Full wwPDB NMR Structure Validation Report (i)

Mar 3, 2022 – 12:17 PM EST

PDB ID	:	2HST
Title	:	Solution structure of the middle domain of human eukaryotic translation termination factor eRF1
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Deposited on	:	2006-07-23

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 (i) symbol.

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

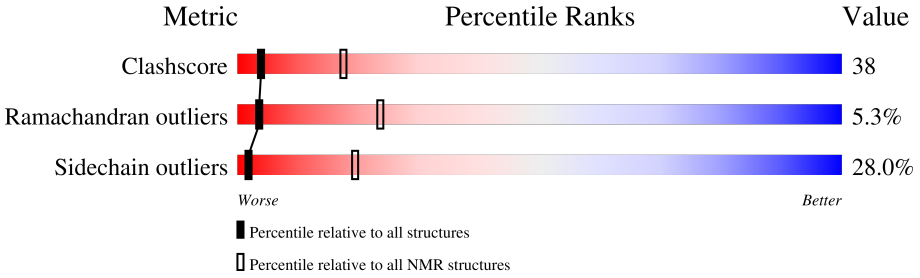
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	143	27% 38% 10% • 19% 5%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:143-A:176, A:197-A:271 (109)	0.22	11

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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2121 atoms, of which 1068 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	136	2121	664	1068	188	199	2	0

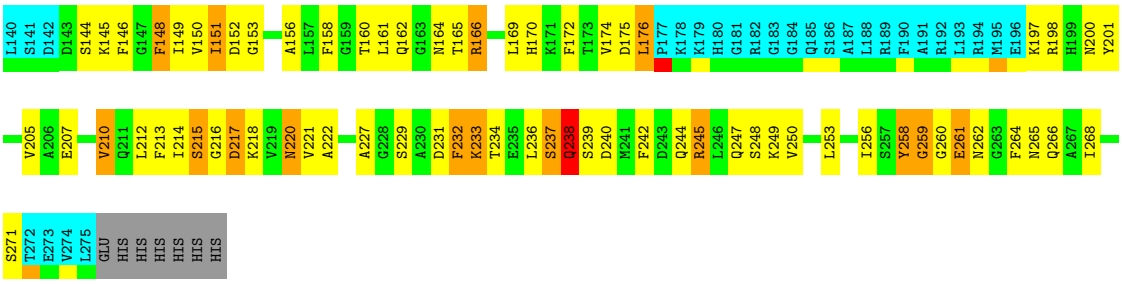
4 Residue-property plots (i)

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: Eukaryotic peptide chain release factor subunit 1

Chain A: 27% 38% 10% • 19% 5%



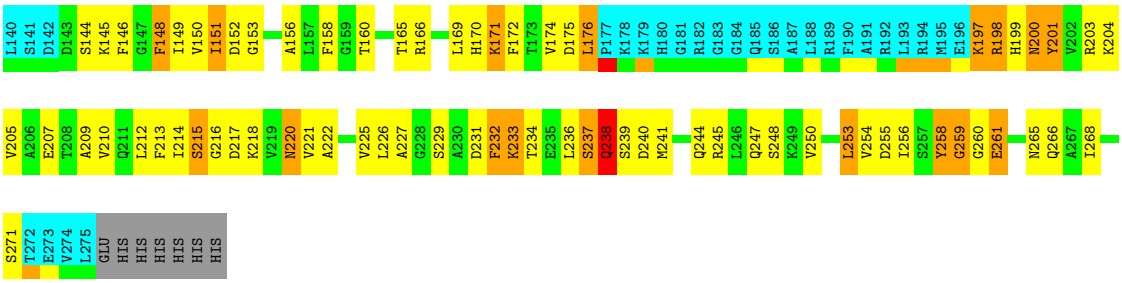
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Eukaryotic peptide chain release factor subunit 1

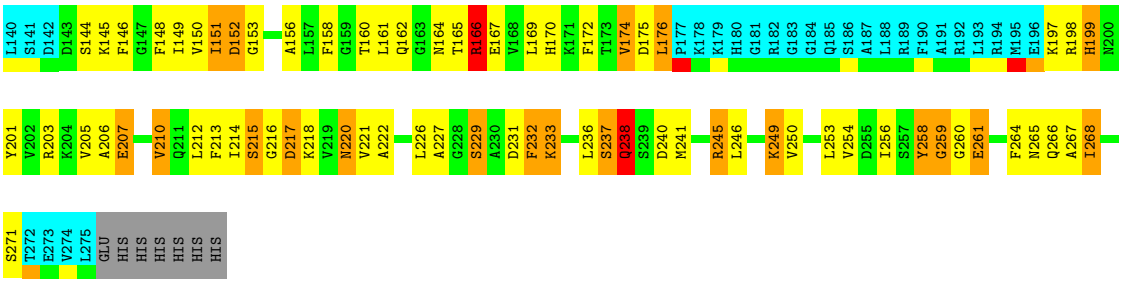
Chain A: 25% 38% 12% • 19% 5%



4.2.2 Score per residue for model 2

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

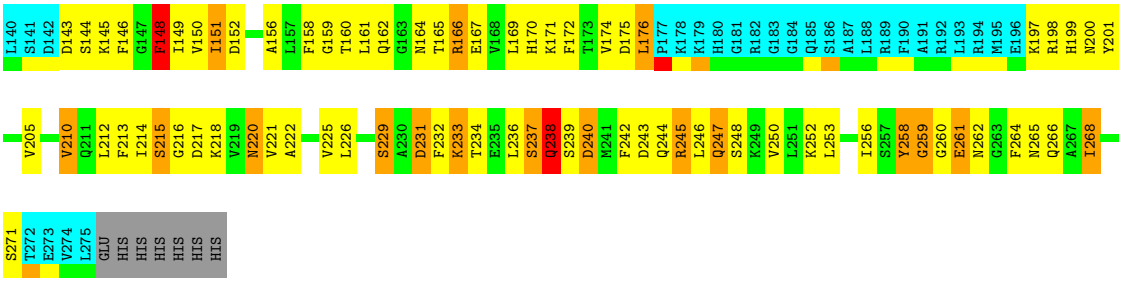
Chain A: 27% 34% 14% • 19% 5%



4.2.3 Score per residue for model 3

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

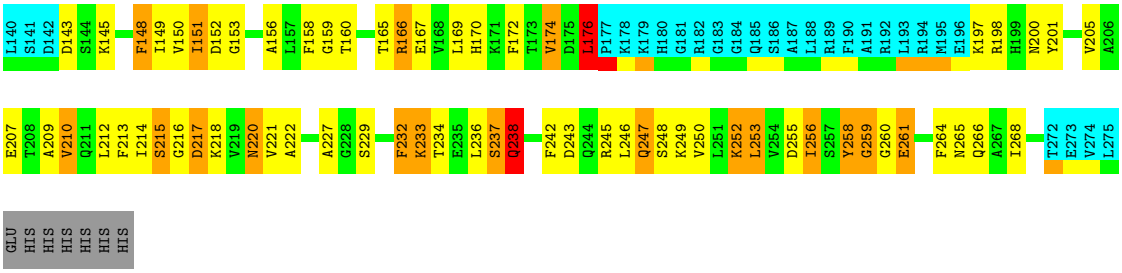
Chain A: 23% 40% 12% • 19% 5%



4.2.4 Score per residue for model 4

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

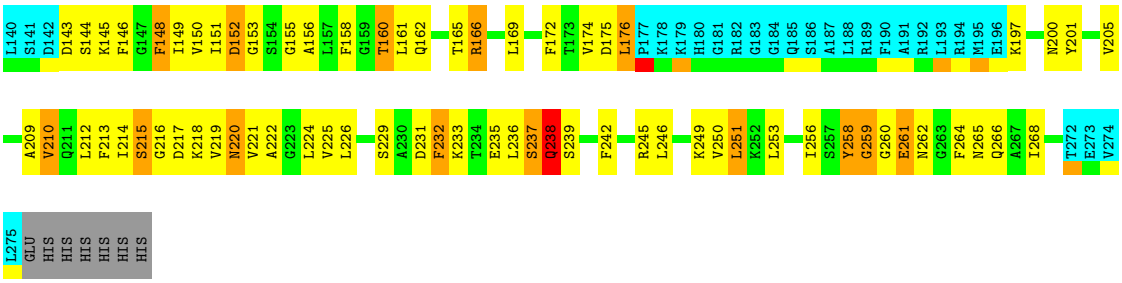
Chain A: 30% 32% 13% • 19% 5%



4.2.5 Score per residue for model 5

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

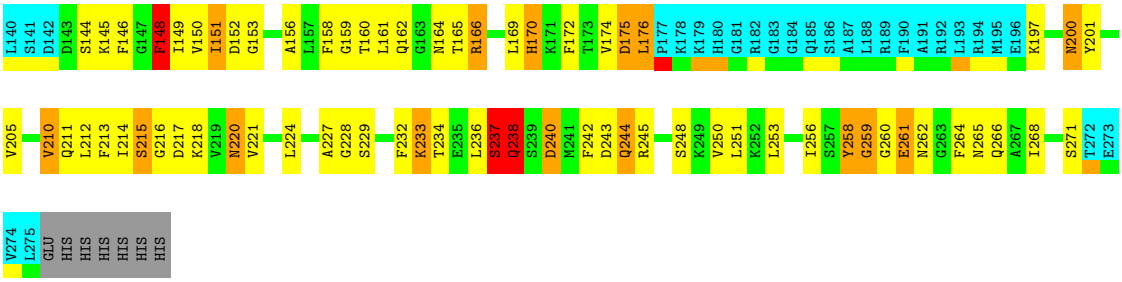
Chain A: 28% 38% 10% • 19% 5%



4.2.6 Score per residue for model 6

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

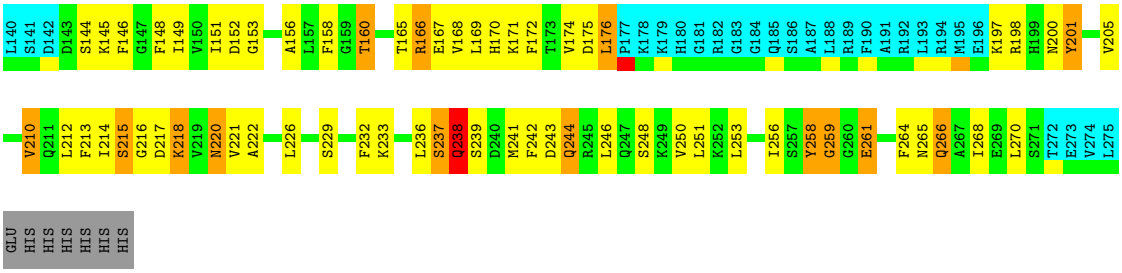
Chain A: 28% 36% 10% • 19% 5%



4.2.7 Score per residue for model 7

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

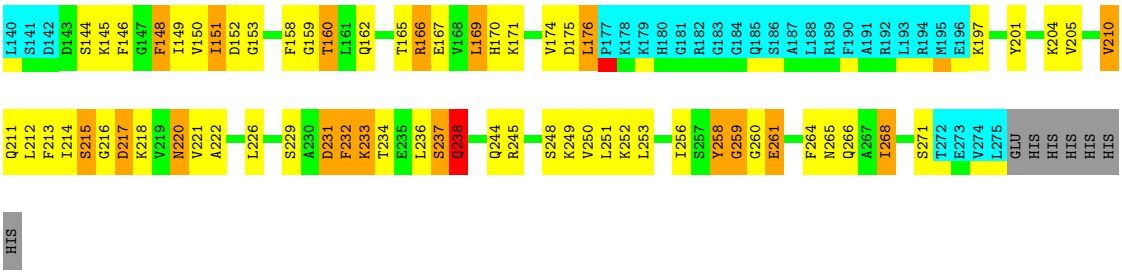
Chain A: 31% 34% 10% • 19% 5%



4.2.8 Score per residue for model 8

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

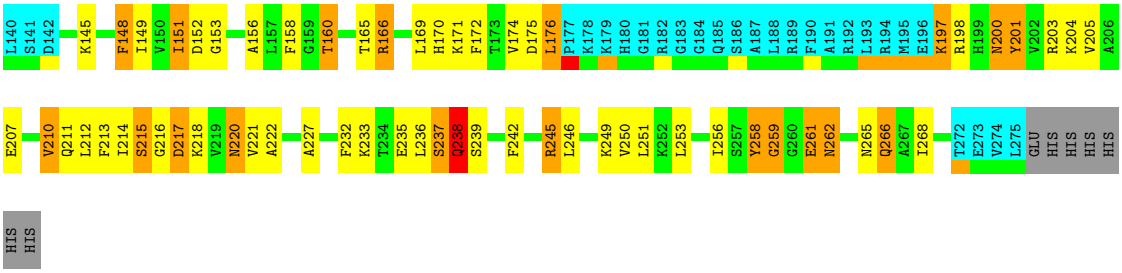
Chain A: 31% 32% 13% • 19% 5%



4.2.9 Score per residue for model 9

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

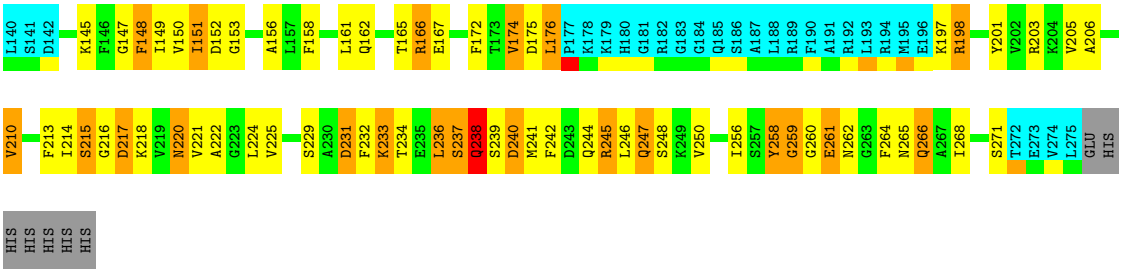
Chain A: 34% 29% 13% • 19% 5%



4.2.10 Score per residue for model 10

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

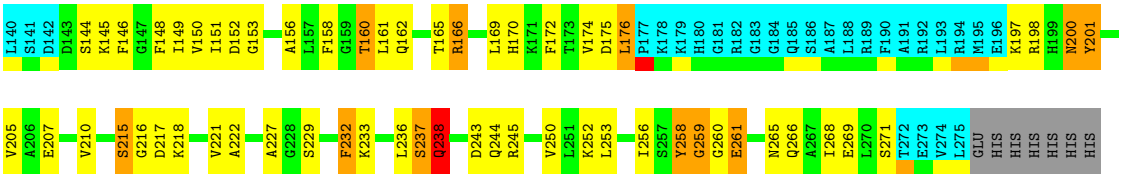
Chain A: 30% 31% 15% • 19% 5%



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

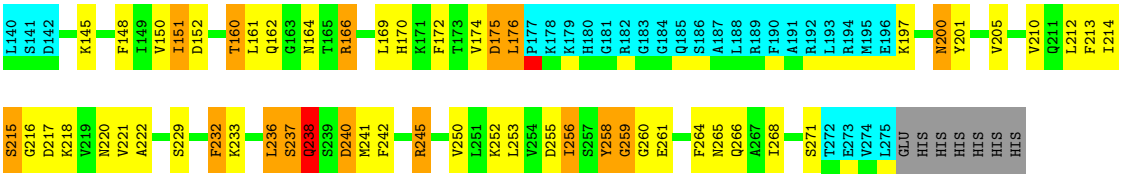
Chain A: 36% 32% 8% • 19% 5%



4.2.12 Score per residue for model 12

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

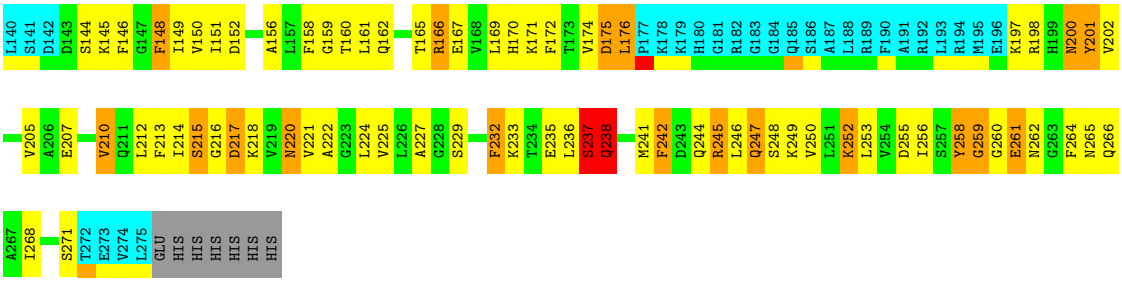
Chain A: 38% 27% 10% • 19% 5%



4.2.13 Score per residue for model 13

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

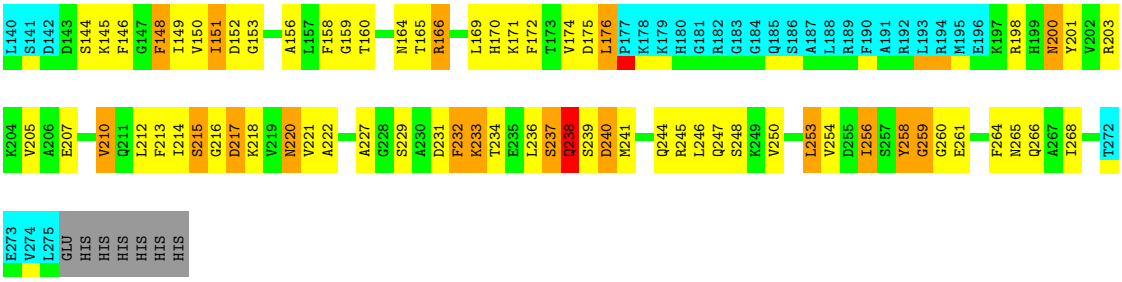
Chain A: 24% 38% 13% • 19% 5%



4.2.14 Score per residue for model 14

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

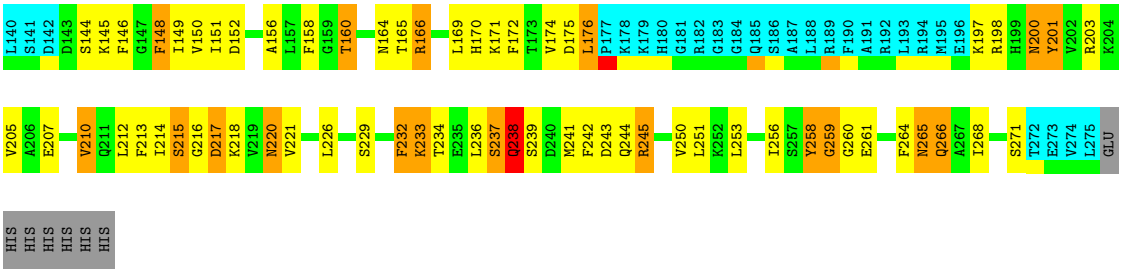
Chain A: 28% 36% 12% • 19% 5%



4.2.15 Score per residue for model 15

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

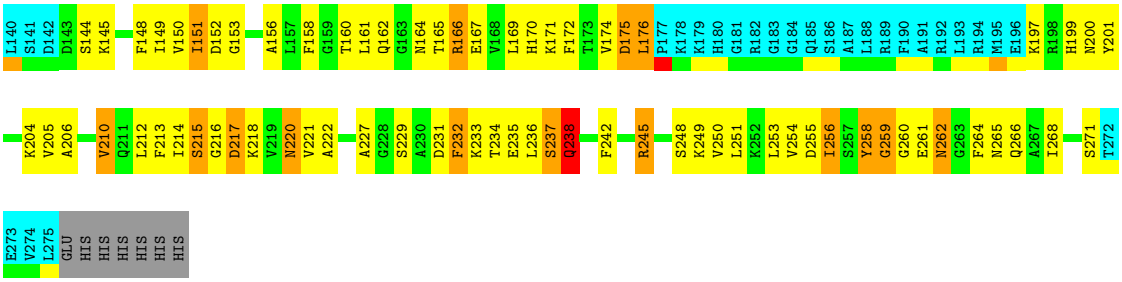
Chain A: 31% 32% 13% • 19% 5%



4.2.16 Score per residue for model 16

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

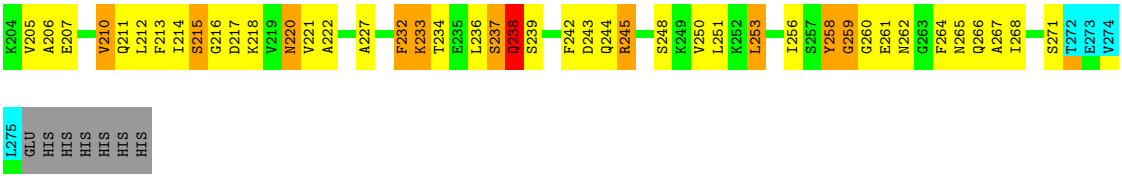
Chain A: 26% 39% 10% • 19% 5%



4.2.17 Score per residue for model 17

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

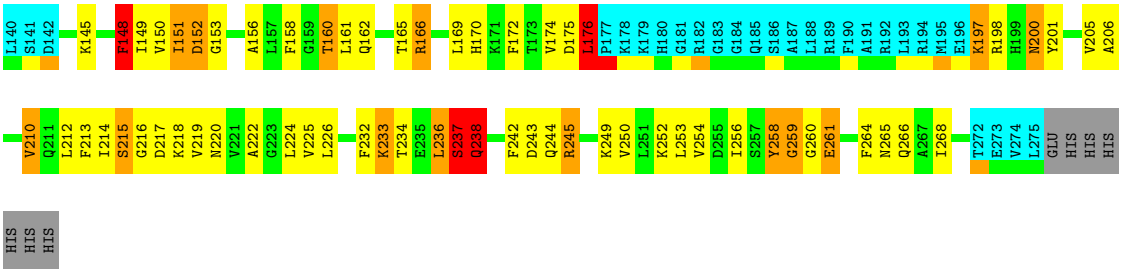
Chain A: 27% 36% 12% • 19% 5%



4.2.18 Score per residue for model 18

• Molecule 1: Eukaryotic peptide chain release factor subunit 1

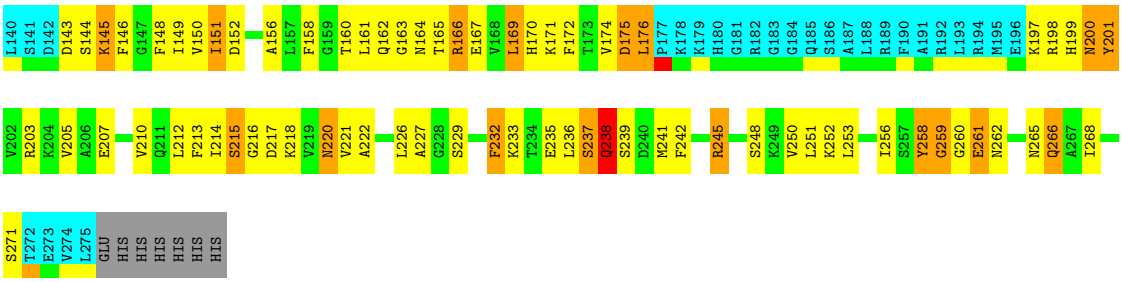
Chain A: 31% 32% 10% • 19% 5%



4.2.19 Score per residue for model 19

• Molecule 1: Eukaryotic peptide chain release factor subunit 1

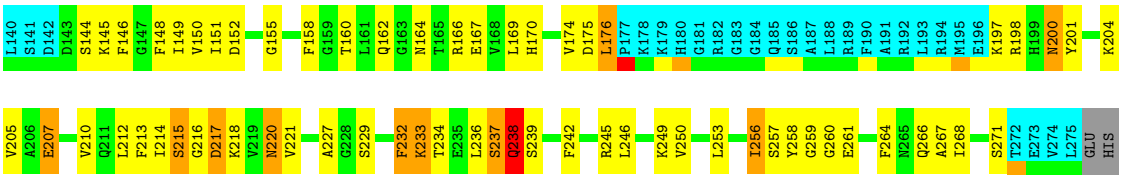
Chain A: 25% 38% 12% • 19% 5%



4.2.20 Score per residue for model 20

• Molecule 1: Eukaryotic peptide chain release factor subunit 1

Chain A: 32% 36% 7% • 19% 5%



HIS HIS HIS HIS HIS

4.2.21 Score per residue for model 21

• Molecule 1: Eukaryotic peptide chain release factor subunit 1

Chain A: 28% 33% 14% • 19% 5%

L140 S141 D142 D143 S144 K145 F148 I149 V150 I151 D152 G153 A156 L157 F158 G159 T160 L161 Q162 G163 N164 T165 R166 L169 H170 K171 F172 T173 V174 D175 L176 P177 K178 K179 H180 G181 R182 G183 G184 Q185 S186 A187 L188 R189 F190 A191 R192 L193 R194 M195 E196 K197 N200 Y201 V205

A206 V210 Q211 L212 F213 I214 S215 G216 D217 K218 V219 N220 V221 A222 L226 A227 G228 S229 A230 D231 F232 K233 T234 E235 L236 S237 Q238 S239 D240 Q244 R245 L246 Q247 S248 K249 V250 L251 K252 L253 I256 S257 Y258 G259 G260 E261 N262 G263 F264 N265 Q266 A267 I268 T272 E273 V274

L275 GLU HIS HIS HIS HIS HIS HIS

4.2.22 Score per residue for model 22

• Molecule 1: Eukaryotic peptide chain release factor subunit 1

Chain A: 29% 31% 15% • 19% 5%

L140 S141 D142 D143 S144 K145 F146 G147 F148 I149 V150 I151 D152 G153 S154 G155 A156 L157 F158 G159 T160 L161 Q162 G163 N164 T165 R166 L169 H170 K171 F172 T173 V174 D175 L176 P177 K178 K179 H180 G181 R182 G183 G184 Q185 S186 A187 L188 R189 F190 A191 R192 L193 R194 M195 E196 K197 R198 H199 N200

Y201 V205 V210 Q211 L212 F213 I214 S215 G216 D217 K218 V219 N220 V221 A222 L226 A227 G228 S229 F232 K233 T234 E235 L236 S237 Q238 M241 F242 D243 Q244 R245 L246 Q247 V250 L253 V254 D255 I256 S257 Y258 G259 G260 E261 N262 G263 F264 N265 Q266 A267 I268 T272 E273

V274 L275 GLU HIS HIS HIS HIS HIS HIS

4.2.23 Score per residue for model 23

• Molecule 1: Eukaryotic peptide chain release factor subunit 1

Chain A: 34% 31% 11% • 19% 5%

L140 S141 D142 K145 F148 I149 V150 I151 D152 A156 L157 F158 G159 T160 L161 Q162 T165 R166 L169 H170 K171 F172 T173 V174 D175 L176 P177 K178 K179 H180 G181 R182 G183 G184 Q185 S186 A187 L188 R189 F190 A191 R192 L193 R194 M195 E196 K197 R198 H199 N200 Y201 V205 A206 E207

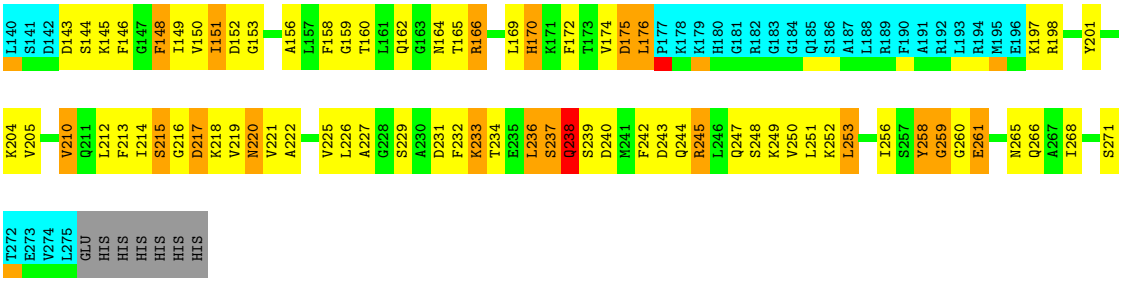
V210 F213 I214 S215 G216 D217 K218 V219 N220 V221 L224 A227 D231 F232 K233 T234 E235 L236 S237 Q238 D243 Q244 R245 L246 Q247 S248 K249 V250 L253 V254 D255 I256 S257 Y258 G259 G260 E261 N262 N265 Q266 A267 I268 S271 T272 E273 V274 L275 GLU HIS HIS HIS

HIS HIS HIS

4.2.24 Score per residue for model 24

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

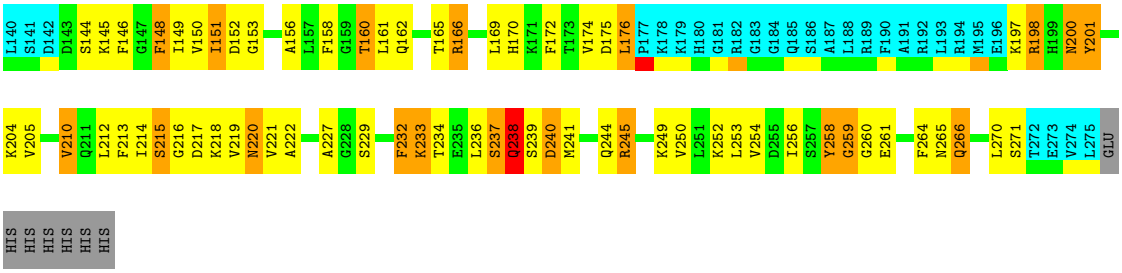
Chain A: 24% 38% 13% • 19% 5%



4.2.25 Score per residue for model 25

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

Chain A: 29% 34% 13% • 19% 5%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 50 calculated structures, 25 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CNS	structure solution	1.1
XPLOR-NIH	refinement	2.11.2

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.73±0.01	0±0/852 (0.0± 0.0%)	0.98±0.01	0±1/1147 (0.0± 0.0%)
All	All	0.73	0/21300 (0.0%)	0.98	10/28675 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.0±0.2
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	148	PHE	CB-CG-CD1	-6.26	116.42	120.80	10	8
1	A	176	LEU	CB-CA-C	5.14	119.96	110.20	4	2

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	166	ARG	Sidechain	1

6.2 Too-close contacts (i)

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	840	843	843	63±9
All	All	21000	21075	21075	1581

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 38.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:238:GLN:O	1:A:238:GLN:NE2	0.91	2.04	7	25
1:A:156:ALA:HB3	1:A:172:PHE:CZ	0.86	2.06	21	22
1:A:247:GLN:HE21	1:A:247:GLN:N	0.85	1.69	21	5
1:A:166:ARG:NH1	1:A:268:ILE:HD12	0.85	1.86	15	1
1:A:253:LEU:N	1:A:253:LEU:HD23	0.83	1.88	4	5
1:A:166:ARG:NH1	1:A:167:GLU:N	0.79	2.30	4	4
1:A:153:GLY:O	1:A:176:LEU:HD11	0.79	1.76	9	14
1:A:166:ARG:NH1	1:A:167:GLU:H	0.77	1.77	4	4
1:A:253:LEU:HD22	1:A:253:LEU:N	0.77	1.94	24	1
1:A:160:THR:OG1	1:A:169:LEU:HD13	0.75	1.82	15	9
1:A:215:SER:O	1:A:217:ASP:N	0.75	2.19	4	25
1:A:215:SER:O	1:A:218:LYS:N	0.73	2.21	18	25
1:A:247:GLN:N	1:A:247:GLN:NE2	0.73	2.37	10	4
1:A:244:GLN:O	1:A:247:GLN:NE2	0.73	2.22	21	5
1:A:266:GLN:NE2	1:A:270:LEU:HD11	0.72	2.00	7	2
1:A:149:ILE:HG23	1:A:158:PHE:CZ	0.72	2.20	24	22
1:A:201:TYR:CZ	1:A:205:VAL:HG21	0.71	2.20	13	22
1:A:264:PHE:CZ	1:A:268:ILE:HD11	0.71	2.20	16	2
1:A:236:LEU:O	1:A:237:SER:O	0.71	2.08	20	25
1:A:247:GLN:NE2	1:A:247:GLN:H	0.71	1.83	22	5
1:A:247:GLN:HE21	1:A:248:SER:H	0.70	1.30	10	3
1:A:166:ARG:CZ	1:A:264:PHE:CZ	0.69	2.76	2	4
1:A:160:THR:O	1:A:166:ARG:NH2	0.69	2.26	17	3
1:A:237:SER:O	1:A:238:GLN:O	0.68	2.10	15	25
1:A:166:ARG:HH11	1:A:166:ARG:CB	0.68	2.00	7	3
1:A:265:ASN:ND2	1:A:266:GLN:N	0.68	2.42	15	1
1:A:166:ARG:NH2	1:A:264:PHE:CE1	0.68	2.62	2	4
1:A:247:GLN:HE21	1:A:248:SER:N	0.68	1.87	10	3
1:A:166:ARG:NH1	1:A:166:ARG:HB2	0.67	2.04	17	7
1:A:233:LYS:CD	1:A:233:LYS:H	0.67	2.02	17	2
1:A:166:ARG:NH2	1:A:264:PHE:CZ	0.67	2.63	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:201:TYR:O	1:A:205:VAL:HG23	0.66	1.89	17	21
1:A:166:ARG:NH1	1:A:166:ARG:CB	0.66	2.58	4	4
1:A:262:ASN:HD22	1:A:262:ASN:N	0.66	1.88	16	1
1:A:160:THR:OG1	1:A:169:LEU:HD22	0.66	1.90	20	7
1:A:198:ARG:NH1	1:A:232:PHE:CZ	0.65	2.65	1	1
1:A:250:VAL:O	1:A:250:VAL:HG13	0.64	1.92	3	25
1:A:166:ARG:NH1	1:A:268:ILE:HD13	0.64	2.06	17	2
1:A:253:LEU:HD12	1:A:253:LEU:N	0.64	2.07	13	7
1:A:213:PHE:O	1:A:220:ASN:ND2	0.64	2.30	18	1
1:A:247:GLN:NE2	1:A:247:GLN:N	0.64	2.45	22	1
1:A:201:TYR:CE1	1:A:205:VAL:CG2	0.63	2.81	2	24
1:A:238:GLN:OE1	1:A:241:MET:N	0.63	2.30	7	3
1:A:232:PHE:O	1:A:236:LEU:N	0.63	2.32	3	20
1:A:153:GLY:O	1:A:176:LEU:HD21	0.63	1.94	16	11
1:A:160:THR:OG1	1:A:169:LEU:HD21	0.63	1.94	4	1
1:A:151:ILE:O	1:A:151:ILE:HG23	0.63	1.94	21	12
1:A:166:ARG:HH11	1:A:166:ARG:CG	0.62	2.07	7	4
1:A:243:ASP:O	1:A:247:GLN:NE2	0.62	2.32	4	3
1:A:166:ARG:HH11	1:A:166:ARG:CA	0.62	2.07	2	4
1:A:166:ARG:CB	1:A:166:ARG:HH11	0.62	2.07	4	1
1:A:166:ARG:NH1	1:A:166:ARG:CA	0.62	2.63	4	4
1:A:198:ARG:NH2	1:A:232:PHE:CE2	0.61	2.68	2	1
1:A:199:HIS:CE1	1:A:241:MET:SD	0.61	2.93	2	2
1:A:151:ILE:HD12	1:A:205:VAL:HG11	0.61	1.72	12	11
1:A:233:LYS:CD	1:A:233:LYS:N	0.61	2.62	17	3
1:A:200:ASN:H	1:A:200:ASN:HD22	0.61	1.36	19	21
1:A:253:LEU:O	1:A:253:LEU:HD12	0.61	1.95	17	1
1:A:174:VAL:O	1:A:174:VAL:HG13	0.61	1.96	7	16
1:A:160:THR:OG1	1:A:169:LEU:HD11	0.61	1.96	4	4
1:A:233:LYS:NZ	1:A:254:VAL:N	0.61	2.49	18	2
1:A:219:VAL:HG11	1:A:249:LYS:NZ	0.61	2.11	5	4
1:A:244:GLN:C	1:A:247:GLN:HE22	0.60	1.99	22	3
1:A:226:LEU:HD12	1:A:253:LEU:HD12	0.60	1.74	24	1
1:A:145:LYS:O	1:A:222:ALA:HB3	0.60	1.97	9	16
1:A:166:ARG:HH11	1:A:167:GLU:N	0.59	1.92	4	4
1:A:262:ASN:N	1:A:262:ASN:ND2	0.59	2.48	16	1
1:A:252:LYS:C	1:A:253:LEU:HD12	0.59	2.18	19	7
1:A:266:GLN:HE22	1:A:270:LEU:HD11	0.59	1.56	7	2
1:A:166:ARG:CG	1:A:166:ARG:HH11	0.58	2.11	16	3
1:A:175:ASP:O	1:A:176:LEU:O	0.58	2.21	14	12
1:A:233:LYS:O	1:A:236:LEU:N	0.58	2.37	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:253:LEU:HD23	1:A:253:LEU:H	0.58	1.57	22	3
1:A:150:VAL:HG13	1:A:256:ILE:HD13	0.58	1.75	23	4
1:A:247:GLN:HE21	1:A:247:GLN:CA	0.58	2.12	10	4
1:A:262:ASN:O	1:A:266:GLN:NE2	0.58	2.37	6	12
1:A:152:ASP:O	1:A:201:TYR:OH	0.58	2.18	1	21
1:A:166:ARG:NH1	1:A:268:ILE:CD1	0.58	2.67	17	2
1:A:262:ASN:HD22	1:A:262:ASN:H	0.58	1.42	9	1
1:A:264:PHE:CE1	1:A:268:ILE:HD11	0.57	2.33	16	6
1:A:166:ARG:NH1	1:A:166:ARG:O	0.57	2.37	9	5
1:A:247:GLN:NE2	1:A:248:SER:H	0.57	1.97	10	3
1:A:258:TYR:CD1	1:A:258:TYR:O	0.57	2.58	21	24
1:A:261:GLU:O	1:A:265:ASN:ND2	0.57	2.38	23	23
1:A:199:HIS:ND1	1:A:241:MET:CE	0.57	2.68	1	1
1:A:234:THR:OG1	1:A:253:LEU:HD12	0.57	1.99	16	3
1:A:145:LYS:O	1:A:222:ALA:N	0.57	2.37	16	12
1:A:166:ARG:HH12	1:A:167:GLU:H	0.57	1.40	3	3
1:A:253:LEU:N	1:A:253:LEU:CD2	0.56	2.60	4	5
1:A:148:PHE:N	1:A:159:GLY:O	0.56	2.39	8	8
1:A:258:TYR:C	1:A:258:TYR:CD1	0.56	2.78	14	3
1:A:197:LYS:N	1:A:197:LYS:CD	0.56	2.69	1	1
1:A:161:LEU:HD23	1:A:162:GLN:N	0.56	2.15	16	13
1:A:166:ARG:HH11	1:A:166:ARG:C	0.56	2.04	2	3
1:A:166:ARG:NE	1:A:265:ASN:OD1	0.56	2.38	22	2
1:A:160:THR:HG1	1:A:169:LEU:HD22	0.56	1.61	7	2
1:A:156:ALA:HB3	1:A:172:PHE:CE2	0.55	2.36	18	7
1:A:253:LEU:H	1:A:253:LEU:HD23	0.55	1.60	16	8
1:A:258:TYR:CD1	1:A:258:TYR:C	0.55	2.80	23	21
1:A:166:ARG:NE	1:A:264:PHE:CZ	0.55	2.74	15	7
1:A:260:GLY:O	1:A:264:PHE:N	0.55	2.34	4	5
1:A:261:GLU:OE1	1:A:262:ASN:ND2	0.55	2.40	22	1
1:A:237:SER:O	1:A:238:GLN:C	0.55	2.45	13	25
1:A:212:LEU:O	1:A:220:ASN:ND2	0.55	2.40	18	14
1:A:240:ASP:N	1:A:240:ASP:OD1	0.55	2.41	10	5
1:A:166:ARG:NH2	1:A:268:ILE:HD11	0.54	2.17	4	1
1:A:236:LEU:O	1:A:237:SER:C	0.54	2.45	24	24
1:A:238:GLN:CD	1:A:241:MET:H	0.54	2.05	7	3
1:A:152:ASP:O	1:A:201:TYR:CZ	0.54	2.60	17	21
1:A:144:SER:O	1:A:146:PHE:CE2	0.54	2.61	7	7
1:A:200:ASN:H	1:A:200:ASN:ND2	0.54	2.01	9	19
1:A:160:THR:OG1	1:A:169:LEU:HD12	0.54	2.03	19	1
1:A:245:ARG:HE	1:A:245:ARG:CA	0.54	2.16	3	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:237:SER:O	1:A:238:GLN:NE2	0.53	2.39	18	4
1:A:210:VAL:O	1:A:214:ILE:N	0.53	2.40	2	24
1:A:236:LEU:O	1:A:238:GLN:NE2	0.53	2.41	1	12
1:A:156:ALA:O	1:A:172:PHE:CD1	0.53	2.62	25	4
1:A:228:GLY:O	1:A:233:LYS:NZ	0.53	2.42	6	1
1:A:143:ASP:CG	1:A:163:GLY:H	0.53	2.07	21	2
1:A:239:SER:OG	1:A:244:GLN:NE2	0.52	2.42	17	4
1:A:166:ARG:O	1:A:166:ARG:NH1	0.52	2.41	19	5
1:A:260:GLY:O	1:A:264:PHE:CB	0.52	2.57	14	9
1:A:206:ALA:O	1:A:210:VAL:HG13	0.52	2.04	16	6
1:A:217:ASP:N	1:A:217:ASP:OD1	0.52	2.42	14	4
1:A:166:ARG:CG	1:A:166:ARG:NH1	0.52	2.72	16	3
1:A:162:GLN:NE2	1:A:167:GLU:OE2	0.52	2.43	19	1
1:A:164:ASN:ND2	1:A:164:ASN:N	0.52	2.57	6	1
1:A:144:SER:O	1:A:146:PHE:CE1	0.52	2.62	11	6
1:A:244:GLN:HE21	1:A:244:GLN:N	0.52	2.02	14	1
1:A:166:ARG:HB2	1:A:268:ILE:HD13	0.52	1.82	16	1
1:A:258:TYR:O	1:A:259:GLY:C	0.52	2.49	14	24
1:A:144:SER:O	1:A:146:PHE:CD1	0.51	2.63	11	5
1:A:169:LEU:O	1:A:170:HIS:CD2	0.51	2.63	13	2
1:A:233:LYS:HZ3	1:A:254:VAL:N	0.51	2.03	1	1
1:A:234:THR:OG1	1:A:253:LEU:HD22	0.51	2.05	21	1
1:A:150:VAL:HG11	1:A:260:GLY:HA2	0.51	1.81	17	22
1:A:213:PHE:C	1:A:220:ASN:ND2	0.51	2.63	20	23
1:A:169:LEU:O	1:A:170:HIS:ND1	0.51	2.43	23	3
1:A:171:LYS:N	1:A:171:LYS:CD	0.51	2.74	1	1
1:A:175:ASP:N	1:A:175:ASP:OD1	0.51	2.43	6	1
1:A:238:GLN:OE1	1:A:241:MET:SD	0.51	2.68	14	1
1:A:149:ILE:HD13	1:A:226:LEU:CD2	0.51	2.36	5	1
1:A:175:ASP:OD1	1:A:175:ASP:N	0.51	2.43	24	2
1:A:255:ASP:OD1	1:A:256:ILE:N	0.51	2.43	22	3
1:A:233:LYS:HZ1	1:A:254:VAL:N	0.51	2.04	18	1
1:A:158:PHE:CD1	1:A:158:PHE:N	0.51	2.77	20	2
1:A:233:LYS:NZ	1:A:234:THR:OG1	0.51	2.40	15	2
1:A:149:ILE:HG23	1:A:158:PHE:CE2	0.51	2.41	24	3
1:A:257:SER:O	1:A:258:TYR:CD1	0.50	2.64	20	1
1:A:158:PHE:O	1:A:169:LEU:HD23	0.50	2.06	22	1
1:A:145:LYS:O	1:A:222:ALA:CB	0.50	2.60	16	18
1:A:160:THR:O	1:A:166:ARG:NH1	0.50	2.41	4	2
1:A:150:VAL:HG13	1:A:256:ILE:HG21	0.50	1.84	14	2
1:A:160:THR:OG1	1:A:169:LEU:CD1	0.50	2.60	23	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:165:THR:HG22	1:A:166:ARG:N	0.50	2.20	14	3
1:A:201:TYR:CZ	1:A:205:VAL:CG2	0.50	2.95	10	7
1:A:151:ILE:HG12	1:A:205:VAL:HG11	0.50	1.83	17	6
1:A:247:GLN:NE2	1:A:248:SER:N	0.50	2.57	10	2
1:A:143:ASP:OD2	1:A:163:GLY:N	0.49	2.42	19	2
1:A:151:ILE:HG13	1:A:205:VAL:HG11	0.49	1.84	22	1
1:A:267:ALA:O	1:A:271:SER:N	0.49	2.42	2	3
1:A:170:HIS:HB2	1:A:212:LEU:HD21	0.49	1.84	12	11
1:A:237:SER:C	1:A:247:GLN:NE2	0.49	2.66	14	3
1:A:224:LEU:H	1:A:251:LEU:HB2	0.49	1.65	5	1
1:A:149:ILE:HD11	1:A:224:LEU:HD22	0.49	1.84	13	3
1:A:149:ILE:HD12	1:A:226:LEU:HD23	0.49	1.84	19	2
1:A:260:GLY:O	1:A:264:PHE:HB2	0.49	2.07	20	2
1:A:233:LYS:CD	1:A:234:THR:H	0.49	2.21	3	3
1:A:153:GLY:N	1:A:198:ARG:NH2	0.49	2.59	18	1
1:A:237:SER:OG	1:A:238:GLN:N	0.49	2.45	17	2
1:A:160:THR:OG1	1:A:169:LEU:CG	0.49	2.60	4	1
1:A:166:ARG:CZ	1:A:268:ILE:HD13	0.49	2.37	17	2
1:A:250:VAL:O	1:A:250:VAL:CG1	0.49	2.61	17	24
1:A:166:ARG:HB2	1:A:166:ARG:HH11	0.49	1.65	17	2
1:A:243:ASP:OD1	1:A:244:GLN:N	0.48	2.47	11	7
1:A:174:VAL:O	1:A:174:VAL:CG1	0.48	2.61	3	24
1:A:151:ILE:CD1	1:A:205:VAL:HG11	0.48	2.39	11	7
1:A:234:THR:OG1	1:A:253:LEU:CD1	0.48	2.62	23	2
1:A:209:ALA:O	1:A:213:PHE:N	0.48	2.47	4	3
1:A:166:ARG:HH21	1:A:268:ILE:HD11	0.48	1.66	4	3
1:A:233:LYS:HD3	1:A:234:THR:H	0.48	1.69	17	2
1:A:265:ASN:ND2	1:A:265:ASN:C	0.48	2.66	15	1
1:A:148:PHE:CE1	1:A:225:VAL:HG11	0.48	2.43	3	6
1:A:160:THR:OG1	1:A:169:LEU:CD2	0.48	2.62	4	5
1:A:199:HIS:ND1	1:A:199:HIS:C	0.48	2.66	2	2
1:A:233:LYS:NZ	1:A:253:LEU:HD12	0.48	2.23	15	1
1:A:149:ILE:HD13	1:A:226:LEU:HD23	0.47	1.85	5	1
1:A:244:GLN:NE2	1:A:244:GLN:N	0.47	2.62	8	1
1:A:261:GLU:CD	1:A:262:ASN:N	0.47	2.67	22	1
1:A:151:ILE:O	1:A:151:ILE:CG2	0.47	2.62	21	12
1:A:245:ARG:CA	1:A:245:ARG:NE	0.47	2.77	19	7
1:A:162:GLN:CG	1:A:162:GLN:O	0.47	2.62	23	2
1:A:152:ASP:O	1:A:155:GLY:O	0.47	2.33	22	3
1:A:224:LEU:O	1:A:251:LEU:CB	0.47	2.62	5	1
1:A:233:LYS:CG	1:A:234:THR:N	0.47	2.78	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:237:SER:CA	1:A:247:GLN:HE22	0.47	2.22	14	3
1:A:247:GLN:NE2	1:A:247:GLN:CA	0.47	2.77	10	3
1:A:167:GLU:N	1:A:167:GLU:CD	0.47	2.68	13	1
1:A:245:ARG:O	1:A:245:ARG:NE	0.47	2.48	21	2
1:A:201:TYR:CE1	1:A:205:VAL:HG21	0.47	2.44	15	9
1:A:246:LEU:O	1:A:249:LYS:N	0.47	2.36	2	3
1:A:145:LYS:NZ	1:A:220:ASN:O	0.47	2.39	14	2
1:A:252:LYS:C	1:A:253:LEU:HD23	0.47	2.30	4	1
1:A:264:PHE:O	1:A:268:ILE:HD12	0.47	2.09	17	2
1:A:145:LYS:NZ	1:A:162:GLN:OE1	0.47	2.48	16	1
1:A:166:ARG:CB	1:A:268:ILE:HD13	0.47	2.40	12	5
1:A:237:SER:O	1:A:242:PHE:CB	0.47	2.62	24	3
1:A:233:LYS:HZ3	1:A:253:LEU:HD12	0.47	1.68	15	1
1:A:224:LEU:O	1:A:251:LEU:HB2	0.47	2.10	5	1
1:A:149:ILE:O	1:A:227:ALA:O	0.46	2.32	2	15
1:A:213:PHE:CA	1:A:220:ASN:ND2	0.46	2.78	9	17
1:A:199:HIS:ND1	1:A:241:MET:SD	0.46	2.88	2	1
1:A:170:HIS:ND1	1:A:212:LEU:HD11	0.46	2.25	25	2
1:A:200:ASN:ND2	1:A:200:ASN:N	0.46	2.64	9	11
1:A:231:ASP:N	1:A:231:ASP:OD1	0.46	2.48	3	1
1:A:239:SER:O	1:A:242:PHE:O	0.46	2.33	9	9
1:A:237:SER:O	1:A:242:PHE:HB2	0.46	2.10	15	7
1:A:242:PHE:CE2	1:A:246:LEU:HD13	0.46	2.45	5	2
1:A:262:ASN:H	1:A:262:ASN:ND2	0.46	2.09	9	1
1:A:243:ASP:CB	1:A:246:LEU:HD12	0.46	2.41	7	1
1:A:257:SER:C	1:A:258:TYR:CG	0.46	2.88	20	1
1:A:203:ARG:O	1:A:207:GLU:N	0.46	2.42	1	7
1:A:200:ASN:N	1:A:200:ASN:ND2	0.46	2.64	19	1
1:A:245:ARG:HE	1:A:245:ARG:C	0.46	2.14	17	5
1:A:166:ARG:NH1	1:A:166:ARG:CG	0.46	2.78	3	2
1:A:160:THR:OG1	1:A:169:LEU:HD23	0.46	2.10	25	1
1:A:268:ILE:O	1:A:271:SER:C	0.46	2.54	19	11
1:A:147:GLY:O	1:A:224:LEU:HD23	0.46	2.11	10	1
1:A:198:ARG:CG	1:A:198:ARG:HH11	0.45	2.24	1	1
1:A:231:ASP:OD1	1:A:233:LYS:NZ	0.45	2.42	8	1
1:A:262:ASN:ND2	1:A:262:ASN:N	0.45	2.65	9	2
1:A:244:GLN:N	1:A:244:GLN:NE2	0.45	2.64	14	1
1:A:229:SER:O	1:A:232:PHE:N	0.45	2.49	2	5
1:A:253:LEU:N	1:A:253:LEU:CD1	0.45	2.80	19	7
1:A:149:ILE:CD1	1:A:224:LEU:HD22	0.45	2.41	10	1
1:A:240:ASP:OD1	1:A:240:ASP:N	0.45	2.48	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:233:LYS:CD	1:A:254:VAL:O	0.45	2.65	25	2
1:A:252:LYS:C	1:A:253:LEU:HD13	0.45	2.32	24	1
1:A:149:ILE:HD12	1:A:226:LEU:CD2	0.45	2.41	7	2
1:A:245:ARG:CA	1:A:245:ARG:HE	0.45	2.25	9	3
1:A:253:LEU:HD22	1:A:253:LEU:H	0.45	1.70	24	1
1:A:160:THR:HG1	1:A:169:LEU:HD11	0.44	1.72	4	1
1:A:237:SER:C	1:A:247:GLN:HE22	0.44	2.14	1	1
1:A:213:PHE:HA	1:A:220:ASN:ND2	0.44	2.27	9	4
1:A:213:PHE:HA	1:A:220:ASN:HD22	0.44	1.73	7	13
1:A:244:GLN:N	1:A:244:GLN:CD	0.44	2.71	8	1
1:A:161:LEU:HD23	1:A:161:LEU:C	0.44	2.33	2	2
1:A:233:LYS:O	1:A:234:THR:C	0.44	2.56	24	3
1:A:144:SER:O	1:A:146:PHE:CD2	0.43	2.70	14	4
1:A:162:GLN:O	1:A:162:GLN:CG	0.43	2.66	25	6
1:A:165:THR:HG22	1:A:167:GLU:OE2	0.43	2.13	16	1
1:A:153:GLY:C	1:A:176:LEU:HD11	0.43	2.33	9	1
1:A:260:GLY:O	1:A:262:ASN:N	0.43	2.51	23	1
1:A:160:THR:HG1	1:A:169:LEU:HD21	0.43	1.72	4	1
1:A:162:GLN:OE1	1:A:167:GLU:OE2	0.43	2.36	8	1
1:A:253:LEU:HD23	1:A:253:LEU:N	0.43	2.26	16	1
1:A:238:GLN:OE1	1:A:241:MET:CG	0.43	2.66	12	1
1:A:201:TYR:CD2	1:A:201:TYR:C	0.43	2.91	13	1
1:A:201:TYR:CD2	1:A:202:VAL:N	0.43	2.86	13	1
1:A:151:ILE:CG2	1:A:151:ILE:O	0.43	2.66	24	1
1:A:167:GLU:OE1	1:A:167:GLU:N	0.43	2.52	10	1
1:A:151:ILE:HD13	1:A:152:ASP:N	0.43	2.28	10	2
1:A:233:LYS:HZ2	1:A:254:VAL:CA	0.43	2.27	2	1
1:A:166:ARG:HH11	1:A:166:ARG:HG3	0.43	1.74	7	1
1:A:152:ASP:O	1:A:201:TYR:CE2	0.42	2.72	4	1
1:A:231:ASP:O	1:A:235:GLU:OE1	0.42	2.36	16	1
1:A:149:ILE:O	1:A:227:ALA:N	0.42	2.51	4	5
1:A:169:LEU:O	1:A:170:HIS:CG	0.42	2.72	8	1
1:A:156:ALA:HB2	1:A:201:TYR:OH	0.42	2.14	10	1
1:A:151:ILE:HD13	1:A:201:TYR:OH	0.42	2.14	23	1
1:A:264:PHE:O	1:A:268:ILE:HG12	0.42	2.15	7	1
1:A:207:GLU:O	1:A:207:GLU:OE1	0.42	2.38	20	1
1:A:210:VAL:CG2	1:A:211:GLN:N	0.42	2.82	9	5
1:A:169:LEU:CD1	1:A:169:LEU:N	0.42	2.83	5	1
1:A:175:ASP:O	1:A:175:ASP:OD1	0.42	2.38	7	1
1:A:158:PHE:O	1:A:169:LEU:HB2	0.42	2.14	8	1
1:A:214:ILE:HG23	1:A:218:LYS:O	0.42	2.15	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:244:GLN:O	1:A:247:GLN:OE1	0.42	2.37	10	1
1:A:233:LYS:CD	1:A:234:THR:N	0.42	2.83	3	1
1:A:143:ASP:OD1	1:A:144:SER:O	0.42	2.37	5	1
1:A:166:ARG:HB3	1:A:268:ILE:HD13	0.42	1.92	18	1
1:A:257:SER:OG	1:A:258:TYR:N	0.42	2.52	20	1
1:A:149:ILE:HG23	1:A:158:PHE:CE1	0.41	2.51	18	3
1:A:203:ARG:CZ	1:A:207:GLU:OE1	0.41	2.68	14	1
1:A:153:GLY:O	1:A:176:LEU:CD1	0.41	2.60	9	1
1:A:233:LYS:NZ	1:A:254:VAL:C	0.41	2.73	16	1
1:A:151:ILE:HG21	1:A:236:LEU:HD11	0.41	1.91	17	2
1:A:200:ASN:HD22	1:A:200:ASN:N	0.41	2.10	19	1
1:A:151:ILE:CD1	1:A:201:TYR:OH	0.41	2.69	22	1
1:A:198:ARG:NH1	1:A:198:ARG:CG	0.41	2.82	23	2
1:A:213:PHE:O	1:A:220:ASN:CG	0.41	2.58	18	1
1:A:237:SER:CA	1:A:247:GLN:NE2	0.41	2.83	24	2
1:A:166:ARG:CZ	1:A:166:ARG:HB2	0.41	2.45	4	1
1:A:233:LYS:NZ	1:A:255:ASP:N	0.41	2.69	16	1
1:A:219:VAL:HG11	1:A:249:LYS:HZ1	0.41	1.75	18	1
1:A:166:ARG:NE	1:A:264:PHE:CE2	0.41	2.89	4	1
1:A:241:MET:O	1:A:242:PHE:O	0.41	2.38	13	1
1:A:151:ILE:HD12	1:A:205:VAL:HG21	0.41	1.93	8	1
1:A:224:LEU:HD12	1:A:249:LYS:HB2	0.41	1.92	18	1
1:A:238:GLN:O	1:A:238:GLN:CD	0.41	2.58	19	1
1:A:231:ASP:OD2	1:A:234:THR:CB	0.41	2.69	8	1
1:A:160:THR:CB	1:A:169:LEU:HD13	0.41	2.46	13	1
1:A:238:GLN:NE2	1:A:242:PHE:H	0.40	2.14	7	1
1:A:150:VAL:CG1	1:A:259:GLY:O	0.40	2.68	23	1
1:A:164:ASN:O	1:A:164:ASN:OD1	0.40	2.39	15	1
1:A:158:PHE:O	1:A:169:LEU:CB	0.40	2.69	19	1
1:A:233:LYS:CG	1:A:234:THR:H	0.40	2.29	16	1
1:A:231:ASP:OD1	1:A:231:ASP:N	0.40	2.54	10	2
1:A:165:THR:CG2	1:A:166:ARG:N	0.40	2.83	14	1
1:A:156:ALA:HB3	1:A:172:PHE:CE1	0.40	2.49	21	1
1:A:166:ARG:HH11	1:A:166:ARG:HG2	0.40	1.75	10	1
1:A:233:LYS:HZ3	1:A:253:LEU:CD1	0.40	2.29	15	1
1:A:245:ARG:NE	1:A:245:ARG:CA	0.40	2.84	21	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	109/143 (76%)	98±1 (90±1%)	5±1 (4±1%)	6±0 (5±0%)	3 23
All	All	2725/3575 (76%)	2459 (90%)	122 (4%)	144 (5%)	3 23

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	176	LEU	25
1	A	216	GLY	25
1	A	237	SER	25
1	A	238	GLN	25
1	A	259	GLY	25
1	A	261	GLU	16
1	A	242	PHE	3

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	91/120 (76%)	65±3 (72±4%)	26±3 (28±4%)	2 19
All	All	2275/3000 (76%)	1637 (72%)	638 (28%)	2 19

All 66 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	148	PHE	25
1	A	166	ARG	25
1	A	215	SER	25

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Mol	Chain	Res	Type	Models (Total)
1	A	238	GLN	25
1	A	256	ILE	25
1	A	221	VAL	24
1	A	233	LYS	24
1	A	245	ARG	24
1	A	258	TYR	24
1	A	220	ASN	22
1	A	151	ILE	21
1	A	232	PHE	21
1	A	210	VAL	21
1	A	165	THR	19
1	A	229	SER	18
1	A	266	GLN	17
1	A	175	ASP	16
1	A	160	THR	16
1	A	198	ARG	14
1	A	217	ASP	14
1	A	200	ASN	12
1	A	170	HIS	11
1	A	171	LYS	11
1	A	248	SER	11
1	A	164	ASN	11
1	A	251	LEU	11
1	A	201	TYR	10
1	A	231	ASP	9
1	A	240	ASP	9
1	A	204	LYS	7
1	A	253	LEU	6
1	A	199	HIS	6
1	A	207	GLU	6
1	A	226	LEU	6
1	A	249	LYS	6
1	A	169	LEU	6
1	A	247	GLN	6
1	A	145	LYS	6
1	A	246	LEU	5
1	A	235	GLU	5
1	A	236	LEU	5
1	A	255	ASP	4
1	A	152	ASP	4
1	A	174	VAL	4
1	A	237	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	261	GLU	4
1	A	197	LYS	3
1	A	268	ILE	3
1	A	143	ASP	3
1	A	252	LYS	3
1	A	244	GLN	3
1	A	218	LYS	2
1	A	262	ASN	2
1	A	241	MET	2
1	A	271	SER	1
1	A	168	VAL	1
1	A	203	ARG	1
1	A	225	VAL	1
1	A	239	SER	1
1	A	269	GLU	1
1	A	172	PHE	1
1	A	265	ASN	1
1	A	144	SER	1
1	A	243	ASP	1
1	A	242	PHE	1
1	A	167	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 (i)

No chemical shift data were provided