



Full wwPDB NMR Structure Validation Report ⓘ

Mar 20, 2026 – 05:04 AM UTC

PDB ID : 2KFU / pdb_00002kfu
BMRB ID : 16248
Title : PknB-phosphorylated Rv1827
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Deposited on : 2009-02-27

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
Mogul : 2022.3.0, CSD as543be (2022)
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

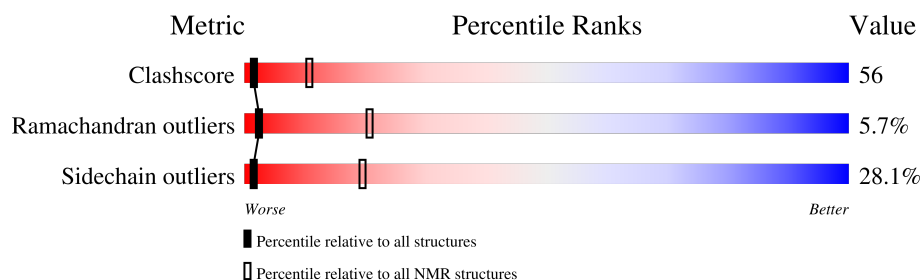
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	162	16% 29% 13% 42%

2 Ensemble composition and analysis

This entry contains 19 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:23-A:26, A:55-A:82, A:86-A:147 (94)	0.46	17

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2206 atoms, of which 989 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Rv1827 pThr 22.

Mol	Chain	Residues	Atoms								Trace
1	A	162	Total	C	H	N	O	P	S		0
			2206	745	989	210	260	1	1		

There is a discrepancy between the modelled and reference sequences:

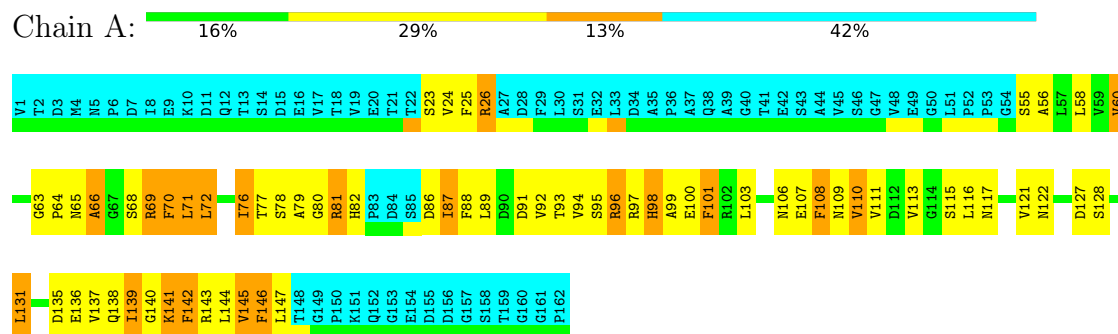
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	MET	engineered mutation	UNP P64897

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: Rv1827 pThr 22

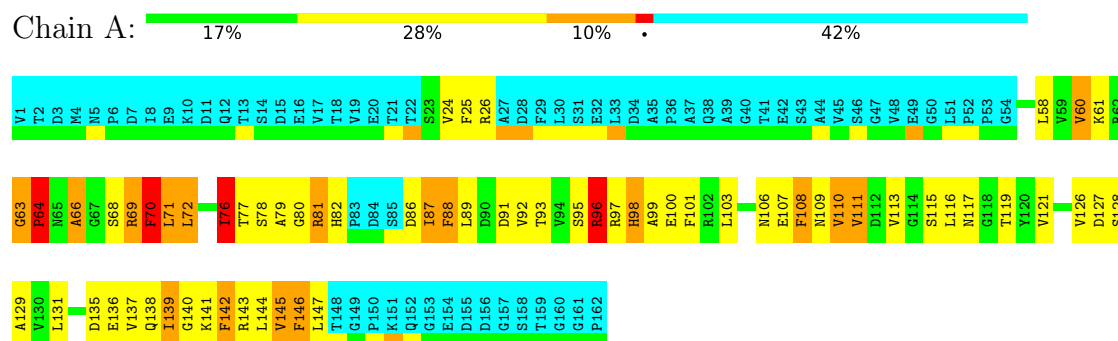


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

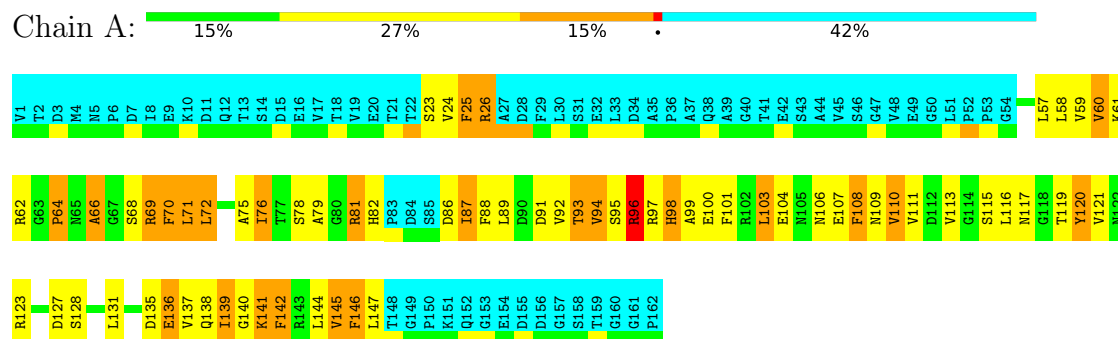
4.2.1 Score per residue for model 1

- Molecule 1: Rv1827 pThr 22



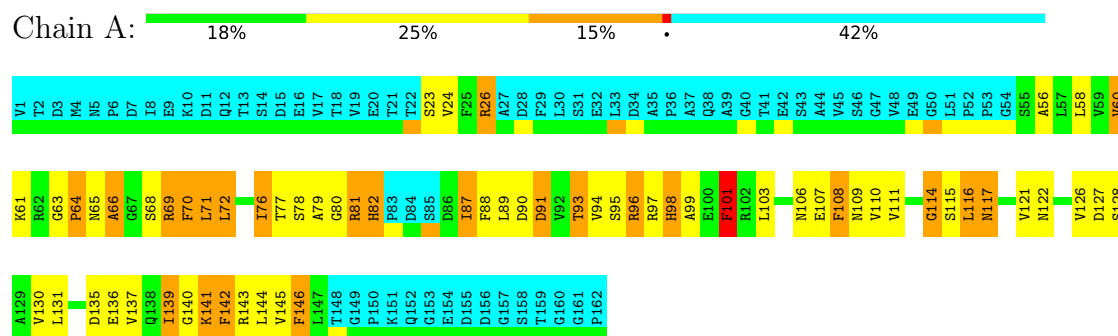
4.2.2 Score per residue for model 2

- Molecule 1: Rv1827 pThr 22



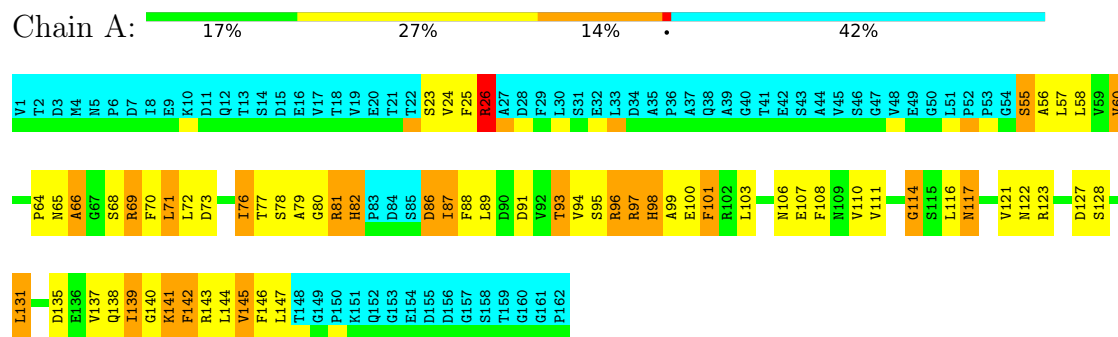
4.2.3 Score per residue for model 3

- Molecule 1: Rv1827 pThr 22



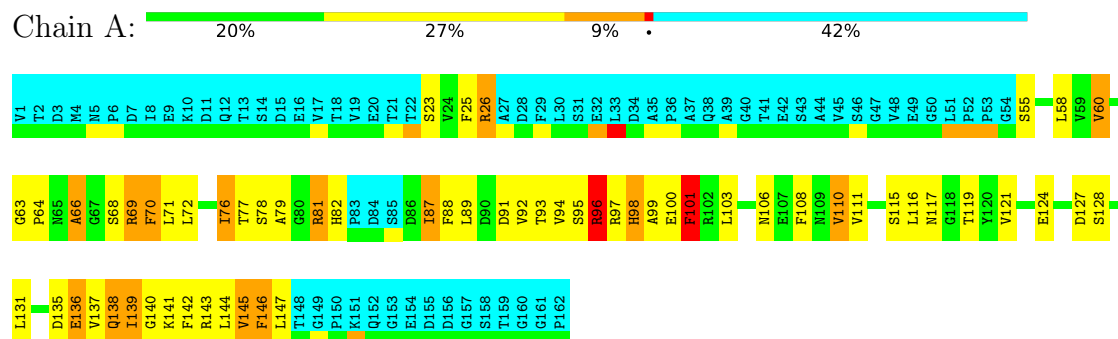
4.2.4 Score per residue for model 4

- Molecule 1: Rv1827 pThr 22



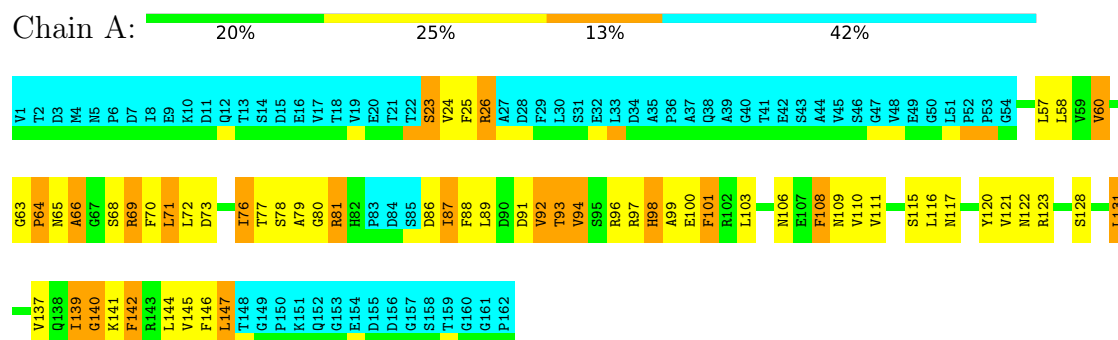
4.2.5 Score per residue for model 5

- Molecule 1: Rv1827 pThr 22



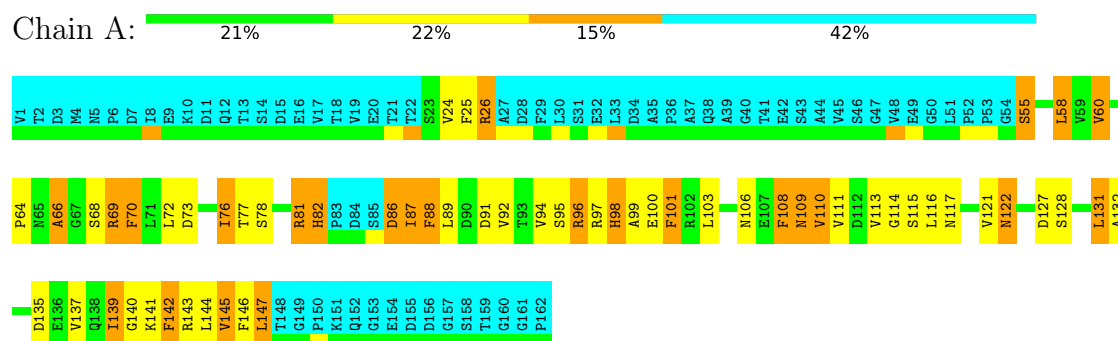
4.2.6 Score per residue for model 6

- Molecule 1: Rv1827 pThr 22



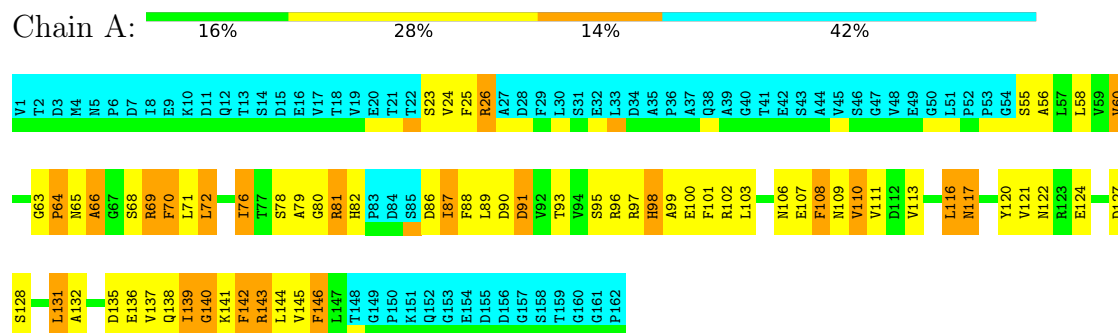
4.2.7 Score per residue for model 7

- Molecule 1: Rv1827 pThr 22



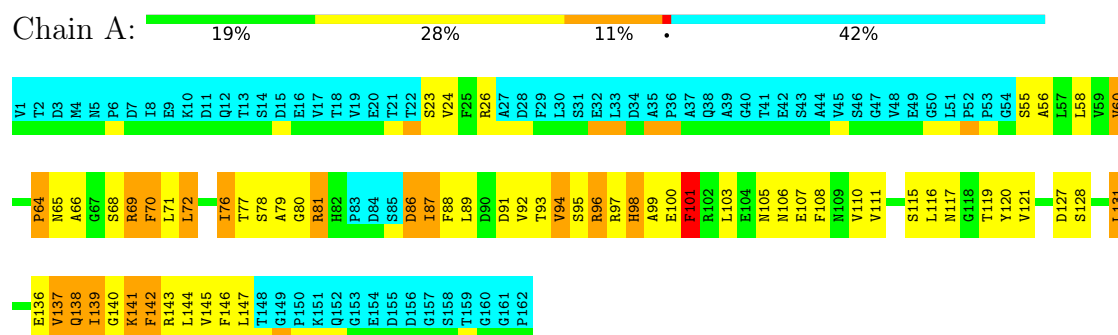
4.2.8 Score per residue for model 8

- Molecule 1: Rv1827 pThr 22



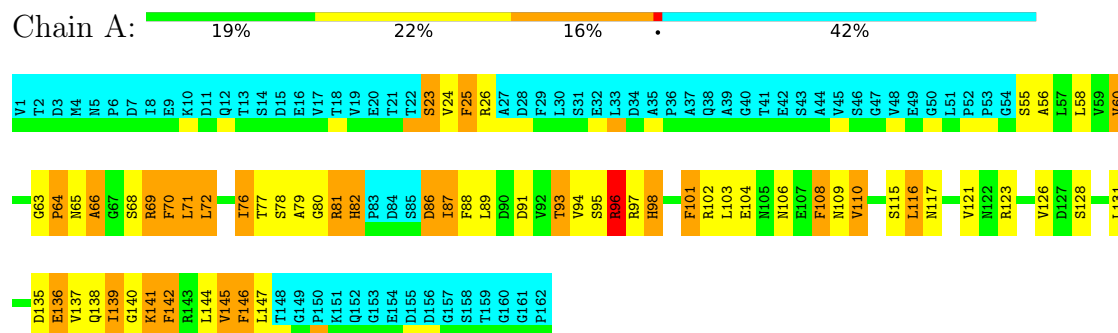
4.2.9 Score per residue for model 9

- Molecule 1: Rv1827 pThr 22



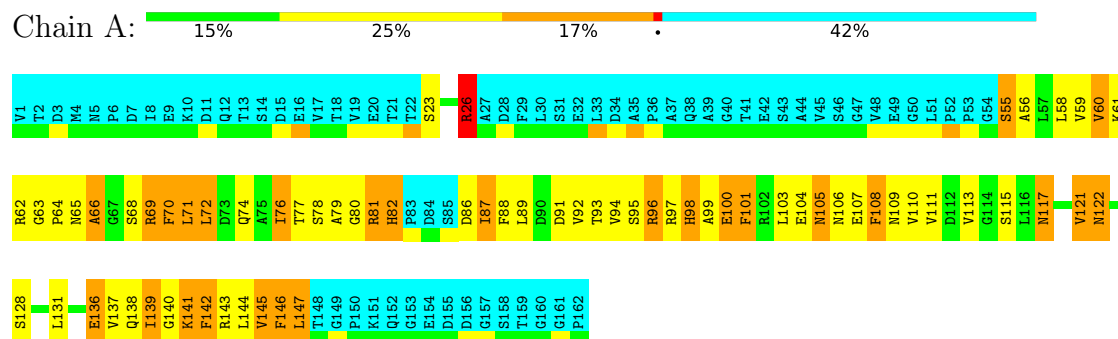
4.2.10 Score per residue for model 10

- Molecule 1: Rv1827 pThr 22



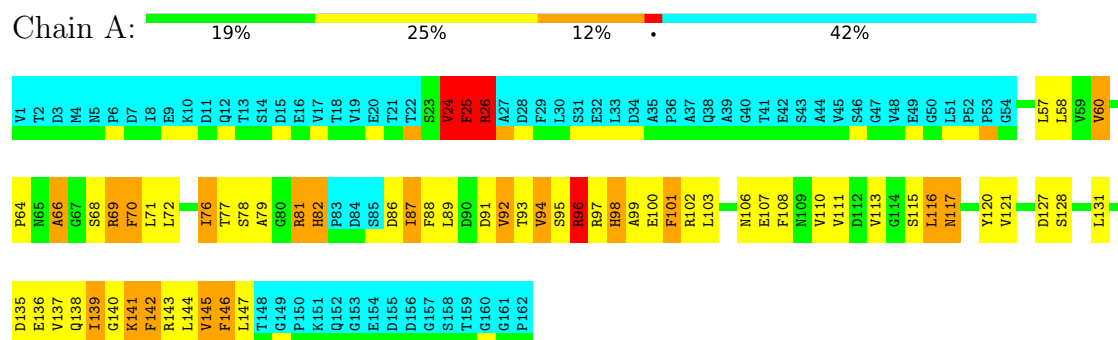
4.2.11 Score per residue for model 11

- Molecule 1: Rv1827 pThr 22



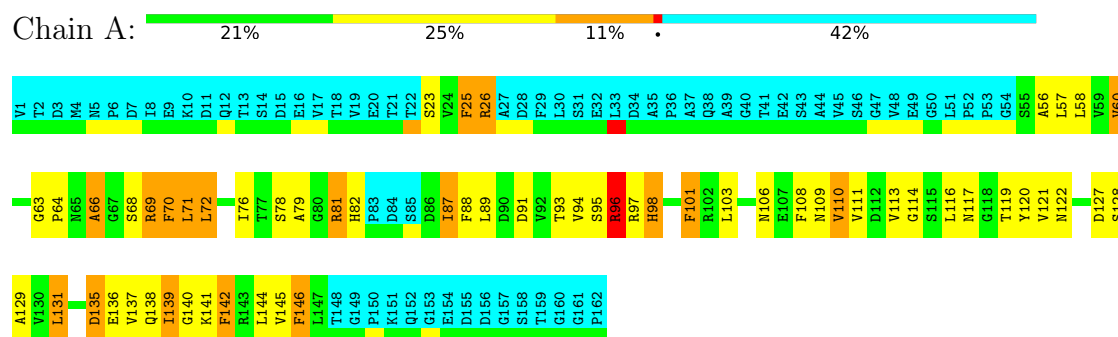
4.2.12 Score per residue for model 12

- Molecule 1: Rv1827 pThr 22



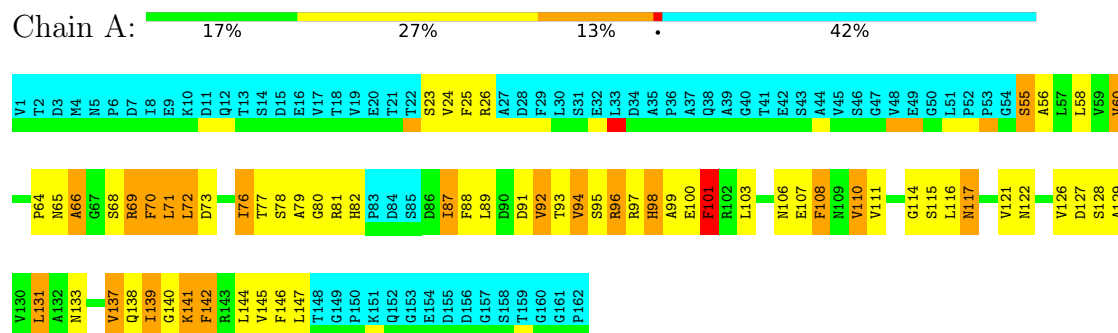
4.2.13 Score per residue for model 13

- Molecule 1: Rv1827 pThr 22



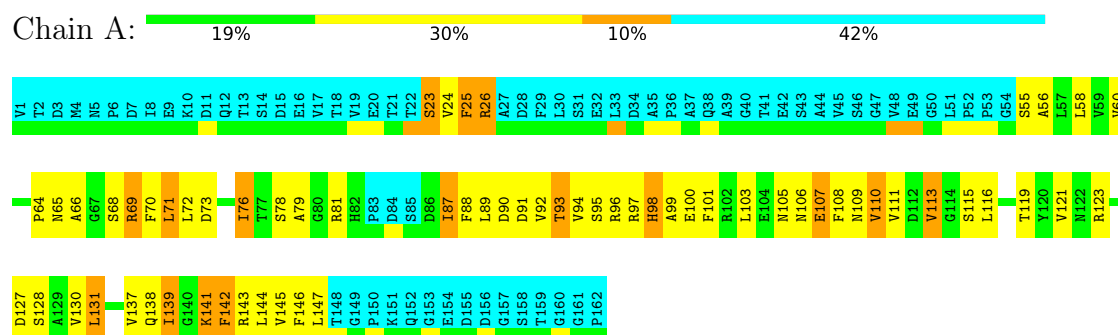
4.2.14 Score per residue for model 14

- Molecule 1: Rv1827 pThr 22



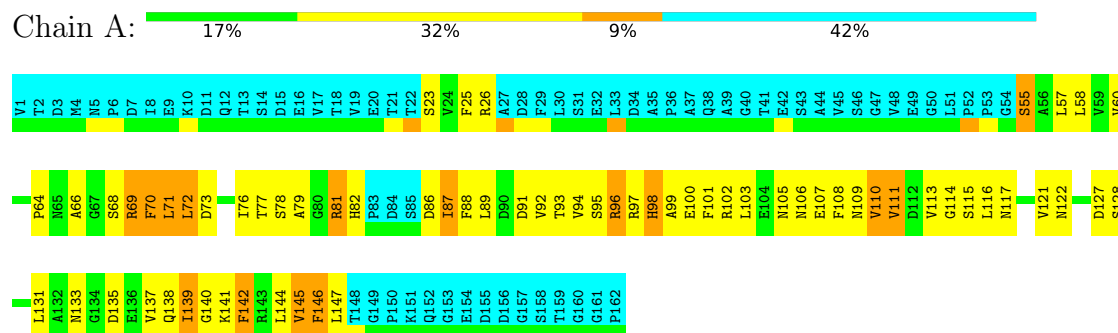
4.2.15 Score per residue for model 15

- Molecule 1: Rv1827 pThr 22



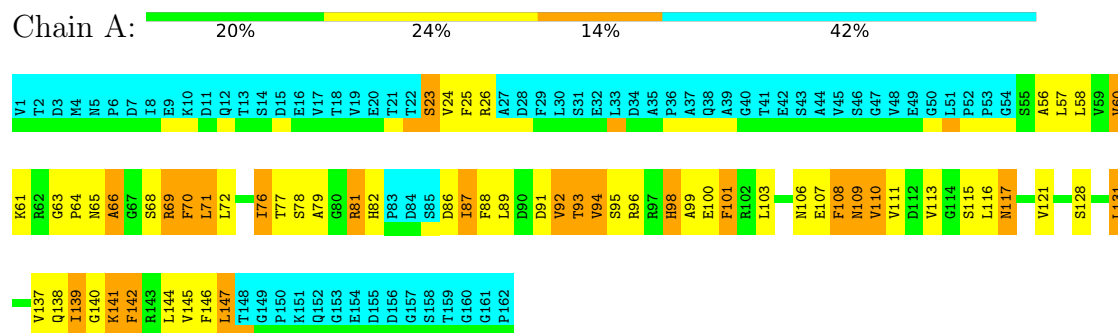
4.2.16 Score per residue for model 16

- Molecule 1: Rv1827 pThr 22



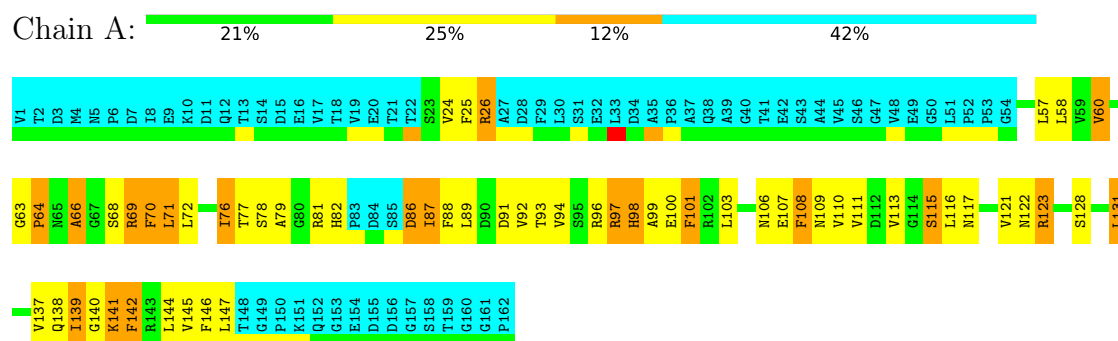
4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Rv1827 pThr 22



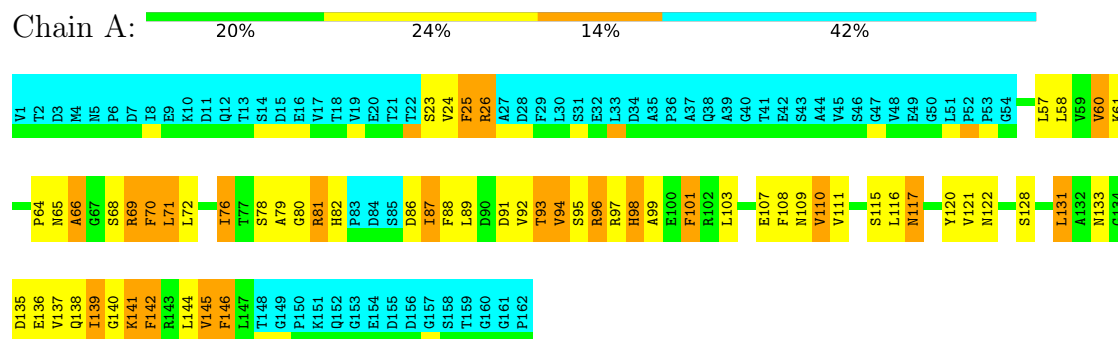
4.2.18 Score per residue for model 18

- Molecule 1: Rv1827 pThr 22



4.2.19 Score per residue for model 19

- Molecule 1: Rv1827 pThr 22



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 19 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
ARIA 1.2	structure solution	
ARIA 1.2	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	1833
Number of shifts mapped to atoms	1676
Number of unparsed shifts	0
Number of shifts with mapping errors	157
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	0.64±0.02	0±0/748 (0.0± 0.0%)	0.86±0.03	0±1/1014 (0.0± 0.1%)
All	All	0.64	0/14212 (0.0%)	0.86	3/19266 (0.0%)

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	63	GLY	CA-C-N	5.63	126.88	119.84	1	1
1	A	63	GLY	C-N-CA	5.63	126.88	119.84	1	1
1	A	70	PHE	CA-CB-CG	5.05	118.86	113.80	1	1

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	736	634	731	82±8
All	All	13984	12046	13889	1555

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 56.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LEU:HG	1:A:139:ILE:HD11	1.08	1.25	19	10
1:A:58:LEU:HG	1:A:146:PHE:HB3	1.06	1.28	13	10
1:A:64:PRO:HG2	1:A:141:LYS:HG3	1.05	1.24	11	16
1:A:64:PRO:HG3	1:A:141:LYS:HG3	1.02	1.31	9	2
1:A:98:HIS:HB2	1:A:115:SER:HB2	0.95	1.39	17	13
1:A:121:VAL:HG22	1:A:137:VAL:HG23	0.91	1.43	9	2
1:A:96:ARG:HG2	1:A:97:ARG:HD2	0.90	1.38	11	1
1:A:60:VAL:HG11	1:A:89:LEU:HD21	0.89	1.44	10	5
1:A:121:VAL:HG22	1:A:137:VAL:HG13	0.89	1.40	13	14
1:A:101:PHE:HD1	1:A:110:VAL:HG13	0.86	1.30	8	2
1:A:121:VAL:HG12	1:A:137:VAL:HG13	0.84	1.48	11	1
1:A:60:VAL:HG11	1:A:89:LEU:HD11	0.81	1.51	5	7
1:A:99:ALA:HA	1:A:111:VAL:O	0.81	1.76	9	14
1:A:60:VAL:HG12	1:A:144:LEU:HG	0.80	1.53	9	14
1:A:81:ARG:HD2	1:A:96:ARG:HA	0.80	1.51	16	8
1:A:137:VAL:HG12	1:A:144:LEU:HB2	0.79	1.51	9	2
1:A:26:ARG:HB3	1:A:141:LYS:HB2	0.78	1.53	12	11
1:A:89:LEU:HD11	1:A:144:LEU:HD21	0.78	1.53	1	1
1:A:110:VAL:O	1:A:128:SER:HA	0.78	1.78	12	19
1:A:101:PHE:CD1	1:A:110:VAL:HG13	0.78	2.13	8	3
1:A:60:VAL:HG22	1:A:68:SER:H	0.76	1.39	19	17
1:A:108:PHE:HB2	1:A:131:LEU:HD13	0.76	1.57	11	3
1:A:101:PHE:CZ	1:A:110:VAL:HB	0.76	2.15	15	1
1:A:58:LEU:HD21	1:A:131:LEU:HD11	0.76	1.57	15	2
1:A:24:VAL:HA	1:A:117:ASN:OD1	0.75	1.80	6	2
1:A:98:HIS:CG	1:A:139:ILE:HB	0.75	2.17	5	18
1:A:72:LEU:HG	1:A:101:PHE:CD1	0.75	2.16	3	5
1:A:89:LEU:HG	1:A:139:ILE:CD1	0.73	2.14	6	6
1:A:101:PHE:HA	1:A:109:ASN:O	0.72	1.84	13	6
1:A:60:VAL:HA	1:A:144:LEU:HA	0.72	1.61	11	17
1:A:72:LEU:HD11	1:A:101:PHE:HB3	0.72	1.62	8	1
1:A:65:ASN:HB3	1:A:142:PHE:HE2	0.72	1.44	9	1
1:A:60:VAL:HG22	1:A:144:LEU:HG	0.71	1.61	16	2
1:A:78:SER:HB2	1:A:82:HIS:NE2	0.71	2.00	7	5
1:A:103:LEU:HD21	1:A:106:ASN:HA	0.70	1.61	5	17
1:A:103:LEU:HD11	1:A:106:ASN:HA	0.70	1.63	2	1
1:A:80:GLY:HA2	1:A:89:LEU:HD23	0.70	1.63	3	5
1:A:98:HIS:CD2	1:A:139:ILE:HB	0.70	2.22	7	7
1:A:58:LEU:HB2	1:A:70:PHE:HD1	0.70	1.47	15	1
1:A:137:VAL:CG1	1:A:144:LEU:HD13	0.69	2.17	9	2
1:A:72:LEU:HG	1:A:101:PHE:CG	0.69	2.23	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:ASP:HB2	1:A:146:PHE:HE1	0.69	1.47	5	4
1:A:72:LEU:HD22	1:A:101:PHE:CG	0.69	2.22	19	7
1:A:81:ARG:HA	1:A:91:ASP:HA	0.69	1.63	4	17
1:A:76:ILE:HA	1:A:101:PHE:O	0.69	1.88	14	14
1:A:24:VAL:HG12	1:A:25:PHE:H	0.69	1.48	12	1
1:A:82:HIS:CE1	1:A:96:ARG:HD3	0.68	2.23	8	1
1:A:58:LEU:HB2	1:A:70:PHE:CD1	0.68	2.23	15	3
1:A:94:VAL:HG23	1:A:115:SER:HA	0.68	1.66	14	2
1:A:120:TYR:HB2	1:A:138:GLN:HB3	0.68	1.66	8	3
1:A:117:ASN:HB3	1:A:140:GLY:O	0.67	1.90	11	9
1:A:60:VAL:HG12	1:A:144:LEU:CG	0.67	2.19	9	14
1:A:96:ARG:HG3	1:A:97:ARG:HG2	0.67	1.66	7	1
1:A:98:HIS:HB2	1:A:115:SER:HB3	0.67	1.66	1	1
1:A:58:LEU:HD11	1:A:101:PHE:CZ	0.67	2.25	2	5
1:A:80:GLY:HA3	1:A:97:ARG:HA	0.66	1.68	11	4
1:A:89:LEU:HD12	1:A:142:PHE:CD2	0.66	2.25	16	6
1:A:77:THR:HB	1:A:86:ASP:HB2	0.65	1.67	6	2
1:A:23:SER:O	1:A:93:THR:HA	0.65	1.92	11	8
1:A:96:ARG:HG2	1:A:97:ARG:HG2	0.65	1.67	12	2
1:A:69:ARG:O	1:A:87:ILE:HB	0.65	1.91	17	13
1:A:78:SER:HB2	1:A:82:HIS:CE1	0.65	2.27	10	3
1:A:58:LEU:HD11	1:A:131:LEU:HD11	0.65	1.67	12	2
1:A:131:LEU:HB3	1:A:146:PHE:CD2	0.65	2.26	9	8
1:A:142:PHE:CD1	1:A:142:PHE:N	0.64	2.65	11	19
1:A:89:LEU:HB3	1:A:142:PHE:CZ	0.64	2.26	8	14
1:A:23:SER:HB2	1:A:92:VAL:O	0.64	1.92	6	4
1:A:96:ARG:NE	1:A:97:ARG:HB3	0.64	2.08	19	1
1:A:64:PRO:CG	1:A:141:LYS:HG3	0.64	2.23	15	6
1:A:72:LEU:HD23	1:A:101:PHE:CD1	0.64	2.27	12	1
1:A:58:LEU:HG	1:A:146:PHE:HB2	0.64	1.69	15	2
1:A:79:ALA:HA	1:A:87:ILE:HG23	0.63	1.68	9	17
1:A:120:TYR:HB3	1:A:123:ARG:HA	0.63	1.70	6	1
1:A:111:VAL:HG12	1:A:113:VAL:HG13	0.63	1.70	17	4
1:A:60:VAL:HG12	1:A:144:LEU:HD23	0.63	1.69	1	2
1:A:111:VAL:HA	1:A:127:ASP:O	0.63	1.94	13	13
1:A:72:LEU:HD12	1:A:131:LEU:HD12	0.63	1.71	19	1
1:A:24:VAL:HG21	1:A:117:ASN:HB2	0.63	1.69	2	1
1:A:81:ARG:HB2	1:A:91:ASP:O	0.63	1.93	8	2
1:A:136:GLU:HB2	1:A:144:LEU:O	0.63	1.94	19	3
1:A:82:HIS:CE1	1:A:96:ARG:HG3	0.62	2.29	5	1
1:A:117:ASN:HB2	1:A:140:GLY:O	0.62	1.94	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:HG	1:A:146:PHE:HB3	0.62	1.71	11	1
1:A:101:PHE:HE1	1:A:110:VAL:HG22	0.62	1.55	13	3
1:A:81:ARG:H	1:A:94:VAL:HB	0.62	1.53	13	6
1:A:139:ILE:HG23	1:A:144:LEU:HD13	0.62	1.70	1	7
1:A:70:PHE:HD2	1:A:101:PHE:HB2	0.62	1.55	8	1
1:A:96:ARG:HD3	1:A:97:ARG:HD2	0.62	1.71	13	3
1:A:64:PRO:HD2	1:A:142:PHE:CD2	0.61	2.30	15	13
1:A:69:ARG:O	1:A:69:ARG:HD2	0.61	1.95	16	3
1:A:24:VAL:CG2	1:A:117:ASN:HB2	0.61	2.26	2	1
1:A:89:LEU:HD12	1:A:139:ILE:HG12	0.61	1.72	9	5
1:A:121:VAL:HG23	1:A:137:VAL:HG22	0.61	1.73	1	2
1:A:60:VAL:HG12	1:A:144:LEU:CD2	0.61	2.26	2	15
1:A:81:ARG:HB3	1:A:94:VAL:O	0.61	1.95	9	8
1:A:135:ASP:HB3	1:A:146:PHE:CE1	0.61	2.30	12	6
1:A:78:SER:O	1:A:87:ILE:HG23	0.61	1.96	16	18
1:A:93:THR:HB	1:A:141:LYS:HD3	0.61	1.73	4	1
1:A:131:LEU:CD2	1:A:146:PHE:HB2	0.60	2.26	8	7
1:A:101:PHE:CE1	1:A:110:VAL:HG22	0.60	2.30	13	3
1:A:135:ASP:HB2	1:A:146:PHE:CE1	0.60	2.31	10	4
1:A:58:LEU:O	1:A:69:ARG:HA	0.60	1.96	18	14
1:A:72:LEU:HB3	1:A:108:PHE:CD2	0.60	2.31	2	2
1:A:57:LEU:HA	1:A:72:LEU:HG	0.60	1.71	17	5
1:A:26:ARG:CB	1:A:141:LYS:HB2	0.60	2.26	7	4
1:A:103:LEU:HD12	1:A:108:PHE:CE2	0.60	2.31	16	2
1:A:136:GLU:HB3	1:A:145:VAL:HB	0.60	1.74	1	1
1:A:141:LYS:H	1:A:142:PHE:HD1	0.60	1.40	11	7
1:A:65:ASN:HB2	1:A:142:PHE:HE2	0.60	1.57	19	7
1:A:117:ASN:ND2	1:A:117:ASN:H	0.60	1.95	9	1
1:A:135:ASP:HB3	1:A:146:PHE:HE1	0.60	1.55	16	3
1:A:60:VAL:HG22	1:A:144:LEU:CG	0.59	2.27	16	2
1:A:76:ILE:HD11	1:A:100:GLU:HB2	0.59	1.74	4	13
1:A:87:ILE:HD11	1:A:89:LEU:HD21	0.59	1.74	7	7
1:A:65:ASN:HB2	1:A:90:ASP:HB2	0.59	1.73	3	3
1:A:26:ARG:HH22	1:A:143:ARG:HB2	0.59	1.56	7	1
1:A:79:ALA:HB3	1:A:99:ALA:O	0.59	1.98	15	4
1:A:98:HIS:CB	1:A:139:ILE:HB	0.59	2.26	3	11
1:A:80:GLY:CA	1:A:89:LEU:HD23	0.59	2.28	3	4
1:A:76:ILE:HD13	1:A:102:ARG:HB3	0.59	1.73	16	1
1:A:121:VAL:HG12	1:A:122:ASN:HD22	0.59	1.57	4	2
1:A:64:PRO:HG3	1:A:141:LYS:CG	0.59	2.18	9	1
1:A:99:ALA:CB	1:A:110:VAL:HG23	0.58	2.28	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:GLU:HG3	1:A:109:ASN:HD21	0.58	1.58	2	3
1:A:77:THR:OG1	1:A:101:PHE:HB3	0.58	1.98	6	11
1:A:64:PRO:HD3	1:A:141:LYS:O	0.58	1.98	8	5
1:A:58:LEU:HD21	1:A:101:PHE:CE1	0.58	2.33	1	5
1:A:111:VAL:HG22	1:A:128:SER:HB3	0.58	1.75	4	4
1:A:131:LEU:HG	1:A:146:PHE:CD1	0.58	2.33	15	8
1:A:26:ARG:HG2	1:A:26:ARG:HH11	0.58	1.57	4	1
1:A:58:LEU:HD12	1:A:72:LEU:HD11	0.58	1.74	5	6
1:A:60:VAL:HB	1:A:144:LEU:HG	0.58	1.74	13	2
1:A:97:ARG:HG3	1:A:113:VAL:HG21	0.58	1.75	16	4
1:A:101:PHE:CE1	1:A:110:VAL:HB	0.58	2.34	15	1
1:A:58:LEU:HG	1:A:146:PHE:CB	0.58	2.23	19	2
1:A:64:PRO:HG2	1:A:141:LYS:CG	0.58	2.17	11	5
1:A:60:VAL:HG21	1:A:68:SER:HB2	0.58	1.75	16	2
1:A:81:ARG:O	1:A:81:ARG:HD2	0.58	1.98	6	6
1:A:98:HIS:HB2	1:A:115:SER:OG	0.58	1.98	18	1
1:A:64:PRO:CG	1:A:141:LYS:HE2	0.58	2.29	4	8
1:A:71:LEU:O	1:A:77:THR:HG21	0.58	1.98	16	4
1:A:24:VAL:HB	1:A:116:LEU:HD23	0.58	1.75	18	5
1:A:70:PHE:HA	1:A:87:ILE:HB	0.57	1.75	19	6
1:A:63:GLY:H	1:A:66:ALA:HB2	0.57	1.59	10	8
1:A:71:LEU:HD23	1:A:71:LEU:O	0.57	1.99	13	9
1:A:58:LEU:HD11	1:A:101:PHE:CE2	0.57	2.35	13	4
1:A:72:LEU:CD1	1:A:101:PHE:HB3	0.57	2.30	13	4
1:A:60:VAL:CG2	1:A:66:ALA:HA	0.56	2.30	1	13
1:A:68:SER:HB2	1:A:89:LEU:HD21	0.56	1.77	1	3
1:A:70:PHE:CZ	1:A:144:LEU:HD22	0.56	2.35	15	1
1:A:121:VAL:HG13	1:A:137:VAL:HG22	0.56	1.77	13	5
1:A:64:PRO:HG2	1:A:141:LYS:HE2	0.56	1.78	5	3
1:A:146:PHE:O	1:A:147:LEU:HD13	0.56	2.00	18	5
1:A:25:PHE:O	1:A:141:LYS:HB2	0.56	2.00	2	1
1:A:26:ARG:HG2	1:A:64:PRO:CD	0.56	2.31	1	1
1:A:81:ARG:O	1:A:96:ARG:HA	0.56	2.01	1	4
1:A:70:PHE:HE1	1:A:144:LEU:CD2	0.56	2.14	1	3
1:A:101:PHE:CZ	1:A:103:LEU:HB2	0.56	2.36	11	5
1:A:72:LEU:HA	1:A:101:PHE:CD2	0.56	2.35	12	3
1:A:117:ASN:ND2	1:A:138:GLN:HE22	0.55	1.99	14	2
1:A:56:ALA:HB1	1:A:146:PHE:CE1	0.55	2.36	17	2
1:A:60:VAL:HG23	1:A:66:ALA:HA	0.55	1.77	8	15
1:A:96:ARG:CD	1:A:97:ARG:HD2	0.55	2.30	13	1
1:A:71:LEU:O	1:A:71:LEU:HD13	0.55	2.02	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LEU:CD1	1:A:72:LEU:HD21	0.55	2.31	2	6
1:A:72:LEU:HA	1:A:101:PHE:CE2	0.55	2.37	14	10
1:A:101:PHE:CE1	1:A:108:PHE:HB3	0.55	2.36	19	9
1:A:117:ASN:HD21	1:A:140:GLY:HA2	0.55	1.61	9	1
1:A:89:LEU:CD2	1:A:139:ILE:HD11	0.55	2.31	14	1
1:A:60:VAL:HG21	1:A:89:LEU:HD11	0.55	1.79	16	2
1:A:60:VAL:CG2	1:A:68:SER:HB2	0.55	2.31	15	2
1:A:24:VAL:O	1:A:25:PHE:HB2	0.55	2.02	6	6
1:A:60:VAL:CG1	1:A:144:LEU:HG	0.55	2.30	11	12
1:A:121:VAL:HG12	1:A:122:ASN:ND2	0.55	2.17	14	3
1:A:108:PHE:C	1:A:109:ASN:HD22	0.55	2.09	13	3
1:A:56:ALA:O	1:A:72:LEU:HB2	0.54	2.03	14	6
1:A:122:ASN:HD22	1:A:122:ASN:N	0.54	1.99	7	2
1:A:72:LEU:HD23	1:A:108:PHE:CB	0.54	2.32	10	4
1:A:96:ARG:HE	1:A:97:ARG:N	0.54	2.00	19	2
1:A:70:PHE:CD1	1:A:70:PHE:N	0.54	2.75	13	13
1:A:89:LEU:CG	1:A:139:ILE:HD11	0.54	2.22	3	4
1:A:72:LEU:CD1	1:A:131:LEU:HD12	0.54	2.33	19	1
1:A:63:GLY:HA3	1:A:142:PHE:HA	0.54	1.78	1	1
1:A:89:LEU:HD13	1:A:142:PHE:CG	0.54	2.37	1	5
1:A:93:THR:HG21	1:A:141:LYS:HE2	0.54	1.80	10	3
1:A:69:ARG:N	1:A:69:ARG:HD3	0.54	2.17	13	11
1:A:70:PHE:HE1	1:A:144:LEU:HD22	0.54	1.63	1	1
1:A:89:LEU:HD12	1:A:139:ILE:CG1	0.54	2.32	10	5
1:A:89:LEU:C	1:A:91:ASP:H	0.54	2.11	6	18
1:A:103:LEU:HA	1:A:107:GLU:O	0.54	2.03	12	10
1:A:68:SER:HB3	1:A:89:LEU:CD2	0.54	2.33	10	1
1:A:57:LEU:HA	1:A:72:LEU:HD13	0.54	1.79	12	1
1:A:24:VAL:HB	1:A:116:LEU:HD12	0.54	1.80	3	3
1:A:60:VAL:HG22	1:A:144:LEU:CD2	0.53	2.32	15	2
1:A:58:LEU:HD12	1:A:72:LEU:HD21	0.53	1.79	2	4
1:A:58:LEU:HD11	1:A:131:LEU:HD21	0.53	1.80	7	4
1:A:146:PHE:O	1:A:147:LEU:HD22	0.53	2.03	15	4
1:A:26:ARG:HD2	1:A:26:ARG:O	0.53	2.03	1	1
1:A:99:ALA:HB2	1:A:110:VAL:HG23	0.53	1.81	16	3
1:A:103:LEU:HD13	1:A:108:PHE:CD1	0.53	2.38	19	1
1:A:24:VAL:HG22	1:A:116:LEU:HD11	0.53	1.80	12	2
1:A:139:ILE:O	1:A:142:PHE:HD1	0.53	1.85	1	14
1:A:65:ASN:HB3	1:A:142:PHE:CE2	0.53	2.34	9	1
1:A:82:HIS:CE1	1:A:97:ARG:HB3	0.53	2.38	2	1
1:A:89:LEU:HD12	1:A:142:PHE:CG	0.53	2.38	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:LEU:HG	1:A:101:PHE:CD2	0.53	2.39	16	3
1:A:101:PHE:HE1	1:A:108:PHE:HA	0.53	1.63	11	1
1:A:136:GLU:HG2	1:A:143:ARG:NH1	0.53	2.18	11	1
1:A:97:ARG:HD3	1:A:100:GLU:HB3	0.53	1.79	2	2
1:A:60:VAL:CG1	1:A:68:SER:HB2	0.53	2.34	2	5
1:A:77:THR:CG2	1:A:86:ASP:HB3	0.52	2.35	11	3
1:A:77:THR:O	1:A:100:GLU:HA	0.52	2.04	7	5
1:A:70:PHE:HB2	1:A:72:LEU:HD11	0.52	1.81	12	1
1:A:103:LEU:HD12	1:A:108:PHE:CE1	0.52	2.40	15	1
1:A:60:VAL:CB	1:A:144:LEU:HG	0.52	2.35	5	11
1:A:117:ASN:HD22	1:A:140:GLY:N	0.52	2.03	11	1
1:A:81:ARG:HG2	1:A:91:ASP:OD1	0.52	2.05	1	3
1:A:101:PHE:HE2	1:A:131:LEU:HB2	0.52	1.65	1	1
1:A:81:ARG:HD2	1:A:96:ARG:CA	0.52	2.33	13	3
1:A:101:PHE:HE2	1:A:108:PHE:HB2	0.52	1.65	8	1
1:A:121:VAL:HB	1:A:137:VAL:HG13	0.52	1.82	17	1
1:A:139:ILE:HD13	1:A:144:LEU:HD11	0.51	1.81	3	1
1:A:58:LEU:HA	1:A:146:PHE:HA	0.51	1.82	2	10
1:A:89:LEU:HD12	1:A:139:ILE:CD1	0.51	2.35	17	1
1:A:104:GLU:O	1:A:107:GLU:HG2	0.51	2.05	2	1
1:A:64:PRO:CB	1:A:141:LYS:HE3	0.51	2.35	9	1
1:A:94:VAL:HG22	1:A:140:GLY:CA	0.51	2.35	10	1
1:A:89:LEU:HB3	1:A:142:PHE:CE2	0.51	2.40	7	1
1:A:58:LEU:CG	1:A:146:PHE:HB3	0.51	2.26	19	2
1:A:60:VAL:HB	1:A:68:SER:H	0.51	1.66	15	2
1:A:76:ILE:HG13	1:A:102:ARG:HB3	0.51	1.81	8	1
1:A:121:VAL:HG22	1:A:137:VAL:CG2	0.51	2.34	14	2
1:A:78:SER:HB3	1:A:82:HIS:CE1	0.51	2.41	8	6
1:A:77:THR:HB	1:A:86:ASP:CB	0.51	2.35	7	4
1:A:60:VAL:HG11	1:A:89:LEU:CD2	0.51	2.29	10	2
1:A:24:VAL:HG22	1:A:116:LEU:CD1	0.51	2.36	1	2
1:A:56:ALA:CB	1:A:131:LEU:HD13	0.51	2.36	8	2
1:A:96:ARG:NE	1:A:97:ARG:HG2	0.50	2.21	1	2
1:A:87:ILE:HG13	1:A:87:ILE:O	0.50	2.04	16	4
1:A:96:ARG:NH2	1:A:97:ARG:HG2	0.50	2.21	2	1
1:A:68:SER:HB3	1:A:89:LEU:CD1	0.50	2.36	7	1
1:A:89:LEU:HD13	1:A:142:PHE:CD1	0.50	2.41	17	2
1:A:139:ILE:HD13	1:A:139:ILE:O	0.50	2.06	15	2
1:A:26:ARG:HG2	1:A:26:ARG:NH1	0.50	2.22	4	1
1:A:132:ALA:HB3	1:A:146:PHE:CE1	0.50	2.40	8	1
1:A:117:ASN:ND2	1:A:140:GLY:HA2	0.50	2.22	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:PHE:N	1:A:70:PHE:HD1	0.50	2.03	13	7
1:A:26:ARG:HG2	1:A:64:PRO:HD2	0.50	1.82	1	1
1:A:60:VAL:HG13	1:A:68:SER:C	0.50	2.32	1	1
1:A:139:ILE:HG23	1:A:144:LEU:CD1	0.50	2.37	5	7
1:A:139:ILE:CD1	1:A:144:LEU:HD11	0.50	2.36	3	1
1:A:121:VAL:HB	1:A:126:VAL:HG11	0.50	1.83	3	1
1:A:81:ARG:HG2	1:A:91:ASP:HA	0.50	1.84	7	1
1:A:77:THR:HG22	1:A:86:ASP:HB3	0.50	1.82	11	2
1:A:93:THR:O	1:A:116:LEU:HB3	0.49	2.07	1	1
1:A:79:ALA:O	1:A:97:ARG:HA	0.49	2.08	15	5
1:A:65:ASN:CB	1:A:142:PHE:HE2	0.49	2.21	14	6
1:A:58:LEU:CD1	1:A:72:LEU:HD11	0.49	2.38	15	2
1:A:72:LEU:CD2	1:A:131:LEU:HD12	0.49	2.37	10	1
1:A:87:ILE:HD11	1:A:89:LEU:CD2	0.49	2.38	12	5
1:A:126:VAL:HG21	1:A:129:ALA:HB2	0.49	1.83	14	2
1:A:93:THR:HG1	1:A:142:PHE:HE1	0.49	1.50	14	2
1:A:87:ILE:O	1:A:87:ILE:HG13	0.49	2.07	17	8
1:A:94:VAL:HG22	1:A:140:GLY:HA3	0.49	1.85	2	3
1:A:140:GLY:O	1:A:141:LYS:HB3	0.48	2.08	2	1
1:A:139:ILE:HD12	1:A:144:LEU:HD21	0.48	1.84	3	1
1:A:70:PHE:CE1	1:A:144:LEU:HD22	0.48	2.43	1	1
1:A:26:ARG:HB3	1:A:141:LYS:O	0.48	2.08	13	3
1:A:89:LEU:HB3	1:A:142:PHE:CE1	0.48	2.44	15	5
1:A:96:ARG:HE	1:A:97:ARG:HB3	0.48	1.67	19	1
1:A:136:GLU:HA	1:A:145:VAL:HA	0.48	1.86	2	6
1:A:79:ALA:HB1	1:A:87:ILE:HG12	0.48	1.85	18	3
1:A:75:ALA:O	1:A:103:LEU:HB2	0.48	2.09	2	1
1:A:100:GLU:O	1:A:111:VAL:HG22	0.48	2.09	5	1
1:A:137:VAL:HG13	1:A:144:LEU:HD13	0.48	1.85	9	2
1:A:98:HIS:CE1	1:A:119:THR:HG23	0.47	2.43	1	6
1:A:131:LEU:HD23	1:A:146:PHE:HB2	0.47	1.84	16	4
1:A:144:LEU:N	1:A:144:LEU:HD12	0.47	2.24	13	5
1:A:72:LEU:HD13	1:A:108:PHE:CB	0.47	2.39	7	5
1:A:26:ARG:NH2	1:A:143:ARG:HB2	0.47	2.22	7	1
1:A:98:HIS:CD2	1:A:139:ILE:HG22	0.47	2.44	13	1
1:A:59:VAL:HG22	1:A:69:ARG:HB3	0.47	1.85	2	1
1:A:57:LEU:HA	1:A:72:LEU:CD2	0.47	2.40	16	3
1:A:99:ALA:HB3	1:A:110:VAL:HG12	0.47	1.85	8	2
1:A:93:THR:CG2	1:A:141:LYS:HE2	0.47	2.38	10	3
1:A:58:LEU:HD21	1:A:110:VAL:CG1	0.47	2.39	11	1
1:A:82:HIS:CE1	1:A:96:ARG:HG2	0.47	2.45	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:ALA:CA	1:A:87:ILE:HG23	0.47	2.40	6	8
1:A:98:HIS:CD2	1:A:139:ILE:HG21	0.47	2.44	3	1
1:A:72:LEU:HD23	1:A:131:LEU:HD11	0.47	1.86	8	1
1:A:80:GLY:HA2	1:A:139:ILE:HD11	0.47	1.86	9	2
1:A:70:PHE:HE1	1:A:144:LEU:HD23	0.47	1.68	13	1
1:A:103:LEU:C	1:A:103:LEU:HD23	0.47	2.35	16	6
1:A:72:LEU:CD1	1:A:131:LEU:HD21	0.47	2.40	5	1
1:A:101:PHE:CE2	1:A:108:PHE:HB2	0.47	2.45	8	1
1:A:64:PRO:HG2	1:A:141:LYS:HD2	0.47	1.84	1	1
1:A:137:VAL:HG12	1:A:144:LEU:CB	0.47	2.36	14	1
1:A:70:PHE:O	1:A:72:LEU:HD22	0.47	2.10	2	2
1:A:122:ASN:HA	1:A:136:GLU:OE2	0.47	2.09	11	1
1:A:57:LEU:HA	1:A:72:LEU:CD1	0.47	2.40	12	1
1:A:93:THR:HB	1:A:141:LYS:CD	0.47	2.39	4	1
1:A:60:VAL:HG11	1:A:89:LEU:CD1	0.46	2.39	3	1
1:A:55:SER:HB3	1:A:73:ASP:HB2	0.46	1.86	7	5
1:A:26:ARG:HD2	1:A:26:ARG:C	0.46	2.35	12	1
1:A:100:GLU:CD	1:A:102:ARG:HH21	0.46	2.18	12	1
1:A:24:VAL:HA	1:A:141:LYS:HD2	0.46	1.85	8	1
1:A:61:LYS:HB2	1:A:145:VAL:CG1	0.46	2.40	19	1
1:A:137:VAL:HG13	1:A:139:ILE:HG22	0.46	1.87	9	1
1:A:68:SER:HB3	1:A:89:LEU:HD21	0.46	1.86	10	1
1:A:58:LEU:HD12	1:A:58:LEU:N	0.46	2.26	16	6
1:A:141:LYS:N	1:A:142:PHE:CD1	0.46	2.83	10	3
1:A:70:PHE:O	1:A:72:LEU:HD13	0.46	2.11	3	1
1:A:69:ARG:HH21	1:A:71:LEU:HB2	0.46	1.70	11	1
1:A:98:HIS:CB	1:A:115:SER:HB2	0.46	2.38	3	2
1:A:81:ARG:N	1:A:94:VAL:HG13	0.46	2.26	17	2
1:A:93:THR:HG21	1:A:141:LYS:HE3	0.46	1.88	1	1
1:A:96:ARG:CZ	1:A:97:ARG:HG2	0.46	2.40	9	3
1:A:136:GLU:HA	1:A:144:LEU:O	0.46	2.10	11	2
1:A:137:VAL:HG12	1:A:144:LEU:HD13	0.46	1.86	9	2
1:A:24:VAL:O	1:A:141:LYS:HD3	0.46	2.11	12	1
1:A:81:ARG:N	1:A:96:ARG:O	0.46	2.49	11	4
1:A:126:VAL:HG21	1:A:129:ALA:CB	0.46	2.41	14	1
1:A:121:VAL:O	1:A:124:GLU:HG2	0.46	2.11	5	2
1:A:71:LEU:HD21	1:A:73:ASP:HB2	0.45	1.86	6	1
1:A:59:VAL:HG12	1:A:147:LEU:HD23	0.45	1.88	11	1
1:A:121:VAL:HG22	1:A:137:VAL:CG1	0.45	2.39	19	2
1:A:111:VAL:O	1:A:111:VAL:HG23	0.45	2.11	19	2
1:A:60:VAL:HG21	1:A:89:LEU:HD21	0.45	1.87	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:ASP:O	1:A:145:VAL:HA	0.45	2.11	7	2
1:A:71:LEU:HD11	1:A:73:ASP:HB3	0.45	1.88	6	1
1:A:87:ILE:HD11	1:A:89:LEU:HD23	0.45	1.88	16	1
1:A:60:VAL:CG1	1:A:89:LEU:HD21	0.45	2.30	10	1
1:A:26:ARG:HH12	1:A:138:GLN:NE2	0.45	2.09	1	1
1:A:56:ALA:HB3	1:A:131:LEU:HD13	0.45	1.87	8	1
1:A:72:LEU:HG	1:A:101:PHE:HD2	0.45	1.72	16	2
1:A:137:VAL:O	1:A:144:LEU:HB2	0.45	2.12	5	2
1:A:136:GLU:OE1	1:A:143:ARG:HD3	0.45	2.10	12	1
1:A:57:LEU:HA	1:A:72:LEU:HD22	0.45	1.88	16	1
1:A:69:ARG:HD2	1:A:69:ARG:C	0.45	2.36	16	2
1:A:95:SER:HB3	1:A:114:GLY:O	0.45	2.12	3	1
1:A:26:ARG:HG3	1:A:141:LYS:HB2	0.45	1.88	1	1
1:A:121:VAL:HB	1:A:126:VAL:HG13	0.45	1.89	10	1
1:A:145:VAL:HG22	1:A:147:LEU:CD2	0.45	2.42	11	2
1:A:101:PHE:CD1	1:A:101:PHE:C	0.45	2.94	12	1
1:A:72:LEU:CD2	1:A:131:LEU:HD21	0.45	2.42	3	2
1:A:58:LEU:HD21	1:A:110:VAL:HG11	0.45	1.88	12	2
1:A:72:LEU:HD22	1:A:101:PHE:CD1	0.44	2.46	17	4
1:A:72:LEU:HG	1:A:101:PHE:HB2	0.44	1.89	12	1
1:A:101:PHE:CE1	1:A:103:LEU:HB2	0.44	2.47	12	1
1:A:101:PHE:CE1	1:A:110:VAL:HG12	0.44	2.47	1	2
1:A:55:SER:CB	1:A:73:ASP:HB2	0.44	2.42	14	1
1:A:24:VAL:HG23	1:A:117:ASN:HB3	0.44	1.88	9	1
1:A:80:GLY:HA3	1:A:94:VAL:HG11	0.44	1.90	10	1
1:A:74:GLN:O	1:A:101:PHE:HE2	0.44	1.95	11	1
1:A:105:ASN:O	1:A:106:ASN:HB3	0.44	2.12	15	1
1:A:61:LYS:HB2	1:A:145:VAL:HG12	0.44	1.89	19	1
1:A:98:HIS:HB3	1:A:139:ILE:HB	0.44	1.89	13	1
1:A:109:ASN:OD1	1:A:130:VAL:HB	0.44	2.13	3	1
1:A:145:VAL:HG22	1:A:147:LEU:HD22	0.44	1.89	11	1
1:A:97:ARG:HH11	1:A:113:VAL:HG21	0.44	1.73	12	1
1:A:76:ILE:HD13	1:A:102:ARG:CB	0.44	2.42	16	1
1:A:72:LEU:HD12	1:A:146:PHE:HE1	0.44	1.73	17	1
1:A:68:SER:HB2	1:A:89:LEU:CD2	0.44	2.42	4	3
1:A:117:ASN:ND2	1:A:141:LYS:HA	0.44	2.28	2	1
1:A:97:ARG:HG2	1:A:113:VAL:HG21	0.44	1.89	18	1
1:A:60:VAL:HG13	1:A:68:SER:HB2	0.43	1.90	2	1
1:A:93:THR:HG21	1:A:142:PHE:CZ	0.43	2.48	12	2
1:A:23:SER:HB2	1:A:93:THR:HG22	0.43	1.90	13	1
1:A:70:PHE:HB2	1:A:72:LEU:HD21	0.43	1.89	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:HIS:O	1:A:88:PHE:HB3	0.43	2.13	7	1
1:A:82:HIS:HD2	1:A:87:ILE:O	0.43	1.96	17	3
1:A:62:ARG:HA	1:A:66:ALA:CB	0.43	2.44	2	1
1:A:103:LEU:HD13	1:A:104:GLU:N	0.43	2.28	2	1
1:A:24:VAL:HB	1:A:116:LEU:CD2	0.43	2.44	10	1
1:A:120:TYR:CE2	1:A:123:ARG:HA	0.43	2.48	2	1
1:A:81:ARG:N	1:A:94:VAL:HB	0.43	2.27	15	3
1:A:122:ASN:O	1:A:123:ARG:HB2	0.43	2.13	4	2
1:A:92:VAL:HG12	1:A:92:VAL:O	0.43	2.12	11	1
1:A:139:ILE:O	1:A:139:ILE:HD13	0.43	2.13	2	1
1:A:104:GLU:C	1:A:105:ASN:HD22	0.43	2.21	11	1
1:A:98:HIS:HA	1:A:115:SER:HB3	0.43	1.91	10	1
1:A:78:SER:HA	1:A:100:GLU:HB3	0.43	1.91	11	1
1:A:70:PHE:CE1	1:A:144:LEU:CD2	0.43	3.02	16	1
1:A:98:HIS:CB	1:A:115:SER:HB3	0.43	2.39	1	1
1:A:26:ARG:HB2	1:A:141:LYS:HB2	0.43	1.89	7	1
1:A:70:PHE:O	1:A:72:LEU:HD12	0.43	2.13	12	1
1:A:63:GLY:O	1:A:66:ALA:N	0.42	2.52	1	1
1:A:117:ASN:HB2	1:A:140:GLY:C	0.42	2.39	7	2
1:A:64:PRO:HD2	1:A:141:LYS:O	0.42	2.14	1	1
1:A:60:VAL:CA	1:A:144:LEU:HG	0.42	2.45	7	1
1:A:138:GLN:HA	1:A:142:PHE:O	0.42	2.14	9	1
1:A:72:LEU:HD22	1:A:131:LEU:CD2	0.42	2.44	12	1
1:A:60:VAL:HB	1:A:68:SER:N	0.42	2.29	15	2
1:A:108:PHE:HB2	1:A:131:LEU:HD23	0.42	1.91	15	1
1:A:101:PHE:O	1:A:101:PHE:CG	0.42	2.71	14	2
1:A:62:ARG:HA	1:A:66:ALA:HB1	0.42	1.91	2	1
1:A:131:LEU:HB3	1:A:146:PHE:CE2	0.42	2.47	9	2
1:A:98:HIS:CD2	1:A:139:ILE:CG2	0.42	3.02	14	3
1:A:70:PHE:CD2	1:A:87:ILE:HG12	0.42	2.48	15	1
1:A:98:HIS:HB2	1:A:115:SER:CB	0.42	2.40	1	1
1:A:24:VAL:HB	1:A:116:LEU:CD1	0.42	2.42	3	1
1:A:99:ALA:HB1	1:A:111:VAL:O	0.42	2.15	15	1
1:A:24:VAL:CB	1:A:116:LEU:HD12	0.42	2.45	19	1
1:A:141:LYS:HG2	1:A:142:PHE:CE1	0.42	2.50	2	1
1:A:97:ARG:HG3	1:A:113:VAL:CG2	0.42	2.44	8	3
1:A:87:ILE:CD1	1:A:89:LEU:HD21	0.42	2.45	5	1
1:A:78:SER:HB2	1:A:82:HIS:HE2	0.42	1.70	7	1
1:A:72:LEU:HD12	1:A:72:LEU:N	0.42	2.30	12	1
1:A:56:ALA:HB1	1:A:146:PHE:CZ	0.42	2.50	17	2
1:A:64:PRO:HG2	1:A:141:LYS:CD	0.42	2.45	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:THR:HB	1:A:117:ASN:HD21	0.42	1.74	1	1
1:A:79:ALA:CB	1:A:87:ILE:HG12	0.42	2.45	18	2
1:A:93:THR:CG2	1:A:141:LYS:HD3	0.42	2.45	19	3
1:A:26:ARG:HG2	1:A:64:PRO:HD3	0.42	1.90	16	1
1:A:103:LEU:HD12	1:A:107:GLU:O	0.42	2.15	19	1
1:A:72:LEU:HD12	1:A:101:PHE:HB3	0.42	1.92	16	2
1:A:89:LEU:C	1:A:91:ASP:N	0.42	2.77	3	5
1:A:95:SER:HB2	1:A:114:GLY:O	0.42	2.15	4	1
1:A:70:PHE:N	1:A:70:PHE:CD1	0.42	2.88	17	2
1:A:131:LEU:HG	1:A:146:PHE:HB2	0.42	1.91	19	2
1:A:70:PHE:CE2	1:A:79:ALA:HB1	0.42	2.49	15	1
1:A:98:HIS:HB3	1:A:139:ILE:HG13	0.41	1.92	9	1
1:A:121:VAL:HB	1:A:126:VAL:CG1	0.41	2.45	3	1
1:A:138:GLN:OE1	1:A:142:PHE:N	0.41	2.52	11	1
1:A:121:VAL:CG2	1:A:126:VAL:HG22	0.41	2.45	14	1
1:A:72:LEU:CD2	1:A:101:PHE:HB3	0.41	2.45	15	1
1:A:109:ASN:OD1	1:A:130:VAL:HG22	0.41	2.14	15	1
1:A:72:LEU:HB3	1:A:108:PHE:CD1	0.41	2.50	15	1
1:A:71:LEU:HD13	1:A:71:LEU:O	0.41	2.16	11	1
1:A:97:ARG:HD2	1:A:113:VAL:HG11	0.41	1.92	15	1
1:A:116:LEU:C	1:A:116:LEU:HD13	0.41	2.41	1	1
1:A:111:VAL:HG12	1:A:128:SER:HB2	0.41	1.91	5	1
1:A:60:VAL:CG2	1:A:144:LEU:HG	0.41	2.41	16	1
1:A:71:LEU:HB3	1:A:86:ASP:HB3	0.41	1.91	19	1
1:A:80:GLY:O	1:A:88:PHE:HA	0.41	2.15	1	1
1:A:117:ASN:HD22	1:A:140:GLY:HA2	0.41	1.75	5	1
1:A:26:ARG:HG2	1:A:141:LYS:O	0.41	2.16	9	1
1:A:78:SER:C	1:A:87:ILE:HG23	0.41	2.41	2	1
1:A:58:LEU:HD12	1:A:58:LEU:H	0.41	1.75	7	1
1:A:94:VAL:HB	1:A:140:GLY:HA2	0.41	1.93	9	1
1:A:25:PHE:HB3	1:A:141:LYS:HE3	0.41	1.92	13	1
1:A:60:VAL:HA	1:A:144:LEU:HG	0.41	1.93	16	1
1:A:121:VAL:CG2	1:A:137:VAL:HG22	0.41	2.44	1	1
1:A:24:VAL:HG23	1:A:116:LEU:CD2	0.41	2.46	15	1
1:A:25:PHE:O	1:A:141:LYS:HD3	0.41	2.15	1	1
1:A:136:GLU:CD	1:A:143:ARG:HD3	0.41	2.40	1	1
1:A:98:HIS:HE1	1:A:119:THR:HG23	0.41	1.75	2	1
1:A:121:VAL:CG2	1:A:137:VAL:HG13	0.41	2.44	2	1
1:A:102:ARG:HG2	1:A:104:GLU:HG3	0.41	1.93	10	1
1:A:25:PHE:O	1:A:141:LYS:HB3	0.41	2.16	16	1
1:A:58:LEU:N	1:A:58:LEU:HD12	0.41	2.31	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:GLN:HG2	1:A:142:PHE:O	0.41	2.16	2	1
1:A:102:ARG:HD2	1:A:111:VAL:HG21	0.41	1.93	8	1
1:A:109:ASN:HA	1:A:129:ALA:O	0.41	2.16	13	1
1:A:89:LEU:HD22	1:A:89:LEU:N	0.41	2.31	14	1
1:A:117:ASN:CG	1:A:138:GLN:HE22	0.41	2.24	14	1
1:A:72:LEU:HD23	1:A:131:LEU:HD12	0.40	1.92	10	1
1:A:72:LEU:N	1:A:72:LEU:HD13	0.40	2.32	16	1
1:A:117:ASN:ND2	1:A:140:GLY:N	0.40	2.69	4	1
1:A:58:LEU:HD22	1:A:70:PHE:CE2	0.40	2.52	10	1
1:A:58:LEU:CD2	1:A:131:LEU:HD11	0.40	2.46	18	1
1:A:131:LEU:HA	1:A:146:PHE:CD2	0.40	2.51	11	1
1:A:69:ARG:C	1:A:87:ILE:HD13	0.40	2.41	19	1
1:A:61:LYS:O	1:A:62:ARG:HG3	0.40	2.16	11	1
1:A:26:ARG:NH1	1:A:63:GLY:HA2	0.40	2.32	13	1
1:A:70:PHE:CD1	1:A:87:ILE:HG12	0.40	2.51	16	1
1:A:98:HIS:CD2	1:A:139:ILE:CB	0.40	3.01	7	1
1:A:58:LEU:HD11	1:A:101:PHE:CE1	0.40	2.50	8	1
1:A:69:ARG:HD3	1:A:69:ARG:N	0.40	2.31	9	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	94/162 (58%)	75±2 (79±2%)	14±2 (15±2%)	5±2 (6±2%)	2	21
All	All	1786/3078 (58%)	1419 (79%)	265 (15%)	102 (6%)	2	21

All 18 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	66	ALA	18
1	A	25	PHE	12
1	A	141	LYS	11
1	A	64	PRO	8

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Mol	Chain	Res	Type	Models (Total)
1	A	96	ARG	8
1	A	23	SER	7
1	A	92	VAL	7
1	A	101	PHE	6
1	A	114	GLY	6
1	A	86	ASP	5
1	A	26	ARG	4
1	A	61	LYS	2
1	A	91	ASP	2
1	A	140	GLY	2
1	A	76	ILE	1
1	A	93	THR	1
1	A	24	VAL	1
1	A	95	SER	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	80/133 (60%)	58±2 (72±3%)	22±2 (28±3%)	1	19
All	All	1520/2527 (60%)	1093 (72%)	427 (28%)	1	19

All 53 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	69	ARG	19
1	A	87	ILE	19
1	A	88	PHE	19
1	A	98	HIS	19
1	A	139	ILE	19
1	A	145	VAL	19
1	A	70	PHE	18
1	A	76	ILE	18
1	A	142	PHE	18
1	A	60	VAL	17
1	A	81	ARG	16

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Mol	Chain	Res	Type	Models (Total)
1	A	96	ARG	16
1	A	71	LEU	14
1	A	26	ARG	13
1	A	108	PHE	12
1	A	110	VAL	12
1	A	101	PHE	12
1	A	146	PHE	11
1	A	131	LEU	11
1	A	72	LEU	10
1	A	93	THR	10
1	A	117	ASN	9
1	A	55	SER	9
1	A	94	VAL	8
1	A	122	ASN	8
1	A	82	HIS	7
1	A	86	ASP	6
1	A	136	GLU	6
1	A	147	LEU	6
1	A	109	ASN	5
1	A	116	LEU	4
1	A	138	GLN	4
1	A	120	TYR	3
1	A	97	ARG	3
1	A	105	ASN	3
1	A	123	ARG	3
1	A	61	LYS	2
1	A	111	VAL	2
1	A	143	ARG	2
1	A	137	VAL	2
1	A	64	PRO	1
1	A	77	THR	1
1	A	103	LEU	1
1	A	58	LEU	1
1	A	100	GLU	1
1	A	121	VAL	1
1	A	24	VAL	1
1	A	25	PHE	1
1	A	135	ASP	1
1	A	107	GLU	1
1	A	113	VAL	1
1	A	141	LYS	1
1	A	115	SER	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	TPO	A	22	1	8,10,11	1.30±0.09	1±0 (6±6%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	TPO	A	22	1	10,14,16	1.73±0.13	1±0 (10±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	22	1	-	0±0,9,11,13	-

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	22	TPO	P-OG1	3.16	1.65	1.59	7	10

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	22	TPO	P-OG1-CB	5.88	107.36	123.33	11	19
1	A	22	TPO	O-C-CA	2.01	119.59	124.77	1	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 90% for the well-defined parts and 89% 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	1833
Number of shifts mapped to atoms	1676
Number of unparsed shifts	0
Number of shifts with mapping errors	157
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	15

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 157 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	VAL	H	8.226	0.0	1
1	A	3	ASP	HB3	2.523	0.0	2
1	A	4	MET	HA2	3.944	0.0	2
1	A	4	MET	HA3	3.944	0.0	2
1	A	5	ASN	HB3	3.804	0.0	2
1	A	7	ASP	HB3	2.612	0.0	2
1	A	8	ILE	HG13	1.163	0.0	2
1	A	9	GLU	HB3	1.937	0.0	2
1	A	9	GLU	HG3	2.205	0.0	2
1	A	10	LYS	HB3	1.706	0.0	2
1	A	10	LYS	HD3	1.658	0.0	2
1	A	10	LYS	HE3	3.009	0.0	2
1	A	10	LYS	HG3	1.451	0.0	2
1	A	11	ASP	HB3	2.741	0.0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	GLN	HB3	1.94	0.0	2
1	A	12	GLN	HG3	2.328	0.0	2
1	A	14	SER	HB3	3.81	0.0	2
1	A	15	ASP	HB3	2.589	0.0	2
1	A	16	GLU	HB3	1.883	0.0	2
1	A	16	GLU	HG3	2.206	0.0	2
1	A	23	SER	HB3	3.485	0.0	2
1	A	25	PHE	HB3	2.75	0.0	2
1	A	26	ARG	HB3	1.383	0.0	2
1	A	26	ARG	HD3	2.839	0.0	2
1	A	26	ARG	HG3	0.882	0.0	2
1	A	28	ASP	HB3	2.414	0.0	2
1	A	29	PHE	HB3	2.81	0.0	2
1	A	30	LEU	HB3	1.493	0.0	2
1	A	31	SER	HB3	3.796	0.0	2
1	A	32	GLU	HB3	1.887	0.0	2
1	A	32	GLU	HG3	2.226	0.0	2
1	A	33	LEU	HB3	1.49	0.0	2
1	A	34	ASP	HB3	2.59	0.0	2
1	A	36	PRO	HB3	1.849	0.0	2
1	A	36	PRO	HD3	3.575	0.0	2
1	A	36	PRO	HG3	1.957	0.0	2
1	A	38	GLN	HB3	1.941	0.0	2
1	A	38	GLN	HG3	2.332	0.0	2
1	A	42	GLU	HB3	1.893	0.0	2
1	A	42	GLU	HG3	2.231	0.0	2
1	A	43	SER	HB3	3.805	0.0	2
1	A	46	SER	HB3	3.852	0.0	2
1	A	49	GLU	HB3	1.885	0.0	2
1	A	49	GLU	HG3	2.222	0.0	2
1	A	51	LEU	HB3	1.375	0.0	2
1	A	52	PRO	HD3	3.743	0.0	2
1	A	53	PRO	HB3	1.816	0.0	2
1	A	53	PRO	HD3	3.562	0.0	2
1	A	53	PRO	HG3	1.95	0.0	2
1	A	55	SER	HB3	3.753	0.0	2
1	A	57	LEU	HB3	1.207	0.0	2
1	A	58	LEU	HB3	1.194	0.0	2
1	A	61	LYS	HB3	1.668	0.0	2
1	A	61	LYS	HD3	1.368	0.0	2
1	A	61	LYS	HE3	2.863	0.0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	61	LYS	HG3	1.571	0.0	2
1	A	62	ARG	HD3	3.074	0.0	2
1	A	62	ARG	HG3	1.358	0.0	2
1	A	64	PRO	HB3	1.846	0.0	2
1	A	64	PRO	HD3	2.316	0.0	2
1	A	64	PRO	HG3	1.678	0.0	2
1	A	65	ASN	HB3	2.831	0.0	2
1	A	68	SER	HB3	3.572	0.0	2
1	A	69	ARG	HB3	1.549	0.0	2
1	A	69	ARG	HD3	3.013	0.0	2
1	A	69	ARG	HG3	1.434	0.0	2
1	A	70	PHE	HB3	2.778	0.0	2
1	A	71	LEU	HB3	1.385	0.0	2
1	A	72	LEU	HB3	1.224	0.0	2
1	A	73	ASP	HB3	2.489	0.0	2
1	A	74	GLN	HB3	1.965	0.0	2
1	A	74	GLN	HG3	2.373	0.0	2
1	A	76	ILE	HG13	1.519	0.0	2
1	A	78	SER	HB3	4.005	0.0	2
1	A	81	ARG	HB3	1.696	0.0	2
1	A	81	ARG	HD3	3.103	0.0	2
1	A	81	ARG	HG3	1.509	0.0	2
1	A	82	HIS	HB3	2.764	0.0	2
1	A	83	PRO	HB3	1.706	0.0	2
1	A	83	PRO	HD3	2.331	0.0	2
1	A	83	PRO	HG3	1.648	0.0	2
1	A	84	ASP	HB3	2.684	0.0	2
1	A	85	SER	HB3	3.561	0.0	2
1	A	86	ASP	HB3	2.784	0.0	2
1	A	87	ILE	HG13	0.347	0.0	2
1	A	88	PHE	HB3	2.958	0.0	2
1	A	89	LEU	HB3	0.199	0.0	2
1	A	90	ASP	HB3	1.63	0.0	2
1	A	91	ASP	HB3	2.38	0.0	2
1	A	95	SER	HB3	3.482	0.0	2
1	A	96	ARG	HB3	2.011	0.0	2
1	A	96	ARG	HD3	2.882	0.0	2
1	A	96	ARG	HG3	1.757	0.0	2
1	A	97	ARG	HB3	1.359	0.0	2
1	A	97	ARG	HD3	3.059	0.0	2
1	A	97	ARG	HG3	1.338	0.0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	HIS	HB3	3.179	0.0	2
1	A	100	GLU	HB3	1.581	0.0	2
1	A	100	GLU	HG3	1.993	0.0	2
1	A	101	PHE	HB3	2.528	0.0	2
1	A	102	ARG	HB3	1.7	0.0	2
1	A	102	ARG	HD3	3.02	0.0	2
1	A	102	ARG	HG3	1.465	0.0	2
1	A	103	LEU	HB3	0.938	0.0	2
1	A	104	GLU	HB3	1.74	0.0	2
1	A	104	GLU	HG3	2.017	0.0	2
1	A	105	ASN	HB3	2.699	0.0	2
1	A	106	ASN	HB3	2.898	0.0	2
1	A	107	GLU	HB3	1.886	0.0	2
1	A	107	GLU	HG3	2.254	0.0	2
1	A	108	PHE	HB3	2.508	0.0	2
1	A	109	ASN	HB3	2.253	0.0	2
1	A	112	ASP	HB3	2.37	0.0	2
1	A	115	SER	HB3	2.943	0.0	2
1	A	116	LEU	HB3	1.694	0.0	2
1	A	117	ASN	HB3	2.993	0.0	2
1	A	120	TYR	HB3	2.371	0.0	2
1	A	122	ASN	HB3	2.794	0.0	2
1	A	123	ARG	HB3	1.365	0.0	2
1	A	123	ARG	HD3	2.823	0.0	2
1	A	123	ARG	HG3	0.849	0.0	2
1	A	124	GLU	HB3	1.852	0.0	2
1	A	124	GLU	HG3	2.238	0.0	2
1	A	125	PRO	HB3	1.622	0.0	2
1	A	125	PRO	HD3	3.859	0.0	2
1	A	125	PRO	HG3	2.055	0.0	2
1	A	127	ASP	HB3	2.628	0.0	2
1	A	128	SER	HB3	3.733	0.0	2
1	A	131	LEU	HB3	0.048	0.0	2
1	A	133	ASN	HB3	2.705	0.0	2
1	A	135	ASP	HB3	2.345	0.0	2
1	A	136	GLU	HB3	1.967	0.0	2
1	A	136	GLU	HG3	2.031	0.0	2
1	A	138	GLN	HB3	2.226	0.0	2
1	A	138	GLN	HG3	2.198	0.0	2
1	A	139	ILE	HG13	0.852	0.0	2
1	A	141	LYS	HB3	0.824	0.0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	141	LYS	HD3	1.268	0.0	2
1	A	141	LYS	HE3	2.442	0.0	2
1	A	141	LYS	HG3	0.646	0.0	2
1	A	142	PHE	HB3	2.541	0.0	2
1	A	143	ARG	HB3	1.727	0.0	2
1	A	143	ARG	HD3	3.096	0.0	2
1	A	143	ARG	HG3	1.447	0.0	2
1	A	144	LEU	HB3	1.442	0.0	2
1	A	146	PHE	HB3	2.558	0.0	2
1	A	147	LEU	HB3	1.272	0.0	2
1	A	150	PRO	HB3	1.826	0.0	2
1	A	150	PRO	HD3	3.446	0.0	2
1	A	150	PRO	HG3	1.96	0.0	2
1	A	152	GLN	HB3	1.908	0.0	2
1	A	152	GLN	HG3	2.3	0.0	2
1	A	154	GLU	HB3	1.889	0.0	2
1	A	154	GLU	HG3	2.231	0.0	2
1	A	155	ASP	HB3	2.728	0.0	2
1	A	156	ASP	HB3	2.677	0.0	2
1	A	158	SER	HB3	3.841	0.0	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	153	-0.16 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	138	0.23 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	157	0.03 ± 0.10	None needed (< 0.5 ppm)
^{15}N	152	-1.04 ± 0.23	Should be applied

7.1.3 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 90%, i.e. 1177 atoms were assigned a chemical shift out of a possible 1302. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	472/473 (100%)	193/193 (100%)	187/188 (99%)	92/92 (100%)

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	Total	¹H	¹³C	¹⁵N
Sidechain	637/734 (87%)	436/476 (92%)	184/220 (84%)	17/38 (45%)
Aromatic	68/95 (72%)	34/47 (72%)	32/44 (73%)	2/4 (50%)
Overall	1177/1302 (90%)	663/716 (93%)	403/452 (89%)	111/134 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1818 atoms were assigned a chemical shift out of a possible 2048. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	780/803 (97%)	318/329 (97%)	310/322 (96%)	152/152 (100%)
Sidechain	960/1140 (84%)	656/737 (89%)	286/359 (80%)	18/44 (41%)
Aromatic	78/105 (74%)	39/52 (75%)	37/49 (76%)	2/4 (50%)
Overall	1818/2048 (89%)	1013/1118 (91%)	633/730 (87%)	172/200 (86%)

7.1.4 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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	148	THR	HG1	6.83	0.08 – 2.19	27.0
1	A	123	ARG	NE	116.17	76.53 – 92.65	19.6
1	A	26	ARG	NE	115.93	76.53 – 92.65	19.4
1	A	143	ARG	NE	115.68	76.53 – 92.65	19.3
1	A	96	ARG	NE	115.20	76.53 – 92.65	19.0
1	A	97	ARG	NE	114.95	76.53 – 92.65	18.8
1	A	102	ARG	NE	114.95	76.53 – 92.65	18.8
1	A	81	ARG	NE	114.23	76.53 – 92.65	18.4
1	A	69	ARG	NE	113.98	76.53 – 92.65	18.2
1	A	5	ASN	CB	63.66	30.50 – 46.89	15.2
1	A	82	HIS	CE1	117.40	126.08 – 149.12	-8.8
1	A	98	HIS	CE1	117.40	126.08 – 149.12	-8.8
1	A	95	SER	H	11.64	5.45 – 11.10	6.0
1	A	52	PRO	CD	44.49	45.11 – 55.58	-5.6
1	A	4	MET	CA	45.11	45.26 – 67.07	-5.1

7.1.5 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. 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:

