



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 10:15 AM UTC

PDB ID : 2HST / pdb_00002hst
Title : Solution structure of the middle domain of human eukaryotic translation termination factor eRF1
Authors : Polshakov, V.I.; Birdsall, B.; Kisselev, L.L.
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 ⓘ 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

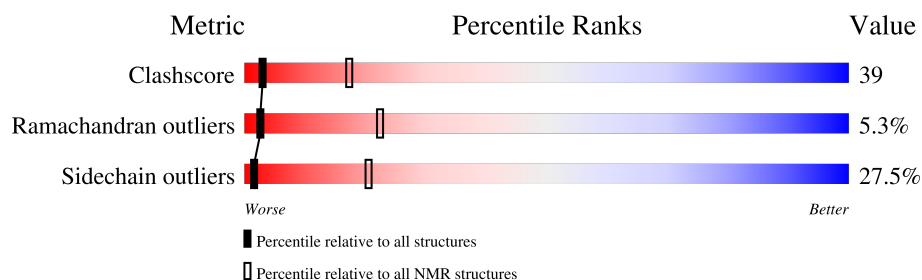
1 Overall quality at a glance

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	143	

2 Ensemble composition and analysis

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)	0.39	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.

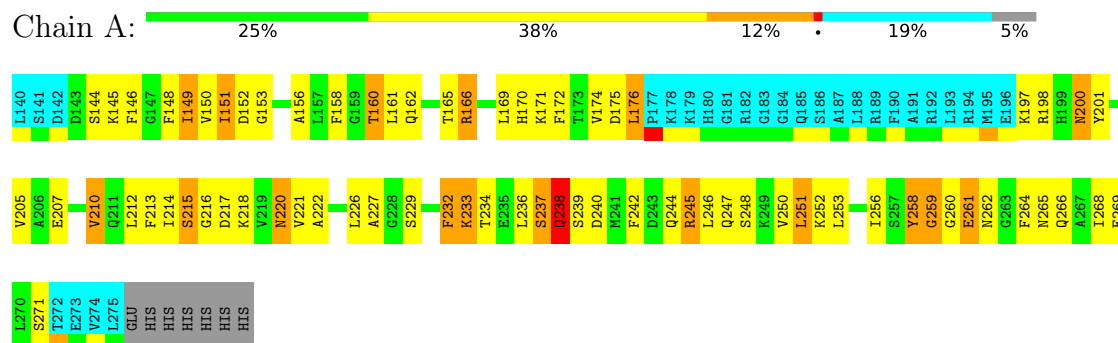
Mol	Chain	Residues	Atoms						Trace
1	A	136	Total	C	H	N	O	S	0
			2121	664	1068	188	199	2	

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: Eukaryotic peptide chain release factor subunit 1

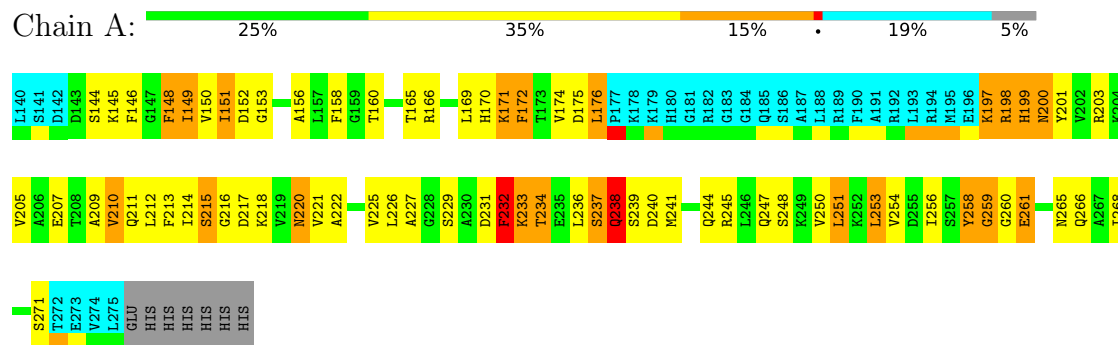


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

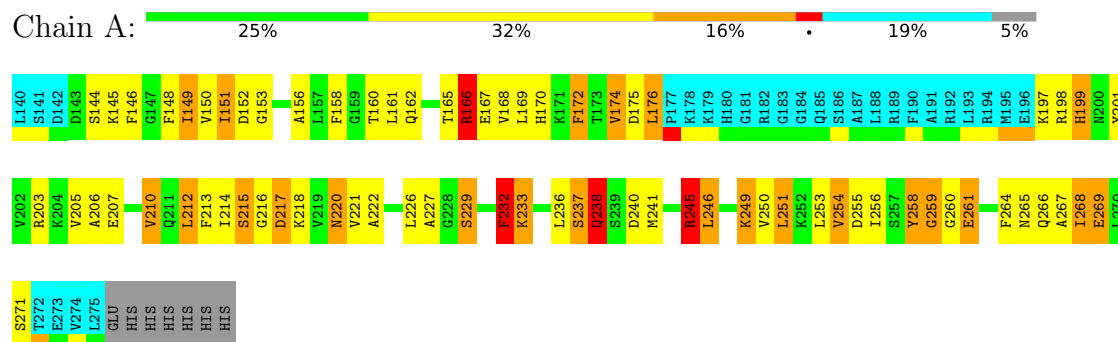
4.2.1 Score per residue for model 1

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



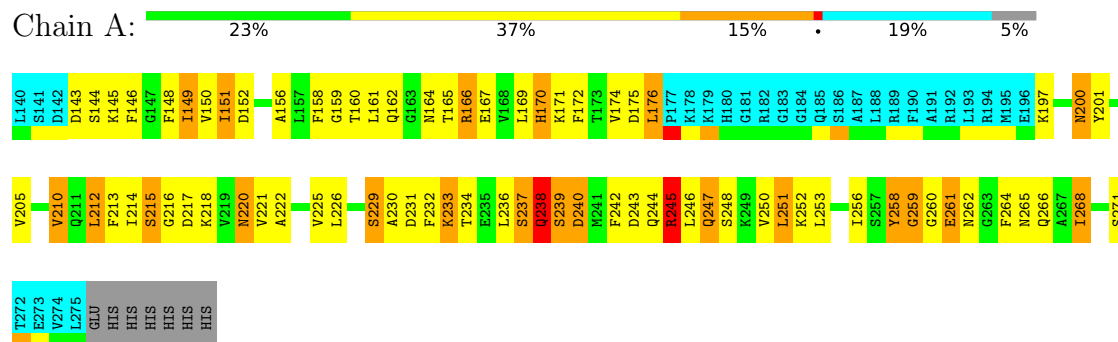
4.2.2 Score per residue for model 2

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



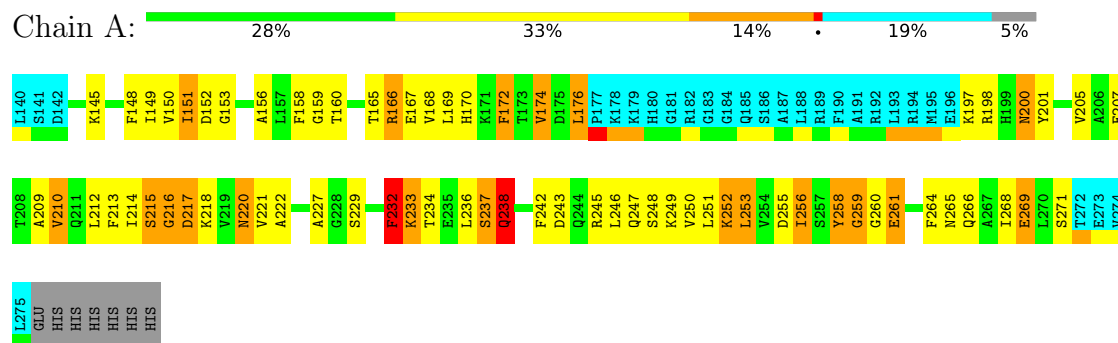
4.2.3 Score per residue for model 3

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



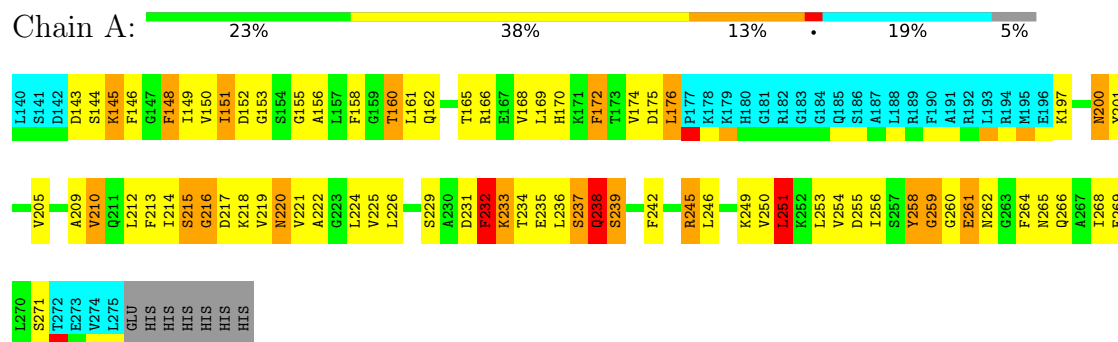
4.2.4 Score per residue for model 4

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



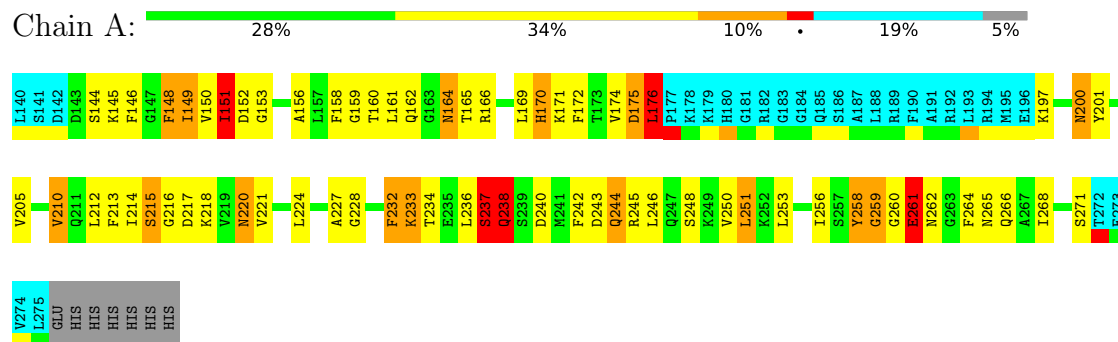
4.2.5 Score per residue for model 5

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



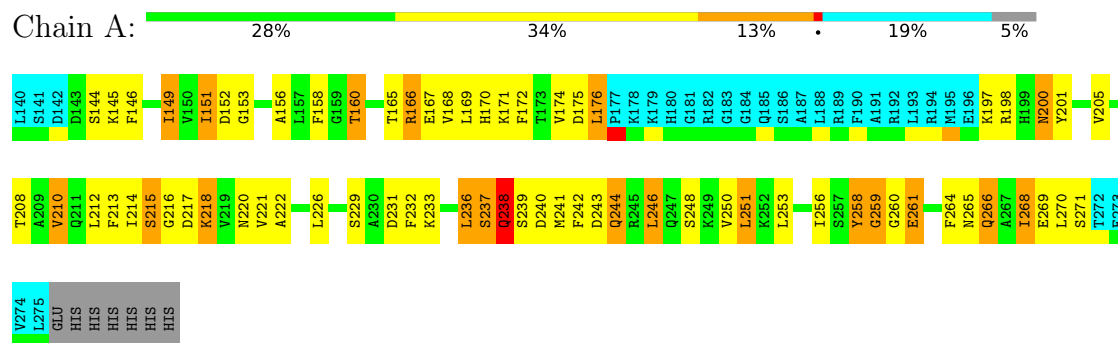
4.2.6 Score per residue for model 6

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



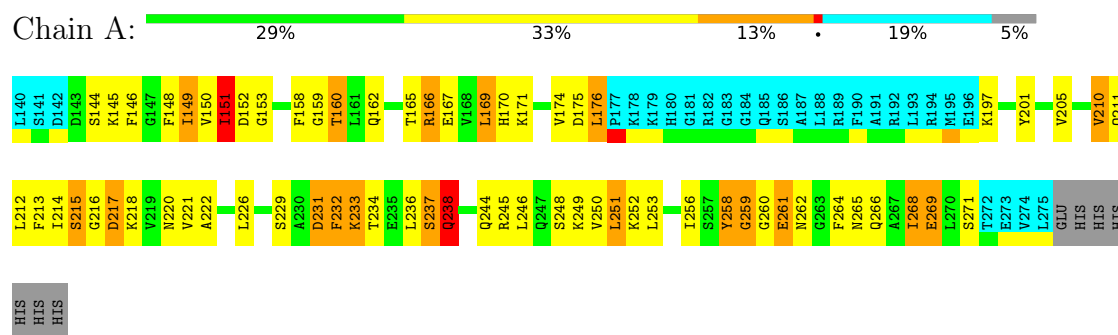
4.2.7 Score per residue for model 7

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



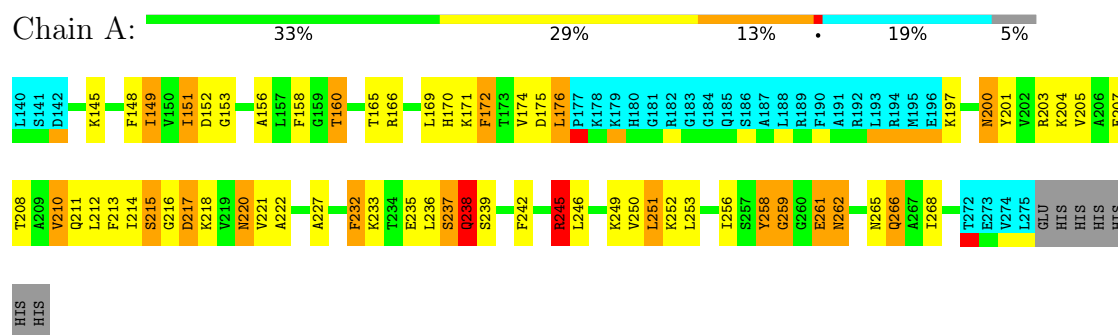
4.2.8 Score per residue for model 8

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



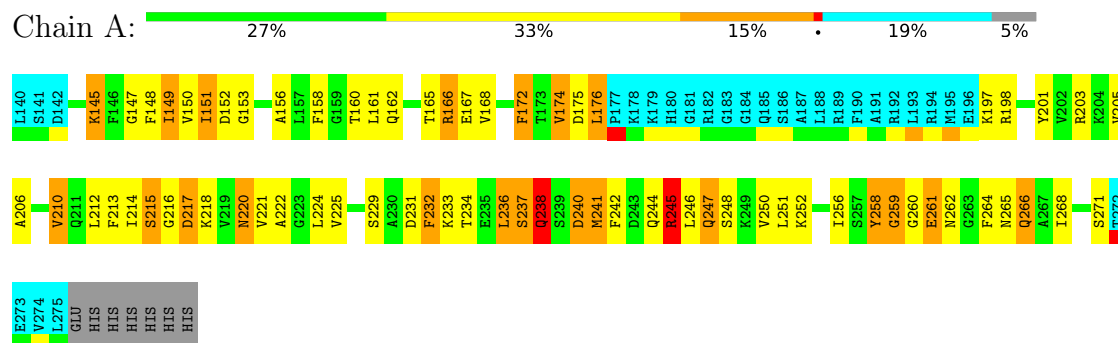
4.2.9 Score per residue for model 9

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



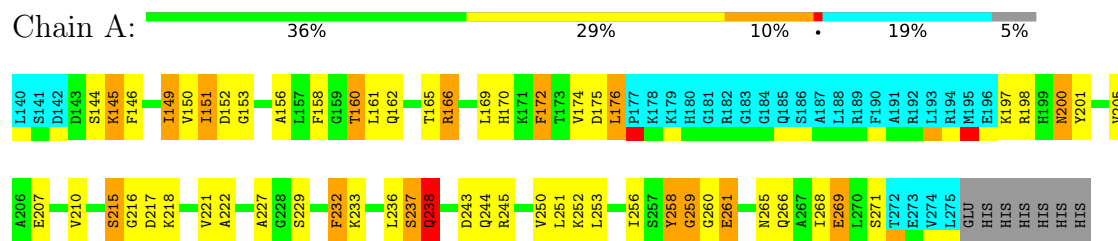
4.2.10 Score per residue for model 10

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



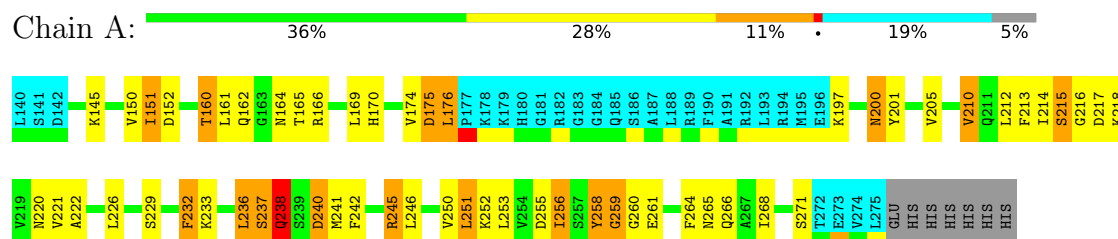
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



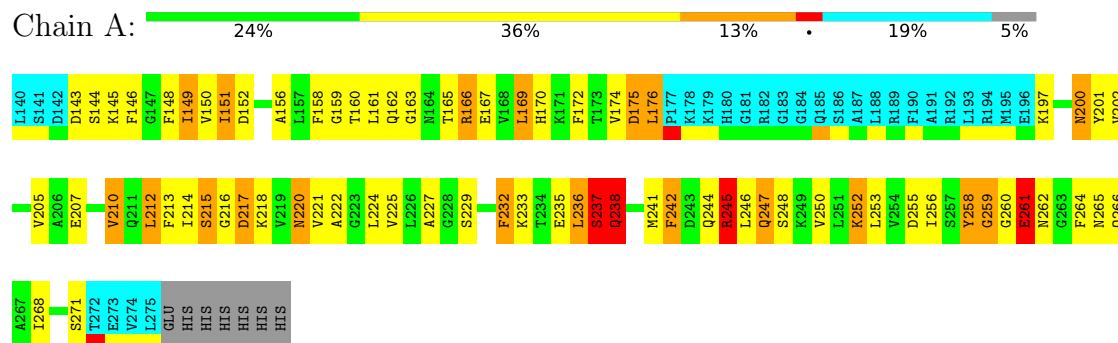
4.2.12 Score per residue for model 12

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



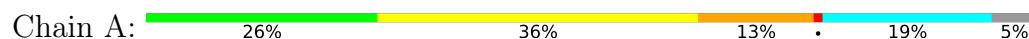
4.2.13 Score per residue for model 13

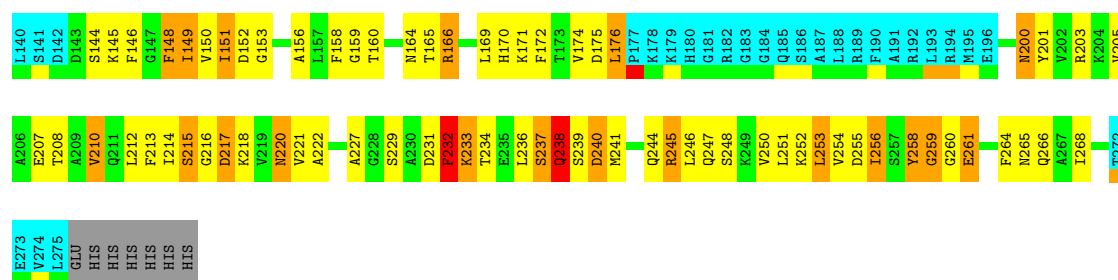
- Molecule 1: Eukaryotic peptide chain release factor subunit 1



4.2.14 Score per residue for model 14

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

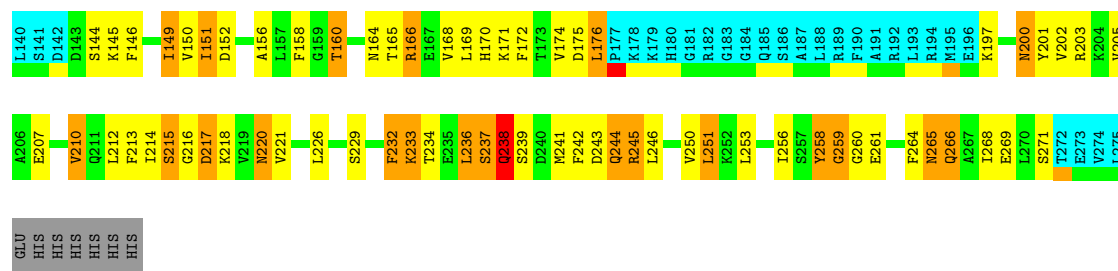




4.2.15 Score per residue for model 15

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

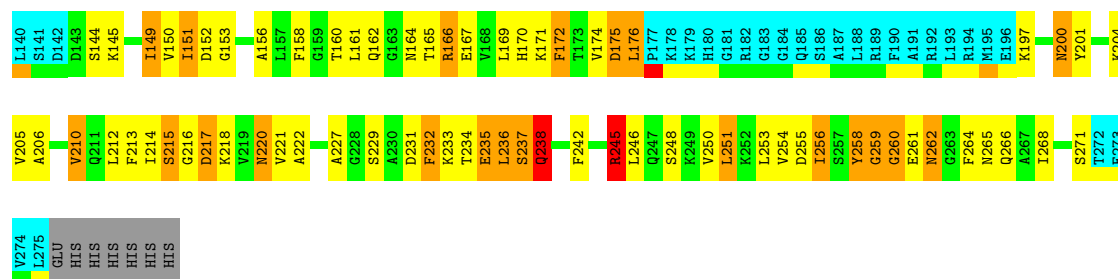
Chain A: 29% 31% 15% 19% 5%



4.2.16 Score per residue for model 16

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

Chain A: 27% 33% 15% 19% 5%

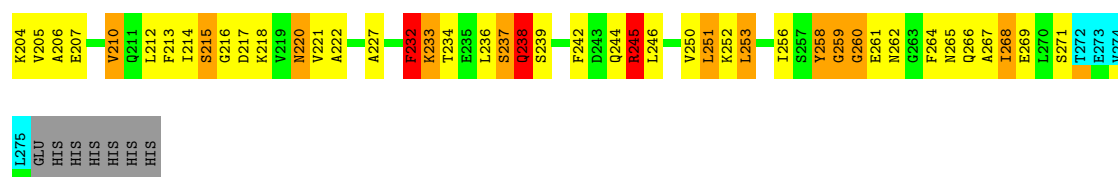


4.2.17 Score per residue for model 17

- Molecule 1: Eukaryotic peptide chain release factor subunit 1

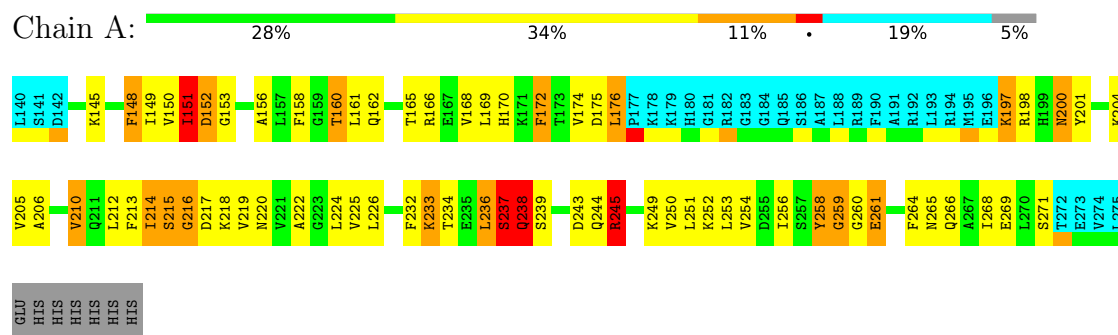
Chain A: 27% 34% 13% 19% 5%





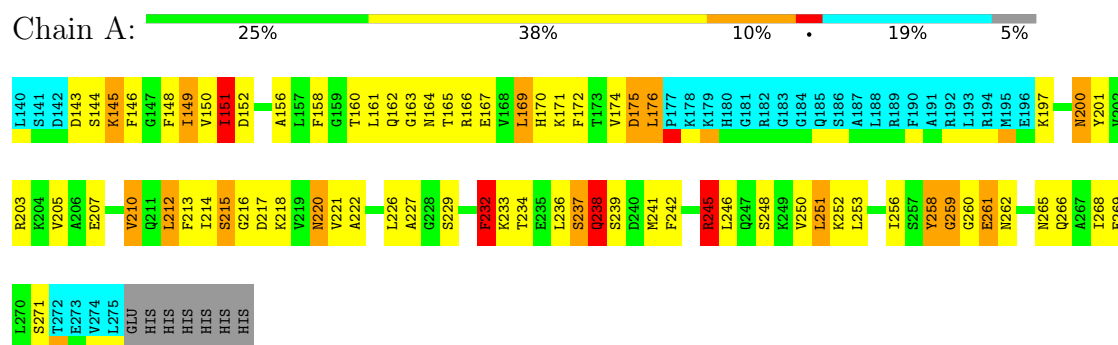
4.2.18 Score per residue for model 18

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



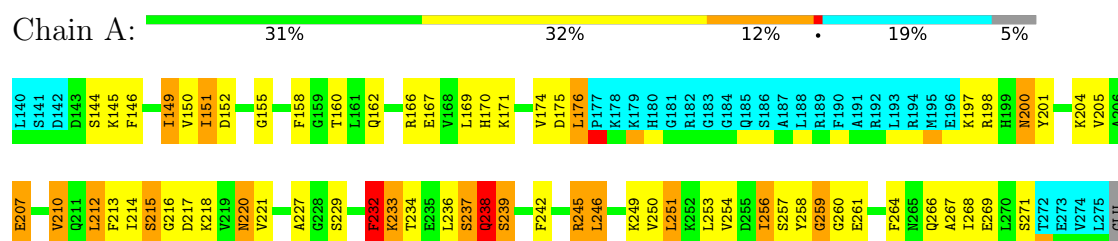
4.2.19 Score per residue for model 19

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



4.2.20 Score per residue for model 20

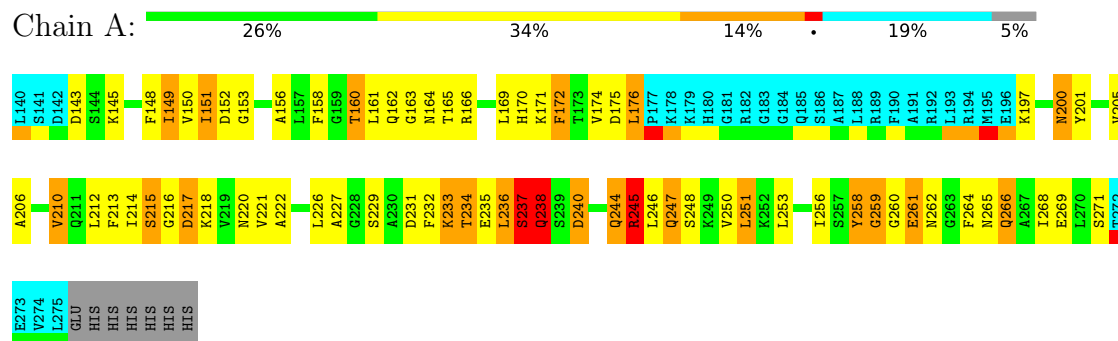
- Molecule 1: Eukaryotic peptide chain release factor subunit 1



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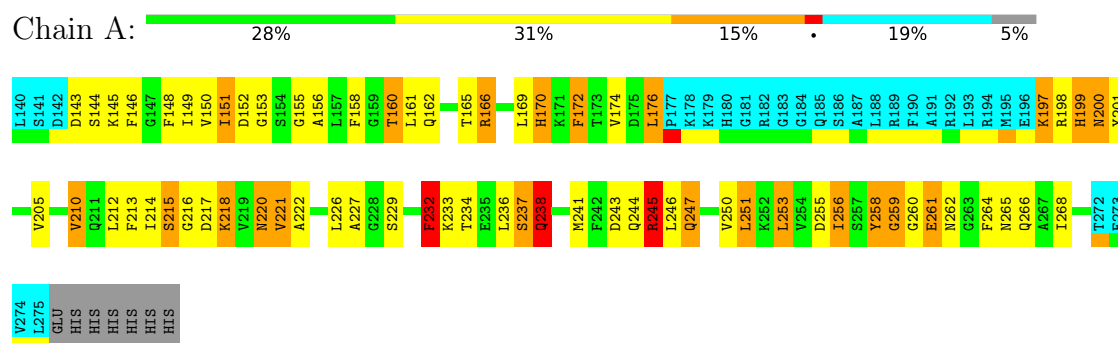
4.2.21 Score per residue for model 21

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



4.2.22 Score per residue for model 22

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



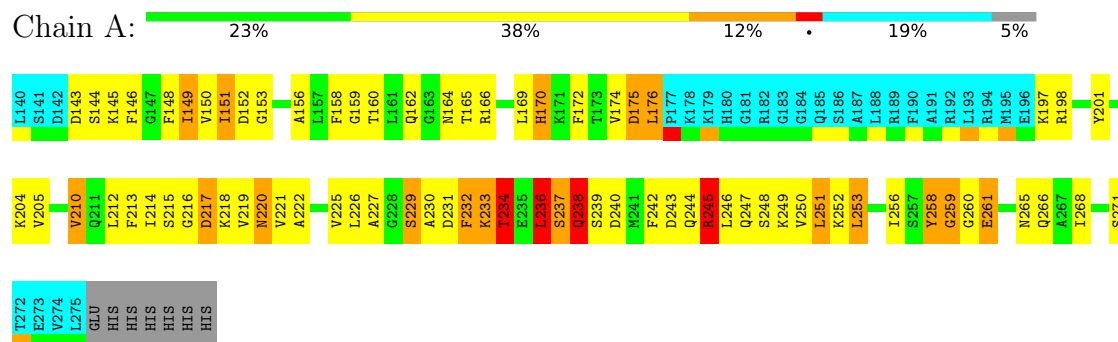
4.2.23 Score per residue for model 23

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



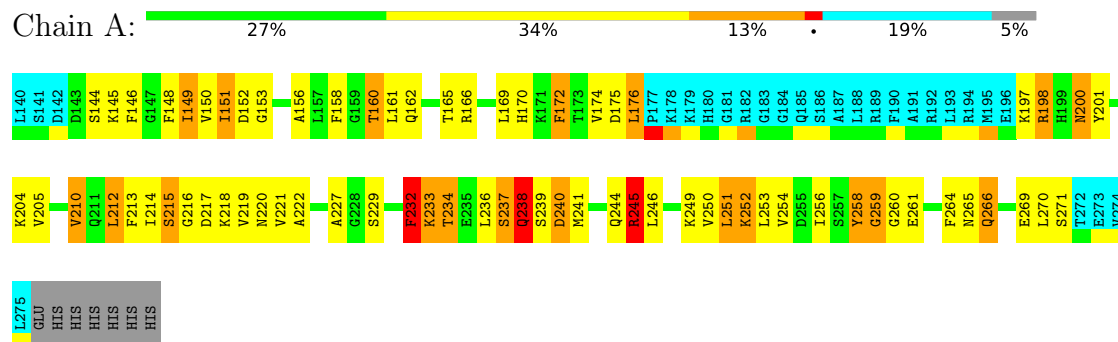
4.2.24 Score per residue for model 24

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



4.2.25 Score per residue for model 25

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



5 Refinement protocol and experimental data overview ⓘ

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	0.90±0.02	1±0/852 (0.1± 0.0%)	1.42±0.02	6±2/1147 (0.5± 0.1%)
All	All	0.90	25/21300 (0.1%)	1.42	145/28675 (0.5%)

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

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	251	LEU	CA-C	7.55	1.60	1.53	9	23
1	A	251	LEU	N-CA	5.15	1.52	1.46	23	1
1	A	176	LEU	CA-C	5.08	1.59	1.52	6	1

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	260	GLY	N-CA-C	9.87	119.19	110.21	16	2
1	A	232	PHE	CA-CB-CG	-7.68	106.12	113.80	20	23
1	A	245	ARG	N-CA-C	7.00	118.99	111.36	16	17
1	A	148	PHE	CA-CB-CG	-6.73	107.07	113.80	17	13
1	A	269	GLU	N-CA-C	-6.72	103.88	111.07	20	12
1	A	251	LEU	N-CA-C	6.62	121.30	111.96	9	22
1	A	246	LEU	N-CA-C	6.51	118.45	111.36	22	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	172	PHE	N-CA-C	6.47	118.05	108.60	4	13
1	A	149	ILE	N-CA-C	6.06	116.92	107.28	3	20
1	A	234	THR	N-CA-C	-5.90	104.85	111.28	25	4
1	A	151	ILE	N-CA-C	5.89	116.36	108.11	6	6
1	A	221	VAL	N-CA-C	5.87	117.21	108.46	22	1
1	A	261	GLU	N-CA-C	5.78	117.25	111.07	14	3
1	A	239	SER	N-CA-C	5.54	117.31	111.28	3	4
1	A	268	ILE	CB-CA-C	-5.42	104.82	112.14	7	1
1	A	236	LEU	CA-C-O	-5.20	115.04	120.55	24	1
1	A	170	HIS	CA-CB-CG	-5.11	108.69	113.80	5	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	66±10
All	All	21000	21075	21075	1640

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 39.

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:244:GLN:C	1:A:247:GLN:HE22	0.65	1.99	22	3
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:252:LYS:C	1:A:253:LEU:HD12	0.64	2.18	19	7
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:199:HIS:ND1	1:A:241:MET:HE2	0.62	2.08	1	1
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:258:TYR:CD1	1:A:258:TYR:C	0.61	2.78	14	19
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:166:ARG:HH11	1:A:166:ARG:C	0.61	2.04	2	4
1:A:219:VAL:HG11	1:A:249:LYS:NZ	0.61	2.11	5	4
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:237:SER:O	1:A:238:GLN:C	0.59	2.44	10	25
1:A:236:LEU:O	1:A:237:SER:C	0.59	2.45	24	25
1:A:262:ASN:N	1:A:262:ASN:ND2	0.59	2.48	16	1
1:A:238:GLN:CD	1:A:241:MET:H	0.59	2.05	7	3
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
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:258:TYR:C	1:A:258:TYR:CD1	0.58	2.80	10	5
1:A:152:ASP:O	1:A:201:TYR:OH	0.58	2.18	1	22
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:233:LYS:HZ3	1:A:254:VAL:C	0.57	2.07	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:143:ASP:CG	1:A:163:GLY:H	0.57	2.07	21	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:258:TYR:O	1:A:259:GLY:C	0.56	2.49	14	25
1:A:148:PHE:N	1:A:159:GLY:O	0.56	2.39	8	8
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:NE	1:A:265:ASN:OD1	0.56	2.38	22	2
1:A:213:PHE:C	1:A:220:ASN:ND2	0.56	2.63	20	23
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: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: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	4
1:A:166:ARG:NH2	1:A:268:ILE:HD11	0.54	2.17	4	1
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:237:SER:C	1:A:247:GLN:NE2	0.54	2.66	14	3
1:A:245:ARG:HE	1:A:245:ARG:CA	0.54	2.16	3	11
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:239:SER:OG	1:A:244:GLN:NE2	0.52	2.42	17	4
1:A:199:HIS:ND1	1:A:199:HIS:C	0.52	2.66	2	2
1:A:166:ARG:O	1:A:166:ARG:NH1	0.52	2.41	19	5
1:A:261:GLU:CD	1:A:262:ASN:N	0.52	2.67	22	2
1:A:260:GLY:O	1:A:264:PHE:CB	0.52	2.57	14	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:167:GLU:N	1:A:167:GLU:CD	0.52	2.68	13	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:233:LYS:HZ3	1:A:254:VAL:N	0.52	2.03	1	1
1:A:252:LYS:C	1:A:253:LEU:HD23	0.52	2.30	4	1
1:A:265:ASN:ND2	1:A:265:ASN:C	0.52	2.66	15	1
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:HZ1	1:A:254:VAL:N	0.51	2.03	18	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: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: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:257:SER:C	1:A:258:TYR:CG	0.51	2.88	20	1
1:A:149:ILE:HG23	1:A:158:PHE:CE2	0.51	2.41	24	3
1:A:268:ILE:O	1:A:271:SER:C	0.50	2.54	19	18
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:245:ARG:HE	1:A:245:ARG:C	0.50	2.14	17	6
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
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:252:LYS:C	1:A:253:LEU:HD13	0.50	2.32	24	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:237:SER:C	1:A:247:GLN:HE22	0.49	2.14	1	3
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:244:GLN:CD	1:A:244:GLN:N	0.49	2.71	8	1
1:A:250:VAL:O	1:A:250:VAL:CG1	0.49	2.61	17	24
1:A:161:LEU:HD23	1:A:161:LEU:C	0.49	2.33	2	3
1:A:166:ARG:HB2	1:A:166:ARG:HH11	0.49	1.65	17	2
1:A:233:LYS:O	1:A:234:THR:C	0.49	2.56	24	4
1:A:240:ASP:OD1	1:A:240:ASP:N	0.48	2.46	21	4
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:153:GLY:C	1:A:176:LEU:HD11	0.48	2.33	9	1
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:201:TYR:CD2	1:A:201:TYR:C	0.48	2.91	13	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: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:N	1:A:244:GLN:NE2	0.47	2.62	8	2
1:A:151:ILE:O	1:A:151:ILE:CG2	0.47	2.62	21	13
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
1:A:237:SER:CA	1:A:247:GLN:HE22	0.47	2.22	14	3
1:A:245:ARG:O	1:A:245:ARG:NE	0.47	2.48	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:233:LYS:HZ1	1:A:253:LEU:HD12	0.47	1.68	15	1
1:A:237:SER:O	1:A:242:PHE:CB	0.47	2.62	24	3
1:A:213:PHE:O	1:A:220:ASN:CG	0.47	2.58	18	1
1:A:224:LEU:O	1:A:251:LEU:HB2	0.47	2.10	5	1
1:A:247:GLN:NE2	1:A:247:GLN:CA	0.47	2.77	10	3
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:164:ASN:ND2	1:A:164:ASN:N	0.46	2.57	6	1
1:A:233:LYS:HZ2	1:A:255:ASP:HA	0.46	1.70	5	2
1:A:262:ASN:H	1:A:262:ASN:ND2	0.46	2.09	9	1
1:A:166:ARG:NH1	1:A:166:ARG:C	0.46	2.72	2	1
1:A:243:ASP:CB	1:A:246:LEU:HD12	0.46	2.41	7	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: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: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:238:GLN:O	1:A:238:GLN:CD	0.45	2.58	19	3
1:A:233:LYS:NZ	1:A:254:VAL:C	0.45	2.73	16	1
1:A:233:LYS:NZ	1:A:254:VAL:O	0.45	2.47	18	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:233:LYS:CD	1:A:254:VAL:O	0.45	2.65	25	2
1:A:149:ILE:HD12	1:A:226:LEU:CD2	0.45	2.41	7	2
1:A:168:VAL:C	1:A:169:LEU:HD12	0.45	2.37	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:245:ARG:CA	1:A:245:ARG:HE	0.45	2.25	9	3
1:A:262:ASN:ND2	1:A:262:ASN:N	0.45	2.65	9	2
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:232:PHE:O	1:A:233:LYS:C	0.44	2.60	14	1
1:A:213:PHE:HA	1:A:220:ASN:ND2	0.44	2.27	9	4
1:A:260:GLY:O	1:A:261:GLU:C	0.44	2.60	18	6
1:A:213:PHE:HA	1:A:220:ASN:HD22	0.44	1.73	7	13
1:A:233:LYS:HZ2	1:A:254:VAL:C	0.44	2.19	16	1
1:A:175:ASP:C	1:A:176:LEU:O	0.44	2.60	3	4
1:A:144:SER:O	1:A:146:PHE:CD2	0.43	2.70	14	4
1:A:166:ARG:C	1:A:167:GLU:CD	0.43	2.86	10	4
1:A:162:GLN:O	1:A:162:GLN:CG	0.43	2.66	25	6
1:A:233:LYS:HZ3	1:A:255:ASP:N	0.43	2.10	2	1
1:A:165:THR:HG22	1:A:167:GLU:OE2	0.43	2.13	16	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:202:VAL:N	0.43	2.86	13	1
1:A:219:VAL:HG11	1:A:249:LYS:HZ3	0.43	1.73	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:215:SER:O	1:A:216:GLY:C	0.43	2.62	18	3
1:A:229:SER:C	1:A:231:ASP:N	0.43	2.77	7	2
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:261:GLU:CD	1:A:261:GLU:C	0.42	2.87	22	1
1:A:264:PHE:O	1:A:268:ILE:HG12	0.42	2.15	7	1
1:A:238:GLN:OE1	1:A:241:MET:HE2	0.42	2.13	10	1
1:A:143:ASP:CG	1:A:163:GLY:N	0.42	2.75	21	2
1:A:207:GLU:O	1:A:207:GLU:OE1	0.42	2.38	20	1
1:A:151:ILE:C	1:A:152:ASP:OD1	0.42	2.62	21	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:158:PHE:O	1:A:169:LEU:HB2	0.42	2.14	8	1
1:A:164:ASN:O	1:A:164:ASN:CG	0.42	2.62	15	1
1:A:214:ILE:HG23	1:A:218:LYS:O	0.42	2.15	8	1
1:A:244:GLN:O	1:A:247:GLN:OE1	0.42	2.37	10	1
1:A:217:ASP:O	1:A:217:ASP:CG	0.42	2.62	18	2
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:210:VAL:CG2	1:A:211:GLN:N	0.42	2.82	9	2
1:A:166:ARG:HB3	1:A:268:ILE:HD13	0.42	1.92	18	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: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:257:SER:OG	1:A:258:TYR:N	0.41	2.52	20	1
1:A:237:SER:CA	1:A:247:GLN:NE2	0.41	2.83	24	2
1:A:268:ILE:O	1:A:269:GLU:C	0.41	2.63	4	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:230:ALA:C	1:A:231:ASP:OD1	0.41	2.64	3	1
1:A:175:ASP:O	1:A:175:ASP:CG	0.41	2.63	7	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: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:229:SER:O	1:A:230:ALA:C	0.40	2.64	24	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:145:LYS:HZ2	1:A:160:THR:HG21	0.40	1.76	10	1
1:A:166:ARG:HH11	1:A:166:ARG:HG2	0.40	1.75	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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%)	2	22
All	All	2725/3575 (76%)	2459 (90%)	122 (4%)	144 (5%)	2	22

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%)	66±3 (72±3%)	25±3 (28±3%)	1	20
All	All	2275/3000 (76%)	1649 (72%)	626 (28%)	1	20

All 67 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	151	ILE	25
1	A	210	VAL	25
1	A	238	GLN	25
1	A	256	ILE	25
1	A	215	SER	24
1	A	221	VAL	24
1	A	245	ARG	24
1	A	258	TYR	24
1	A	233	LYS	22
1	A	165	THR	20
1	A	200	ASN	19
1	A	246	LEU	19
1	A	251	LEU	18
1	A	220	ASN	17
1	A	229	SER	17
1	A	175	ASP	16
1	A	266	GLN	16
1	A	160	THR	16
1	A	166	ARG	15
1	A	232	PHE	13
1	A	170	HIS	12
1	A	171	LYS	12
1	A	217	ASP	12
1	A	248	SER	10
1	A	240	ASP	9
1	A	164	ASN	9
1	A	236	LEU	9
1	A	252	LYS	8
1	A	145	LYS	8
1	A	198	ARG	7
1	A	253	LEU	7
1	A	212	LEU	7
1	A	226	LEU	7
1	A	169	LEU	7
1	A	204	LYS	7
1	A	231	ASP	6
1	A	168	VAL	6
1	A	247	GLN	5
1	A	207	GLU	5
1	A	235	GLU	5
1	A	199	HIS	4
1	A	174	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	249	LYS	4
1	A	268	ILE	4
1	A	237	SER	4
1	A	244	GLN	4
1	A	261	GLU	4
1	A	197	LYS	3
1	A	254	VAL	3
1	A	255	ASP	3
1	A	234	THR	3
1	A	208	THR	3
1	A	269	GLU	3
1	A	143	ASP	2
1	A	218	LYS	2
1	A	262	ASN	2
1	A	241	MET	2
1	A	211	GLN	1
1	A	148	PHE	1
1	A	203	ARG	1
1	A	225	VAL	1
1	A	202	VAL	1
1	A	265	ASN	1
1	A	144	SER	1
1	A	152	ASP	1
1	A	214	ILE	1
1	A	167	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 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