Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 07:03 AM EDT

PDB ID	:	1KLP
Title	:	The Solution Structure of Acyl Carrier Protein from Mycobacterium tuberculosis
Authors	:	Wong, H.C.; Liu, G.; Zhang, Y.-M.; Rock, C.O.; Zheng, J.
Deposited on	:	2001-12-12

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 (i) 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 (i)) were used in the production of this report:

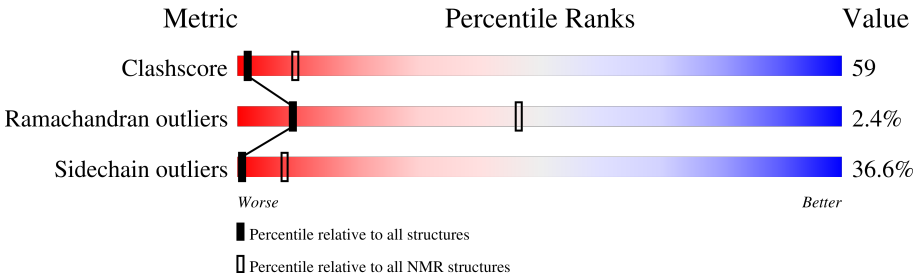
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	115	11% 44% 10% 34%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 16 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 target function*.

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:4-A:79 (76)	0.34	16

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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1615 atoms, of which 738 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	115	1615	545	738	138	192	2	0

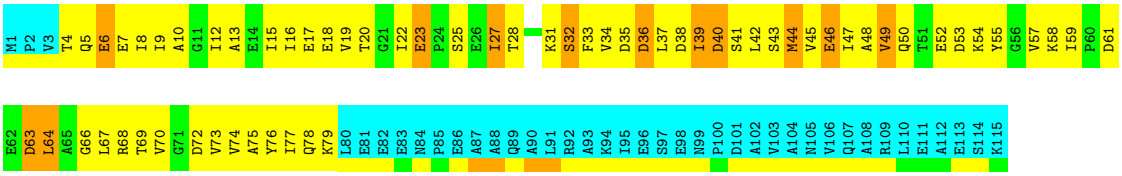
4 Residue-property plots (i)

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: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

Chain A: 11% 44% 10% 34%



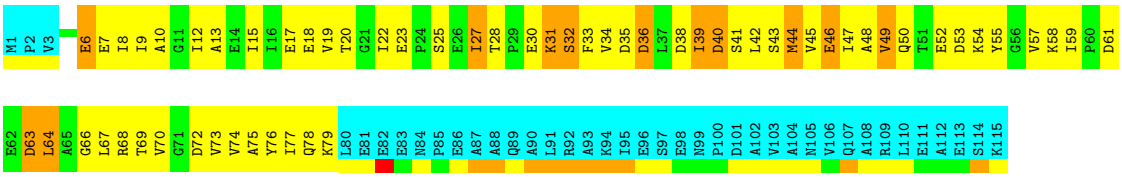
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

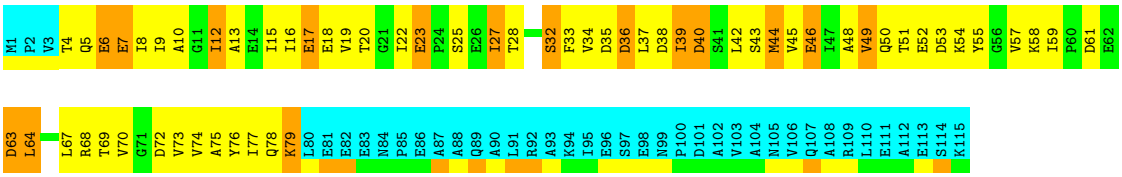
Chain A: 14% 42% 10% 34%



4.2.2 Score per residue for model 2

• Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

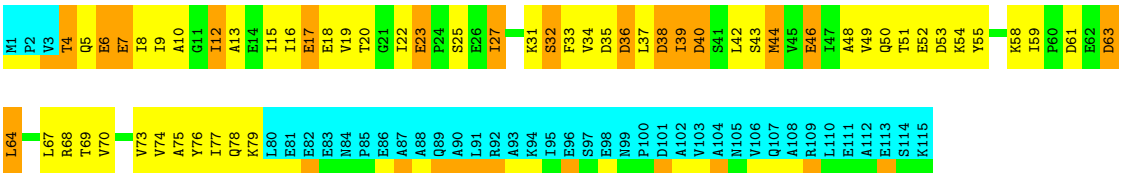
Chain A: 14% 38% 14% 34%



4.2.3 Score per residue for model 3

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

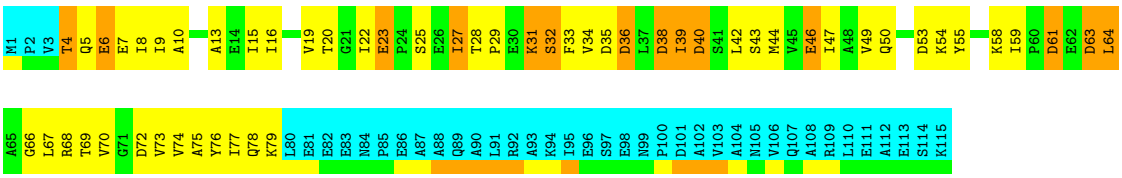
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

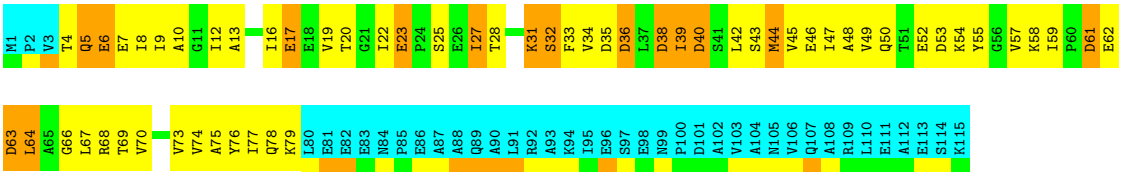
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

Chain A: 17% 34% 16% 34%

M1 P2 V3 T4 Q5 E6 E7 I8 I9 A10 A13 E17 E18 V19 T20 G21 I22 E23 P24 S25 E26 I27 T28 K31 S32 F33 V34 D35 D36 L37 D38 I39 D40 S41 L42 S43 M44 V45 E46 I47 A48 V49 Q50 T51 E52 D53 K54 Y55 G56 V57 K58 D61 E62 D63 L64

L67 R68 T69 V70 G71 D72 V73 V74 A75 Y76 I77 Q78 K79 L80 E81 E82 E83 N84 P85 E86 A87 A88 Q89 A90 L91 R92 A93 K94 I95 E96 S97 E98 N99 P100 D101 A102 V103 A104 N105 V106 Q107 A108 R109 L110 E111 A112 E113 S114 K115

4.2.7 Score per residue for model 7

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

Chain A: 12% 39% 15% 34%

M1 P2 V3 T4 Q5 E6 E7 I8 I9 A10 G11 I12 A13 E14 I15 I16 E17 E18 V19 T20 G21 I22 E23 P24 S25 E26 I27 E30 K31 S32 F33 V34 D35 D36 L37 D38 I39 D40 S41 L42 S43 M44 V45 E46 I47 A48 V49 Q50 T51 E52 D53 K54 Y55 G56 V57 K58 I59 P60 D61

E62 D63 L64 A65 G66 L67 R68 T69 V70 G71 D72 V73 V74 A75 Y76 I77 Q78 K79 L80 E81 E82 E83 N84 P85 E86 A87 A88 Q89 A90 L91 R92 A93 K94 I95 E96 S97 E98 N99 P100 D101 A102 V103 A104 N105 V106 Q107 A108 R109 L110 E111 A112 E113 S114 K115

4.2.8 Score per residue for model 8

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

Chain A: 18% 35% 13% 34%

M1 P2 V3 E6 E7 I8 I9 A10 G11 I12 E17 E18 V19 I22 E23 P24 S25 E26 I27 T28 P29 E30 K31 S32 F33 V34 D35 D36 L37 D38 I39 D40 S41 L42 S43 M44 V45 E46 I47 A48 V49 Q50 T51 E52 D53 K54 Y55 K58 I59 P60 D61 E62 D63 L64 A65 G66

L67 R68 T69 V70 G71 D72 V73 V74 A75 Y76 I77 Q78 K79 L80 E81 E82 E83 N84 P85 E86 A87 A88 Q89 A90 L91 R92 A93 K94 I95 E96 S97 E98 N99 P100 D101 A102 V103 A104 N105 V106 Q107 A108 R109 L110 E111 A112 E113 S114 K115

4.2.9 Score per residue for model 9

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

Chain A: 12% 39% 15% 34%

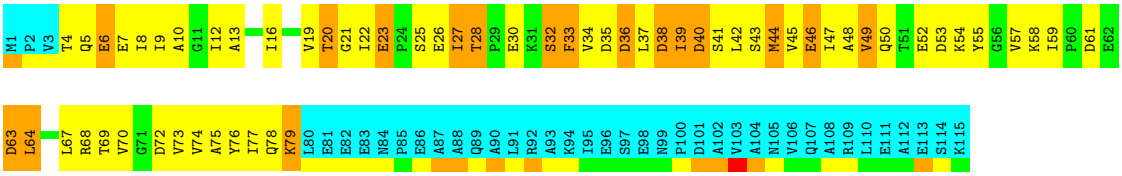
M1 P2 V3 T4 Q5 E6 E7 I8 I9 A10 G11 I12 A13 E14 I15 I16 E17 E18 V19 T20 G21 I22 E23 P24 S25 E26 I27 T28 K31 S32 F33 V34 D35 D36 L37 D38 I39 D40 S41 L42 S43 M44 V45 E46 I47 A48 V49 Q50 T51 E52 D53 K54 Y55 G56 V57 K58 I59 P60 D61

E62 D63 L64 A65 G66 L67 R68 T69 V70 G71 D72 V73 V74 A75 Y76 I77 Q78 K79 L80 E81 E82 E83 N84 P85 E86 A87 A88 Q89 A90 L91 R92 A93 K94 I95 E96 S97 E98 N99 P100 D101 A102 V103 A104 N105 V106 Q107 A108 R109 L110 E111 A112 E113 S114 K115

4.2.10 Score per residue for model 10

• Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

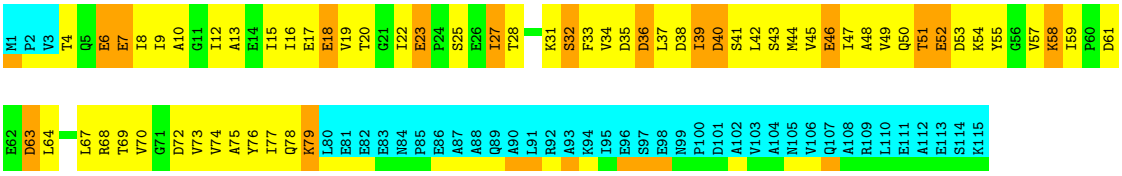
Chain A: 13% 38% 15% 34%



4.2.11 Score per residue for model 11

• Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

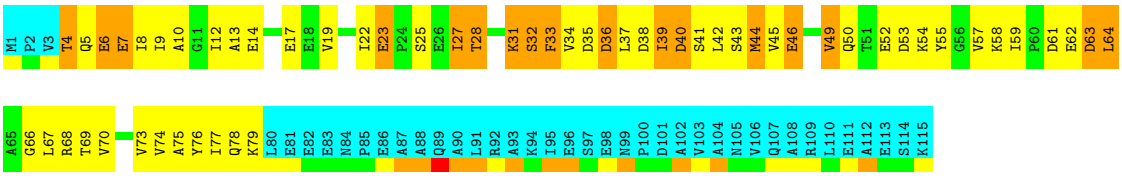
Chain A: 12% 41% 13% 34%



4.2.12 Score per residue for model 12

• Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

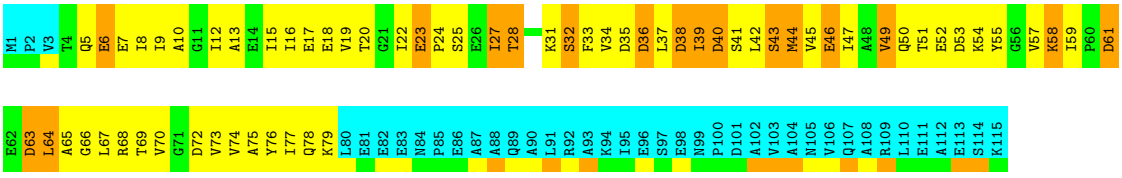
Chain A: 16% 36% 15% 34%



4.2.13 Score per residue for model 13

• Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

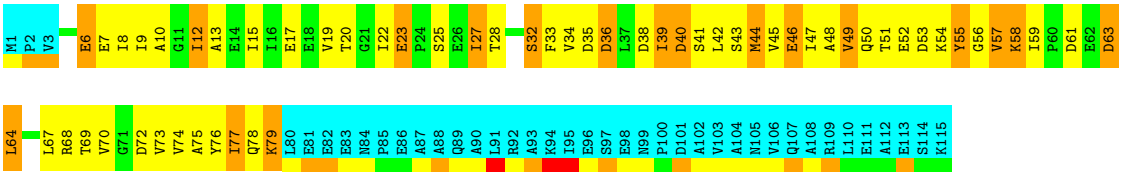
Chain A: 10% 41% 15% 34%



4.2.14 Score per residue for model 14

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

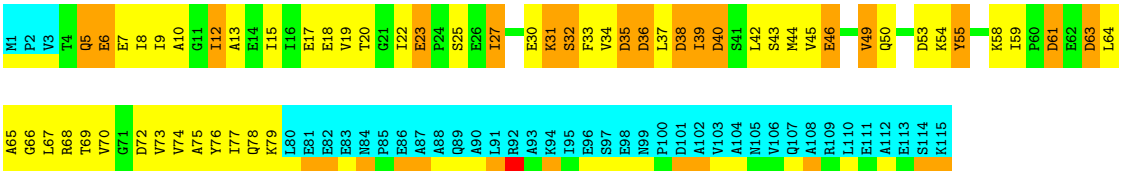
Chain A: 16% 35% 16% 34%



4.2.15 Score per residue for model 15

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

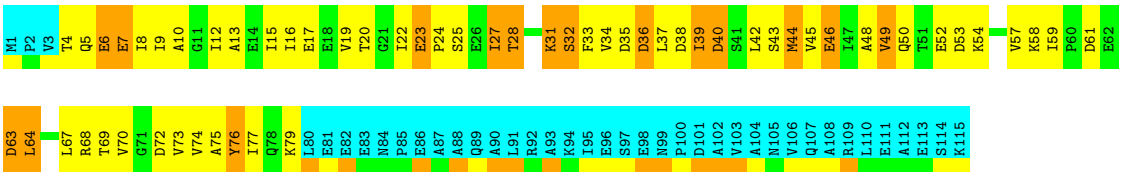
Chain A: 17% 35% 15% 34%



4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

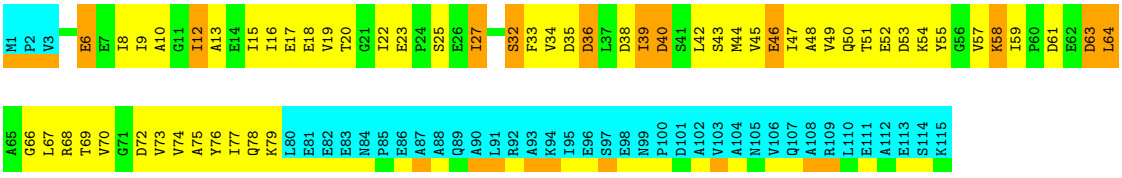
Chain A: 16% 37% 14% 34%



4.2.17 Score per residue for model 17

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

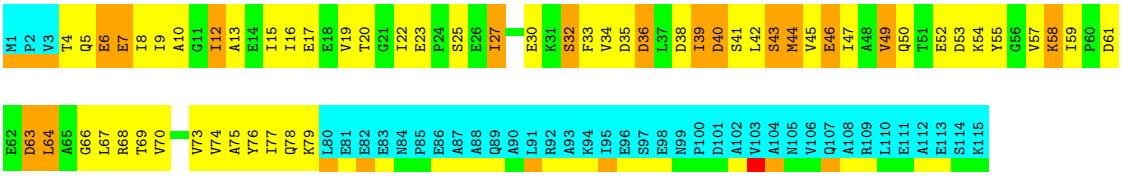
Chain A: 17% 40% 10% 34%



4.2.18 Score per residue for model 18

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

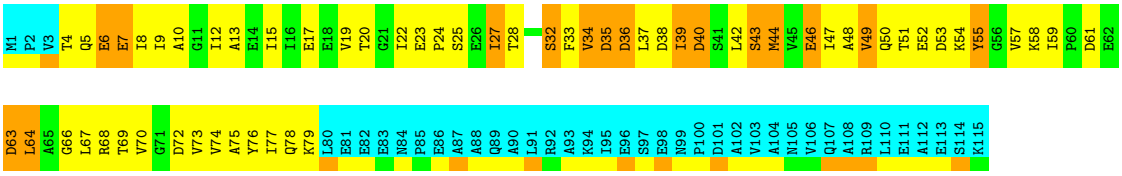
Chain A: 16% 37% 13% 34%



4.2.19 Score per residue for model 19

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

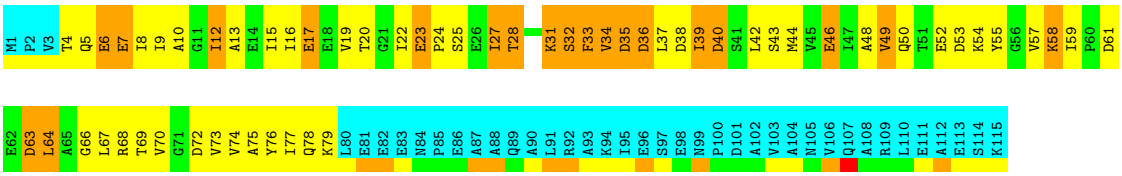
Chain A: 14% 38% 14% 34%



4.2.20 Score per residue for model 20

- Molecule 1: MEROMYCOLATE EXTENSION ACYL CARRIER PROTEIN

Chain A: 14% 35% 17% 34%



5 Refinement protocol and experimental data overview (i)

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

Of the 320 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
DYANA	refinement	1.5

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	581	501	576	69±8
All	All	11620	10020	11520	1374

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 59.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ILE:HD12	1:A:74:VAL:HG13	1.09	1.25	9	19
1:A:8:ILE:CD1	1:A:74:VAL:HG13	0.97	1.88	10	20
1:A:8:ILE:HG21	1:A:74:VAL:HG22	0.96	1.36	15	14
1:A:67:LEU:HD21	1:A:76:TYR:CD2	0.92	2.00	16	13
1:A:48:ALA:HB1	1:A:52:GLU:OE2	0.89	1.66	16	5
1:A:48:ALA:HB1	1:A:52:GLU:OE1	0.89	1.67	3	8
1:A:69:THR:O	1:A:73:VAL:HG23	0.88	1.69	7	20
1:A:8:ILE:HD12	1:A:74:VAL:CG1	0.88	1.95	19	20
1:A:70:VAL:O	1:A:74:VAL:HG23	0.85	1.71	12	15
1:A:19:VAL:HG12	1:A:43:SER:OG	0.82	1.74	19	20
1:A:67:LEU:HD21	1:A:76:TYR:CG	0.81	2.10	9	13
1:A:59:ILE:HD11	1:A:77:ILE:HD11	0.81	1.53	16	9
1:A:59:ILE:HD11	1:A:77:ILE:CD1	0.81	2.05	16	12
1:A:31:LYS:NZ	1:A:37:LEU:HD23	0.81	1.90	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:LEU:HD13	1:A:73:VAL:HG13	0.80	1.52	3	18
1:A:27:ILE:O	1:A:28:THR:HG23	0.79	1.78	10	6
1:A:67:LEU:HD13	1:A:73:VAL:HA	0.77	1.56	20	19
1:A:67:LEU:HB3	1:A:73:VAL:HG22	0.75	1.58	20	20
1:A:59:ILE:HD11	1:A:77:ILE:HG12	0.75	1.57	9	10
1:A:59:ILE:HD11	1:A:77:ILE:CG1	0.74	2.12	14	12
1:A:6:GLU:O	1:A:10:ALA:HB3	0.73	1.83	15	20
1:A:67:LEU:HD22	1:A:72:ASP:O	0.73	1.83	6	13
1:A:33:PHE:CZ	1:A:64:LEU:HD11	0.73	2.18	20	6
1:A:32:SER:HA	1:A:69:THR:HG22	0.72	1.62	11	17
1:A:63:ASP:CB	1:A:76:TYR:CE2	0.71	2.72	15	6
1:A:39:ILE:O	1:A:39:ILE:HD13	0.71	1.85	7	20
1:A:75:ALA:HB1	1:A:79:LYS:HG3	0.69	1.62	8	11
1:A:33:PHE:CD2	1:A:44:MET:CE	0.69	2.75	20	2
1:A:59:ILE:HG22	1:A:59:ILE:O	0.69	1.88	1	5
1:A:33:PHE:CD2	1:A:44:MET:HE1	0.69	2.22	20	2
1:A:31:LYS:O	1:A:69:THR:HG22	0.68	1.88	20	6
1:A:19:VAL:HG11	1:A:46:GLU:CB	0.68	2.18	10	13
1:A:41:SER:O	1:A:45:VAL:HG23	0.68	1.88	8	11
1:A:75:ALA:HB1	1:A:79:LYS:CD	0.68	2.19	5	1
1:A:67:LEU:CD2	1:A:76:TYR:CD2	0.67	2.77	16	13
1:A:20:THR:HG23	1:A:47:ILE:HD11	0.67	1.67	5	10
1:A:9:ILE:O	1:A:13:ALA:HB2	0.67	1.89	16	18
1:A:33:PHE:CD1	1:A:44:MET:HE2	0.66	2.26	11	1
1:A:20:THR:HG22	1:A:43:SER:HB3	0.65	1.67	6	6
1:A:16:ILE:HD12	1:A:27:ILE:CG1	0.65	2.22	13	7
1:A:75:ALA:HB1	1:A:79:LYS:CG	0.64	2.22	8	4
1:A:52:GLU:HA	1:A:57:VAL:HG22	0.64	1.69	6	12
1:A:31:LYS:HZ3	1:A:37:LEU:HD21	0.64	1.50	15	1
1:A:64:LEU:HD13	1:A:64:LEU:O	0.63	1.93	18	18
1:A:63:ASP:CG	1:A:76:TYR:CE2	0.62	2.72	20	16
1:A:4:THR:HG22	1:A:7:GLU:OE1	0.62	1.94	11	2
1:A:63:ASP:OD1	1:A:76:TYR:CE2	0.61	2.53	2	8
1:A:33:PHE:CD1	1:A:44:MET:SD	0.61	2.94	6	6
1:A:67:LEU:CD1	1:A:73:VAL:HG13	0.61	2.26	3	14
1:A:20:THR:HG22	1:A:39:ILE:HG13	0.61	1.71	10	1
1:A:20:THR:HB	1:A:22:ILE:HD12	0.60	1.73	10	1
1:A:63:ASP:CG	1:A:76:TYR:CD2	0.60	2.74	8	9
1:A:33:PHE:CE1	1:A:44:MET:SD	0.60	2.94	16	8
1:A:33:PHE:CE2	1:A:44:MET:SD	0.60	2.94	10	3
1:A:33:PHE:CZ	1:A:44:MET:SD	0.60	2.94	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ILE:HD12	1:A:27:ILE:HG12	0.60	1.71	13	5
1:A:39:ILE:O	1:A:40:ASP:CB	0.60	2.50	20	20
1:A:37:LEU:HD13	1:A:44:MET:CE	0.59	2.27	7	1
1:A:32:SER:O	1:A:33:PHE:CB	0.59	2.51	11	20
1:A:8:ILE:HD13	1:A:77:ILE:HD12	0.59	1.72	10	7
1:A:15:ILE:HG23	1:A:50:GLN:NE2	0.58	2.13	9	7
1:A:63:ASP:OD1	1:A:76:TYR:CE1	0.58	2.56	4	1
1:A:4:THR:HG23	1:A:5:GLN:N	0.58	2.14	3	6
1:A:19:VAL:HG11	1:A:46:GLU:HB3	0.58	1.76	10	2
1:A:75:ALA:HB1	1:A:79:LYS:HD2	0.57	1.74	5	1
1:A:63:ASP:OD1	1:A:76:TYR:CD2	0.57	2.56	7	6
1:A:72:ASP:OD1	1:A:76:TYR:CE1	0.57	2.57	19	1
1:A:39:ILE:CG2	1:A:44:MET:SD	0.57	2.92	7	1
1:A:20:THR:HG21	1:A:44:MET:HE1	0.57	1.77	7	1
1:A:8:ILE:CG2	1:A:74:VAL:HG22	0.57	2.23	15	10
1:A:20:THR:HG22	1:A:43:SER:CB	0.57	2.29	13	10
1:A:67:LEU:HD13	1:A:73:VAL:CG1	0.57	2.29	3	6
1:A:20:THR:HG22	1:A:43:SER:OG	0.56	2.00	17	8
1:A:63:ASP:CG	1:A:76:TYR:CZ	0.56	2.79	6	6
1:A:31:LYS:HZ2	1:A:37:LEU:HD23	0.56	1.58	20	1
1:A:51:THR:HG22	1:A:57:VAL:HG21	0.56	1.76	14	4
1:A:63:ASP:OD1	1:A:76:TYR:CZ	0.55	2.60	4	3
1:A:6:GLU:O	1:A:10:ALA:CB	0.55	2.55	15	20
1:A:33:PHE:CG	1:A:44:MET:SD	0.55	2.99	20	2
1:A:20:THR:HG21	1:A:44:MET:CE	0.55	2.31	7	1
1:A:63:ASP:HB2	1:A:76:TYR:CE2	0.55	2.37	15	4
1:A:16:ILE:HG23	1:A:20:THR:OG1	0.55	2.02	10	2
1:A:8:ILE:HG21	1:A:74:VAL:CG2	0.54	2.24	15	1
1:A:46:GLU:O	1:A:49:VAL:HG12	0.54	2.03	1	14
1:A:31:LYS:HZ1	1:A:37:LEU:HD23	0.54	1.62	20	1
1:A:33:PHE:CD2	1:A:44:MET:SD	0.53	3.01	10	3
1:A:75:ALA:O	1:A:79:LYS:N	0.53	2.41	6	20
1:A:19:VAL:CG1	1:A:43:SER:OG	0.53	2.57	17	20
1:A:33:PHE:CE2	1:A:64:LEU:HD11	0.53	2.39	20	1
1:A:33:PHE:O	1:A:37:LEU:HD12	0.53	2.04	19	6
1:A:70:VAL:O	1:A:74:VAL:N	0.53	2.42	19	16
1:A:55:TYR:CD1	1:A:57:VAL:CG1	0.52	2.93	10	2
1:A:31:LYS:NZ	1:A:37:LEU:HD21	0.52	2.18	15	1
1:A:39:ILE:HD12	1:A:43:SER:HB2	0.52	1.80	7	9
1:A:67:LEU:HD22	1:A:72:ASP:C	0.52	2.24	10	11
1:A:59:ILE:HG22	1:A:64:LEU:HD23	0.52	1.82	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:VAL:CG1	1:A:77:ILE:HG23	0.52	2.34	11	1
1:A:9:ILE:O	1:A:13:ALA:CB	0.52	2.58	15	17
1:A:20:THR:HG23	1:A:47:ILE:CD1	0.52	2.35	6	2
1:A:17:GLU:CB	1:A:22:ILE:O	0.52	2.58	2	17
1:A:4:THR:HG22	1:A:5:GLN:H	0.52	1.64	19	2
1:A:75:ALA:O	1:A:79:LYS:CG	0.52	2.58	20	6
1:A:4:THR:HG22	1:A:7:GLU:CD	0.52	2.25	20	1
1:A:37:LEU:CD1	1:A:44:MET:SD	0.52	2.98	11	7
1:A:20:THR:HG22	1:A:39:ILE:CG1	0.52	2.35	10	1
1:A:34:VAL:HG12	1:A:35:ASP:N	0.51	2.20	3	20
1:A:57:VAL:HG12	1:A:58:LYS:H	0.51	1.63	11	1
1:A:41:SER:O	1:A:45:VAL:CG2	0.51	2.59	6	10
1:A:79:LYS:N	1:A:79:LYS:HZ3	0.51	2.03	8	1
1:A:16:ILE:O	1:A:21:GLY:N	0.51	2.44	10	1
1:A:39:ILE:O	1:A:39:ILE:CD1	0.51	2.59	8	20
1:A:17:GLU:CG	1:A:22:ILE:O	0.51	2.58	17	13
1:A:33:PHE:O	1:A:44:MET:CE	0.51	2.59	20	2
1:A:19:VAL:HG21	1:A:46:GLU:HB3	0.50	1.82	10	1
1:A:33:PHE:CG	1:A:44:MET:HE2	0.50	2.42	11	1
1:A:58:LYS:O	1:A:59:ILE:CG1	0.50	2.59	18	5
1:A:27:ILE:O	1:A:28:THR:CG2	0.50	2.59	16	4
1:A:12:ILE:O	1:A:15:ILE:N	0.49	2.45	16	10
1:A:59:ILE:CD1	1:A:77:ILE:HD11	0.49	2.34	16	1
1:A:63:ASP:HB3	1:A:76:TYR:CE2	0.49	2.42	12	2
1:A:31:LYS:O	1:A:69:THR:CG2	0.49	2.58	20	2
1:A:27:ILE:N	1:A:27:ILE:CD1	0.49	2.76	8	17
1:A:63:ASP:OD2	1:A:76:TYR:CD2	0.49	2.65	15	5
1:A:4:THR:CG2	1:A:5:GLN:N	0.49	2.75	3	3
1:A:8:ILE:CD1	1:A:74:VAL:CG1	0.49	2.88	15	1
1:A:74:VAL:CG1	1:A:78:GLN:NE2	0.48	2.76	13	2
1:A:59:ILE:O	1:A:59:ILE:CG2	0.48	2.59	1	3
1:A:79:LYS:N	1:A:79:LYS:NZ	0.48	2.61	9	1
1:A:22:ILE:CG2	1:A:23:GLU:N	0.48	2.77	18	18
1:A:19:VAL:HG11	1:A:46:GLU:HB2	0.48	1.81	10	5
1:A:76:TYR:CD1	1:A:76:TYR:O	0.48	2.67	5	1
1:A:22:ILE:HG22	1:A:23:GLU:N	0.48	2.23	6	20
1:A:20:THR:CG2	1:A:43:SER:OG	0.48	2.62	20	3
1:A:8:ILE:HD13	1:A:74:VAL:HG13	0.48	1.84	15	1
1:A:50:GLN:O	1:A:54:LYS:N	0.47	2.45	9	20
1:A:48:ALA:CB	1:A:52:GLU:OE1	0.47	2.60	20	1
1:A:75:ALA:O	1:A:79:LYS:CB	0.47	2.62	15	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ALA:HB1	1:A:24:PRO:O	0.47	2.10	16	2
1:A:63:ASP:O	1:A:66:GLY:N	0.47	2.48	4	4
1:A:67:LEU:CD2	1:A:72:ASP:O	0.47	2.63	8	3
1:A:43:SER:O	1:A:46:GLU:N	0.47	2.47	20	10
1:A:20:THR:OG1	1:A:47:ILE:HD11	0.47	2.08	10	1
1:A:16:ILE:CG2	1:A:20:THR:OG1	0.47	2.62	7	4
1:A:34:VAL:O	1:A:36:ASP:N	0.46	2.48	15	20
1:A:74:VAL:O	1:A:77:ILE:N	0.46	2.46	6	4
1:A:34:VAL:O	1:A:38:ASP:N	0.46	2.48	12	13
1:A:55:TYR:CD1	1:A:57:VAL:HG13	0.46	2.45	10	2
1:A:37:LEU:HD13	1:A:44:MET:HE1	0.46	1.88	7	1
1:A:34:VAL:C	1:A:36:ASP:N	0.46	2.69	19	20
1:A:70:VAL:HG12	1:A:74:VAL:CG2	0.45	2.41	19	3
1:A:4:THR:OG1	1:A:5:GLN:N	0.45	2.49	20	1
1:A:78:GLN:O	1:A:79:LYS:C	0.45	2.53	19	12
1:A:33:PHE:HZ	1:A:64:LEU:HD11	0.45	1.70	2	1
1:A:33:PHE:CG	1:A:44:MET:HE1	0.45	2.46	6	2
1:A:58:LYS:CG	1:A:58:LYS:O	0.45	2.64	17	1
1:A:51:THR:HG22	1:A:57:VAL:CG2	0.45	2.42	14	2
1:A:64:LEU:HD22	1:A:67:LEU:HD12	0.45	1.89	14	3
1:A:6:GLU:O	1:A:10:ALA:N	0.45	2.48	12	16
1:A:70:VAL:O	1:A:74:VAL:CG2	0.45	2.58	20	2
1:A:75:ALA:O	1:A:77:ILE:N	0.44	2.50	8	3
1:A:75:ALA:C	1:A:77:ILE:N	0.44	2.69	8	6
1:A:67:LEU:HD11	1:A:76:TYR:HD2	0.44	1.72	20	1
1:A:34:VAL:O	1:A:35:ASP:C	0.44	2.56	18	20
1:A:7:GLU:CG	1:A:55:TYR:OH	0.44	2.65	7	2
1:A:16:ILE:O	1:A:20:THR:OG1	0.44	2.32	3	4
1:A:37:LEU:HD13	1:A:44:MET:CG	0.44	2.43	12	1
1:A:70:VAL:O	1:A:73:VAL:N	0.44	2.51	19	2
1:A:39:ILE:HG22	1:A:44:MET:SD	0.44	2.53	7	1
1:A:75:ALA:CA	1:A:79:LYS:HG2	0.44	2.42	8	1
1:A:57:VAL:CG1	1:A:77:ILE:CG2	0.44	2.96	11	1
1:A:16:ILE:HD12	1:A:27:ILE:HG13	0.44	1.88	20	1
1:A:63:ASP:OD2	1:A:76:TYR:CG	0.44	2.71	4	2
1:A:67:LEU:HD13	1:A:73:VAL:HG22	0.43	1.90	19	3
1:A:5:GLN:HG3	1:A:9:ILE:CD1	0.43	2.43	19	6
1:A:58:LYS:O	1:A:58:LYS:NZ	0.43	2.49	11	1
1:A:75:ALA:O	1:A:79:LYS:HB2	0.43	2.13	15	1
1:A:37:LEU:HD11	1:A:44:MET:CE	0.43	2.44	16	1
1:A:67:LEU:HD11	1:A:76:TYR:CD2	0.43	2.49	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:GLN:O	1:A:9:ILE:N	0.43	2.52	5	3
1:A:58:LYS:O	1:A:58:LYS:CD	0.43	2.67	13	1
1:A:67:LEU:CD2	1:A:76:TYR:CG	0.43	2.95	9	1
1:A:51:THR:O	1:A:57:VAL:HG23	0.43	2.14	11	1
1:A:16:ILE:HG22	1:A:22:ILE:HB	0.42	1.91	10	1
1:A:46:GLU:O	1:A:49:VAL:N	0.42	2.51	13	2
1:A:5:GLN:CD	1:A:9:ILE:CD1	0.42	2.88	15	1
1:A:4:THR:N	1:A:7:GLU:HB2	0.42	2.29	18	2
1:A:31:LYS:NZ	1:A:37:LEU:CD2	0.42	2.75	20	1
1:A:32:SER:HB3	1:A:35:ASP:CB	0.42	2.45	19	11
1:A:61:ASP:C	1:A:63:ASP:N	0.42	2.71	13	4
1:A:66:GLY:O	1:A:67:LEU:C	0.42	2.58	20	13
1:A:5:GLN:C	1:A:7:GLU:N	0.42	2.73	19	5
1:A:48:ALA:C	1:A:50:GLN:N	0.42	2.73	16	7
1:A:31:LYS:CE	1:A:36:ASP:OD1	0.42	2.67	1	1
1:A:36:ASP:O	1:A:37:LEU:C	0.42	2.58	10	4
1:A:33:PHE:CG	1:A:44:MET:CE	0.42	3.02	11	2
1:A:46:GLU:O	1:A:47:ILE:C	0.42	2.58	13	3
1:A:55:TYR:CD1	1:A:57:VAL:HG12	0.41	2.50	1	1
1:A:61:ASP:O	1:A:63:ASP:N	0.41	2.53	13	3
1:A:33:PHE:CE2	1:A:44:MET:HE3	0.41	2.50	11	1
1:A:67:LEU:HD13	1:A:73:VAL:CA	0.41	2.41	12	2
1:A:5:GLN:CD	1:A:9:ILE:HD11	0.41	2.35	15	1
1:A:48:ALA:CB	1:A:52:GLU:OE2	0.41	2.59	1	1
1:A:4:THR:HG22	1:A:5:GLN:N	0.41	2.31	2	1
1:A:40:ASP:O	1:A:44:MET:SD	0.41	2.79	7	1
1:A:20:THR:CG2	1:A:44:MET:CE	0.41	2.99	7	1
1:A:7:GLU:CD	1:A:55:TYR:OH	0.41	2.59	3	1
1:A:37:LEU:CD1	1:A:44:MET:CG	0.41	2.98	3	2
1:A:9:ILE:CD1	1:A:29:PRO:HG3	0.41	2.45	4	1
1:A:37:LEU:HD12	1:A:44:MET:SD	0.41	2.56	20	2
1:A:57:VAL:HG11	1:A:77:ILE:HD13	0.41	1.92	11	1
1:A:58:LYS:O	1:A:58:LYS:CG	0.41	2.69	14	1
1:A:69:THR:O	1:A:72:ASP:N	0.41	2.54	16	1
1:A:32:SER:CB	1:A:35:ASP:HB3	0.41	2.46	7	1
1:A:33:PHE:HA	1:A:37:LEU:HD12	0.41	1.91	8	1
1:A:32:SER:O	1:A:33:PHE:HB2	0.41	2.16	20	1
1:A:34:VAL:CG1	1:A:35:ASP:N	0.40	2.85	3	1
1:A:53:ASP:O	1:A:54:LYS:C	0.40	2.59	6	1
1:A:39:ILE:HD12	1:A:43:SER:CB	0.40	2.46	2	1
1:A:15:ILE:O	1:A:18:GLU:N	0.40	2.48	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:CG2	1:A:47:ILE:HA	0.40	2.47	13	1
1:A:64:LEU:CD2	1:A:67:LEU:HD12	0.40	2.47	3	1
1:A:64:LEU:O	1:A:64:LEU:HD13	0.40	2.17	5	1
1:A:63:ASP:C	1:A:65:ALA:N	0.40	2.74	13	2
1:A:56:GLY:O	1:A:57:VAL:C	0.40	2.60	14	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	76/115 (66%)	56±2 (74±2%)	18±2 (24±2%)	2±1 (2±1%)	9	46
All	All	1520/2300 (66%)	1123 (74%)	361 (24%)	36 (2%)	9	46

All 8 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	40	ASP	20
1	A	31	LYS	5
1	A	57	VAL	3
1	A	35	ASP	3
1	A	24	PRO	2
1	A	5	GLN	1
1	A	76	TYR	1
1	A	77	ILE	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	66/97 (68%)	42±2 (63±2%)	24±2 (37±2%)	1 8
All	All	1320/1940 (68%)	837 (63%)	483 (37%)	1 8

All 40 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	6	GLU	20
1	A	25	SER	20
1	A	27	ILE	20
1	A	32	SER	20
1	A	36	ASP	20
1	A	39	ILE	20
1	A	42	LEU	20
1	A	46	GLU	20
1	A	49	VAL	20
1	A	53	ASP	20
1	A	58	LYS	20
1	A	61	ASP	20
1	A	63	ASP	20
1	A	68	ARG	20
1	A	64	LEU	19
1	A	7	GLU	18
1	A	44	MET	17
1	A	38	ASP	16
1	A	12	ILE	15
1	A	28	THR	15
1	A	23	GLU	14
1	A	18	GLU	11
1	A	55	TYR	11
1	A	31	LYS	10
1	A	30	GLU	6
1	A	17	GLU	6
1	A	4	THR	6
1	A	33	PHE	6
1	A	45	VAL	5
1	A	79	LYS	5
1	A	43	SER	5
1	A	34	VAL	4
1	A	52	GLU	4
1	A	51	THR	3
1	A	62	GLU	2
1	A	20	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	26	GLU	1
1	A	14	GLU	1
1	A	5	GLN	1
1	A	76	TYR	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

No chemical shift data were provided