



Full wwPDB NMR Structure Validation Report ⓘ

Apr 21, 2024 – 02:54 PM EDT

PDB ID : 2HQN
Title : Structure of a Atypical Orphan Response Regulator Protein Revealed a New Phosphorylation-Independent Regulatory Mechanism
Authors : Hong, E.; Lee, W.
Deposited on : 2006-07-19

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

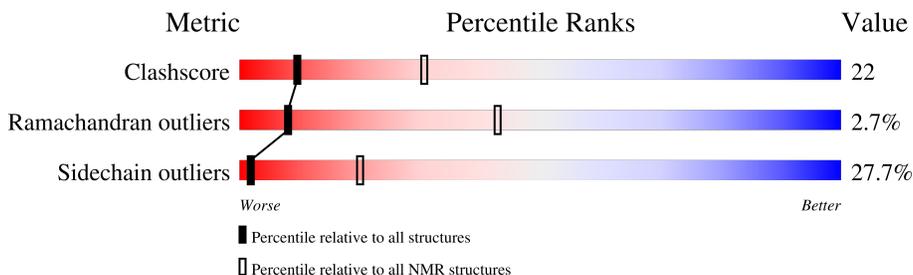
1 Overall quality at a glance

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	109	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:120-A:217 (98)	0.29	3

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1760 atoms, of which 886 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative TRANSCRIPTIONAL REGULATOR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	109	1760	550	886	153	167	4	0

There are 4 discrepancies between the modelled and reference sequences:

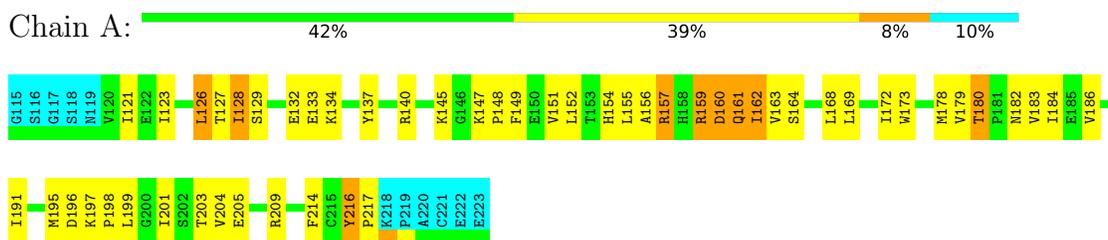
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	GLY	-	cloning artifact	UNP Q9ZM42
A	116	SER	-	cloning artifact	UNP Q9ZM42
A	117	GLY	-	cloning artifact	UNP Q9ZM42
A	118	SER	-	cloning artifact	UNP Q9ZM42

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

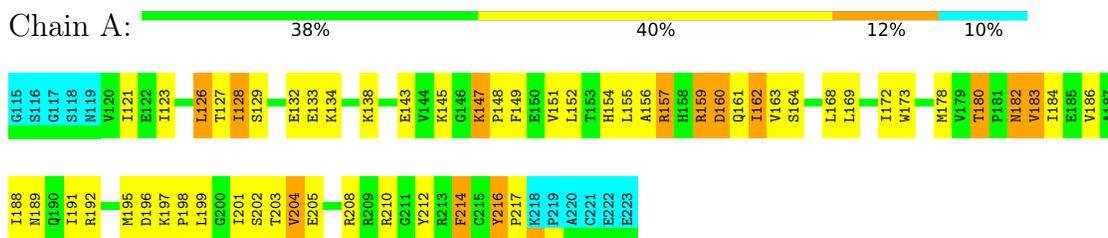


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

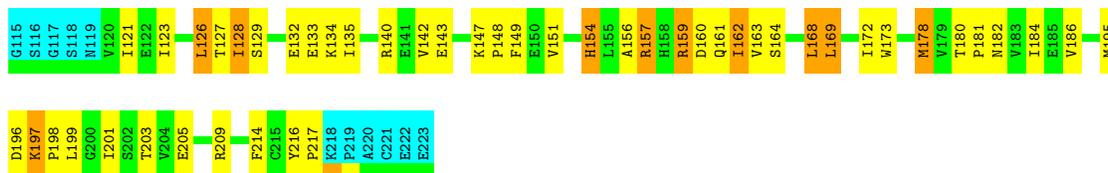
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



4.2.2 Score per residue for model 2

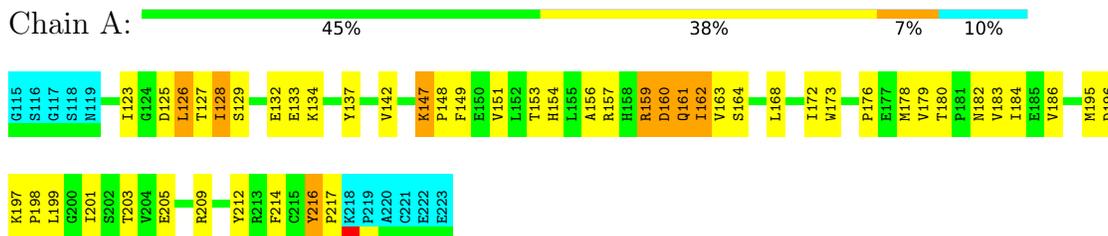
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR





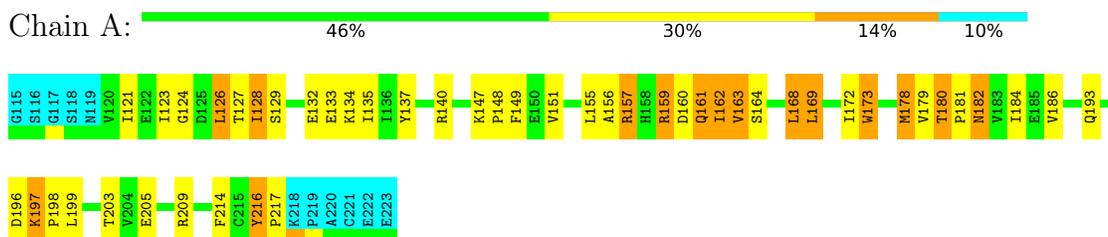
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



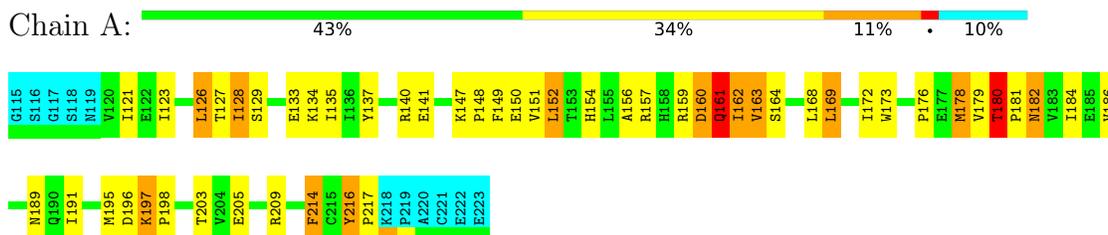
4.2.4 Score per residue for model 4

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



4.2.5 Score per residue for model 5

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

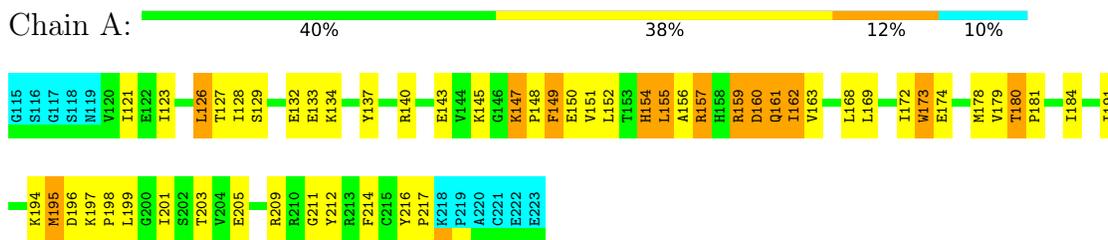


4.2.6 Score per residue for model 6

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

4.2.10 Score per residue for model 10

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



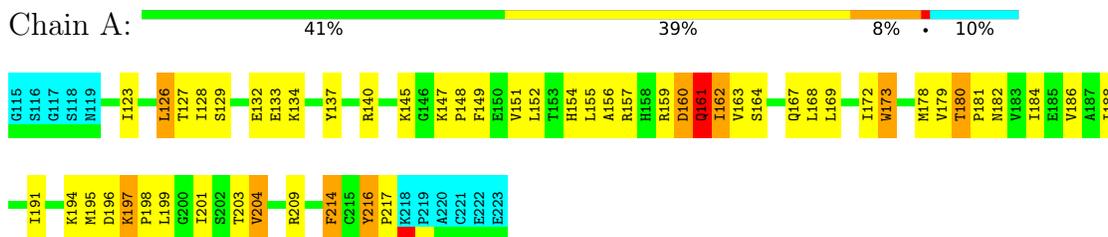
4.2.11 Score per residue for model 11

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



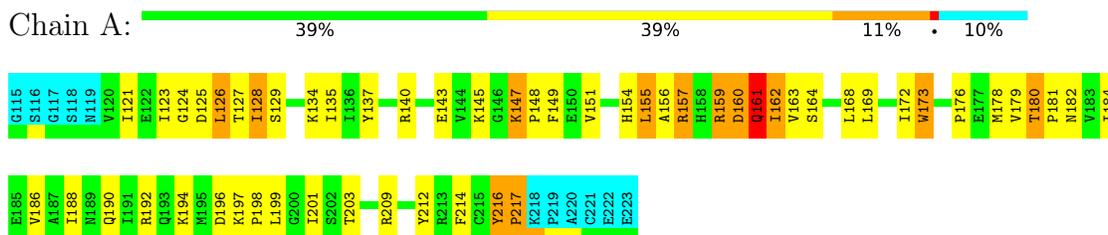
4.2.12 Score per residue for model 12

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



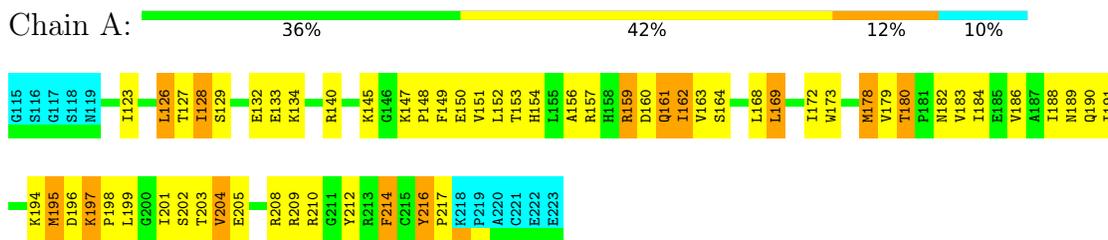
4.2.13 Score per residue for model 13

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



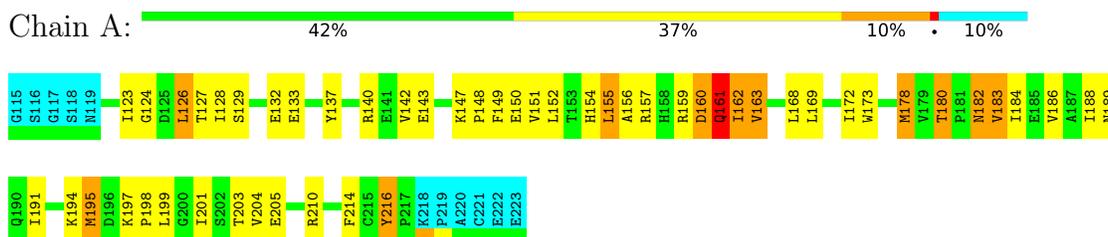
4.2.14 Score per residue for model 14

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



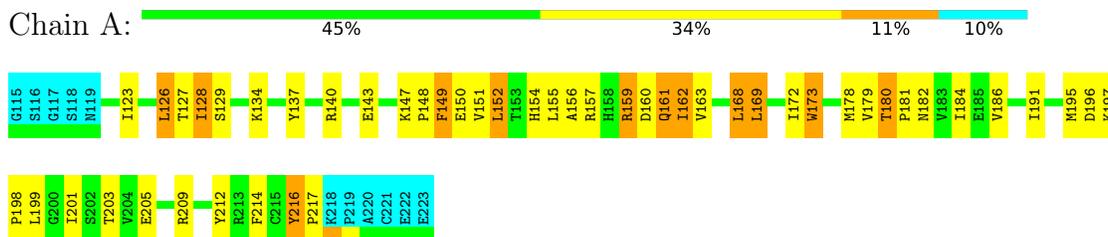
4.2.15 Score per residue for model 15

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



4.2.16 Score per residue for model 16

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



4.2.17 Score per residue for model 17

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



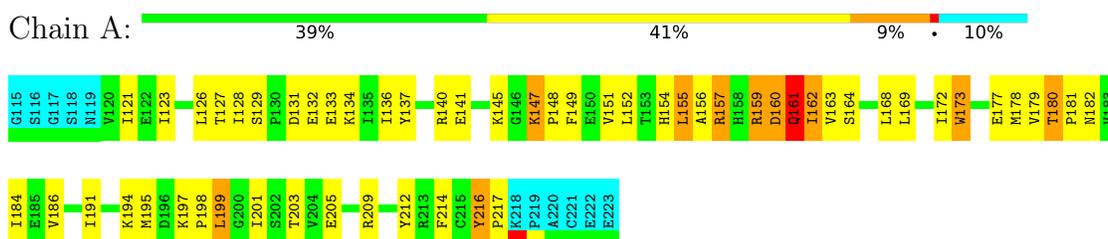
4.2.18 Score per residue for model 18

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



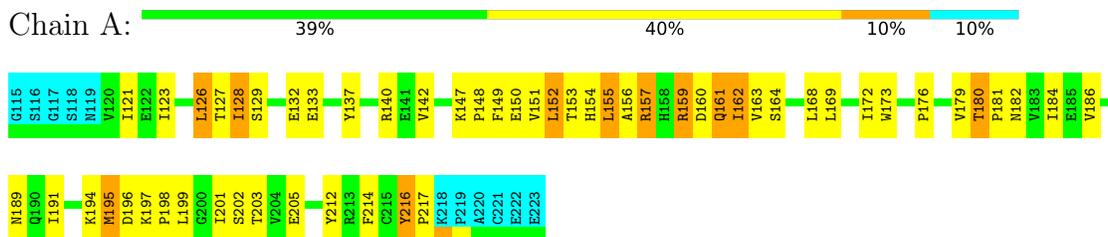
4.2.19 Score per residue for model 19

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



4.2.20 Score per residue for model 20

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

No chemical shift data was provided.

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	801	822	822	36±4
All	All	16020	16440	16440	725

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:VAL:HG12	1:A:172:ILE:HG21	1.06	1.26	9	20
1:A:142:VAL:HG21	1:A:199:LEU:HD21	0.95	1.35	15	7
1:A:163:VAL:HG11	1:A:168:LEU:HD12	0.88	1.46	8	4
1:A:152:LEU:HD22	1:A:191:ILE:HG21	0.86	1.45	16	2
1:A:155:LEU:HD11	1:A:168:LEU:HD13	0.84	1.48	20	1
1:A:126:LEU:HD13	1:A:216:TYR:CZ	0.77	2.15	18	11
1:A:168:LEU:HD22	1:A:184:ILE:HD12	0.70	1.62	3	18
1:A:152:LEU:HD13	1:A:214:PHE:CE2	0.70	2.22	20	7
1:A:126:LEU:HD13	1:A:216:TYR:CE1	0.68	2.22	6	10
1:A:151:VAL:HG12	1:A:172:ILE:CG2	0.67	2.14	9	20
1:A:126:LEU:HD22	1:A:216:TYR:CD2	0.67	2.25	1	18
1:A:147:LYS:N	1:A:148:PRO:HD2	0.67	2.05	15	20
1:A:152:LEU:HD13	1:A:191:ILE:HG13	0.67	1.64	16	2
1:A:123:ILE:HD12	1:A:156:ALA:O	0.67	1.90	11	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:LEU:HD21	1:A:168:LEU:HD21	0.67	1.66	15	4
1:A:151:VAL:CG1	1:A:172:ILE:HG21	0.66	2.20	19	20
1:A:126:LEU:HD13	1:A:216:TYR:CE2	0.65	2.27	2	9
1:A:126:LEU:HD12	1:A:137:TYR:HB2	0.65	1.69	10	12
1:A:188:ILE:HG23	1:A:204:VAL:CG2	0.64	2.21	1	7
1:A:169:LEU:HD11	1:A:181:PRO:HA	0.63	1.71	8	9
1:A:188:ILE:HG23	1:A:204:VAL:HG21	0.62	1.71	14	7
1:A:126:LEU:HD22	1:A:216:TYR:CE2	0.62	2.30	6	12
1:A:156:ALA:HB2	1:A:214:PHE:CZ	0.62	2.30	4	17
1:A:195:MET:HE1	1:A:201:ILE:HD11	0.61	1.72	14	2
1:A:168:LEU:HD13	1:A:184:ILE:HG23	0.61	1.72	19	3
1:A:151:VAL:O	1:A:155:LEU:HD23	0.60	1.96	11	1
1:A:182:ASN:O	1:A:186:VAL:HG23	0.60	1.96	3	19
1:A:195:MET:CE	1:A:201:ILE:HD11	0.60	2.27	20	4
1:A:195:MET:CE	1:A:199:LEU:HD22	0.59	2.27	11	1
1:A:121:ILE:HG21	1:A:157:ARG:CD	0.59	2.28	19	6
1:A:199:LEU:HD22	1:A:201:ILE:HG12	0.58	1.74	19	1
1:A:121:ILE:HD12	1:A:157:ARG:HB3	0.57	1.77	2	5
1:A:203:THR:HG22	1:A:216:TYR:CE1	0.57	2.34	10	5
1:A:159:ARG:O	1:A:160:ASP:C	0.57	2.43	15	20
1:A:147:LYS:N	1:A:148:PRO:CD	0.56	2.68	15	20
1:A:203:THR:HG22	1:A:216:TYR:CZ	0.56	2.34	13	12
1:A:123:ILE:CG2	1:A:126:LEU:HD23	0.56	2.30	18	5
1:A:199:LEU:O	1:A:201:ILE:HG23	0.56	2.01	3	12
1:A:142:VAL:CG2	1:A:199:LEU:HD21	0.56	2.23	15	1
1:A:126:LEU:HD11	1:A:135:ILE:CG2	0.55	2.30	18	3
1:A:148:PRO:O	1:A:151:VAL:HG22	0.55	2.01	9	17
1:A:137:TYR:CE2	1:A:201:ILE:HG21	0.55	2.36	20	2
1:A:162:ILE:O	1:A:162:ILE:CG2	0.54	2.55	10	20
1:A:163:VAL:HG12	1:A:212:TYR:O	0.54	2.03	16	10
1:A:195:MET:HE2	1:A:199:LEU:HD12	0.54	1.78	15	1
1:A:151:VAL:O	1:A:155:LEU:HD22	0.53	2.02	15	4
1:A:178:MET:O	1:A:180:THR:HG23	0.53	2.03	2	19
1:A:168:LEU:O	1:A:168:LEU:HD12	0.53	2.02	20	1
1:A:162:ILE:HD13	1:A:163:VAL:N	0.53	2.19	7	3
1:A:172:ILE:O	1:A:173:TRP:C	0.53	2.47	8	20
1:A:203:THR:HG22	1:A:216:TYR:CE2	0.53	2.39	12	6
1:A:126:LEU:HD21	1:A:128:ILE:CG2	0.52	2.34	5	15
1:A:121:ILE:HG21	1:A:157:ARG:HG2	0.52	1.80	17	2
1:A:195:MET:HE3	1:A:201:ILE:HD11	0.52	1.81	20	1
1:A:121:ILE:HG21	1:A:157:ARG:HD2	0.52	1.80	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:LEU:HD21	1:A:168:LEU:CD2	0.52	2.33	15	4
1:A:195:MET:CE	1:A:199:LEU:HD12	0.51	2.35	2	5
1:A:126:LEU:HD21	1:A:128:ILE:HG23	0.51	1.83	5	8
1:A:155:LEU:CD1	1:A:168:LEU:HD13	0.51	2.31	20	1
1:A:123:ILE:HD13	1:A:160:ASP:HB3	0.51	1.81	4	1
1:A:163:VAL:HG11	1:A:168:LEU:CD1	0.51	2.31	8	2
1:A:196:ASP:OD1	1:A:203:THR:HG23	0.50	2.06	4	1
1:A:154:HIS:HB3	1:A:172:ILE:HD11	0.50	1.82	2	5
1:A:169:LEU:CA	1:A:184:ILE:HD11	0.50	2.37	11	1
1:A:152:LEU:HD22	1:A:191:ILE:CG2	0.50	2.30	18	2
1:A:201:ILE:HD13	1:A:216:TYR:CE1	0.50	2.41	13	1
1:A:179:VAL:C	1:A:180:THR:HG23	0.49	2.27	5	10
1:A:126:LEU:HD22	1:A:216:TYR:CD1	0.49	2.41	2	1
1:A:169:LEU:HD23	1:A:183:VAL:HG12	0.49	1.82	11	1
1:A:152:LEU:HG	1:A:191:ILE:HG21	0.49	1.85	15	13
1:A:195:MET:HE2	1:A:199:LEU:HD22	0.49	1.84	11	1
1:A:188:ILE:HG23	1:A:204:VAL:HG23	0.49	1.84	12	2
1:A:121:ILE:HG21	1:A:157:ARG:HD3	0.48	1.84	18	1
1:A:188:ILE:HG22	1:A:192:ARG:HD2	0.48	1.85	18	1
1:A:126:LEU:HD11	1:A:135:ILE:HG23	0.48	1.85	18	2
1:A:152:LEU:HD11	1:A:188:ILE:HD13	0.48	1.84	18	1
1:A:121:ILE:HD13	1:A:157:ARG:HG2	0.48	1.85	7	3
1:A:197:LYS:CB	1:A:198:PRO:CD	0.47	2.92	16	20
1:A:153:THR:O	1:A:156:ALA:HB3	0.47	2.09	14	7
1:A:168:LEU:HG	1:A:184:ILE:HD12	0.47	1.86	20	1
1:A:168:LEU:HD22	1:A:184:ILE:CD1	0.47	2.38	7	7
1:A:197:LYS:N	1:A:198:PRO:HD2	0.47	2.25	18	20
1:A:169:LEU:CD1	1:A:183:VAL:HG12	0.47	2.39	6	6
1:A:155:LEU:HD13	1:A:159:ARG:CG	0.47	2.38	20	1
1:A:159:ARG:NH2	1:A:168:LEU:HD11	0.47	2.25	17	2
1:A:176:PRO:O	1:A:179:VAL:HG12	0.46	2.11	11	4
1:A:169:LEU:HA	1:A:184:ILE:HD11	0.45	1.88	11	1
1:A:180:THR:CB	1:A:181:PRO:HD2	0.45	2.42	20	1
1:A:126:LEU:HD22	1:A:216:TYR:CE1	0.45	2.47	2	1
1:A:151:VAL:HG12	1:A:172:ILE:HG13	0.44	1.89	11	1
1:A:121:ILE:HG21	1:A:157:ARG:NE	0.44	2.27	13	1
1:A:155:LEU:CD2	1:A:168:LEU:HD21	0.44	2.41	15	1
1:A:126:LEU:HD12	1:A:137:TYR:CD1	0.44	2.48	13	2
1:A:123:ILE:HG23	1:A:126:LEU:HB3	0.44	1.90	19	1
1:A:152:LEU:HD13	1:A:214:PHE:HE2	0.44	1.69	10	2
1:A:188:ILE:HG22	1:A:192:ARG:HD3	0.43	1.90	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ILE:H	1:A:128:ILE:HD13	0.43	1.73	1	1
1:A:195:MET:HE3	1:A:199:LEU:HD22	0.43	1.89	12	1
1:A:132:GLU:O	1:A:133:GLU:C	0.43	2.57	15	17
1:A:148:PRO:O	1:A:151:VAL:CG2	0.43	2.66	19	6
1:A:155:LEU:O	1:A:159:ARG:CB	0.43	2.66	9	1
1:A:155:LEU:HD12	1:A:159:ARG:CD	0.43	2.44	11	1
1:A:160:ASP:O	1:A:161:GLN:CB	0.42	2.66	9	10
1:A:162:ILE:O	1:A:162:ILE:HG23	0.42	2.13	5	4
1:A:163:VAL:HG22	1:A:167:GLN:HB2	0.42	1.90	12	1
1:A:128:ILE:HG22	1:A:135:ILE:HG23	0.42	1.91	5	7
1:A:195:MET:C	1:A:198:PRO:HD2	0.42	2.34	11	7
1:A:123:ILE:HD13	1:A:160:ASP:OD2	0.42	2.14	18	1
1:A:123:ILE:O	1:A:126:LEU:HB3	0.42	2.14	10	3
1:A:155:LEU:HD23	1:A:159:ARG:HH11	0.42	1.75	15	1
1:A:152:LEU:CD2	1:A:191:ILE:HG21	0.42	2.32	16	1
1:A:142:VAL:HG21	1:A:199:LEU:HD11	0.42	1.92	6	1
1:A:155:LEU:HD21	1:A:168:LEU:CG	0.42	2.45	13	2
1:A:179:VAL:HG13	1:A:180:THR:N	0.41	2.30	11	1
1:A:169:LEU:HG	1:A:184:ILE:HD11	0.41	1.91	19	1
1:A:173:TRP:NE1	1:A:179:VAL:HG11	0.41	2.31	20	1
1:A:213:ARG:O	1:A:213:ARG:CG	0.41	2.69	17	2
1:A:149:PHE:N	1:A:191:ILE:HD11	0.41	2.30	18	3
1:A:151:VAL:HG12	1:A:172:ILE:CB	0.41	2.46	11	4
1:A:169:LEU:HD12	1:A:183:VAL:HG12	0.41	1.93	1	1
1:A:195:MET:O	1:A:199:LEU:HB2	0.41	2.15	1	1
1:A:126:LEU:CD2	1:A:128:ILE:HG23	0.41	2.45	5	1
1:A:188:ILE:HG22	1:A:192:ARG:CD	0.40	2.47	13	1
1:A:206:THR:O	1:A:206:THR:HG23	0.40	2.16	8	1
1:A:199:LEU:HD23	1:A:201:ILE:HG12	0.40	1.93	13	1
1:A:136:ILE:HD13	1:A:141:GLU:HA	0.40	1.94	19	1
1:A:159:ARG:CG	1:A:163:VAL:HB	0.40	2.46	11	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	98/109 (90%)	83±1 (85±1%)	12±2 (12±2%)	3±1 (3±1%)	8	43
All	All	1960/2180 (90%)	1667 (85%)	241 (12%)	52 (3%)	8	43

All 7 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	161	GLN	20
1	A	217	PRO	18
1	A	160	ASP	6
1	A	124	GLY	5
1	A	180	THR	1
1	A	211	GLY	1
1	A	176	PRO	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	90/98 (92%)	65±3 (72±3%)	25±3 (28±3%)	2	20
All	All	1800/1960 (92%)	1301 (72%)	499 (28%)	2	20

All 56 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	127	THR	20
1	A	128	ILE	20
1	A	129	SER	20
1	A	149	PHE	20
1	A	162	ILE	20
1	A	126	LEU	19
1	A	157	ARG	19
1	A	140	ARG	18
1	A	134	LYS	17
1	A	164	SER	17
1	A	216	TYR	17

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Mol	Chain	Res	Type	Models (Total)
1	A	154	HIS	17
1	A	180	THR	16
1	A	161	GLN	16
1	A	205	GLU	15
1	A	209	ARG	14
1	A	159	ARG	13
1	A	196	ASP	13
1	A	155	LEU	12
1	A	195	MET	12
1	A	145	LYS	11
1	A	169	LEU	10
1	A	194	LYS	10
1	A	150	GLU	9
1	A	143	GLU	8
1	A	214	PHE	8
1	A	173	TRP	8
1	A	197	LYS	7
1	A	147	LYS	6
1	A	204	VAL	6
1	A	210	ARG	6
1	A	168	LEU	6
1	A	178	MET	6
1	A	183	VAL	5
1	A	189	ASN	5
1	A	125	ASP	5
1	A	199	LEU	5
1	A	152	LEU	5
1	A	160	ASP	4
1	A	182	ASN	4
1	A	163	VAL	4
1	A	138	LYS	3
1	A	202	SER	3
1	A	174	GLU	3
1	A	190	GLN	3
1	A	208	ARG	2
1	A	213	ARG	2
1	A	131	ASP	2
1	A	193	GLN	1
1	A	133	GLU	1
1	A	141	GLU	1
1	A	201	ILE	1
1	A	123	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	132	GLU	1
1	A	192	ARG	1
1	A	177	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

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