



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 08:25 pm BST

PDB ID : 1QLC
Title : Solution structure of the second PDZ domain of Postsynaptic Density-95
Authors : Tochio, H.; Hung, F.; Li, M.; Zhang, M.
Deposited on : 1999-08-25

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 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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

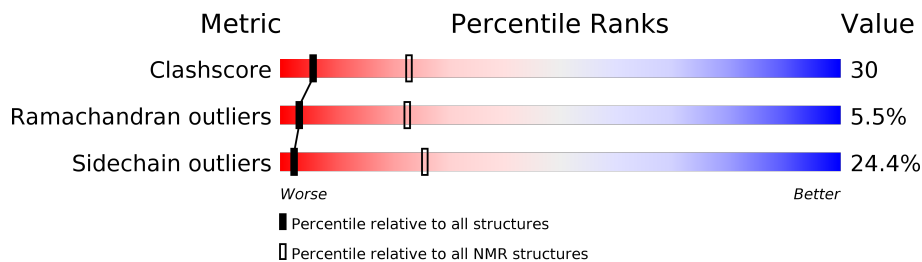
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	95	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 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:158-A:245 (88)	0.21	16

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1428 atoms, of which 727 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called POSTSYNAPTIC DENSITY PROTEIN 95.

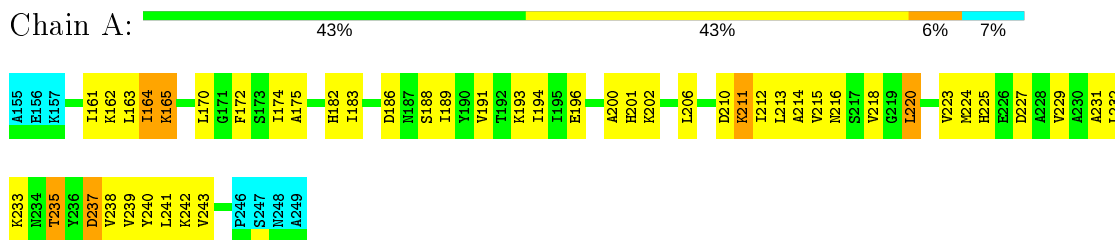
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	95	1428	444	727	121	134	2	0

4 Residue-property plots

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: POSTSYNAPTIC DENSITY PROTEIN 95

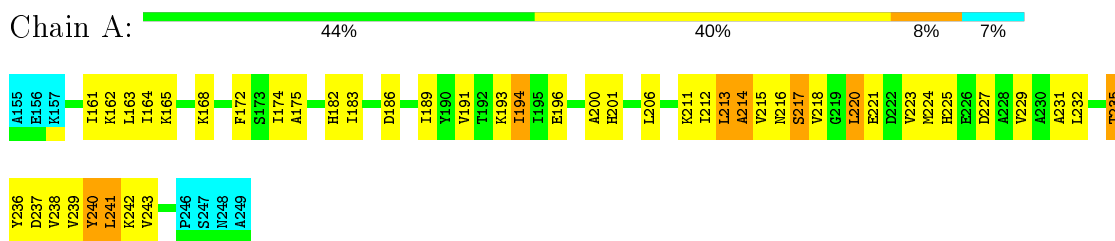


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

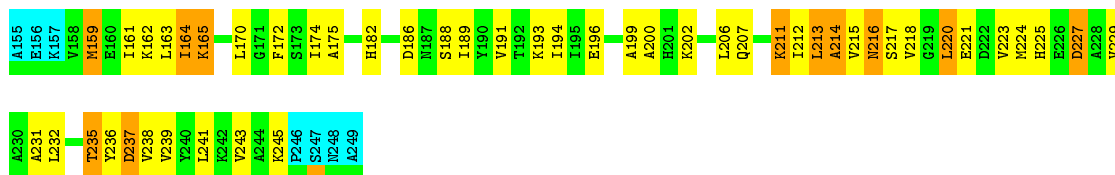
- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



4.2.2 Score per residue for model 2

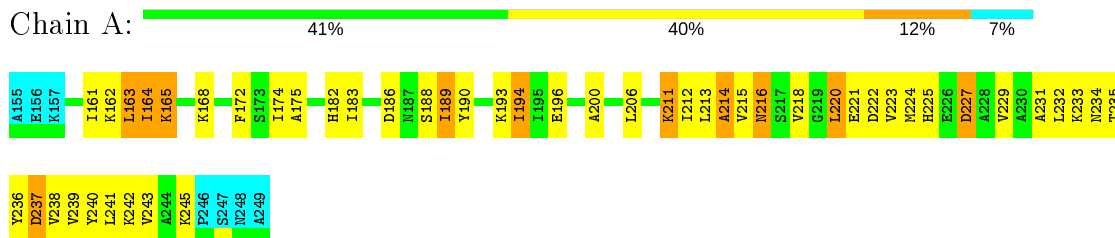
- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95





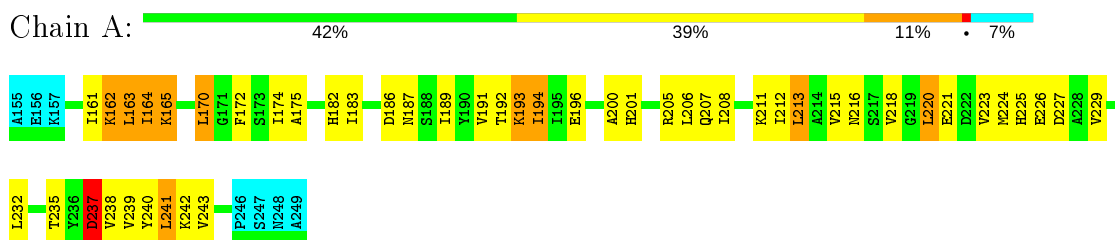
4.2.3 Score per residue for model 3

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



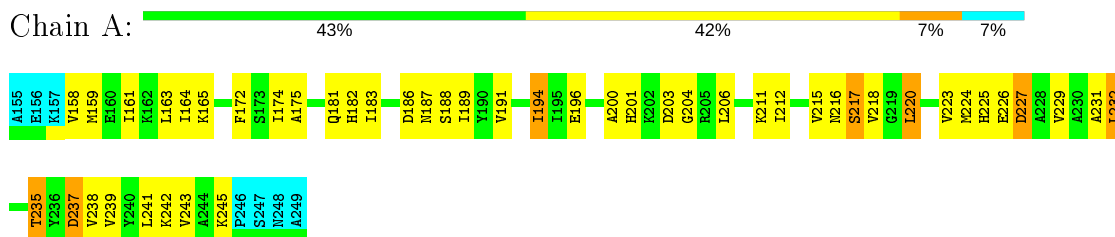
4.2.4 Score per residue for model 4

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



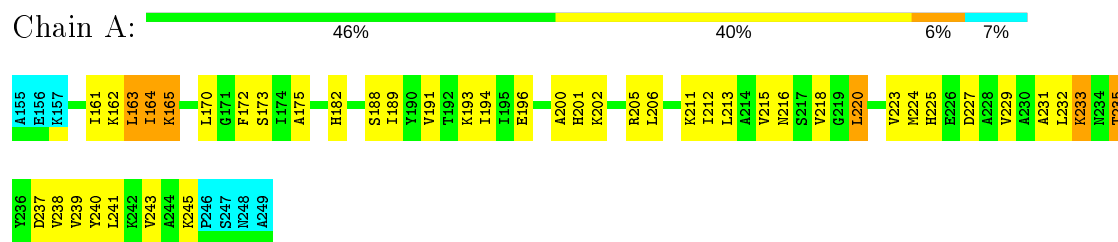
4.2.5 Score per residue for model 5

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



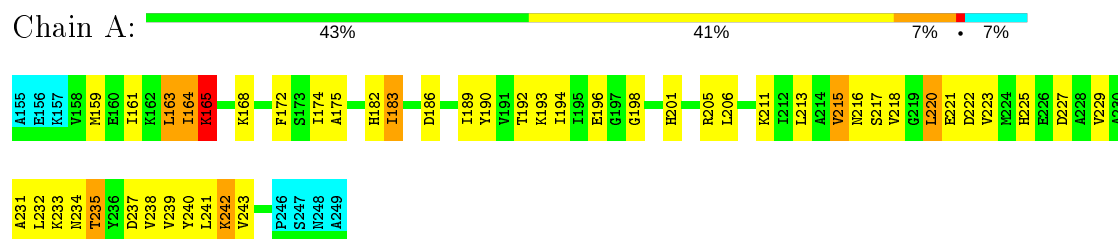
4.2.6 Score per residue for model 6

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



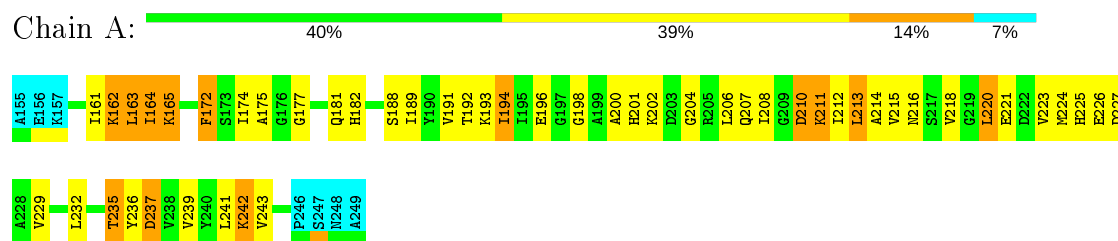
4.2.7 Score per residue for model 7

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



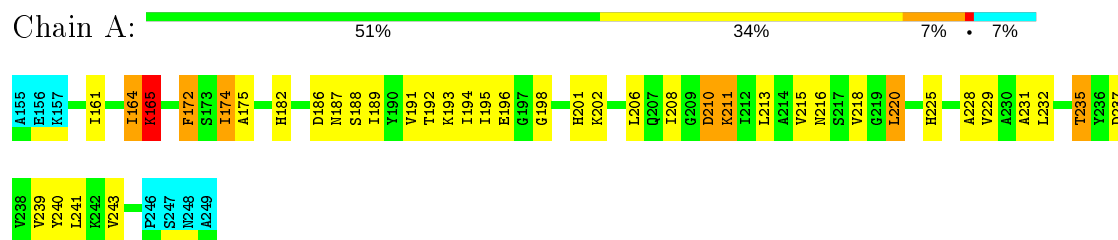
4.2.8 Score per residue for model 8

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



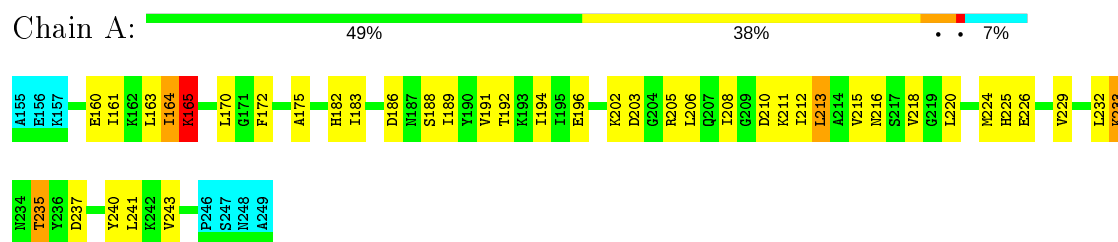
4.2.9 Score per residue for model 9

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



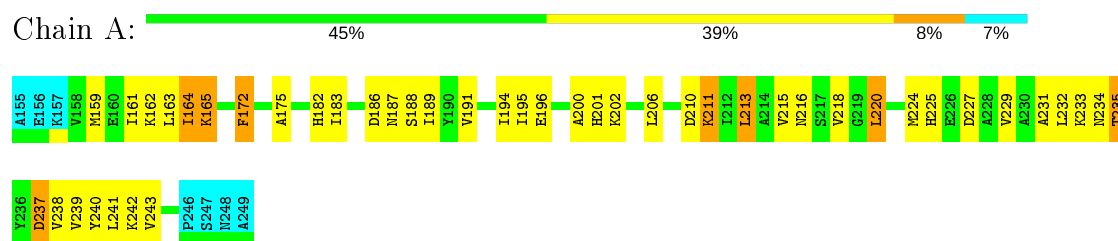
4.2.10 Score per residue for model 10

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



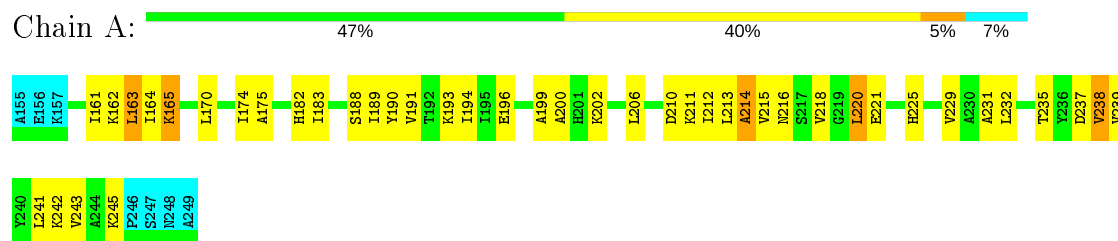
4.2.11 Score per residue for model 11

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



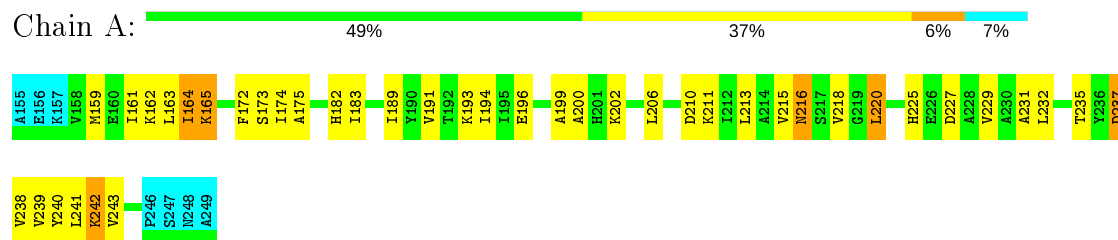
4.2.12 Score per residue for model 12

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



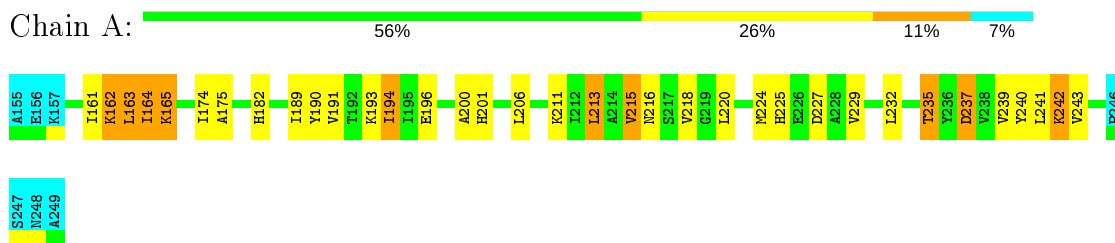
4.2.13 Score per residue for model 13

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



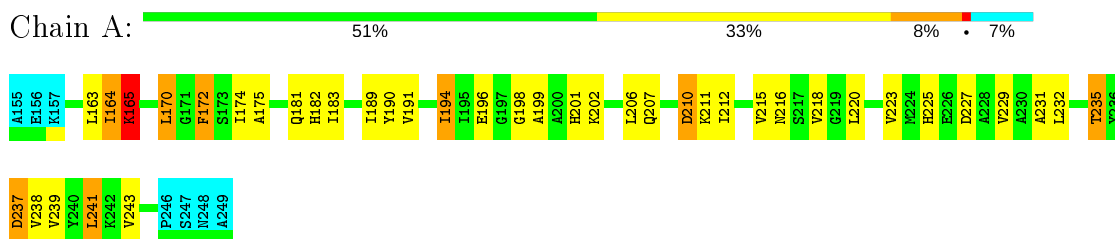
4.2.14 Score per residue for model 14

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



4.2.15 Score per residue for model 15

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



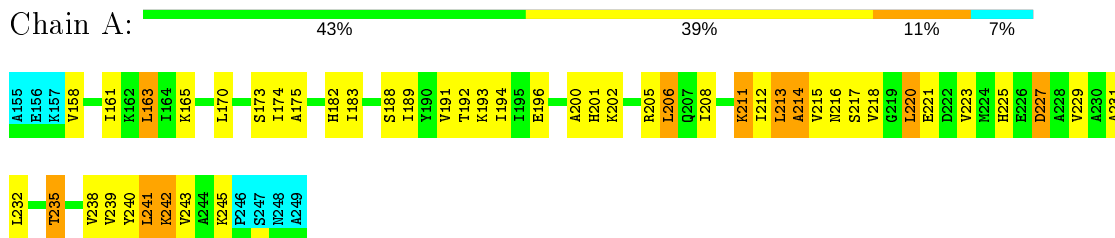
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



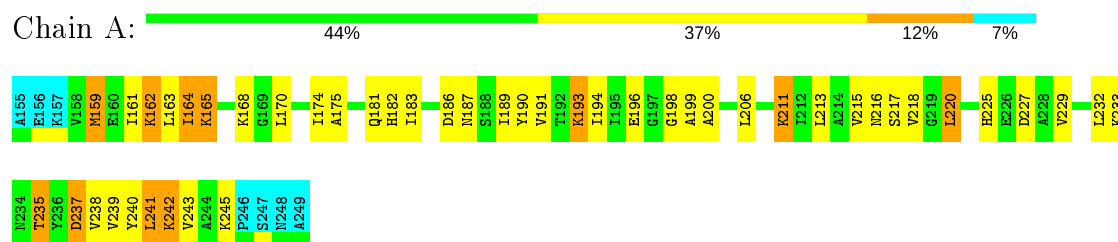
4.2.17 Score per residue for model 17

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



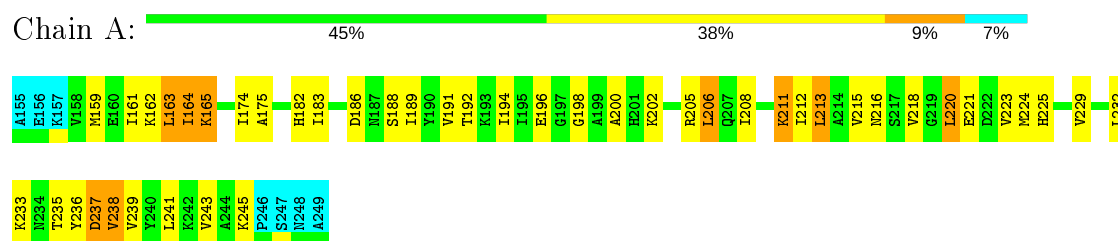
4.2.18 Score per residue for model 18

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



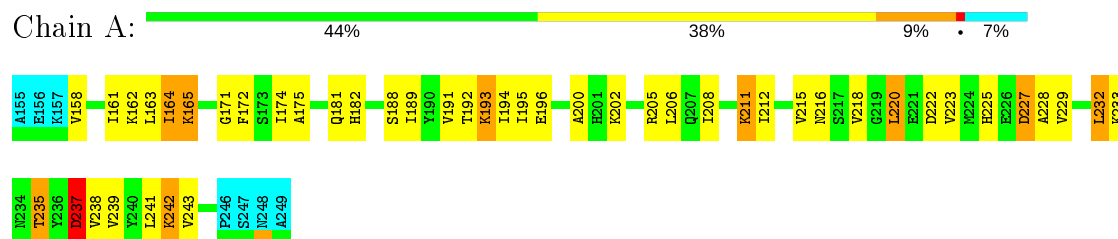
4.2.19 Score per residue for model 19

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



4.2.20 Score per residue for model 20

- Molecule 1: POSTSYNAPTIC DENSITY PROTEIN 95



5 Refinement protocol and experimental data overview

The models were refined using the following method: ?.

Of the ? 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
X-PLOR	refinement	3.8

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	651	678	678	40±7
All	All	13020	13560	13560	794

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:ILE:HG21	1:A:206:LEU:HD23	1.10	1.20	3	13
1:A:163:LEU:HD11	1:A:241:LEU:HD11	1.05	1.26	1	8
1:A:235:THR:HG21	1:A:239:VAL:HG21	0.95	1.38	1	17
1:A:200:ALA:HB1	1:A:206:LEU:HD21	0.86	1.45	16	7
1:A:164:ILE:HD12	1:A:238:VAL:HG22	0.85	1.48	1	2
1:A:220:LEU:HD22	1:A:231:ALA:HB1	0.84	1.49	3	5
1:A:161:ILE:HG22	1:A:163:LEU:HD21	0.83	1.49	16	13
1:A:220:LEU:O	1:A:223:VAL:HG12	0.82	1.74	16	5
1:A:175:ALA:O	1:A:189:ILE:HD13	0.81	1.74	1	20
1:A:212:ILE:HD13	1:A:243:VAL:CG2	0.80	2.06	6	13
1:A:175:ALA:HB2	1:A:192:THR:CG2	0.80	2.06	10	2
1:A:215:VAL:HG22	1:A:241:LEU:HD23	0.79	1.53	8	5
1:A:164:ILE:HD13	1:A:165:LYS:N	0.78	1.94	14	15
1:A:225:HIS:O	1:A:229:VAL:HG23	0.78	1.78	20	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:211:LYS:O	1:A:243:VAL:HG23	0.78	1.78	7	3
1:A:161:ILE:HG22	1:A:163:LEU:CD2	0.77	2.09	17	7
1:A:206:LEU:HD12	1:A:206:LEU:O	0.75	1.82	8	2
1:A:164:ILE:CD1	1:A:238:VAL:HG22	0.74	2.12	1	2
1:A:206:LEU:O	1:A:206:LEU:HD12	0.73	1.83	18	3
1:A:215:VAL:HG13	1:A:241:LEU:CD2	0.72	2.14	1	6
1:A:215:VAL:HG23	1:A:220:LEU:HD21	0.72	1.60	6	5
1:A:162:LYS:O	1:A:163:LEU:HD23	0.72	1.84	11	10
1:A:235:THR:CG2	1:A:239:VAL:HG21	0.71	2.15	5	17
1:A:215:VAL:CG2	1:A:220:LEU:HD21	0.71	2.16	1	10
1:A:161:ILE:HD13	1:A:206:LEU:HB3	0.71	1.63	10	4
1:A:211:LYS:O	1:A:243:VAL:HG13	0.70	1.87	20	17
1:A:213:LEU:HD21	1:A:242:LYS:CG	0.70	2.17	13	5
1:A:215:VAL:HG13	1:A:241:LEU:HG	0.69	1.62	13	11
1:A:213:LEU:O	1:A:213:LEU:HD12	0.69	1.87	19	3
1:A:163:LEU:HD12	1:A:170:LEU:HD22	0.69	1.63	12	2
1:A:163:LEU:HD22	1:A:200:ALA:HA	0.69	1.64	2	9
1:A:174:ILE:HG21	1:A:232:LEU:HD11	0.68	1.64	18	15
1:A:161:ILE:CG2	1:A:206:LEU:HD23	0.68	2.11	18	11
1:A:163:LEU:CD1	1:A:241:LEU:HD11	0.68	2.18	2	5
1:A:162:LYS:C	1:A:163:LEU:HD23	0.68	2.09	3	12
1:A:215:VAL:O	1:A:218:VAL:HG12	0.67	1.88	13	20
1:A:215:VAL:HG13	1:A:241:LEU:HD23	0.67	1.67	10	4
1:A:170:LEU:O	1:A:199:ALA:HB3	0.67	1.90	12	5
1:A:175:ALA:HB1	1:A:182:HIS:CG	0.67	2.24	12	20
1:A:215:VAL:HG12	1:A:239:VAL:CG2	0.67	2.20	7	13
1:A:161:ILE:CG2	1:A:163:LEU:HD21	0.66	2.19	16	7
1:A:163:LEU:HD21	1:A:170:LEU:HD23	0.66	1.66	15	1
1:A:210:ASP:OD2	1:A:243:VAL:HG21	0.66	1.91	9	1
1:A:220:LEU:HD22	1:A:231:ALA:CB	0.65	2.21	17	5
1:A:161:ILE:HG21	1:A:206:LEU:HD22	0.65	1.68	17	3
1:A:220:LEU:HD23	1:A:231:ALA:HB3	0.65	1.67	12	4
1:A:163:LEU:HD11	1:A:241:LEU:CD1	0.65	2.21	5	5
1:A:163:LEU:HD21	1:A:241:LEU:CD1	0.65	2.22	14	1
1:A:161:ILE:HG21	1:A:206:LEU:CD2	0.64	2.23	13	8
1:A:210:ASP:CG	1:A:243:VAL:HG21	0.63	2.14	9	1
1:A:161:ILE:CG2	1:A:206:LEU:HD22	0.62	2.25	17	1
1:A:193:LYS:C	1:A:194:ILE:HD13	0.62	2.14	4	8
1:A:211:LYS:O	1:A:243:VAL:HG22	0.61	1.95	15	17
1:A:229:VAL:HA	1:A:232:LEU:HD12	0.61	1.72	17	6
1:A:218:VAL:HG13	1:A:220:LEU:CD2	0.60	2.26	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:213:LEU:HD21	1:A:242:LYS:HG2	0.60	1.72	14	7
1:A:218:VAL:HG11	1:A:231:ALA:O	0.59	1.97	9	4
1:A:163:LEU:HD12	1:A:170:LEU:HD12	0.59	1.74	6	2
1:A:213:LEU:HD21	1:A:242:LYS:HG3	0.59	1.75	13	4
1:A:175:ALA:HB2	1:A:192:THR:HG22	0.59	1.72	7	2
1:A:161:ILE:O	1:A:241:LEU:HD12	0.58	1.98	14	2
1:A:194:ILE:HG22	1:A:201:HIS:HB2	0.58	1.73	15	12
1:A:212:ILE:HA	1:A:243:VAL:HG22	0.58	1.75	20	6
1:A:215:VAL:HG13	1:A:241:LEU:HD22	0.58	1.75	1	2
1:A:174:ILE:HG21	1:A:232:LEU:CD1	0.58	2.28	18	3
1:A:220:LEU:HD12	1:A:221:GLU:N	0.56	2.15	19	5
1:A:162:LYS:NZ	1:A:238:VAL:HG21	0.56	2.15	12	1
1:A:220:LEU:HD23	1:A:231:ALA:CB	0.56	2.31	12	1
1:A:194:ILE:HD12	1:A:206:LEU:CD1	0.55	2.32	18	4
1:A:191:VAL:HG11	1:A:194:ILE:CD1	0.55	2.31	11	16
1:A:175:ALA:HB1	1:A:182:HIS:HB3	0.55	1.78	9	18
1:A:232:LEU:O	1:A:235:THR:HG23	0.55	2.01	15	14
1:A:192:THR:HA	1:A:208:ILE:HG23	0.54	1.77	9	2
1:A:170:LEU:HD21	1:A:239:VAL:HG11	0.54	1.78	12	2
1:A:235:THR:HB	1:A:239:VAL:HG22	0.54	1.78	9	1
1:A:191:VAL:HG21	1:A:206:LEU:HD13	0.54	1.78	13	2
1:A:163:LEU:HD11	1:A:170:LEU:CD1	0.54	2.33	10	1
1:A:163:LEU:HD11	1:A:170:LEU:HG	0.53	1.78	15	1
1:A:215:VAL:CG2	1:A:220:LEU:HD11	0.53	2.33	1	3
1:A:175:ALA:HB1	1:A:182:HIS:CB	0.53	2.34	15	19
1:A:241:LEU:HD12	1:A:241:LEU:N	0.53	2.19	7	1
1:A:194:ILE:HD12	1:A:206:LEU:HD12	0.53	1.81	10	5
1:A:158:VAL:HG23	1:A:243:VAL:O	0.53	2.03	17	1
1:A:192:THR:C	1:A:208:ILE:HD12	0.52	2.25	10	2
1:A:165:LYS:HE2	1:A:170:LEU:HD22	0.52	1.80	4	2
1:A:191:VAL:HG11	1:A:194:ILE:HD11	0.52	1.79	18	6
1:A:232:LEU:HD12	1:A:233:LYS:N	0.52	2.20	10	2
1:A:212:ILE:HD13	1:A:243:VAL:HG22	0.51	1.82	2	6
1:A:158:VAL:HG11	1:A:242:LYS:HD2	0.50	1.82	5	1
1:A:215:VAL:HG12	1:A:239:VAL:HG21	0.50	1.84	7	3
1:A:213:LEU:O	1:A:214:ALA:HB2	0.50	2.07	1	5
1:A:183:ILE:HD11	1:A:190:TYR:CB	0.49	2.38	15	2
1:A:215:VAL:HG21	1:A:220:LEU:HD11	0.49	1.84	1	3
1:A:215:VAL:CG2	1:A:241:LEU:HD23	0.49	2.37	20	2
1:A:171:GLY:C	1:A:195:ILE:HD13	0.49	2.28	20	1
1:A:235:THR:HG21	1:A:239:VAL:CG1	0.49	2.38	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:ALA:HB1	1:A:182:HIS:CD2	0.49	2.43	7	10
1:A:213:LEU:HD11	1:A:242:LYS:HG2	0.49	1.84	18	1
1:A:215:VAL:HG21	1:A:220:LEU:HD21	0.48	1.84	20	3
1:A:240:TYR:C	1:A:241:LEU:HD23	0.48	2.30	1	1
1:A:163:LEU:HD21	1:A:241:LEU:HD13	0.48	1.84	14	1
1:A:163:LEU:HD13	1:A:172:PHE:CE1	0.47	2.44	1	1
1:A:175:ALA:CB	1:A:182:HIS:CD2	0.47	2.97	7	18
1:A:223:VAL:HG21	1:A:227:ASP:CB	0.47	2.39	20	8
1:A:170:LEU:HD21	1:A:239:VAL:CG1	0.47	2.39	12	2
1:A:206:LEU:HD12	1:A:206:LEU:C	0.47	2.30	18	2
1:A:162:LYS:CG	1:A:238:VAL:HG22	0.47	2.40	19	1
1:A:215:VAL:CB	1:A:220:LEU:HD21	0.47	2.40	1	1
1:A:241:LEU:N	1:A:241:LEU:HD12	0.46	2.25	4	2
1:A:206:LEU:HD23	1:A:206:LEU:H	0.46	1.70	6	1
1:A:164:ILE:HD13	1:A:165:LYS:H	0.46	1.67	20	4
1:A:163:LEU:CD2	1:A:170:LEU:HD23	0.46	2.39	15	1
1:A:191:VAL:HG21	1:A:206:LEU:HD12	0.46	1.86	16	2
1:A:189:ILE:HG21	1:A:220:LEU:HD22	0.46	1.88	8	1
1:A:161:ILE:HG23	1:A:204:GLY:CA	0.45	2.41	5	2
1:A:163:LEU:CD1	1:A:172:PHE:CE1	0.45	2.99	13	3
1:A:189:ILE:HD11	1:A:228:ALA:CB	0.45	2.41	20	1
1:A:216:ASN:HB2	1:A:239:VAL:HG23	0.45	1.89	13	1
1:A:215:VAL:CG1	1:A:239:VAL:HG22	0.45	2.42	17	4
1:A:220:LEU:N	1:A:220:LEU:HD23	0.45	2.26	2	1
1:A:183:ILE:HD11	1:A:190:TYR:HB2	0.45	1.89	12	1
1:A:162:LYS:CD	1:A:240:TYR:CE2	0.45	3.00	13	1
1:A:174:ILE:CD1	1:A:228:ALA:HB3	0.45	2.42	9	1
1:A:163:LEU:HG	1:A:239:VAL:HG13	0.44	1.89	7	2
1:A:191:VAL:CG1	1:A:194:ILE:HD11	0.44	2.42	18	3
1:A:165:LYS:N	1:A:237:ASP:O	0.44	2.50	8	10
1:A:183:ILE:CD1	1:A:190:TYR:CD1	0.44	3.00	16	2
1:A:210:ASP:OD2	1:A:243:VAL:HG11	0.44	2.13	8	1
1:A:158:VAL:HG11	1:A:242:LYS:HE2	0.44	1.89	20	1
1:A:172:PHE:N	1:A:195:ILE:HD13	0.43	2.28	9	2
1:A:212:ILE:HD13	1:A:243:VAL:HG21	0.43	1.86	20	1
1:A:194:ILE:HD13	1:A:194:ILE:N	0.43	2.28	4	1
1:A:195:ILE:HD12	1:A:195:ILE:N	0.43	2.28	11	1
1:A:239:VAL:HG13	1:A:239:VAL:O	0.43	2.12	7	1
1:A:190:TYR:CD1	1:A:190:TYR:N	0.43	2.86	14	1
1:A:191:VAL:CG1	1:A:194:ILE:CD1	0.43	2.97	17	14
1:A:215:VAL:HG22	1:A:241:LEU:CD2	0.43	2.35	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:215:VAL:HG12	1:A:239:VAL:HG22	0.42	1.90	19	2
1:A:161:ILE:HG22	1:A:241:LEU:HD12	0.42	1.91	19	1
1:A:164:ILE:HD13	1:A:238:VAL:HG22	0.42	1.88	5	1
1:A:161:ILE:O	1:A:241:LEU:N	0.42	2.52	13	1
1:A:215:VAL:HG22	1:A:241:LEU:HD22	0.42	1.92	1	1
1:A:236:TYR:N	1:A:236:TYR:CD1	0.42	2.87	1	1
1:A:172:PHE:CD2	1:A:206:LEU:HD11	0.42	2.50	15	1
1:A:241:LEU:N	1:A:241:LEU:HD23	0.42	2.30	15	1
1:A:215:VAL:CG1	1:A:239:VAL:CG2	0.42	2.98	18	7
1:A:159:MET:SD	1:A:161:ILE:HD11	0.42	2.54	2	1
1:A:215:VAL:HB	1:A:220:LEU:HD21	0.42	1.92	1	1
1:A:212:ILE:HG21	1:A:220:LEU:HD21	0.42	1.90	8	1
1:A:241:LEU:HD12	1:A:241:LEU:H	0.42	1.74	14	2
1:A:192:THR:O	1:A:208:ILE:HD13	0.42	2.15	9	4
1:A:215:VAL:CG1	1:A:241:LEU:HD22	0.42	2.45	1	1
1:A:215:VAL:O	1:A:217:SER:N	0.42	2.53	2	5
1:A:159:MET:O	1:A:243:VAL:HG12	0.42	2.15	18	1
1:A:223:VAL:CG2	1:A:227:ASP:CB	0.41	2.98	5	6
1:A:172:PHE:HB3	1:A:200:ALA:HB3	0.41	1.91	8	2
1:A:210:ASP:OD1	1:A:243:VAL:HG11	0.41	2.13	15	1
1:A:235:THR:HG21	1:A:239:VAL:HG11	0.41	1.90	15	1
1:A:161:ILE:HG22	1:A:163:LEU:HD23	0.41	1.91	7	1
1:A:177:GLY:O	1:A:181:GLN:CG	0.41	2.68	8	1
1:A:163:LEU:HD11	1:A:170:LEU:CG	0.41	2.44	15	1
1:A:163:LEU:HD21	1:A:241:LEU:HD12	0.41	1.92	19	1
1:A:175:ALA:CB	1:A:182:HIS:CG	0.41	3.01	12	2
1:A:163:LEU:CD2	1:A:241:LEU:HD11	0.41	2.45	15	1
1:A:162:LYS:HD2	1:A:240:TYR:CE2	0.41	2.51	13	1
1:A:239:VAL:O	1:A:239:VAL:HG13	0.41	2.16	14	1
1:A:164:ILE:HD12	1:A:238:VAL:CG2	0.41	2.34	1	1
1:A:208:ILE:N	1:A:208:ILE:HD13	0.41	2.30	10	1
1:A:235:THR:HG21	1:A:239:VAL:CG2	0.41	2.33	11	1
1:A:213:LEU:HD12	1:A:213:LEU:O	0.41	2.16	3	1
1:A:216:ASN:OD1	1:A:239:VAL:HG23	0.41	2.16	3	1
1:A:175:ALA:N	1:A:190:TYR:O	0.41	2.54	7	3
1:A:206:LEU:HD22	1:A:241:LEU:HD12	0.40	1.93	15	1
1:A:173:SER:N	1:A:193:LYS:O	0.40	2.55	17	1
1:A:206:LEU:H	1:A:206:LEU:HD23	0.40	1.75	16	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/95 (93%)	71±2 (80±2%)	13±2 (14±2%)	5±1 (5±1%)	3	23
All	All	1760/1900 (93%)	1413 (80%)	251 (14%)	96 (5%)	3	23

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	216	ASN	20
1	A	196	GLU	20
1	A	237	ASP	19
1	A	235	THR	15
1	A	165	LYS	6
1	A	214	ALA	6
1	A	198	GLY	6
1	A	181	GLN	1
1	A	199	ALA	1
1	A	222	ASP	1
1	A	188	SER	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	68/73 (93%)	51±3 (76±5%)	17±3 (24±5%)	2	26
All	All	1360/1460 (93%)	1028 (76%)	332 (24%)	2	26

All 46 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	165	LYS	20
1	A	220	LEU	20
1	A	164	ILE	17
1	A	238	VAL	14
1	A	202	LYS	13
1	A	227	ASP	13
1	A	224	MET	12
1	A	213	LEU	12
1	A	183	ILE	12
1	A	186	ASP	12
1	A	172	PHE	11
1	A	240	TYR	11
1	A	188	SER	11
1	A	211	LYS	10
1	A	163	LEU	10
1	A	245	LYS	9
1	A	242	LYS	9
1	A	159	MET	8
1	A	233	LYS	8
1	A	193	LYS	8
1	A	205	ARG	8
1	A	194	ILE	7
1	A	210	ASP	7
1	A	241	LEU	5
1	A	237	ASP	5
1	A	187	ASN	5
1	A	168	LYS	5
1	A	162	LYS	5
1	A	221	GLU	5
1	A	236	TYR	4
1	A	207	GLN	4
1	A	217	SER	4
1	A	226	GLU	4
1	A	181	GLN	3
1	A	234	ASN	3
1	A	232	LEU	2
1	A	215	VAL	2
1	A	206	LEU	2
1	A	222	ASP	2
1	A	170	LEU	2
1	A	203	ASP	2
1	A	173	SER	2
1	A	189	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	160	GLU	1
1	A	174	ILE	1
1	A	216	ASN	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