HG3	0.67	1.65	3	7
2:B:96:GLN:HG2	2:B:103:ILE:HG12	0.67	1.66	10	3
1:A:83:LEU:HD13	1:A:105:ASN:HD21	0.67	1.47	6	2
2:B:14:SER:HB3	2:B:22:PHE:HE1	0.67	1.50	20	2
2:B:43:LYS:HE2	2:B:43:LYS:HA	0.67	1.66	6	10
2:B:44:ASN:HB2	2:B:47:GLU:HG3	0.67	1.67	18	8
1:A:23:ASP:HA	1:A:33:PRO:HG3	0.66	1.65	4	1
2:B:10:THR:HB	2:B:112:ASN:HB3	0.66	1.67	4	4
1:A:36:LEU:HA	1:A:39:ARG:HG2	0.66	1.68	3	2
1:A:6:LYS:HB2	1:A:107:VAL:HB	0.65	1.69	4	1
2:B:8:GLN:HB3	2:B:28:ARG:HG2	0.65	1.67	10	1
1:A:84:GLU:HG3	1:A:106:TYR:HB2	0.64	1.69	16	1
2:B:11:GLU:HB3	2:B:111:THR:HG23	0.63	1.70	14	1
1:A:39:ARG:HD2	1:A:44:PHE:HE2	0.63	1.53	10	2
1:A:6:LYS:HB2	1:A:28:LEU:HD21	0.63	1.70	12	2
1:A:91:TYR:HA	1:A:98:PRO:HA	0.63	1.70	8	1
2:B:8:GLN:HG3	2:B:28:ARG:HA	0.63	1.71	2	2
2:B:68:LYS:HE2	2:B:103:ILE:HD11	0.63	1.68	6	1
1:A:92:ASN:HB2	1:A:99:GLN:HB2	0.63	1.69	7	4
1:A:83:LEU:HD23	1:A:105:ASN:HB3	0.62	1.71	8	3
2:B:13:ILE:HG12	2:B:109:THR:HG23	0.62	1.69	14	2
1:A:9:LEU:HD21	1:A:102:MET:HB3	0.61	1.72	17	1
1:A:83:LEU:HG	1:A:107:VAL:HG13	0.61	1.71	10	1
1:A:89:VAL:HG22	1:A:101:ILE:HG23	0.61	1.72	19	4
2:B:25:VAL:HG21	2:B:40:LEU:HB2	0.61	1.72	11	6
1:A:12:HIS:HA	1:A:17:LYS:O	0.61	1.96	8	14
2:B:15:ARG:HD3	2:B:24:PHE:HB3	0.60	1.73	19	3
1:A:46:HIS:HD2	1:A:73:MET:HA	0.60	1.55	16	3
1:A:46:HIS:CD2	1:A:73:MET:HA	0.60	2.31	16	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:ARG:HG2	2:B:107:ILE:HG12	0.60	1.73	15	1
1:A:72:ARG:HB2	1:A:80:TYR:HB3	0.60	1.74	15	1
1:A:12:HIS:O	1:A:101:ILE:HB	0.59	1.97	17	1
2:B:77:ARG:HB3	2:B:85:TRP:HB3	0.59	1.74	4	2
1:A:7:THR:HB	2:B:95:PHE:CE2	0.59	2.32	3	2
1:A:13:SER:HB3	1:A:100:CYS:HA	0.59	1.73	5	1
2:B:94:THR:HB	2:B:96:GLN:OE1	0.59	1.96	9	3
1:A:64:GLY:HA2	1:A:89:VAL:HB	0.59	1.74	10	2
1:A:40:SER:HB2	1:A:43:GLU:HG2	0.59	1.75	17	2
2:B:15:ARG:HD2	2:B:24:PHE:HB3	0.59	1.75	17	1
1:A:106:TYR:HB3	2:B:98:PRO:HB3	0.58	1.75	1	1
2:B:8:GLN:HB2	2:B:31:ALA:HB3	0.58	1.74	12	1
1:A:100:CYS:HB3	2:B:109:THR:HG21	0.58	1.75	17	1
1:A:8:PHE:CE1	1:A:25:ILE:HB	0.58	2.33	3	5
1:A:40:SER:HB2	1:A:43:GLU:HG3	0.58	1.76	6	3
1:A:46:HIS:CB	1:A:49:ASP:HB2	0.58	2.29	18	2
1:A:81:VAL:HG12	1:A:83:LEU:HD13	0.57	1.76	11	2
1:A:33:PRO:O	1:A:37:LEU:HG	0.57	1.99	2	4
1:A:83:LEU:HB3	1:A:107:VAL:HA	0.57	1.75	6	3
1:A:86:GLN:HB3	1:A:104:VAL:HB	0.57	1.74	10	2
2:B:79:ARG:HB2	2:B:85:TRP:CZ3	0.57	2.34	15	8
2:B:93:PHE:HB3	2:B:107:ILE:HD12	0.57	1.75	6	1
1:A:100:CYS:HB3	2:B:13:ILE:HD11	0.57	1.76	13	1
1:A:21:CYS:SG	1:A:36:LEU:HB2	0.57	2.40	5	6
1:A:81:VAL:HB	1:A:83:LEU:HD13	0.57	1.76	4	2
2:B:13:ILE:HG23	2:B:107:ILE:HG23	0.56	1.77	15	1
1:A:39:ARG:HD2	1:A:44:PHE:CE2	0.56	2.35	10	1
1:A:11:ARG:HG3	1:A:20:TYR:HB3	0.56	1.77	5	1
2:B:15:ARG:HH12	2:B:24:PHE:HB3	0.56	1.61	20	1
2:B:15:ARG:NH1	2:B:24:PHE:HB3	0.56	2.16	20	1
1:A:28:LEU:HD13	1:A:107:VAL:HG21	0.56	1.78	14	5
1:A:97:GLN:HB2	1:A:98:PRO:HD2	0.56	1.77	8	1
2:B:105:TYR:HE1	2:B:107:ILE:HG23	0.56	1.60	18	1
2:B:10:THR:HG22	2:B:32:THR:HG23	0.56	1.78	6	3
2:B:64:VAL:HA	2:B:67:LEU:HD12	0.55	1.76	20	2
2:B:50:HIS:HB3	2:B:53:ASP:HB2	0.55	1.77	10	5
1:A:6:LYS:HD3	1:A:24:ARG:HG2	0.55	1.78	12	1
2:B:8:GLN:HB3	2:B:28:ARG:HA	0.55	1.78	12	1
2:B:10:THR:HG22	2:B:32:THR:HA	0.55	1.76	10	3
1:A:79:GLY:HA3	1:A:111:ILE:HG23	0.55	1.79	15	1
2:B:67:LEU:HB3	2:B:70:GLN:HB3	0.54	1.80	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:ASN:HB2	1:A:99:GLN:HG3	0.54	1.80	13	1
1:A:11:ARG:HG3	1:A:102:MET:HG2	0.54	1.79	15	1
2:B:16:HIS:CB	2:B:22:PHE:HA	0.54	2.33	7	1
1:A:23:ASP:HA	1:A:33:PRO:CG	0.54	2.33	4	1
1:A:46:HIS:HB3	1:A:49:ASP:OD1	0.53	2.04	15	4
1:A:70:GLN:HB3	1:A:82:TRP:HB3	0.53	1.79	14	1
1:A:51:GLU:O	1:A:55:LYS:HG2	0.53	2.03	9	2
2:B:11:GLU:HG3	2:B:111:THR:HG23	0.53	1.80	10	1
1:A:89:VAL:HG22	1:A:101:ILE:HG12	0.53	1.79	6	6
1:A:28:LEU:HD22	1:A:107:VAL:HG21	0.53	1.80	4	2
2:B:11:GLU:HB3	2:B:111:THR:HG22	0.53	1.80	13	1
2:B:95:PHE:HB3	2:B:105:TYR:O	0.53	2.04	8	1
2:B:12:PHE:HB3	2:B:28:ARG:HB3	0.53	1.79	3	2
2:B:33:VAL:HG12	2:B:86:LEU:HD21	0.53	1.79	7	2
2:B:37:PRO:O	2:B:41:LEU:HG	0.52	2.03	2	12
1:A:81:VAL:HG22	1:A:111:ILE:HG23	0.52	1.81	1	2
2:B:11:GLU:HA	2:B:110:ASN:O	0.52	2.04	18	4
1:A:46:HIS:HA	1:A:72:ARG:O	0.52	2.03	10	1
2:B:30:VAL:HG13	2:B:36:GLN:HE22	0.52	1.63	19	3
1:A:68:SER:HB2	1:A:85:THR:HB	0.52	1.81	8	2
1:A:73:MET:O	1:A:80:TYR:HA	0.52	2.05	5	2
1:A:12:HIS:HB2	1:A:101:ILE:HB	0.51	1.82	16	2
1:A:8:PHE:HB2	1:A:22:ASP:HB3	0.51	1.81	11	5
1:A:73:MET:HB2	1:A:83:LEU:HD11	0.51	1.81	6	1
1:A:9:LEU:HG	2:B:107:ILE:HD13	0.51	1.82	4	1
2:B:71:VAL:HB	2:B:93:PHE:HD1	0.51	1.66	8	1
1:A:10:SER:HB3	1:A:103:CYS:HB2	0.51	1.82	1	1
1:A:99:GLN:HE21	1:A:99:GLN:HA	0.51	1.65	10	1
2:B:73:SER:HA	2:B:91:SER:HA	0.51	1.83	8	9
1:A:83:LEU:HD11	1:A:107:VAL:HG13	0.51	1.83	17	1
2:B:65:VAL:HA	2:B:94:THR:HG21	0.51	1.81	17	1
2:B:8:GLN:HB2	2:B:28:ARG:HG2	0.51	1.83	7	2
2:B:14:SER:HB2	2:B:108:CYS:SG	0.50	2.46	12	3
2:B:97:ASN:HB3	2:B:99:TYR:CD2	0.50	2.42	6	1
1:A:71:TYR:O	1:A:82:TRP:HA	0.50	2.07	9	10
1:A:65:GLN:HA	1:A:87:GLY:O	0.50	2.07	20	5
2:B:11:GLU:O	2:B:28:ARG:HD3	0.50	2.06	9	2
2:B:11:GLU:O	2:B:28:ARG:HD2	0.50	2.07	5	1
1:A:70:GLN:HG2	1:A:82:TRP:HE3	0.50	1.66	3	1
1:A:18:PHE:HB3	1:A:37:LEU:HA	0.50	1.84	17	1
1:A:11:ARG:CB	1:A:20:TYR:HB3	0.50	2.36	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:16:HIS:HB3	2:B:22:PHE:HA	0.50	1.83	7	1
2:B:11:GLU:HB2	2:B:111:THR:HG23	0.50	1.83	8	3
2:B:16:HIS:O	2:B:105:TYR:HB2	0.50	2.07	7	3
2:B:33:VAL:HG11	2:B:78:PHE:HD2	0.50	1.67	7	1
2:B:87:TRP:H	2:B:114:LYS:HG3	0.49	1.66	15	1
1:A:9:LEU:HD23	2:B:95:PHE:HZ	0.49	1.67	1	1
2:B:97:ASN:ND2	2:B:99:TYR:HB2	0.49	2.22	18	1
1:A:88:THR:HG21	2:B:71:VAL:HG11	0.49	1.84	17	1
1:A:70:GLN:HG2	1:A:84:GLU:HG3	0.49	1.83	10	1
2:B:90:THR:CG2	2:B:108:CYS:HB3	0.49	2.37	10	5
1:A:40:SER:HB3	1:A:43:GLU:HG3	0.49	1.84	9	1
1:A:21:CYS:HB2	1:A:33:PRO:HB3	0.49	1.85	19	1
1:A:6:LYS:HB3	1:A:28:LEU:HD21	0.49	1.85	9	1
1:A:99:GLN:HG3	1:A:100:CYS:SG	0.49	2.48	8	2
2:B:71:VAL:HB	2:B:93:PHE:HD2	0.49	1.67	1	5
1:A:104:VAL:HG21	2:B:93:PHE:CE1	0.49	2.43	20	2
1:A:92:ASN:HB3	1:A:95:ASN:HB2	0.49	1.84	2	1
1:A:26:THR:HG23	1:A:32:HIS:HA	0.48	1.85	8	1
2:B:90:THR:CG2	2:B:108:CYS:HB2	0.48	2.38	3	1
1:A:34:GLU:HA	1:A:37:LEU:HD12	0.48	1.84	16	2
2:B:80:SER:OG	2:B:84:GLU:HG3	0.48	2.08	14	2
1:A:104:VAL:HG13	2:B:95:PHE:CZ	0.48	2.44	10	1
1:A:46:HIS:HB3	1:A:49:ASP:HB3	0.48	1.86	14	1
1:A:25:ILE:HD11	1:A:29:ILE:HD12	0.48	1.84	14	3
1:A:8:PHE:CD1	1:A:22:ASP:HB3	0.48	2.44	6	1
1:A:83:LEU:HB3	1:A:105:ASN:HD21	0.48	1.69	4	1
1:A:86:GLN:HG2	1:A:106:TYR:HE2	0.48	1.69	4	1
2:B:61:PHE:O	2:B:64:VAL:HG12	0.48	2.09	10	12
1:A:85:THR:HA	1:A:104:VAL:O	0.48	2.09	12	2
1:A:8:PHE:HB3	1:A:24:ARG:HB2	0.48	1.85	13	1
2:B:71:VAL:HB	2:B:93:PHE:CD2	0.47	2.44	2	5
2:B:44:ASN:HB3	2:B:46:VAL:HG12	0.47	1.87	16	3
1:A:81:VAL:HG22	1:A:111:ILE:HG12	0.47	1.86	12	1
2:B:68:LYS:HB3	2:B:96:GLN:HE22	0.47	1.68	19	2
1:A:84:GLU:O	1:A:105:ASN:HA	0.47	2.08	3	2
1:A:48:LEU:H	1:A:48:LEU:HD23	0.47	1.70	1	2
2:B:10:THR:HG23	2:B:32:THR:HA	0.47	1.86	9	1
1:A:84:GLU:HB2	1:A:106:TYR:HB2	0.47	1.86	12	2
1:A:6:LYS:HE2	1:A:24:ARG:HG2	0.47	1.87	9	1
1:A:32:HIS:CD2	1:A:35:GLU:HB2	0.47	2.45	9	1
1:A:21:CYS:HB2	1:A:33:PRO:HA	0.47	1.85	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:TYR:OH	2:B:15:ARG:HD2	0.47	2.09	5	1
1:A:70:GLN:HG3	1:A:84:GLU:HG2	0.47	1.86	11	1
2:B:25:VAL:HG12	2:B:26:ASP:H	0.47	1.70	20	1
2:B:53:ASP:HB3	2:B:76:PHE:HB2	0.46	1.87	3	2
1:A:36:LEU:HD23	1:A:44:PHE:HZ	0.46	1.69	5	1
1:A:7:THR:HG23	1:A:106:TYR:HA	0.46	1.88	8	1
1:A:11:ARG:HD3	2:B:13:ILE:HD12	0.46	1.86	14	1
2:B:96:GLN:HG3	2:B:103:ILE:HG12	0.46	1.87	9	1
2:B:14:SER:HB3	2:B:22:PHE:CE2	0.46	2.45	6	4
1:A:84:GLU:HG3	1:A:108:LEU:HD12	0.46	1.86	12	1
1:A:83:LEU:HG	1:A:107:VAL:HG22	0.46	1.87	19	2
2:B:77:ARG:HA	2:B:86:LEU:O	0.46	2.11	4	3
2:B:63:GLN:O	2:B:67:LEU:HG	0.45	2.11	15	2
2:B:92:SER:HA	2:B:108:CYS:HA	0.45	1.88	3	1
1:A:83:LEU:HD21	1:A:107:VAL:HG22	0.45	1.88	2	1
2:B:14:SER:HB2	2:B:108:CYS:HB2	0.45	1.88	15	1
2:B:87:TRP:HB2	2:B:114:LYS:HB3	0.45	1.88	20	2
2:B:87:TRP:HB2	2:B:114:LYS:HB2	0.45	1.88	3	2
1:A:9:LEU:H	1:A:22:ASP:HB2	0.45	1.71	2	1
1:A:83:LEU:HD22	1:A:107:VAL:HG22	0.45	1.89	5	1
1:A:90:ILE:HD11	2:B:71:VAL:HG11	0.45	1.89	20	1
2:B:17:ASN:ND2	2:B:21:ILE:HB	0.45	2.27	4	1
1:A:48:LEU:HG	1:A:49:ASP:N	0.45	2.27	4	1
1:A:95:ASN:HB3	1:A:97:GLN:HG2	0.44	1.88	14	1
1:A:93:PRO:HD2	2:B:111:THR:HG21	0.44	1.89	20	1
2:B:80:SER:HB3	2:B:86:LEU:HD21	0.44	1.88	13	2
1:A:25:ILE:HG23	1:A:31:TYR:O	0.44	2.12	5	1
2:B:9:PRO:HB2	2:B:11:GLU:HG2	0.44	1.90	14	1
1:A:70:GLN:HG2	1:A:84:GLU:CG	0.44	2.43	10	1
2:B:38:GLN:HA	2:B:41:LEU:HD12	0.44	1.89	20	3
1:A:81:VAL:HG13	1:A:111:ILE:HG12	0.44	1.88	18	2
1:A:32:HIS:CD2	1:A:33:PRO:HD2	0.44	2.47	7	1
2:B:92:SER:HA	2:B:107:ILE:O	0.44	2.13	14	1
1:A:41:ALA:O	1:A:45:TYR:HB2	0.44	2.13	10	1
1:A:60:LEU:HD21	1:A:87:GLY:HA3	0.44	1.90	20	1
1:A:108:LEU:HD12	2:B:98:PRO:HB2	0.44	1.90	17	1
2:B:93:PHE:HB3	2:B:107:ILE:HB	0.44	1.90	8	1
1:A:6:LYS:HA	2:B:97:ASN:OD1	0.43	2.12	5	1
2:B:14:SER:HB3	2:B:25:VAL:HA	0.43	1.88	9	1
1:A:83:LEU:HD11	1:A:107:VAL:HG22	0.43	1.90	3	1
1:A:11:ARG:O	1:A:18:PHE:HA	0.43	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:TYR:HA	1:A:37:LEU:CD2	0.43	2.43	1	1
2:B:9:PRO:HD2	2:B:28:ARG:HG2	0.43	1.89	9	2
1:A:36:LEU:O	1:A:39:ARG:HG2	0.43	2.13	20	1
1:A:89:VAL:HG13	1:A:101:ILE:HG12	0.43	1.89	20	1
2:B:29:CYS:HA	2:B:32:THR:OG1	0.43	2.12	2	1
2:B:61:PHE:O	2:B:65:VAL:HG23	0.43	2.13	9	4
2:B:73:SER:HB3	2:B:89:ARG:HD2	0.43	1.90	3	1
2:B:80:SER:HB3	2:B:86:LEU:HD23	0.43	1.90	4	1
1:A:84:GLU:HB2	1:A:106:TYR:CE1	0.43	2.49	18	1
1:A:48:LEU:HD23	1:A:48:LEU:H	0.43	1.72	15	2
2:B:80:SER:OG	2:B:84:GLU:HG2	0.43	2.14	11	2
2:B:79:ARG:HA	2:B:84:GLU:O	0.43	2.14	9	3
1:A:17:LYS:HB2	1:A:39:ARG:O	0.43	2.14	13	1
2:B:12:PHE:HB2	2:B:26:ASP:CB	0.43	2.44	16	5
1:A:18:PHE:HB3	1:A:21:CYS:SG	0.43	2.54	15	1
2:B:65:VAL:O	2:B:68:LYS:HG3	0.43	2.14	6	2
1:A:101:ILE:HG22	1:A:103:CYS:SG	0.43	2.54	9	1
2:B:10:THR:HG21	2:B:112:ASN:HB2	0.43	1.89	12	1
1:A:7:THR:HB	2:B:95:PHE:CZ	0.43	2.49	16	1
2:B:96:GLN:HB3	2:B:103:ILE:HA	0.42	1.91	12	1
1:A:11:ARG:CZ	1:A:100:CYS:HB2	0.42	2.43	8	1
1:A:32:HIS:HB3	1:A:35:GLU:HB2	0.42	1.91	8	1
2:B:22:PHE:HB2	2:B:40:LEU:O	0.42	2.13	3	1
2:B:33:VAL:HG23	2:B:35:TYR:H	0.42	1.74	5	1
1:A:90:ILE:HG22	1:A:100:CYS:HB2	0.42	1.92	14	1
2:B:75:MET:HE3	2:B:87:TRP:HB3	0.42	1.91	17	1
1:A:8:PHE:HB2	1:A:22:ASP:CB	0.42	2.43	13	1
2:B:90:THR:HG22	2:B:108:CYS:HB2	0.42	1.92	3	1
1:A:21:CYS:HB2	1:A:33:PRO:CB	0.42	2.44	19	1
2:B:30:VAL:O	2:B:34:GLY:HA2	0.42	2.14	11	1
2:B:77:ARG:HD2	2:B:85:TRP:HB3	0.42	1.91	8	1
1:A:92:ASN:HD21	1:A:94:ARG:NH2	0.42	2.12	18	1
1:A:67:VAL:HG13	1:A:86:GLN:HB3	0.42	1.91	4	1
1:A:98:PRO:HB2	1:A:101:ILE:HD11	0.42	1.92	17	1
2:B:33:VAL:O	2:B:80:SER:HB2	0.41	2.14	20	1
1:A:93:PRO:HG2	2:B:113:VAL:HA	0.41	1.92	1	1
1:A:89:VAL:HG11	1:A:98:PRO:HB3	0.41	1.93	19	1
1:A:49:ASP:O	1:A:53:MET:HG2	0.41	2.16	16	1
1:A:72:ARG:HA	1:A:81:VAL:O	0.41	2.15	15	1
2:B:13:ILE:CD1	2:B:109:THR:HG23	0.41	2.45	9	1
1:A:87:GLY:HA2	1:A:103:CYS:HA	0.41	1.92	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:ASN:HB2	1:A:97:GLN:HG2	0.41	1.92	3	1
2:B:105:TYR:CE1	2:B:107:ILE:HG23	0.41	2.47	18	1
1:A:8:PHE:HB2	1:A:22:ASP:CG	0.41	2.36	17	1
2:B:114:LYS:HA	2:B:114:LYS:HD3	0.41	1.73	11	1
1:A:11:ARG:HA	1:A:101:ILE:O	0.41	2.16	20	1
2:B:17:ASN:HD21	2:B:21:ILE:HB	0.41	1.75	4	1
2:B:91:SER:O	2:B:108:CYS:HA	0.41	2.16	12	1
1:A:18:PHE:HB2	1:A:36:LEU:O	0.41	2.16	12	1
2:B:50:HIS:CD2	2:B:51:PRO:HD2	0.41	2.51	17	2
2:B:12:PHE:CB	2:B:28:ARG:HB2	0.41	2.44	10	1
1:A:33:PRO:HA	1:A:36:LEU:HD12	0.41	1.93	10	1
2:B:87:TRP:HB2	2:B:114:LYS:CG	0.41	2.46	15	1
1:A:22:ASP:O	1:A:33:PRO:HG3	0.41	2.16	7	1
2:B:11:GLU:CB	2:B:111:THR:HG22	0.40	2.45	13	1
2:B:13:ILE:HG22	2:B:15:ARG:HG3	0.40	1.93	11	1
1:A:104:VAL:HG13	2:B:95:PHE:HE1	0.40	1.75	2	1
2:B:105:TYR:HE1	2:B:107:ILE:HG12	0.40	1.76	12	1
2:B:114:LYS:HE3	2:B:114:LYS:HA	0.40	1.92	8	1
1:A:93:PRO:HA	1:A:96:LEU:HD23	0.40	1.93	7	1
1:A:8:PHE:CE1	1:A:21:CYS:HB2	0.40	2.51	20	1
1:A:108:LEU:HD21	2:B:98:PRO:HG2	0.40	1.92	18	1
1:A:40:SER:HB3	1:A:43:GLU:HG2	0.40	1.92	15	1
2:B:50:HIS:HB2	2:B:77:ARG:O	0.40	2.17	1	1
2:B:16:HIS:HD2	2:B:108:CYS:SG	0.40	2.39	14	1
2:B:22:PHE:HB3	2:B:25:VAL:HG22	0.40	1.94	16	1
2:B:58:ARG:O	2:B:62:GLN:HG2	0.40	2.17	3	1
1:A:99:GLN:HG2	1:A:100:CYS:SG	0.40	2.56	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	105/107 (98%)	94±3 (90±2%)	10±3 (9±3%)	1±1 (1±1%)	26	73
2	B	106/108 (98%)	100±2 (94±2%)	6±2 (5±2%)	1±0 (1±0%)	29	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4220/4300 (98%)	3878 (92%)	305 (7%)	37 (1%)	26 73

All 5 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	68	LYS	17
1	A	77	HIS	11
1	A	46	HIS	6
1	A	14	MET	2
2	B	113	VAL	1

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	97/97 (100%)	84±3 (87±3%)	13±3 (13±3%)	9 50
2	B	103/103 (100%)	94±2 (91±2%)	9±2 (9±2%)	16 61
All	All	4000/4000 (100%)	3557 (89%)	443 (11%)	12 55

All 93 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)
2	B	10	THR	20
2	B	94	THR	20
1	A	45	TYR	20
1	A	19	THR	18
1	A	62	THR	16
2	B	57	LEU	15
1	A	26	THR	15
2	B	111	THR	13
1	A	55	LYS	11
2	B	23	THR	10
2	B	86	LEU	10
2	B	96	GLN	10

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Mol	Chain	Res	Type	Models (Total)
1	A	40	SER	10
1	A	49	ASP	10
2	B	114	LYS	9
2	B	100	SER	9
1	A	53	MET	9
1	A	35	GLU	8
2	B	102	GLU	8
1	A	7	THR	8
1	A	21	CYS	8
1	A	48	LEU	7
1	A	81	VAL	7
1	A	17	LYS	7
1	A	110	GLU	7
1	A	46	HIS	7
2	B	107	ILE	6
1	A	32	HIS	6
2	B	11	GLU	6
1	A	50	SER	5
1	A	11	ARG	5
1	A	71	TYR	5
1	A	23	ASP	5
2	B	14	SER	4
1	A	99	GLN	4
1	A	9	LEU	4
2	B	32	THR	4
2	B	109	THR	4
1	A	54	THR	4
2	B	13	ILE	4
1	A	83	LEU	3
1	A	52	ASN	3
1	A	94	ARG	3
1	A	31	TYR	3
1	A	95	ASN	3
1	A	16	MET	3
2	B	80	SER	3
2	B	28	ARG	3
1	A	39	ARG	2
2	B	8	GLN	2
2	B	95	PHE	2
2	B	90	THR	2
1	A	100	CYS	2
1	A	105	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	15	ASP	2
2	B	7	CYS	2
2	B	27	HIS	2
2	B	97	ASN	2
1	A	88	THR	2
2	B	93	PHE	2
2	B	15	ARG	2
1	A	68	SER	2
1	A	109	SER	2
1	A	13	SER	2
1	A	108	LEU	1
1	A	36	LEU	1
2	B	112	ASN	1
1	A	51	GLU	1
2	B	64	VAL	1
2	B	104	GLU	1
1	A	22	ASP	1
1	A	102	MET	1
2	B	25	VAL	1
1	A	20	TYR	1
1	A	44	PHE	1
1	A	34	GLU	1
1	A	8	PHE	1
2	B	89	ARG	1
1	A	106	TYR	1
2	B	113	VAL	1
2	B	91	SER	1
2	B	29	CYS	1
1	A	24	ARG	1
1	A	18	PHE	1
2	B	24	PHE	1
1	A	14	MET	1
1	A	104	VAL	1
2	B	77	ARG	1
2	B	16	HIS	1
2	B	61	PHE	1
2	B	83	GLN	1
1	A	10	SER	1
2	B	35	TYR	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 carbohydrates 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](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided