



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 07:51 PM BST

PDB ID : 2DJY
Title : Solution structure of Smurf2 WW3 domain-Smad7 PY peptide complex
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Deposited on : 2006-04-06

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

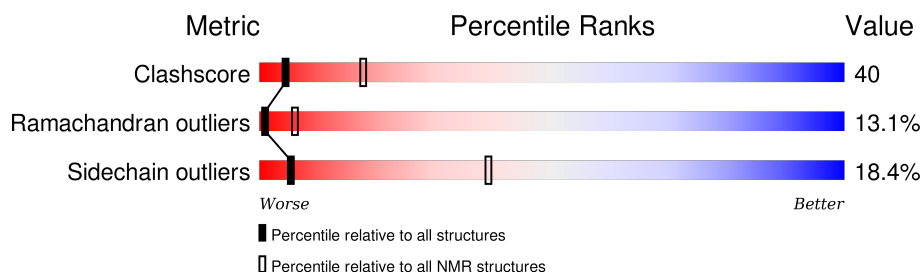
1 Overall quality at a glance

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	42	
2	B	20	

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:299-A:330, B:208-B:217 (42)	0.23	1

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 5 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 2, 5, 7, 12, 13, 15, 16, 19, 20, 22, 29
2	17, 18, 24, 26, 27
3	6, 10, 11, 14
4	25, 30
5	8, 9
Single-model clusters	3; 4; 21; 23; 28

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 852 atoms, of which 371 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Smad ubiquitination regulatory factor 2.

Mol	Chain	Residues	Atoms					Trace
1	A	42	Total	C	H	N	O	0
			590	203	263	62	62	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	GLY	-	CLONING ARTIFACT	UNP Q9HAU4
A	293	PRO	-	CLONING ARTIFACT	UNP Q9HAU4
A	294	LEU	-	CLONING ARTIFACT	UNP Q9HAU4
A	295	GLY	-	CLONING ARTIFACT	UNP Q9HAU4
A	296	SER	-	CLONING ARTIFACT	UNP Q9HAU4

- Molecule 2 is a protein called Mothers against decapentaplegic homolog 7.

Mol	Chain	Residues	Atoms						Trace
2	B	20	Total	C	H	N	O	S	0
			262	98	108	23	32	1	

There are 5 discrepancies between the modelled and reference sequences:

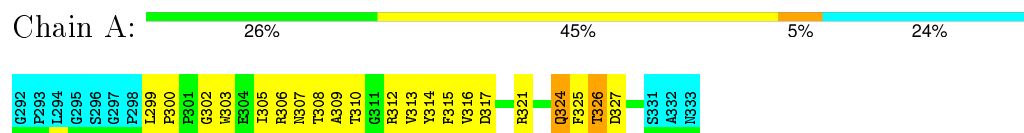
Chain	Residue	Modelled	Actual	Comment	Reference
B	198	GLY	-	CLONING ARTIFACT	UNP O15105
B	199	PRO	-	CLONING ARTIFACT	UNP O15105
B	200	LEU	-	CLONING ARTIFACT	UNP O15105
B	201	GLY	-	CLONING ARTIFACT	UNP O15105
B	202	SER	-	CLONING ARTIFACT	UNP O15105

4 Residue-property plots [i](#)

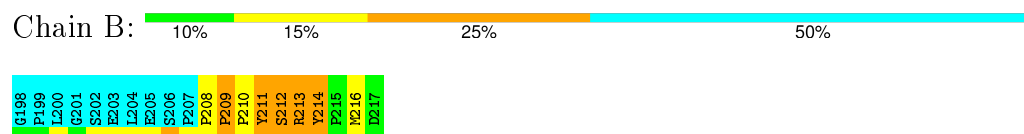
4.1 Average score per residue in the NMR ensemble

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: Smad ubiquitination regulatory factor 2



- Molecule 2: Mothers against decapentaplegic homolog 7

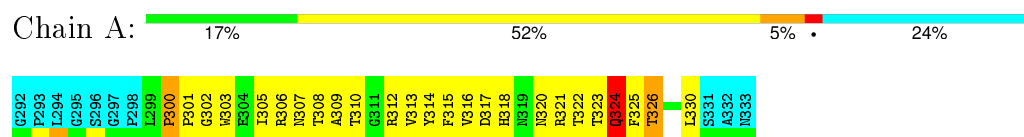


4.2 Scores per residue for each member of the ensemble

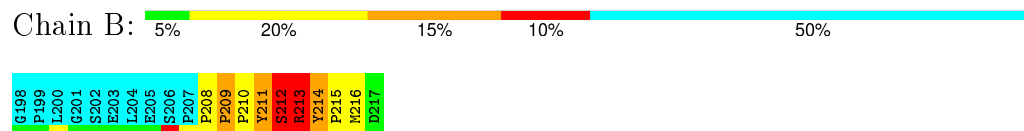
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Smad ubiquitination regulatory factor 2

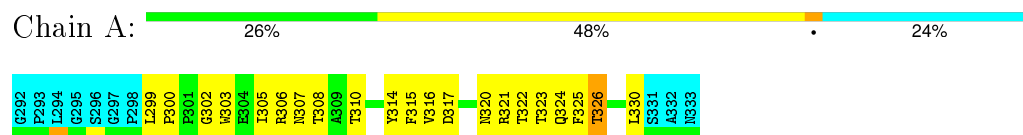


- Molecule 2: Mothers against decapentaplegic homolog 7

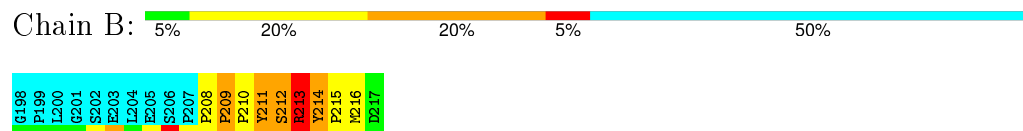


4.2.2 Score per residue for model 2

- Molecule 1: Smad ubiquitination regulatory factor 2

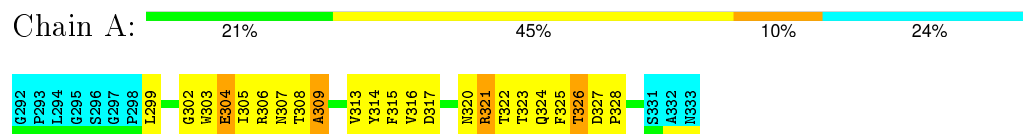


- Molecule 2: Mothers against decapentaplegic homolog 7

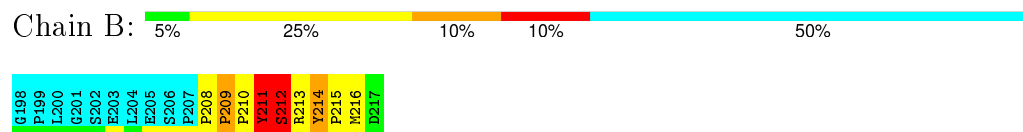


4.2.3 Score per residue for model 3

- Molecule 1: Smad ubiquitination regulatory factor 2

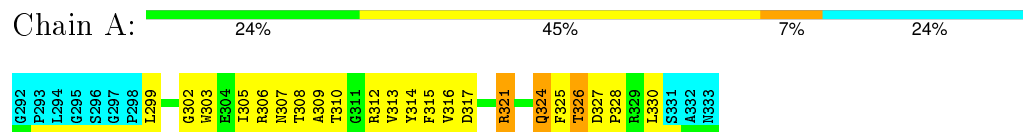


- Molecule 2: Mothers against decapentaplegic homolog 7

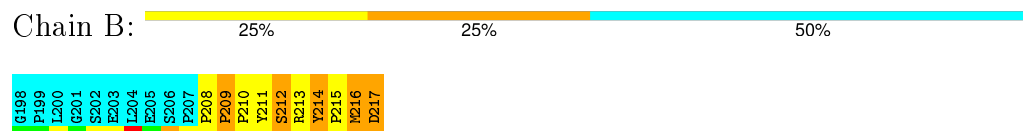


4.2.4 Score per residue for model 4

- Molecule 1: Smad ubiquitination regulatory factor 2

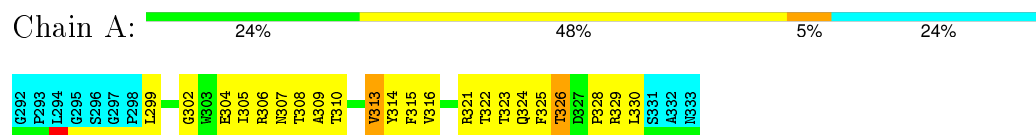


- Molecule 2: Mothers against decapentaplegic homolog 7

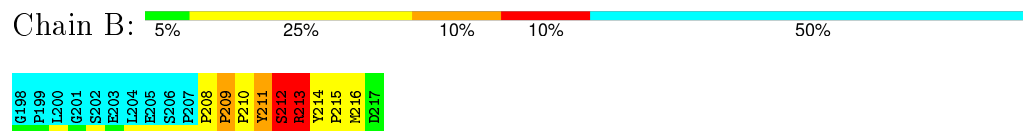


4.2.5 Score per residue for model 5

- Molecule 1: Smad ubiquitination regulatory factor 2

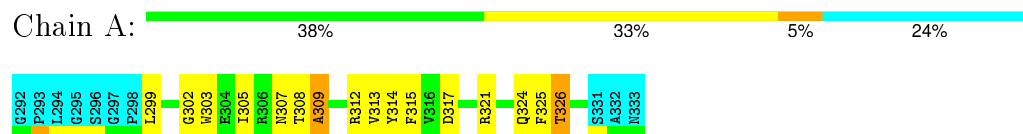


- Molecule 2: Mothers against decapentaplegic homolog 7

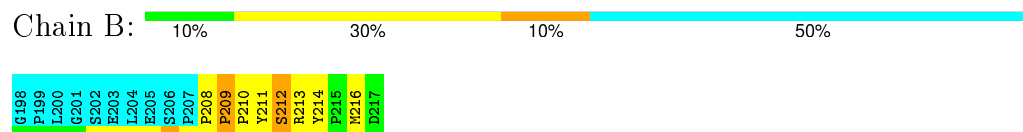


4.2.6 Score per residue for model 6

- Molecule 1: Smad ubiquitination regulatory factor 2

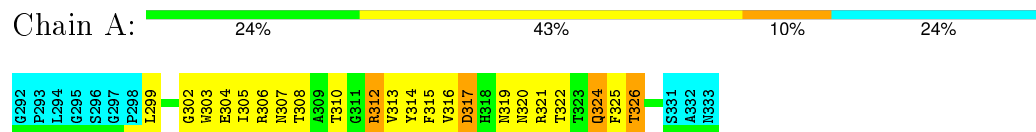


- Molecule 2: Mothers against decapentaplegic homolog 7

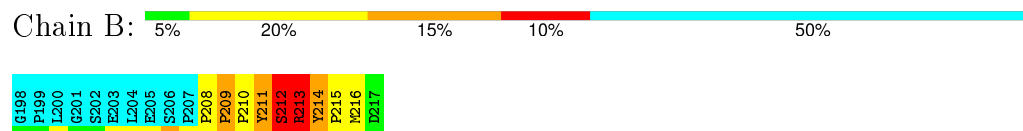


4.2.7 Score per residue for model 7

- Molecule 1: Smad ubiquitination regulatory factor 2

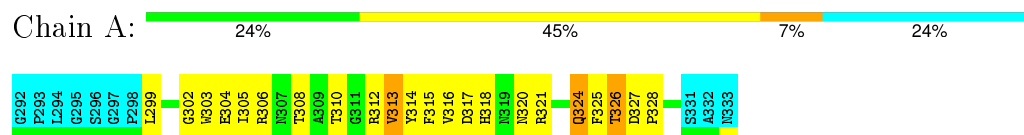


- Molecule 2: Mothers against decapentaplegic homolog 7

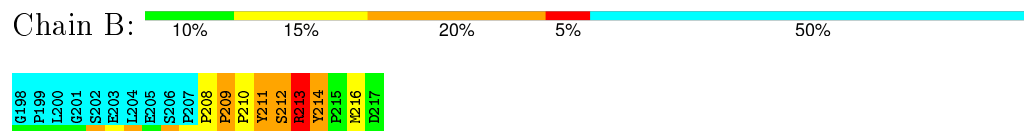


4.2.8 Score per residue for model 8

- Molecule 1: Smad ubiquitination regulatory factor 2

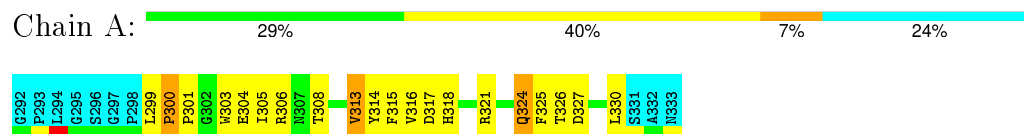


- Molecule 2: Mothers against decapentaplegic homolog 7

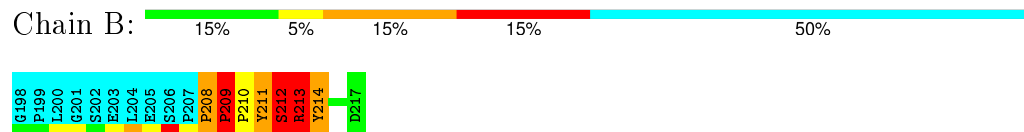


4.2.9 Score per residue for model 9

- Molecule 1: Smad ubiquitination regulatory factor 2

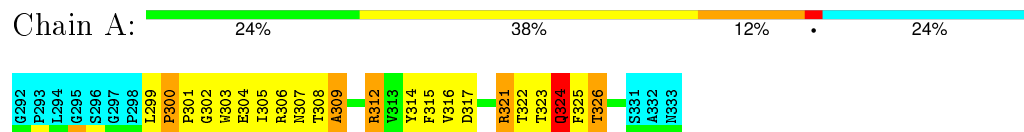


- Molecule 2: Mothers against decapentaplegic homolog 7

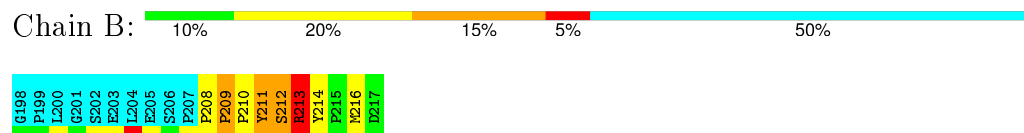


4.2.10 Score per residue for model 10

- Molecule 1: Smad ubiquitination regulatory factor 2

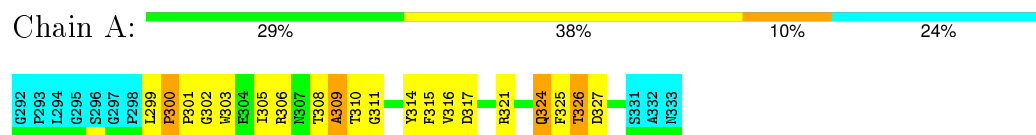


- Molecule 2: Mothers against decapentaplegic homolog 7

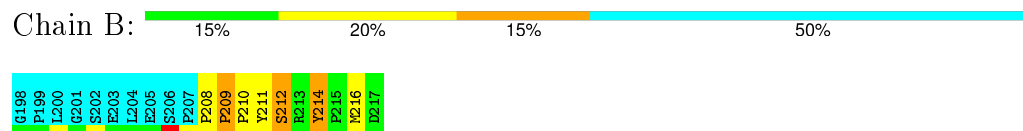


4.2.11 Score per residue for model 11

- Molecule 1: Smad ubiquitination regulatory factor 2

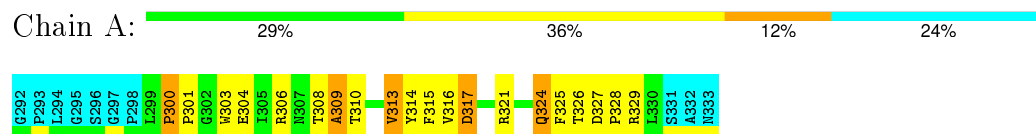


- Molecule 2: Mothers against decapentaplegic homolog 7

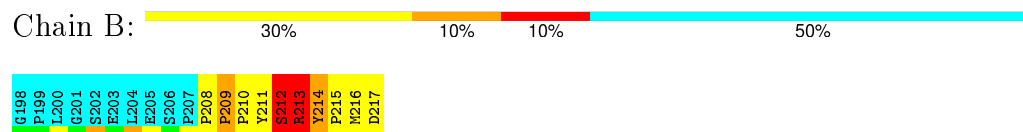


4.2.12 Score per residue for model 12

- Molecule 1: Smad ubiquitination regulatory factor 2

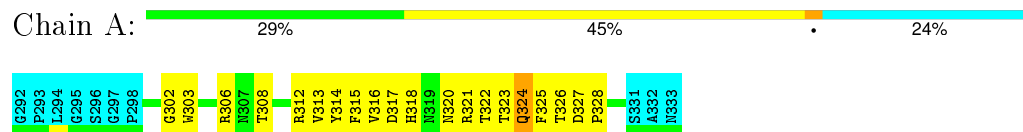


- Molecule 2: Mothers against decapentaplegic homolog 7

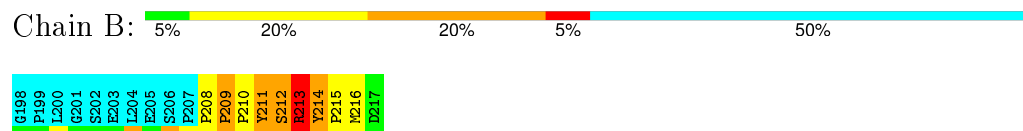


4.2.13 Score per residue for model 13

- Molecule 1: Smad ubiquitination regulatory factor 2

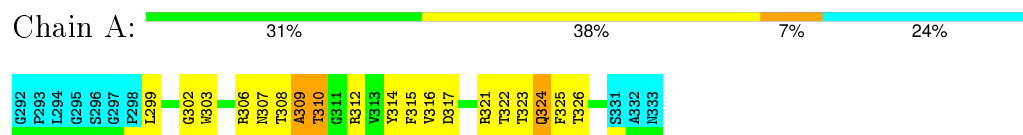


- Molecule 2: Mothers against decapentaplegic homolog 7

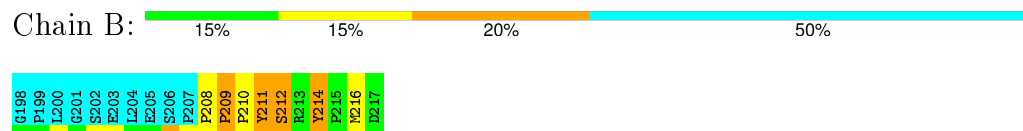


4.2.14 Score per residue for model 14

- Molecule 1: Smad ubiquitination regulatory factor 2

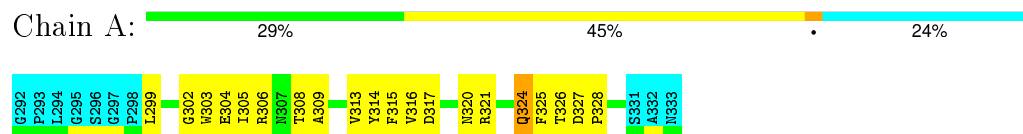


- Molecule 2: Mothers against decapentaplegic homolog 7

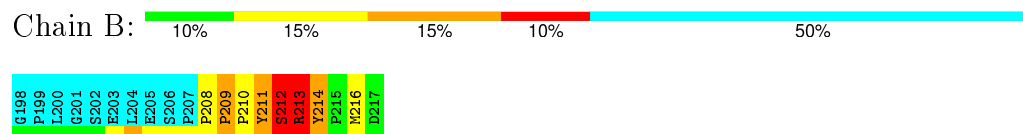


4.2.15 Score per residue for model 15

- Molecule 1: Smad ubiquitination regulatory factor 2

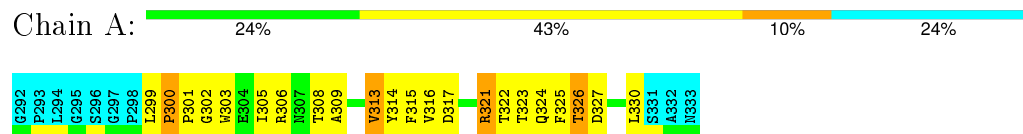


- Molecule 2: Mothers against decapentaplegic homolog 7

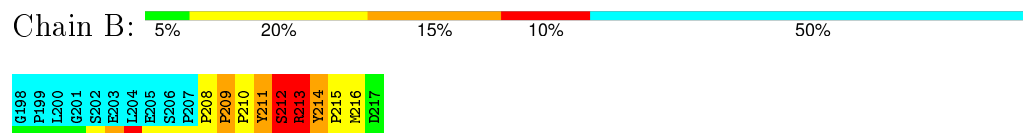


4.2.16 Score per residue for model 16

- Molecule 1: Smad ubiquitination regulatory factor 2

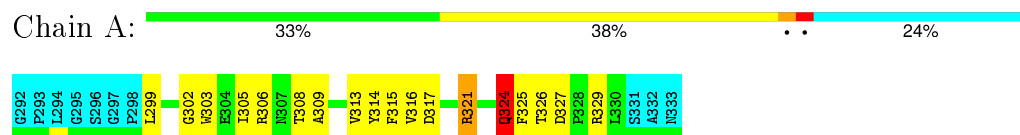


- Molecule 2: Mothers against decapentaplegic homolog 7

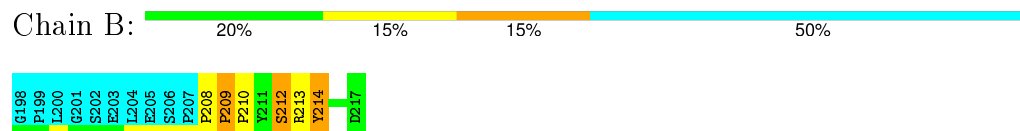


4.2.17 Score per residue for model 17

- Molecule 1: Smad ubiquitination regulatory factor 2

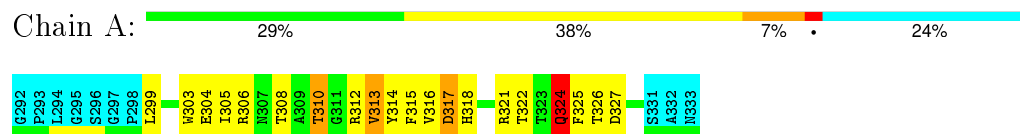


- Molecule 2: Mothers against decapentaplegic homolog 7

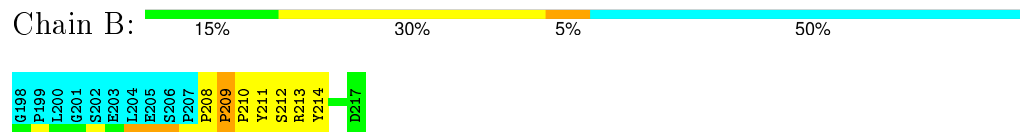


4.2.18 Score per residue for model 18

- Molecule 1: Smad ubiquitination regulatory factor 2

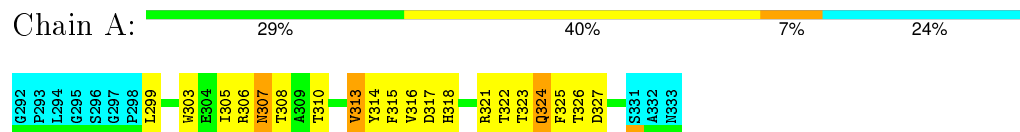


- Molecule 2: Mothers against decapentaplegic homolog 7

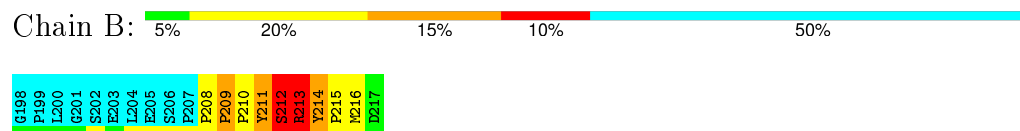


4.2.19 Score per residue for model 19

- Molecule 1: Smad ubiquitination regulatory factor 2

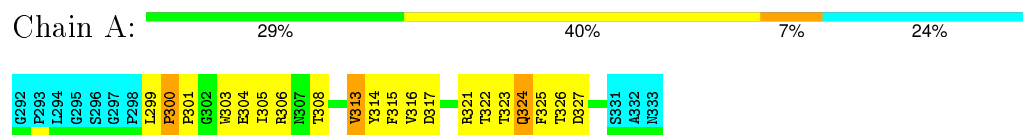


- Molecule 2: Mothers against decapentaplegic homolog 7

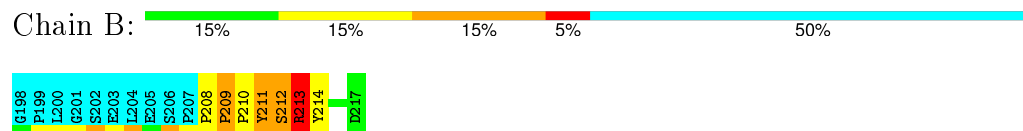


4.2.20 Score per residue for model 20

- Molecule 1: Smad ubiquitination regulatory factor 2

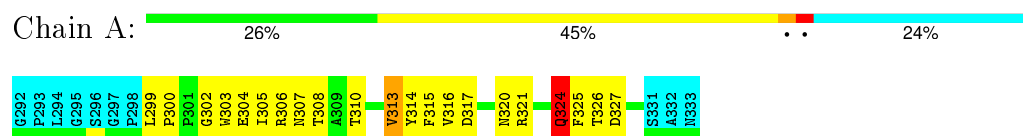


- Molecule 2: Mothers against decapentaplegic homolog 7

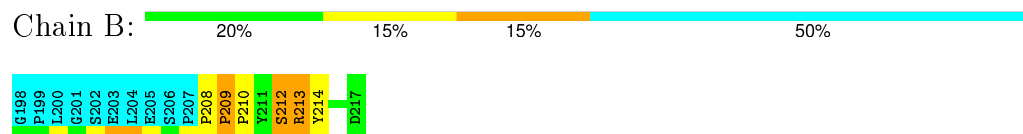


4.2.21 Score per residue for model 21

- Molecule 1: Smad ubiquitination regulatory factor 2

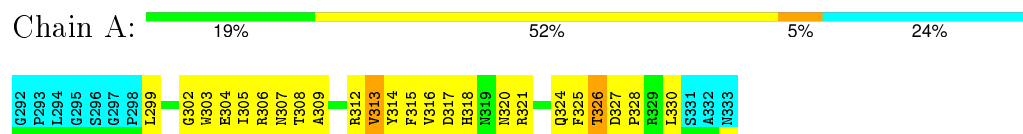


- Molecule 2: Mothers against decapentaplegic homolog 7

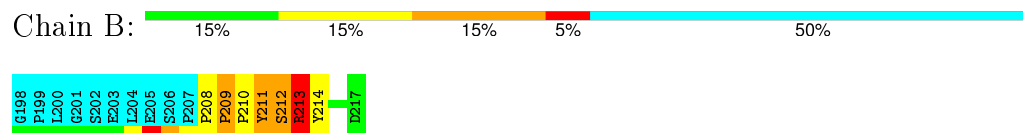


4.2.22 Score per residue for model 22

- Molecule 1: Smad ubiquitination regulatory factor 2

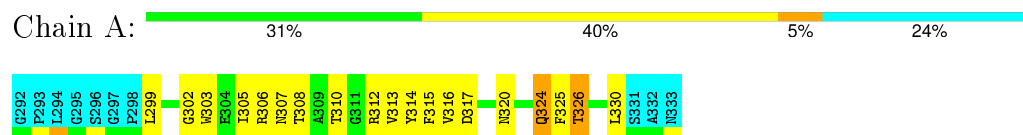


- Molecule 2: Mothers against decapentaplegic homolog 7

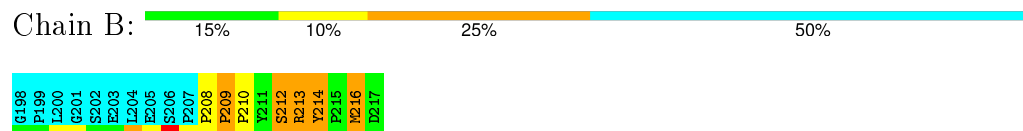


4.2.23 Score per residue for model 23

- Molecule 1: Smad ubiquitination regulatory factor 2

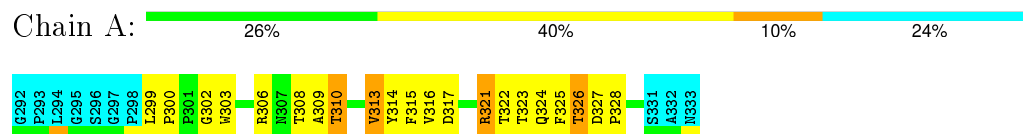


- Molecule 2: Mothers against decapentaplegic homolog 7

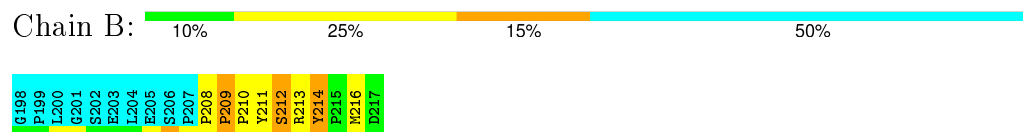


4.2.24 Score per residue for model 24

- Molecule 1: Smad ubiquitination regulatory factor 2

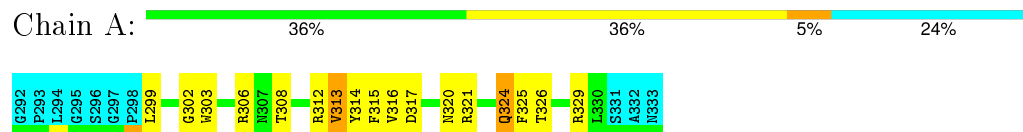


- Molecule 2: Mothers against decapentaplegic homolog 7

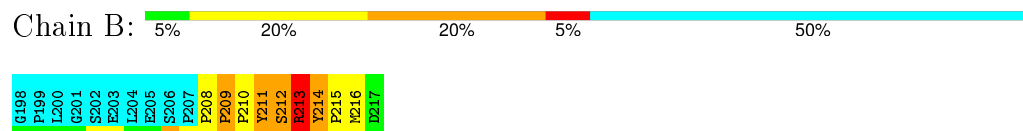


4.2.25 Score per residue for model 25

- Molecule 1: Smad ubiquitination regulatory factor 2

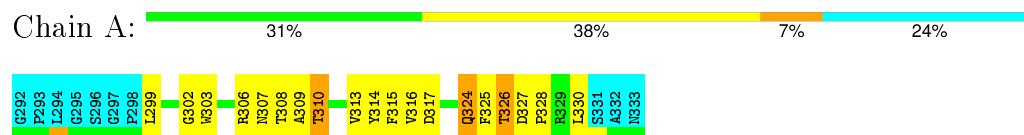


- Molecule 2: Mothers against decapentaplegic homolog 7

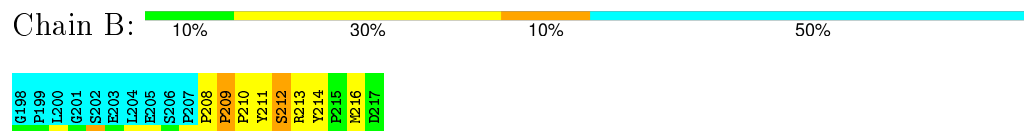


4.2.26 Score per residue for model 26

- Molecule 1: Smad ubiquitination regulatory factor 2

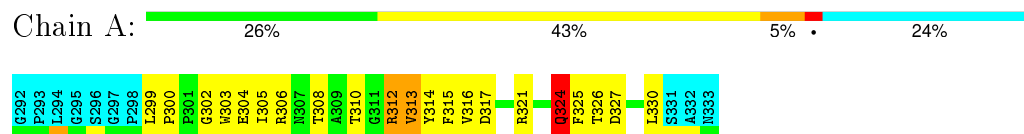


- Molecule 2: Mothers against decapentaplegic homolog 7

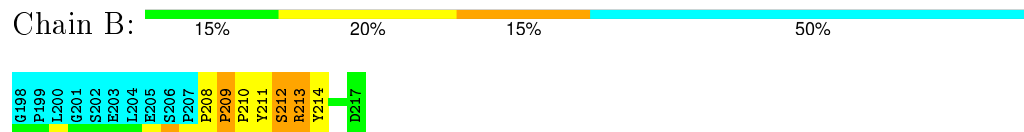


4.2.27 Score per residue for model 27

- Molecule 1: Smad ubiquitination regulatory factor 2

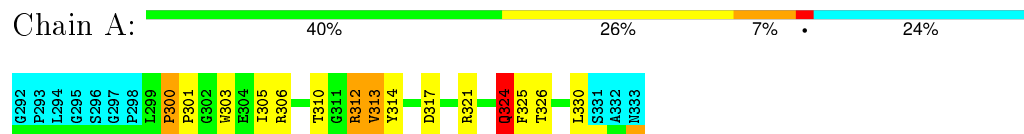


- Molecule 2: Mothers against decapentaplegic homolog 7

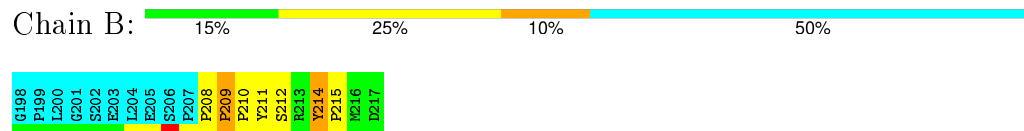


4.2.28 Score per residue for model 28

- Molecule 1: Smad ubiquitination regulatory factor 2

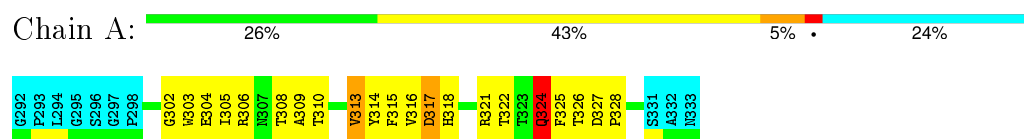


- Molecule 2: Mothers against decapentaplegic homolog 7

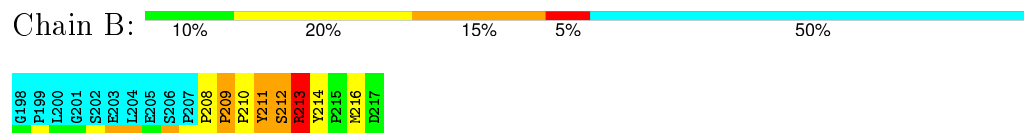


4.2.29 Score per residue for model 29

- Molecule 1: Smad ubiquitination regulatory factor 2

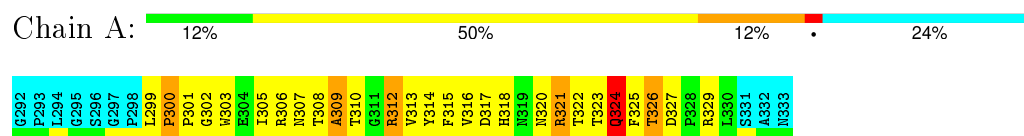


- Molecule 2: Mothers against decapentaplegic homolog 7

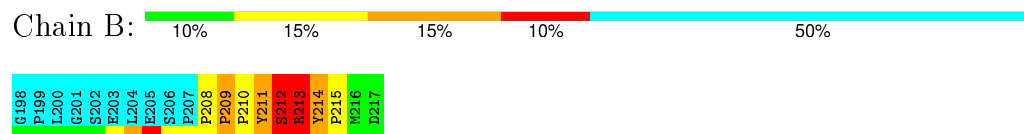


4.2.30 Score per residue for model 30

- Molecule 1: Smad ubiquitination regulatory factor 2



- Molecule 2: Mothers against decapentaplegic homolog 7



5 Refinement protocol and experimental data overview

Of the 200 calculated structures, 30 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	refinement	1.2

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	267	216	254	20±4
2	B	86	56	77	14±2
All	All	10590	8160	9930	823

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:306:ARG:CZ	1:A:316:VAL:HG21	0.81	2.06	21	4
1:A:308:THR:HG22	2:B:209:PRO:HG3	0.72	1.61	19	4
1:A:306:ARG:HD2	1:A:316:VAL:HG21	0.69	1.63	26	6
1:A:299:LEU:HD11	1:A:305:ILE:HG13	0.68	1.64	18	9
1:A:308:THR:HG22	2:B:209:PRO:CD	0.68	2.19	29	24
1:A:306:ARG:NH1	1:A:316:VAL:HG21	0.66	2.05	21	4
1:A:306:ARG:O	1:A:313:VAL:HG12	0.62	1.94	25	9
1:A:299:LEU:HD21	1:A:315:PHE:CE2	0.61	2.30	6	17
1:A:308:THR:HG22	2:B:209:PRO:HD3	0.61	1.71	29	15
1:A:305:ILE:HG23	1:A:313:VAL:CG2	0.60	2.27	23	6
1:A:314:TYR:CE2	1:A:316:VAL:HG22	0.59	2.33	2	23
1:A:299:LEU:HD21	1:A:315:PHE:HE2	0.58	1.59	23	13
1:A:314:TYR:CZ	2:B:209:PRO:HG2	0.57	2.35	27	30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:299:LEU:HD11	1:A:305:ILE:CG1	0.57	2.29	30	11
1:A:317:ASP:N	1:A:317:ASP:OD1	0.55	2.39	7	2
2:B:214:TYR:CD1	2:B:214:TYR:N	0.55	2.73	24	18
2:B:214:TYR:N	2:B:214:TYR:CD1	0.55	2.73	23	12
1:A:314:TYR:CE1	2:B:209:PRO:HG2	0.55	2.36	16	3
1:A:306:ARG:O	1:A:313:VAL:HG23	0.55	2.01	3	2
1:A:299:LEU:HD12	1:A:304:GLU:HA	0.53	1.78	18	8
1:A:317:ASP:OD1	1:A:317:ASP:N	0.53	2.42	18	1
1:A:305:ILE:CD1	1:A:315:PHE:CE2	0.53	2.91	3	1
1:A:306:ARG:NH1	1:A:316:VAL:HG11	0.52	2.20	17	2
2:B:209:PRO:HB2	2:B:210:PRO:CD	0.51	2.36	19	25
1:A:308:THR:CG2	2:B:209:PRO:CD	0.50	2.89	22	11
2:B:209:PRO:CB	2:B:210:PRO:CD	0.50	2.90	27	30
2:B:212:SER:O	2:B:213:ARG:CB	0.50	2.59	21	14
1:A:308:THR:HG22	2:B:209:PRO:CG	0.50	2.36	27	6
1:A:313:VAL:O	1:A:325:PHE:CE1	0.49	2.66	19	6
1:A:303:TRP:CZ3	1:A:324:GLN:OE1	0.49	2.66	21	16
1:A:303:TRP:CH2	1:A:317:ASP:OD2	0.49	2.66	7	4
1:A:318:HIS:CE1	2:B:213:ARG:CD	0.49	2.96	13	2
1:A:306:ARG:O	1:A:314:TYR:CD1	0.49	2.66	9	6
1:A:313:VAL:O	1:A:325:PHE:CD1	0.49	2.66	29	9
1:A:300:PRO:CB	1:A:301:PRO:CD	0.48	2.92	20	9
2:B:212:SER:O	2:B:213:ARG:CG	0.48	2.61	20	17
1:A:303:TRP:CZ2	1:A:317:ASP:OD2	0.48	2.66	10	17
1:A:315:PHE:CD1	1:A:326:THR:O	0.48	2.67	7	13
2:B:211:TYR:CG	2:B:212:SER:N	0.48	2.80	3	1
1:A:315:PHE:CE2	1:A:327:ASP:OD1	0.48	2.67	26	2
1:A:316:VAL:HG12	2:B:211:TYR:CD1	0.48	2.44	20	1
1:A:315:PHE:CG	1:A:326:THR:O	0.47	2.67	24	3
1:A:315:PHE:N	1:A:315:PHE:CD1	0.47	2.82	19	4
1:A:314:TYR:CE2	2:B:209:PRO:HG2	0.47	2.44	24	17
1:A:303:TRP:CE2	1:A:317:ASP:OD1	0.47	2.68	8	4
1:A:305:ILE:HG22	1:A:306:ARG:N	0.47	2.25	4	3
1:A:317:ASP:OD1	1:A:322:THR:HG22	0.47	2.09	29	1
1:A:314:TYR:CG	2:B:209:PRO:HD2	0.46	2.45	27	3
1:A:318:HIS:CE1	2:B:213:ARG:HD2	0.46	2.44	13	2
1:A:306:ARG:CZ	1:A:316:VAL:CG2	0.46	2.91	23	3
2:B:214:TYR:CB	2:B:215:PRO:CD	0.46	2.92	25	3
1:A:315:PHE:CZ	1:A:327:ASP:CB	0.46	2.99	4	2
1:A:315:PHE:CD1	1:A:315:PHE:N	0.46	2.84	18	4
2:B:208:PRO:O	2:B:209:PRO:O	0.46	2.34	9	27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:325:PHE:CD1	2:B:208:PRO:HG3	0.46	2.46	29	30
1:A:312:ARG:HD3	1:A:325:PHE:CE2	0.46	2.46	4	3
1:A:308:THR:O	1:A:310:THR:HG22	0.46	2.11	18	1
1:A:317:ASP:OD2	1:A:322:THR:HG22	0.46	2.11	29	1
1:A:306:ARG:HB3	1:A:314:TYR:CE1	0.45	2.47	27	2
1:A:305:ILE:HD11	1:A:315:PHE:CE2	0.45	2.46	3	1
2:B:212:SER:O	2:B:214:TYR:N	0.45	2.49	18	9
1:A:312:ARG:CD	1:A:325:PHE:CE2	0.45	2.99	4	1
1:A:308:THR:O	1:A:309:ALA:HB3	0.44	2.13	15	6
1:A:308:THR:O	1:A:309:ALA:HB2	0.44	2.12	30	7
1:A:312:ARG:NE	1:A:325:PHE:CE2	0.44	2.85	27	1
1:A:312:ARG:CZ	1:A:313:VAL:HG23	0.44	2.42	28	1
1:A:299:LEU:HD11	1:A:305:ILE:HG12	0.44	1.87	3	1
2:B:211:TYR:O	2:B:213:ARG:N	0.44	2.51	20	17
2:B:214:TYR:HB3	2:B:215:PRO:CD	0.44	2.42	25	11
1:A:318:HIS:CE1	2:B:213:ARG:HD3	0.44	2.48	9	7
1:A:305:ILE:CG2	1:A:313:VAL:CG2	0.44	2.96	6	2
1:A:303:TRP:CZ2	1:A:317:ASP:CG	0.44	2.92	9	17
1:A:303:TRP:CE2	1:A:317:ASP:CG	0.44	2.92	14	2
1:A:321:ARG:HD2	2:B:211:TYR:CE2	0.44	2.48	29	3
2:B:212:SER:OG	2:B:213:ARG:N	0.43	2.51	20	1
2:B:216:MET:O	2:B:216:MET:CG	0.43	2.66	7	5
1:A:307:ASN:OD1	1:A:313:VAL:N	0.43	2.51	21	3
1:A:317:ASP:O	1:A:321:ARG:N	0.43	2.52	20	4
1:A:314:TYR:CE2	1:A:316:VAL:CG2	0.43	3.02	2	1
1:A:317:ASP:OD2	1:A:320:ASN:ND2	0.43	2.52	8	11
1:A:306:ARG:NH1	2:B:213:ARG:O	0.43	2.51	24	3
1:A:303:TRP:CH2	1:A:317:ASP:CG	0.43	2.92	28	1
1:A:306:ARG:CZ	2:B:213:ARG:O	0.43	2.67	18	4
2:B:212:SER:O	2:B:213:ARG:HB2	0.43	2.13	4	1
1:A:317:ASP:OD2	1:A:322:THR:CG2	0.43	2.67	29	1
1:A:315:PHE:CE2	1:A:327:ASP:CG	0.43	2.92	30	10
1:A:326:THR:HG22	1:A:330:LEU:HD12	0.43	1.89	5	1
1:A:317:ASP:OD1	1:A:322:THR:N	0.43	2.52	29	1
2:B:209:PRO:HB2	2:B:210:PRO:HD2	0.43	1.89	16	6
1:A:305:ILE:O	1:A:306:ARG:CG	0.43	2.67	28	9
1:A:314:TYR:HB3	1:A:325:PHE:CE1	0.43	2.48	9	2
2:B:209:PRO:HB3	2:B:216:MET:O	0.43	2.13	8	3
2:B:216:MET:CG	2:B:216:MET:O	0.43	2.66	5	4
1:A:303:TRP:CZ3	1:A:317:ASP:CG	0.43	2.92	12	2
1:A:315:PHE:CZ	1:A:327:ASP:CG	0.43	2.92	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:299:LEU:HD12	1:A:304:GLU:CA	0.43	2.43	3	2
2:B:214:TYR:O	2:B:216:MET:CE	0.43	2.67	10	10
1:A:319:ASN:OD1	1:A:320:ASN:N	0.43	2.52	7	1
1:A:305:ILE:CG2	1:A:306:ARG:N	0.43	2.82	4	1
2:B:211:TYR:C	2:B:211:TYR:CD1	0.42	2.92	3	1
1:A:315:PHE:CD2	1:A:328:PRO:HD2	0.42	2.49	8	5
2:B:211:TYR:CD2	2:B:212:SER:N	0.42	2.87	29	2
1:A:308:THR:O	1:A:310:THR:N	0.42	2.52	2	7
1:A:327:ASP:OD2	1:A:329:ARG:NE	0.42	2.52	12	1
1:A:321:ARG:HA	2:B:211:TYR:CD1	0.42	2.50	20	1
1:A:327:ASP:OD2	1:A:329:ARG:CZ	0.42	2.67	17	1
1:A:306:ARG:NH2	2:B:213:ARG:O	0.42	2.52	9	3
1:A:304:GLU:OE2	1:A:306:ARG:NH2	0.42	2.52	29	3
1:A:299:LEU:HD22	1:A:328:PRO:HG2	0.42	1.91	26	1
1:A:300:PRO:CB	1:A:301:PRO:HD2	0.42	2.44	12	7
1:A:299:LEU:CD2	1:A:327:ASP:OD1	0.42	2.68	19	2
1:A:309:ALA:CB	2:B:217:ASP:O	0.42	2.67	4	1
1:A:317:ASP:CG	1:A:322:THR:HG23	0.42	2.34	18	1
1:A:314:TYR:HB3	1:A:325:PHE:CD1	0.42	2.50	17	3
1:A:304:GLU:OE2	1:A:306:ARG:CZ	0.42	2.68	12	3
1:A:303:TRP:CG	1:A:328:PRO:HG3	0.42	2.50	24	4
1:A:321:ARG:HB3	2:B:211:TYR:CD2	0.42	2.50	3	6
1:A:303:TRP:CE3	1:A:317:ASP:HB3	0.42	2.49	29	1
1:A:322:THR:OG1	1:A:323:THR:N	0.42	2.53	2	12
1:A:315:PHE:CZ	1:A:327:ASP:HB2	0.42	2.50	30	8
1:A:304:GLU:OE1	1:A:306:ARG:NH2	0.42	2.53	8	1
1:A:315:PHE:CE2	1:A:327:ASP:HA	0.42	2.50	3	2
2:B:209:PRO:CB	2:B:216:MET:O	0.41	2.67	23	2
1:A:303:TRP:CZ3	1:A:317:ASP:HB2	0.41	2.51	20	3
1:A:299:LEU:HD23	1:A:329:ARG:CD	0.41	2.45	30	1
2:B:211:TYR:CE1	2:B:212:SER:O	0.41	2.74	3	1
2:B:212:SER:OG	2:B:216:MET:CE	0.41	2.69	23	1
1:A:303:TRP:CD2	1:A:328:PRO:HG3	0.41	2.51	13	4
1:A:306:ARG:NE	2:B:213:ARG:O	0.41	2.53	9	1
1:A:304:GLU:OE2	1:A:306:ARG:NH1	0.41	2.53	10	1
2:B:208:PRO:HA	2:B:209:PRO:HD2	0.41	1.80	24	6
1:A:321:ARG:HD2	2:B:211:TYR:CZ	0.41	2.51	20	1
1:A:318:HIS:CE1	2:B:213:ARG:NE	0.41	2.89	13	1
1:A:307:ASN:N	1:A:307:ASN:OD1	0.41	2.54	19	1
1:A:306:ARG:CZ	2:B:214:TYR:O	0.41	2.69	23	1
1:A:312:ARG:HD2	1:A:325:PHE:CE2	0.41	2.50	28	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:309:ALA:HB3	2:B:217:ASP:O	0.41	2.15	4	1
1:A:321:ARG:HA	2:B:211:TYR:CD2	0.41	2.50	4	1
1:A:309:ALA:O	1:A:310:THR:CB	0.41	2.69	30	1
1:A:299:LEU:HD21	1:A:327:ASP:OD1	0.41	2.15	24	1
1:A:325:PHE:CE1	2:B:208:PRO:HA	0.41	2.51	14	7
1:A:306:ARG:NE	1:A:314:TYR:OH	0.41	2.50	24	1
2:B:214:TYR:HB3	2:B:215:PRO:HD2	0.40	1.93	5	2
2:B:217:ASP:N	2:B:217:ASP:OD1	0.40	2.54	12	1
2:B:211:TYR:O	2:B:211:TYR:CG	0.40	2.73	4	1
2:B:214:TYR:O	2:B:216:MET:HE3	0.40	2.16	3	1
1:A:306:ARG:CB	1:A:314:TYR:CZ	0.40	3.05	27	1
1:A:327:ASP:O	1:A:330:LEU:N	0.40	2.52	22	1
1:A:308:THR:CG2	2:B:209:PRO:HD3	0.40	2.44	6	1
1:A:303:TRP:CZ3	1:A:317:ASP:HB3	0.40	2.51	29	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	32/42 (76%)	23±2 (72±5%)	7±2 (20±7%)	2±1 (7±4%)	3	17
2	B	9/20 (45%)	3±1 (33±7%)	3±1 (33±16%)	3±1 (34±13%)	0	0
All	All	1230/1860 (66%)	785 (64%)	284 (23%)	161 (13%)	1	6

All 13 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	209	PRO	29
2	B	211	TYR	25
1	A	302	GLY	24
2	B	212	SER	19
2	B	213	ARG	19
1	A	324	GLN	16
1	A	300	PRO	13

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Mol	Chain	Res	Type	Models (Total)
1	A	309	ALA	10
1	A	330	LEU	2
1	A	312	ARG	1
1	A	311	GLY	1
1	A	310	THR	1
2	B	208	PRO	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	29/35 (83%)	24±1 (83±4%)	5±1 (17±4%)	6	42
2	B	10/18 (56%)	8±1 (77±11%)	2±1 (23±11%)	3	30
All	All	1170/1590 (74%)	955 (82%)	215 (18%)	5	39

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	326	THR	30
1	A	324	GLN	30
1	A	321	ARG	23
2	B	213	ARG	22
2	B	212	SER	20
2	B	214	TYR	20
1	A	313	VAL	17
1	A	310	THR	14
1	A	312	ARG	13
1	A	307	ASN	12
1	A	317	ASP	4
2	B	216	MET	3
1	A	304	GLU	2
2	B	209	PRO	2
1	A	322	THR	1
2	B	211	TYR	1
2	B	217	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 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