Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 08:22 PM BST

PDB ID	:	2EQS
Title	:	Solution structure of the S1 RNA binding domain of human ATP-dependent RNA helicase DHX8
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Deposited on	:	2007-03-30

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 (i) symbol.

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

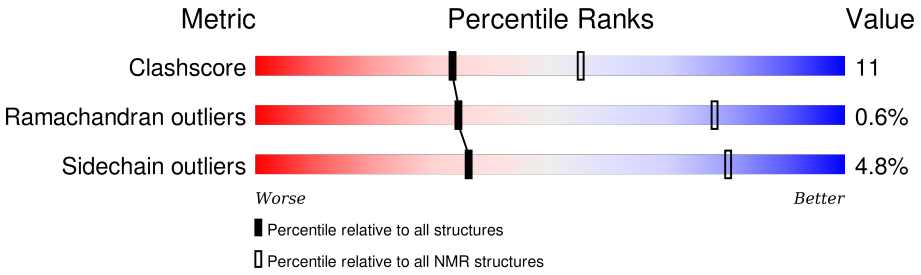
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	103	62% 14% 24%

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:260-A:300, A:309-A:345 (78)	0.26	17

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1601 atoms, of which 806 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms						Trace
1	A	103	Total	C	H	N	O	S	0
			1601	488	806	149	155	3	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	GLY	-	EXPRESSION TAG	UNP Q14562
A	254	SER	-	EXPRESSION TAG	UNP Q14562
A	255	SER	-	EXPRESSION TAG	UNP Q14562
A	256	GLY	-	EXPRESSION TAG	UNP Q14562
A	257	SER	-	EXPRESSION TAG	UNP Q14562
A	258	SER	-	EXPRESSION TAG	UNP Q14562
A	259	GLY	-	EXPRESSION TAG	UNP Q14562

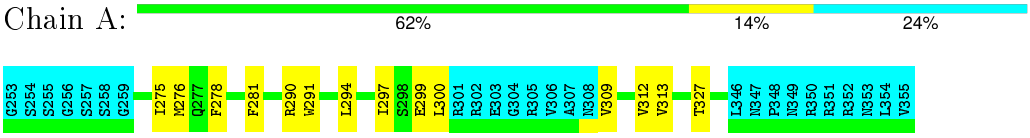
4 Residue-property plots

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: ATP-dependent RNA helicase DHX8

Chain A:



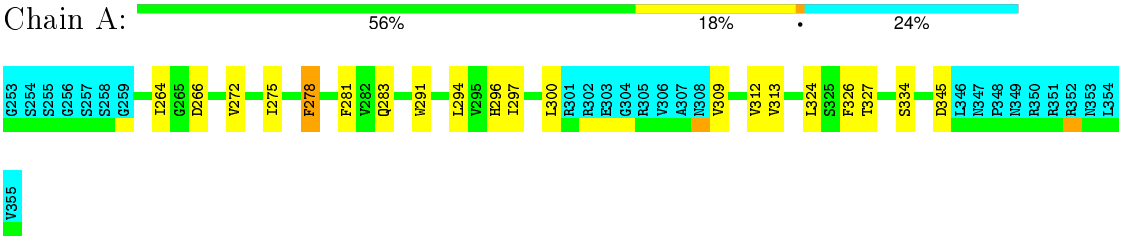
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: ATP-dependent RNA helicase DHX8

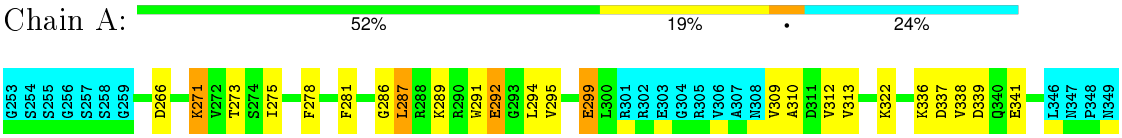
Chain A:

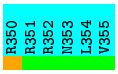


4.2.2 Score per residue for model 2

- Molecule 1: ATP-dependent RNA helicase DHX8

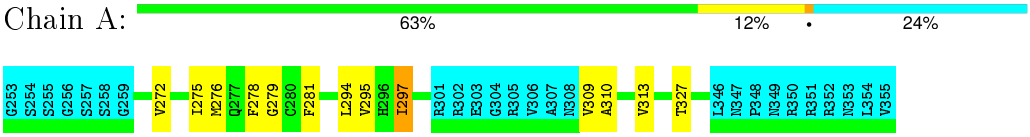
Chain A:





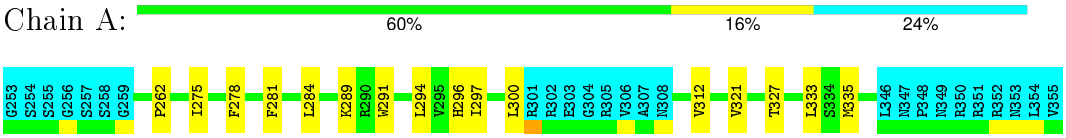
4.2.3 Score per residue for model 3

• Molecule 1: ATP-dependent RNA helicase DHX8



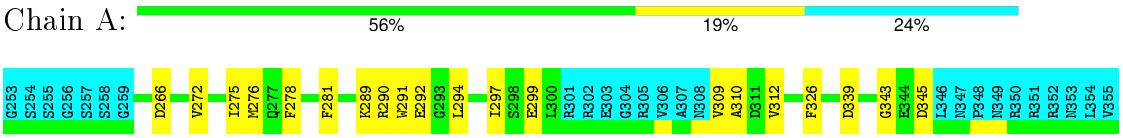
4.2.4 Score per residue for model 4

• Molecule 1: ATP-dependent RNA helicase DHX8



4.2.5 Score per residue for model 5

• Molecule 1: ATP-dependent RNA helicase DHX8



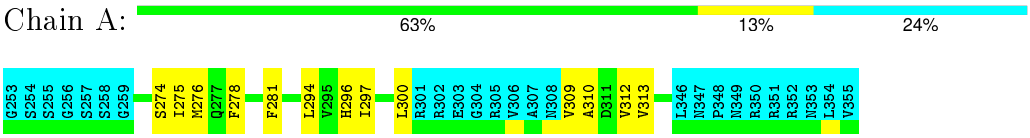
4.2.6 Score per residue for model 6

• Molecule 1: ATP-dependent RNA helicase DHX8

4.2.7 Score per residue for model 7

• Molecule 1: ATP-dependent RNA helicase DHX8

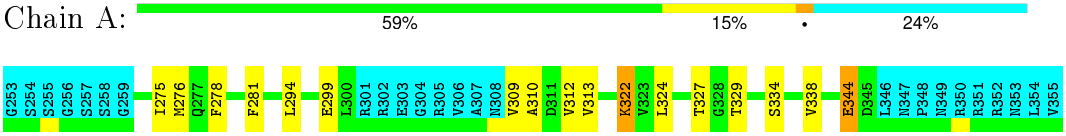
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: ATP-dependent RNA helicase DHX8

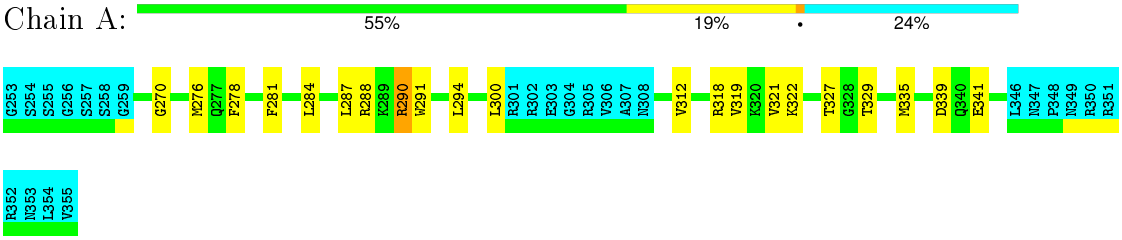
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: ATP-dependent RNA helicase DHX8

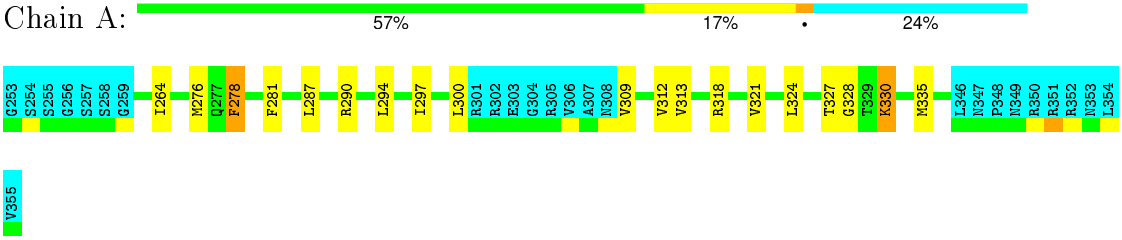
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: ATP-dependent RNA helicase DHX8

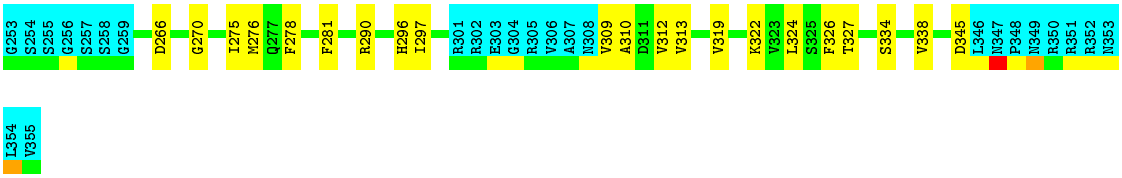
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: ATP-dependent RNA helicase DHX8

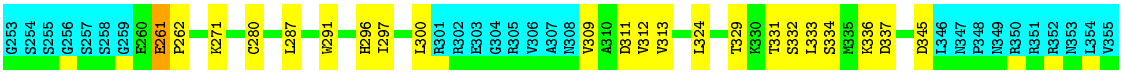
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: ATP-dependent RNA helicase DHX8

Chain A:



4.2.13 Score per residue for model 13

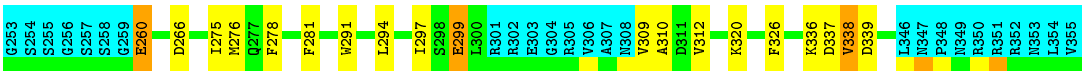
- Molecule 1: ATP-dependent RNA helicase DHX8

Chain A:

4.2.14 Score per residue for model 14

- Molecule 1: ATP-dependent RNA helicase DHX8

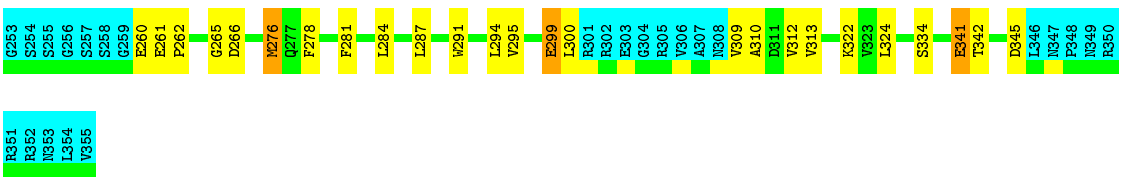
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: ATP-dependent RNA helicase DHX8

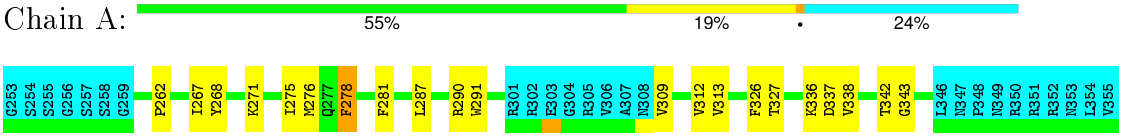
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: ATP-dependent RNA helicase DHX8

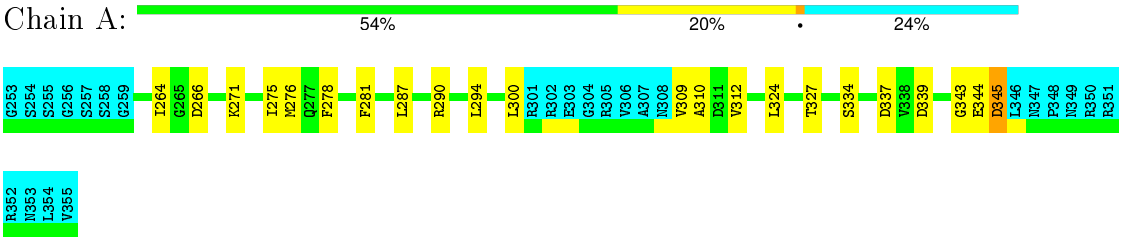
Chain A:



4.2.17 Score per residue for model 17 (medoid)

• Molecule 1: ATP-dependent RNA helicase DHX8

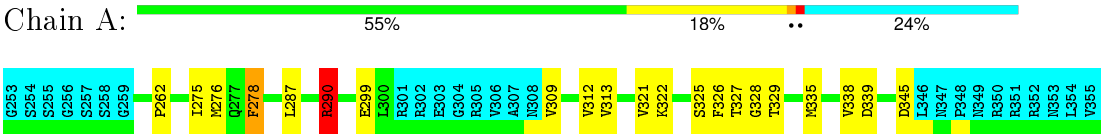
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: ATP-dependent RNA helicase DHX8

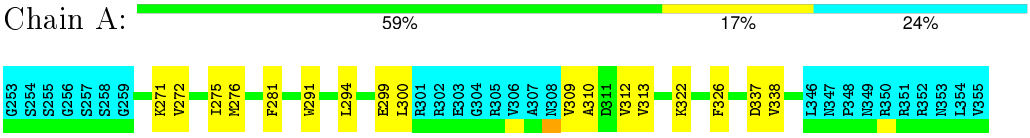
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: ATP-dependent RNA helicase DHX8

Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: ATP-dependent RNA helicase DHX8

Chain A:


G253
S254
S255
G256
S257
S258
G259
T275
M276
Q277
F278
G279
C280
L284
W291
L300
R301
R302
E303
G304
R305
V306
A307
N308
V309
A310
D311
V312
V313
V321
L324
T327
L333
S334
L346
N347
P348
N349
R350
R351
R352
N353
L354
V355

5 Refinement protocol and experimental data overview

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

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

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. 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	606	614	614	13±3
All	All	12120	12280	12280	266

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:300:LEU:HD13	1:A:312:VAL:HG11	0.93	1.37	20	7
1:A:297:ILE:HD13	1:A:297:ILE:O	0.71	1.85	3	1
1:A:281:PHE:CE1	1:A:294:LEU:HD13	0.71	2.20	1	5
1:A:309:VAL:HG12	1:A:313:VAL:HG22	0.68	1.64	19	12
1:A:284:LEU:HD12	1:A:291:TRP:HB2	0.65	1.66	15	4
1:A:281:PHE:CD1	1:A:294:LEU:HD13	0.63	2.28	1	1
1:A:264:ILE:HG23	1:A:324:LEU:O	0.60	1.96	1	3
1:A:291:TRP:CH2	1:A:326:PHE:CE1	0.60	2.90	14	2
1:A:276:MET:SD	1:A:281:PHE:CE2	0.60	2.95	14	3
1:A:321:VAL:HG12	1:A:335:MET:HG2	0.58	1.74	9	4
1:A:276:MET:SD	1:A:278:PHE:CZ	0.58	2.97	14	2
1:A:276:MET:CE	1:A:281:PHE:CD2	0.58	2.86	13	1
1:A:276:MET:CB	1:A:278:PHE:CE1	0.58	2.86	15	2
1:A:276:MET:SD	1:A:278:PHE:CE2	0.57	2.97	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:324:LEU:HD11	1:A:334:SER:HB2	0.57	1.75	20	4
1:A:320:LYS:C	1:A:338:VAL:HG11	0.56	2.21	14	1
1:A:332:SER:O	1:A:333:LEU:HD23	0.55	2.02	12	1
1:A:321:VAL:HG21	1:A:333:LEU:HD13	0.55	1.77	20	1
1:A:324:LEU:HD11	1:A:334:SER:HB3	0.55	1.77	13	1
1:A:275:ILE:HG23	1:A:309:VAL:CG1	0.55	2.31	5	2
1:A:276:MET:SD	1:A:281:PHE:CD2	0.55	3.00	13	3
1:A:281:PHE:CZ	1:A:294:LEU:HD13	0.54	2.38	17	1
1:A:329:THR:O	1:A:329:THR:HG22	0.53	2.03	9	2
1:A:275:ILE:N	1:A:275:ILE:HD12	0.53	2.18	2	5
1:A:262:PRO:HG2	1:A:326:PHE:CD2	0.53	2.38	18	1
1:A:341:GLU:CA	1:A:341:GLU:OE1	0.53	2.57	15	1
1:A:271:LYS:NZ	1:A:273:THR:HG22	0.53	2.19	2	1
1:A:324:LEU:HD11	1:A:334:SER:OG	0.52	2.04	1	1
1:A:262:PRO:CG	1:A:326:PHE:CD2	0.52	2.92	18	1
1:A:272:VAL:HG11	1:A:275:ILE:HD11	0.51	1.82	1	4
1:A:309:VAL:CG1	1:A:313:VAL:HG22	0.51	2.34	19	2
1:A:309:VAL:O	1:A:312:VAL:N	0.51	2.44	5	8
1:A:275:ILE:HG23	1:A:309:VAL:HG12	0.51	1.83	13	2
1:A:297:ILE:HD12	1:A:309:VAL:HG23	0.51	1.81	14	1
1:A:261:GLU:OE1	1:A:261:GLU:CA	0.51	2.59	12	1
1:A:321:VAL:HG12	1:A:335:MET:CG	0.50	2.36	9	2
1:A:276:MET:HB3	1:A:278:PHE:CZ	0.50	2.40	20	12
1:A:299:GLU:N	1:A:299:GLU:CD	0.50	2.65	2	1
1:A:322:LYS:N	1:A:338:VAL:HG21	0.50	2.22	8	2
1:A:327:THR:O	1:A:327:THR:HG23	0.50	2.07	4	5
1:A:295:VAL:CG1	1:A:299:GLU:O	0.50	2.60	15	2
1:A:337:ASP:O	1:A:338:VAL:CG2	0.50	2.60	14	1
1:A:276:MET:CE	1:A:294:LEU:CD1	0.49	2.89	10	3
1:A:261:GLU:OE1	1:A:261:GLU:N	0.49	2.44	12	1
1:A:291:TRP:CH2	1:A:326:PHE:CZ	0.49	3.00	14	3
1:A:297:ILE:HD13	1:A:297:ILE:C	0.49	2.27	3	1
1:A:289:LYS:HE2	1:A:291:TRP:CZ2	0.49	2.43	2	1
1:A:327:THR:O	1:A:328:GLY:C	0.49	2.50	10	1
1:A:276:MET:O	1:A:309:VAL:HG21	0.49	2.07	20	1
1:A:276:MET:HE1	1:A:281:PHE:CD2	0.48	2.42	13	1
1:A:344:GLU:N	1:A:344:GLU:OE1	0.48	2.47	8	1
1:A:284:LEU:HD12	1:A:291:TRP:CB	0.48	2.35	15	1
1:A:324:LEU:HD21	1:A:334:SER:HB3	0.48	1.84	11	1
1:A:344:GLU:CD	1:A:345:ASP:N	0.48	2.66	17	1
1:A:336:LYS:O	1:A:338:VAL:N	0.48	2.46	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:321:VAL:HG23	1:A:333:LEU:HD22	0.48	1.86	20	1
1:A:327:THR:HG23	1:A:327:THR:O	0.48	2.08	20	3
1:A:284:LEU:HD21	1:A:333:LEU:HD22	0.48	1.86	4	1
1:A:289:LYS:HG2	1:A:291:TRP:CZ2	0.48	2.43	13	1
1:A:312:VAL:HG12	1:A:313:VAL:HG13	0.48	1.86	19	5
1:A:276:MET:HG2	1:A:278:PHE:CZ	0.48	2.43	15	4
1:A:337:ASP:O	1:A:338:VAL:HG23	0.47	2.09	14	1
1:A:322:LYS:CB	1:A:338:VAL:CG2	0.47	2.92	8	1
1:A:275:ILE:HD12	1:A:275:ILE:N	0.47	2.25	8	6
1:A:276:MET:CB	1:A:278:PHE:CZ	0.47	2.98	20	2
1:A:276:MET:HE1	1:A:281:PHE:CG	0.47	2.44	13	2
1:A:283:GLN:NE2	1:A:291:TRP:O	0.47	2.48	1	1
1:A:299:GLU:N	1:A:299:GLU:OE1	0.47	2.48	19	1
1:A:291:TRP:CZ2	1:A:326:PHE:CZ	0.47	3.03	6	1
1:A:276:MET:O	1:A:309:VAL:CG2	0.47	2.62	20	1
1:A:262:PRO:HB2	1:A:323:VAL:HG21	0.47	1.87	13	1
1:A:281:PHE:CE2	1:A:294:LEU:HD13	0.46	2.45	17	6
1:A:289:LYS:HG2	1:A:291:TRP:CE2	0.46	2.45	13	1
1:A:276:MET:HB3	1:A:278:PHE:CE1	0.46	2.44	3	5
1:A:262:PRO:HD3	1:A:291:TRP:CD1	0.46	2.46	4	2
1:A:275:ILE:HG21	1:A:310:ALA:HA	0.46	1.86	14	2
1:A:326:PHE:C	1:A:326:PHE:CD1	0.46	2.89	1	3
1:A:292:GLU:C	1:A:292:GLU:CD	0.46	2.74	2	1
1:A:280:CYS:HB3	1:A:309:VAL:HG11	0.45	1.88	20	2
1:A:321:VAL:CG2	1:A:333:LEU:HD22	0.45	2.41	20	1
1:A:272:VAL:CG1	1:A:275:ILE:HD11	0.45	2.41	5	3
1:A:267:ILE:C	1:A:268:TYR:CD1	0.45	2.89	16	1
1:A:300:LEU:HB3	1:A:312:VAL:HG11	0.45	1.88	4	2
1:A:287:LEU:O	1:A:290:ARG:NH2	0.45	2.50	6	3
1:A:299:GLU:O	1:A:300:LEU:HD23	0.45	2.11	6	1
1:A:336:LYS:O	1:A:337:ASP:C	0.45	2.55	2	2
1:A:299:GLU:O	1:A:336:LYS:CG	0.45	2.65	14	1
1:A:281:PHE:CE1	1:A:294:LEU:HB2	0.45	2.46	7	2
1:A:309:VAL:O	1:A:310:ALA:C	0.45	2.55	11	4
1:A:276:MET:CG	1:A:278:PHE:CZ	0.45	2.99	15	1
1:A:278:PHE:O	1:A:297:ILE:N	0.44	2.50	6	2
1:A:296:HIS:CE1	1:A:297:ILE:HG22	0.44	2.47	7	4
1:A:337:ASP:O	1:A:337:ASP:CG	0.44	2.56	14	1
1:A:276:MET:CB	1:A:278:PHE:CE2	0.44	3.01	10	1
1:A:260:GLU:CD	1:A:260:GLU:C	0.44	2.76	14	1
1:A:272:VAL:HG11	1:A:275:ILE:CD1	0.44	2.43	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:309:VAL:HG12	1:A:313:VAL:CG2	0.44	2.42	12	1
1:A:345:ASP:OD1	1:A:345:ASP:C	0.43	2.57	11	1
1:A:326:PHE:CD1	1:A:326:PHE:C	0.43	2.92	16	1
1:A:262:PRO:HD3	1:A:291:TRP:NE1	0.43	2.29	15	2
1:A:265:GLY:O	1:A:322:LYS:NZ	0.43	2.50	15	1
1:A:286:GLY:O	1:A:287:LEU:C	0.43	2.56	2	2
1:A:327:THR:O	1:A:329:THR:N	0.43	2.52	18	1
1:A:327:THR:OG1	1:A:330:LYS:CB	0.42	2.66	10	1
1:A:272:VAL:CG1	1:A:275:ILE:CD1	0.42	2.97	3	3
1:A:278:PHE:CD1	1:A:278:PHE:N	0.42	2.87	16	1
1:A:336:LYS:C	1:A:338:VAL:N	0.42	2.71	16	1
1:A:276:MET:SD	1:A:276:MET:N	0.42	2.92	11	2
1:A:300:LEU:HD11	1:A:309:VAL:HG22	0.42	1.90	12	1
1:A:329:THR:HG22	1:A:329:THR:O	0.42	2.15	8	1
1:A:322:LYS:HB2	1:A:338:VAL:CG2	0.42	2.45	11	4
1:A:292:GLU:C	1:A:292:GLU:OE2	0.42	2.58	2	1
1:A:262:PRO:HD3	1:A:287:LEU:HD13	0.42	1.92	15	1
1:A:324:LEU:HD21	1:A:334:SER:HB2	0.41	1.92	8	1
1:A:289:LYS:CD	1:A:291:TRP:CZ2	0.41	3.03	5	1
1:A:278:PHE:N	1:A:278:PHE:CD1	0.41	2.89	1	1
1:A:260:GLU:OE2	1:A:260:GLU:C	0.41	2.59	14	1
1:A:339:ASP:CG	1:A:341:GLU:CD	0.41	2.79	2	1
1:A:283:GLN:NE2	1:A:291:TRP:C	0.41	2.74	1	1
1:A:287:LEU:O	1:A:288:ARG:C	0.41	2.59	9	1
1:A:318:ARG:CZ	1:A:318:ARG:HB2	0.41	2.46	9	1
1:A:279:GLY:CA	1:A:295:VAL:O	0.41	2.69	3	1
1:A:341:GLU:OE1	1:A:341:GLU:N	0.41	2.53	15	1
1:A:291:TRP:CE3	1:A:331:THR:OG1	0.41	2.71	12	1
1:A:276:MET:HE3	1:A:294:LEU:CD1	0.41	2.46	3	1
1:A:339:ASP:OD2	1:A:341:GLU:N	0.40	2.54	9	1
1:A:260:GLU:O	1:A:261:GLU:OE1	0.40	2.39	15	1
1:A:342:THR:HG23	1:A:343:GLY:N	0.40	2.31	16	1
1:A:337:ASP:C	1:A:338:VAL:HG23	0.40	2.37	14	1
1:A:284:LEU:HD21	1:A:333:LEU:CD2	0.40	2.45	4	1
1:A:339:ASP:O	1:A:343:GLY:N	0.40	2.54	17	2
1:A:270:GLY:O	1:A:319:VAL:O	0.40	2.40	9	2

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	78/103 (76%)	69±3 (88±3%)	9±2 (11±3%)	1±1 (1±1%)	34 78
All	All	1560/2060 (76%)	1372 (88%)	178 (11%)	10 (1%)	34 78

All 6 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	287	LEU	3
1	A	290	ARG	2
1	A	296	HIS	2
1	A	338	VAL	1
1	A	337	ASP	1
1	A	328	GLY	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	69/89 (78%)	66±1 (95±2%)	3±1 (5±2%)	36 80
All	All	1380/1780 (78%)	1314 (95%)	66 (5%)	36 80

All 25 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	266	ASP	8
1	A	290	ARG	7
1	A	278	PHE	6
1	A	271	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	299	GLU	6
1	A	345	ASP	5
1	A	327	THR	3
1	A	292	GLU	3
1	A	289	LYS	2
1	A	322	LYS	2
1	A	311	ASP	2
1	A	276	MET	2
1	A	288	ARG	2
1	A	260	GLU	1
1	A	344	GLU	1
1	A	318	ARG	1
1	A	297	ILE	1
1	A	337	ASP	1
1	A	274	SER	1
1	A	325	SER	1
1	A	261	GLU	1
1	A	277	GLN	1
1	A	330	LYS	1
1	A	342	THR	1
1	A	341	GLU	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 carbohydrates 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