Full wwPDB NMR Structure Validation Report (i)

Apr 2, 2024 – 10:20 AM EDT

PDB ID	:	1AF8
Title	:	ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN FROM STREPTOMYCES COELICOLOR A3(2), NMR, 24 STRUCTURES
Authors	:	Crump, M.P.; Crosby, J.; Dempsey, C.E.; Parkinson, J.A.; Murray, M.; Hopwood, D.A.; Simpson, T.J.
Deposited on	:	1997-03-23

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:

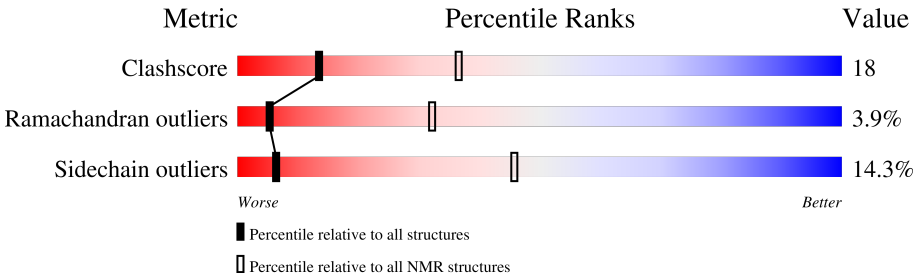
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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	86	44% 36% 5% 15%

2 Ensemble composition and analysis (i)

This entry contains 24 models. Model 11 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:4-A:18, A:29-A:86 (73)	1.32	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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1277 atoms, of which 630 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	86	1277	397	630	108	139	3	0

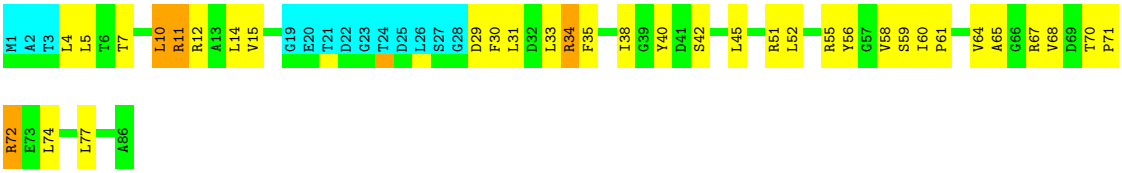
4 Residue-property plots (i)

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: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

Chain A: 44% 36% 5% 15%



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

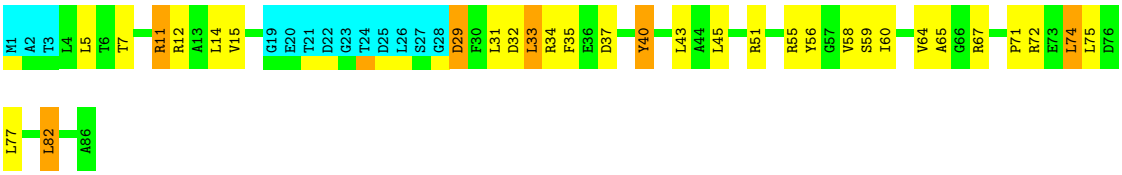
• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

Chain A: 49% 28% 7% • 15%

4.2.2 Score per residue for model 2

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

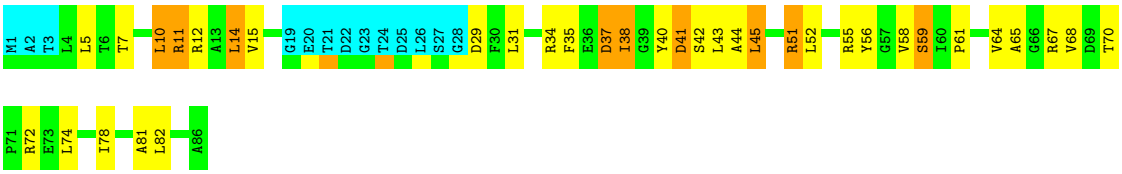
Chain A: 49% 29% 7% 15%



4.2.3 Score per residue for model 3

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

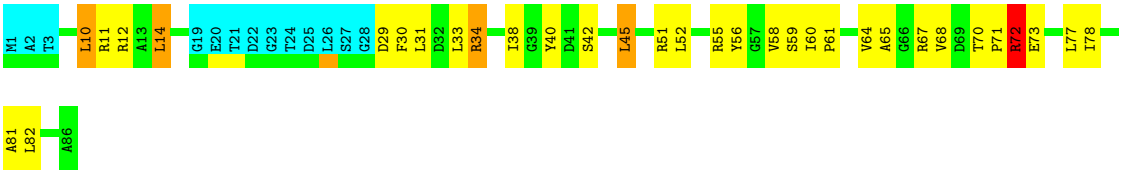
Chain A: 43% 31% 10% 15%



4.2.4 Score per residue for model 4

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

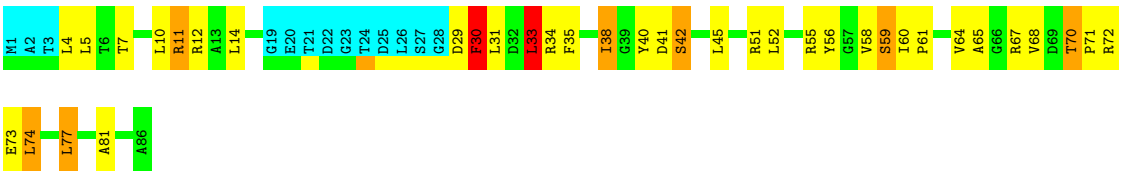
Chain A: 47% 33% 5% • 15%



4.2.5 Score per residue for model 5

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

Chain A: 42% 33% 8% • 15%



4.2.6 Score per residue for model 6

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

Chain A: 47% 36% •• 15%

M1 A2 T3 L4 L5 T6 T7 D8 D9 L10 R11 R12 A13 L14 V15 G19 E20 T21 D22 G23 T24 D25 L26 S27 G28 D29 F30 L31 R34 F35 E36 D41 S42 L45 R51 R55 Y56 G57 V58 S59 I60 P61 V64 A65 G66 R67 V68 D69 T70 P71 R72 L77

A81 A86

4.2.7 Score per residue for model 7

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

Chain A: 44% 30% 9% • 15%

M1 A2 T3 L4 L5 T6 T7 D8 D9 L10 R11 R12 A13 L14 G19 E20 T21 D22 G23 T24 D25 L26 S27 G28 D29 F30 L31 D32 L33 R34 F35 E36 D37 I38 G39 Y40 D41 S42 L45 M46 E47 R51 S54 R55 Y56 G57 V58 S59 I60 P61 V64 A65 G66 R67 V68

D69 T70 P71 R72 A81 A86

4.2.8 Score per residue for model 8

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

Chain A: 41% 34% 10% 15%

M1 A2 T3 L4 L5 T6 T7 L10 R11 R12 A13 L14 V15 E16 G19 E20 T21 D22 G23 T24 D25 L26 S27 G28 D29 F30 L31 R34 F35 E36 D37 I38 G39 Y40 D41 S42 L43 A44 L45 M46 A50 R51 L52 E53 S54 R55 V58 S59 I60 P61 V64 A65 G66 R67

V68 P71 R72 E73 L74 I78 A86

4.2.9 Score per residue for model 9

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

Chain A: 47% 33% • • 15%

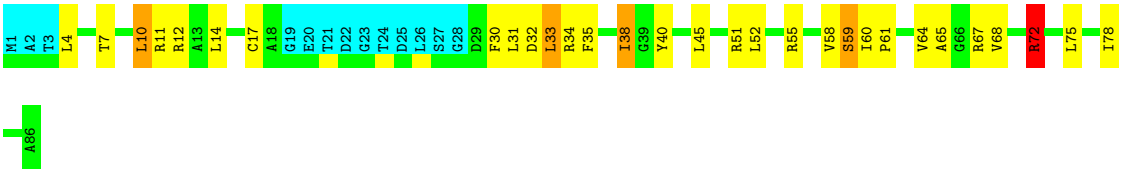
M1 A2 T3 T7 L10 R11 R12 A13 L14 V15 G19 E20 T21 D22 G23 T24 D25 L26 S27 G28 D29 F30 L31 D32 L33 R34 F35 E36 D37 I38 S42 L45 R51 R55 Y56 G57 V58 S59 I60 P61 D62 D63 V64 A65 G66 R67 V68 D69 T70 P71 R72 E73 L74

L77 A81 A86

4.2.10 Score per residue for model 10

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

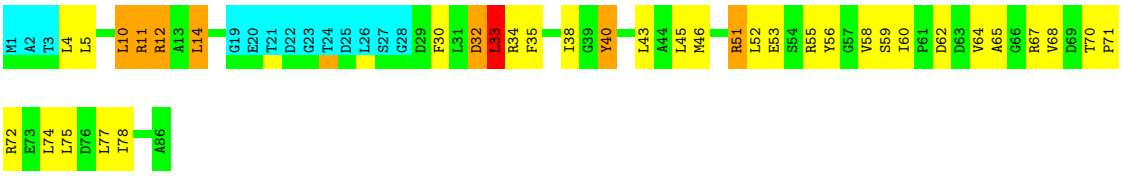
Chain A: 50% 29% 5% • 15%



4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

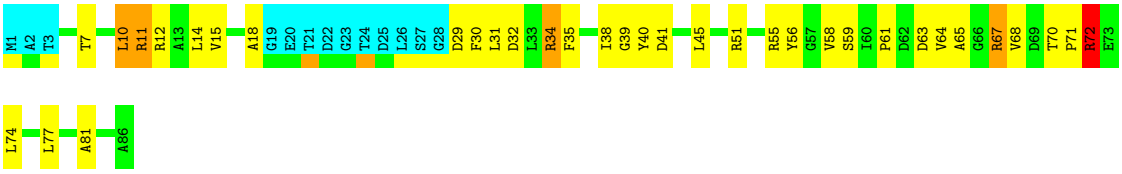
Chain A: 43% 33% 8% • 15%



4.2.12 Score per residue for model 12

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

Chain A: 44% 35% 5% • 15%



4.2.13 Score per residue for model 13

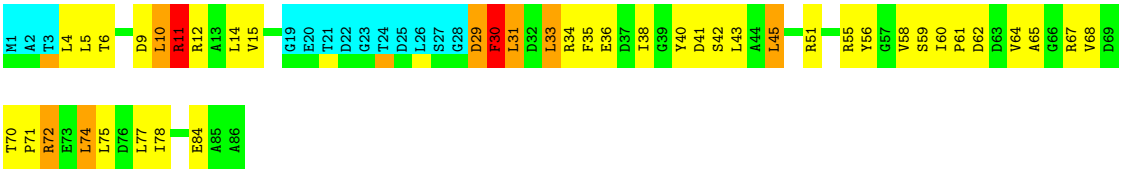
• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

Chain A: 42% 35% 8% 15%

4.2.14 Score per residue for model 14

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

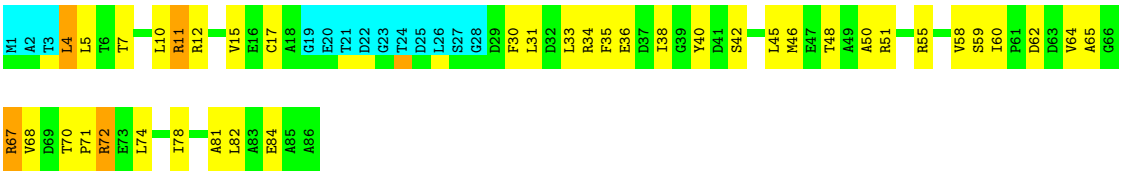
Chain A: 36% 38% 8% • 15%



4.2.15 Score per residue for model 15

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

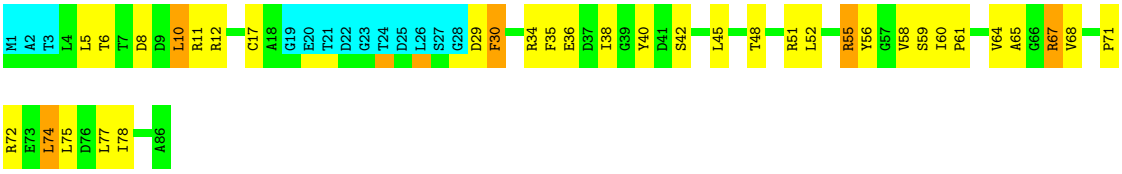
Chain A: 40% 41% 5% 15%



4.2.16 Score per residue for model 16

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

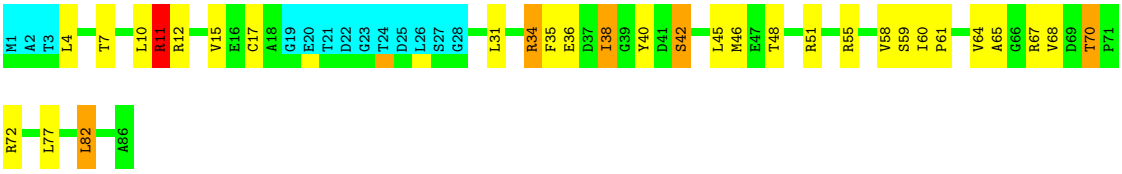
Chain A: 44% 35% 6% 15%



4.2.17 Score per residue for model 17

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

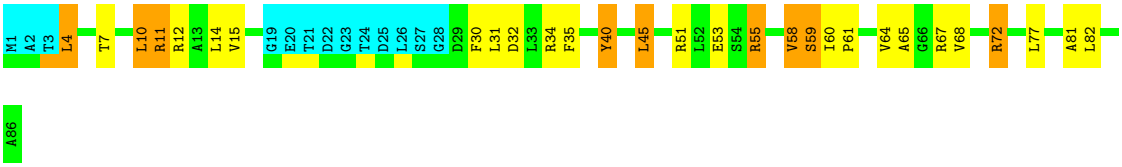
Chain A: 49% 29% 6% • 15%



4.2.18 Score per residue for model 18

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

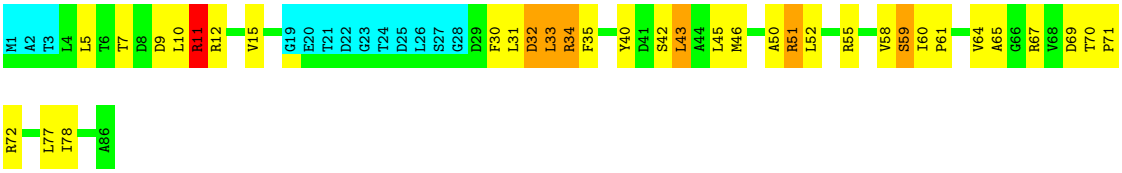
Chain A: 51% 23% 10% 15%



4.2.19 Score per residue for model 19

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

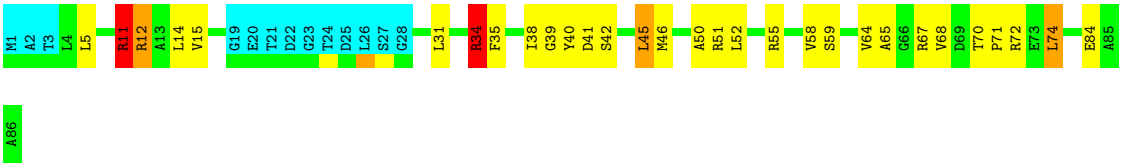
Chain A: 44% 33% 7% • 15%



4.2.20 Score per residue for model 20

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

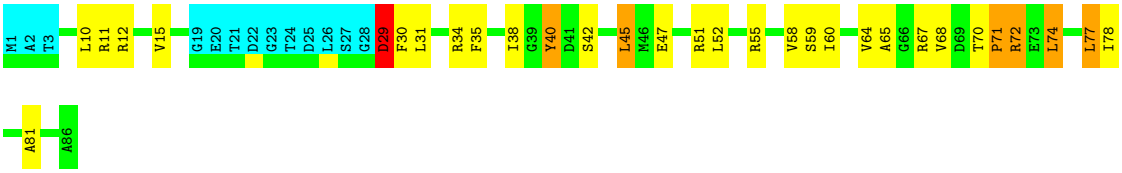
Chain A: 50% 29% • • 15%



4.2.21 Score per residue for model 21

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

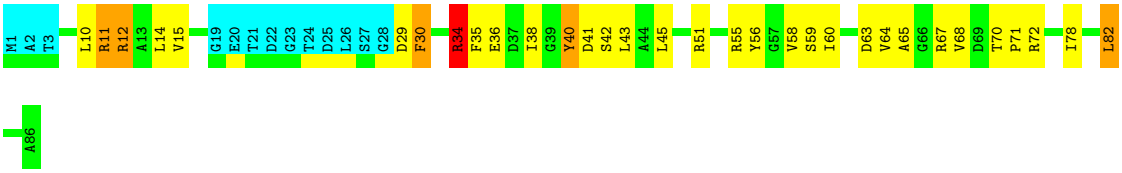
Chain A: 49% 28% 7% • 15%



4.2.22 Score per residue for model 22

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

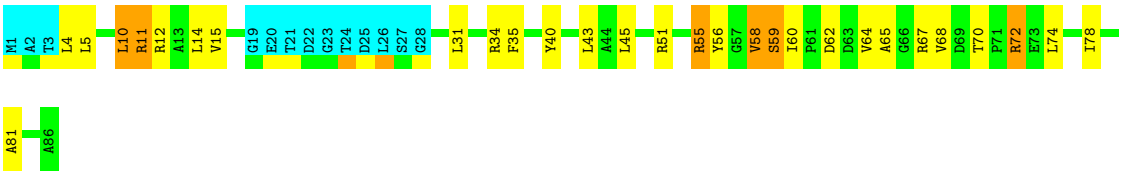
Chain A: 48% 30% 6% • 15%



4.2.23 Score per residue for model 23

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

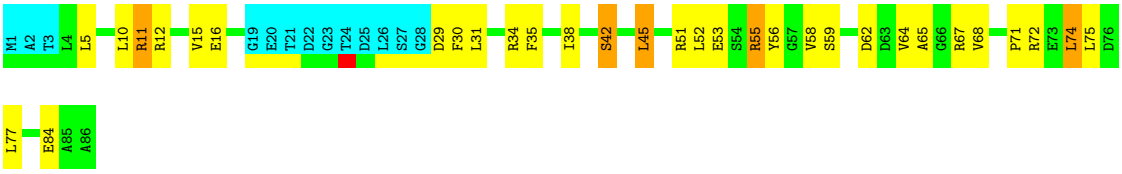
Chain A: 51% 27% 7% 15%



4.2.24 Score per residue for model 24

• Molecule 1: ACTINORHODIN POLYKETIDE SYNTHASE ACYL CARRIER PROTEIN

Chain A: 48% 31% 6% 15%



5 Refinement protocol and experimental data overview (i)

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

Of the 30 calculated structures, 24 were deposited, based on the following criterion: *FEWEST RESTRAINT VIOLATIONS*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	

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.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	7.0±0.0
All	All	0	168

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	11	ARG	Sidechain	24
1	A	12	ARG	Sidechain	24
1	A	34	ARG	Sidechain	24
1	A	51	ARG	Sidechain	24
1	A	55	ARG	Sidechain	24
1	A	67	ARG	Sidechain	24
1	A	72	ARG	Sidechain	24

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	562	554	554	20±5
All	All	13488	13296	13296	481

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ILE:HD11	1:A:40:TYR:CE2	0.87	2.03	17	6
1:A:14:LEU:HD21	1:A:35:PHE:CE1	0.84	2.07	3	3
1:A:35:PHE:CE2	1:A:45:LEU:HD22	0.84	2.08	21	20
1:A:38:ILE:HD11	1:A:40:TYR:CD2	0.81	2.10	22	6
1:A:11:ARG:O	1:A:15:VAL:HG23	0.79	1.78	15	17
1:A:58:VAL:HG23	1:A:81:ALA:HB2	0.79	1.54	9	1
1:A:58:VAL:HG21	1:A:81:ALA:HB1	0.77	1.56	6	2
1:A:58:VAL:HG11	1:A:78:ILE:HG23	0.77	1.56	16	5
1:A:58:VAL:HG23	1:A:81:ALA:CB	0.77	2.09	18	3
1:A:38:ILE:O	1:A:38:ILE:HD13	0.74	1.82	10	3
1:A:10:LEU:HD12	1:A:14:LEU:HD12	0.74	1.60	13	13
1:A:35:PHE:CE1	1:A:45:LEU:HD13	0.73	2.19	3	1
1:A:58:VAL:HG11	1:A:78:ILE:CG2	0.72	2.14	16	1
1:A:17:CYS:SG	1:A:48:THR:HG21	0.71	2.25	15	1
1:A:17:CYS:SG	1:A:48:THR:HG23	0.71	2.26	16	1
1:A:58:VAL:CG2	1:A:81:ALA:HB3	0.69	2.18	23	2
1:A:33:LEU:HD22	1:A:70:THR:HG22	0.69	1.63	5	1
1:A:10:LEU:HD13	1:A:11:ARG:N	0.69	2.03	7	1
1:A:35:PHE:CD2	1:A:45:LEU:HD22	0.68	2.23	12	15
1:A:61:PRO:HB3	1:A:77:LEU:HD12	0.68	1.66	5	1
1:A:10:LEU:HD22	1:A:10:LEU:O	0.67	1.88	7	1
1:A:43:LEU:O	1:A:43:LEU:HD23	0.67	1.89	2	1
1:A:42:SER:O	1:A:45:LEU:HD23	0.66	1.91	3	1
1:A:5:LEU:HD22	1:A:9:ASP:CG	0.66	2.10	6	2
1:A:61:PRO:O	1:A:65:ALA:HB3	0.66	1.90	14	8
1:A:74:LEU:HA	1:A:77:LEU:HD12	0.66	1.65	16	4
1:A:14:LEU:HD23	1:A:40:TYR:CE1	0.66	2.26	8	1
1:A:74:LEU:O	1:A:78:ILE:HD12	0.66	1.90	14	3
1:A:73:GLU:O	1:A:77:LEU:HD23	0.65	1.92	5	1
1:A:33:LEU:HD22	1:A:70:THR:CG2	0.65	2.21	5	1
1:A:68:VAL:HG11	1:A:74:LEU:HD11	0.64	1.67	14	2
1:A:30:PHE:CE1	1:A:31:LEU:HD21	0.64	2.28	5	1
1:A:68:VAL:HG21	1:A:74:LEU:CD1	0.64	2.23	20	4
1:A:4:LEU:HD22	1:A:4:LEU:N	0.63	2.08	14	2
1:A:7:THR:HG21	1:A:31:LEU:HD11	0.63	1.69	10	1
1:A:4:LEU:HD11	1:A:82:LEU:HD13	0.63	1.70	15	1
1:A:34:ARG:O	1:A:38:ILE:HG22	0.62	1.94	1	3
1:A:4:LEU:HD13	1:A:4:LEU:N	0.62	2.08	18	1
1:A:35:PHE:CZ	1:A:74:LEU:HD22	0.62	2.30	21	2
1:A:58:VAL:CG2	1:A:60:ILE:HD13	0.62	2.24	11	1
1:A:31:LEU:HD13	1:A:72:ARG:CD	0.61	2.26	23	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ILE:N	1:A:61:PRO:CD	0.60	2.64	8	6
1:A:14:LEU:O	1:A:18:ALA:HB2	0.60	1.95	12	1
1:A:64:VAL:CG2	1:A:77:LEU:HD11	0.60	2.26	6	1
1:A:5:LEU:HD21	1:A:56:TYR:CE2	0.60	2.31	23	6
1:A:14:LEU:HD23	1:A:40:TYR:CE2	0.60	2.31	7	3
1:A:31:LEU:HD13	1:A:72:ARG:HD3	0.60	1.72	12	2
1:A:41:ASP:C	1:A:45:LEU:HD21	0.60	2.17	6	1
1:A:45:LEU:HD13	1:A:68:VAL:CG1	0.59	2.27	14	2
1:A:4:LEU:HD13	1:A:82:LEU:HB3	0.59	1.74	1	1
1:A:38:ILE:HD11	1:A:40:TYR:HB3	0.59	1.75	3	1
1:A:58:VAL:HG22	1:A:59:SER:N	0.59	2.13	18	15
1:A:31:LEU:HD23	1:A:71:PRO:HB2	0.58	1.73	21	3
1:A:7:THR:HA	1:A:10:LEU:HD12	0.58	1.74	7	1
1:A:10:LEU:O	1:A:14:LEU:HD12	0.58	1.99	8	1
1:A:60:ILE:HD11	1:A:78:ILE:HA	0.58	1.74	22	1
1:A:32:ASP:HB3	1:A:33:LEU:HD23	0.58	1.76	11	2
1:A:5:LEU:HD12	1:A:9:ASP:HB3	0.58	1.76	19	1
1:A:60:ILE:O	1:A:60:ILE:HG23	0.57	1.98	14	6
1:A:60:ILE:HG21	1:A:77:LEU:HD21	0.57	1.76	21	1
1:A:58:VAL:CG2	1:A:81:ALA:HB2	0.57	2.27	9	1
1:A:10:LEU:HD22	1:A:10:LEU:C	0.57	2.19	7	1
1:A:65:ALA:O	1:A:68:VAL:HG12	0.57	1.99	10	4
1:A:68:VAL:O	1:A:68:VAL:HG13	0.57	1.99	15	21
1:A:68:VAL:HG11	1:A:74:LEU:CD1	0.56	2.30	5	4
1:A:10:LEU:HB3	1:A:75:LEU:HD13	0.56	1.77	14	4
1:A:58:VAL:HG11	1:A:78:ILE:HD12	0.56	1.77	11	1
1:A:5:LEU:HD23	1:A:5:LEU:N	0.56	2.16	19	2
1:A:59:SER:O	1:A:60:ILE:HD13	0.56	2.00	17	1
1:A:7:THR:HG22	1:A:30:PHE:CZ	0.56	2.35	19	4
1:A:58:VAL:HG21	1:A:81:ALA:CB	0.55	2.31	5	1
1:A:33:LEU:HA	1:A:70:THR:HG22	0.55	1.78	14	1
1:A:5:LEU:O	1:A:75:LEU:HD11	0.55	2.02	2	2
1:A:82:LEU:O	1:A:82:LEU:HD13	0.55	2.02	2	1
1:A:53:GLU:HA	1:A:58:VAL:HG12	0.55	1.78	18	1
1:A:33:LEU:HD12	1:A:70:THR:HG23	0.55	1.78	14	1
1:A:33:LEU:HD21	1:A:36:GLU:HB2	0.54	1.78	14	1
1:A:46:MET:O	1:A:50:ALA:HB2	0.53	2.03	19	5
1:A:68:VAL:HG21	1:A:74:LEU:HD13	0.53	1.79	20	4
1:A:40:TYR:HB3	1:A:45:LEU:HD23	0.53	1.81	4	2
1:A:10:LEU:HD21	1:A:31:LEU:HD21	0.53	1.80	14	2
1:A:7:THR:HG23	1:A:31:LEU:HD11	0.53	1.81	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ILE:HG23	1:A:40:TYR:CD1	0.53	2.38	4	1
1:A:30:PHE:CZ	1:A:31:LEU:HD21	0.52	2.39	14	1
1:A:10:LEU:HD13	1:A:31:LEU:HD21	0.52	1.81	21	1
1:A:7:THR:HG22	1:A:30:PHE:HZ	0.52	1.64	18	3
1:A:7:THR:CG2	1:A:31:LEU:HD11	0.52	2.34	10	4
1:A:31:LEU:HD13	1:A:72:ARG:HD2	0.52	1.82	23	3
1:A:32:ASP:O	1:A:33:LEU:HD23	0.52	2.05	19	1
1:A:52:LEU:O	1:A:52:LEU:HD23	0.51	2.04	20	1
1:A:5:LEU:HD11	1:A:56:TYR:CZ	0.51	2.40	14	2
1:A:58:VAL:HG23	1:A:81:ALA:HB3	0.51	1.82	3	1
1:A:38:ILE:HD13	1:A:40:TYR:CD2	0.51	2.41	5	1
1:A:71:PRO:HA	1:A:74:LEU:HD21	0.51	1.82	21	2
1:A:43:LEU:HD12	1:A:43:LEU:N	0.51	2.20	3	1
1:A:58:VAL:CG2	1:A:81:ALA:HB1	0.51	2.34	5	3
1:A:30:PHE:CD1	1:A:30:PHE:N	0.51	2.78	8	1
1:A:10:LEU:CD1	1:A:14:LEU:HD12	0.51	2.34	23	3
1:A:10:LEU:HD12	1:A:14:LEU:CD1	0.50	2.35	8	2
1:A:60:ILE:C	1:A:60:ILE:HD12	0.50	2.27	8	1
1:A:31:LEU:HD23	1:A:71:PRO:HG2	0.50	1.83	4	3
1:A:58:VAL:HG11	1:A:78:ILE:CD1	0.50	2.36	11	2
1:A:40:TYR:CD2	1:A:41:ASP:N	0.50	2.80	3	1
1:A:38:ILE:HD13	1:A:38:ILE:C	0.50	2.26	10	3
1:A:35:PHE:CZ	1:A:45:LEU:HD13	0.50	2.40	3	1
1:A:52:LEU:HD21	1:A:56:TYR:CE2	0.49	2.41	5	1
1:A:78:ILE:HG22	1:A:82:LEU:HD12	0.49	1.83	15	2
1:A:6:THR:HG23	1:A:8:ASP:H	0.49	1.68	16	1
1:A:78:ILE:HG22	1:A:82:LEU:CD1	0.49	2.37	15	1
1:A:5:LEU:HD21	1:A:56:TYR:HE2	0.49	1.68	13	1
1:A:68:VAL:HG11	1:A:74:LEU:HD13	0.48	1.84	1	3
1:A:56:TYR:HB3	1:A:82:LEU:HD11	0.48	1.85	22	1
1:A:30:PHE:O	1:A:30:PHE:CD2	0.48	2.67	16	2
1:A:14:LEU:HD21	1:A:35:PHE:CD1	0.48	2.43	3	1
1:A:38:ILE:HG22	1:A:38:ILE:O	0.48	2.08	11	1
1:A:45:LEU:HD11	1:A:68:VAL:CG1	0.48	2.38	20	1
1:A:7:THR:CG2	1:A:30:PHE:CE1	0.48	2.97	5	1
1:A:58:VAL:HG21	1:A:81:ALA:HB3	0.47	1.85	23	1
1:A:4:LEU:HD12	1:A:82:LEU:HB3	0.47	1.86	17	1
1:A:45:LEU:HD11	1:A:68:VAL:HG12	0.47	1.86	17	4
1:A:5:LEU:HD23	1:A:5:LEU:H	0.47	1.67	16	2
1:A:35:PHE:CZ	1:A:74:LEU:CD2	0.47	2.97	21	2
1:A:10:LEU:HD22	1:A:14:LEU:HD12	0.47	1.87	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:O	1:A:33:LEU:HD23	0.47	2.10	14	1
1:A:5:LEU:HD13	1:A:56:TYR:CE2	0.47	2.45	11	1
1:A:10:LEU:HD13	1:A:10:LEU:C	0.46	2.30	7	1
1:A:38:ILE:HD11	1:A:40:TYR:CE1	0.46	2.45	14	2
1:A:14:LEU:HD13	1:A:34:ARG:NE	0.46	2.25	20	2
1:A:10:LEU:CD2	1:A:14:LEU:HD12	0.46	2.41	22	1
1:A:40:TYR:HE2	1:A:45:LEU:HD22	0.46	1.70	3	1
1:A:30:PHE:CZ	1:A:31:LEU:CD2	0.46	2.98	14	1
1:A:6:THR:O	1:A:75:LEU:HD11	0.46	2.10	13	3
1:A:31:LEU:HD23	1:A:71:PRO:CG	0.46	2.40	4	2
1:A:41:ASP:O	1:A:45:LEU:HD23	0.46	2.11	12	1
1:A:32:ASP:O	1:A:33:LEU:CB	0.45	2.64	19	1
1:A:35:PHE:CZ	1:A:45:LEU:CD1	0.45	3.00	3	1
1:A:31:LEU:HD13	1:A:72:ARG:HG3	0.45	1.88	14	1
1:A:68:VAL:HG22	1:A:70:THR:O	0.45	2.12	14	4
1:A:29:ASP:O	1:A:30:PHE:CD1	0.45	2.70	16	3
1:A:31:LEU:HD13	1:A:72:ARG:HE	0.45	1.71	7	2
1:A:60:ILE:N	1:A:61:PRO:HD3	0.45	2.26	6	1
1:A:53:GLU:OE1	1:A:58:VAL:HG13	0.45	2.11	11	1
1:A:41:ASP:CG	1:A:44:ALA:HB3	0.45	2.32	3	1
1:A:38:ILE:CD1	1:A:40:TYR:CD2	0.45	2.99	17	1
1:A:10:LEU:O	1:A:10:LEU:HD23	0.45	2.11	24	1
1:A:52:LEU:HD22	1:A:52:LEU:N	0.45	2.26	21	1
1:A:64:VAL:HG13	1:A:65:ALA:N	0.45	2.26	9	24
1:A:52:LEU:HD22	1:A:55:ARG:NH2	0.45	2.26	16	1
1:A:7:THR:CG2	1:A:30:PHE:CZ	0.45	2.99	5	1
1:A:4:LEU:HD11	1:A:82:LEU:HD23	0.45	1.89	18	1
1:A:68:VAL:HG21	1:A:74:LEU:HD12	0.44	1.88	5	2
1:A:53:GLU:HG2	1:A:78:ILE:HD13	0.44	1.90	8	1
1:A:55:ARG:NE	1:A:56:TYR:CE1	0.44	2.85	16	1
1:A:5:LEU:HD22	1:A:9:ASP:OD2	0.44	2.12	6	1
1:A:10:LEU:HD23	1:A:10:LEU:C	0.44	2.33	5	1
1:A:43:LEU:O	1:A:43:LEU:HD13	0.44	2.13	8	2
1:A:10:LEU:HD23	1:A:10:LEU:O	0.44	2.13	19	2
1:A:32:ASP:CB	1:A:33:LEU:HD23	0.44	2.43	2	2
1:A:35:PHE:CD1	1:A:45:LEU:HD22	0.44	2.48	20	1
1:A:38:ILE:HD12	1:A:38:ILE:C	0.44	2.33	20	1
1:A:58:VAL:CG1	1:A:78:ILE:HG23	0.43	2.43	10	1
1:A:38:ILE:CD1	1:A:40:TYR:CE2	0.43	2.99	15	2
1:A:52:LEU:HD12	1:A:52:LEU:N	0.43	2.28	3	1
1:A:41:ASP:O	1:A:42:SER:CB	0.43	2.66	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:VAL:CG1	1:A:77:LEU:HD21	0.43	2.43	1	1
1:A:29:ASP:O	1:A:30:PHE:CB	0.43	2.67	5	1
1:A:58:VAL:HG12	1:A:61:PRO:HB3	0.43	1.88	9	1
1:A:4:LEU:N	1:A:4:LEU:CD2	0.43	2.80	17	2
1:A:29:ASP:O	1:A:30:PHE:CG	0.43	2.72	4	3
1:A:30:PHE:CE1	1:A:31:LEU:CD2	0.43	2.99	5	1
1:A:58:VAL:HG13	1:A:59:SER:H	0.43	1.73	23	1
1:A:64:VAL:HG21	1:A:77:LEU:HD11	0.43	1.89	6	1
1:A:5:LEU:HD21	1:A:56:TYR:CE1	0.43	2.49	14	1
1:A:5:LEU:N	1:A:5:LEU:CD2	0.43	2.82	16	2
1:A:29:ASP:O	1:A:30:PHE:CD2	0.43	2.72	21	1
1:A:5:LEU:HD22	1:A:9:ASP:CB	0.43	2.44	7	1
1:A:58:VAL:O	1:A:81:ALA:HB1	0.43	2.13	7	1
1:A:58:VAL:HG13	1:A:59:SER:N	0.42	2.29	17	5
1:A:4:LEU:HD12	1:A:4:LEU:N	0.42	2.29	10	1
1:A:41:ASP:OD2	1:A:44:ALA:HB2	0.42	2.13	13	1
1:A:58:VAL:HG22	1:A:59:SER:H	0.42	1.75	1	1
1:A:38:ILE:CG2	1:A:40:TYR:CD1	0.42	3.02	4	1
1:A:56:TYR:CD1	1:A:56:TYR:N	0.42	2.86	12	1
1:A:33:LEU:HD12	1:A:70:THR:CG2	0.42	2.44	14	1
1:A:30:PHE:O	1:A:31:LEU:HD23	0.42	2.14	5	1
1:A:4:LEU:N	1:A:4:LEU:HD23	0.42	2.29	8	1
1:A:14:LEU:CD2	1:A:40:TYR:CE1	0.42	3.01	8	1
1:A:60:ILE:HD12	1:A:61:PRO:N	0.42	2.30	8	1
1:A:14:LEU:HD13	1:A:34:ARG:HE	0.42	1.74	22	1
1:A:10:LEU:HD12	1:A:10:LEU:C	0.42	2.35	10	1
1:A:40:TYR:O	1:A:45:LEU:HD23	0.42	2.15	1	1
1:A:17:CYS:SG	1:A:52:LEU:HD11	0.42	2.54	10	1
1:A:38:ILE:CD1	1:A:40:TYR:CE1	0.42	3.02	16	1
1:A:58:VAL:HG23	1:A:81:ALA:HB1	0.42	1.88	18	1
1:A:58:VAL:CG2	1:A:59:SER:N	0.42	2.83	18	1
1:A:13:ALA:HB1	1:A:52:LEU:HD21	0.41	1.90	1	1
1:A:30:PHE:CD1	1:A:31:LEU:HG	0.41	2.49	5	1
1:A:33:LEU:HD22	1:A:36:GLU:CD	0.41	2.36	15	1
1:A:17:CYS:HB3	1:A:48:THR:HG21	0.41	1.92	17	1
1:A:29:ASP:O	1:A:30:PHE:HB3	0.41	2.15	5	1
1:A:61:PRO:CB	1:A:64:VAL:CG1	0.41	2.99	18	1
1:A:45:LEU:HD13	1:A:68:VAL:HG11	0.41	1.91	14	1
1:A:45:LEU:C	1:A:45:LEU:HD12	0.41	2.36	12	1
1:A:45:LEU:CD1	1:A:68:VAL:CG1	0.41	2.99	14	1
1:A:30:PHE:CE2	1:A:31:LEU:HD21	0.41	2.51	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:O	1:A:56:TYR:CD1	0.41	2.74	4	1
1:A:10:LEU:HB2	1:A:75:LEU:HD13	0.41	1.93	16	1
1:A:61:PRO:CB	1:A:65:ALA:CB	0.41	2.98	6	1
1:A:64:VAL:CG1	1:A:77:LEU:HD11	0.41	2.46	14	1
1:A:30:PHE:O	1:A:30:PHE:CG	0.40	2.73	22	1
1:A:35:PHE:CD1	1:A:40:TYR:CZ	0.40	3.09	3	1
1:A:52:LEU:CD1	1:A:56:TYR:CD1	0.40	3.03	13	1
1:A:35:PHE:O	1:A:40:TYR:CD1	0.40	2.75	14	1
1:A:60:ILE:O	1:A:60:ILE:CG2	0.40	2.69	14	1
1:A:58:VAL:CG2	1:A:81:ALA:CB	0.40	3.00	21	1
1:A:10:LEU:HD13	1:A:31:LEU:CD2	0.40	2.46	17	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	72/86 (84%)	58±3 (80±4%)	11±3 (16±4%)	3±1 (4±2%)	5	32
All	All	1728/2064 (84%)	1388 (80%)	273 (16%)	67 (4%)	5	32

All 16 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	42	SER	15
1	A	71	PRO	13
1	A	29	ASP	6
1	A	59	SER	5
1	A	37	ASP	4
1	A	30	PHE	3
1	A	33	LEU	3
1	A	58	VAL	3
1	A	39	GLY	3
1	A	40	TYR	3
1	A	57	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	63	ASP	2
1	A	34	ARG	2
1	A	31	LEU	1
1	A	38	ILE	1
1	A	32	ASP	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	59/68 (87%)	51±2 (86±4%)	8±2 (14±4%)	6 46
All	All	1416/1632 (87%)	1214 (86%)	202 (14%)	6 46

All 42 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	70	THR	16
1	A	10	LEU	15
1	A	74	LEU	11
1	A	77	LEU	9
1	A	33	LEU	9
1	A	11	ARG	8
1	A	40	TYR	7
1	A	45	LEU	7
1	A	43	LEU	7
1	A	34	ARG	6
1	A	29	ASP	6
1	A	38	ILE	6
1	A	4	LEU	6
1	A	62	ASP	6
1	A	14	LEU	5
1	A	82	LEU	5
1	A	41	ASP	5
1	A	12	ARG	5
1	A	51	ARG	4
1	A	72	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	30	PHE	4
1	A	36	GLU	4
1	A	55	ARG	4
1	A	59	SER	4
1	A	52	LEU	4
1	A	84	GLU	4
1	A	32	ASP	3
1	A	46	MET	3
1	A	67	ARG	3
1	A	37	ASP	2
1	A	73	GLU	2
1	A	6	THR	2
1	A	47	GLU	2
1	A	16	GLU	2
1	A	53	GLU	2
1	A	5	LEU	2
1	A	60	ILE	2
1	A	42	SER	2
1	A	54	SER	1
1	A	9	ASP	1
1	A	69	ASP	1
1	A	63	ASP	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