



Full wwPDB NMR Structure Validation Report ⓘ

May 30, 2020 – 03:53 pm BST

PDB ID : 2NBQ
Title : NMR Structure of the C-Terminal Domain of human APOBEC3B
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Deposited on : 2016-03-09

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

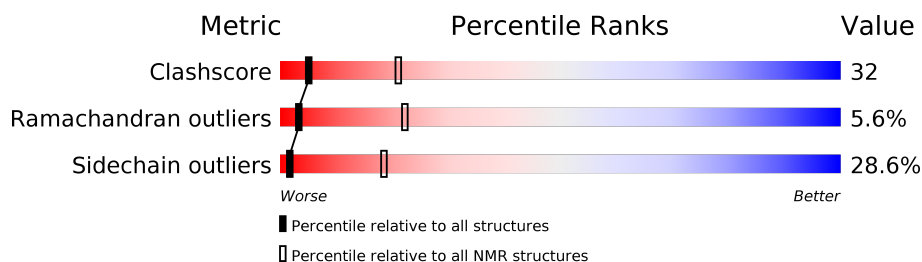
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 64%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	205	

2 Ensemble composition and analysis

This entry contains 30 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: *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:191-A:202, A:214-A:240, A:252-A:377 (165)	0.45	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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	6, 7, 8, 15, 16, 20, 23, 24, 25, 27
2	1, 4, 5, 11, 12, 17, 19, 22, 28, 30
3	14, 18, 21, 26
4	3, 9, 10
5	13, 29
Single-model clusters	2

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3208 atoms, of which 1563 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA dC->dU-editing enzyme APOBEC-3B.

Mol	Chain	Residues	Atoms						Trace
1	A	197	Total	C	H	N	O	S	0
			3207	1055	1563	282	294	13	

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	MET	-	EXPRESSION TAG	UNP Q9UH17
A	383	LEU	-	EXPRESSION TAG	UNP Q9UH17
A	384	GLU	-	EXPRESSION TAG	UNP Q9UH17
A	385	HIS	-	EXPRESSION TAG	UNP Q9UH17
A	386	HIS	-	EXPRESSION TAG	UNP Q9UH17
A	387	HIS	-	EXPRESSION TAG	UNP Q9UH17
A	388	HIS	-	EXPRESSION TAG	UNP Q9UH17
A	389	HIS	-	EXPRESSION TAG	UNP Q9UH17
A	390	HIS	-	EXPRESSION TAG	UNP Q9UH17

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

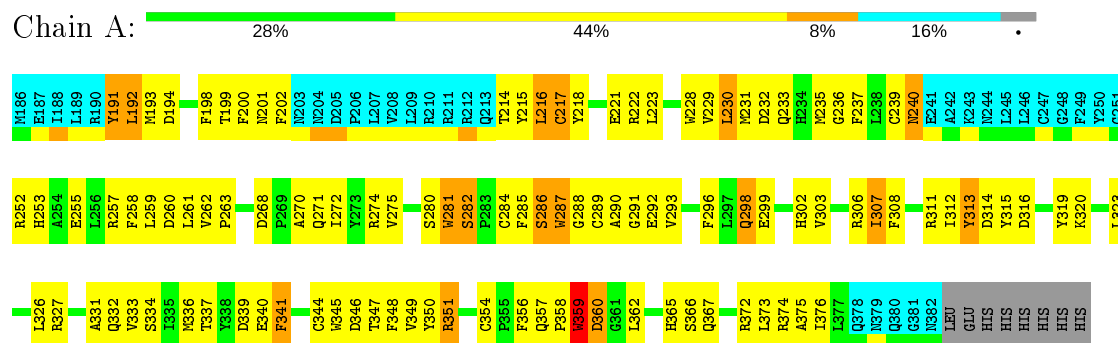
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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: DNA dC->dU-editing enzyme APOBEC-3B

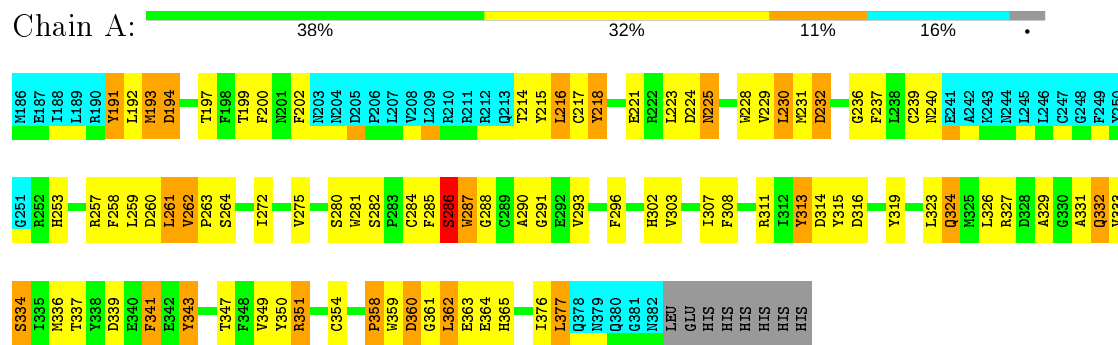


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

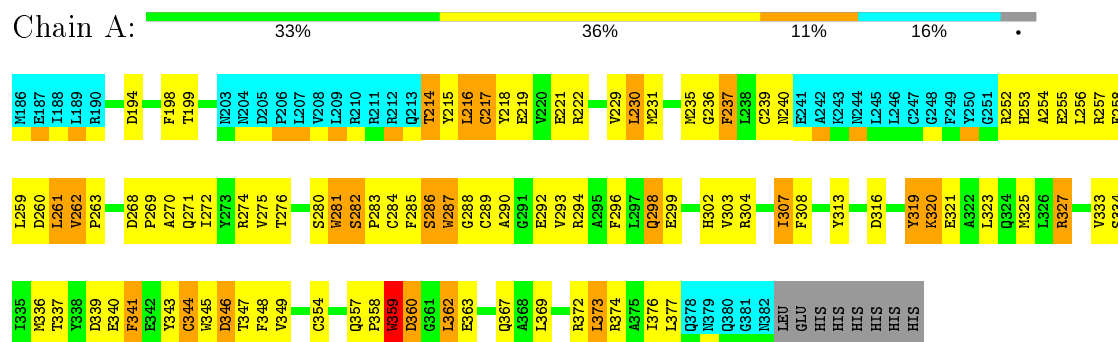
4.2.1 Score per residue for model 1

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



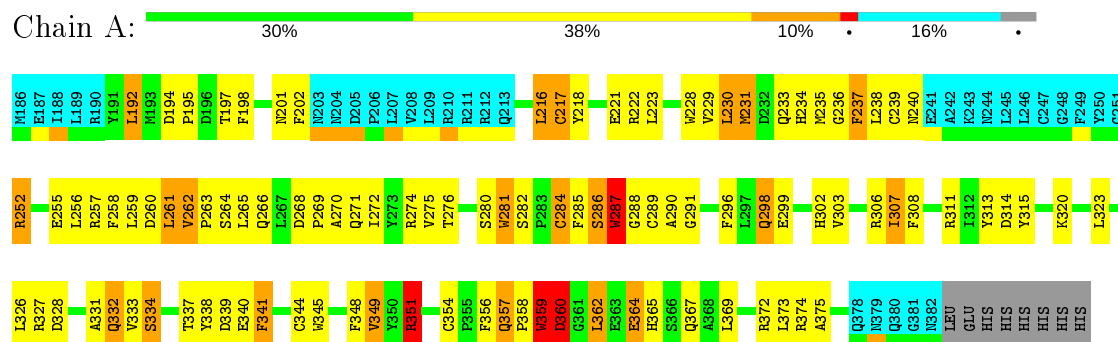
4.2.2 Score per residue for model 2

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



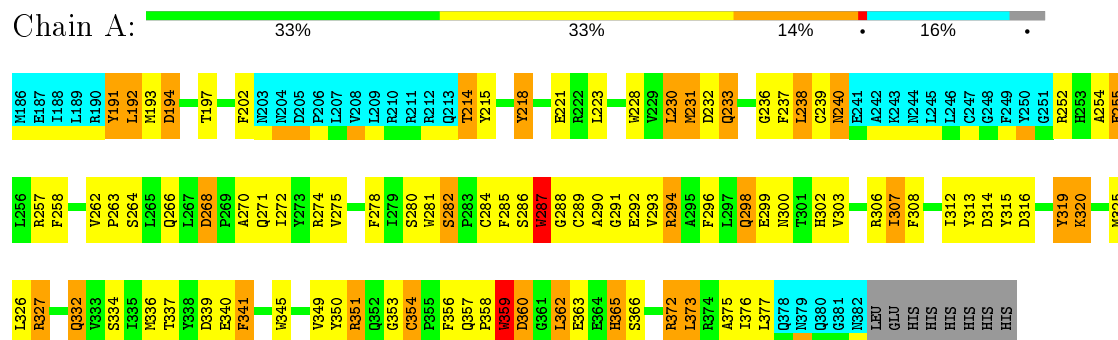
4.2.5 Score per residue for model 5

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



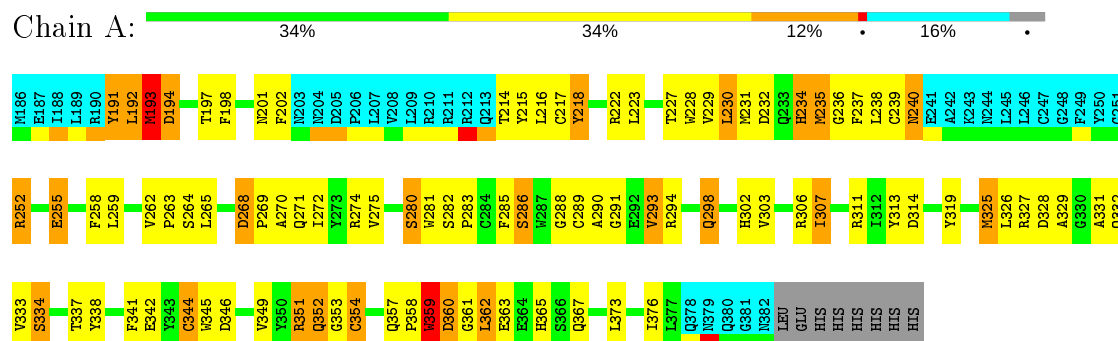
4.2.6 Score per residue for model 6

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



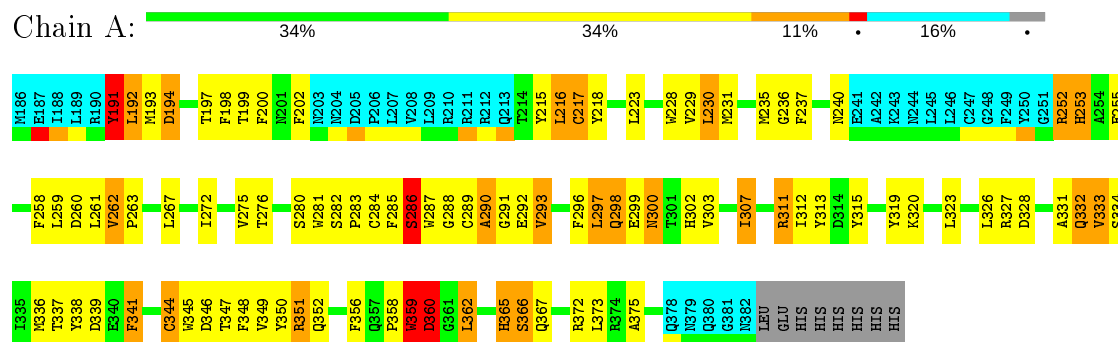
4.2.7 Score per residue for model 7

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



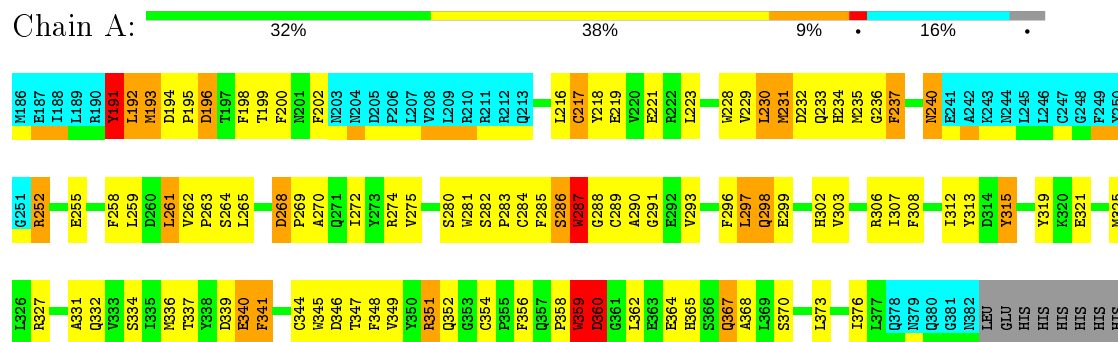
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



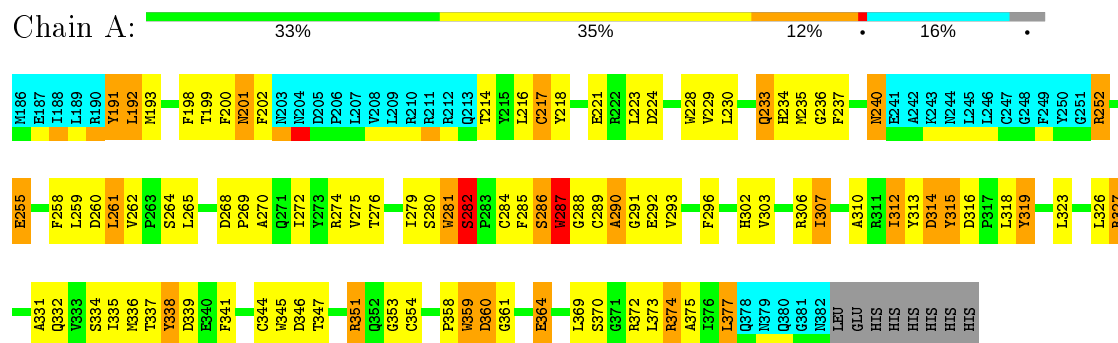
4.2.12 Score per residue for model 12

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



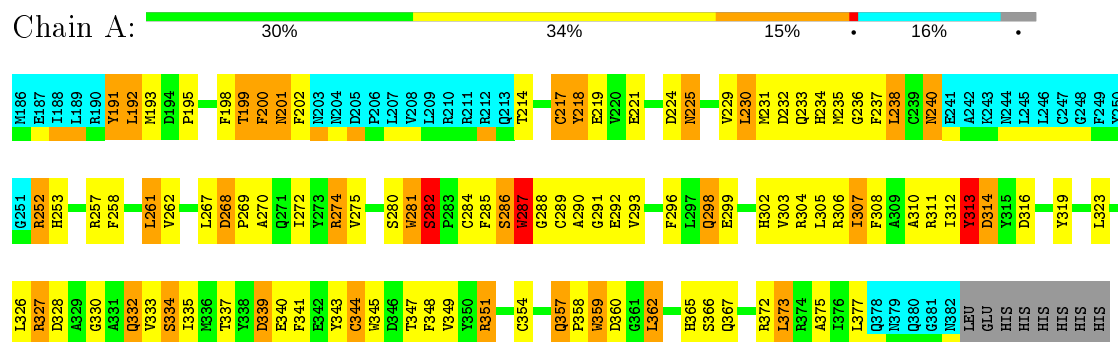
4.2.13 Score per residue for model 13

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



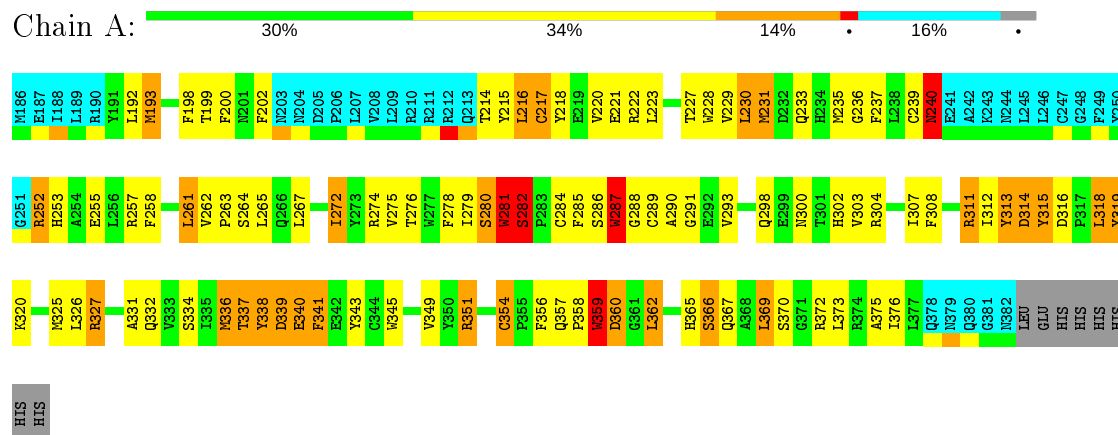
4.2.14 Score per residue for model 14

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



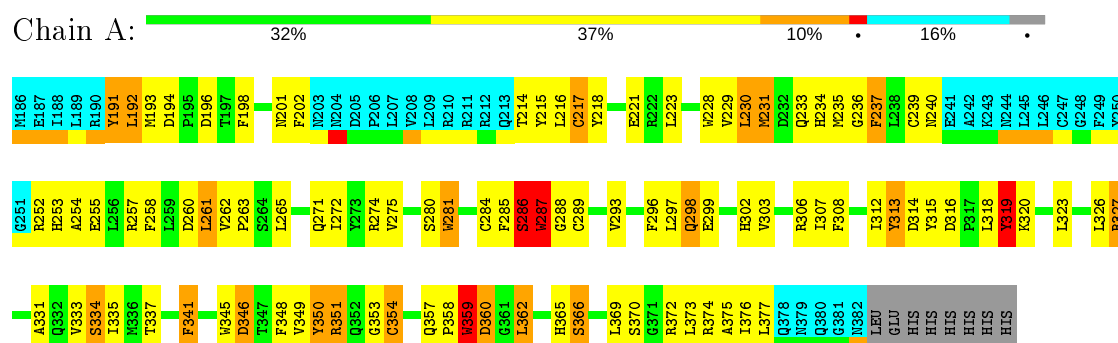
4.2.15 Score per residue for model 15

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



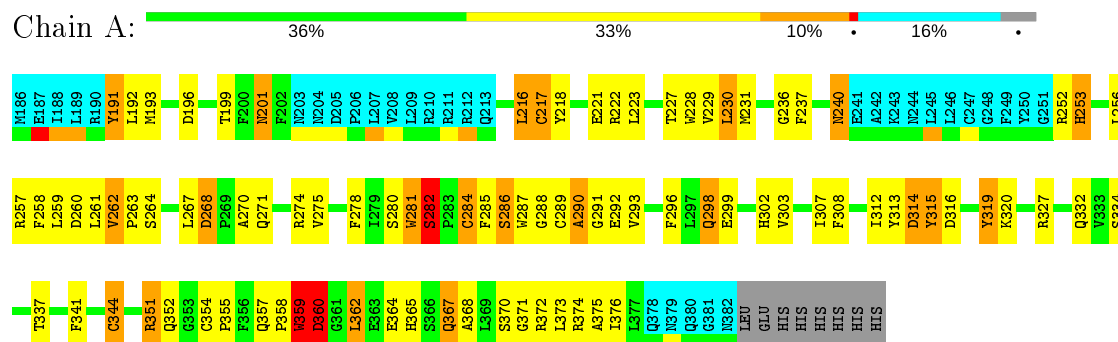
4.2.16 Score per residue for model 16

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



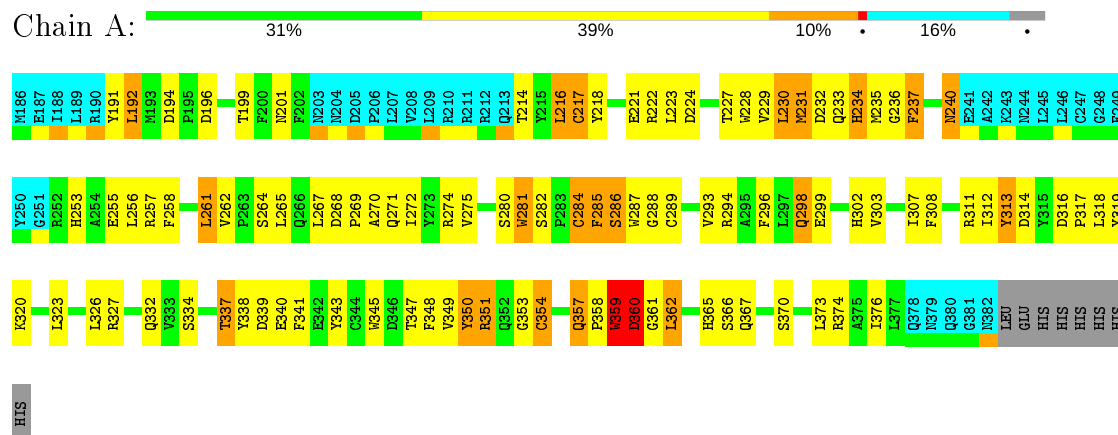
4.2.17 Score per residue for model 17

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



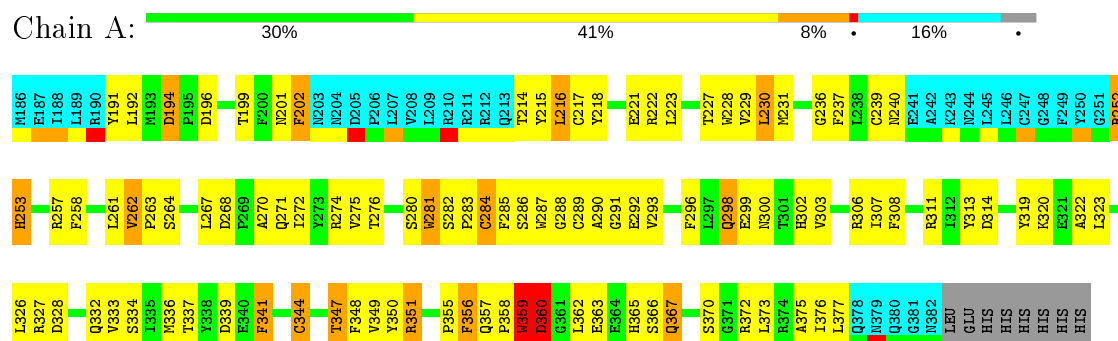
4.2.18 Score per residue for model 18

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



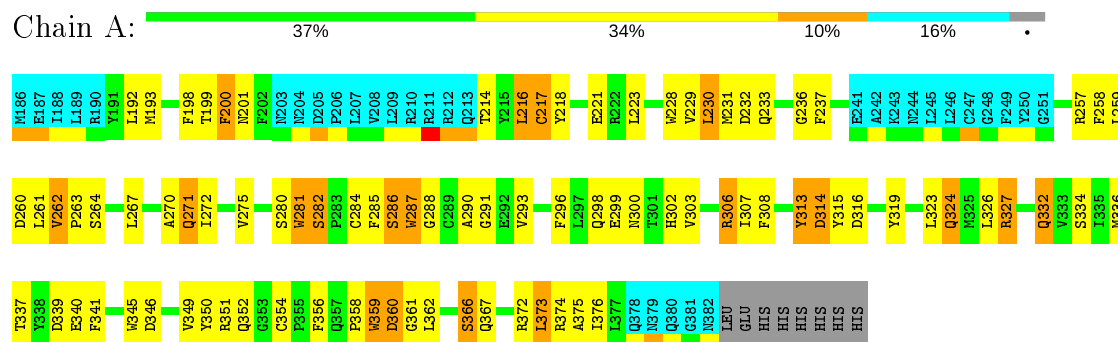
4.2.19 Score per residue for model 19

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



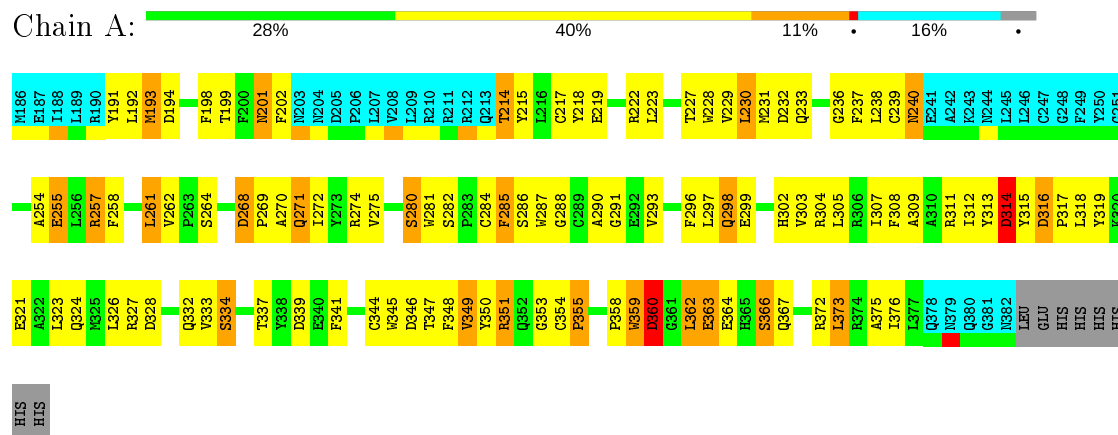
4.2.20 Score per residue for model 20

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



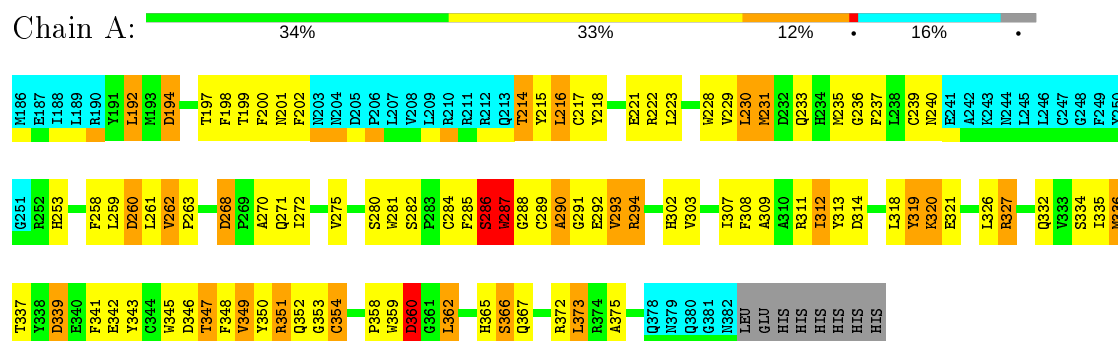
4.2.21 Score per residue for model 21

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



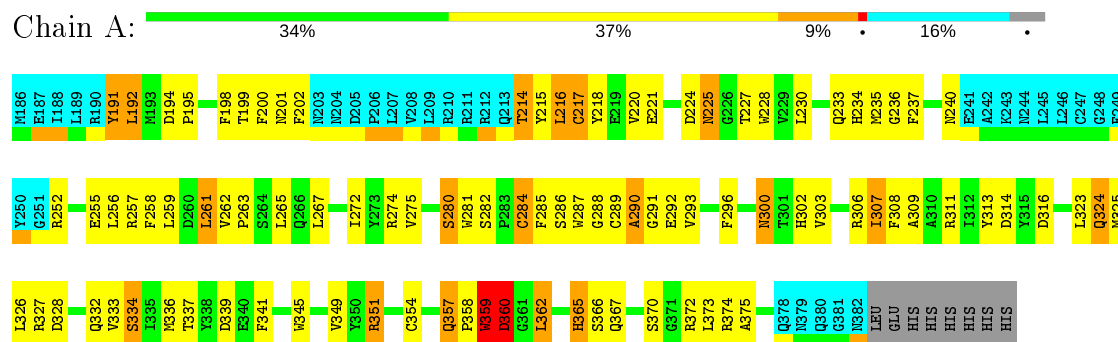
4.2.22 Score per residue for model 22

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



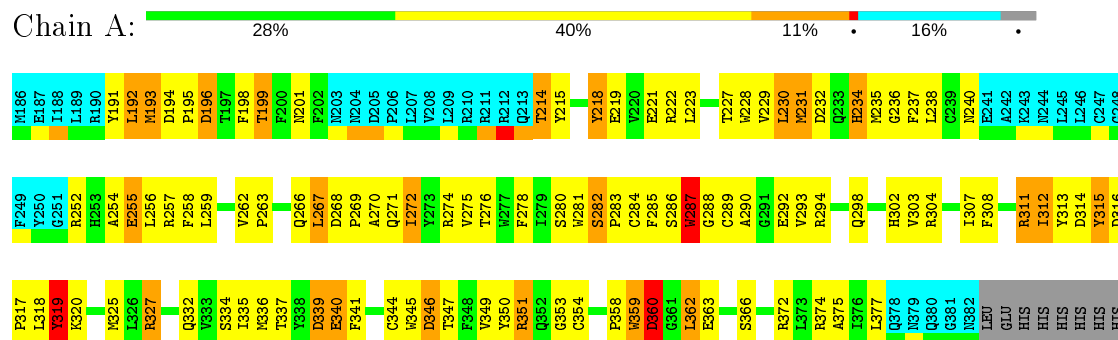
4.2.23 Score per residue for model 23

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



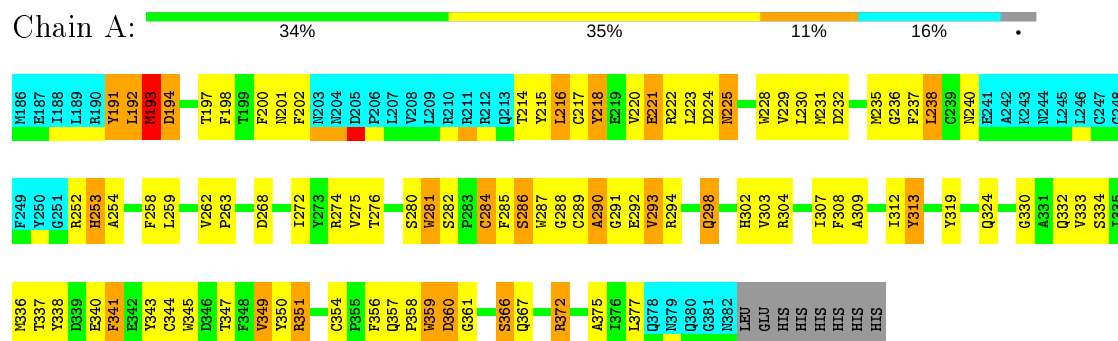
4.2.24 Score per residue for model 24

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



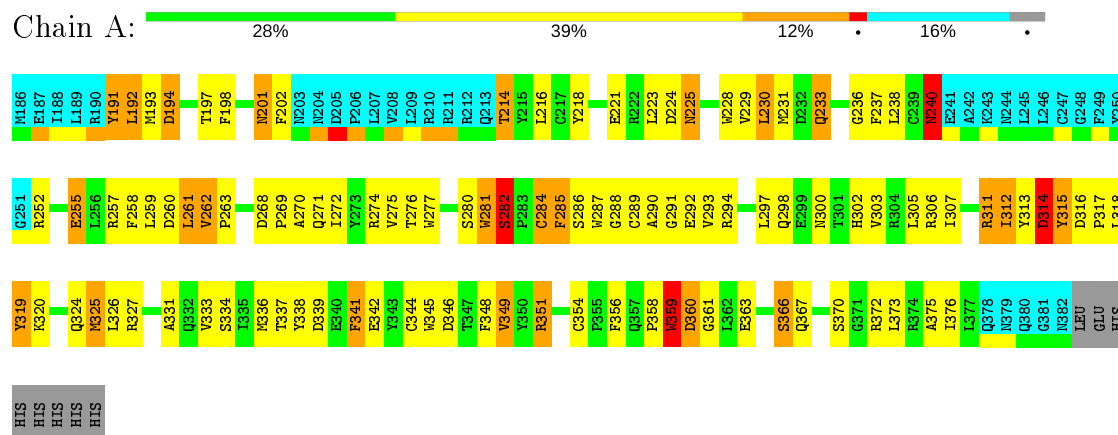
4.2.25 Score per residue for model 25

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



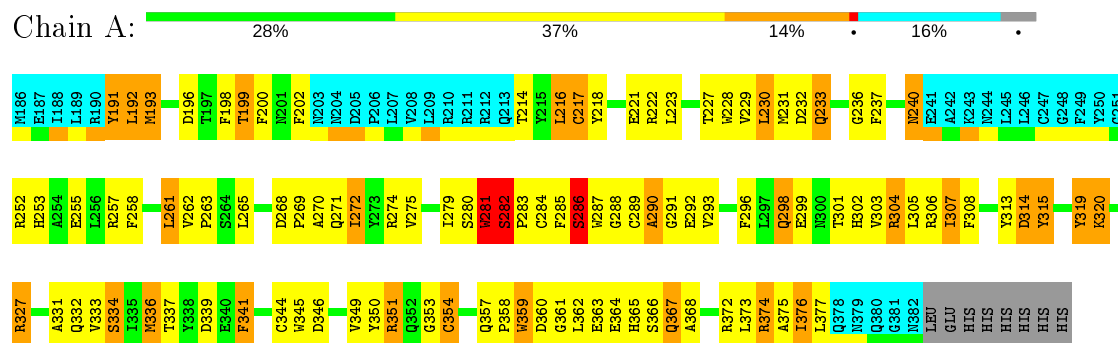
4.2.26 Score per residue for model 26

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



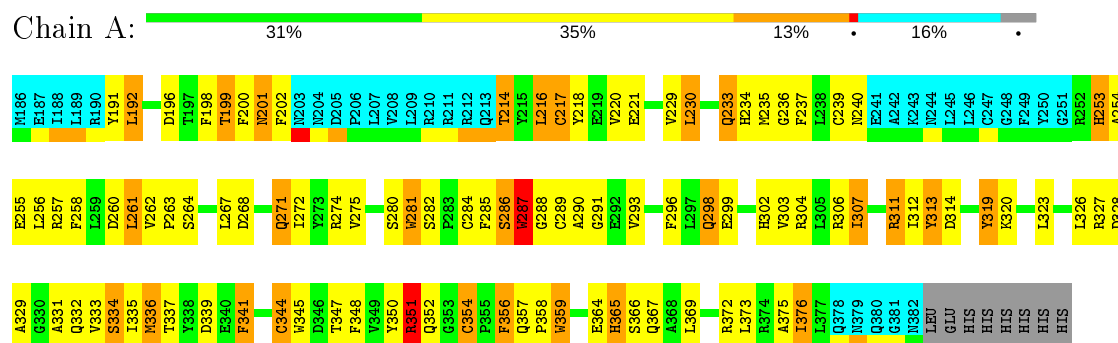
4.2.27 Score per residue for model 27

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



4.2.28 Score per residue for model 28

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



5 Refinement protocol and experimental data overview

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

Of the 256 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
XPLOR-NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	2
Total number of shifts	2228
Number of shifts mapped to atoms	2228
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	64%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	1382	1298	1298	87±10
All	All	41490	38940	38940	2604

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:335:ILE:HD11	1:A:369:LEU:HD23	0.85	1.46	16	4
1:A:327:ARG:CZ	1:A:377:LEU:HD11	0.81	2.06	13	2
1:A:312:ILE:HD12	1:A:312:ILE:H	0.80	1.36	3	1
1:A:307:ILE:HD12	1:A:307:ILE:N	0.79	1.92	11	4
1:A:238:LEU:N	1:A:238:LEU:HD23	0.79	1.91	6	1
1:A:312:ILE:HD13	1:A:312:ILE:O	0.77	1.78	10	1
1:A:238:LEU:HD23	1:A:238:LEU:N	0.76	1.94	14	1
1:A:312:ILE:H	1:A:312:ILE:HD12	0.76	1.39	13	1
1:A:327:ARG:HH11	1:A:377:LEU:HD11	0.74	1.39	16	1
1:A:297:LEU:CD2	1:A:331:ALA:HB2	0.72	2.14	12	4
1:A:351:ARG:NE	1:A:351:ARG:H	0.72	1.83	27	9
1:A:362:LEU:O	1:A:362:LEU:HD12	0.72	1.85	24	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:259:LEU:HD22	1:A:292:GLU:OE1	0.72	1.84	25	1
1:A:362:LEU:HD12	1:A:362:LEU:O	0.71	1.85	22	2
1:A:365:HIS:CE1	1:A:369:LEU:HD23	0.71	2.20	15	1
1:A:302:HIS:CD2	1:A:302:HIS:H	0.71	2.04	3	1
1:A:307:ILE:N	1:A:307:ILE:HD13	0.71	2.01	9	6
1:A:312:ILE:N	1:A:312:ILE:HD12	0.70	2.01	13	1
1:A:307:ILE:HD13	1:A:307:ILE:N	0.70	2.02	7	8
1:A:351:ARG:H	1:A:351:ARG:NE	0.69	1.84	7	11
1:A:341:PHE:CE2	1:A:362:LEU:HD21	0.69	2.23	6	3
1:A:216:LEU:HD12	1:A:217:CYS:N	0.68	2.01	9	24
1:A:312:ILE:HD12	1:A:312:ILE:N	0.68	2.02	3	2
1:A:285:PHE:CD2	1:A:286:SER:N	0.67	2.62	6	13
1:A:255:GLU:CD	1:A:255:GLU:H	0.67	1.93	8	7
1:A:351:ARG:N	1:A:351:ARG:NE	0.67	2.42	19	10
1:A:335:ILE:CD1	1:A:369:LEU:HD23	0.67	2.19	16	4
1:A:285:PHE:CD1	1:A:286:SER:N	0.67	2.63	1	17
1:A:296:PHE:CZ	1:A:300:ASN:ND2	0.67	2.62	30	1
1:A:351:ARG:NE	1:A:351:ARG:N	0.66	2.43	10	11
1:A:312:ILE:N	1:A:312:ILE:HD13	0.66	2.06	22	1
1:A:220:VAL:O	1:A:230:LEU:HD23	0.65	1.90	25	2
1:A:284:CYS:SG	1:A:285:PHE:N	0.65	2.70	12	16
1:A:192:LEU:N	1:A:192:LEU:HD23	0.65	2.05	25	4
1:A:358:PRO:O	1:A:360:ASP:N	0.65	2.30	27	24
1:A:240:ASN:H	1:A:240:ASN:ND2	0.65	1.88	27	3
1:A:351:ARG:HE	1:A:351:ARG:H	0.65	1.33	12	1
1:A:285:PHE:CG	1:A:286:SER:N	0.64	2.65	21	19
1:A:222:ARG:O	1:A:229:VAL:HG22	0.64	1.93	18	13
1:A:216:LEU:C	1:A:216:LEU:HD12	0.64	2.14	18	19
1:A:362:LEU:C	1:A:362:LEU:HD12	0.64	2.13	24	7
1:A:341:PHE:CD2	1:A:362:LEU:HD21	0.63	2.28	9	5
1:A:312:ILE:HD11	1:A:369:LEU:CD2	0.63	2.23	3	1
1:A:259:LEU:HD21	1:A:292:GLU:O	0.63	1.93	9	2
1:A:261:LEU:C	1:A:261:LEU:HD23	0.63	2.13	21	7
1:A:327:ARG:NH1	1:A:377:LEU:HD11	0.63	2.08	13	2
1:A:345:TRP:NE1	1:A:351:ARG:NH1	0.63	2.46	7	7
1:A:261:LEU:HD23	1:A:262:VAL:N	0.63	2.08	27	19
1:A:302:HIS:CD2	1:A:302:HIS:N	0.63	2.66	3	1
1:A:237:PHE:N	1:A:237:PHE:CD1	0.63	2.67	16	14
1:A:287:TRP:CD1	1:A:288:GLY:N	0.63	2.67	8	11
1:A:253:HIS:CD2	1:A:253:HIS:N	0.62	2.67	17	6
1:A:351:ARG:H	1:A:351:ARG:HE	0.62	1.36	30	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:240:ASN:ND2	1:A:240:ASN:H	0.62	1.92	15	4
1:A:364:GLU:O	1:A:367:GLN:NE2	0.62	2.32	12	3
1:A:327:ARG:NE	1:A:377:LEU:HD11	0.62	2.10	14	3
1:A:345:TRP:CD1	1:A:351:ARG:NH1	0.62	2.67	21	6
1:A:367:GLN:NE2	1:A:368:ALA:N	0.62	2.47	27	2
1:A:201:ASN:ND2	1:A:215:TYR:CD1	0.62	2.67	19	2
1:A:319:TYR:CD1	1:A:320:LYS:N	0.62	2.67	29	5
1:A:367:GLN:NE2	1:A:367:GLN:N	0.62	2.48	9	3
1:A:351:ARG:NH2	1:A:354:CYS:N	0.62	2.47	27	7
1:A:298:GLN:NE2	1:A:299:GLU:N	0.62	2.48	9	1
1:A:320:LYS:HZ2	1:A:376:ILE:CD1	0.62	2.07	28	1
1:A:351:ARG:N	1:A:351:ARG:HE	0.62	1.93	30	4
1:A:274:ARG:NE	1:A:306:ARG:NH1	0.62	2.48	23	1
1:A:327:ARG:NH2	1:A:377:LEU:HD21	0.62	2.09	2	1
1:A:193:MET:N	1:A:237:PHE:CZ	0.62	2.68	7	10
1:A:259:LEU:H	1:A:259:LEU:HD22	0.62	1.54	5	4
1:A:281:TRP:NE1	1:A:311:ARG:NH1	0.62	2.48	24	1
1:A:238:LEU:H	1:A:238:LEU:HD23	0.62	1.55	14	1
1:A:240:ASN:N	1:A:240:ASN:ND2	0.62	2.47	4	3
1:A:198:PHE:CE2	1:A:202:PHE:CE2	0.62	2.88	29	2
1:A:258:PHE:CE2	1:A:262:VAL:CG2	0.62	2.82	12	14
1:A:228:TRP:CD1	1:A:274:ARG:NH2	0.61	2.68	12	5
1:A:306:ARG:NH1	1:A:332:GLN:NE2	0.61	2.47	20	1
1:A:351:ARG:HE	1:A:353:GLY:H	0.61	1.38	24	1
1:A:270:ALA:HB3	1:A:271:GLN:OE1	0.61	1.95	26	3
1:A:200:PHE:CD2	1:A:201:ASN:N	0.61	2.68	8	1
1:A:319:TYR:CG	1:A:320:LYS:N	0.61	2.67	30	3
1:A:261:LEU:HD23	1:A:261:LEU:C	0.61	2.16	18	12
1:A:237:PHE:CD1	1:A:237:PHE:N	0.61	2.68	5	13
1:A:281:TRP:CE2	1:A:311:ARG:NH2	0.61	2.67	7	1
1:A:351:ARG:NH1	1:A:354:CYS:N	0.61	2.48	8	3
1:A:311:ARG:NH2	1:A:365:HIS:CD2	0.61	2.68	11	1
1:A:200:PHE:CD1	1:A:201:ASN:N	0.61	2.69	20	1
1:A:274:ARG:NH2	1:A:304:ARG:NH2	0.61	2.49	28	1
1:A:306:ARG:NH2	1:A:332:GLN:NE2	0.61	2.47	5	1
1:A:216:LEU:HD12	1:A:216:LEU:C	0.61	2.16	1	4
1:A:259:LEU:HD22	1:A:259:LEU:H	0.61	1.54	7	3
1:A:238:LEU:N	1:A:238:LEU:CD2	0.61	2.64	6	2
1:A:362:LEU:HD12	1:A:362:LEU:C	0.61	2.16	22	6
1:A:258:PHE:CE1	1:A:262:VAL:CG2	0.61	2.84	25	4
1:A:351:ARG:HE	1:A:351:ARG:N	0.61	1.92	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:252:ARG:NH2	1:A:257:ARG:NE	0.60	2.49	23	1
1:A:222:ARG:NH2	1:A:231:MET:SD	0.60	2.75	25	3
1:A:358:PRO:O	1:A:359:TRP:CD1	0.60	2.55	8	9
1:A:235:MET:SD	1:A:236:GLY:N	0.59	2.75	24	4
1:A:336:MET:SD	1:A:341:PHE:CZ	0.59	2.95	25	7
1:A:367:GLN:OE1	1:A:367:GLN:N	0.59	2.34	17	2
1:A:198:PHE:CE1	1:A:202:PHE:CE1	0.59	2.89	23	4
1:A:307:ILE:CD1	1:A:307:ILE:N	0.59	2.65	11	9
1:A:193:MET:SD	1:A:237:PHE:CD2	0.59	2.95	15	1
1:A:313:TYR:O	1:A:313:TYR:CG	0.59	2.54	21	1
1:A:220:VAL:CG2	1:A:265:LEU:HD13	0.59	2.27	15	5
1:A:230:LEU:HD13	1:A:231:MET:N	0.59	2.13	7	25
1:A:336:MET:SD	1:A:341:PHE:CE2	0.59	2.96	19	10
1:A:217:CYS:SG	1:A:348:PHE:CD2	0.59	2.96	22	6
1:A:255:GLU:OE1	1:A:289:CYS:SG	0.59	2.61	16	4
1:A:193:MET:SD	1:A:237:PHE:CD1	0.59	2.95	30	2
1:A:259:LEU:HD22	1:A:259:LEU:N	0.58	2.13	11	4
1:A:281:TRP:NE1	1:A:311:ARG:NH2	0.58	2.51	7	1
1:A:240:ASN:N	1:A:240:ASN:HD22	0.58	1.93	27	2
1:A:192:LEU:HD11	1:A:350:TYR:H	0.58	1.57	27	1
1:A:326:LEU:HD23	1:A:326:LEU:C	0.58	2.19	22	10
1:A:215:TYR:CZ	1:A:239:CYS:SG	0.58	2.96	15	2
1:A:307:ILE:H	1:A:307:ILE:HD12	0.58	1.58	11	2
1:A:278:PHE:CE2	1:A:336:MET:SD	0.58	2.96	24	1
1:A:217:CYS:SG	1:A:348:PHE:CE1	0.58	2.95	5	4
1:A:326:LEU:HD23	1:A:327:ARG:N	0.58	2.13	22	1
1:A:255:GLU:H	1:A:255:GLU:CD	0.58	2.00	24	2
1:A:240:ASN:HD22	1:A:253:HIS:N	0.58	1.97	16	1
1:A:201:ASN:ND2	1:A:202:PHE:CD2	0.58	2.72	4	1
1:A:217:CYS:SG	1:A:348:PHE:CZ	0.57	2.95	3	1
1:A:372:ARG:O	1:A:375:ALA:HB3	0.57	1.99	25	19
1:A:259:LEU:N	1:A:259:LEU:HD22	0.57	2.13	4	3
1:A:297:LEU:HD12	1:A:304:ARG:HH12	0.57	1.59	30	1
1:A:270:ALA:HB1	1:A:271:GLN:NE2	0.57	2.14	8	4
1:A:252:ARG:CD	1:A:252:ARG:N	0.57	2.67	12	1
1:A:239:CYS:SG	1:A:240:ASN:N	0.57	2.77	22	2
1:A:240:ASN:HD22	1:A:240:ASN:H	0.57	1.40	18	2
1:A:274:ARG:NH2	1:A:306:ARG:CZ	0.57	2.67	16	4
1:A:253:HIS:N	1:A:253:HIS:CD2	0.57	2.70	25	5
1:A:231:MET:SD	1:A:233:GLN:NE2	0.57	2.77	18	1
1:A:312:ILE:N	1:A:312:ILE:CD1	0.57	2.66	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:198:PHE:CE2	1:A:202:PHE:CE1	0.57	2.92	14	7
1:A:198:PHE:CZ	1:A:202:PHE:CD2	0.57	2.93	22	3
1:A:252:ARG:CZ	1:A:257:ARG:NE	0.57	2.67	23	1
1:A:312:ILE:H	1:A:312:ILE:CD1	0.57	2.12	24	1
1:A:367:GLN:CD	1:A:368:ALA:N	0.57	2.57	17	3
1:A:252:ARG:N	1:A:252:ARG:CD	0.57	2.67	14	1
1:A:312:ILE:CG2	1:A:319:TYR:CE2	0.57	2.88	18	1
1:A:281:TRP:CE2	1:A:282:SER:O	0.57	2.58	3	13
1:A:356:PHE:CE1	1:A:357:GLN:O	0.57	2.58	28	3
1:A:286:SER:O	1:A:288:GLY:N	0.57	2.38	8	30
1:A:294:ARG:O	1:A:298:GLN:NE2	0.57	2.38	7	2
1:A:351:ARG:HH21	1:A:354:CYS:N	0.56	1.98	27	5
1:A:281:TRP:O	1:A:309:ALA:HB1	0.56	2.00	23	4
1:A:359:TRP:NE1	1:A:362:LEU:CB	0.56	2.68	24	3
1:A:217:CYS:SG	1:A:348:PHE:CE2	0.56	2.95	2	2
1:A:318:LEU:N	1:A:318:LEU:HD12	0.56	2.15	22	1
1:A:344:CYS:SG	1:A:345:TRP:N	0.56	2.78	14	8
1:A:327:ARG:NE	1:A:377:LEU:HD22	0.56	2.15	8	1
1:A:372:ARG:CD	1:A:372:ARG:N	0.56	2.68	25	1
1:A:351:ARG:N	1:A:351:ARG:CD	0.56	2.69	11	2
1:A:262:VAL:N	1:A:263:PRO:CD	0.56	2.69	25	16
1:A:191:TYR:O	1:A:193:MET:N	0.56	2.38	27	1
1:A:335:ILE:HD11	1:A:373:LEU:HD23	0.56	1.78	22	3
1:A:296:PHE:CD1	1:A:300:ASN:OD1	0.56	2.59	30	1
1:A:195:PRO:CG	1:A:351:ARG:NH2	0.56	2.69	14	1
1:A:201:ASN:ND2	1:A:202:PHE:CD1	0.55	2.74	14	3
1:A:218:TYR:CD2	1:A:236:GLY:O	0.55	2.59	29	29
1:A:351:ARG:CD	1:A:351:ARG:N	0.55	2.70	24	3
1:A:326:LEU:C	1:A:326:LEU:HD23	0.55	2.22	6	7
1:A:252:ARG:NH2	1:A:257:ARG:HE	0.55	2.00	23	1
1:A:312:ILE:O	1:A:314:ASP:N	0.55	2.39	3	5
1:A:376:ILE:N	1:A:376:ILE:HD13	0.55	2.17	4	2
1:A:341:PHE:CD1	1:A:356:PHE:CE2	0.55	2.94	26	2
1:A:280:SER:O	1:A:281:TRP:CG	0.55	2.60	22	17
1:A:313:TYR:O	1:A:315:TYR:N	0.55	2.40	21	11
1:A:192:LEU:HD11	1:A:347:THR:O	0.55	2.02	19	2
1:A:271:GLN:H	1:A:271:GLN:NE2	0.55	2.00	28	1
1:A:358:PRO:O	1:A:359:TRP:CG	0.55	2.59	29	1
1:A:280:SER:O	1:A:281:TRP:CD1	0.55	2.60	23	17
1:A:235:MET:SD	1:A:347:THR:HG22	0.55	2.42	28	2
1:A:286:SER:OG	1:A:287:TRP:N	0.55	2.40	24	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:240:ASN:ND2	1:A:240:ASN:N	0.55	2.54	6	1
1:A:365:HIS:CE1	1:A:369:LEU:HD13	0.55	2.37	16	1
1:A:360:ASP:O	1:A:362:LEU:N	0.55	2.40	29	1
1:A:272:ILE:HG23	1:A:272:ILE:O	0.54	2.02	26	14
1:A:272:ILE:O	1:A:272:ILE:HG23	0.54	2.02	5	13
1:A:286:SER:O	1:A:291:GLY:N	0.54	2.40	4	18
1:A:287:TRP:N	1:A:287:TRP:CD1	0.54	2.69	10	1
1:A:239:CYS:SG	1:A:240:ASN:ND2	0.54	2.80	15	1
1:A:274:ARG:NE	1:A:306:ARG:HH11	0.54	2.00	23	1
1:A:217:CYS:SG	1:A:348:PHE:CD1	0.54	2.95	18	5
1:A:222:ARG:NH2	1:A:271:GLN:NE2	0.54	2.56	7	1
1:A:192:LEU:HD13	1:A:348:PHE:O	0.54	2.02	4	6
1:A:313:TYR:O	1:A:313:TYR:CD2	0.54	2.60	21	1
1:A:193:MET:N	1:A:237:PHE:CE1	0.54	2.76	13	7
1:A:364:GLU:O	1:A:367:GLN:OE1	0.54	2.26	17	1
1:A:296:PHE:O	1:A:299:GLU:N	0.54	2.41	10	19
1:A:258:PHE:O	1:A:261:LEU:N	0.54	2.40	2	21
1:A:289:CYS:O	1:A:292:GLU:N	0.54	2.39	29	12
1:A:341:PHE:CD1	1:A:356:PHE:CZ	0.54	2.96	11	9
1:A:332:GLN:NE2	1:A:333:VAL:H	0.54	2.00	1	1
1:A:312:ILE:CD1	1:A:312:ILE:N	0.54	2.70	22	4
1:A:359:TRP:O	1:A:361:GLY:N	0.54	2.41	13	8
1:A:198:PHE:CE1	1:A:202:PHE:CD2	0.54	2.96	11	2
1:A:201:ASN:ND2	1:A:202:PHE:CE1	0.54	2.75	23	1
1:A:306:ARG:C	1:A:307:ILE:HD13	0.54	2.23	4	13
1:A:270:ALA:HB3	1:A:271:GLN:NE2	0.54	2.18	20	3
1:A:221:GLU:N	1:A:221:GLU:OE1	0.54	2.41	13	4
1:A:265:LEU:N	1:A:265:LEU:CD1	0.54	2.71	16	1
1:A:312:ILE:H	1:A:312:ILE:HD13	0.54	1.61	24	1
1:A:351:ARG:NE	1:A:354:CYS:O	0.54	2.41	28	1
1:A:350:TYR:CG	1:A:350:TYR:O	0.54	2.60	3	1
1:A:285:PHE:CZ	1:A:286:SER:OG	0.53	2.61	2	2
1:A:346:ASP:OD1	1:A:347:THR:N	0.53	2.41	4	3
1:A:214:THR:HG23	1:A:215:TYR:N	0.53	2.18	7	3
1:A:239:CYS:SG	1:A:257:ARG:NH1	0.53	2.81	19	1
1:A:228:TRP:HE1	1:A:274:ARG:NH1	0.53	2.01	30	1
1:A:357:GLN:O	1:A:357:GLN:NE2	0.53	2.41	14	1
1:A:296:PHE:CD2	1:A:297:LEU:HD12	0.53	2.38	11	3
1:A:274:ARG:NE	1:A:306:ARG:NH2	0.53	2.56	12	1
1:A:307:ILE:N	1:A:307:ILE:CD1	0.53	2.66	3	7
1:A:316:ASP:O	1:A:319:TYR:CE2	0.53	2.61	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:372:ARG:O	1:A:375:ALA:N	0.53	2.41	23	12
1:A:315:TYR:O	1:A:315:TYR:CD2	0.53	2.62	20	1
1:A:234:HIS:ND1	1:A:265:LEU:O	0.53	2.42	13	2
1:A:315:TYR:O	1:A:315:TYR:CG	0.53	2.61	8	2
1:A:281:TRP:NE1	1:A:282:SER:O	0.53	2.41	10	5
1:A:366:SER:OG	1:A:367:GLN:NE2	0.53	2.42	30	7
1:A:274:ARG:HH12	1:A:304:ARG:NH1	0.53	2.01	27	1
1:A:359:TRP:NE1	1:A:362:LEU:HD23	0.53	2.18	11	7
1:A:313:TYR:O	1:A:316:ASP:N	0.53	2.41	4	3
1:A:214:THR:O	1:A:240:ASN:ND2	0.53	2.41	18	3
1:A:319:TYR:CD1	1:A:319:TYR:O	0.53	2.62	25	2
1:A:362:LEU:O	1:A:365:HIS:ND1	0.53	2.41	23	1
1:A:300:ASN:HD22	1:A:303:VAL:CG1	0.53	2.17	30	1
1:A:314:ASP:N	1:A:314:ASP:OD1	0.53	2.42	27	1
1:A:289:CYS:O	1:A:291:GLY:N	0.53	2.42	11	11
1:A:219:GLU:OE1	1:A:347:THR:HG21	0.53	2.03	21	3
1:A:317:PRO:O	1:A:319:TYR:N	0.53	2.42	21	1
1:A:312:ILE:HD13	1:A:312:ILE:N	0.53	2.19	24	1
1:A:240:ASN:OD1	1:A:252:ARG:NE	0.53	2.42	25	1
1:A:357:GLN:O	1:A:359:TRP:CE3	0.53	2.62	16	14
1:A:364:GLU:OE1	1:A:364:GLU:N	0.53	2.42	5	1
1:A:365:HIS:ND1	1:A:366:SER:N	0.53	2.57	23	4
1:A:218:TYR:C	1:A:218:TYR:CD1	0.53	2.83	9	14
1:A:200:PHE:O	1:A:200:PHE:CD1	0.53	2.62	11	3
1:A:359:TRP:CD1	1:A:362:LEU:HD23	0.53	2.38	19	2
1:A:366:SER:OG	1:A:367:GLN:N	0.53	2.42	19	1
1:A:268:ASP:OD1	1:A:268:ASP:N	0.53	2.42	22	2
1:A:215:TYR:CE1	1:A:239:CYS:SG	0.53	3.00	2	2
1:A:268:ASP:O	1:A:270:ALA:N	0.53	2.42	27	12
1:A:361:GLY:O	1:A:365:HIS:CG	0.53	2.62	7	4
1:A:351:ARG:HH21	1:A:353:GLY:CA	0.53	2.17	7	7
1:A:240:ASN:ND2	1:A:252:ARG:O	0.53	2.42	11	5
1:A:346:ASP:O	1:A:350:TYR:CD2	0.53	2.62	16	1
1:A:327:ARG:NH2	1:A:332:GLN:OE1	0.53	2.42	14	1
1:A:194:ASP:OD2	1:A:197:THR:N	0.53	2.42	7	3
1:A:367:GLN:OE1	1:A:368:ALA:N	0.53	2.42	17	1
1:A:281:TRP:NE1	1:A:311:ARG:CZ	0.53	2.71	24	1
1:A:370:SER:O	1:A:374:ARG:NH1	0.53	2.42	13	1
1:A:256:LEU:HD11	1:A:292:GLU:OE1	0.52	2.05	2	1
1:A:271:GLN:N	1:A:271:GLN:OE1	0.52	2.42	3	4
1:A:281:TRP:CD2	1:A:313:TYR:CE2	0.52	2.96	30	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:351:ARG:NH1	1:A:354:CYS:O	0.52	2.42	10	2
1:A:222:ARG:NH1	1:A:271:GLN:OE1	0.52	2.42	9	1
1:A:361:GLY:O	1:A:365:HIS:ND1	0.52	2.43	9	1
1:A:311:ARG:NH2	1:A:365:HIS:NE2	0.52	2.58	4	1
1:A:373:LEU:O	1:A:376:ILE:N	0.52	2.42	18	8
1:A:307:ILE:O	1:A:308:PHE:CD1	0.52	2.62	15	17
1:A:254:ALA:O	1:A:257:ARG:N	0.52	2.42	21	4
1:A:349:VAL:O	1:A:351:ARG:NH1	0.52	2.42	24	1
1:A:323:LEU:O	1:A:326:LEU:N	0.52	2.42	20	16
1:A:282:SER:OG	1:A:319:TYR:CG	0.52	2.62	9	1
1:A:324:GLN:NE2	1:A:376:ILE:O	0.52	2.42	20	2
1:A:356:PHE:O	1:A:356:PHE:CG	0.52	2.61	19	1
1:A:320:LYS:O	1:A:324:GLN:NE2	0.52	2.42	30	1
1:A:191:TYR:O	1:A:237:PHE:CZ	0.52	2.62	27	1
1:A:198:PHE:CZ	1:A:202:PHE:CE1	0.52	2.97	26	5
1:A:253:HIS:O	1:A:256:LEU:N	0.52	2.42	18	1
1:A:313:TYR:O	1:A:313:TYR:CD1	0.52	2.62	23	1
1:A:202:PHE:O	1:A:311:ARG:NH2	0.52	2.42	1	1
1:A:198:PHE:CZ	1:A:202:PHE:CZ	0.52	2.98	3	1
1:A:201:ASN:OD1	1:A:202:PHE:CD2	0.52	2.62	13	1
1:A:255:GLU:OE2	1:A:289:CYS:SG	0.52	2.67	5	9
1:A:240:ASN:ND2	1:A:253:HIS:O	0.52	2.42	29	1
1:A:315:TYR:CD2	1:A:316:ASP:OD1	0.52	2.62	1	1
1:A:345:TRP:CZ2	1:A:351:ARG:NE	0.52	2.78	14	1
1:A:258:PHE:O	1:A:260:ASP:N	0.52	2.43	3	6
1:A:358:PRO:C	1:A:359:TRP:CG	0.52	2.83	26	15
1:A:313:TYR:C	1:A:315:TYR:H	0.52	2.09	21	6
1:A:285:PHE:O	1:A:289:CYS:N	0.52	2.42	12	3
1:A:278:PHE:CE1	1:A:340:GLU:OE1	0.52	2.63	15	2
1:A:315:TYR:CG	1:A:315:TYR:O	0.52	2.63	29	4
1:A:308:PHE:CD2	1:A:340:GLU:OE1	0.52	2.62	20	1
1:A:271:GLN:OE1	1:A:271:GLN:N	0.52	2.42	24	1
1:A:238:LEU:HD23	1:A:238:LEU:H	0.52	1.62	6	1
1:A:308:PHE:CE1	1:A:340:GLU:OE2	0.52	2.63	6	1
1:A:355:PRO:O	1:A:357:GLN:NE2	0.52	2.43	17	1
1:A:346:ASP:O	1:A:351:ARG:NH1	0.52	2.43	24	1
1:A:222:ARG:NE	1:A:271:GLN:OE1	0.51	2.42	2	1
1:A:218:TYR:CD1	1:A:218:TYR:C	0.51	2.83	3	16
1:A:326:LEU:CD2	1:A:331:ALA:HB3	0.51	2.35	28	8
1:A:194:ASP:OD1	1:A:197:THR:N	0.51	2.43	30	4
1:A:350:TYR:O	1:A:350:TYR:CG	0.51	2.62	21	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:221:GLU:N	1:A:221:GLU:CD	0.51	2.63	28	2
1:A:300:ASN:OD1	1:A:300:ASN:N	0.51	2.42	8	3
1:A:252:ARG:CZ	1:A:257:ARG:CZ	0.51	2.88	23	1
1:A:201:ASN:OD1	1:A:215:TYR:CE2	0.51	2.63	25	1
1:A:319:TYR:OH	1:A:320:LYS:NZ	0.51	2.42	28	2
1:A:192:LEU:N	1:A:192:LEU:CD2	0.51	2.70	25	1
1:A:315:TYR:O	1:A:315:TYR:CD1	0.51	2.64	6	1
1:A:349:VAL:O	1:A:351:ARG:NE	0.51	2.41	10	5
1:A:274:ARG:NH2	1:A:304:ARG:HH21	0.51	2.03	9	1
1:A:367:GLN:HE21	1:A:367:GLN:CA	0.51	2.19	9	1
1:A:227:THR:HG22	1:A:228:TRP:N	0.51	2.21	24	13
1:A:221:GLU:OE1	1:A:221:GLU:N	0.51	2.43	20	4
1:A:296:PHE:O	1:A:298:GLN:N	0.51	2.44	30	14
1:A:286:SER:C	1:A:291:GLY:H	0.51	2.08	30	6
1:A:196:ASP:OD1	1:A:197:THR:N	0.51	2.43	9	1
1:A:318:LEU:N	1:A:318:LEU:CD1	0.51	2.74	22	1
1:A:200:PHE:CD1	1:A:200:PHE:O	0.51	2.64	14	2
1:A:233:GLN:OE1	1:A:233:GLN:N	0.51	2.42	6	1
1:A:287:TRP:C	1:A:287:TRP:CD1	0.51	2.83	13	7
1:A:362:LEU:C	1:A:362:LEU:HD13	0.51	2.26	27	4
1:A:358:PRO:C	1:A:360:ASP:N	0.51	2.64	27	9
1:A:220:VAL:HG21	1:A:265:LEU:HD13	0.51	1.82	15	5
1:A:265:LEU:CD1	1:A:265:LEU:N	0.51	2.74	30	3
1:A:356:PHE:CD1	1:A:357:GLN:N	0.51	2.79	25	1
1:A:316:ASP:O	1:A:318:LEU:N	0.50	2.44	24	6
1:A:308:PHE:CG	1:A:340:GLU:OE2	0.50	2.64	25	1
1:A:286:SER:C	1:A:288:GLY:N	0.50	2.64	30	30
1:A:359:TRP:O	1:A:360:ASP:CB	0.50	2.60	24	7
1:A:238:LEU:CD2	1:A:257:ARG:NE	0.50	2.75	29	1
1:A:268:ASP:N	1:A:268:ASP:OD1	0.50	2.42	12	2
1:A:290:ALA:CB	1:A:322:ALA:HB1	0.50	2.35	8	1
1:A:238:LEU:CD2	1:A:257:ARG:NH1	0.50	2.74	10	1
1:A:201:ASN:ND2	1:A:215:TYR:CG	0.50	2.79	19	1
1:A:228:TRP:NE1	1:A:274:ARG:NH1	0.50	2.59	30	1
1:A:292:GLU:OE1	1:A:292:GLU:N	0.50	2.45	8	1
1:A:292:GLU:CD	1:A:293:VAL:N	0.50	2.65	25	2
1:A:339:ASP:OD1	1:A:340:GLU:N	0.50	2.44	24	2
1:A:193:MET:CE	1:A:237:PHE:CD2	0.50	2.94	25	1
1:A:286:SER:HA	1:A:290:ALA:HB3	0.50	1.83	5	27
1:A:270:ALA:HB3	1:A:271:GLN:HE21	0.50	1.67	5	1
1:A:214:THR:O	1:A:215:TYR:CD2	0.50	2.65	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:351:ARG:H	1:A:351:ARG:HH11	0.50	1.47	25	2
1:A:194:ASP:OD1	1:A:196:ASP:N	0.50	2.45	19	1
1:A:345:TRP:O	1:A:349:VAL:O	0.49	2.30	22	22
1:A:362:LEU:C	1:A:362:LEU:CD1	0.49	2.80	24	8
1:A:300:ASN:HD22	1:A:303:VAL:HG13	0.49	1.67	30	1
1:A:240:ASN:O	1:A:252:ARG:NE	0.49	2.45	27	1
1:A:336:MET:SD	1:A:340:GLU:OE2	0.49	2.70	15	1
1:A:367:GLN:N	1:A:367:GLN:NE2	0.49	2.60	25	2
1:A:222:ARG:HH21	1:A:231:MET:CE	0.49	2.20	29	1
1:A:191:TYR:O	1:A:237:PHE:CE1	0.49	2.65	27	1
1:A:332:GLN:CD	1:A:333:VAL:N	0.49	2.65	11	2
1:A:201:ASN:OD1	1:A:215:TYR:CD2	0.49	2.65	25	1
1:A:214:THR:O	1:A:215:TYR:CD1	0.49	2.65	2	2
1:A:221:GLU:HG3	1:A:230:LEU:HD22	0.49	1.83	30	13
1:A:218:TYR:O	1:A:236:GLY:O	0.49	2.30	17	28
1:A:223:LEU:N	1:A:228:TRP:CZ3	0.49	2.80	30	25
1:A:359:TRP:C	1:A:361:GLY:N	0.49	2.65	26	7
1:A:349:VAL:HG12	1:A:349:VAL:O	0.49	2.07	10	1
1:A:274:ARG:HH11	1:A:304:ARG:NH2	0.49	2.06	2	1
1:A:356:PHE:CG	1:A:356:PHE:O	0.49	2.63	29	2
1:A:304:ARG:NH1	1:A:330:GLY:O	0.49	2.45	14	1
1:A:235:MET:CG	1:A:236:GLY:N	0.49	2.75	13	11
1:A:259:LEU:H	1:A:259:LEU:CD2	0.49	2.20	5	4
1:A:338:TYR:CD2	1:A:339:ASP:N	0.49	2.80	5	3
1:A:352:GLN:OE1	1:A:352:GLN:N	0.49	2.46	7	2
1:A:280:SER:O	1:A:311:ARG:NH1	0.49	2.44	26	2
1:A:367:GLN:CD	1:A:367:GLN:H	0.49	2.08	9	1
1:A:358:PRO:O	1:A:359:TRP:O	0.49	2.30	28	1
1:A:296:PHE:CE2	1:A:300:ASN:ND2	0.49	2.80	30	1
1:A:214:THR:H	1:A:240:ASN:HD21	0.49	1.47	1	1
1:A:319:TYR:C	1:A:319:TYR:CD1	0.49	2.85	9	10
1:A:238:LEU:HD21	1:A:261:LEU:HD13	0.49	1.84	5	2
1:A:306:ARG:HH12	1:A:332:GLN:NE2	0.49	2.05	20	2
1:A:363:GLU:O	1:A:367:GLN:NE2	0.49	2.46	8	1
1:A:282:SER:HG	1:A:319:TYR:CB	0.49	2.21	9	1
1:A:318:LEU:O	1:A:320:LYS:N	0.49	2.45	16	3
1:A:240:ASN:OD1	1:A:240:ASN:N	0.49	2.43	22	2
1:A:218:TYR:CE2	1:A:261:LEU:HD11	0.48	2.43	3	1
1:A:285:PHE:CD2	1:A:318:LEU:HD22	0.48	2.43	3	1
1:A:351:ARG:NH2	1:A:353:GLY:C	0.48	2.67	27	5
1:A:365:HIS:ND1	1:A:365:HIS:C	0.48	2.65	23	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:ARG:NH2	1:A:271:GLN:HE21	0.48	2.06	7	1
1:A:274:ARG:NH2	1:A:304:ARG:HE	0.48	2.06	15	1
1:A:363:GLU:C	1:A:367:GLN:NE2	0.48	2.66	21	1
1:A:274:ARG:NH1	1:A:305:LEU:C	0.48	2.67	9	1
1:A:340:GLU:O	1:A:344:CYS:SG	0.48	2.70	9	1
1:A:285:PHE:O	1:A:288:GLY:N	0.48	2.46	3	6
1:A:296:PHE:C	1:A:298:GLN:N	0.48	2.67	21	17
1:A:287:TRP:CD1	1:A:287:TRP:C	0.48	2.86	24	4
1:A:363:GLU:H	1:A:363:GLU:CD	0.48	2.12	6	3
1:A:351:ARG:HE	1:A:352:GLN:H	0.48	1.51	17	1
1:A:192:LEU:HD13	1:A:350:TYR:CD1	0.48	2.43	24	1
1:A:324:GLN:NE2	1:A:376:ILE:HG22	0.48	2.23	30	1
1:A:313:TYR:C	1:A:315:TYR:N	0.48	2.67	27	13
1:A:358:PRO:C	1:A:360:ASP:H	0.48	2.12	25	9
1:A:307:ILE:HG22	1:A:308:PHE:N	0.48	2.22	18	13
1:A:300:ASN:N	1:A:300:ASN:ND2	0.48	2.60	11	1
1:A:235:MET:C	1:A:235:MET:SD	0.48	2.92	24	2
1:A:294:ARG:NE	1:A:298:GLN:OE1	0.48	2.46	26	1
1:A:308:PHE:CE2	1:A:340:GLU:OE2	0.48	2.67	2	1
1:A:197:THR:HG23	1:A:198:PHE:N	0.48	2.23	5	1
1:A:351:ARG:NH1	1:A:353:GLY:C	0.48	2.67	8	2
1:A:296:PHE:CD1	1:A:296:PHE:C	0.48	2.87	9	2
1:A:233:GLN:C	1:A:234:HIS:CD2	0.48	2.87	12	7
1:A:216:LEU:CD1	1:A:216:LEU:C	0.48	2.81	23	6
1:A:196:ASP:N	1:A:196:ASP:OD1	0.48	2.46	12	1
1:A:274:ARG:NH1	1:A:276:THR:OG1	0.48	2.46	24	1
1:A:321:GLU:N	1:A:321:GLU:OE1	0.48	2.47	12	1
1:A:311:ARG:HH21	1:A:365:HIS:CD2	0.48	2.27	4	1
1:A:367:GLN:CD	1:A:367:GLN:N	0.48	2.67	9	4
1:A:352:GLN:N	1:A:352:GLN:CD	0.48	2.66	17	2
1:A:233:GLN:CD	1:A:233:GLN:H	0.48	2.08	26	2
1:A:305:LEU:O	1:A:331:ALA:HB1	0.48	2.09	29	2
1:A:219:GLU:OE1	1:A:230:LEU:HD21	0.48	2.08	10	2
1:A:306:ARG:NH2	1:A:332:GLN:HE22	0.48	2.06	5	1
1:A:311:ARG:NH1	1:A:313:TYR:CE2	0.48	2.82	8	1
1:A:319:TYR:CD1	1:A:319:TYR:C	0.48	2.87	11	4
1:A:314:ASP:OD1	1:A:314:ASP:N	0.48	2.47	1	1
1:A:229:VAL:O	1:A:229:VAL:CG2	0.48	2.62	30	8
1:A:271:GLN:N	1:A:271:GLN:CD	0.48	2.66	8	5
1:A:359:TRP:C	1:A:361:GLY:H	0.48	2.12	20	8
1:A:278:PHE:CE1	1:A:340:GLU:CD	0.48	2.87	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:351:ARG:HH12	1:A:353:GLY:CA	0.48	2.20	13	1
1:A:258:PHE:C	1:A:260:ASP:N	0.48	2.67	3	10
1:A:216:LEU:C	1:A:216:LEU:CD1	0.48	2.81	18	10
1:A:255:GLU:CD	1:A:289:CYS:SG	0.48	2.92	8	4
1:A:259:LEU:CD2	1:A:259:LEU:H	0.48	2.21	7	2
1:A:281:TRP:O	1:A:281:TRP:CD1	0.48	2.67	15	2
1:A:305:LEU:O	1:A:331:ALA:CB	0.48	2.62	29	1
1:A:281:TRP:O	1:A:282:SER:O	0.47	2.32	3	11
1:A:280:SER:O	1:A:281:TRP:CB	0.47	2.62	17	11
1:A:214:THR:HG22	1:A:215:TYR:N	0.47	2.23	15	3
1:A:198:PHE:CE2	1:A:202:PHE:CD2	0.47	3.01	28	1
1:A:307:ILE:HD11	1:A:331:ALA:HB1	0.47	1.86	4	2
1:A:346:ASP:O	1:A:350:TYR:CE1	0.47	2.67	10	1
1:A:315:TYR:CD1	1:A:315:TYR:N	0.47	2.77	24	1
1:A:358:PRO:O	1:A:359:TRP:C	0.47	2.53	23	13
1:A:198:PHE:CE1	1:A:202:PHE:CE2	0.47	3.02	21	1
1:A:367:GLN:N	1:A:367:GLN:CD	0.47	2.68	28	8
1:A:225:ASN:O	1:A:225:ASN:CG	0.47	2.53	23	3
1:A:252:ARG:NH2	1:A:257:ARG:NH2	0.47	2.63	23	1
1:A:364:GLU:CD	1:A:364:GLU:H	0.47	2.13	1	1
1:A:233:GLN:H	1:A:233:GLN:CD	0.47	2.13	27	1
1:A:351:ARG:CA	1:A:351:ARG:HE	0.47	2.22	22	3
1:A:363:GLU:CD	1:A:363:GLU:H	0.47	2.13	7	1
1:A:351:ARG:HE	1:A:354:CYS:CB	0.47	2.23	15	1
1:A:300:ASN:ND2	1:A:300:ASN:N	0.47	2.61	23	1
1:A:294:ARG:CZ	1:A:298:GLN:OE1	0.47	2.62	25	2
1:A:304:ARG:NH2	1:A:330:GLY:O	0.47	2.48	25	1
1:A:338:TYR:CE2	1:A:342:GLU:OE2	0.47	2.68	26	1
1:A:364:GLU:CG	1:A:365:HIS:N	0.47	2.77	28	1
1:A:253:HIS:ND1	1:A:255:GLU:CD	0.47	2.68	29	1
1:A:235:MET:SD	1:A:235:MET:C	0.47	2.93	7	2
1:A:337:THR:O	1:A:339:ASP:N	0.47	2.48	15	1
1:A:359:TRP:HE1	1:A:362:LEU:CA	0.47	2.22	24	2
1:A:351:ARG:CG	1:A:352:GLN:N	0.47	2.78	28	1
1:A:239:CYS:O	1:A:254:ALA:HB2	0.47	2.10	4	1
1:A:198:PHE:C	1:A:198:PHE:CD1	0.47	2.88	7	3
1:A:255:GLU:CD	1:A:255:GLU:N	0.47	2.67	9	3
1:A:214:THR:CG2	1:A:215:TYR:N	0.47	2.78	15	3
1:A:324:GLN:CD	1:A:324:GLN:N	0.47	2.68	23	1
1:A:233:GLN:N	1:A:233:GLN:CD	0.47	2.67	26	1
1:A:240:ASN:ND2	1:A:253:HIS:C	0.47	2.68	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:201:ASN:CG	1:A:202:PHE:N	0.47	2.68	4	1
1:A:221:GLU:OE1	1:A:274:ARG:O	0.47	2.33	28	14
1:A:227:THR:CG2	1:A:228:TRP:N	0.47	2.78	24	7
1:A:261:LEU:CD2	1:A:261:LEU:C	0.47	2.82	18	7
1:A:286:SER:OG	1:A:325:MET:CE	0.47	2.62	15	4
1:A:339:ASP:CG	1:A:340:GLU:N	0.47	2.68	4	3
1:A:300:ASN:N	1:A:300:ASN:OD1	0.47	2.47	15	3
1:A:225:ASN:CG	1:A:225:ASN:O	0.47	2.52	26	3
1:A:356:PHE:C	1:A:356:PHE:CD1	0.47	2.87	29	1
1:A:324:GLN:NE2	1:A:377:LEU:C	0.47	2.68	1	1
1:A:327:ARG:CD	1:A:327:ARG:C	0.47	2.83	20	2
1:A:225:ASN:OD1	1:A:225:ASN:O	0.47	2.33	9	1
1:A:298:GLN:C	1:A:298:GLN:NE2	0.47	2.69	9	1
1:A:271:GLN:CD	1:A:271:GLN:N	0.46	2.68	6	1
1:A:239:CYS:SG	1:A:240:ASN:OD1	0.46	2.73	22	1
1:A:274:ARG:HH21	1:A:304:ARG:NH2	0.46	2.09	28	1
1:A:362:LEU:HD13	1:A:362:LEU:C	0.46	2.29	6	2
1:A:281:TRP:CD2	1:A:282:SER:O	0.46	2.68	3	1
1:A:232:ASP:N	1:A:232:ASP:OD1	0.46	2.48	10	1
1:A:257:ARG:N	1:A:257:ARG:CD	0.46	2.78	15	1
1:A:317:PRO:C	1:A:319:TYR:N	0.46	2.68	21	1
1:A:359:TRP:HE1	1:A:362:LEU:CB	0.46	2.22	24	2
1:A:327:ARG:NE	1:A:377:LEU:HD21	0.46	2.25	13	1
1:A:315:TYR:N	1:A:315:TYR:CD1	0.46	2.82	3	1
1:A:333:VAL:CG2	1:A:334:SER:N	0.46	2.77	28	11
1:A:281:TRP:CD1	1:A:282:SER:O	0.46	2.69	9	4
1:A:361:GLY:O	1:A:365:HIS:CD2	0.46	2.68	1	2
1:A:191:TYR:C	1:A:192:LEU:HD22	0.46	2.31	21	2
1:A:271:GLN:N	1:A:271:GLN:NE2	0.46	2.62	28	1
1:A:234:HIS:CE1	1:A:265:LEU:O	0.46	2.69	5	1
1:A:327:ARG:C	1:A:327:ARG:CD	0.46	2.84	30	3
1:A:340:GLU:OE1	1:A:340:GLU:N	0.46	2.49	12	1
1:A:338:TYR:C	1:A:338:TYR:CD1	0.46	2.88	13	4
1:A:376:ILE:N	1:A:376:ILE:CD1	0.46	2.78	29	1
1:A:312:ILE:HG21	1:A:319:TYR:CE2	0.46	2.46	4	1
1:A:224:ASP:O	1:A:225:ASN:OD1	0.46	2.34	26	6
1:A:229:VAL:CG2	1:A:229:VAL:O	0.46	2.64	11	7
1:A:297:LEU:HD21	1:A:305:LEU:HB3	0.46	1.87	9	1
1:A:253:HIS:C	1:A:255:GLU:N	0.46	2.68	18	1
1:A:376:ILE:N	1:A:376:ILE:HD12	0.46	2.26	29	1
1:A:229:VAL:HG23	1:A:229:VAL:O	0.46	2.10	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:319:TYR:O	1:A:319:TYR:CD1	0.46	2.69	15	1
1:A:351:ARG:H	1:A:351:ARG:CZ	0.46	2.23	13	2
1:A:197:THR:CG2	1:A:198:PHE:N	0.46	2.78	5	1
1:A:240:ASN:CB	1:A:254:ALA:N	0.46	2.79	16	1
1:A:258:PHE:C	1:A:258:PHE:CD1	0.46	2.89	19	2
1:A:339:ASP:O	1:A:342:GLU:N	0.46	2.49	22	1
1:A:360:ASP:C	1:A:362:LEU:N	0.46	2.69	29	1
1:A:214:THR:N	1:A:240:ASN:HD21	0.46	2.09	1	1
1:A:198:PHE:CD1	1:A:198:PHE:C	0.46	2.88	8	4
1:A:279:ILE:CG1	1:A:280:SER:N	0.46	2.79	9	8
1:A:296:PHE:CD1	1:A:296:PHE:O	0.46	2.69	1	2
1:A:282:SER:OG	1:A:319:TYR:CD2	0.46	2.63	6	1
1:A:289:CYS:C	1:A:291:GLY:N	0.46	2.68	11	6
1:A:370:SER:OG	1:A:371:GLY:N	0.46	2.49	17	1
1:A:281:TRP:HE1	1:A:311:ARG:NH1	0.46	2.08	24	1
1:A:214:THR:H	1:A:240:ASN:ND2	0.45	2.09	22	3
1:A:253:HIS:O	1:A:255:GLU:N	0.45	2.50	18	1
1:A:362:LEU:CD1	1:A:362:LEU:C	0.45	2.82	14	9
1:A:308:PHE:CD1	1:A:340:GLU:OE2	0.45	2.70	25	2
1:A:222:ARG:NH2	1:A:271:GLN:CD	0.45	2.70	9	1
1:A:228:TRP:CD1	1:A:274:ARG:NH1	0.45	2.84	17	1
1:A:318:LEU:O	1:A:321:GLU:N	0.45	2.47	22	1
1:A:351:ARG:NH2	1:A:353:GLY:CA	0.45	2.79	18	8
1:A:261:LEU:C	1:A:261:LEU:CD2	0.45	2.84	27	8
1:A:292:GLU:OE1	1:A:292:GLU:CA	0.45	2.63	8	1
1:A:312:ILE:CG2	1:A:319:TYR:OH	0.45	2.64	15	2
1:A:274:ARG:NE	1:A:306:ARG:HH21	0.45	2.09	12	1
1:A:307:ILE:O	1:A:308:PHE:CG	0.45	2.70	15	1
1:A:307:ILE:C	1:A:308:PHE:CD1	0.45	2.89	18	1
1:A:274:ARG:CZ	1:A:306:ARG:NH2	0.45	2.80	12	1
1:A:351:ARG:HE	1:A:351:ARG:CA	0.45	2.23	17	1
1:A:296:PHE:C	1:A:296:PHE:CD1	0.45	2.88	29	3
1:A:370:SER:OG	1:A:374:ARG:NH1	0.45	2.49	30	1
1:A:373:LEU:HD22	1:A:376:ILE:HD12	0.45	1.88	6	1
1:A:326:LEU:O	1:A:329:ALA:N	0.45	2.45	1	3
1:A:225:ASN:O	1:A:225:ASN:OD1	0.45	2.34	10	1
1:A:201:ASN:CG	1:A:215:TYR:CD2	0.45	2.89	16	1
1:A:347:THR:O	1:A:350:TYR:CE2	0.45	2.70	1	1
1:A:345:TRP:NE1	1:A:351:ARG:CD	0.45	2.80	13	1
1:A:260:ASP:OD1	1:A:260:ASP:N	0.45	2.49	5	1
1:A:363:GLU:O	1:A:366:SER:N	0.45	2.49	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:306:ARG:HH22	1:A:332:GLN:HE22	0.45	1.55	5	1
1:A:351:ARG:HH12	1:A:353:GLY:C	0.45	2.15	13	2
1:A:259:LEU:CD2	1:A:259:LEU:N	0.45	2.79	22	2
1:A:258:PHE:CE1	1:A:262:VAL:HG21	0.45	2.46	24	1
1:A:369:LEU:CD2	1:A:372:ARG:NH2	0.45	2.80	2	1
1:A:268:ASP:O	1:A:271:GLN:OE1	0.45	2.34	18	3
1:A:224:ASP:O	1:A:225:ASN:ND2	0.45	2.50	10	1
1:A:235:MET:SD	1:A:347:THR:CG2	0.45	3.05	11	4
1:A:351:ARG:CG	1:A:351:ARG:O	0.45	2.64	26	1
1:A:262:VAL:N	1:A:263:PRO:HD2	0.45	2.27	16	8
1:A:325:MET:C	1:A:325:MET:SD	0.44	2.95	2	2
1:A:296:PHE:CE1	1:A:300:ASN:OD1	0.44	2.71	3	2
1:A:367:GLN:OE1	1:A:367:GLN:CA	0.44	2.65	8	1
1:A:307:ILE:CD1	1:A:331:ALA:HB1	0.44	2.42	15	1
1:A:316:ASP:C	1:A:318:LEU:N	0.44	2.71	24	5
1:A:268:ASP:O	1:A:271:GLN:NE2	0.44	2.49	28	1
1:A:222:ARG:HH21	1:A:271:GLN:HE21	0.44	1.54	7	1
1:A:318:LEU:C	1:A:320:LYS:N	0.44	2.68	16	3
1:A:311:ARG:C	1:A:312:ILE:HD13	0.44	2.33	22	1
1:A:268:ASP:C	1:A:270:ALA:N	0.44	2.71	26	12
1:A:240:ASN:N	1:A:240:ASN:OD1	0.44	2.48	8	1
1:A:258:PHE:CD1	1:A:258:PHE:C	0.44	2.91	22	3
1:A:220:VAL:O	1:A:231:MET:SD	0.44	2.75	30	1
1:A:327:ARG:HH11	1:A:377:LEU:CD1	0.44	2.18	16	1
1:A:311:ARG:C	1:A:312:ILE:HD12	0.44	2.33	21	1
1:A:232:ASP:OD1	1:A:232:ASP:N	0.44	2.48	1	1
1:A:364:GLU:C	1:A:367:GLN:OE1	0.44	2.56	17	1
1:A:274:ARG:HE	1:A:306:ARG:NH1	0.44	2.09	23	1
1:A:240:ASN:ND2	1:A:253:HIS:N	0.44	2.65	25	1
1:A:351:ARG:CG	1:A:352:GLN:H	0.44	2.25	28	1
1:A:333:VAL:HG22	1:A:334:SER:N	0.44	2.27	1	7
1:A:255:GLU:N	1:A:255:GLU:CD	0.44	2.69	8	1
1:A:259:LEU:HD11	1:A:296:PHE:CD2	0.44	2.48	23	2
1:A:240:ASN:O	1:A:252:ARG:O	0.44	2.35	16	2
1:A:304:ARG:CG	1:A:305:LEU:N	0.44	2.81	21	2
1:A:309:ALA:C	1:A:336:MET:SD	0.44	2.95	22	1
1:A:195:PRO:O	1:A:199:THR:HG23	0.44	2.12	23	1
1:A:268:ASP:C	1:A:270:ALA:H	0.44	2.16	5	12
1:A:191:TYR:O	1:A:192:LEU:O	0.44	2.36	3	15
1:A:272:ILE:O	1:A:272:ILE:CG2	0.44	2.66	7	5
1:A:258:PHE:CE1	1:A:262:VAL:HG22	0.44	2.47	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:364:GLU:OE1	1:A:364:GLU:CA	0.44	2.64	5	1
1:A:359:TRP:O	1:A:360:ASP:OD1	0.44	2.36	23	2
1:A:278:PHE:CE2	1:A:344:CYS:CB	0.44	3.01	17	1
1:A:367:GLN:CA	1:A:367:GLN:OE1	0.44	2.65	17	1
1:A:218:TYR:CD1	1:A:219:GLU:N	0.44	2.86	14	3
1:A:253:HIS:H	1:A:253:HIS:CD2	0.44	2.31	28	1
1:A:233:GLN:NE2	1:A:233:GLN:H	0.44	2.10	30	1
1:A:342:GLU:OE2	1:A:342:GLU:O	0.44	2.36	30	1
1:A:360:ASP:O	1:A:364:GLU:OE1	0.44	2.36	13	1
1:A:351:ARG:HH21	1:A:353:GLY:C	0.44	2.17	7	2
1:A:363:GLU:O	1:A:367:GLN:OE1	0.44	2.35	19	2
1:A:198:PHE:CZ	1:A:202:PHE:CE2	0.44	3.06	11	2
1:A:358:PRO:CB	1:A:362:LEU:HD23	0.44	2.43	1	1
1:A:234:HIS:CD2	1:A:234:HIS:N	0.43	2.86	7	1
1:A:277:TRP:CE2	1:A:305:LEU:HD11	0.43	2.48	26	1
1:A:201:ASN:OD1	1:A:280:SER:CB	0.43	2.66	28	1
1:A:350:TYR:C	1:A:350:TYR:CD1	0.43	2.87	28	1
1:A:272:ILE:CG2	1:A:272:ILE:O	0.43	2.66	2	7
1:A:300:ASN:HD22	1:A:300:ASN:N	0.43	2.11	23	2
1:A:337:THR:C	1:A:339:ASP:N	0.43	2.71	15	1
1:A:261:LEU:HD21	1:A:265:LEU:HD21	0.43	1.90	18	1
1:A:237:PHE:C	1:A:238:LEU:HD22	0.43	2.33	21	1
1:A:335:ILE:O	1:A:335:ILE:CG2	0.43	2.66	24	2
1:A:364:GLU:CD	1:A:364:GLU:N	0.43	2.71	13	1
1:A:296:PHE:O	1:A:300:ASN:OD1	0.43	2.35	30	1
1:A:231:MET:CE	1:A:234:HIS:CE1	0.43	3.01	18	3
1:A:289:CYS:O	1:A:292:GLU:OE2	0.43	2.36	11	1
1:A:297:LEU:HD11	1:A:331:ALA:HB2	0.43	1.90	16	1
1:A:281:TRP:CZ3	1:A:313:TYR:CB	0.43	3.02	13	3
1:A:285:PHE:CD1	1:A:322:ALA:HB2	0.43	2.48	19	1
1:A:372:ARG:CG	1:A:372:ARG:HH11	0.43	2.26	25	1
1:A:230:LEU:HD13	1:A:231:MET:H	0.43	1.74	2	16
1:A:343:TYR:O	1:A:347:THR:OG1	0.43	2.36	14	5
1:A:294:ARG:C	1:A:294:ARG:CD	0.43	2.87	6	1
1:A:232:ASP:O	1:A:232:ASP:OD1	0.43	2.36	7	1
1:A:217:CYS:SG	1:A:278:PHE:O	0.43	2.69	15	1
1:A:363:GLU:O	1:A:366:SER:CB	0.43	2.67	19	1
1:A:274:ARG:CZ	1:A:306:ARG:NH1	0.43	2.81	23	1
1:A:366:SER:O	1:A:370:SER:OG	0.43	2.37	4	4
1:A:266:GLN:O	1:A:268:ASP:OD1	0.43	2.36	6	1
1:A:239:CYS:C	1:A:240:ASN:HD22	0.43	2.16	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:TYR:CD2	1:A:235:MET:O	0.43	2.71	30	1
1:A:372:ARG:HG3	1:A:376:ILE:HD11	0.43	1.89	4	1
1:A:351:ARG:CZ	1:A:351:ARG:H	0.43	2.27	7	1
1:A:307:ILE:CG2	1:A:308:PHE:N	0.43	2.82	29	3
1:A:267:LEU:O	1:A:268:ASP:OD1	0.43	2.36	9	4
1:A:366:SER:CB	1:A:367:GLN:NE2	0.43	2.82	18	2
1:A:362:LEU:O	1:A:366:SER:OG	0.43	2.37	21	1
1:A:252:ARG:NH2	1:A:257:ARG:CZ	0.43	2.82	23	1
1:A:332:GLN:NE2	1:A:333:VAL:N	0.43	2.67	1	1
1:A:343:TYR:O	1:A:346:ASP:OD1	0.43	2.36	4	1
1:A:350:TYR:CE1	1:A:353:GLY:N	0.43	2.87	27	1
1:A:363:GLU:O	1:A:366:SER:OG	0.43	2.37	27	1
1:A:351:ARG:HE	1:A:352:GLN:N	0.43	2.12	17	1
1:A:285:PHE:CE2	1:A:286:SER:OG	0.43	2.66	20	2
1:A:274:ARG:NH2	1:A:304:ARG:HH11	0.43	2.11	21	1
1:A:282:SER:OG	1:A:319:TYR:CD1	0.43	2.64	24	1
1:A:336:MET:SD	1:A:341:PHE:CD2	0.43	3.12	30	1
1:A:274:ARG:C	1:A:274:ARG:CD	0.43	2.87	14	1
1:A:283:PRO:O	1:A:284:CYS:O	0.43	2.37	10	3
1:A:367:GLN:O	1:A:370:SER:OG	0.43	2.37	23	4
1:A:306:ARG:CZ	1:A:332:GLN:NE2	0.43	2.82	5	1
1:A:195:PRO:CB	1:A:351:ARG:NH2	0.43	2.81	5	1
1:A:326:LEU:C	1:A:326:LEU:CD2	0.43	2.88	6	11
1:A:252:ARG:CG	1:A:252:ARG:HH11	0.43	2.27	7	1
1:A:335:ILE:O	1:A:335:ILE:HG23	0.43	2.14	24	1
1:A:281:TRP:CE3	1:A:313:TYR:CD2	0.42	3.06	30	1
1:A:326:LEU:CD2	1:A:326:LEU:C	0.42	2.87	3	3
1:A:221:GLU:OE2	1:A:274:ARG:O	0.42	2.37	25	2
1:A:346:ASP:O	1:A:350:TYR:CE2	0.42	2.72	8	1
1:A:265:LEU:HD12	1:A:265:LEU:N	0.42	2.29	16	1
1:A:195:PRO:O	1:A:199:THR:OG1	0.42	2.37	24	2
1:A:192:LEU:O	1:A:193:MET:O	0.42	2.37	4	2
1:A:360:ASP:OD1	1:A:363:GLU:OE1	0.42	2.36	26	1
1:A:198:PHE:CE2	1:A:202:PHE:CD1	0.42	3.07	14	1
1:A:286:SER:C	1:A:288:GLY:H	0.42	2.18	27	4
1:A:281:TRP:O	1:A:282:SER:C	0.42	2.58	26	6
1:A:367:GLN:CA	1:A:367:GLN:NE2	0.42	2.82	9	1
1:A:351:ARG:HH21	1:A:353:GLY:N	0.42	2.12	21	2
1:A:221:GLU:OE2	1:A:221:GLU:N	0.42	2.52	23	1
1:A:192:LEU:CD2	1:A:192:LEU:N	0.42	2.82	30	1
1:A:194:ASP:OD2	1:A:197:THR:CB	0.42	2.68	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:192:LEU:HD13	1:A:350:TYR:H	0.42	1.74	8	1
1:A:358:PRO:CB	1:A:362:LEU:HD21	0.42	2.45	11	1
1:A:316:ASP:O	1:A:319:TYR:CD2	0.42	2.72	20	1
1:A:286:SER:CA	1:A:291:GLY:H	0.42	2.28	6	2
1:A:288:GLY:O	1:A:292:GLU:OE1	0.42	2.36	6	1
1:A:297:LEU:HD21	1:A:331:ALA:HB2	0.42	1.87	11	1
1:A:307:ILE:HD13	1:A:326:LEU:HD21	0.42	1.91	22	3
1:A:194:ASP:OD1	1:A:196:ASP:OD1	0.42	2.37	24	1
1:A:194:ASP:OD1	1:A:197:THR:CB	0.42	2.67	30	2
1:A:281:TRP:CE3	1:A:313:TYR:CE2	0.42	3.07	30	1
1:A:259:LEU:N	1:A:259:LEU:CD2	0.42	2.80	4	1
1:A:286:SER:O	1:A:287:TRP:C	0.42	2.58	22	7
1:A:290:ALA:O	1:A:293:VAL:N	0.42	2.51	7	1
1:A:214:THR:O	1:A:240:ASN:OD1	0.42	2.37	23	2
1:A:327:ARG:HH21	1:A:377:LEU:HD21	0.42	1.71	2	1
1:A:221:GLU:OE2	1:A:276:THR:OG1	0.42	2.37	15	2
1:A:360:ASP:O	1:A:363:GLU:OE2	0.42	2.37	24	1
1:A:372:ARG:NH1	1:A:372:ARG:CG	0.42	2.80	25	1
1:A:357:GLN:CD	1:A:357:GLN:N	0.42	2.73	14	2
1:A:324:GLN:O	1:A:328:ASP:OD1	0.42	2.38	3	1
1:A:282:SER:OG	1:A:319:TYR:CB	0.42	2.68	9	1
1:A:326:LEU:HD23	1:A:326:LEU:O	0.42	2.15	9	2
1:A:337:THR:OG1	1:A:340:GLU:OE1	0.42	2.37	18	1
1:A:281:TRP:C	1:A:281:TRP:CD2	0.42	2.90	3	1
1:A:366:SER:O	1:A:370:SER:CB	0.42	2.68	8	4
1:A:296:PHE:CZ	1:A:300:ASN:CG	0.42	2.93	30	1
1:A:258:PHE:O	1:A:262:VAL:HG23	0.41	2.15	28	3
1:A:193:MET:SD	1:A:237:PHE:CG	0.41	3.13	10	1
1:A:307:ILE:N	1:A:307:ILE:HD12	0.41	2.30	12	1
1:A:345:TRP:CH2	1:A:349:VAL:HG11	0.41	2.50	23	1
1:A:372:ARG:O	1:A:375:ALA:CB	0.41	2.68	29	1
1:A:299:GLU:O	1:A:299:GLU:OE1	0.41	2.37	30	1
1:A:240:ASN:OD1	1:A:252:ARG:O	0.41	2.37	5	2
1:A:351:ARG:CA	1:A:351:ARG:NE	0.41	2.83	7	1
1:A:233:GLN:O	1:A:234:HIS:CD2	0.41	2.72	14	2
1:A:262:VAL:O	1:A:265:LEU:N	0.41	2.50	12	1
1:A:316:ASP:C	1:A:318:LEU:H	0.41	2.18	24	3
1:A:376:ILE:CD1	1:A:376:ILE:H	0.41	2.27	4	1
1:A:278:PHE:CD1	1:A:336:MET:SD	0.41	3.14	6	1
1:A:314:ASP:C	1:A:316:ASP:H	0.41	2.19	15	5
1:A:344:CYS:O	1:A:347:THR:N	0.41	2.52	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:327:ARG:HE	1:A:327:ARG:C	0.41	2.19	29	1
1:A:286:SER:N	1:A:290:ALA:HB3	0.41	2.30	13	1
1:A:365:HIS:HD1	1:A:366:SER:N	0.41	2.13	23	1
1:A:274:ARG:HH21	1:A:304:ARG:HE	0.41	1.58	15	1
1:A:191:TYR:CE2	1:A:235:MET:O	0.41	2.73	30	1
1:A:221:GLU:CD	1:A:274:ARG:O	0.41	2.59	13	1
1:A:338:TYR:CE2	1:A:342:GLU:OE1	0.41	2.74	7	1
1:A:255:GLU:CG	1:A:289:CYS:SG	0.41	3.09	8	1
1:A:350:TYR:CD2	1:A:350:TYR:O	0.41	2.73	18	1
1:A:252:ARG:HH22	1:A:257:ARG:HH21	0.41	1.58	23	1
1:A:356:PHE:CG	1:A:357:GLN:N	0.41	2.89	25	1
1:A:252:ARG:CD	1:A:252:ARG:H	0.41	2.27	12	1
1:A:327:ARG:NH1	1:A:377:LEU:HD21	0.41	2.31	16	1
1:A:266:GLN:O	1:A:267:LEU:O	0.41	2.39	24	1
1:A:216:LEU:HD23	1:A:254:ALA:CB	0.41	2.46	9	2
1:A:369:LEU:HD12	1:A:369:LEU:N	0.41	2.30	5	1
1:A:252:ARG:NH1	1:A:252:ARG:CG	0.41	2.81	7	1
1:A:218:TYR:OH	1:A:265:LEU:CD2	0.41	2.69	7	1
1:A:281:TRP:CD2	1:A:282:SER:N	0.41	2.89	9	1
1:A:315:TYR:O	1:A:316:ASP:OD1	0.41	2.39	16	1
1:A:231:MET:CE	1:A:234:HIS:NE2	0.41	2.83	18	1
1:A:333:VAL:O	1:A:377:LEU:HD21	0.41	2.16	19	1
1:A:360:ASP:C	1:A:362:LEU:H	0.41	2.19	22	1
1:A:335:ILE:HG23	1:A:335:ILE:O	0.41	2.15	29	1
1:A:300:ASN:CG	1:A:300:ASN:O	0.41	2.58	30	1
1:A:376:ILE:CD1	1:A:376:ILE:N	0.41	2.80	4	1
1:A:345:TRP:CZ2	1:A:351:ARG:CD	0.41	3.04	14	1
1:A:364:GLU:O	1:A:365:HIS:C	0.41	2.59	12	2
1:A:240:ASN:OD1	1:A:252:ARG:CZ	0.41	2.68	25	1
1:A:274:ARG:HH21	1:A:304:ARG:CZ	0.41	2.29	28	1
1:A:336:MET:CE	1:A:341:PHE:CZ	0.41	3.04	29	1
1:A:290:ALA:O	1:A:294:ARG:N	0.41	2.54	30	1
1:A:229:VAL:O	1:A:229:VAL:HG23	0.40	2.16	16	1
1:A:293:VAL:CG1	1:A:294:ARG:N	0.40	2.84	22	1
1:A:325:MET:SD	1:A:325:MET:O	0.40	2.79	23	1
1:A:201:ASN:HD21	1:A:280:SER:CB	0.40	2.28	29	1
1:A:216:LEU:HD23	1:A:254:ALA:HB1	0.40	1.93	9	1
1:A:337:THR:O	1:A:338:TYR:C	0.40	2.60	9	1
1:A:354:CYS:O	1:A:355:PRO:O	0.40	2.39	21	1
1:A:286:SER:OG	1:A:325:MET:SD	0.40	2.75	26	1
1:A:323:LEU:HD21	1:A:373:LEU:HD11	0.40	1.94	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:PHE:CE1	1:A:340:GLU:OE1	0.40	2.75	6	1
1:A:259:LEU:HD21	1:A:296:PHE:HB2	0.40	1.92	30	1
1:A:311:ARG:HH12	1:A:365:HIS:CE1	0.40	2.33	14	1
1:A:265:LEU:O	1:A:266:GLN:C	0.40	2.60	5	1
1:A:278:PHE:CE1	1:A:336:MET:SD	0.40	3.15	6	1
1:A:224:ASP:O	1:A:225:ASN:CG	0.40	2.59	10	1
1:A:367:GLN:NE2	1:A:368:ALA:H	0.40	2.15	12	1
1:A:274:ARG:NH2	1:A:306:ARG:NE	0.40	2.70	19	1
1:A:192:LEU:HD22	1:A:192:LEU:N	0.40	2.31	30	1
1:A:255:GLU:CA	1:A:255:GLU:OE1	0.40	2.68	7	1
1:A:312:ILE:CG2	1:A:319:TYR:CE1	0.40	3.05	16	1
1:A:238:LEU:CD1	1:A:254:ALA:HB1	0.40	2.47	25	1
1:A:194:ASP:OD1	1:A:197:THR:OG1	0.40	2.37	1	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	165/205 (80%)	131±4 (80±2%)	25±3 (15±2%)	9±2 (6±1%)	3	22
All	All	4950/6150 (80%)	3936 (80%)	738 (15%)	276 (6%)	3	22

All 34 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	TRP	28
1	A	359	TRP	27
1	A	360	ASP	26
1	A	192	LEU	22
1	A	281	TRP	20
1	A	286	SER	14
1	A	269	PRO	12
1	A	314	ASP	12
1	A	282	SER	11

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Mol	Chain	Res	Type	Models (Total)
1	A	284	CYS	10
1	A	290	ALA	9
1	A	191	TYR	8
1	A	240	ASN	8
1	A	193	MET	7
1	A	267	LEU	7
1	A	313	TYR	6
1	A	358	PRO	5
1	A	355	PRO	5
1	A	283	PRO	5
1	A	259	LEU	5
1	A	317	PRO	4
1	A	285	PHE	4
1	A	297	LEU	4
1	A	351	ARG	3
1	A	270	ALA	3
1	A	336	MET	2
1	A	319	TYR	2
1	A	361	GLY	1
1	A	271	GLN	1
1	A	318	LEU	1
1	A	338	TYR	1
1	A	349	VAL	1
1	A	253	HIS	1
1	A	195	PRO	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	146/182 (80%)	104±4 (71±3%)	42±4 (29±3%)	2	18
All	All	4380/5460 (80%)	3129 (71%)	1251 (29%)	2	18

All 118 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	302	HIS	30
1	A	303	VAL	30
1	A	275	VAL	30
1	A	334	SER	30
1	A	337	THR	30
1	A	282	SER	29
1	A	327	ARG	29
1	A	230	LEU	29
1	A	341	PHE	29
1	A	351	ARG	28
1	A	293	VAL	28
1	A	332	GLN	27
1	A	354	CYS	24
1	A	298	GLN	23
1	A	373	LEU	22
1	A	339	ASP	22
1	A	216	LEU	21
1	A	217	CYS	21
1	A	194	ASP	20
1	A	359	TRP	19
1	A	313	TYR	19
1	A	362	LEU	19
1	A	261	LEU	19
1	A	314	ASP	18
1	A	199	THR	17
1	A	252	ARG	16
1	A	319	TYR	16
1	A	240	ASN	16
1	A	191	TYR	16
1	A	214	THR	15
1	A	307	ILE	15
1	A	312	ILE	15
1	A	344	CYS	15
1	A	366	SER	15
1	A	264	SER	15
1	A	320	LYS	14
1	A	268	ASP	14
1	A	346	ASP	14
1	A	232	ASP	13
1	A	360	ASP	13
1	A	257	ARG	13
1	A	262	VAL	12
1	A	374	ARG	12

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Mol	Chain	Res	Type	Models (Total)
1	A	365	HIS	12
1	A	193	MET	12
1	A	287	TRP	11
1	A	201	ASN	11
1	A	328	ASP	11
1	A	233	GLN	10
1	A	315	TYR	10
1	A	286	SER	10
1	A	200	PHE	10
1	A	311	ARG	9
1	A	231	MET	9
1	A	284	CYS	9
1	A	196	ASP	9
1	A	350	TYR	8
1	A	218	TYR	8
1	A	336	MET	8
1	A	271	GLN	8
1	A	255	GLU	8
1	A	352	GLN	7
1	A	239	CYS	7
1	A	276	THR	7
1	A	260	ASP	7
1	A	324	GLN	6
1	A	281	TRP	6
1	A	225	ASN	6
1	A	325	MET	6
1	A	376	ILE	6
1	A	238	LEU	6
1	A	367	GLN	6
1	A	294	ARG	5
1	A	349	VAL	5
1	A	237	PHE	5
1	A	253	HIS	5
1	A	357	GLN	5
1	A	318	LEU	5
1	A	316	ASP	5
1	A	340	GLU	5
1	A	256	LEU	5
1	A	363	GLU	5
1	A	343	TYR	5
1	A	280	SER	4
1	A	229	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	272	ILE	4
1	A	377	LEU	4
1	A	333	VAL	4
1	A	356	PHE	4
1	A	364	GLU	4
1	A	304	ARG	4
1	A	300	ASN	3
1	A	372	ARG	3
1	A	215	TYR	3
1	A	234	HIS	3
1	A	292	GLU	3
1	A	192	LEU	3
1	A	370	SER	3
1	A	321	GLU	2
1	A	347	THR	2
1	A	296	PHE	2
1	A	369	LEU	2
1	A	224	ASP	2
1	A	274	ARG	2
1	A	267	LEU	2
1	A	306	ARG	2
1	A	222	ARG	1
1	A	323	LEU	1
1	A	308	PHE	1
1	A	266	GLN	1
1	A	279	ILE	1
1	A	202	PHE	1
1	A	301	THR	1
1	A	299	GLU	1
1	A	221	GLU	1
1	A	259	LEU	1
1	A	235	MET	1
1	A	338	TYR	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 [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 61% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1840
Number of shifts mapped to atoms	1840
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	11

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	187	-0.40 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	171	0.57 ± 0.10	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	180	-0.12 ± 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 64%, i.e. 1362 atoms were assigned a chemical shift out of a possible 2129. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	613/811 (76%)	304/323 (94%)	156/330 (47%)	153/158 (97%)
Sidechain	632/1030 (61%)	387/607 (64%)	236/373 (63%)	9/50 (18%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	117/288 (41%)	111/152 (73%)	0/126 (0%)	6/10 (60%)
Overall	1362/2129 (64%)	802/1082 (74%)	392/829 (47%)	168/218 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 61%, i.e. 1569 atoms were assigned a chemical shift out of a possible 2560. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	703/969 (73%)	347/386 (90%)	181/394 (46%)	175/189 (93%)
Sidechain	749/1286 (58%)	458/758 (60%)	278/457 (61%)	13/71 (18%)
Aromatic	117/305 (38%)	111/161 (69%)	0/134 (0%)	6/10 (60%)
Overall	1569/2560 (61%)	916/1305 (70%)	459/985 (47%)	194/270 (72%)

7.1.4 Statistically unusual chemical shifts ⓘ

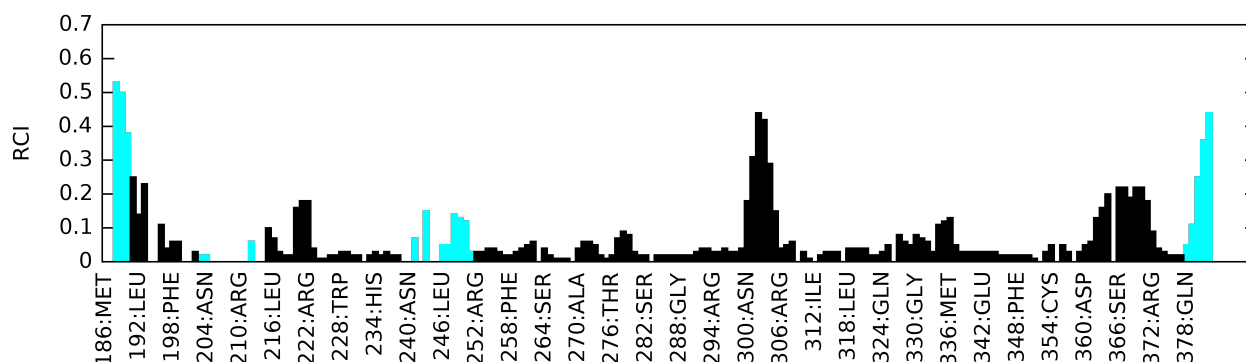
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	351	ARG	HD3	0.32	4.36 – 1.86	-11.2
1	A	277	TRP	HE1	5.50	12.85 – 7.35	-8.4
1	A	255	GLU	H	12.41	11.34 – 5.34	6.8
1	A	223	LEU	HD23	-0.84	2.14 – -0.66	-5.6
1	A	223	LEU	HD21	-0.84	2.14 – -0.66	-5.6
1	A	223	LEU	HD22	-0.84	2.14 – -0.66	-5.6
1	A	351	ARG	HD2	1.85	4.27 – 1.97	-5.5
1	A	277	TRP	NE1	118.98	139.19 – 119.59	-5.3
1	A	347	THR	HG21	-0.03	2.29 – -0.01	-5.1
1	A	347	THR	HG22	-0.03	2.29 – -0.01	-5.1
1	A	347	THR	HG23	-0.03	2.29 – -0.01	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1_dup*

7.2.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	388
Number of shifts mapped to atoms	388
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	170	0.25 ± 0.32	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 15%, i.e. 329 atoms were assigned a chemical shift out of a possible 2129. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	291/811 (36%)	145/323 (45%)	0/330 (0%)	146/158 (92%)
Sidechain	26/1030 (3%)	17/607 (3%)	0/373 (0%)	9/50 (18%)
Aromatic	12/288 (4%)	6/152 (4%)	0/126 (0%)	6/10 (60%)
Overall	329/2129 (15%)	168/1082 (16%)	0/829 (0%)	161/218 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 15%, i.e. 378 atoms were assigned a chemical shift out of a possible 2560. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	329/969 (34%)	164/386 (42%)	0/394 (0%)	165/189 (87%)
Sidechain	37/1286 (3%)	24/758 (3%)	0/457 (0%)	13/71 (18%)
Aromatic	12/305 (4%)	6/161 (4%)	0/134 (0%)	6/10 (60%)
Overall	378/2560 (15%)	194/1305 (15%)	0/985 (0%)	184/270 (68%)

7.2.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	277	TRP	HE1	5.52	12.85 – 7.35	-8.3
1	A	255	GLU	H	12.56	11.34 – 5.34	7.0
1	A	277	TRP	NE1	119.18	139.19 – 119.59	-5.2

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

