



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:23 PM UTC

PDB ID : 2MTG / pdb_00002mtg
BMRB ID : 25160
Title : Solution structure of the RRM1 of human LARP6
Authors : Martino, L.; Atkinson, A.R.; Kelly, G.; Conte, M.R.
Deposited on : 2014-08-18

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

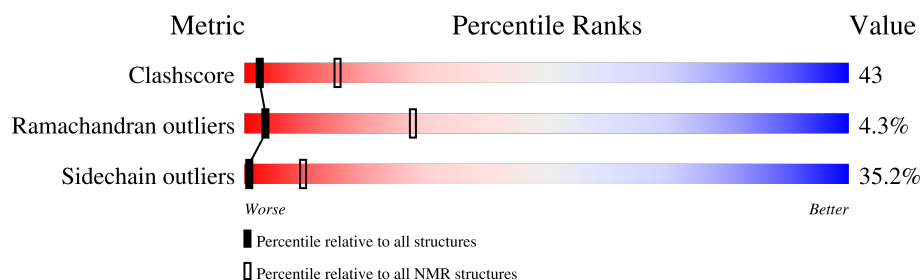
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	119	24% 51% 9% • 13% •

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:183-A:199, A:208-A:291 (101)	0.69	1

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1884 atoms, of which 964 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called La-related protein 6.

Mol	Chain	Residues	Atoms						Trace
1	A	116	Total	C	H	N	O	S	0
			1884	591	964	157	166	6	

There is a discrepancy between the modelled and reference sequences:

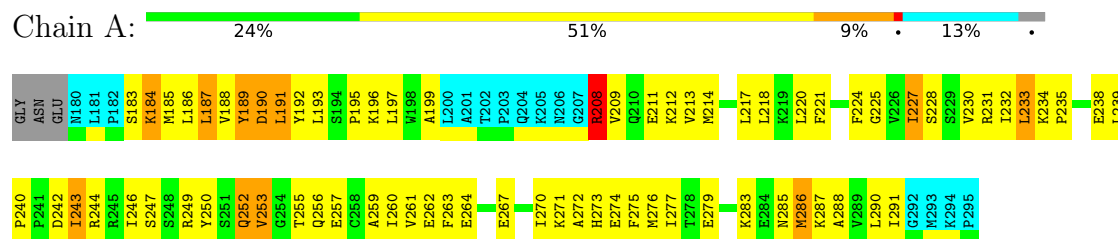
Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLY	-	expression tag	UNP Q9BRS8

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: La-related protein 6

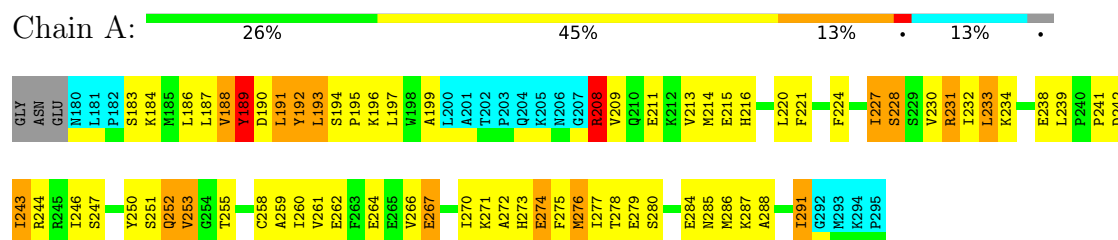


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

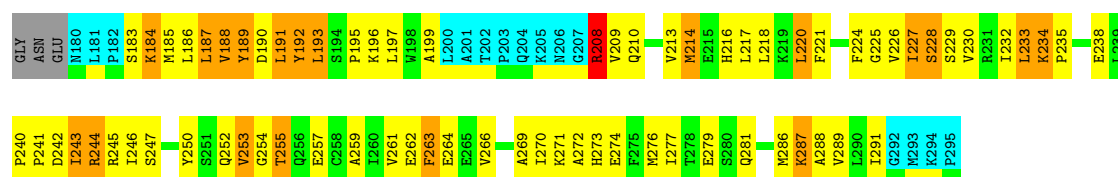
- Molecule 1: La-related protein 6



4.2.2 Score per residue for model 2

- Molecule 1: La-related protein 6

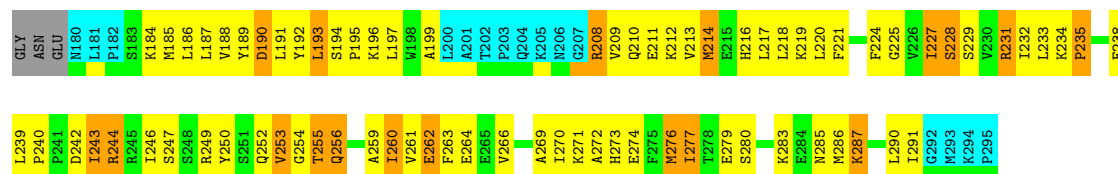




4.2.3 Score per residue for model 3

- Molecule 1: La-related protein 6

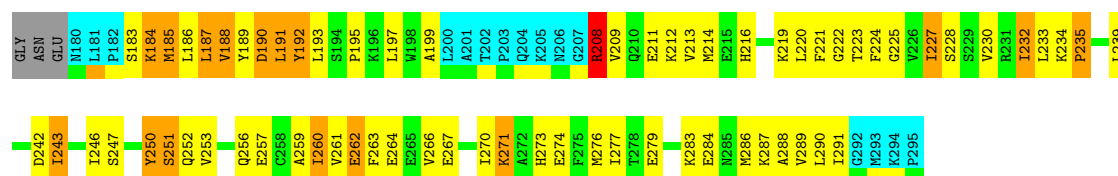
Chain A: 21% 49% 15% 13% .



4.2.4 Score per residue for model 4

- Molecule 1: La-related protein 6

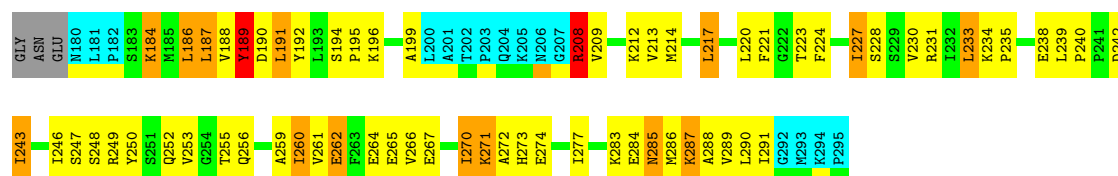
Chain A: 27% 44% 13% . 13% .



4.2.5 Score per residue for model 5

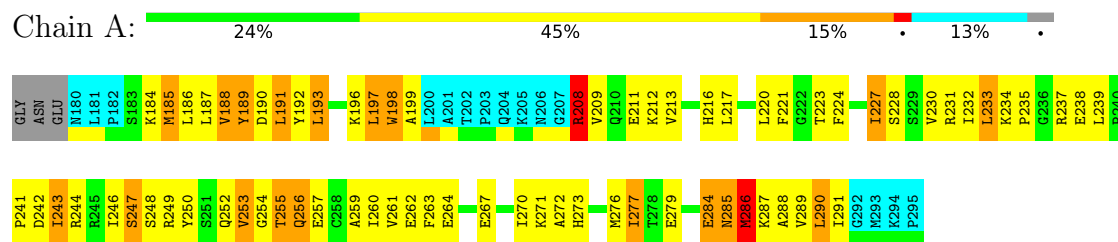
- Molecule 1: La-related protein 6

Chain A: 29% 42% 12% . 13% .



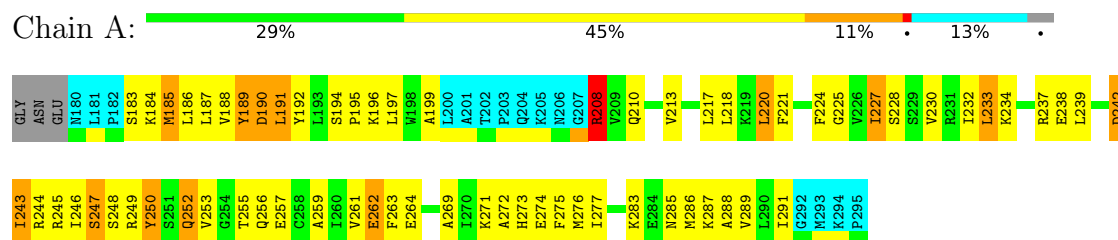
4.2.6 Score per residue for model 6

- Molecule 1: La-related protein 6



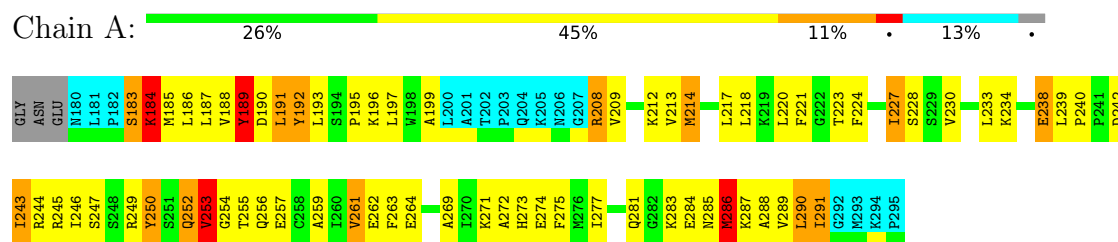
4.2.7 Score per residue for model 7

- Molecule 1: La-related protein 6



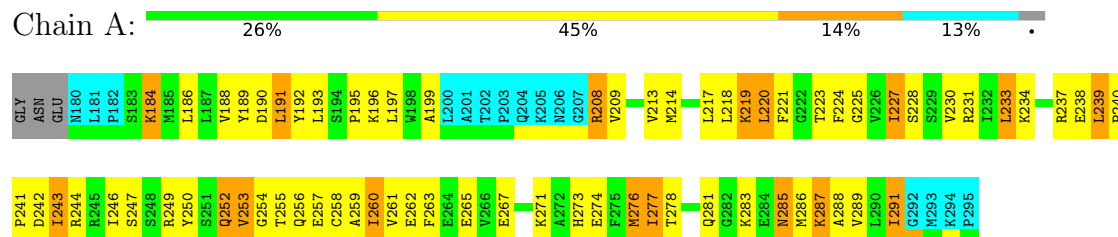
4.2.8 Score per residue for model 8

- Molecule 1: La-related protein 6



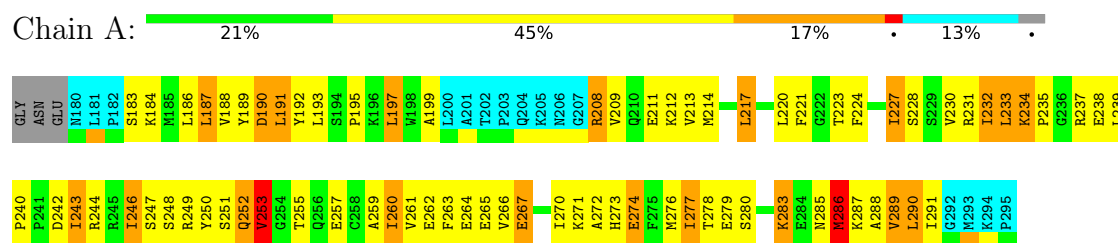
4.2.9 Score per residue for model 9

- Molecule 1: La-related protein 6



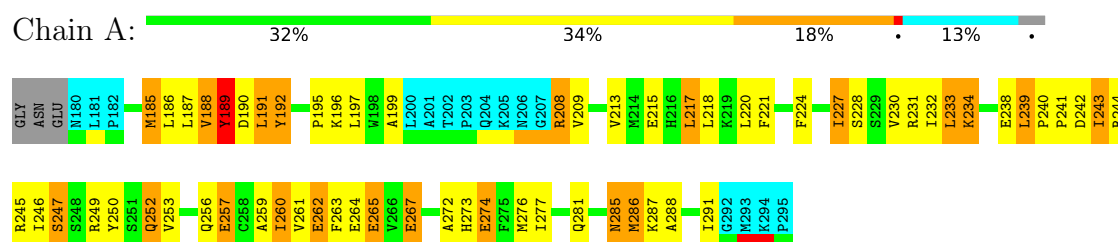
4.2.10 Score per residue for model 10

- Molecule 1: La-related protein 6



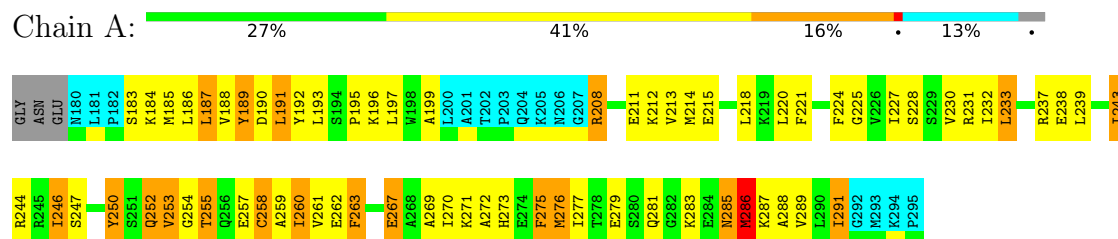
4.2.11 Score per residue for model 11

- Molecule 1: La-related protein 6



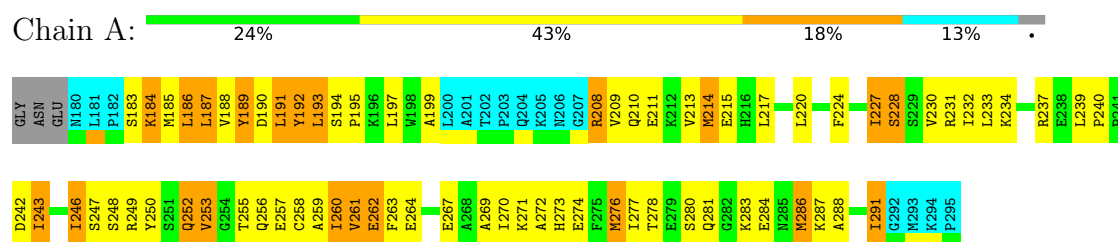
4.2.12 Score per residue for model 12

- Molecule 1: La-related protein 6



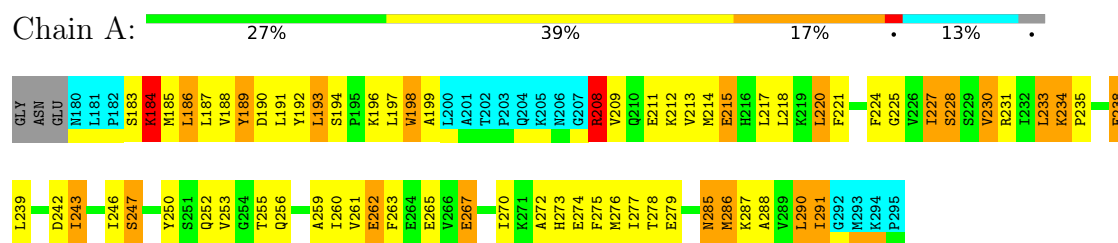
4.2.13 Score per residue for model 13

- Molecule 1: La-related protein 6



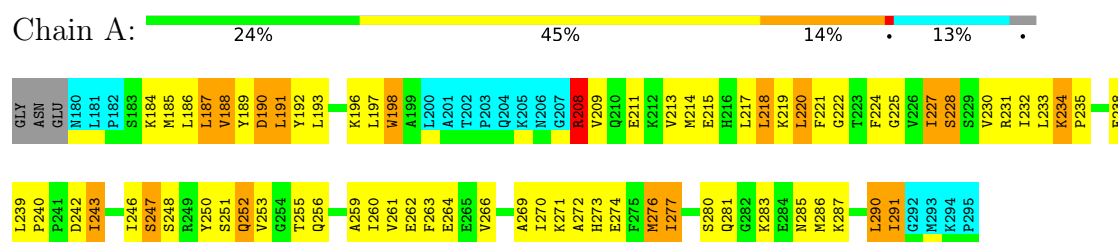
4.2.14 Score per residue for model 14

- Molecule 1: La-related protein 6



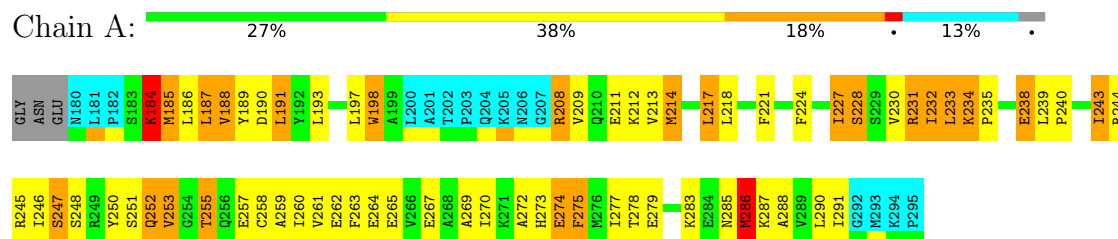
4.2.15 Score per residue for model 15

- Molecule 1: La-related protein 6



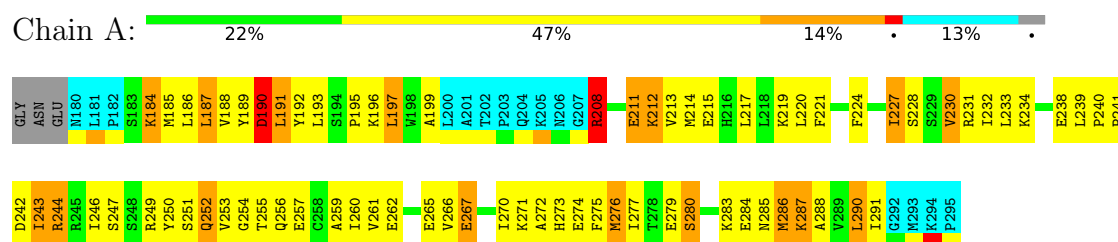
4.2.16 Score per residue for model 16

- Molecule 1: La-related protein 6



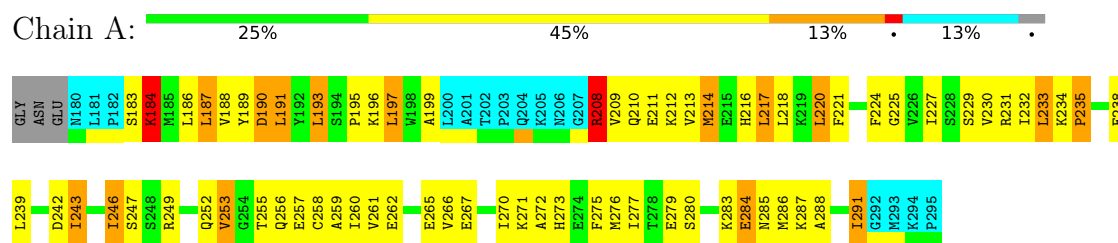
4.2.17 Score per residue for model 17

- Molecule 1: La-related protein 6



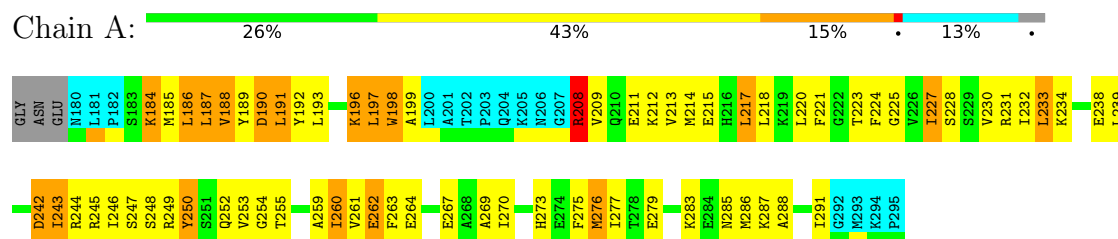
4.2.18 Score per residue for model 18

- Molecule 1: La-related protein 6



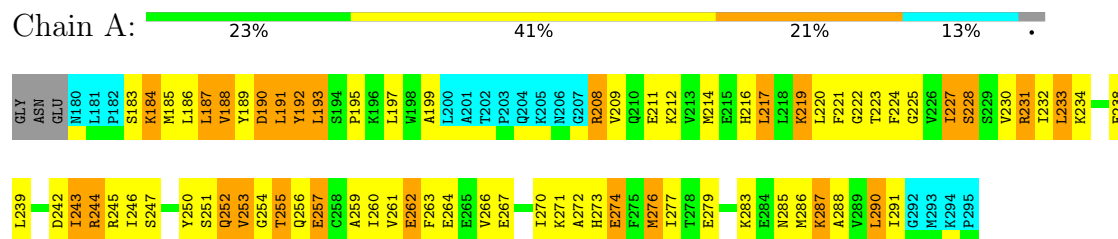
4.2.19 Score per residue for model 19

- Molecule 1: La-related protein 6



4.2.20 Score per residue for model 20

- Molecule 1: La-related protein 6



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 100 calculated structures, 20 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
CNS	structure solution	1.21
CNS	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1254
Number of shifts mapped to atoms	1254
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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	0.35±0.01	0±0/826 (0.0± 0.0%)	0.72±0.03	1±1/1112 (0.1± 0.1%)
All	All	0.35	0/16520 (0.0%)	0.72	12/22240 (0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	189	TYR	N-CA-C	7.38	120.07	108.79	5	8
1	A	239	LEU	CA-C-N	5.13	123.36	119.66	11	2
1	A	239	LEU	C-N-CA	5.13	123.36	119.66	11	2

There are no chirality outliers.

There are no planarity outliers.

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	811	848	846	71±8
All	All	16220	16960	16920	1419

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 43.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:LEU:HD21	1:A:288:ALA:HB1	0.98	1.35	12	11
1:A:230:VAL:HG12	1:A:261:VAL:HG12	0.96	1.33	2	2
1:A:277:ILE:HD13	1:A:278:THR:N	0.93	1.78	9	1
1:A:230:VAL:HG22	1:A:261:VAL:HG12	0.88	1.45	4	10
1:A:188:VAL:HG22	1:A:259:ALA:HB3	0.86	1.45	12	8
1:A:191:LEU:HD22	1:A:191:LEU:O	0.85	1.71	5	5
1:A:188:VAL:CG2	1:A:259:ALA:HB3	0.83	2.03	5	17
1:A:189:TYR:O	1:A:286:MET:HA	0.82	1.74	2	2
1:A:191:LEU:HD13	1:A:191:LEU:H	0.81	1.33	2	9
1:A:195:PRO:O	1:A:199:ALA:HB3	0.81	1.75	7	15
1:A:191:LEU:HD22	1:A:192:TYR:N	0.80	1.90	2	9
1:A:273:HIS:O	1:A:277:ILE:HD12	0.80	1.76	9	1
1:A:197:LEU:HD11	1:A:209:VAL:HG13	0.80	1.51	19	1
1:A:224:PHE:CD1	1:A:272:ALA:HB2	0.79	2.12	18	11
1:A:197:LEU:HD12	1:A:209:VAL:HG23	0.79	1.50	15	1
1:A:190:ASP:OD2	1:A:253:VAL:HG21	0.79	1.76	19	3
1:A:224:PHE:CE1	1:A:272:ALA:HB2	0.78	2.12	2	8
1:A:221:PHE:HB2	1:A:227:ILE:HD11	0.78	1.54	7	5
1:A:243:ILE:HG21	1:A:258:CYS:SG	0.78	2.19	18	2
1:A:214:MET:HE1	1:A:230:VAL:HG23	0.77	1.56	2	1
1:A:188:VAL:HG13	1:A:191:LEU:HD12	0.77	1.57	2	1
1:A:243:ILE:HG22	1:A:247:SER:OG	0.77	1.80	2	2
1:A:189:TYR:CE1	1:A:289:VAL:HG23	0.76	2.15	7	5
1:A:267:GLU:O	1:A:270:ILE:HG22	0.76	1.79	12	1
1:A:197:LEU:HD21	1:A:209:VAL:HG13	0.76	1.58	3	1
1:A:191:LEU:HD12	1:A:192:TYR:N	0.76	1.95	14	2
1:A:233:LEU:HD21	1:A:243:ILE:HD12	0.76	1.55	3	1
1:A:221:PHE:CB	1:A:227:ILE:HD11	0.76	2.10	7	8
1:A:187:LEU:HD23	1:A:291:ILE:HD11	0.76	1.57	7	2
1:A:219:LYS:O	1:A:223:THR:HG23	0.76	1.81	20	3
1:A:261:VAL:HG11	1:A:263:PHE:CZ	0.75	2.16	10	2
1:A:197:LEU:HD22	1:A:209:VAL:HG13	0.75	1.56	14	2
1:A:214:MET:HE1	1:A:230:VAL:CG2	0.75	2.11	2	1
1:A:217:LEU:HD23	1:A:286:MET:HE1	0.75	1.57	7	1
1:A:191:LEU:C	1:A:191:LEU:HD13	0.75	2.06	16	5
1:A:193:LEU:HD13	1:A:255:THR:HG21	0.74	1.60	15	3
1:A:227:ILE:HG21	1:A:230:VAL:HG22	0.74	1.59	5	10
1:A:192:TYR:O	1:A:197:LEU:HD12	0.74	1.80	4	3
1:A:270:ILE:HD12	1:A:271:LYS:N	0.74	1.97	1	2
1:A:233:LEU:C	1:A:233:LEU:HD22	0.74	2.08	16	1
1:A:213:VAL:HG12	1:A:217:LEU:HD11	0.74	1.60	14	2
1:A:186:LEU:HD12	1:A:186:LEU:O	0.73	1.83	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:190:ASP:CG	1:A:253:VAL:HG11	0.73	2.08	15	7
1:A:190:ASP:O	1:A:286:MET:N	0.73	2.21	17	13
1:A:191:LEU:HD13	1:A:191:LEU:N	0.73	1.99	11	8
1:A:188:VAL:HB	1:A:259:ALA:HB3	0.73	1.60	7	3
1:A:233:LEU:CD1	1:A:239:LEU:HD23	0.72	2.14	5	17
1:A:190:ASP:OD2	1:A:193:LEU:HD22	0.72	1.84	16	2
1:A:192:TYR:HA	1:A:197:LEU:HD13	0.72	1.59	11	2
1:A:188:VAL:HG22	1:A:259:ALA:CB	0.71	2.16	12	7
1:A:191:LEU:HD23	1:A:213:VAL:HG11	0.71	1.62	2	2
1:A:186:LEU:O	1:A:261:VAL:HG22	0.71	1.85	9	6
1:A:276:MET:CE	1:A:286:MET:HE2	0.71	2.16	11	1
1:A:273:HIS:CE1	1:A:277:ILE:HD13	0.71	2.20	19	3
1:A:227:ILE:CG2	1:A:261:VAL:HG23	0.71	2.16	8	1
1:A:273:HIS:CD2	1:A:277:ILE:HD12	0.71	2.20	11	1
1:A:273:HIS:CD2	1:A:290:LEU:HD13	0.71	2.21	15	1
1:A:189:TYR:O	1:A:191:LEU:HD13	0.71	1.86	20	2
1:A:209:VAL:O	1:A:213:VAL:HG12	0.70	1.86	15	5
1:A:190:ASP:CB	1:A:253:VAL:HG11	0.70	2.16	20	7
1:A:230:VAL:HG13	1:A:261:VAL:HG12	0.70	1.60	9	3
1:A:188:VAL:CG1	1:A:191:LEU:HD12	0.70	2.16	2	1
1:A:267:GLU:HA	1:A:270:ILE:HD12	0.69	1.64	10	7
1:A:220:LEU:O	1:A:220:LEU:HD13	0.69	1.87	1	1
1:A:192:TYR:HB2	1:A:209:VAL:HG21	0.69	1.63	4	3
1:A:227:ILE:HG23	1:A:263:PHE:CE1	0.69	2.22	19	5
1:A:188:VAL:HG23	1:A:259:ALA:HB3	0.69	1.62	1	8
1:A:189:TYR:CE2	1:A:287:LYS:HB2	0.69	2.21	9	3
1:A:188:VAL:HG13	1:A:276:MET:HE1	0.69	1.63	4	6
1:A:186:LEU:HD12	1:A:290:LEU:HD22	0.69	1.64	6	2
1:A:276:MET:HE3	1:A:286:MET:HG3	0.69	1.64	6	1
1:A:190:ASP:OD1	1:A:193:LEU:HD13	0.68	1.88	16	1
1:A:213:VAL:O	1:A:217:LEU:HD13	0.67	1.90	3	3
1:A:277:ILE:HD13	1:A:278:THR:H	0.67	1.47	9	1
1:A:266:VAL:O	1:A:270:ILE:HG23	0.67	1.90	18	2
1:A:197:LEU:CD1	1:A:209:VAL:HG23	0.67	2.18	15	1
1:A:263:PHE:CE2	1:A:269:ALA:HB2	0.67	2.25	12	2
1:A:188:VAL:CG1	1:A:276:MET:HE1	0.67	2.19	4	2
1:A:187:LEU:HD23	1:A:291:ILE:HG21	0.66	1.67	13	1
1:A:221:PHE:CG	1:A:227:ILE:HD11	0.66	2.25	4	3
1:A:186:LEU:CD2	1:A:269:ALA:HB1	0.66	2.19	3	1
1:A:190:ASP:OD1	1:A:193:LEU:HD23	0.66	1.90	14	1
1:A:189:TYR:CE2	1:A:250:TYR:CZ	0.66	2.84	2	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:276:MET:HE2	1:A:286:MET:SD	0.66	2.30	12	1
1:A:193:LEU:HD22	1:A:255:THR:HB	0.65	1.67	3	2
1:A:187:LEU:HD23	1:A:291:ILE:CD1	0.65	2.21	5	2
1:A:213:VAL:HG12	1:A:217:LEU:CD1	0.65	2.20	14	1
1:A:190:ASP:OD1	1:A:253:VAL:HG21	0.65	1.90	20	2
1:A:227:ILE:HG23	1:A:263:PHE:CD1	0.65	2.27	9	5
1:A:191:LEU:HG	1:A:213:VAL:HG23	0.65	1.69	16	1
1:A:186:LEU:CD1	1:A:290:LEU:HD12	0.65	2.21	17	1
1:A:189:TYR:CD2	1:A:287:LYS:HB2	0.64	2.27	7	1
1:A:192:TYR:CE2	1:A:209:VAL:HG21	0.64	2.28	6	3
1:A:215:GLU:HA	1:A:218:LEU:HD12	0.64	1.69	12	2
1:A:233:LEU:HD22	1:A:240:PRO:HD2	0.64	1.67	3	1
1:A:192:TYR:HA	1:A:197:LEU:HD22	0.64	1.68	19	1
1:A:273:HIS:O	1:A:277:ILE:HG12	0.64	1.93	18	10
1:A:217:LEU:HD23	1:A:221:PHE:CZ	0.64	2.28	19	2
1:A:232:ILE:HG22	1:A:259:ALA:CB	0.63	2.23	11	10
1:A:189:TYR:CD1	1:A:189:TYR:N	0.63	2.66	12	5
1:A:209:VAL:O	1:A:213:VAL:HG22	0.63	1.94	9	8
1:A:190:ASP:OD2	1:A:253:VAL:HG12	0.63	1.93	5	1
1:A:227:ILE:HG21	1:A:230:VAL:CG2	0.63	2.23	11	3
1:A:240:PRO:HD2	1:A:243:ILE:HD11	0.63	1.69	16	3
1:A:217:LEU:CD2	1:A:286:MET:HE1	0.62	2.23	7	2
1:A:197:LEU:CD2	1:A:209:VAL:HG13	0.62	2.24	6	1
1:A:190:ASP:OD2	1:A:255:THR:HG22	0.62	1.94	20	1
1:A:186:LEU:HD13	1:A:269:ALA:HB1	0.62	1.70	19	3
1:A:266:VAL:HG12	1:A:270:ILE:HG23	0.62	1.70	18	1
1:A:232:ILE:HG22	1:A:259:ALA:HB1	0.62	1.70	19	5
1:A:221:PHE:HB3	1:A:227:ILE:HD11	0.62	1.71	4	4
1:A:276:MET:HE1	1:A:287:LYS:O	0.62	1.94	12	1
1:A:276:MET:HE3	1:A:286:MET:HG2	0.62	1.71	7	7
1:A:187:LEU:HD11	1:A:243:ILE:CG2	0.62	2.24	11	1
1:A:247:SER:HA	1:A:250:TYR:CZ	0.62	2.30	2	11
1:A:186:LEU:HD23	1:A:269:ALA:HB1	0.62	1.70	3	1
1:A:266:VAL:HG22	1:A:270:ILE:HG23	0.61	1.72	1	1
1:A:189:TYR:HB2	1:A:287:LYS:CB	0.61	2.26	3	5
1:A:273:HIS:NE2	1:A:277:ILE:HD11	0.61	2.11	3	5
1:A:193:LEU:HD21	1:A:255:THR:OG1	0.61	1.95	14	1
1:A:267:GLU:O	1:A:270:ILE:HG13	0.61	1.96	1	1
1:A:197:LEU:HD23	1:A:209:VAL:HG23	0.61	1.72	18	1
1:A:197:LEU:C	1:A:197:LEU:HD13	0.60	2.20	2	7
1:A:243:ILE:N	1:A:243:ILE:HD13	0.60	2.10	2	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:LEU:HD12	1:A:290:LEU:HD12	0.60	1.72	14	2
1:A:187:LEU:HB3	1:A:291:ILE:HD11	0.60	1.73	5	4
1:A:190:ASP:HB3	1:A:253:VAL:HG11	0.60	1.73	18	1
1:A:243:ILE:HA	1:A:246:ILE:HG22	0.60	1.73	12	11
1:A:189:TYR:CD2	1:A:253:VAL:HG21	0.60	2.31	11	4
1:A:191:LEU:HD13	1:A:192:TYR:N	0.60	2.11	5	1
1:A:276:MET:HE3	1:A:286:MET:CG	0.60	2.26	6	4
1:A:187:LEU:HD13	1:A:243:ILE:HG22	0.60	1.74	12	2
1:A:185:MET:HE2	1:A:291:ILE:HD11	0.60	1.72	13	1
1:A:266:VAL:HG23	1:A:290:LEU:HD21	0.60	1.73	17	2
1:A:233:LEU:HD21	1:A:243:ILE:CD1	0.60	2.27	3	1
1:A:232:ILE:HD11	1:A:234:LYS:NZ	0.60	2.12	13	1
1:A:187:LEU:HD22	1:A:243:ILE:CG2	0.59	2.27	5	1
1:A:193:LEU:HB2	1:A:255:THR:HG21	0.59	1.72	8	1
1:A:217:LEU:HD21	1:A:221:PHE:CE2	0.59	2.32	16	1
1:A:253:VAL:HG13	1:A:284:GLU:HB3	0.59	1.73	17	1
1:A:187:LEU:HA	1:A:259:ALA:O	0.59	1.97	18	9
1:A:233:LEU:HD22	1:A:233:LEU:O	0.59	1.96	16	1
1:A:274:GLU:O	1:A:278:THR:HG23	0.59	1.97	1	2
1:A:291:ILE:C	1:A:291:ILE:HD13	0.59	2.22	9	4
1:A:189:TYR:HB2	1:A:287:LYS:CA	0.59	2.27	20	6
1:A:276:MET:HE2	1:A:288:ALA:HB2	0.59	1.72	10	5
1:A:186:LEU:HD12	1:A:290:LEU:CD2	0.59	2.28	8	1
1:A:187:LEU:HD23	1:A:291:ILE:HB	0.59	1.75	1	3
1:A:190:ASP:OD2	1:A:253:VAL:HG11	0.58	1.98	7	1
1:A:191:LEU:HB3	1:A:286:MET:HE3	0.58	1.73	11	2
1:A:273:HIS:NE2	1:A:277:ILE:HG21	0.58	2.13	9	2
1:A:220:LEU:O	1:A:224:PHE:CD2	0.58	2.56	18	3
1:A:243:ILE:O	1:A:247:SER:N	0.58	2.37	1	19
1:A:189:TYR:HE1	1:A:289:VAL:HG23	0.58	1.59	7	3
1:A:217:LEU:HD21	1:A:221:PHE:CD2	0.58	2.34	8	2
1:A:189:TYR:HD2	1:A:253:VAL:HG21	0.58	1.57	11	3
1:A:273:HIS:CD2	1:A:274:GLU:N	0.58	2.72	11	1
1:A:221:PHE:CD2	1:A:227:ILE:HD11	0.58	2.32	18	4
1:A:291:ILE:N	1:A:291:ILE:HD13	0.58	2.14	15	1
1:A:191:LEU:HB3	1:A:286:MET:HG2	0.57	1.76	13	1
1:A:188:VAL:HG21	1:A:259:ALA:HB3	0.57	1.77	17	3
1:A:191:LEU:H	1:A:191:LEU:CD1	0.57	2.11	2	1
1:A:233:LEU:HD12	1:A:233:LEU:O	0.57	1.98	17	5
1:A:209:VAL:O	1:A:213:VAL:HG23	0.57	1.99	6	3
1:A:191:LEU:HD22	1:A:213:VAL:HG11	0.57	1.76	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:234:LYS:CG	1:A:235:PRO:HD2	0.57	2.30	10	3
1:A:233:LEU:HD13	1:A:238:GLU:O	0.57	2.00	7	4
1:A:233:LEU:HD11	1:A:258:CYS:HB2	0.57	1.76	16	1
1:A:186:LEU:HD21	1:A:288:ALA:CB	0.57	2.28	18	6
1:A:189:TYR:HB2	1:A:287:LYS:C	0.57	2.25	19	6
1:A:189:TYR:OH	1:A:250:TYR:CE2	0.57	2.58	4	2
1:A:189:TYR:HB2	1:A:287:LYS:HB2	0.56	1.76	4	1
1:A:263:PHE:CD2	1:A:269:ALA:HB2	0.56	2.35	3	5
1:A:189:TYR:CG	1:A:287:LYS:HB3	0.56	2.35	3	1
1:A:227:ILE:CG2	1:A:261:VAL:HG13	0.56	2.30	10	3
1:A:263:PHE:HD2	1:A:269:ALA:HB2	0.56	1.60	13	4
1:A:189:TYR:OH	1:A:289:VAL:HG22	0.56	1.99	7	1
1:A:266:VAL:CG2	1:A:290:LEU:HD21	0.56	2.30	10	3
1:A:224:PHE:CZ	1:A:272:ALA:HB1	0.56	2.35	20	1
1:A:189:TYR:CD2	1:A:287:LYS:CB	0.56	2.89	7	1
1:A:186:LEU:HD11	1:A:273:HIS:ND1	0.56	2.15	4	1
1:A:197:LEU:HG	1:A:209:VAL:HG23	0.56	1.77	20	1
1:A:189:TYR:C	1:A:191:LEU:HD13	0.56	2.26	12	3
1:A:276:MET:HE1	1:A:287:LYS:C	0.55	2.26	13	2
1:A:260:ILE:N	1:A:260:ILE:HD13	0.55	2.17	13	1
1:A:224:PHE:CD2	1:A:272:ALA:HB2	0.55	2.36	10	1
1:A:189:TYR:N	1:A:287:LYS:O	0.55	2.39	4	8
1:A:189:TYR:O	1:A:191:LEU:N	0.55	2.38	20	4
1:A:276:MET:SD	1:A:288:ALA:HB2	0.55	2.42	4	1
1:A:190:ASP:CG	1:A:255:THR:HG22	0.55	2.26	6	1
1:A:187:LEU:HD13	1:A:243:ILE:CG2	0.55	2.31	18	2
1:A:190:ASP:HB2	1:A:253:VAL:HG11	0.55	1.79	10	8
1:A:291:ILE:HD13	1:A:291:ILE:C	0.55	2.26	14	1
1:A:276:MET:CE	1:A:288:ALA:HB2	0.55	2.32	2	4
1:A:192:TYR:HE2	1:A:209:VAL:HG21	0.55	1.60	14	2
1:A:243:ILE:O	1:A:247:SER:CB	0.55	2.55	15	16
1:A:242:ASP:O	1:A:246:ILE:HG22	0.54	2.02	17	16
1:A:188:VAL:HG13	1:A:276:MET:CE	0.54	2.32	18	3
1:A:189:TYR:CZ	1:A:287:LYS:CB	0.54	2.91	8	4
1:A:197:LEU:HD13	1:A:197:LEU:O	0.54	2.03	2	1
1:A:273:HIS:CE1	1:A:277:ILE:HD11	0.54	2.37	15	1
1:A:240:PRO:O	1:A:243:ILE:HD13	0.54	2.03	17	1
1:A:273:HIS:O	1:A:277:ILE:HB	0.54	2.03	13	8
1:A:190:ASP:OD1	1:A:255:THR:HG23	0.54	2.02	7	1
1:A:187:LEU:HD11	1:A:250:TYR:HE2	0.54	1.63	12	1
1:A:187:LEU:HD11	1:A:250:TYR:CE2	0.54	2.38	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:LEU:HD23	1:A:291:ILE:CG2	0.54	2.33	13	1
1:A:276:MET:HE3	1:A:288:ALA:HB2	0.54	1.80	1	2
1:A:266:VAL:HG22	1:A:270:ILE:HG13	0.53	1.78	2	2
1:A:233:LEU:HB2	1:A:238:GLU:O	0.53	2.03	16	13
1:A:266:VAL:O	1:A:270:ILE:HG22	0.53	2.03	4	1
1:A:187:LEU:C	1:A:187:LEU:HD12	0.53	2.28	5	2
1:A:253:VAL:HG12	1:A:253:VAL:O	0.53	2.03	5	1
1:A:259:ALA:C	1:A:260:ILE:HD13	0.53	2.28	11	2
1:A:186:LEU:HD22	1:A:288:ALA:HB1	0.53	1.80	5	1
1:A:191:LEU:HD22	1:A:191:LEU:C	0.53	2.28	5	3
1:A:185:MET:SD	1:A:291:ILE:HG21	0.53	2.43	4	1
1:A:233:LEU:HD13	1:A:239:LEU:HA	0.53	1.80	12	4
1:A:233:LEU:HD13	1:A:258:CYS:O	0.53	2.04	16	1
1:A:277:ILE:HG22	1:A:287:LYS:HG3	0.53	1.81	18	1
1:A:247:SER:HA	1:A:250:TYR:CE2	0.53	2.39	15	7
1:A:243:ILE:HG22	1:A:247:SER:HB2	0.53	1.81	4	2
1:A:217:LEU:HD21	1:A:286:MET:HE1	0.53	1.79	19	1
1:A:193:LEU:HD22	1:A:284:GLU:HG3	0.53	1.80	1	1
1:A:224:PHE:CG	1:A:272:ALA:HB2	0.52	2.39	13	4
1:A:189:TYR:CB	1:A:287:LYS:HG3	0.52	2.33	17	1
1:A:190:ASP:OD1	1:A:255:THR:HG21	0.52	2.04	10	1
1:A:221:PHE:O	1:A:225:GLY:O	0.52	2.28	19	8
1:A:192:TYR:HE1	1:A:209:VAL:HG21	0.52	1.64	10	1
1:A:189:TYR:CE2	1:A:250:TYR:CE1	0.52	2.98	3	1
1:A:217:LEU:HD11	1:A:286:MET:HE1	0.52	1.82	6	1
1:A:187:LEU:HD12	1:A:259:ALA:O	0.52	2.04	11	1
1:A:273:HIS:HD2	1:A:277:ILE:HD12	0.52	1.64	11	1
1:A:189:TYR:CE2	1:A:250:TYR:CE2	0.52	2.97	12	3
1:A:227:ILE:HD12	1:A:227:ILE:H	0.52	1.63	17	1
1:A:224:PHE:CE2	1:A:272:ALA:HB1	0.52	2.40	20	1
1:A:261:VAL:HG11	1:A:263:PHE:CE1	0.52	2.40	3	2
1:A:191:LEU:HD22	1:A:191:LEU:H	0.52	1.65	11	2
1:A:243:ILE:HG21	1:A:258:CYS:HB3	0.52	1.81	1	1
1:A:240:PRO:HD2	1:A:243:ILE:CG1	0.52	2.35	11	4
1:A:188:VAL:HG23	1:A:259:ALA:CB	0.52	2.34	1	3
1:A:232:ILE:HG22	1:A:259:ALA:HB2	0.52	1.81	11	3
1:A:189:TYR:CB	1:A:287:LYS:HB3	0.51	2.35	19	3
1:A:213:VAL:HG12	1:A:217:LEU:HD13	0.51	1.82	6	1
1:A:263:PHE:CD1	1:A:269:ALA:HB2	0.51	2.40	16	1
1:A:224:PHE:CE1	1:A:272:ALA:CB	0.51	2.93	1	8
1:A:189:TYR:CZ	1:A:250:TYR:CE2	0.51	2.98	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:193:LEU:HA	1:A:198:TRP:CB	0.51	2.36	15	5
1:A:233:LEU:HD11	1:A:258:CYS:CB	0.51	2.35	16	1
1:A:189:TYR:HB2	1:A:287:LYS:HB3	0.51	1.82	3	4
1:A:187:LEU:CB	1:A:291:ILE:HD11	0.51	2.36	19	3
1:A:273:HIS:ND1	1:A:277:ILE:HD12	0.51	2.20	5	1
1:A:228:SER:N	1:A:262:GLU:O	0.51	2.41	9	12
1:A:190:ASP:CG	1:A:284:GLU:O	0.51	2.54	5	1
1:A:190:ASP:CG	1:A:253:VAL:CG1	0.51	2.84	6	7
1:A:227:ILE:HG21	1:A:230:VAL:HG13	0.51	1.81	17	1
1:A:253:VAL:O	1:A:253:VAL:HG12	0.51	2.05	17	4
1:A:217:LEU:HD12	1:A:286:MET:CE	0.51	2.36	17	1
1:A:280:SER:CB	1:A:286:MET:O	0.51	2.59	1	3
1:A:285:ASN:O	1:A:287:LYS:HG2	0.51	2.06	10	2
1:A:227:ILE:HG21	1:A:230:VAL:HG23	0.51	1.82	11	1
1:A:263:PHE:CE1	1:A:269:ALA:HB2	0.51	2.41	16	1
1:A:231:ARG:O	1:A:260:ILE:N	0.51	2.44	14	11
1:A:273:HIS:ND1	1:A:274:GLU:N	0.51	2.58	5	1
1:A:193:LEU:HD13	1:A:255:THR:CB	0.51	2.36	8	1
1:A:190:ASP:OD1	1:A:253:VAL:HG11	0.51	2.05	17	1
1:A:184:LYS:HB2	1:A:266:VAL:HG22	0.51	1.82	18	1
1:A:231:ARG:O	1:A:260:ILE:HG13	0.50	2.06	3	1
1:A:261:VAL:HG21	1:A:263:PHE:CZ	0.50	2.42	8	1
1:A:217:LEU:HG	1:A:286:MET:HE1	0.50	1.82	3	1
1:A:224:PHE:CZ	1:A:272:ALA:CB	0.50	2.94	6	4
1:A:273:HIS:CG	1:A:274:GLU:N	0.50	2.79	20	3
1:A:193:LEU:HD13	1:A:255:THR:CG2	0.50	2.36	13	1
1:A:234:LYS:HG3	1:A:235:PRO:HD2	0.50	1.83	3	2
1:A:250:TYR:C	1:A:250:TYR:CD1	0.50	2.89	12	5
1:A:228:SER:CB	1:A:262:GLU:O	0.50	2.59	8	17
1:A:233:LEU:HD21	1:A:258:CYS:SG	0.50	2.47	18	1
1:A:191:LEU:HB2	1:A:286:MET:HE3	0.50	1.82	19	1
1:A:275:PHE:C	1:A:275:PHE:CD1	0.50	2.89	12	1
1:A:222:GLY:HA2	1:A:225:GLY:O	0.50	2.06	20	2
1:A:189:TYR:CZ	1:A:287:LYS:HB3	0.50	2.42	11	4
1:A:191:LEU:CD2	1:A:192:TYR:N	0.50	2.75	20	6
1:A:191:LEU:N	1:A:191:LEU:CD1	0.49	2.71	11	5
1:A:224:PHE:CD1	1:A:272:ALA:CB	0.49	2.95	5	1
1:A:250:TYR:HD1	1:A:250:TYR:O	0.49	1.90	2	7
1:A:243:ILE:O	1:A:247:SER:HB2	0.49	2.07	9	2
1:A:193:LEU:HD13	1:A:255:THR:HB	0.49	1.83	8	2
1:A:191:LEU:HD23	1:A:213:VAL:CG1	0.49	2.35	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:221:PHE:CE2	1:A:261:VAL:HG11	0.49	2.41	16	2
1:A:185:MET:O	1:A:291:ILE:HG22	0.49	2.07	17	5
1:A:233:LEU:HD22	1:A:240:PRO:CD	0.49	2.38	13	5
1:A:241:PRO:HA	1:A:244:ARG:HG2	0.49	1.85	2	6
1:A:273:HIS:CE1	1:A:277:ILE:CD1	0.49	2.96	15	3
1:A:233:LEU:C	1:A:233:LEU:CD2	0.49	2.81	16	1
1:A:221:PHE:HA	1:A:224:PHE:CZ	0.49	2.42	6	7
1:A:224:PHE:CD1	1:A:224:PHE:C	0.49	2.91	18	6
1:A:189:TYR:N	1:A:189:TYR:HD1	0.49	2.05	12	2
1:A:233:LEU:HD21	1:A:260:ILE:HD11	0.49	1.84	5	2
1:A:274:GLU:O	1:A:278:THR:HG22	0.49	2.07	14	3
1:A:189:TYR:CZ	1:A:250:TYR:CD2	0.49	3.00	16	1
1:A:220:LEU:O	1:A:224:PHE:CE2	0.48	2.66	2	5
1:A:221:PHE:O	1:A:225:GLY:C	0.48	2.56	7	2
1:A:184:LYS:CB	1:A:266:VAL:HG22	0.48	2.38	18	1
1:A:197:LEU:C	1:A:197:LEU:CD1	0.48	2.86	2	2
1:A:189:TYR:CB	1:A:287:LYS:HB2	0.48	2.37	4	1
1:A:217:LEU:HD21	1:A:221:PHE:CZ	0.48	2.43	11	1
1:A:190:ASP:HB2	1:A:253:VAL:CG1	0.48	2.38	8	6
1:A:217:LEU:HD23	1:A:221:PHE:CE2	0.48	2.43	20	1
1:A:186:LEU:HB3	1:A:261:VAL:HG23	0.48	1.86	1	4
1:A:190:ASP:OD1	1:A:255:THR:HG22	0.48	2.08	2	2
1:A:243:ILE:HG21	1:A:258:CYS:CB	0.48	2.38	16	1
1:A:250:TYR:O	1:A:250:TYR:CD1	0.48	2.67	10	8
1:A:217:LEU:HD12	1:A:286:MET:HE1	0.48	1.84	8	1
1:A:187:LEU:HG	1:A:289:VAL:HG12	0.48	1.85	10	1
1:A:189:TYR:CE2	1:A:287:LYS:HB3	0.48	2.43	18	2
1:A:185:MET:O	1:A:291:ILE:HG12	0.48	2.07	7	2
1:A:253:VAL:HG12	1:A:284:GLU:HB2	0.48	1.84	18	1
1:A:186:LEU:HB3	1:A:261:VAL:CG2	0.48	2.39	14	3
1:A:242:ASP:OD2	1:A:291:ILE:HD12	0.48	2.09	5	1
1:A:240:PRO:HD2	1:A:243:ILE:CD1	0.48	2.38	17	1
1:A:243:ILE:HD13	1:A:243:ILE:H	0.48	1.69	17	5
1:A:191:LEU:CD2	1:A:191:LEU:C	0.48	2.87	7	3
1:A:276:MET:HE2	1:A:287:LYS:C	0.48	2.33	2	2
1:A:232:ILE:HD11	1:A:234:LYS:HZ3	0.48	1.68	13	1
1:A:188:VAL:HG12	1:A:189:TYR:N	0.47	2.24	3	2
1:A:221:PHE:CE1	1:A:286:MET:HE1	0.47	2.45	9	1
1:A:185:MET:HE2	1:A:242:ASP:OD2	0.47	2.08	17	1
1:A:188:VAL:C	1:A:189:TYR:CD1	0.47	2.93	12	2
1:A:191:LEU:HD11	1:A:197:LEU:HD13	0.47	1.86	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:PRO:HA	1:A:199:ALA:HB3	0.47	1.85	4	2
1:A:187:LEU:HD21	1:A:289:VAL:CG1	0.47	2.40	10	1
1:A:250:TYR:O	1:A:250:TYR:HD1	0.47	1.91	10	2
1:A:253:VAL:O	1:A:255:THR:HG22	0.47	2.10	17	2
1:A:246:ILE:CG2	1:A:247:SER:N	0.47	2.77	18	18
1:A:266:VAL:O	1:A:270:ILE:N	0.47	2.46	2	2
1:A:188:VAL:CB	1:A:259:ALA:HB3	0.47	2.39	3	6
1:A:191:LEU:HD12	1:A:191:LEU:C	0.47	2.34	3	2
1:A:187:LEU:HD22	1:A:243:ILE:HG22	0.47	1.85	5	1
1:A:250:TYR:C	1:A:250:TYR:HD1	0.47	2.18	12	2
1:A:188:VAL:O	1:A:258:CYS:HA	0.47	2.10	13	1
1:A:197:LEU:HD12	1:A:209:VAL:CG2	0.47	2.31	15	1
1:A:187:LEU:CA	1:A:259:ALA:O	0.47	2.63	16	1
1:A:191:LEU:HD11	1:A:213:VAL:CG1	0.47	2.40	5	2
1:A:193:LEU:O	1:A:198:TRP:CE3	0.47	2.68	16	4
1:A:220:LEU:O	1:A:224:PHE:CZ	0.47	2.68	7	1
1:A:283:LYS:O	1:A:285:ASN:N	0.47	2.47	7	3
1:A:233:LEU:HD11	1:A:243:ILE:HG13	0.47	1.87	12	3
1:A:189:TYR:OH	1:A:289:VAL:CG2	0.47	2.62	4	1
1:A:270:ILE:HG13	1:A:271:LYS:N	0.47	2.25	5	1
1:A:217:LEU:HD22	1:A:221:PHE:CE2	0.47	2.45	7	1
1:A:197:LEU:HD11	1:A:209:VAL:HG22	0.47	1.85	8	2
1:A:213:VAL:HG22	1:A:217:LEU:HD13	0.47	1.85	10	1
1:A:190:ASP:OD1	1:A:193:LEU:HB2	0.47	2.09	10	2
1:A:191:LEU:C	1:A:191:LEU:CD1	0.47	2.86	5	4
1:A:221:PHE:CD2	1:A:227:ILE:CD1	0.46	2.99	5	3
1:A:270:ILE:HD12	1:A:270:ILE:C	0.46	2.34	1	2
1:A:267:GLU:O	1:A:270:ILE:CG1	0.46	2.64	5	2
1:A:189:TYR:CB	1:A:287:LYS:CG	0.46	2.93	17	1
1:A:193:LEU:HD12	1:A:255:THR:HB	0.46	1.86	20	1
1:A:269:ALA:O	1:A:273:HIS:N	0.46	2.49	3	2
1:A:189:TYR:CG	1:A:287:LYS:HB2	0.46	2.45	7	2
1:A:191:LEU:O	1:A:197:LEU:HD22	0.46	2.11	17	1
1:A:192:TYR:CD1	1:A:197:LEU:CD2	0.46	2.99	19	1
1:A:291:ILE:HG23	1:A:291:ILE:O	0.46	2.10	18	2
1:A:191:LEU:HD23	1:A:286:MET:SD	0.46	2.51	19	1
1:A:191:LEU:HD22	1:A:192:TYR:H	0.46	1.71	8	4
1:A:189:TYR:CD1	1:A:287:LYS:HB3	0.46	2.45	12	1
1:A:266:VAL:HG22	1:A:270:ILE:CD1	0.46	2.41	15	1
1:A:277:ILE:HD13	1:A:277:ILE:C	0.46	2.32	9	1
1:A:287:LYS:CG	1:A:288:ALA:N	0.46	2.79	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:TYR:CZ	1:A:287:LYS:HB2	0.46	2.46	14	3
1:A:266:VAL:HG12	1:A:270:ILE:CG2	0.46	2.38	18	1
1:A:213:VAL:HG23	1:A:214:MET:N	0.46	2.26	3	6
1:A:227:ILE:HG23	1:A:263:PHE:CE2	0.46	2.46	20	1
1:A:188:VAL:HG12	1:A:259:ALA:N	0.45	2.26	2	1
1:A:188:VAL:HG23	1:A:191:LEU:HD11	0.45	1.87	12	1
1:A:197:LEU:HD21	1:A:213:VAL:CG1	0.45	2.41	17	1
1:A:192:TYR:CD1	1:A:192:TYR:C	0.45	2.95	1	3
1:A:235:PRO:HD3	1:A:256:GLN:O	0.45	2.12	3	3
1:A:187:LEU:HD12	1:A:188:VAL:N	0.45	2.26	13	2
1:A:189:TYR:CE1	1:A:288:ALA:CA	0.45	3.00	7	1
1:A:230:VAL:CG1	1:A:261:VAL:HG12	0.45	2.31	17	1
1:A:193:LEU:HD23	1:A:193:LEU:O	0.45	2.10	20	1
1:A:193:LEU:HD12	1:A:255:THR:CG2	0.45	2.41	20	2
1:A:234:LYS:CB	1:A:235:PRO:HD2	0.45	2.42	2	1
1:A:246:ILE:O	1:A:250:TYR:CD2	0.45	2.70	13	3
1:A:189:TYR:CZ	1:A:287:LYS:HG2	0.45	2.47	6	2
1:A:189:TYR:HB2	1:A:287:LYS:O	0.45	2.11	19	3
1:A:186:LEU:C	1:A:186:LEU:HD23	0.45	2.37	9	2
1:A:233:LEU:HD11	1:A:239:LEU:HD23	0.45	1.87	13	1
1:A:187:LEU:HD12	1:A:188:VAL:O	0.45	2.11	13	1
1:A:188:VAL:HG23	1:A:276:MET:HE1	0.45	1.89	2	1
1:A:261:VAL:CG1	1:A:263:PHE:CZ	0.45	3.00	3	2
1:A:189:TYR:HB2	1:A:287:LYS:N	0.45	2.27	20	2
1:A:217:LEU:CD2	1:A:221:PHE:CZ	0.45	2.99	10	3
1:A:193:LEU:HD12	1:A:198:TRP:CD1	0.45	2.47	14	1
1:A:244:ARG:O	1:A:248:SER:CB	0.45	2.65	16	1
1:A:239:LEU:O	1:A:244:ARG:CD	0.45	2.65	3	6
1:A:217:LEU:CD1	1:A:286:MET:HE1	0.45	2.41	6	2
1:A:233:LEU:HD23	1:A:260:ILE:HD11	0.45	1.89	13	1
1:A:246:ILE:HG23	1:A:247:SER:N	0.44	2.26	3	1
1:A:270:ILE:HG23	1:A:271:LYS:N	0.44	2.27	4	1
1:A:189:TYR:CD2	1:A:250:TYR:CZ	0.44	3.05	12	1
1:A:217:LEU:CD2	1:A:221:PHE:CG	0.44	2.99	17	1
1:A:190:ASP:OD1	1:A:193:LEU:CB	0.44	2.65	12	1
1:A:189:TYR:CE2	1:A:287:LYS:HG2	0.44	2.47	13	2
1:A:213:VAL:HG13	1:A:214:MET:N	0.44	2.27	8	4
1:A:198:TRP:CZ3	1:A:199:ALA:HB2	0.44	2.48	14	3
1:A:243:ILE:N	1:A:243:ILE:CD1	0.44	2.78	2	6
1:A:285:ASN:O	1:A:286:MET:C	0.44	2.60	14	9
1:A:230:VAL:CG2	1:A:261:VAL:HG12	0.44	2.33	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:230:VAL:HG13	1:A:261:VAL:CG1	0.44	2.43	13	1
1:A:186:LEU:HD11	1:A:273:HIS:HB3	0.44	1.88	20	1
1:A:192:TYR:CE1	1:A:193:LEU:HD12	0.44	2.47	2	1
1:A:187:LEU:HD12	1:A:187:LEU:C	0.44	2.37	13	1
1:A:191:LEU:O	1:A:191:LEU:HD13	0.44	2.12	16	1
1:A:189:TYR:OH	1:A:289:VAL:HB	0.44	2.12	12	1
1:A:233:LEU:O	1:A:233:LEU:HD13	0.44	2.12	16	1
1:A:243:ILE:HB	1:A:247:SER:HB2	0.44	1.90	17	1
1:A:186:LEU:HD23	1:A:187:LEU:N	0.44	2.28	20	1
1:A:224:PHE:CZ	1:A:272:ALA:HB2	0.43	2.48	6	2
1:A:187:LEU:CD1	1:A:243:ILE:CG2	0.43	2.95	11	1
1:A:280:SER:HB3	1:A:286:MET:O	0.43	2.12	17	1
1:A:273:HIS:O	1:A:277:ILE:N	0.43	2.44	5	2
1:A:189:TYR:HB3	1:A:287:LYS:HG3	0.43	1.88	17	1
1:A:277:ILE:CG2	1:A:288:ALA:O	0.43	2.67	19	3
1:A:235:PRO:CG	1:A:256:GLN:O	0.43	2.65	5	1
1:A:245:ARG:O	1:A:249:ARG:CB	0.43	2.66	7	1
1:A:253:VAL:O	1:A:255:THR:N	0.43	2.52	20	5
1:A:189:TYR:CE1	1:A:289:VAL:CG2	0.43	2.98	7	1
1:A:265:GLU:HB3	1:A:267:GLU:CG	0.43	2.44	11	1
1:A:221:PHE:HA	1:A:224:PHE:CE2	0.43	2.48	16	1
1:A:285:ASN:O	1:A:287:LYS:CG	0.43	2.66	1	2
1:A:270:ILE:HA	1:A:273:HIS:CD2	0.43	2.48	5	1
1:A:227:ILE:HG23	1:A:261:VAL:HG13	0.43	1.90	11	1
1:A:225:GLY:O	1:A:263:PHE:CZ	0.43	2.72	14	1
1:A:266:VAL:HG13	1:A:270:ILE:HD12	0.43	1.88	2	1
1:A:273:HIS:CD2	1:A:273:HIS:C	0.43	2.97	14	1
1:A:273:HIS:NE2	1:A:277:ILE:CD1	0.43	2.82	6	3
1:A:189:TYR:CZ	1:A:250:TYR:CZ	0.43	3.07	10	1
1:A:253:VAL:HG13	1:A:287:LYS:HE3	0.43	1.91	1	1
1:A:186:LEU:O	1:A:261:VAL:CG2	0.43	2.66	4	3
1:A:273:HIS:ND1	1:A:290:LEU:HD23	0.43	2.28	6	1
1:A:221:PHE:HE2	1:A:261:VAL:HG11	0.43	1.73	16	1
1:A:190:ASP:CG	1:A:253:VAL:HG21	0.43	2.39	18	1
1:A:190:ASP:O	1:A:190:ASP:CG	0.43	2.60	14	1
1:A:275:PHE:CD1	1:A:275:PHE:C	0.43	2.97	1	6
1:A:291:ILE:C	1:A:291:ILE:CD1	0.43	2.91	9	3
1:A:189:TYR:HE1	1:A:289:VAL:HG12	0.43	1.73	9	1
1:A:189:TYR:CE1	1:A:289:VAL:HB	0.43	2.49	10	1
1:A:191:LEU:HA	1:A:286:MET:HG2	0.43	1.90	15	1
1:A:186:LEU:HD12	1:A:290:LEU:HG	0.43	1.90	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:273:HIS:CD2	1:A:288:ALA:O	0.42	2.72	12	2
1:A:188:VAL:CG1	1:A:189:TYR:N	0.42	2.82	3	1
1:A:277:ILE:HD11	1:A:288:ALA:O	0.42	2.14	11	1
1:A:185:MET:HE3	1:A:260:ILE:CG2	0.42	2.44	15	1
1:A:224:PHE:C	1:A:224:PHE:CD1	0.42	2.97	16	1
1:A:183:SER:O	1:A:184:LYS:HD3	0.42	2.15	7	2
1:A:242:ASP:O	1:A:246:ILE:CG2	0.42	2.66	7	4
1:A:185:MET:HE2	1:A:291:ILE:HG21	0.42	1.91	11	1
1:A:189:TYR:O	1:A:191:LEU:CD1	0.42	2.63	20	1
1:A:189:TYR:CD2	1:A:287:LYS:HG3	0.42	2.49	5	2
1:A:192:TYR:CE1	1:A:209:VAL:HG21	0.42	2.48	10	1
1:A:217:LEU:HD11	1:A:286:MET:SD	0.42	2.55	5	1
1:A:280:SER:OG	1:A:287:LYS:CD	0.42	2.67	10	1
1:A:217:LEU:CD2	1:A:221:PHE:CE2	0.42	3.03	20	1
1:A:250:TYR:CD1	1:A:250:TYR:O	0.42	2.72	12	2
1:A:224:PHE:CE2	1:A:272:ALA:CB	0.42	3.02	10	1
1:A:217:LEU:CD2	1:A:221:PHE:CD1	0.42	3.02	17	1
1:A:191:LEU:HD21	1:A:257:GLU:HG2	0.42	1.91	8	1
1:A:243:ILE:CD1	1:A:260:ILE:HD11	0.42	2.45	9	1
1:A:261:VAL:CG1	1:A:263:PHE:CD1	0.42	3.02	11	1
1:A:273:HIS:O	1:A:277:ILE:CB	0.42	2.67	13	2
1:A:191:LEU:H	1:A:191:LEU:HD22	0.42	1.75	1	1
1:A:226:VAL:HG12	1:A:227:ILE:N	0.42	2.29	2	1
1:A:189:TYR:O	1:A:190:ASP:C	0.42	2.63	4	3
1:A:190:ASP:OD2	1:A:253:VAL:CG2	0.42	2.66	7	1
1:A:217:LEU:HD22	1:A:221:PHE:CE1	0.42	2.50	14	1
1:A:191:LEU:O	1:A:191:LEU:CD2	0.42	2.61	16	1
1:A:230:VAL:HA	1:A:260:ILE:O	0.42	2.15	20	2
1:A:232:ILE:O	1:A:232:ILE:HG23	0.42	2.15	2	2
1:A:276:MET:O	1:A:280:SER:CB	0.42	2.68	15	2
1:A:192:TYR:CD2	1:A:257:GLU:OE1	0.42	2.73	8	1
1:A:227:ILE:HG23	1:A:263:PHE:CD2	0.42	2.49	16	1
1:A:188:VAL:CG2	1:A:259:ALA:N	0.42	2.83	8	1
1:A:188:VAL:HG22	1:A:259:ALA:N	0.42	2.30	8	1
1:A:191:LEU:HB2	1:A:213:VAL:HG13	0.42	1.92	12	1
1:A:243:ILE:CB	1:A:247:SER:HB3	0.42	2.45	16	1
1:A:272:ALA:O	1:A:275:PHE:CD1	0.42	2.73	16	1
1:A:185:MET:HE2	1:A:291:ILE:HD13	0.42	1.92	6	1
1:A:227:ILE:CG2	1:A:261:VAL:CG1	0.41	2.98	3	1
1:A:235:PRO:CD	1:A:256:GLN:O	0.41	2.69	4	1
1:A:231:ARG:CG	1:A:260:ILE:HB	0.41	2.45	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:LEU:HD12	1:A:286:MET:HE3	0.41	1.91	17	1
1:A:190:ASP:CG	1:A:253:VAL:CB	0.41	2.93	20	1
1:A:213:VAL:CG2	1:A:214:MET:N	0.41	2.82	19	1
1:A:189:TYR:CE1	1:A:288:ALA:C	0.41	2.98	7	1
1:A:242:ASP:O	1:A:246:ILE:CG1	0.41	2.68	10	1
1:A:184:LYS:HG2	1:A:184:LYS:O	0.41	2.16	18	1
1:A:276:MET:CE	1:A:287:LYS:O	0.41	2.68	19	1
1:A:276:MET:HE3	1:A:287:LYS:C	0.41	2.40	3	1
1:A:213:VAL:CG1	1:A:217:LEU:HD13	0.41	2.46	6	1
1:A:253:VAL:C	1:A:255:THR:H	0.41	2.23	20	1
1:A:289:VAL:CG1	1:A:290:LEU:N	0.41	2.83	4	1
1:A:190:ASP:O	1:A:190:ASP:OD1	0.41	2.39	11	1
1:A:253:VAL:HG12	1:A:255:THR:HG22	0.41	1.91	17	1
1:A:191:LEU:CD1	1:A:197:LEU:HD13	0.41	2.46	19	1
1:A:273:HIS:CE1	1:A:274:GLU:HG2	0.41	2.51	5	1
1:A:189:TYR:CE1	1:A:287:LYS:C	0.41	2.99	11	1
1:A:189:TYR:CD2	1:A:287:LYS:HB3	0.41	2.51	18	1
1:A:192:TYR:CD1	1:A:257:GLU:OE2	0.41	2.74	4	1
1:A:195:PRO:CA	1:A:199:ALA:HB3	0.41	2.45	4	1
1:A:217:LEU:CD2	1:A:221:PHE:CE1	0.41	3.04	5	1
1:A:183:SER:O	1:A:184:LYS:CG	0.41	2.69	8	2
1:A:189:TYR:CE2	1:A:287:LYS:CG	0.41	3.03	13	2
1:A:186:LEU:CD2	1:A:288:ALA:HB1	0.41	2.41	18	2
1:A:217:LEU:HD23	1:A:221:PHE:CE1	0.41	2.51	18	1
1:A:189:TYR:CE1	1:A:287:LYS:HB2	0.41	2.50	1	1
1:A:253:VAL:C	1:A:255:THR:N	0.41	2.79	2	2
1:A:276:MET:HE2	1:A:287:LYS:O	0.41	2.16	2	1
1:A:234:LYS:HE2	1:A:234:LYS:N	0.41	2.31	11	1
1:A:188:VAL:CG2	1:A:191:LEU:HD11	0.41	2.45	12	1
1:A:190:ASP:OD2	1:A:253:VAL:CG1	0.41	2.69	14	1
1:A:189:TYR:CZ	1:A:289:VAL:CG1	0.41	3.04	2	1
1:A:227:ILE:HG21	1:A:261:VAL:HG12	0.41	1.93	13	1
1:A:232:ILE:HA	1:A:259:ALA:HA	0.40	1.93	12	1
1:A:192:TYR:CG	1:A:257:GLU:OE2	0.40	2.74	20	1
1:A:227:ILE:CG2	1:A:230:VAL:HG22	0.40	2.40	5	1
1:A:192:TYR:CD1	1:A:257:GLU:HG3	0.40	2.52	11	1
1:A:218:LEU:O	1:A:222:GLY:N	0.40	2.54	15	1
1:A:190:ASP:HB3	1:A:253:VAL:CG1	0.40	2.46	17	1
1:A:190:ASP:OD1	1:A:253:VAL:CG2	0.40	2.67	20	1
1:A:190:ASP:CB	1:A:253:VAL:CG1	0.40	3.00	2	1
1:A:253:VAL:O	1:A:284:GLU:HB2	0.40	2.17	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:188:VAL:HG13	1:A:259:ALA:HB3	0.40	1.92	10	1
1:A:212:LYS:O	1:A:216:HIS:CD2	0.40	2.74	3	1
1:A:220:LEU:HD11	1:A:275:PHE:CE1	0.40	2.52	17	1
1:A:194:SER:CB	1:A:285:ASN:OD1	0.40	2.70	3	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	101/119 (85%)	88±2 (87±2%)	9±2 (9±2%)	4±1 (4±1%)	3	28
All	All	2020/2380 (85%)	1755 (87%)	179 (9%)	86 (4%)	3	28

All 10 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	208	ARG	20
1	A	252	GLN	19
1	A	184	LYS	15
1	A	254	GLY	9
1	A	190	ASP	8
1	A	286	MET	7
1	A	235	PRO	3
1	A	238	GLU	2
1	A	253	VAL	2
1	A	251	SER	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	90/104 (87%)	58±3 (65±3%)	32±3 (35±3%)	1	10
All	All	1800/2080 (87%)	1166 (65%)	634 (35%)	1	10

All 77 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	243	ILE	20
1	A	191	LEU	18
1	A	227	ILE	18
1	A	234	LYS	17
1	A	220	LEU	16
1	A	233	LEU	15
1	A	264	GLU	15
1	A	211	GLU	14
1	A	271	LYS	14
1	A	252	GLN	13
1	A	253	VAL	13
1	A	274	GLU	13
1	A	279	GLU	13
1	A	187	LEU	13
1	A	214	MET	13
1	A	283	LYS	13
1	A	196	LYS	12
1	A	257	GLU	12
1	A	212	LYS	12
1	A	208	ARG	11
1	A	184	LYS	11
1	A	249	ARG	11
1	A	256	GLN	11
1	A	291	ILE	10
1	A	218	LEU	10
1	A	262	GLU	10
1	A	285	ASN	10
1	A	188	VAL	9
1	A	193	LEU	9
1	A	267	GLU	9
1	A	276	MET	9
1	A	260	ILE	9
1	A	290	LEU	9
1	A	217	LEU	9
1	A	228	SER	8
1	A	183	SER	8

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Mol	Chain	Res	Type	Models (Total)
1	A	255	THR	8
1	A	185	MET	8
1	A	192	TYR	7
1	A	215	GLU	7
1	A	231	ARG	7
1	A	251	SER	7
1	A	281	GLN	7
1	A	248	SER	7
1	A	265	GLU	7
1	A	197	LEU	7
1	A	286	MET	7
1	A	189	TYR	6
1	A	216	HIS	6
1	A	244	ARG	6
1	A	245	ARG	6
1	A	287	LYS	6
1	A	237	ARG	6
1	A	247	SER	6
1	A	194	SER	5
1	A	210	GLN	5
1	A	219	LYS	5
1	A	277	ILE	5
1	A	250	TYR	5
1	A	284	GLU	5
1	A	223	THR	5
1	A	198	TRP	5
1	A	232	ILE	4
1	A	186	LEU	4
1	A	246	ILE	4
1	A	229	SER	3
1	A	242	ASP	3
1	A	238	GLU	3
1	A	263	PHE	2
1	A	261	VAL	2
1	A	258	CYS	2
1	A	275	PHE	2
1	A	230	VAL	2
1	A	190	ASP	2
1	A	270	ILE	1
1	A	289	VAL	1
1	A	280	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: working_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	1254
Number of shifts mapped to atoms	1254
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	112	-0.05 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	104	0.33 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	99	0.22 ± 0.13	None needed (< 0.5 ppm)
^{15}N	103	1.02 ± 0.21	Should be applied

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 81%, i.e. 1176 atoms were assigned a chemical shift out of a possible 1453. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	486/502 (97%)	197/203 (97%)	193/202 (96%)	96/97 (99%)
Sidechain	618/856 (72%)	418/560 (75%)	200/265 (75%)	0/31 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	72/95 (76%)	36/46 (78%)	35/44 (80%)	1/5 (20%)
Overall	1176/1453 (81%)	651/809 (80%)	428/511 (84%)	97/133 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1254 atoms were assigned a chemical shift out of a possible 1647. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	527/573 (92%)	213/232 (92%)	211/232 (91%)	103/109 (94%)
Sidechain	655/979 (67%)	440/640 (69%)	215/303 (71%)	0/36 (0%)
Aromatic	72/95 (76%)	36/46 (78%)	35/44 (80%)	1/5 (20%)
Overall	1254/1647 (76%)	689/918 (75%)	461/579 (80%)	104/150 (69%)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	287	LYS	HB3	-0.15	0.46 – 3.04	-7.4
1	A	252	GLN	CG	28.18	28.36 – 39.21	-5.2
1	A	227	ILE	C	166.40	166.59 – 185.34	-5.1
1	A	231	ARG	CG	33.20	21.24 – 33.19	5.0

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

