



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 12:16 PM UTC

PDB ID : 2CPQ / pdb_00002cpq
Title : Solution structure of the N-terminal KH domain of human FXR1
Authors : Nagata, T.; Muto, Y.; Inoue, M.; Kigawa, T.; Terada, T.; Shirouzu, M.;
Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-05-19

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	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

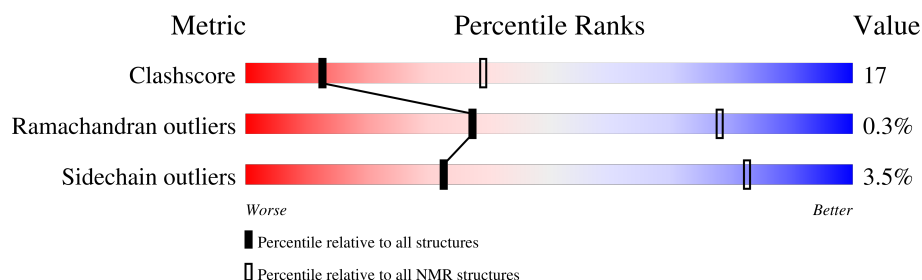
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	91	

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:217-A:280 (64)	0.29	12

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1325 atoms, of which 651 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fragile X mental retardation syndrome related protein 1, isoform b'.

Mol	Chain	Residues	Atoms						Trace
1	A	91	Total	C	H	N	O	S	0
			1325	420	651	116	137	1	

There are 13 discrepancies between the modelled and reference sequences:

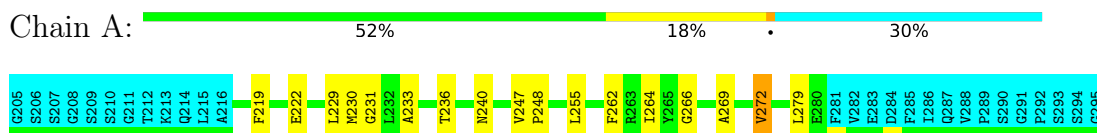
Chain	Residue	Modelled	Actual	Comment	Reference
A	205	GLY	-	cloning artifact	UNP P51114
A	206	SER	-	cloning artifact	UNP P51114
A	207	SER	-	cloning artifact	UNP P51114
A	208	GLY	-	cloning artifact	UNP P51114
A	209	SER	-	cloning artifact	UNP P51114
A	210	SER	-	cloning artifact	UNP P51114
A	211	GLY	-	cloning artifact	UNP P51114
A	290	SER	-	cloning artifact	UNP P51114
A	291	GLY	-	cloning artifact	UNP P51114
A	292	PRO	-	cloning artifact	UNP P51114
A	293	SER	-	cloning artifact	UNP P51114
A	294	SER	-	cloning artifact	UNP P51114
A	295	GLY	-	cloning artifact	UNP P51114

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'

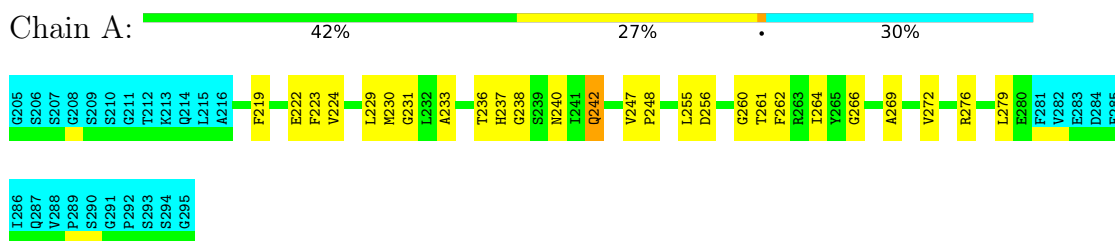


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

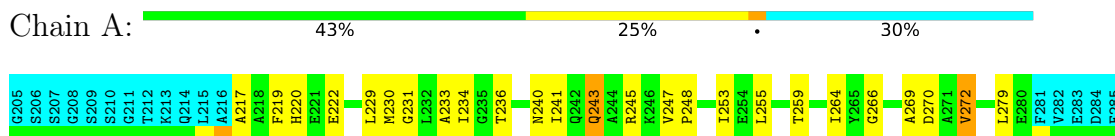
4.2.1 Score per residue for model 1

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



4.2.2 Score per residue for model 2

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



T286
Q287
V288
P289
S290
Q291
P292
S293
S294
Q295

4.2.3 Score per residue for model 3

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'

Chain A: 

G205 S206 S207 G208 S209 S210 G211 T212 K213 Q214 L215 A216 F219 V224 L229 M230 G231 G232 A233 T236 H237 V247 P248 D256 F262 R263 I264 G266 A269 V272 L279 E280 F281 V282 E283 D284 F285 I286 Q287 V288 P289 S290 Q291 P292 S293 S294 G295

4.2.4 Score per residue for model 4

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'

Chain A: 

G205 S206 S207 G208 S209 S210 G211 T212 K213 Q214 L215 A216 E222 L229 M230 G231 L232 A233 T236 H237 V247 P248 D256 F262 R263 I264 G266 V272 L279 E280 F281 V282 E283 D284 F285 I286 Q287 V288 P289 S290 Q291 P292 S293 S294 G295

4.2.5 Score per residue for model 5

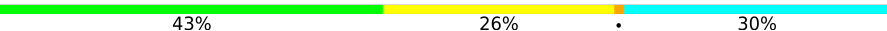
- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'

Chain A: 

G205 S206 S207 G208 S209 S210 G211 T212 K213 Q214 L215 A216 F219 H220 F223 L229 M230 G231 A233 T236 H237 V247 P248 D256 F262 R263 I264 Y265 G266 A269 V272 K273 K274 L279 E280 F281 V282 E283 D284 F285 I286 Q287 V288 P289 S290 Q291 P292 S293 S294 G295

4.2.6 Score per residue for model 6

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'

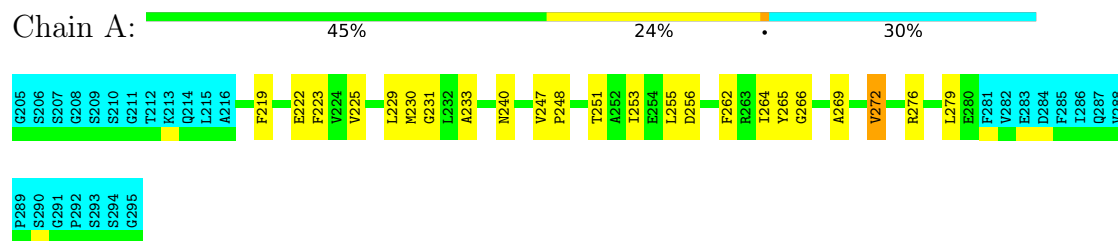
Chain A: 

G205 S206 S207 G208 S209 S210 G211 T212 K213 Q214 L215 A216 F219 F223 V224 D228 L229 M230 G231 L232 G235 T236 H237 Q242 Q243 V247 P248 I253 E254 L255 T261 F262 R263 I264 A269 D270 A271 V272 R276 E280 F281 V282 E283 D284 F285 I286 Q287 V288 P289

S290
Q291
P292
S293
S294
Q295

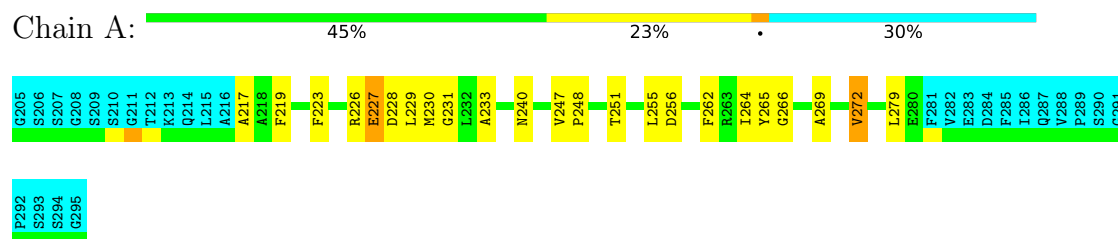
4.2.7 Score per residue for model 7

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



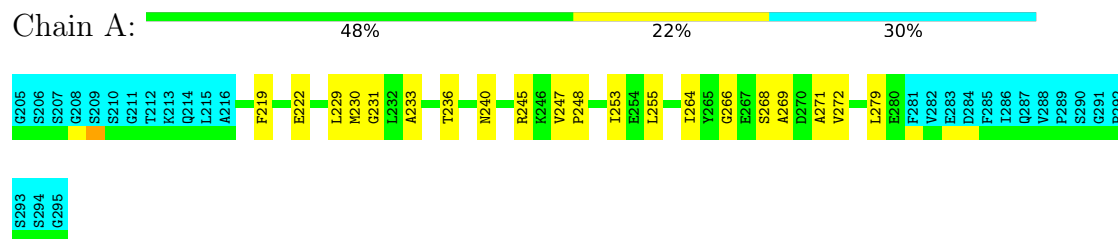
4.2.8 Score per residue for model 8

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



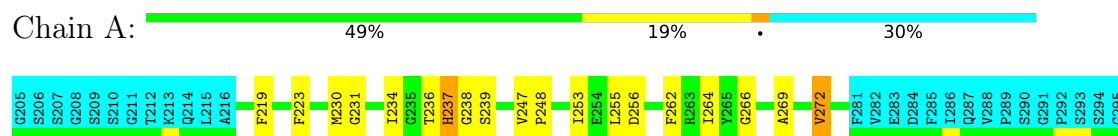
4.2.9 Score per residue for model 9

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



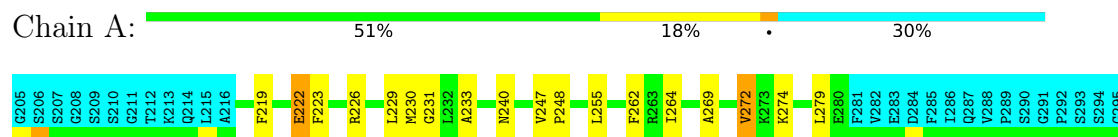
4.2.10 Score per residue for model 10

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



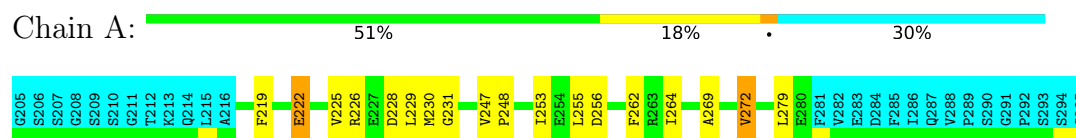
4.2.11 Score per residue for model 11

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



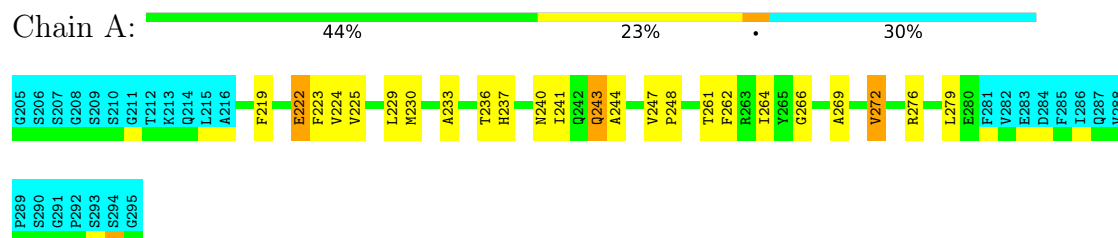
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



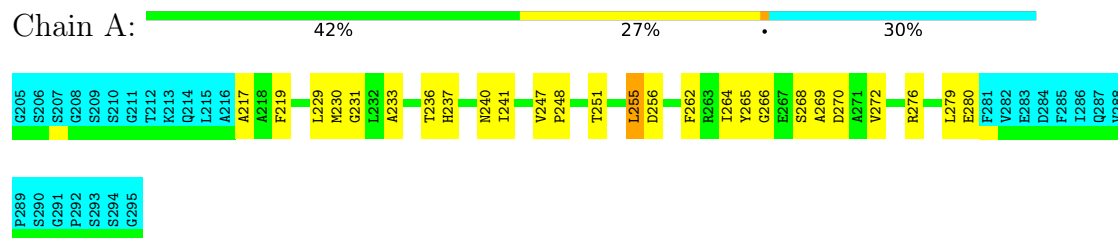
4.2.13 Score per residue for model 13

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



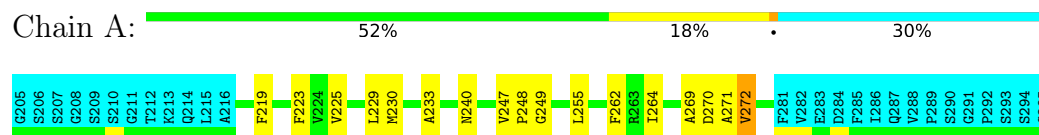
4.2.14 Score per residue for model 14

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



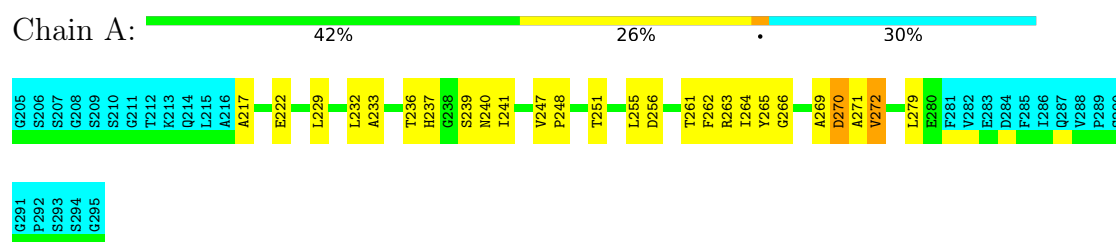
4.2.15 Score per residue for model 15

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



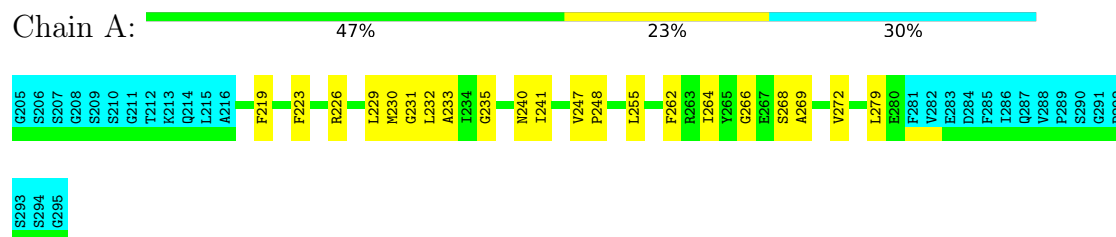
4.2.16 Score per residue for model 16

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



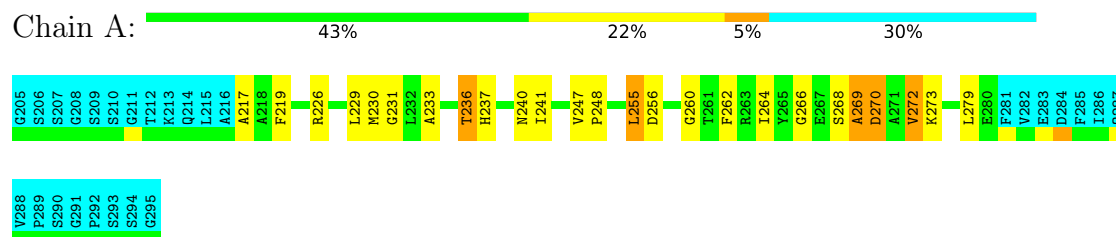
4.2.17 Score per residue for model 17

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



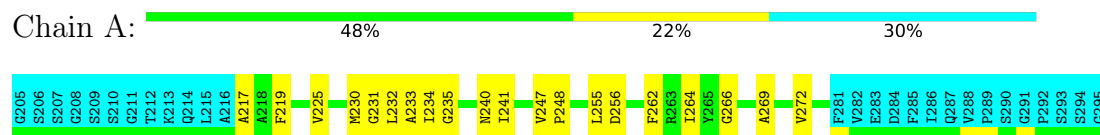
4.2.18 Score per residue for model 18

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



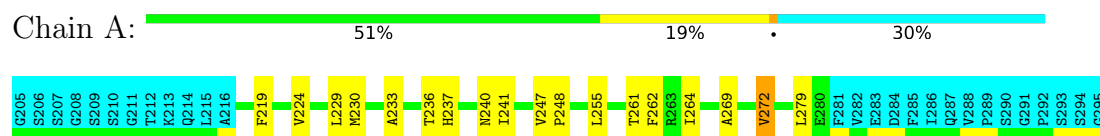
4.2.19 Score per residue for model 19

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



4.2.20 Score per residue for model 20

- Molecule 1: Fragile X mental retardation syndrome related protein 1, isoform b'



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function, structures with the lowest energy, structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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	490	478	478	16±4
All	All	9800	9560	9560	323

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:219:PHE:CD2	1:A:269:ALA:HB2	0.98	1.93	1	18
1:A:230:MET:HE1	1:A:255:LEU:HD11	0.90	1.43	5	8
1:A:264:ILE:HG22	1:A:272:VAL:HG12	0.82	1.51	4	18
1:A:264:ILE:HD11	1:A:279:LEU:HD12	0.81	1.52	9	3
1:A:230:MET:CE	1:A:255:LEU:HD11	0.77	2.09	3	11
1:A:266:GLY:HA3	1:A:272:VAL:HG13	0.74	1.57	9	10
1:A:223:PHE:O	1:A:261:THR:HG23	0.71	1.85	13	1
1:A:262:PHE:CE1	1:A:279:LEU:HD22	0.71	2.21	14	11
1:A:217:ALA:HB1	1:A:266:GLY:O	0.66	1.90	14	4
1:A:253:ILE:HG12	1:A:264:ILE:HG23	0.64	1.70	6	4
1:A:255:LEU:HD22	1:A:262:PHE:CZ	0.63	2.28	15	5
1:A:219:PHE:CE2	1:A:269:ALA:HB2	0.61	2.30	18	1
1:A:255:LEU:HD22	1:A:262:PHE:CE1	0.61	2.31	19	5
1:A:222:GLU:CD	1:A:261:THR:CG2	0.60	2.74	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:264:ILE:CD1	1:A:279:LEU:HD12	0.59	2.25	9	3
1:A:266:GLY:CA	1:A:272:VAL:HG13	0.58	2.28	9	3
1:A:241:ILE:HG12	1:A:279:LEU:HD21	0.58	1.76	5	4
1:A:264:ILE:CG2	1:A:272:VAL:HG12	0.57	2.26	18	12
1:A:222:GLU:CD	1:A:222:GLU:C	0.56	2.74	11	6
1:A:255:LEU:HD12	1:A:256:ASP:N	0.56	2.14	14	3
1:A:255:LEU:HD13	1:A:262:PHE:CZ	0.55	2.36	16	2
1:A:217:ALA:HB1	1:A:266:GLY:C	0.52	2.29	16	3
1:A:247:VAL:HG13	1:A:248:PRO:HD2	0.52	1.82	6	20
1:A:255:LEU:HD12	1:A:256:ASP:H	0.52	1.65	12	3
1:A:266:GLY:N	1:A:272:VAL:CG1	0.51	2.74	9	1
1:A:255:LEU:HD13	1:A:262:PHE:CE1	0.51	2.41	20	2
1:A:255:LEU:HD13	1:A:262:PHE:CE2	0.50	2.40	16	2
1:A:230:MET:HE1	1:A:255:LEU:CD1	0.50	2.28	5	1
1:A:230:MET:O	1:A:231:GLY:C	0.50	2.55	17	15
1:A:222:GLU:OE1	1:A:261:THR:CG2	0.50	2.60	16	1
1:A:224:VAL:HG22	1:A:261:THR:OG1	0.49	2.08	6	5
1:A:244:ALA:O	1:A:247:VAL:HG23	0.49	2.06	13	1
1:A:236:THR:O	1:A:237:HIS:C	0.49	2.55	14	9
1:A:233:ALA:O	1:A:240:ASN:CG	0.49	2.55	5	9
1:A:226:ARG:O	1:A:229:LEU:N	0.49	2.45	8	3
1:A:223:PHE:CE2	1:A:262:PHE:HB2	0.49	2.42	8	6
1:A:242:GLN:OE1	1:A:242:GLN:N	0.49	2.46	1	1
1:A:234:ILE:HG23	1:A:241:ILE:HG13	0.49	1.84	19	2
1:A:232:LEU:O	1:A:235:GLY:N	0.49	2.46	17	3
1:A:243:GLN:NE2	1:A:243:GLN:N	0.48	2.61	2	1
1:A:269:ALA:O	1:A:271:ALA:N	0.48	2.46	16	1
1:A:238:GLY:O	1:A:242:GLN:NE2	0.48	2.47	1	1
1:A:256:ASP:O	1:A:260:GLY:N	0.48	2.47	18	2
1:A:223:PHE:CD1	1:A:223:PHE:N	0.48	2.82	15	1
1:A:236:THR:O	1:A:236:THR:HG23	0.47	2.07	9	2
1:A:226:ARG:O	1:A:228:ASP:N	0.47	2.47	8	1
1:A:262:PHE:CD1	1:A:279:LEU:HD13	0.47	2.44	11	2
1:A:223:PHE:CZ	1:A:262:PHE:CB	0.47	2.98	10	2
1:A:256:ASP:CG	1:A:263:ARG:NH2	0.47	2.73	4	1
1:A:276:ARG:CZ	1:A:280:GLU:OE1	0.47	2.63	6	1
1:A:256:ASP:OD2	1:A:263:ARG:CZ	0.47	2.62	4	1
1:A:255:LEU:HB2	1:A:262:PHE:CE1	0.47	2.45	16	1
1:A:234:ILE:HG22	1:A:238:GLY:HA2	0.46	1.85	10	1
1:A:229:LEU:O	1:A:230:MET:C	0.46	2.59	4	8
1:A:233:ALA:O	1:A:240:ASN:CB	0.46	2.63	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:236:THR:O	1:A:238:GLY:N	0.46	2.48	10	1
1:A:222:GLU:CD	1:A:222:GLU:O	0.46	2.58	1	3
1:A:238:GLY:O	1:A:242:GLN:CD	0.46	2.58	1	1
1:A:222:GLU:OE1	1:A:261:THR:HG22	0.45	2.11	16	1
1:A:222:GLU:CD	1:A:263:ARG:CG	0.45	2.90	16	1
1:A:269:ALA:O	1:A:270:ASP:C	0.45	2.58	16	1
1:A:243:GLN:OE1	1:A:243:GLN:N	0.45	2.49	13	1
1:A:226:ARG:C	1:A:228:ASP:N	0.45	2.72	8	2
1:A:232:LEU:O	1:A:233:ALA:C	0.45	2.60	17	1
1:A:240:ASN:O	1:A:241:ILE:C	0.45	2.58	16	5
1:A:226:ARG:O	1:A:227:GLU:C	0.45	2.60	8	1
1:A:269:ALA:C	1:A:271:ALA:N	0.45	2.73	16	1
1:A:268:SER:O	1:A:269:ALA:C	0.44	2.58	14	4
1:A:233:ALA:O	1:A:240:ASN:ND2	0.44	2.49	18	3
1:A:228:ASP:C	1:A:228:ASP:OD1	0.44	2.59	6	1
1:A:276:ARG:NH1	1:A:280:GLU:CD	0.44	2.75	14	1
1:A:257:GLU:O	1:A:258:ASP:C	0.44	2.61	3	1
1:A:222:GLU:C	1:A:222:GLU:OE2	0.44	2.61	11	2
1:A:268:SER:C	1:A:270:ASP:N	0.44	2.75	18	2
1:A:269:ALA:O	1:A:273:LYS:CG	0.44	2.66	5	2
1:A:251:THR:N	1:A:265:TYR:O	0.44	2.51	7	4
1:A:266:GLY:N	1:A:272:VAL:HG13	0.44	2.28	10	2
1:A:256:ASP:OD1	1:A:263:ARG:NH2	0.44	2.50	4	1
1:A:236:THR:C	1:A:238:GLY:N	0.43	2.76	10	1
1:A:223:PHE:CE1	1:A:276:ARG:HG3	0.43	2.48	7	3
1:A:219:PHE:CG	1:A:269:ALA:N	0.43	2.86	18	1
1:A:223:PHE:CZ	1:A:262:PHE:HB2	0.43	2.49	10	1
1:A:234:ILE:HG22	1:A:234:ILE:O	0.43	2.13	10	1
1:A:222:GLU:OE1	1:A:222:GLU:C	0.43	2.61	12	1
1:A:220:HIS:CD2	1:A:220:HIS:O	0.43	2.72	5	1
1:A:245:ARG:HG3	1:A:253:ILE:HD12	0.43	1.90	2	1
1:A:256:ASP:O	1:A:260:GLY:CA	0.42	2.67	1	1
1:A:220:HIS:O	1:A:220:HIS:CD2	0.42	2.72	2	1
1:A:222:GLU:CG	1:A:263:ARG:HG2	0.42	2.44	4	1
1:A:255:LEU:HD13	1:A:262:PHE:CD1	0.42	2.50	20	1
1:A:242:GLN:O	1:A:243:GLN:C	0.42	2.62	6	1
1:A:255:LEU:HD13	1:A:262:PHE:CD2	0.42	2.49	15	1
1:A:268:SER:O	1:A:270:ASP:N	0.42	2.53	18	2
1:A:236:THR:O	1:A:239:SER:N	0.42	2.53	10	1
1:A:239:SER:O	1:A:240:ASN:C	0.42	2.63	16	1
1:A:222:GLU:CD	1:A:263:ARG:HG3	0.41	2.39	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:ARG:HB2	1:A:229:LEU:HD12	0.41	1.92	12	2
1:A:245:ARG:N	1:A:253:ILE:HD12	0.41	2.31	9	1
1:A:217:ALA:HB1	1:A:266:GLY:N	0.41	2.31	16	2
1:A:268:SER:O	1:A:271:ALA:N	0.41	2.54	9	1
1:A:249:GLY:HA3	1:A:271:ALA:HB2	0.41	1.91	15	1
1:A:234:ILE:O	1:A:240:ASN:N	0.40	2.54	2	1
1:A:262:PHE:CD1	1:A:279:LEU:HD22	0.40	2.51	12	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	64/91 (70%)	57±2 (89±3%)	7±2 (10±3%)	0±0 (0±1%)	37	78
All	All	1280/1820 (70%)	1144 (89%)	132 (10%)	4 (0%)	37	78

All 4 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	227	GLU	1
1	A	237	HIS	1
1	A	270	ASP	1
1	A	269	ALA	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	49/70 (70%)	47±1 (97±2%)	2±1 (3±2%)	32	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	980/1400 (70%)	946 (97%)	34 (3%)	32 82

All 10 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	272	VAL	15
1	A	270	ASP	4
1	A	256	ASP	3
1	A	222	GLU	3
1	A	243	GLN	2
1	A	274	LYS	2
1	A	255	LEU	2
1	A	242	GLN	1
1	A	259	THR	1
1	A	236	THR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided