



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:22 pm BST

PDB ID : 2KID
Title : Solution Structure of the S. Aureus Sortase A-substrate Complex
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Deposited on : 2009-05-01

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

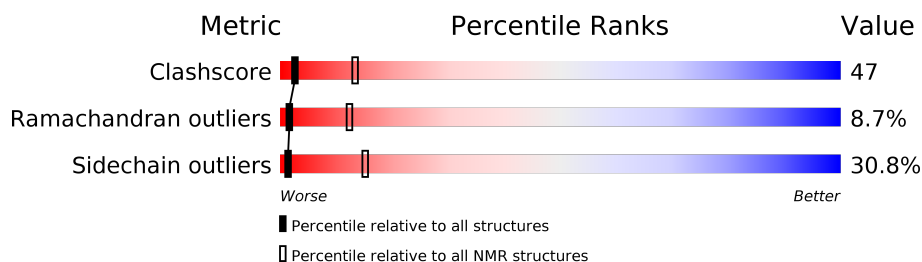
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	148	
2	C	5	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:63-A:206, C:702-C:704 (147)	0.28	11

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

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

The models can be grouped into 5 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2437 atoms, of which 1222 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sortase.

Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2360	743	1183	199	231	4	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	-	initiating methionine	UNP Q9S446

- Molecule 2 is a protein called (PHQ)LPA(B27) peptide.

Mol	Chain	Residues	Atoms						Trace
2	C	5	Total	C	H	N	O	S	0
			76	26	39	4	6	1	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

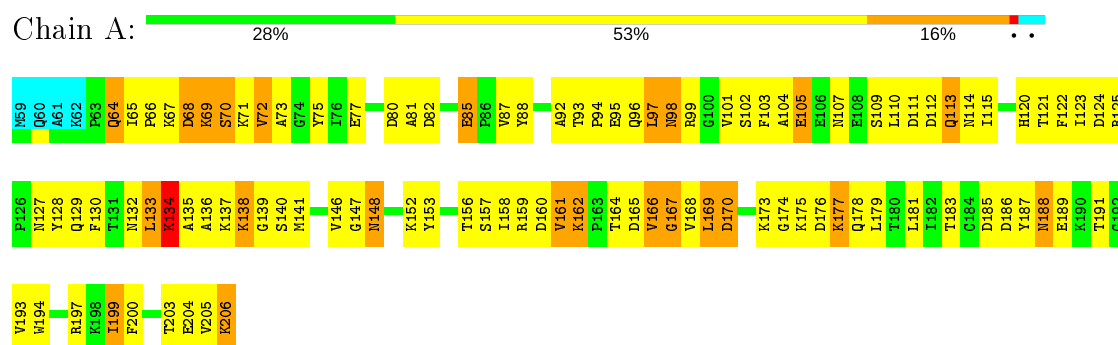
Mol	Chain	Residues	Atoms	
3	A	1	Total	Ca
			1	1

4 Residue-property plots

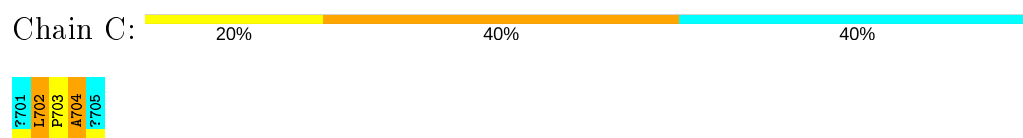
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Sortase



- Molecule 2: (PHQ)LPA(B27) peptide

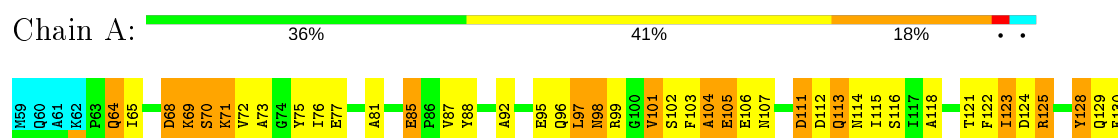


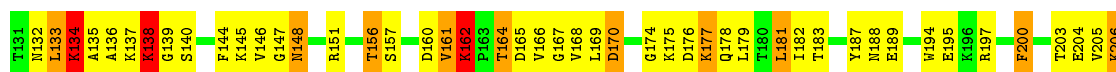
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Sortase





- Molecule 2: (PHQ)LPA(B27) peptide

Chain C: 60% 40%



4.2.2 Score per residue for model 2

- Molecule 1: Sortase

Chain A: 32% 41% 22%



- Molecule 2: (PHQ)LPA(B27) peptide

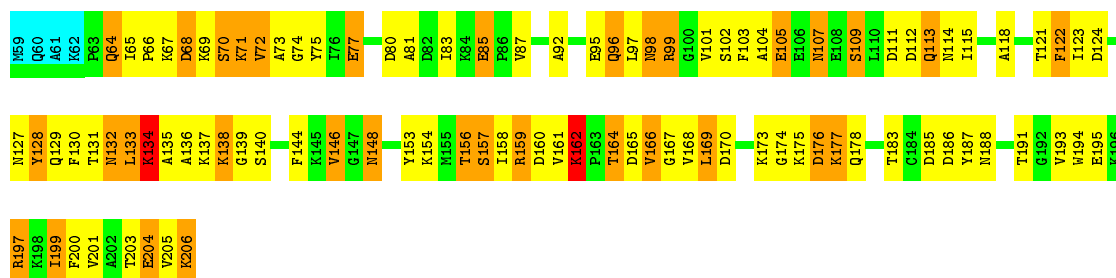
Chain C: 20% 40% 40%



4.2.3 Score per residue for model 3

- Molecule 1: Sortase

Chain A: 32% 42% 22%

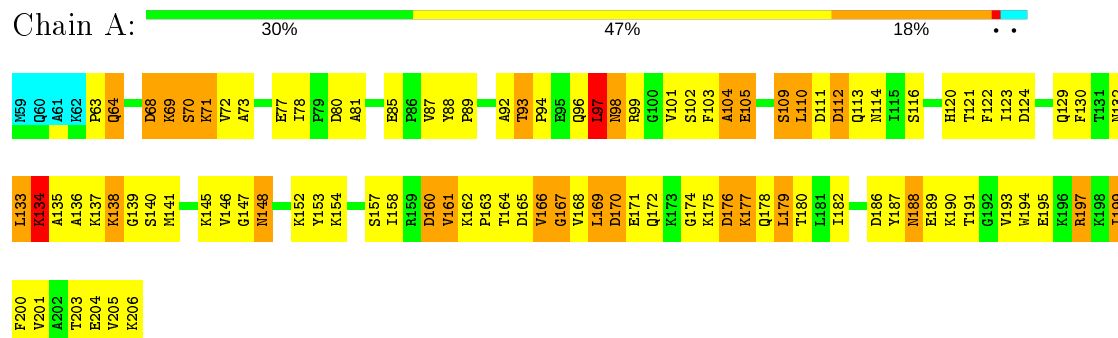


- Molecule 2: (PHQ)LPA(B27) peptide

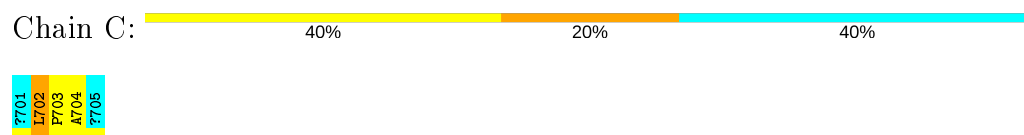


4.2.4 Score per residue for model 4

- Molecule 1: Sortase

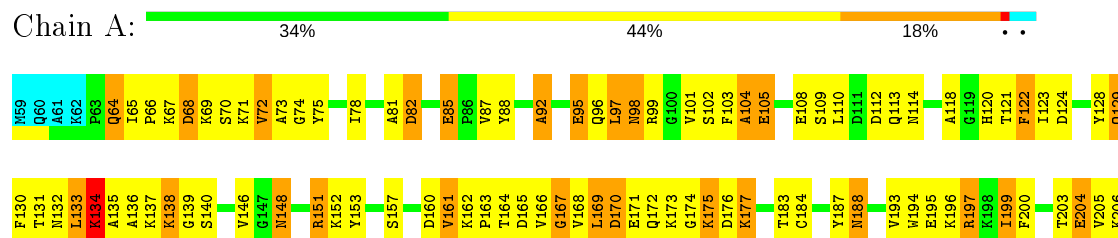


- Molecule 2: (PHQ)LPA(B27) peptide



4.2.5 Score per residue for model 5

- Molecule 1: Sortase

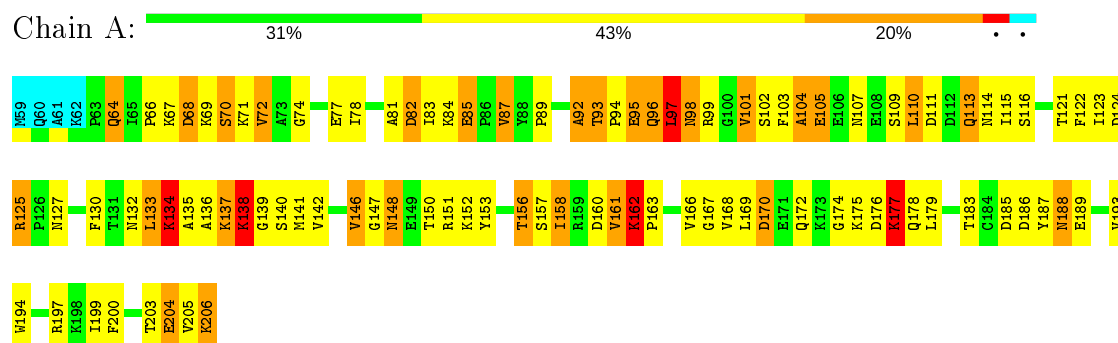


- Molecule 2: (PHQ)LPA(B27) peptide

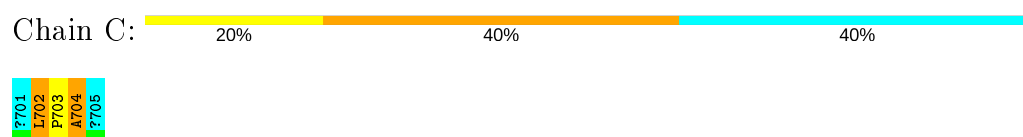


4.2.6 Score per residue for model 6

- Molecule 1: Sortase

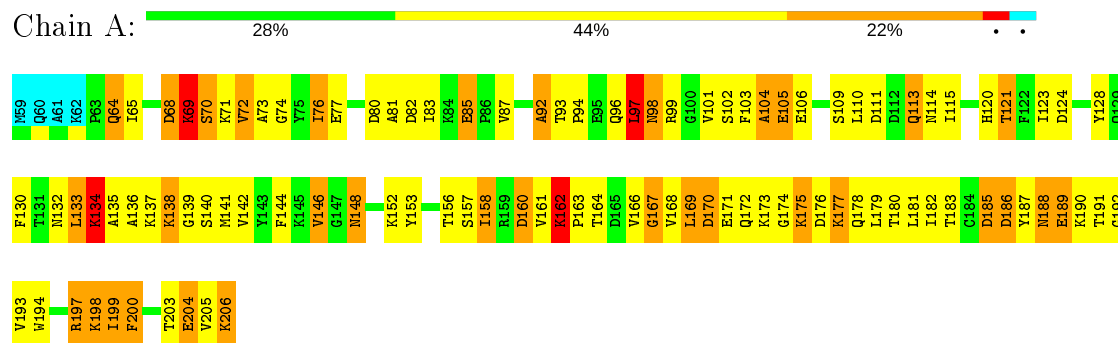


- Molecule 2: (PHQ)LPA(B27) peptide

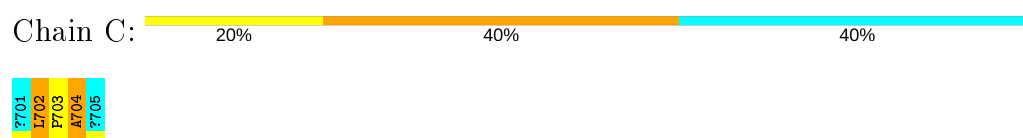


4.2.7 Score per residue for model 7

- Molecule 1: Sortase

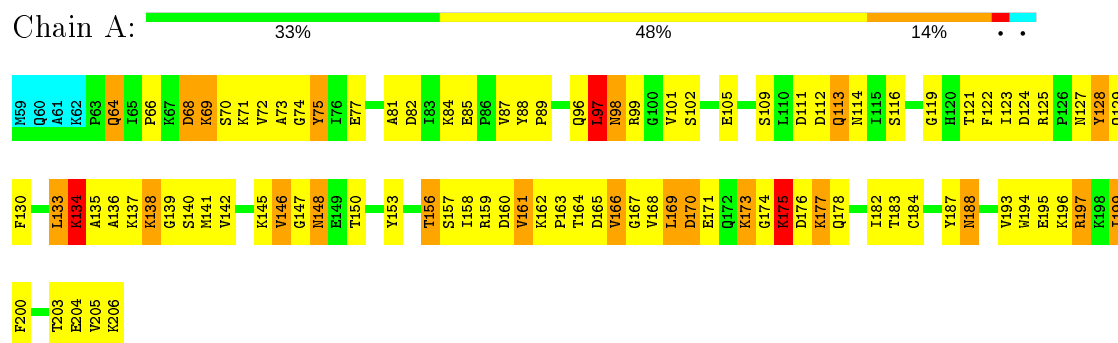


- Molecule 2: (PHQ)LPA(B27) peptide

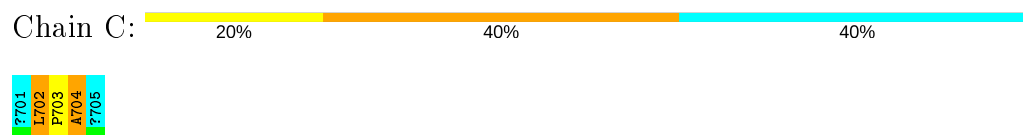


4.2.8 Score per residue for model 8

- Molecule 1: Sortase

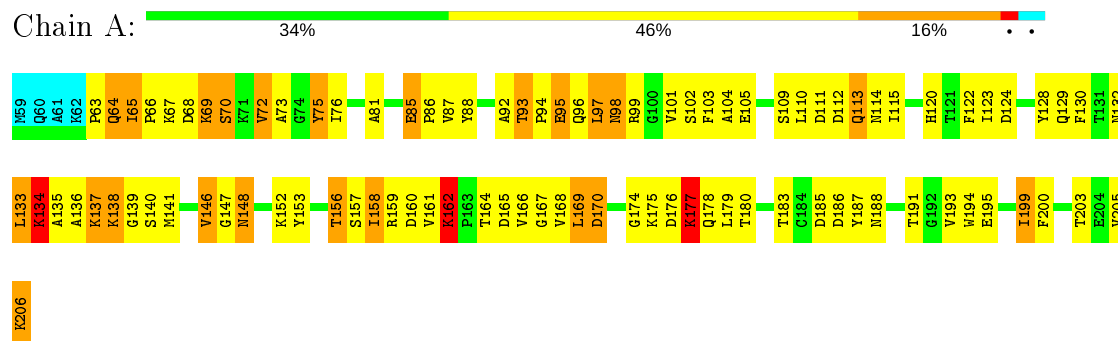


- Molecule 2: (PHQ)LPA(B27) peptide



4.2.9 Score per residue for model 9

- Molecule 1: Sortase

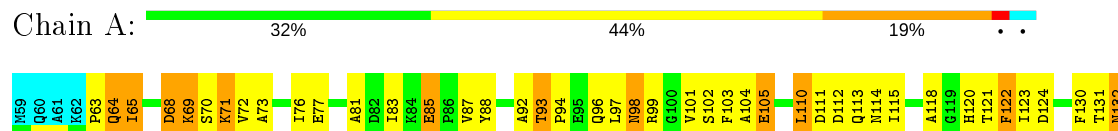


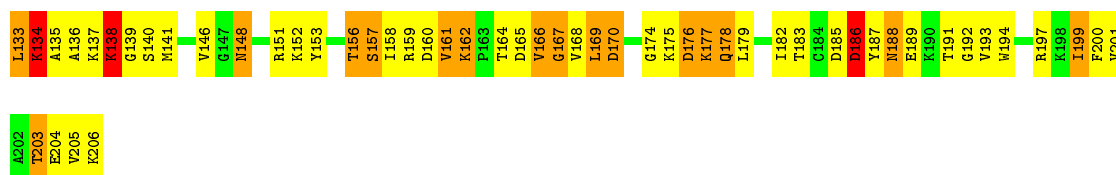
- Molecule 2: (PHQ)LPA(B27) peptide



4.2.10 Score per residue for model 10

- Molecule 1: Sortase





- Molecule 2: (PHQ)LPA(B27) peptide

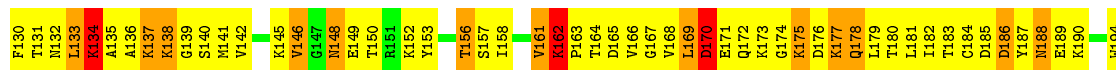
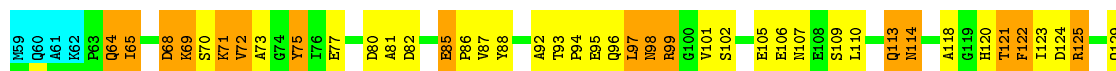
Chain C: 60% 40%



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Sortase

Chain A: 26% 48% 21%



- Molecule 2: (PHQ)LPA(B27) peptide

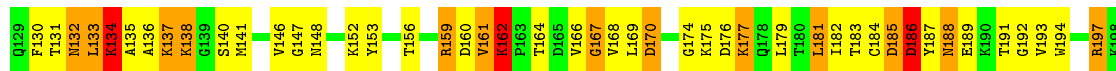
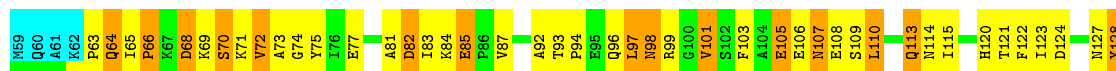
Chain C: 60% 40%

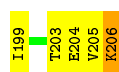


4.2.12 Score per residue for model 12

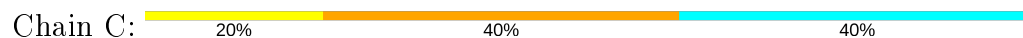
- Molecule 1: Sortase

Chain A: 33% 43% 20%



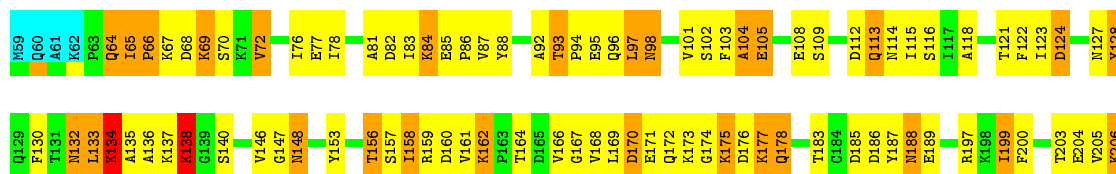


- Molecule 2: (PHQ)LPA(B27) peptide



4.2.13 Score per residue for model 13

- Molecule 1: Sortase



- Molecule 2: (PHQ)LPA(B27) peptide



4.2.14 Score per residue for model 14

- Molecule 1: Sortase



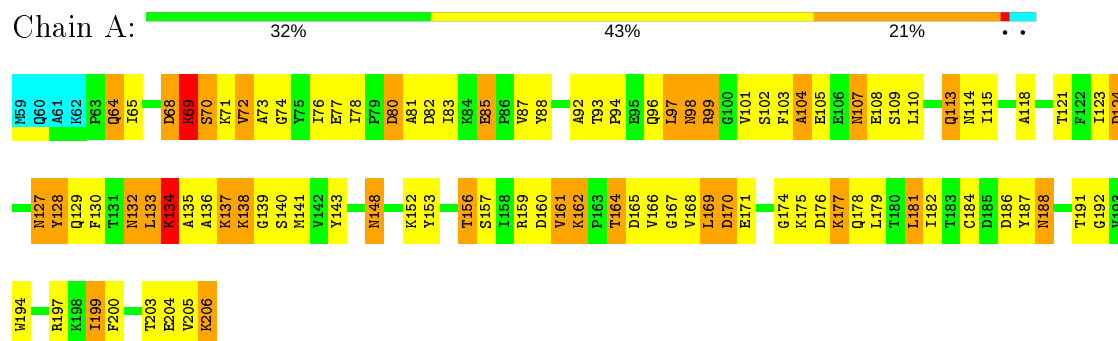
- Molecule 2: (PHQ)LPA(B27) peptide





4.2.15 Score per residue for model 15

- Molecule 1: Sortase

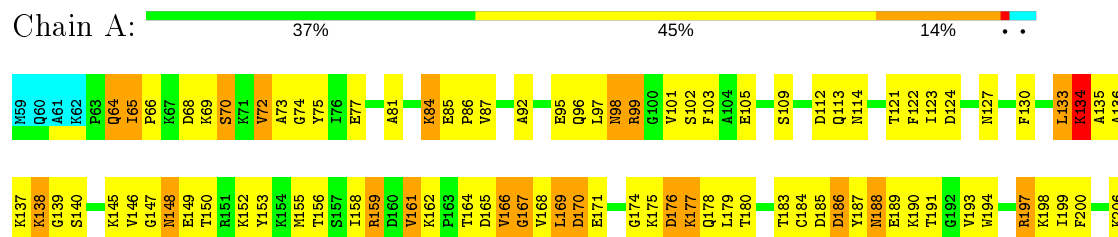


- Molecule 2: (PHQ)LPA(B27) peptide

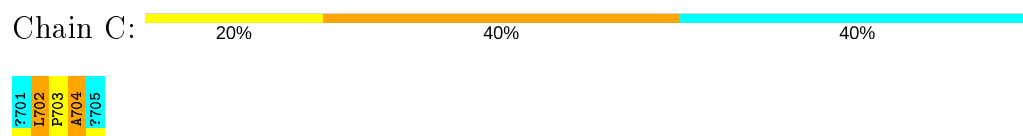


4.2.16 Score per residue for model 16

- Molecule 1: Sortase

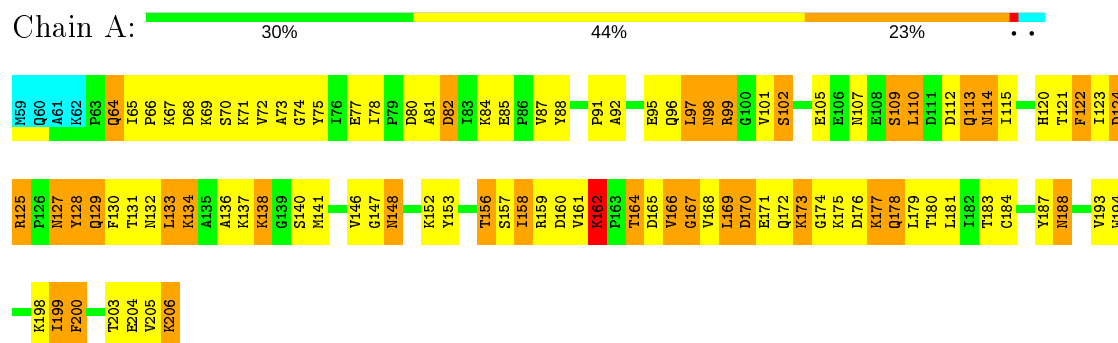


- Molecule 2: (PHQ)LPA(B27) peptide

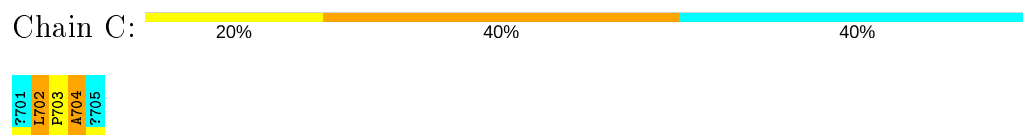


4.2.17 Score per residue for model 17

- Molecule 1: Sortase

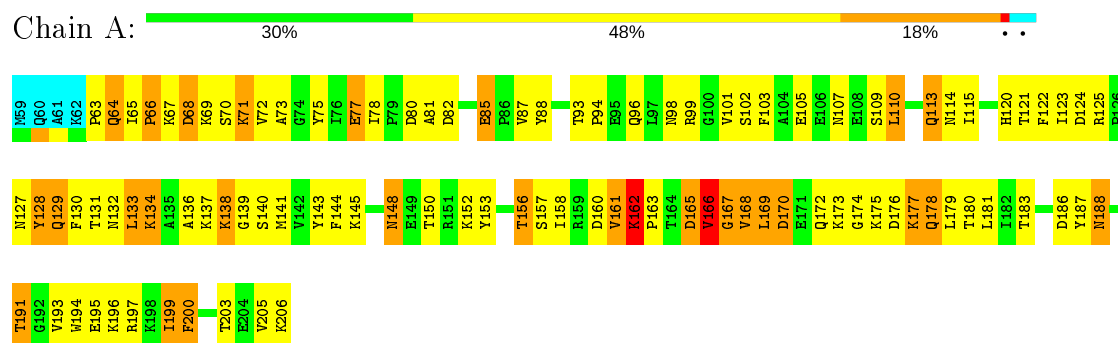


- Molecule 2: (PHQ)LPA(B27) peptide

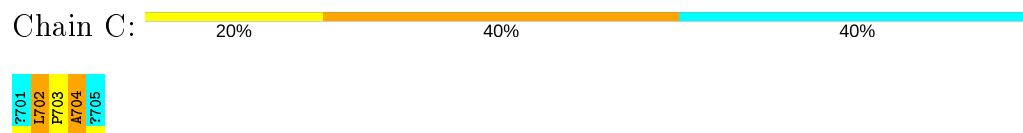


4.2.18 Score per residue for model 18

- Molecule 1: Sortase

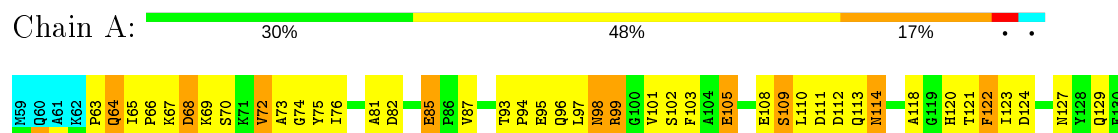


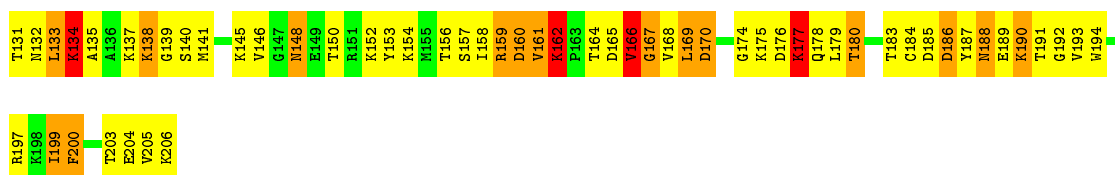
- Molecule 2: (PHQ)LPA(B27) peptide



4.2.19 Score per residue for model 19

- Molecule 1: Sortase





- Molecule 2: (PHQ)LPA(B27) peptide

Chain C: 20% 40% 40%



4.2.20 Score per residue for model 20

- Molecule 1: Sortase

Chain A: 37% 40% 19% . .



- Molecule 2: (PHQ)LPA(B27) peptide

Chain C: 20% 40% 40%



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
ProcheckNMR	refinement	
MOLMOL	structure solution	

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

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1810
Number of shifts mapped to atoms	1806
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	4
Assignment completeness (well-defined parts)	89%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B27, CA, PHQ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1146	1146	1146	106±11
2	C	20	23	22	6±2
All	All	23340	23380	23360	2180

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 47.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:158:ILE:HD12	1:A:159:ARG:N	0.89	1.83	13	3
2:C:702:LEU:HD12	2:C:702:LEU:N	0.85	1.87	10	7
2:C:702:LEU:N	2:C:702:LEU:HD12	0.84	1.88	15	12
1:A:165:ASP:O	1:A:168:VAL:HG23	0.81	1.76	10	2
1:A:133:LEU:HD13	1:A:136:ALA:HB3	0.81	1.50	18	2
1:A:118:ALA:HB1	2:C:704:ALA:HB2	0.79	1.52	1	8
1:A:158:ILE:HD12	1:A:200:PHE:CD1	0.78	2.13	17	2
1:A:158:ILE:HD12	1:A:200:PHE:CD2	0.78	2.13	6	1
1:A:81:ALA:HB2	1:A:136:ALA:HB2	0.76	1.57	12	19
1:A:181:LEU:HD13	1:A:182:ILE:N	0.75	1.95	14	4
1:A:188:ASN:HD21	1:A:192:GLY:N	0.75	1.79	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:LEU:HD23	1:A:182:ILE:N	0.74	1.95	11	2
1:A:63:PRO:O	1:A:110:LEU:HD13	0.74	1.82	10	4
1:A:64:GLN:H	1:A:64:GLN:HE21	0.73	1.26	14	1
1:A:101:VAL:HG11	1:A:130:PHE:CE2	0.73	2.19	5	14
1:A:176:ASP:O	1:A:177:LYS:O	0.73	2.07	20	20
1:A:72:VAL:HG12	1:A:88:TYR:CE1	0.72	2.18	1	10
1:A:188:ASN:ND2	1:A:193:VAL:H	0.72	1.82	16	5
1:A:64:GLN:NE2	1:A:64:GLN:N	0.71	2.39	3	9
1:A:98:ASN:HD21	1:A:99:ARG:NE	0.71	1.84	11	9
1:A:101:VAL:HG23	1:A:101:VAL:O	0.70	1.86	17	7
1:A:160:ASP:O	1:A:161:VAL:HG13	0.70	1.87	7	5
1:A:101:VAL:O	1:A:101:VAL:HG23	0.70	1.86	20	12
1:A:163:PRO:O	2:C:702:LEU:HD11	0.69	1.87	6	2
1:A:65:ILE:HD13	1:A:65:ILE:N	0.69	2.03	10	4
1:A:104:ALA:HB3	1:A:116:SER:OG	0.69	1.87	14	2
1:A:98:ASN:ND2	1:A:99:ARG:NE	0.69	2.41	7	6
1:A:141:MET:SD	1:A:142:VAL:N	0.69	2.66	11	6
1:A:128:TYR:CE2	1:A:129:GLN:NE2	0.69	2.61	8	3
1:A:128:TYR:CZ	1:A:129:GLN:NE2	0.69	2.61	9	1
1:A:110:LEU:HD23	1:A:110:LEU:H	0.69	1.46	12	3
1:A:101:VAL:HG11	1:A:130:PHE:CZ	0.69	2.23	17	3
1:A:166:VAL:O	1:A:168:VAL:N	0.69	2.26	17	20
1:A:114:ASN:ND2	1:A:178:GLN:NE2	0.69	2.40	8	6
1:A:188:ASN:HD21	1:A:192:GLY:H	0.68	1.31	15	2
1:A:64:GLN:N	1:A:64:GLN:NE2	0.68	2.40	6	6
1:A:156:THR:OG1	1:A:203:THR:HG23	0.68	1.88	3	11
1:A:188:ASN:ND2	1:A:192:GLY:N	0.68	2.42	15	5
1:A:64:GLN:NE2	1:A:64:GLN:H	0.68	1.87	18	5
1:A:64:GLN:N	1:A:64:GLN:HE21	0.67	1.87	18	1
1:A:68:ASP:O	1:A:70:SER:N	0.66	2.28	4	20
1:A:68:ASP:C	1:A:70:SER:N	0.66	2.48	2	20
1:A:188:ASN:HD22	1:A:193:VAL:H	0.66	1.33	7	3
1:A:122:PHE:O	1:A:131:THR:HG21	0.66	1.91	17	8
1:A:101:VAL:CG2	1:A:117:ILE:HG22	0.66	2.21	14	1
1:A:162:LYS:CD	1:A:162:LYS:H	0.65	2.01	11	1
1:A:107:ASN:N	1:A:107:ASN:HD22	0.65	1.89	12	2
1:A:107:ASN:H	1:A:107:ASN:ND2	0.65	1.87	14	1
1:A:81:ALA:O	1:A:132:ASN:ND2	0.65	2.30	10	18
1:A:64:GLN:H	1:A:64:GLN:NE2	0.65	1.89	3	8
1:A:197:ARG:HE	2:C:702:LEU:HD13	0.65	1.52	18	3
1:A:181:LEU:HD22	1:A:200:PHE:CE2	0.65	2.27	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:VAL:HG22	1:A:162:LYS:N	0.64	2.07	14	1
1:A:158:ILE:HD12	1:A:200:PHE:CE2	0.64	2.28	6	1
1:A:109:SER:O	1:A:115:ILE:HD11	0.64	1.93	17	2
1:A:130:PHE:CE1	1:A:181:LEU:HD11	0.64	2.28	11	2
1:A:199:ILE:HD12	1:A:199:ILE:C	0.63	2.13	3	5
2:C:702:LEU:CD1	2:C:702:LEU:N	0.63	2.57	15	8
1:A:113:GLN:HE22	1:A:177:LYS:NZ	0.63	1.90	11	1
1:A:95:GLU:O	1:A:98:ASN:ND2	0.63	2.32	19	7
1:A:83:ILE:HD11	1:A:132:ASN:OD1	0.63	1.94	10	6
1:A:98:ASN:ND2	1:A:99:ARG:CZ	0.63	2.62	16	3
1:A:187:TYR:CE2	1:A:188:ASN:O	0.63	2.52	17	4
1:A:203:THR:O	1:A:205:VAL:HG23	0.63	1.94	11	12
1:A:97:LEU:CD2	1:A:120:HIS:CE1	0.63	2.82	17	1
1:A:163:PRO:C	2:C:702:LEU:HD11	0.62	2.14	4	5
1:A:64:GLN:HE21	1:A:64:GLN:N	0.62	1.90	14	1
1:A:134:LYS:H	1:A:134:LYS:CD	0.62	2.08	18	7
1:A:187:TYR:CE1	1:A:188:ASN:O	0.62	2.53	1	16
1:A:64:GLN:NE2	1:A:64:GLN:O	0.62	2.31	4	9
1:A:188:ASN:ND2	1:A:191:THR:OG1	0.62	2.31	16	5
1:A:138:LYS:O	1:A:140:SER:N	0.62	2.33	18	20
1:A:200:PHE:CD1	1:A:200:PHE:N	0.62	2.64	17	10
1:A:96:GLN:HE21	1:A:99:ARG:NH1	0.62	1.93	6	3
1:A:64:GLN:O	1:A:64:GLN:NE2	0.62	2.33	10	8
1:A:114:ASN:ND2	1:A:114:ASN:O	0.61	2.33	17	1
1:A:114:ASN:ND2	1:A:170:ASP:O	0.61	2.34	7	6
2:C:702:LEU:N	2:C:702:LEU:CD1	0.61	2.62	2	9
1:A:98:ASN:HD21	1:A:99:ARG:NH1	0.61	1.92	4	2
1:A:188:ASN:OD1	1:A:190:LYS:N	0.61	2.33	20	4
1:A:157:SER:C	1:A:158:ILE:HD12	0.61	2.15	18	1
1:A:148:ASN:ND2	1:A:148:ASN:C	0.61	2.54	20	8
1:A:114:ASN:OD1	1:A:178:GLN:NE2	0.61	2.33	9	6
1:A:114:ASN:ND2	1:A:169:LEU:O	0.61	2.33	12	4
1:A:73:ALA:N	1:A:87:VAL:O	0.61	2.34	1	17
1:A:96:GLN:O	1:A:98:ASN:N	0.61	2.34	6	18
1:A:133:LEU:O	1:A:135:ALA:N	0.61	2.34	9	17
1:A:64:GLN:CA	1:A:64:GLN:HE21	0.61	2.08	18	4
1:A:92:ALA:O	1:A:97:LEU:HD11	0.60	1.96	20	6
1:A:98:ASN:HD21	1:A:99:ARG:HE	0.60	1.39	8	2
1:A:199:ILE:C	1:A:199:ILE:HD12	0.60	2.16	4	7
1:A:103:PHE:O	1:A:105:GLU:N	0.60	2.34	14	11
1:A:168:VAL:O	1:A:170:ASP:N	0.60	2.35	3	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:ARG:NH2	2:C:703:PRO:O	0.60	2.35	4	5
1:A:99:ARG:CG	1:A:99:ARG:HH11	0.60	2.10	3	3
1:A:114:ASN:ND2	1:A:178:GLN:HE21	0.60	1.93	4	3
1:A:72:VAL:CG2	1:A:74:GLY:O	0.60	2.49	6	7
1:A:161:VAL:HG21	1:A:165:ASP:CB	0.60	2.25	14	1
1:A:98:ASN:OD1	1:A:99:ARG:N	0.60	2.34	14	1
1:A:107:ASN:HD22	1:A:107:ASN:N	0.60	1.94	20	1
1:A:64:GLN:HE21	1:A:64:GLN:H	0.60	1.37	18	1
1:A:68:ASP:C	1:A:70:SER:H	0.60	1.98	11	20
1:A:197:ARG:CG	1:A:197:ARG:HH11	0.60	2.10	18	5
1:A:125:ARG:CG	1:A:125:ARG:HH11	0.60	2.10	8	6
1:A:69:LYS:O	1:A:99:ARG:NH1	0.60	2.35	18	1
1:A:159:ARG:CG	1:A:159:ARG:HH11	0.60	2.09	12	3
1:A:75:TYR:CD2	1:A:85:GLU:O	0.59	2.55	8	7
1:A:65:ILE:HD13	1:A:65:ILE:H	0.59	1.57	14	2
1:A:113:GLN:NE2	1:A:173:LYS:O	0.59	2.35	8	3
1:A:159:ARG:CG	1:A:159:ARG:NH1	0.59	2.65	12	2
1:A:148:ASN:C	1:A:148:ASN:ND2	0.59	2.55	7	11
1:A:64:GLN:CD	1:A:64:GLN:N	0.59	2.56	20	9
1:A:162:LYS:H	1:A:162:LYS:CD	0.59	2.09	14	4
1:A:98:ASN:HD21	1:A:99:ARG:CZ	0.59	2.11	14	4
1:A:99:ARG:HH11	1:A:99:ARG:CG	0.59	2.11	10	5
1:A:152:LYS:N	1:A:206:LYS:OXT	0.59	2.35	16	1
1:A:107:ASN:ND2	1:A:107:ASN:N	0.58	2.50	20	4
1:A:65:ILE:CD1	1:A:65:ILE:H	0.58	2.11	14	1
1:A:197:ARG:HH11	1:A:197:ARG:CG	0.58	2.11	16	4
1:A:189:GLU:H	1:A:189:GLU:CD	0.58	2.00	7	1
1:A:98:ASN:ND2	1:A:99:ARG:HE	0.58	1.96	8	2
1:A:158:ILE:HD12	1:A:159:ARG:H	0.58	1.54	13	3
1:A:72:VAL:HG12	1:A:88:TYR:CZ	0.58	2.33	10	7
1:A:73:ALA:O	1:A:146:VAL:HG23	0.58	1.99	4	5
1:A:63:PRO:O	1:A:110:LEU:CD1	0.58	2.51	19	2
1:A:162:LYS:CD	1:A:162:LYS:N	0.58	2.64	14	2
1:A:188:ASN:HD21	1:A:191:THR:N	0.58	1.95	15	3
1:A:197:ARG:NH2	2:C:702:LEU:O	0.58	2.37	3	1
1:A:64:GLN:N	1:A:64:GLN:CD	0.58	2.57	9	6
1:A:89:PRO:O	1:A:96:GLN:NE2	0.58	2.36	8	3
1:A:141:MET:SD	1:A:153:TYR:O	0.58	2.62	6	5
1:A:137:LYS:O	1:A:138:LYS:O	0.58	2.21	12	20
1:A:110:LEU:N	1:A:110:LEU:HD23	0.57	2.14	19	1
1:A:125:ARG:NH1	1:A:125:ARG:CG	0.57	2.67	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:LYS:H	1:A:134:LYS:CE	0.57	2.11	19	2
1:A:96:GLN:NE2	1:A:99:ARG:NH1	0.57	2.51	6	2
1:A:113:GLN:NE2	1:A:177:LYS:CE	0.57	2.67	11	1
1:A:64:GLN:HE21	1:A:64:GLN:CA	0.57	2.12	3	8
1:A:77:GLU:N	1:A:77:GLU:CD	0.57	2.57	3	2
1:A:197:ARG:CG	1:A:197:ARG:NH1	0.57	2.67	20	5
1:A:171:GLU:N	1:A:172:GLN:OE1	0.57	2.38	7	1
1:A:169:LEU:O	1:A:170:ASP:C	0.57	2.42	19	20
1:A:174:GLY:O	1:A:175:LYS:C	0.57	2.41	4	20
1:A:105:GLU:OE1	1:A:169:LEU:HD13	0.57	1.99	3	1
1:A:99:ARG:NH1	1:A:99:ARG:CG	0.57	2.67	17	6
1:A:123:ILE:HG23	1:A:124:ASP:N	0.57	2.15	10	19
1:A:163:PRO:O	2:C:702:LEU:CD1	0.57	2.52	6	1
1:A:134:LYS:CD	1:A:134:LYS:H	0.57	2.13	17	10
1:A:163:PRO:CA	1:A:197:ARG:HH21	0.57	2.13	11	1
1:A:169:LEU:N	1:A:169:LEU:HD23	0.57	2.15	14	1
1:A:197:ARG:NH1	2:C:704:ALA:O	0.56	2.38	6	3
1:A:120:HIS:N	1:A:129:GLN:OE1	0.56	2.37	14	1
1:A:169:LEU:O	1:A:171:GLU:N	0.56	2.38	11	6
1:A:205:VAL:HG12	1:A:206:LYS:N	0.56	2.14	4	14
1:A:168:VAL:C	1:A:170:ASP:N	0.56	2.58	5	20
1:A:77:GLU:N	1:A:77:GLU:OE1	0.56	2.38	18	2
1:A:107:ASN:H	1:A:107:ASN:HD22	0.56	1.42	14	2
1:A:197:ARG:NE	2:C:702:LEU:HD13	0.56	2.15	5	1
1:A:144:PHE:CZ	1:A:146:VAL:CG1	0.56	2.88	7	1
1:A:197:ARG:NH2	2:C:704:ALA:C	0.56	2.59	7	1
1:A:193:VAL:HG12	1:A:194:TRP:N	0.56	2.14	20	9
2:C:702:LEU:O	2:C:702:LEU:HD12	0.56	1.99	6	1
1:A:68:ASP:N	1:A:68:ASP:OD1	0.56	2.38	18	4
1:A:77:GLU:CD	1:A:77:GLU:N	0.56	2.59	17	2
1:A:160:ASP:OD1	1:A:160:ASP:N	0.56	2.36	7	1
1:A:106:GLU:OE2	1:A:107:ASN:ND2	0.56	2.39	11	1
1:A:140:SER:OG	1:A:155:MET:SD	0.56	2.64	16	1
1:A:168:VAL:C	1:A:170:ASP:H	0.56	2.03	5	16
1:A:64:GLN:HE21	1:A:64:GLN:C	0.56	2.04	18	7
1:A:197:ARG:NH1	1:A:197:ARG:CG	0.56	2.66	18	4
1:A:68:ASP:OD1	1:A:68:ASP:N	0.56	2.39	20	1
1:A:92:ALA:O	1:A:97:LEU:CD1	0.56	2.54	15	10
1:A:98:ASN:ND2	1:A:99:ARG:NH1	0.56	2.54	16	4
1:A:87:VAL:CG1	1:A:103:PHE:CZ	0.56	2.89	13	6
1:A:185:ASP:CG	1:A:198:LYS:HZ2	0.55	2.05	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:188:ASN:ND2	1:A:195:GLU:CD	0.55	2.60	5	10
1:A:74:GLY:C	1:A:75:TYR:CD1	0.55	2.80	19	3
1:A:75:TYR:CE1	1:A:86:PRO:N	0.55	2.74	9	1
1:A:185:ASP:O	1:A:186:ASP:CB	0.55	2.54	12	2
1:A:129:GLN:OE1	1:A:129:GLN:N	0.55	2.39	1	1
1:A:129:GLN:N	1:A:129:GLN:OE1	0.55	2.40	17	2
1:A:113:GLN:CD	1:A:113:GLN:N	0.55	2.60	18	7
1:A:64:GLN:C	1:A:64:GLN:HE21	0.55	2.05	5	6
1:A:166:VAL:C	1:A:168:VAL:N	0.55	2.59	20	20
1:A:133:LEU:HD13	1:A:133:LEU:O	0.55	2.01	6	9
1:A:151:ARG:NH2	1:A:204:GLU:OE2	0.55	2.39	20	1
1:A:132:ASN:O	1:A:132:ASN:ND2	0.55	2.40	13	2
1:A:114:ASN:CG	1:A:178:GLN:NE2	0.55	2.61	4	4
1:A:185:ASP:OD1	1:A:186:ASP:N	0.55	2.36	10	4
1:A:188:ASN:ND2	1:A:188:ASN:C	0.55	2.60	15	1
1:A:159:ARG:NH1	1:A:159:ARG:CG	0.55	2.67	19	2
1:A:133:LEU:CD1	1:A:136:ALA:HB3	0.55	2.27	18	2
1:A:134:LYS:CE	1:A:134:LYS:H	0.54	2.16	18	3
1:A:96:GLN:NE2	1:A:99:ARG:HH12	0.54	2.00	12	2
1:A:131:THR:O	1:A:134:LYS:CD	0.54	2.55	17	3
1:A:125:ARG:CG	1:A:125:ARG:NH1	0.54	2.68	11	4
1:A:113:GLN:N	1:A:113:GLN:CD	0.54	2.60	7	1
1:A:113:GLN:NE2	1:A:177:LYS:NZ	0.54	2.55	11	1
1:A:146:VAL:HG13	1:A:146:VAL:O	0.54	2.02	5	1
1:A:194:TRP:CD1	1:A:194:TRP:N	0.54	2.75	1	7
1:A:156:THR:OG1	1:A:203:THR:CG2	0.54	2.56	3	6
1:A:205:VAL:O	1:A:206:LYS:C	0.54	2.46	18	4
1:A:92:ALA:O	1:A:97:LEU:HD23	0.54	2.02	7	3
1:A:85:GLU:N	1:A:85:GLU:OE2	0.54	2.41	10	1
1:A:188:ASN:ND2	1:A:193:VAL:O	0.54	2.41	16	2
1:A:143:TYR:CE1	1:A:152:LYS:CG	0.54	2.91	18	2
1:A:104:ALA:HB1	2:C:703:PRO:HG3	0.54	1.79	4	5
1:A:183:THR:O	1:A:183:THR:HG23	0.54	2.03	18	4
1:A:183:THR:HG23	1:A:183:THR:O	0.54	2.00	17	5
1:A:168:VAL:HG11	1:A:199:ILE:HG21	0.54	1.80	10	1
1:A:95:GLU:CD	1:A:95:GLU:H	0.54	2.06	5	1
1:A:68:ASP:O	1:A:71:LYS:N	0.54	2.30	11	8
1:A:114:ASN:CG	1:A:178:GLN:HE21	0.54	2.07	4	1
1:A:130:PHE:CD1	1:A:181:LEU:HD11	0.54	2.38	7	1
1:A:132:ASN:ND2	1:A:132:ASN:C	0.54	2.60	13	1
1:A:137:LYS:O	1:A:140:SER:OG	0.53	2.26	16	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:VAL:CG2	1:A:101:VAL:O	0.53	2.55	17	9
1:A:85:GLU:N	1:A:85:GLU:CD	0.53	2.61	10	2
1:A:160:ASP:C	1:A:161:VAL:HG22	0.53	2.23	6	7
1:A:164:THR:O	1:A:164:THR:HG22	0.53	2.04	10	1
1:A:200:PHE:N	1:A:200:PHE:CD1	0.53	2.76	2	7
1:A:194:TRP:N	1:A:194:TRP:CD1	0.53	2.76	18	10
1:A:185:ASP:CG	1:A:186:ASP:N	0.53	2.62	7	3
1:A:98:ASN:HD22	1:A:99:ARG:NH1	0.53	2.00	10	1
1:A:133:LEU:O	1:A:133:LEU:HD13	0.53	2.03	14	3
1:A:152:LYS:O	1:A:205:VAL:N	0.53	2.34	19	8
1:A:159:ARG:HH11	1:A:159:ARG:CG	0.53	2.15	16	1
1:A:149:GLU:CD	1:A:150:THR:N	0.53	2.62	16	1
2:C:703:PRO:O	2:C:704:ALA:O	0.52	2.28	11	13
1:A:169:LEU:HD23	1:A:169:LEU:N	0.52	2.20	3	1
1:A:80:ASP:OD1	1:A:80:ASP:N	0.52	2.37	15	1
1:A:92:ALA:HB1	1:A:97:LEU:HD21	0.52	1.80	1	5
1:A:96:GLN:C	1:A:98:ASN:N	0.52	2.63	5	18
1:A:130:PHE:O	1:A:134:LYS:CE	0.52	2.58	12	6
1:A:101:VAL:O	1:A:101:VAL:CG2	0.52	2.56	20	6
1:A:130:PHE:CE1	1:A:181:LEU:HD21	0.52	2.38	14	1
1:A:199:ILE:HD12	1:A:199:ILE:O	0.52	2.04	2	6
1:A:78:ILE:O	1:A:82:ASP:N	0.52	2.43	15	6
1:A:132:ASN:CG	1:A:132:ASN:O	0.52	2.48	15	3
1:A:99:ARG:CG	1:A:99:ARG:NH1	0.52	2.70	19	2
1:A:114:ASN:C	1:A:114:ASN:HD22	0.52	2.08	2	2
1:A:127:ASN:C	1:A:127:ASN:HD22	0.52	2.08	2	1
1:A:75:TYR:CD1	1:A:75:TYR:N	0.52	2.78	12	3
1:A:183:THR:O	1:A:183:THR:CG2	0.52	2.58	18	1
1:A:133:LEU:C	1:A:135:ALA:N	0.52	2.63	2	17
1:A:205:VAL:CG1	1:A:206:LYS:N	0.52	2.72	10	14
1:A:193:VAL:CG1	1:A:194:TRP:N	0.52	2.73	8	6
1:A:161:VAL:O	1:A:162:LYS:O	0.52	2.28	6	13
1:A:173:LYS:NZ	1:A:176:ASP:O	0.52	2.43	13	1
1:A:127:ASN:O	1:A:128:TYR:O	0.51	2.28	18	8
1:A:185:ASP:CG	1:A:186:ASP:H	0.51	2.08	16	3
1:A:148:ASN:ND2	1:A:148:ASN:O	0.51	2.42	20	4
1:A:148:ASN:CG	1:A:148:ASN:O	0.51	2.48	20	1
1:A:96:GLN:HE21	1:A:99:ARG:HH12	0.51	1.47	20	1
1:A:181:LEU:HD13	1:A:182:ILE:H	0.51	1.65	12	4
1:A:85:GLU:OE2	1:A:129:GLN:O	0.51	2.29	11	5
1:A:152:LYS:C	1:A:153:TYR:CD1	0.51	2.83	2	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:LYS:C	1:A:140:SER:N	0.51	2.64	1	20
1:A:74:GLY:O	1:A:87:VAL:N	0.51	2.43	15	6
1:A:110:LEU:CD2	1:A:110:LEU:N	0.51	2.74	19	2
1:A:114:ASN:ND2	1:A:180:THR:OG1	0.51	2.40	7	2
1:A:151:ARG:NH1	1:A:204:GLU:OE2	0.51	2.44	20	1
1:A:85:GLU:OE2	1:A:128:TYR:O	0.51	2.28	1	2
2:C:702:LEU:O	2:C:703:PRO:O	0.51	2.29	10	7
1:A:159:ARG:O	1:A:160:ASP:OD1	0.51	2.29	14	3
1:A:148:ASN:C	1:A:148:ASN:HD22	0.51	2.09	19	5
1:A:148:ASN:HD22	1:A:148:ASN:C	0.51	2.09	4	8
1:A:83:ILE:CD1	1:A:132:ASN:OD1	0.51	2.59	6	4
1:A:113:GLN:NE2	1:A:114:ASN:N	0.51	2.58	9	1
1:A:132:ASN:O	1:A:132:ASN:CG	0.51	2.49	12	3
1:A:87:VAL:CG1	1:A:103:PHE:CE1	0.51	2.94	2	13
1:A:197:ARG:HE	2:C:702:LEU:HD22	0.51	1.66	8	2
1:A:92:ALA:HB3	2:C:703:PRO:CB	0.51	2.36	15	3
1:A:106:GLU:CG	1:A:107:ASN:N	0.51	2.73	12	1
1:A:85:GLU:OE1	1:A:128:TYR:O	0.50	2.30	15	3
1:A:121:THR:OG1	1:A:134:LYS:NZ	0.50	2.44	11	2
1:A:65:ILE:H	1:A:65:ILE:CD1	0.50	2.17	10	3
1:A:141:MET:SD	1:A:141:MET:C	0.50	2.88	11	2
1:A:168:VAL:HG21	1:A:199:ILE:HG21	0.50	1.82	15	1
1:A:170:ASP:OD1	1:A:180:THR:OG1	0.50	2.28	17	1
1:A:181:LEU:HD22	1:A:200:PHE:CD2	0.50	2.41	7	1
1:A:164:THR:HA	2:C:702:LEU:HD11	0.50	1.84	20	3
1:A:166:VAL:C	1:A:168:VAL:H	0.50	2.10	3	13
1:A:144:PHE:CE2	1:A:146:VAL:HG11	0.50	2.41	3	1
1:A:144:PHE:CZ	1:A:146:VAL:HG11	0.50	2.41	7	1
1:A:101:VAL:CG1	1:A:130:PHE:CZ	0.50	2.93	17	1
1:A:114:ASN:C	1:A:114:ASN:ND2	0.50	2.65	2	2
1:A:113:GLN:NE2	1:A:113:GLN:C	0.50	2.65	9	1
1:A:96:GLN:C	1:A:98:ASN:H	0.50	2.09	11	15
1:A:197:ARG:NE	2:C:702:LEU:HD22	0.50	2.22	8	2
1:A:185:ASP:OD2	1:A:186:ASP:OD1	0.50	2.30	7	1
1:A:105:GLU:OE2	1:A:108:GLU:OE1	0.50	2.29	15	4
1:A:114:ASN:OD1	1:A:178:GLN:OE1	0.50	2.30	17	1
1:A:96:GLN:N	1:A:96:GLN:CD	0.50	2.65	10	4
1:A:123:ILE:CG2	1:A:124:ASP:N	0.50	2.75	10	15
1:A:164:THR:N	2:C:702:LEU:HD11	0.50	2.22	7	2
1:A:160:ASP:O	1:A:161:VAL:CG1	0.50	2.59	7	2
1:A:75:TYR:CE1	1:A:85:GLU:C	0.50	2.84	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:LYS:NZ	1:A:178:GLN:HE21	0.50	2.03	11	1
1:A:85:GLU:OE1	1:A:129:GLN:O	0.50	2.30	18	3
1:A:148:ASN:O	1:A:148:ASN:CG	0.50	2.49	11	2
1:A:169:LEU:O	1:A:170:ASP:OD1	0.50	2.30	17	4
1:A:133:LEU:O	1:A:136:ALA:N	0.50	2.45	2	12
1:A:114:ASN:O	1:A:114:ASN:CG	0.50	2.51	15	2
1:A:72:VAL:CG2	1:A:72:VAL:O	0.49	2.60	1	3
1:A:188:ASN:C	1:A:188:ASN:ND2	0.49	2.65	12	1
1:A:114:ASN:OD1	1:A:170:ASP:O	0.49	2.30	9	4
1:A:113:GLN:HE22	1:A:172:GLN:N	0.49	2.05	13	2
1:A:188:ASN:OD1	1:A:191:THR:N	0.49	2.45	16	4
1:A:176:ASP:OD1	1:A:176:ASP:O	0.49	2.30	9	2
1:A:98:ASN:ND2	1:A:99:ARG:N	0.49	2.60	3	1
1:A:197:ARG:CZ	2:C:702:LEU:HD13	0.49	2.37	11	2
1:A:161:VAL:CG2	1:A:162:LYS:N	0.49	2.75	14	1
1:A:114:ASN:OD1	1:A:169:LEU:O	0.49	2.30	5	1
1:A:114:ASN:OD1	1:A:114:ASN:O	0.49	2.31	4	1
1:A:84:LYS:N	1:A:85:GLU:OE2	0.49	2.43	6	1
1:A:115:ILE:HG22	1:A:115:ILE:O	0.49	2.08	7	7
1:A:128:TYR:CD2	1:A:129:GLN:OE1	0.49	2.66	8	1
1:A:114:ASN:ND2	1:A:178:GLN:CD	0.49	2.66	8	1
1:A:161:VAL:HG21	1:A:168:VAL:CG1	0.49	2.38	9	1
1:A:64:GLN:CA	1:A:64:GLN:NE2	0.49	2.75	6	6
1:A:137:LYS:O	1:A:140:SER:CB	0.49	2.61	12	14
1:A:165:ASP:O	1:A:167:GLY:N	0.49	2.45	18	7
1:A:101:VAL:CG1	1:A:130:PHE:CE2	0.49	2.96	12	10
1:A:134:LYS:CD	1:A:134:LYS:N	0.49	2.75	7	5
1:A:96:GLN:N	1:A:96:GLN:NE2	0.49	2.60	1	1
1:A:138:LYS:C	1:A:140:SER:H	0.49	2.11	16	20
1:A:170:ASP:OD1	1:A:170:ASP:O	0.49	2.31	10	1
1:A:156:THR:CG2	1:A:203:THR:OG1	0.49	2.61	18	2
1:A:107:ASN:ND2	1:A:107:ASN:H	0.49	2.05	2	2
1:A:64:GLN:NE2	1:A:64:GLN:CA	0.49	2.75	3	6
1:A:75:TYR:CD1	1:A:85:GLU:O	0.49	2.66	9	1
1:A:114:ASN:CG	1:A:114:ASN:O	0.49	2.50	12	2
1:A:170:ASP:O	1:A:170:ASP:OD1	0.49	2.31	18	2
1:A:170:ASP:OD2	1:A:180:THR:OG1	0.49	2.30	19	2
1:A:95:GLU:N	1:A:95:GLU:OE1	0.49	2.46	5	1
1:A:64:GLN:O	1:A:65:ILE:C	0.49	2.50	3	15
1:A:188:ASN:ND2	1:A:195:GLU:OE2	0.49	2.46	9	3
1:A:205:VAL:O	1:A:206:LYS:O	0.49	2.30	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:SER:C	1:A:111:ASP:N	0.49	2.65	9	6
1:A:83:ILE:CG1	1:A:132:ASN:OD1	0.49	2.60	12	2
1:A:165:ASP:O	1:A:166:VAL:C	0.48	2.52	16	14
1:A:157:SER:O	1:A:201:VAL:N	0.48	2.44	4	4
1:A:95:GLU:O	1:A:98:ASN:OD1	0.48	2.29	14	1
1:A:103:PHE:C	1:A:105:GLU:N	0.48	2.66	10	10
1:A:92:ALA:O	1:A:97:LEU:HD13	0.48	2.08	5	3
1:A:169:LEU:C	1:A:170:ASP:OD1	0.48	2.52	17	3
1:A:110:LEU:HD23	1:A:110:LEU:N	0.48	2.23	4	1
1:A:182:ILE:HG23	1:A:199:ILE:HG22	0.48	1.83	11	2
1:A:80:ASP:OD1	1:A:80:ASP:O	0.48	2.32	11	1
1:A:96:GLN:CD	1:A:96:GLN:N	0.48	2.67	15	2
1:A:81:ALA:HB2	1:A:136:ALA:CB	0.48	2.38	2	3
1:A:178:GLN:OE1	1:A:180:THR:N	0.48	2.46	11	2
1:A:110:LEU:H	1:A:110:LEU:HD23	0.48	1.68	14	1
1:A:95:GLU:O	1:A:98:ASN:CG	0.48	2.52	14	1
1:A:67:LYS:CG	1:A:67:LYS:O	0.48	2.61	19	2
1:A:78:ILE:HB	1:A:81:ALA:HB3	0.48	1.84	18	6
1:A:188:ASN:C	1:A:188:ASN:OD1	0.48	2.52	10	1
1:A:134:LYS:NZ	1:A:183:THR:OG1	0.48	2.46	12	1
1:A:77:GLU:O	1:A:77:GLU:OE1	0.48	2.31	18	1
1:A:127:ASN:ND2	1:A:127:ASN:O	0.48	2.47	19	1
1:A:146:VAL:O	1:A:147:GLY:C	0.48	2.51	2	11
1:A:133:LEU:HD12	1:A:200:PHE:CZ	0.48	2.44	4	2
1:A:176:ASP:O	1:A:177:LYS:C	0.48	2.51	20	8
1:A:95:GLU:OE2	1:A:96:GLN:OE1	0.48	2.31	9	1
1:A:68:ASP:O	1:A:69:LYS:C	0.48	2.52	4	20
1:A:97:LEU:HD11	1:A:119:GLY:HA2	0.48	1.85	8	1
2:C:703:PRO:O	2:C:704:ALA:C	0.48	2.51	20	5
1:A:113:GLN:C	1:A:113:GLN:HE21	0.48	2.11	9	1
1:A:134:LYS:N	1:A:134:LYS:CD	0.48	2.77	9	9
1:A:113:GLN:NE2	1:A:113:GLN:CA	0.48	2.76	3	1
1:A:151:ARG:NH2	1:A:153:TYR:OH	0.48	2.47	6	1
1:A:161:VAL:HG22	1:A:162:LYS:H	0.48	1.69	14	1
1:A:133:LEU:C	1:A:135:ALA:H	0.48	2.12	19	4
1:A:191:THR:OG1	1:A:193:VAL:HG12	0.47	2.07	4	6
1:A:124:ASP:OD1	1:A:124:ASP:O	0.47	2.31	10	1
1:A:164:THR:N	2:C:702:LEU:HD21	0.47	2.23	20	1
1:A:111:ASP:CG	1:A:151:ARG:HH22	0.47	2.13	10	2
1:A:115:ILE:O	1:A:115:ILE:HG22	0.47	2.09	6	6
1:A:75:TYR:CA	1:A:87:VAL:HG23	0.47	2.39	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:SER:C	1:A:111:ASP:H	0.47	2.12	8	5
1:A:199:ILE:O	1:A:199:ILE:HD12	0.47	2.10	8	1
1:A:111:ASP:OD1	1:A:151:ARG:NH1	0.47	2.47	10	1
1:A:114:ASN:HD22	1:A:178:GLN:CD	0.47	2.12	14	1
1:A:161:VAL:HG21	1:A:168:VAL:HG22	0.47	1.87	16	1
1:A:75:TYR:HA	1:A:87:VAL:HG23	0.47	1.86	8	5
1:A:85:GLU:CB	1:A:86:PRO:CD	0.47	2.93	16	2
1:A:178:GLN:OE1	1:A:179:LEU:N	0.47	2.48	4	2
1:A:76:ILE:CG2	1:A:85:GLU:OE1	0.47	2.63	7	1
1:A:170:ASP:CG	1:A:170:ASP:O	0.47	2.53	19	1
1:A:106:GLU:OE1	1:A:107:ASN:ND2	0.47	2.48	1	1
1:A:189:GLU:N	1:A:189:GLU:CD	0.47	2.66	7	1
1:A:160:ASP:N	1:A:160:ASP:OD1	0.47	2.47	8	1
1:A:107:ASN:N	1:A:107:ASN:ND2	0.47	2.62	14	2
1:A:67:LYS:O	1:A:67:LYS:CG	0.47	2.63	17	1
1:A:188:ASN:HD21	1:A:191:THR:C	0.47	2.13	7	3
1:A:163:PRO:C	1:A:197:ARG:HH21	0.46	2.13	11	1
1:A:197:ARG:NH2	2:C:702:LEU:HD13	0.46	2.25	11	1
1:A:188:ASN:OD1	1:A:188:ASN:C	0.46	2.54	16	1
1:A:144:PHE:O	1:A:150:THR:HG23	0.46	2.10	18	1
1:A:64:GLN:O	1:A:66:PRO:N	0.46	2.48	3	4
1:A:144:PHE:CG	1:A:145:LYS:N	0.46	2.83	18	1
1:A:107:ASN:C	1:A:107:ASN:ND2	0.46	2.68	3	1
1:A:170:ASP:OD2	1:A:178:GLN:NE2	0.46	2.49	8	1
1:A:151:ARG:HH12	1:A:204:GLU:CD	0.46	2.14	20	1
1:A:170:ASP:CG	1:A:180:THR:HG1	0.46	2.13	19	2
1:A:141:MET:C	1:A:141:MET:SD	0.46	2.94	7	2
1:A:85:GLU:OE2	1:A:85:GLU:N	0.46	2.48	7	1
1:A:188:ASN:ND2	1:A:193:VAL:N	0.46	2.60	10	1
1:A:170:ASP:O	1:A:170:ASP:CG	0.46	2.54	8	2
1:A:84:LYS:O	1:A:85:GLU:CD	0.46	2.54	8	2
1:A:96:GLN:OE1	1:A:102:SER:OG	0.46	2.34	8	1
1:A:156:THR:OG1	1:A:203:THR:N	0.46	2.49	10	1
1:A:88:TYR:CE2	1:A:99:ARG:CD	0.46	2.99	17	1
1:A:113:GLN:CA	1:A:113:GLN:NE2	0.46	2.76	4	1
1:A:93:THR:OG1	1:A:96:GLN:OE1	0.46	2.30	15	2
1:A:158:ILE:CD1	1:A:159:ARG:N	0.46	2.71	13	1
1:A:188:ASN:ND2	1:A:192:GLY:H	0.46	2.01	15	1
1:A:114:ASN:OD1	1:A:178:GLN:CD	0.46	2.54	17	2
1:A:133:LEU:HD13	1:A:136:ALA:CB	0.46	2.33	18	1
1:A:199:ILE:CG1	1:A:199:ILE:O	0.46	2.64	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:LYS:CG	1:A:138:LYS:H	0.46	2.23	14	1
1:A:104:ALA:HB1	2:C:703:PRO:HG2	0.46	1.88	14	1
1:A:129:GLN:CD	1:A:129:GLN:N	0.45	2.70	1	1
1:A:199:ILE:CD1	1:A:199:ILE:O	0.45	2.65	2	2
1:A:153:TYR:CD2	1:A:204:GLU:HA	0.45	2.46	19	14
1:A:164:THR:HG22	1:A:164:THR:O	0.45	2.11	16	3
1:A:111:ASP:OD2	1:A:151:ARG:NH2	0.45	2.44	10	1
1:A:72:VAL:O	1:A:72:VAL:CG2	0.45	2.64	10	1
1:A:110:LEU:O	1:A:110:LEU:HD13	0.45	2.11	17	1
1:A:171:GLU:H	1:A:172:GLN:HE21	0.45	1.54	17	1
1:A:133:LEU:O	1:A:134:LYS:C	0.45	2.55	2	10
1:A:168:VAL:O	1:A:169:LEU:C	0.45	2.54	14	5
1:A:197:ARG:CD	2:C:702:LEU:HD22	0.45	2.41	10	1
1:A:75:TYR:N	1:A:145:LYS:O	0.45	2.41	14	2
1:A:81:ALA:O	1:A:82:ASP:CB	0.45	2.65	20	3
1:A:170:ASP:CG	1:A:178:GLN:HE22	0.45	2.13	8	1
1:A:72:VAL:HG23	1:A:72:VAL:O	0.45	2.11	8	2
1:A:94:PRO:O	1:A:95:GLU:C	0.45	2.53	6	2
1:A:98:ASN:ND2	1:A:99:ARG:CD	0.45	2.80	6	1
1:A:134:LYS:H	1:A:134:LYS:HD2	0.45	1.69	14	1
1:A:140:SER:OG	1:A:155:MET:CG	0.45	2.64	16	1
1:A:75:TYR:CD2	1:A:85:GLU:C	0.45	2.90	18	3
1:A:188:ASN:ND2	1:A:191:THR:N	0.45	2.65	12	2
1:A:84:LYS:O	1:A:84:LYS:CG	0.45	2.64	17	1
1:A:75:TYR:CD1	1:A:85:GLU:C	0.45	2.89	9	1
1:A:92:ALA:HB3	2:C:703:PRO:HB3	0.45	1.88	3	3
1:A:168:VAL:O	1:A:170:ASP:CG	0.45	2.54	10	1
1:A:166:VAL:O	1:A:167:GLY:C	0.45	2.56	10	9
1:A:130:PHE:O	1:A:134:LYS:NZ	0.45	2.50	12	4
1:A:178:GLN:OE1	1:A:201:VAL:HG13	0.45	2.12	10	1
1:A:205:VAL:O	1:A:206:LYS:OXT	0.45	2.35	14	1
1:A:92:ALA:HB3	2:C:703:PRO:HB2	0.45	1.89	4	1
1:A:188:ASN:CG	1:A:195:GLU:OE2	0.45	2.56	8	1
1:A:98:ASN:C	1:A:98:ASN:OD1	0.45	2.55	8	3
1:A:95:GLU:O	1:A:99:ARG:NH1	0.44	2.49	6	1
1:A:65:ILE:CD1	1:A:110:LEU:HD13	0.44	2.41	9	2
1:A:165:ASP:O	1:A:165:ASP:OD1	0.44	2.34	16	1
1:A:199:ILE:O	1:A:199:ILE:HG13	0.44	2.13	14	1
1:A:170:ASP:CG	1:A:180:THR:OG1	0.44	2.55	17	1
1:A:134:LYS:HD2	1:A:134:LYS:H	0.44	1.71	18	1
1:A:65:ILE:H	1:A:65:ILE:HD13	0.44	1.65	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:188:ASN:CG	1:A:191:THR:H	0.44	2.15	15	1
1:A:113:GLN:HA	1:A:113:GLN:NE2	0.44	2.27	15	4
1:A:93:THR:O	1:A:94:PRO:C	0.44	2.56	13	13
1:A:110:LEU:HD13	1:A:110:LEU:O	0.44	2.13	6	1
1:A:161:VAL:O	1:A:162:LYS:C	0.44	2.55	6	1
1:A:110:LEU:C	1:A:111:ASP:OD1	0.44	2.55	7	2
1:A:98:ASN:OD1	1:A:98:ASN:C	0.44	2.56	4	1
1:A:114:ASN:ND2	1:A:116:SER:OG	0.44	2.48	6	2
1:A:156:THR:CB	1:A:203:THR:HG23	0.44	2.43	17	1
1:A:104:ALA:HB3	1:A:116:SER:HB2	0.43	1.90	1	1
1:A:160:ASP:C	1:A:161:VAL:CG2	0.43	2.86	4	4
1:A:67:LYS:O	1:A:69:LYS:N	0.43	2.47	20	3
1:A:158:ILE:CD1	1:A:200:PHE:CE2	0.43	3.01	6	1
1:A:204:GLU:OE1	1:A:204:GLU:C	0.43	2.56	4	1
1:A:159:ARG:HG2	1:A:159:ARG:HH11	0.43	1.73	12	1
1:A:137:LYS:O	1:A:138:LYS:C	0.43	2.54	13	3
1:A:95:GLU:O	1:A:99:ARG:NH2	0.43	2.51	16	1
1:A:110:LEU:HD11	1:A:146:VAL:HG21	0.43	1.91	17	1
1:A:152:LYS:CE	1:A:206:LYS:OXT	0.43	2.66	4	1
1:A:114:ASN:HD21	1:A:180:THR:CB	0.43	2.26	7	1
1:A:114:ASN:OD1	1:A:171:GLU:CB	0.43	2.67	15	1
1:A:114:ASN:OD1	1:A:114:ASN:C	0.43	2.56	4	2
1:A:77:GLU:OE1	1:A:77:GLU:CA	0.43	2.62	18	1
1:A:129:GLN:CA	1:A:129:GLN:OE1	0.43	2.66	1	1
1:A:197:ARG:HG2	2:C:702:LEU:HD22	0.43	1.91	12	1
1:A:88:TYR:CD2	1:A:99:ARG:CD	0.43	3.02	15	1
1:A:199:ILE:C	1:A:199:ILE:CD1	0.43	2.86	8	2
1:A:113:GLN:HE21	1:A:177:LYS:CD	0.43	2.27	11	1
1:A:106:GLU:CG	1:A:107:ASN:H	0.43	2.27	12	1
1:A:105:GLU:OE2	1:A:108:GLU:OE2	0.43	2.37	13	1
1:A:114:ASN:HD22	1:A:178:GLN:NE2	0.43	2.08	14	1
1:A:145:LYS:CG	1:A:150:THR:OG1	0.43	2.66	19	1
1:A:65:ILE:H	1:A:65:ILE:HD12	0.43	1.73	7	2
1:A:74:GLY:C	1:A:87:VAL:CG2	0.43	2.87	6	1
1:A:177:LYS:CD	1:A:177:LYS:N	0.43	2.82	9	1
1:A:175:LYS:H	1:A:175:LYS:CD	0.43	2.25	3	1
1:A:103:PHE:O	1:A:104:ALA:C	0.43	2.57	4	3
1:A:197:ARG:HD3	2:C:702:LEU:HD22	0.43	1.91	7	1
1:A:118:ALA:HB1	2:C:704:ALA:CB	0.43	2.44	3	1
1:A:176:ASP:OD1	1:A:176:ASP:N	0.43	2.38	4	2
1:A:162:LYS:N	1:A:162:LYS:CD	0.43	2.79	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:GLN:OE1	1:A:171:GLU:C	0.42	2.57	13	1
1:A:98:ASN:HD22	1:A:99:ARG:CZ	0.42	2.27	16	1
1:A:130:PHE:CE2	1:A:181:LEU:HD11	0.42	2.49	20	2
1:A:103:PHE:C	1:A:105:GLU:H	0.42	2.17	10	3
1:A:81:ALA:C	1:A:82:ASP:OD2	0.42	2.56	12	1
1:A:161:VAL:C	1:A:162:LYS:O	0.42	2.57	18	1
1:A:96:GLN:OE1	1:A:99:ARG:CZ	0.42	2.68	18	1
1:A:151:ARG:CG	1:A:151:ARG:NH1	0.42	2.82	5	2
1:A:199:ILE:CD1	1:A:199:ILE:C	0.42	2.82	3	2
1:A:182:ILE:HG22	1:A:182:ILE:O	0.42	2.13	8	2
1:A:125:ARG:NH1	1:A:127:ASN:OD1	0.42	2.53	6	1
1:A:150:THR:HG22	1:A:150:THR:O	0.42	2.13	8	1
1:A:199:ILE:O	1:A:199:ILE:CG1	0.42	2.68	8	3
1:A:121:THR:HG22	1:A:194:TRP:CZ3	0.42	2.50	14	1
1:A:132:ASN:O	1:A:132:ASN:OD1	0.42	2.37	15	1
1:A:91:PRO:C	1:A:102:SER:HG	0.42	2.17	17	1
1:A:163:PRO:CB	1:A:197:ARG:NH2	0.42	2.82	18	1
1:A:124:ASP:O	1:A:124:ASP:CG	0.42	2.58	3	1
1:A:111:ASP:CG	1:A:151:ARG:HH12	0.42	2.17	10	1
1:A:144:PHE:CE2	1:A:146:VAL:CG1	0.42	3.03	3	1
1:A:188:ASN:OD1	1:A:192:GLY:N	0.42	2.52	10	1
1:A:178:GLN:C	1:A:178:GLN:OE1	0.42	2.58	11	1
1:A:75:TYR:CE2	1:A:86:PRO:N	0.42	2.88	2	2
1:A:67:LYS:C	1:A:69:LYS:H	0.42	2.17	3	1
1:A:183:THR:CG2	1:A:183:THR:O	0.42	2.68	17	1
1:A:70:SER:OG	1:A:99:ARG:NH1	0.42	2.50	5	1
1:A:193:VAL:HG22	1:A:194:TRP:N	0.41	2.30	3	1
1:A:136:ALA:C	1:A:137:LYS:CG	0.41	2.89	6	1
1:A:114:ASN:CG	1:A:170:ASP:O	0.41	2.59	9	3
1:A:128:TYR:CG	1:A:129:GLN:N	0.41	2.88	9	1
1:A:163:PRO:CA	1:A:197:ARG:NH2	0.41	2.83	11	1
1:A:169:LEU:O	1:A:170:ASP:O	0.41	2.38	12	1
1:A:63:PRO:HG2	1:A:110:LEU:HD23	0.41	1.91	9	1
1:A:151:ARG:CZ	1:A:204:GLU:OE2	0.41	2.68	20	1
1:A:113:GLN:NE2	1:A:113:GLN:HA	0.41	2.30	1	3
1:A:71:LYS:O	1:A:71:LYS:CG	0.41	2.69	18	1
1:A:97:LEU:HD23	1:A:120:HIS:CE1	0.41	2.50	17	1
1:A:158:ILE:CD1	1:A:200:PHE:CD1	0.41	2.97	17	1
1:A:164:THR:O	1:A:166:VAL:N	0.41	2.54	3	1
1:A:109:SER:OG	1:A:112:ASP:N	0.41	2.53	4	1
1:A:114:ASN:ND2	1:A:178:GLN:HE22	0.41	2.12	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:PHE:C	1:A:144:PHE:CD1	0.41	2.90	1	1
1:A:181:LEU:HD23	1:A:200:PHE:CD2	0.41	2.50	17	2
1:A:85:GLU:OE2	1:A:130:PHE:CZ	0.41	2.73	18	1
1:A:143:TYR:CZ	1:A:152:LYS:CD	0.41	3.04	20	1
1:A:170:ASP:OD1	1:A:173:LYS:NZ	0.41	2.40	8	1
1:A:84:LYS:C	1:A:85:GLU:CD	0.41	2.78	16	1
1:A:85:GLU:OE2	1:A:130:PHE:CE1	0.41	2.74	18	1
1:A:96:GLN:HE21	1:A:99:ARG:HH11	0.41	1.54	6	1
1:A:176:ASP:C	1:A:177:LYS:O	0.41	2.58	7	2
1:A:81:ALA:HB1	1:A:132:ASN:OD1	0.41	2.15	15	2
1:A:165:ASP:C	1:A:167:GLY:N	0.41	2.72	18	1
1:A:72:VAL:HG23	1:A:87:VAL:H	0.41	1.75	12	1
1:A:81:ALA:HB1	1:A:132:ASN:ND2	0.41	2.30	13	1
1:A:204:GLU:OE1	1:A:204:GLU:O	0.41	2.39	5	1
1:A:83:ILE:HD11	1:A:132:ASN:HB3	0.40	1.92	7	1
1:A:188:ASN:ND2	1:A:191:THR:H	0.40	2.14	15	1
1:A:156:THR:CG2	1:A:203:THR:HG1	0.40	2.29	18	1
1:A:125:ARG:NH1	1:A:125:ARG:HG3	0.40	2.31	8	1
1:A:81:ALA:O	1:A:132:ASN:OD1	0.40	2.40	10	1
1:A:81:ALA:O	1:A:82:ASP:OD2	0.40	2.39	12	1
1:A:150:THR:O	1:A:150:THR:HG22	0.40	2.15	6	1
1:A:96:GLN:NE2	1:A:96:GLN:N	0.40	2.70	6	1
1:A:149:GLU:OE1	1:A:150:THR:N	0.40	2.54	11	1
1:A:124:ASP:O	1:A:125:ARG:CG	0.40	2.70	14	1
1:A:71:LYS:CG	1:A:71:LYS:O	0.40	2.69	14	1
1:A:199:ILE:HG13	1:A:199:ILE:O	0.40	2.15	15	1
1:A:125:ARG:O	1:A:131:THR:CB	0.40	2.70	14	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	143/148 (97%)	108±2 (76±2%)	24±3 (17±2%)	11±1 (8±1%)	2	14
2	C	2/5 (40%)	0±0 (18±24%)	0±0 (8±18%)	2±1 (75±25%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2900/3060 (95%)	2172 (75%)	475 (16%)	253 (9%)	1 12

All 24 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	C	704	ALA	20
1	A	177	LYS	20
1	A	138	LYS	20
1	A	167	GLY	20
1	A	170	ASP	19
1	A	139	GLY	17
1	A	134	LYS	17
1	A	97	LEU	16
1	A	162	LYS	15
1	A	169	LEU	15
1	A	66	PRO	13
1	A	128	TYR	12
1	A	104	ALA	11
2	C	703	PRO	10
1	A	69	LYS	7
1	A	129	GLN	5
1	A	92	ALA	4
1	A	101	VAL	3
1	A	186	ASP	2
1	A	175	LYS	2
1	A	166	VAL	2
1	A	89	PRO	1
1	A	174	GLY	1
1	A	172	GLN	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	127/130 (98%)	88±4 (70±3%)	39±4 (30±3%)	1 15
2	C	2/2 (100%)	1±0 (50±0%)	1±0 (50±0%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2580/2640 (98%)	1786 (69%)	794 (31%)	1 15

All 92 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	64	GLN	20
1	A	134	LYS	20
1	A	148	ASN	20
1	A	133	LEU	20
2	C	702	LEU	20
1	A	121	THR	19
1	A	199	ILE	19
1	A	98	ASN	19
1	A	162	LYS	19
1	A	113	GLN	19
1	A	102	SER	18
1	A	105	GLU	18
1	A	188	ASN	17
1	A	85	GLU	17
1	A	156	THR	17
1	A	122	PHE	16
1	A	109	SER	16
1	A	157	SER	15
1	A	77	GLU	15
1	A	68	ASP	15
1	A	158	ILE	14
1	A	161	VAL	14
1	A	179	LEU	14
1	A	72	VAL	13
1	A	186	ASP	13
1	A	112	ASP	13
1	A	71	LYS	13
1	A	189	GLU	12
1	A	197	ARG	12
1	A	164	THR	12
1	A	146	VAL	11
1	A	166	VAL	11
1	A	184	CYS	10
1	A	110	LEU	10
1	A	178	GLN	10
1	A	70	SER	10

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Mol	Chain	Res	Type	Models (Total)
1	A	82	ASP	10
1	A	206	LYS	10
1	A	80	ASP	9
1	A	141	MET	8
1	A	76	ILE	8
1	A	107	ASN	8
1	A	200	PHE	7
1	A	65	ILE	7
1	A	137	LYS	7
1	A	93	THR	7
1	A	99	ARG	7
1	A	183	THR	7
1	A	159	ARG	6
1	A	173	LYS	6
1	A	125	ARG	6
1	A	75	TYR	6
1	A	132	ASN	6
1	A	69	LYS	6
1	A	175	LYS	6
1	A	97	LEU	5
1	A	145	LYS	5
1	A	204	GLU	5
1	A	196	LYS	5
1	A	124	ASP	5
1	A	160	ASP	5
1	A	185	ASP	5
1	A	114	ASN	4
1	A	176	ASP	4
1	A	67	LYS	4
1	A	177	LYS	4
1	A	127	ASN	4
1	A	138	LYS	4
1	A	198	LYS	4
1	A	190	LYS	3
1	A	154	LYS	3
1	A	203	THR	3
1	A	181	LEU	3
1	A	172	GLN	3
1	A	180	THR	3
1	A	84	LYS	3
1	A	95	GLU	3
1	A	165	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	151	ARG	2
1	A	96	GLN	2
1	A	116	SER	2
1	A	170	ASP	1
1	A	106	GLU	1
1	A	129	GLN	1
1	A	149	GLU	1
1	A	193	VAL	1
1	A	101	VAL	1
1	A	168	VAL	1
1	A	111	ASP	1
1	A	123	ILE	1
1	A	191	THR	1
1	A	87	VAL	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
2	B27	C	705	1,2	5,6,6	0.37±0.02	0±0 (0±0%)

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
2	B27	C	705	1,2	2,7,7	1.71±0.07	0±0 (0±0%)

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
2	B27	C	705	1,2	-	0±0,4,6,6	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

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

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1810
Number of shifts mapped to atoms	1806
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	4
Number of shift outliers (ShiftChecker)	5

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

- No matching atoms found in structure. All 4 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
C	705	B27	HG21	1.29	0.0	1
C	705	B27	HG22	1.29	0.0	1
C	705	B27	HG23	1.29	0.0	1
C	705	B27	H	6.82	0.0	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	150	-0.37 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	140	-0.11 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	137	0.11 ± 0.06	None needed (< 0.5 ppm)
^{15}N	140	-0.40 ± 0.43	None needed (< 0.5 ppm)

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 89%, i.e. 1624 atoms were assigned a chemical shift out of a possible 1828. 18 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	703/715 (98%)	284/284 (100%)	282/294 (96%)	137/137 (100%)
Sidechain	829/1001 (83%)	509/588 (87%)	304/367 (83%)	16/46 (35%)
Aromatic	92/112 (82%)	46/59 (78%)	45/51 (88%)	1/2 (50%)
Overall	1624/1828 (89%)	839/931 (90%)	631/712 (89%)	154/185 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1655 atoms were assigned a chemical shift out of a possible 1881. 18 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	714/735 (97%)	289/292 (99%)	286/302 (95%)	139/141 (99%)
Sidechain	849/1034 (82%)	521/608 (86%)	312/378 (83%)	16/48 (33%)
Aromatic	92/112 (82%)	46/59 (78%)	45/51 (88%)	1/2 (50%)
Overall	1655/1881 (88%)	856/959 (89%)	643/731 (88%)	156/191 (82%)

7.1.4 Statistically unusual chemical shifts [i](#)

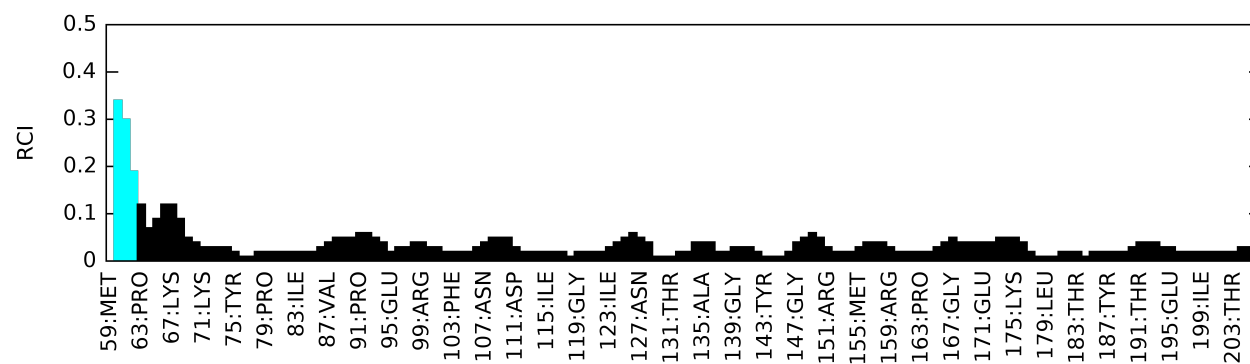
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	151	ARG	NE	121.31	92.63 – 76.73	23.0
1	A	99	ARG	NE	119.85	92.63 – 76.73	22.1
1	A	197	ARG	NE	119.65	92.63 – 76.73	22.0
1	A	133	LEU	HG	-0.56	3.16 – -0.14	-6.3
1	A	113	GLN	H	11.32	11.17 – 5.27	5.3

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

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain C:

