Full wwPDB NMR Structure Validation Report (i)

Feb 12, 2022 – 04:46 PM EST

PDB ID	:	1G47
Title	:	1ST LIM DOMAIN OF PINCH PROTEIN
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Deposited on	:	2000-10-26

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

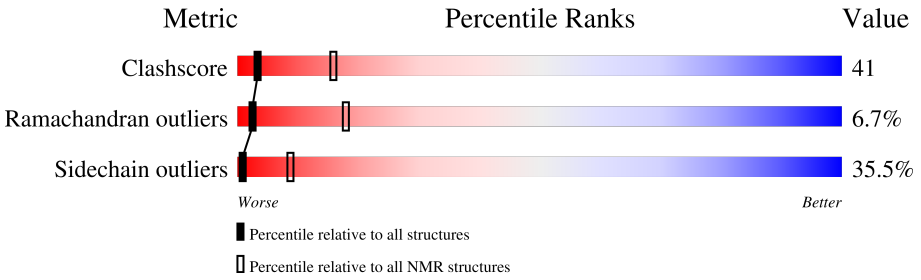
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	77	25% 38% 16% 13% 9%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 6 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:8-A:67 (60)	0.42	7

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 4 single-model clusters were found.

Cluster number	Models
1	6, 7, 8, 11, 13, 16, 18, 24, 25
2	1, 5, 9, 12, 14, 17, 21, 23
3	10, 15, 20, 22
Single-model clusters	2; 3; 4; 19

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1057 atoms, of which 501 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PINCH PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	70	1055	352	501	91	102	9	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ILE	-	cloning artifact	UNP P48059
A	-2	SER	-	cloning artifact	UNP P48059
A	-1	GLU	-	cloning artifact	UNP P48059
A	0	PHE	-	cloning artifact	UNP P48059
A	71	TRP	-	cloning artifact	UNP P48059
A	72	ILE	-	cloning artifact	UNP P48059
A	73	LEU	-	cloning artifact	UNP P48059

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

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: PINCH PROTEIN

Chain A: 25% 38% 16% 13% 9%

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

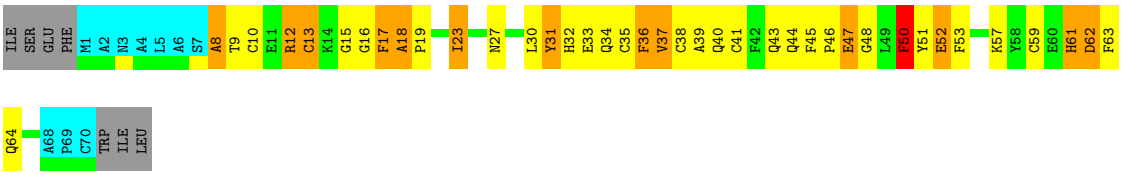
• Molecule 1: PINCH PROTEIN

Chain A: 25% 32% 19% • 13% 9%

4.2.2 Score per residue for model 2

• Molecule 1: PINCH PROTEIN

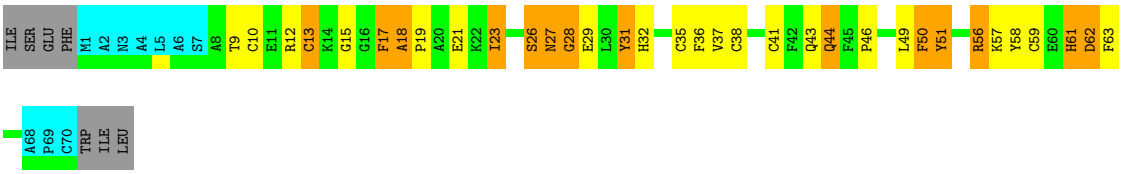
Chain A: 26% 34% 17% • 13% 9%



4.2.3 Score per residue for model 3

- Molecule 1: PINCH PROTEIN

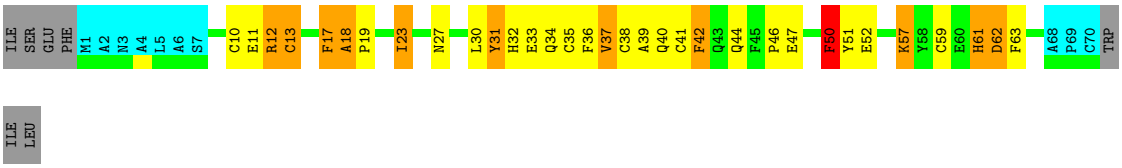
Chain A: 34% 26% 18% 13% 9%



4.2.4 Score per residue for model 4

- Molecule 1: PINCH PROTEIN

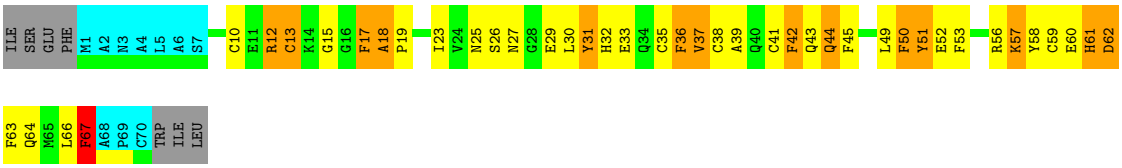
Chain A: 35% 27% 14% • 13% 9%



4.2.5 Score per residue for model 5

- Molecule 1: PINCH PROTEIN

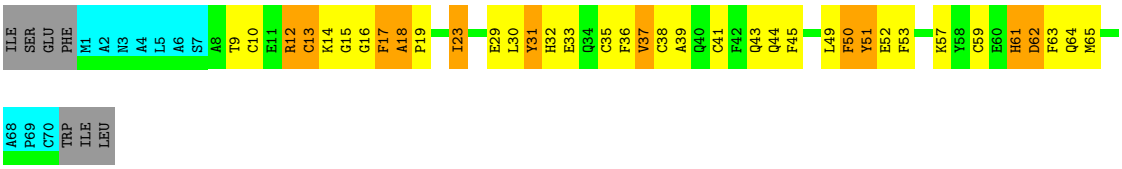
Chain A: 23% 35% 18% • 13% 9%



4.2.6 Score per residue for model 6

- Molecule 1: PINCH PROTEIN

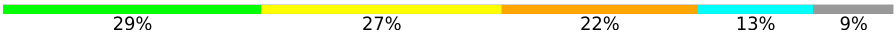
Chain A: 30% 34% 14% 13% 9%

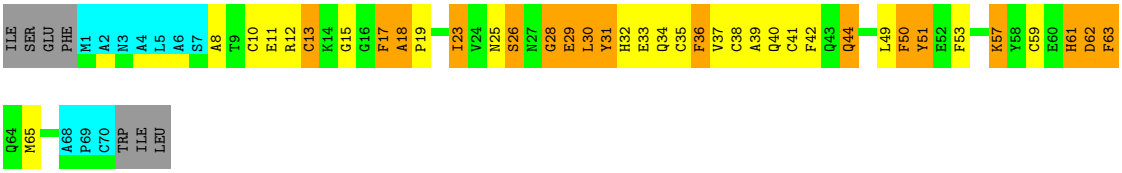


4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: PINCH PROTEIN

Chain A:

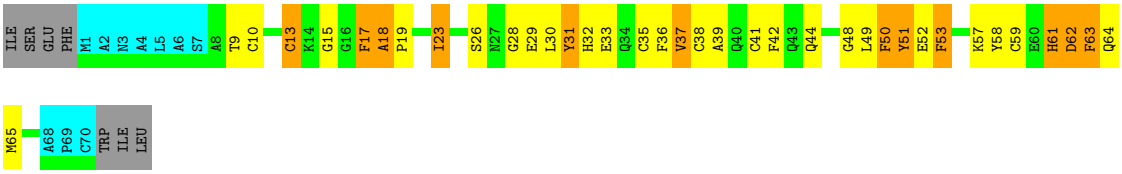




4.2.8 Score per residue for model 8

- Molecule 1: PINCH PROTEIN

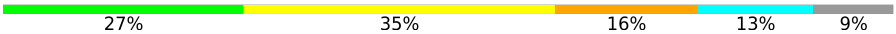
Chain A:

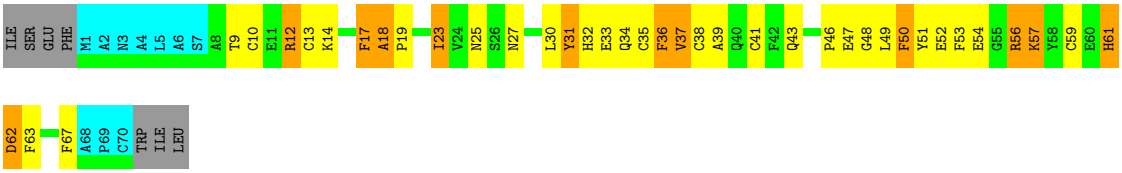


4.2.9 Score per residue for model 9

- Molecule 1: PINCH PROTEIN

Chain A:





4.2.10 Score per residue for model 10

- Molecule 1: PINCH PROTEIN

Chain A: 23% 39% 14% • 13% 9%

ILE SER GLU PHE M1 A2 N3 A4 L5 A6 S7 A8 T9 C10 E11 R12 C13 K14 G15 G16 F17 A18 P19 A20 E21 K22 I23 S26 N27 G28 E29 L30 Y31 H32 C35 F36 V37 C38 C41 F42 Q43 Q44 F45 P46 E47 G48 L49 F50 Y51 E52 F53 E54 G55 R56 K57 Y58 C59

E60 H61 D62 F63 Q64 M65 A68 P69 C70 TRP ILE LEU

4.2.11 Score per residue for model 11

- Molecule 1: PINCH PROTEIN

Chain A: 26% 34% 18% 13% 9%

ILE SER GLU PHE M1 A2 N3 A4 L5 A6 S7 A8 T9 C10 E11 R12 C13 K14 G15 G16 F17 A18 P19 A20 I23 S26 N27 G28 E29 L30 Y31 H32 E33 Q34 C35 F36 V37 C38 A39 Q40 C41 Q44 F45 L49 F50 Y51 E52 K57 Y58 C59 E60 H61 D62 F63 Q64

M65 A68 P69 C70 TRP ILE LEU

4.2.12 Score per residue for model 12

- Molecule 1: PINCH PROTEIN

Chain A: 26% 34% 18% 13% 9%

ILE SER GLU PHE M1 A2 N3 A4 L5 A6 S7 A8 T9 C10 E11 R12 C13 K14 G15 G16 F17 A18 P19 I23 S26 N27 G28 Y31 H32 E33 Q34 C35 F36 V37 C38 A39 Q40 C41 F42 Q43 Q44 F45 P46 E47 G48 L49 F50 Y51 E52 F53 E54 K57 Y58 C59 E60 H61

D62 F63 Q64 F67 A68 P69 C70 TRP ILE LEU

4.2.13 Score per residue for model 13

- Molecule 1: PINCH PROTEIN

Chain A: 31% 30% 17% 13% 9%

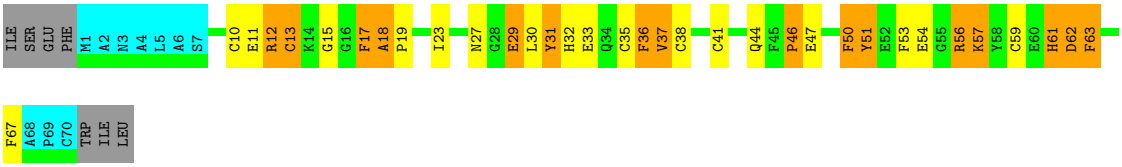
ILE SER GLU PHE M1 A2 N3 A4 L5 A6 S7 C10 E11 R12 C13 K14 G15 G16 F17 A18 P19 I23 V24 N25 S26 N27 G28 E29 L30 Y31 H32 E33 Q34 C35 F36 V37 C38 A39 Q40 C41 Q44 L49 F50 Y51 E52 F53 R56 K57 Y58 C59 E60 H61 D62 F63 Q64

M65 A68 P69 C70 TRP ILE LEU

4.2.14 Score per residue for model 14

- Molecule 1: PINCH PROTEIN

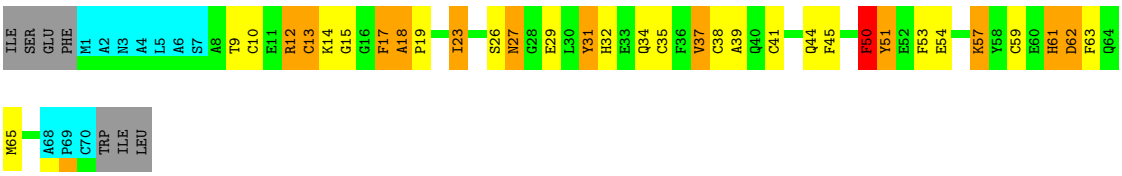
Chain A: 34% 23% 21% 13% 9%



4.2.15 Score per residue for model 15

- Molecule 1: PINCH PROTEIN

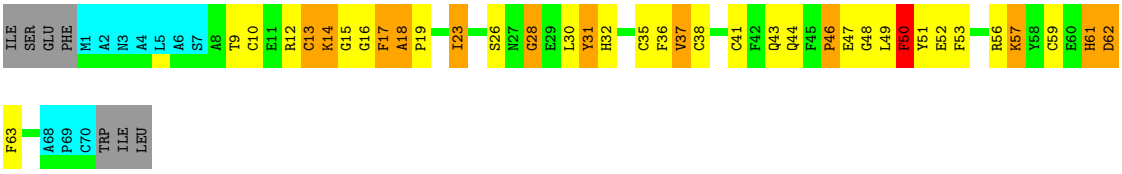
Chain A: 35% 26% 16% • 13% 9%



4.2.16 Score per residue for model 16

- Molecule 1: PINCH PROTEIN

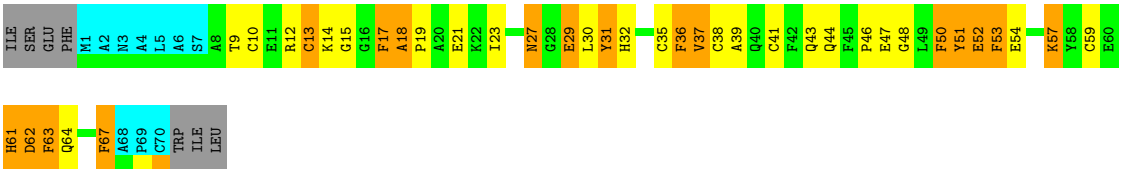
Chain A: 30% 31% 16% • 13% 9%



4.2.17 Score per residue for model 17

- Molecule 1: PINCH PROTEIN

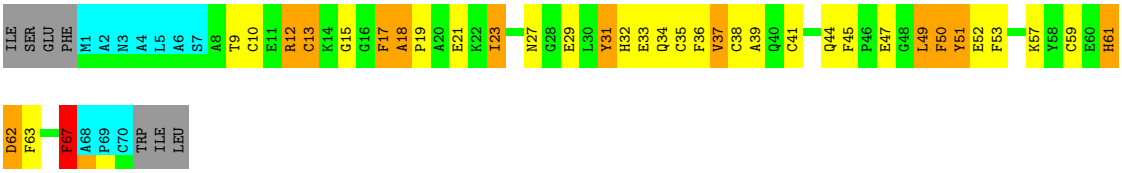
Chain A: 27% 29% 22% 13% 9%



4.2.18 Score per residue for model 18

- Molecule 1: PINCH PROTEIN

Chain A: 31% 30% 16% • 13% 9%



4.2.19 Score per residue for model 19

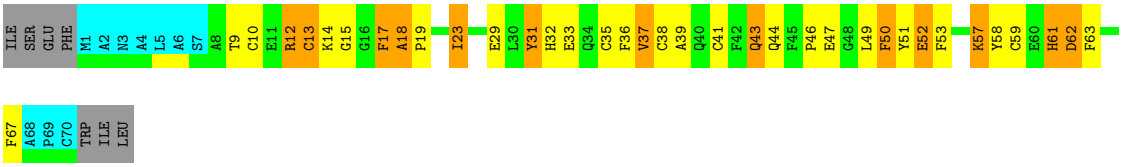
- Molecule 1: PINCH PROTEIN

Chain A: 29% 31% 17% • 13% 9%

4.2.20 Score per residue for model 20

- Molecule 1: PINCH PROTEIN

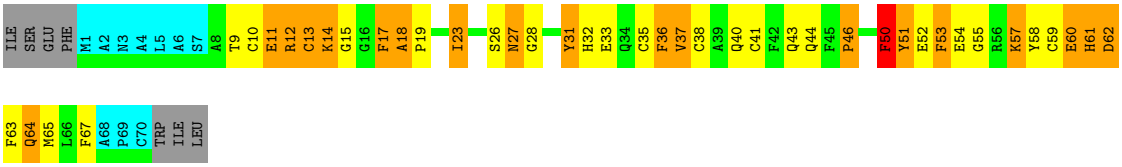
Chain A: 31% 30% 17% 13% 9%



4.2.21 Score per residue for model 21

- Molecule 1: PINCH PROTEIN

Chain A: 23% 29% 25% • 13% 9%



4.2.22 Score per residue for model 22

• Molecule 1: PINCH PROTEIN

Chain A: 22% 36% 18% • 13% 9%

ILE SER GLU PHE M1 A2 N3 A4 L5 A6 S7 A8 T9 C10 E11 R12 C13 K14 G15 G16 F17 A18 P19 A20 E21 K22 I23 S26 N27 G28 E29 L30 Y31 H32 E33 Q34 C35 F36 V37 C38 C41 F42 Q43 Q44 F45 P46 E47 F50 Y51 E52 F53 E54 G55 R56 K57 Y58 C59

E60 H61 D62 F63 Q64 M65 L66 F67 A68 P69 C70 TRP ILE LEU

4.2.23 Score per residue for model 23

• Molecule 1: PINCH PROTEIN

Chain A: 22% 34% 22% 13% 9%

ILE SER GLU PHE M1 A2 N3 A4 L5 A6 S7 A8 T9 C10 E11 R12 C13 K14 G15 G16 F17 A18 P19 A20 E21 K22 I23 V24 N25 S26 N27 G28 E29 L30 Y31 H32 C35 F36 V37 C38 A39 Q40 C41 F42 Q43 Q44 L49 F50 Y51 E52 F53 E54 G55 R56 K57 Y58 C59 E60

H61 D62 F63 Q64 M65 L66 F67 A68 P69 C70 TRP ILE LEU

4.2.24 Score per residue for model 24

• Molecule 1: PINCH PROTEIN

Chain A: 38% 22% 18% 13% 9%

ILE SER GLU PHE M1 A2 N3 A4 L5 A6 S7 C10 E11 R12 C13 K14 G15 G16 F17 A18 P19 I23 S26 N27 G28 Y31 H32 C35 F36 V37 C38 C41 G48 L49 F50 Y51 E52 F53 R56 K57 Y58 C59 E60 H61 D62 F63 F67 A68 P69 C70 TRP

ILE LEU

4.2.25 Score per residue for model 25

• Molecule 1: PINCH PROTEIN

Chain A: 34% 21% 23% 13% 9%

ILE SER GLU PHE M1 A2 N3 A4 L5 A6 S7 A8 T9 C10 E11 R12 C13 K14 G15 G16 F17 A18 P19 I23 V24 N25 S26 N27 G28 Y31 H32 C35 F36 V37 C38 C41 F42 Q43 F50 Y51 E52 F53 E54 K57 Y58 C59 E60 H61 D62 F63 Q64 A68 P69

C70 TRP ILE LEU

5 Refinement protocol and experimental data overview (i)

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

Of the 125 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.843
X-PLOR	refinement	3.843

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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	491	438	438	38±5
All	All	12325	10950	10950	955

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 41.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ALA:N	1:A:57:LYS:HZ1	0.79	1.75	9	2
1:A:31:TYR:CD1	1:A:31:TYR:N	0.76	2.54	18	25
1:A:18:ALA:HB3	1:A:19:PRO:HD3	0.76	1.58	22	25
1:A:12:ARG:HD3	1:A:37:VAL:HG22	0.75	1.56	1	3
1:A:30:LEU:HD22	1:A:30:LEU:N	0.75	1.97	7	10
1:A:38:CYS:HB3	1:A:41:CYS:SG	0.75	2.21	7	25
1:A:37:VAL:HG23	1:A:57:LYS:CE	0.73	2.13	22	15
1:A:37:VAL:HG23	1:A:57:LYS:NZ	0.73	1.99	22	8
1:A:23:ILE:HD11	1:A:30:LEU:HD13	0.72	1.59	17	1
1:A:61:HIS:CG	1:A:62:ASP:N	0.71	2.58	21	25
1:A:12:ARG:NH1	1:A:31:TYR:CD2	0.71	2.59	25	6
1:A:51:TYR:CD2	1:A:58:TYR:HB2	0.71	2.21	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:GLU:C	1:A:30:LEU:HD23	0.71	2.06	13	2
1:A:26:SER:O	1:A:28:GLY:N	0.70	2.23	3	11
1:A:35:CYS:O	1:A:37:VAL:HG22	0.68	1.89	22	8
1:A:39:ALA:HB2	1:A:57:LYS:HG2	0.67	1.65	4	8
1:A:59:CYS:SG	1:A:61:HIS:HB3	0.66	2.30	20	25
1:A:32:HIS:HB2	1:A:35:CYS:SG	0.65	2.31	24	25
1:A:37:VAL:HG23	1:A:57:LYS:HE3	0.65	1.69	5	11
1:A:17:PHE:CE1	1:A:23:ILE:HD12	0.65	2.27	14	2
1:A:39:ALA:HB3	1:A:58:TYR:CE1	0.65	2.26	20	3
1:A:31:TYR:HB2	1:A:36:PHE:CE1	0.65	2.27	9	20
1:A:12:ARG:HG3	1:A:37:VAL:HG21	0.65	1.67	22	5
1:A:39:ALA:CA	1:A:57:LYS:HZ1	0.64	2.05	9	2
1:A:50:PHE:CD2	1:A:59:CYS:HA	0.64	2.27	20	20
1:A:50:PHE:CD1	1:A:51:TYR:N	0.64	2.65	13	20
1:A:58:TYR:CD2	1:A:63:PHE:CE1	0.64	2.85	21	9
1:A:51:TYR:CG	1:A:51:TYR:O	0.63	2.51	8	1
1:A:39:ALA:N	1:A:57:LYS:NZ	0.62	2.47	9	2
1:A:51:TYR:CE2	1:A:58:TYR:CB	0.62	2.82	8	1
1:A:12:ARG:NE	1:A:31:TYR:CD2	0.62	2.68	5	3
1:A:51:TYR:CE2	1:A:58:TYR:HB2	0.62	2.30	8	1
1:A:37:VAL:HG23	1:A:57:LYS:HE2	0.62	1.70	19	5
1:A:51:TYR:CD2	1:A:63:PHE:CD1	0.61	2.89	8	1
1:A:10:CYS:SG	1:A:11:GLU:N	0.60	2.73	22	1
1:A:10:CYS:HB3	1:A:13:CYS:SG	0.60	2.37	4	21
1:A:51:TYR:CE1	1:A:63:PHE:CE1	0.60	2.89	8	2
1:A:36:PHE:CD2	1:A:50:PHE:CE1	0.59	2.90	16	1
1:A:51:TYR:CE2	1:A:63:PHE:CD1	0.59	2.91	8	1
1:A:49:LEU:HD13	1:A:50:PHE:N	0.59	2.13	16	1
1:A:29:GLU:C	1:A:30:LEU:HD13	0.58	2.19	7	1
1:A:26:SER:OG	1:A:27:ASN:N	0.58	2.35	3	1
1:A:17:PHE:CD1	1:A:17:PHE:N	0.57	2.71	17	25
1:A:38:CYS:SG	1:A:62:ASP:HB2	0.57	2.39	9	6
1:A:41:CYS:SG	1:A:43:GLN:HB2	0.57	2.40	10	4
1:A:51:TYR:CZ	1:A:58:TYR:CD2	0.57	2.93	8	1
1:A:38:CYS:SG	1:A:62:ASP:OD1	0.57	2.63	18	1
1:A:39:ALA:HB3	1:A:40:GLN:HE21	0.56	1.61	2	2
1:A:27:ASN:O	1:A:29:GLU:N	0.56	2.39	3	1
1:A:50:PHE:CD1	1:A:50:PHE:N	0.56	2.73	4	15
1:A:49:LEU:HD13	1:A:49:LEU:C	0.56	2.20	7	2
1:A:27:ASN:ND2	1:A:27:ASN:C	0.56	2.58	12	3
1:A:17:PHE:CD1	1:A:23:ILE:HD12	0.56	2.36	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:CYS:SG	1:A:15:GLY:N	0.56	2.79	23	21
1:A:17:PHE:CE1	1:A:23:ILE:HD11	0.55	2.36	15	15
1:A:10:CYS:SG	1:A:31:TYR:HA	0.55	2.42	18	2
1:A:50:PHE:N	1:A:50:PHE:CD1	0.55	2.74	16	1
1:A:27:ASN:N	1:A:31:TYR:OH	0.55	2.40	3	1
1:A:12:ARG:CZ	1:A:31:TYR:CE2	0.55	2.89	5	3
1:A:10:CYS:HA	1:A:17:PHE:CE2	0.55	2.37	21	23
1:A:12:ARG:NH1	1:A:35:CYS:SG	0.54	2.80	19	2
1:A:41:CYS:SG	1:A:43:GLN:CB	0.54	2.95	1	9
1:A:12:ARG:NH1	1:A:31:TYR:CE2	0.54	2.76	14	3
1:A:37:VAL:HG12	1:A:42:PHE:O	0.54	2.02	5	1
1:A:18:ALA:HB3	1:A:19:PRO:CD	0.54	2.33	2	23
1:A:10:CYS:SG	1:A:12:ARG:HG3	0.54	2.42	11	2
1:A:56:ARG:NH1	1:A:56:ARG:CG	0.54	2.71	13	4
1:A:52:GLU:H	1:A:52:GLU:CD	0.54	2.06	2	3
1:A:30:LEU:HD22	1:A:30:LEU:H	0.54	1.61	7	1
1:A:30:LEU:N	1:A:30:LEU:CD2	0.54	2.71	8	10
1:A:56:ARG:CG	1:A:56:ARG:HH11	0.53	2.17	1	9
1:A:12:ARG:NH1	1:A:12:ARG:CG	0.53	2.71	5	5
1:A:17:PHE:CD1	1:A:23:ILE:HD11	0.53	2.38	24	2
1:A:30:LEU:C	1:A:31:TYR:CD1	0.53	2.82	23	4
1:A:50:PHE:CE1	1:A:52:GLU:HB3	0.53	2.38	10	3
1:A:45:PHE:CE2	1:A:59:CYS:CB	0.53	2.92	18	1
1:A:56:ARG:CG	1:A:56:ARG:NH1	0.52	2.71	10	5
1:A:29:GLU:HB3	1:A:31:TYR:CZ	0.52	2.40	22	4
1:A:38:CYS:SG	1:A:40:GLN:OE1	0.52	2.67	21	1
1:A:12:ARG:CG	1:A:12:ARG:HH11	0.52	2.17	5	5
1:A:18:ALA:N	1:A:19:PRO:HD2	0.52	2.20	11	25
1:A:51:TYR:CD2	1:A:58:TYR:CB	0.52	2.92	8	1
1:A:31:TYR:CZ	1:A:52:GLU:CD	0.52	2.83	25	1
1:A:29:GLU:O	1:A:30:LEU:HD23	0.52	2.04	13	2
1:A:35:CYS:O	1:A:37:VAL:N	0.51	2.43	5	7
1:A:41:CYS:SG	1:A:43:GLN:CG	0.51	2.98	20	2
1:A:12:ARG:HE	1:A:37:VAL:CG2	0.51	2.19	4	2
1:A:12:ARG:HB3	1:A:37:VAL:HG21	0.51	1.80	10	1
1:A:12:ARG:CG	1:A:37:VAL:HG21	0.51	2.34	22	2
1:A:11:GLU:HB3	1:A:12:ARG:NH1	0.51	2.21	25	3
1:A:50:PHE:CG	1:A:51:TYR:N	0.51	2.78	4	7
1:A:12:ARG:HG2	1:A:37:VAL:CG2	0.51	2.36	14	2
1:A:27:ASN:ND2	1:A:53:PHE:O	0.51	2.42	21	1
1:A:17:PHE:CD1	1:A:23:ILE:HG12	0.51	2.41	16	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:CYS:SG	1:A:43:GLN:HG3	0.50	2.47	12	1
1:A:39:ALA:HB3	1:A:40:GLN:NE2	0.50	2.22	4	2
1:A:41:CYS:SG	1:A:43:GLN:HB3	0.50	2.47	1	4
1:A:12:ARG:HG2	1:A:12:ARG:NH1	0.50	2.20	6	1
1:A:50:PHE:CG	1:A:59:CYS:HA	0.49	2.42	20	6
1:A:12:ARG:HB2	1:A:37:VAL:HG21	0.49	1.83	19	2
1:A:10:CYS:HA	1:A:17:PHE:CZ	0.49	2.42	14	7
1:A:66:LEU:O	1:A:67:PHE:CG	0.49	2.65	22	1
1:A:29:GLU:O	1:A:31:TYR:CE1	0.49	2.65	19	1
1:A:11:GLU:CD	1:A:11:GLU:C	0.49	2.70	21	1
1:A:51:TYR:CG	1:A:63:PHE:CD1	0.49	3.00	8	1
1:A:27:ASN:O	1:A:28:GLY:C	0.48	2.51	3	1
1:A:36:PHE:HB3	1:A:50:PHE:CE2	0.48	2.43	4	1
1:A:25:ASN:HB2	1:A:30:LEU:HD22	0.48	1.85	13	1
1:A:58:TYR:CG	1:A:63:PHE:CE1	0.48	3.01	20	9
1:A:38:CYS:O	1:A:42:PHE:N	0.48	2.46	4	6
1:A:23:ILE:HG22	1:A:23:ILE:O	0.48	2.07	10	4
1:A:9:THR:C	1:A:17:PHE:CZ	0.48	2.87	23	19
1:A:46:PRO:O	1:A:47:GLU:C	0.48	2.51	2	3
1:A:18:ALA:N	1:A:19:PRO:CD	0.48	2.76	10	25
1:A:57:LYS:NZ	1:A:57:LYS:O	0.48	2.47	9	2
1:A:50:PHE:C	1:A:50:PHE:CD1	0.47	2.86	5	7
1:A:51:TYR:CE2	1:A:63:PHE:HD1	0.47	2.27	8	1
1:A:38:CYS:HB2	1:A:59:CYS:SG	0.47	2.49	22	3
1:A:51:TYR:CD1	1:A:63:PHE:CE1	0.47	3.03	8	1
1:A:66:LEU:C	1:A:67:PHE:CG	0.47	2.86	22	1
1:A:51:TYR:CD1	1:A:63:PHE:CD2	0.47	3.03	1	4
1:A:36:PHE:HB3	1:A:50:PHE:CZ	0.47	2.45	4	5
1:A:12:ARG:HH11	1:A:12:ARG:CB	0.47	2.23	2	1
1:A:12:ARG:HG2	1:A:37:VAL:HG22	0.47	1.86	7	1
1:A:38:CYS:O	1:A:40:GLN:N	0.47	2.48	7	2
1:A:10:CYS:O	1:A:14:LYS:HA	0.47	2.10	22	6
1:A:51:TYR:CZ	1:A:63:PHE:CD1	0.47	3.03	8	1
1:A:18:ALA:H	1:A:19:PRO:HD2	0.46	1.71	10	16
1:A:12:ARG:CZ	1:A:31:TYR:CD2	0.46	2.98	12	1
1:A:17:PHE:CE1	1:A:23:ILE:CD1	0.46	2.98	17	1
1:A:37:VAL:O	1:A:57:LYS:CE	0.46	2.63	21	1
1:A:31:TYR:CB	1:A:36:PHE:CE1	0.46	2.96	9	2
1:A:26:SER:O	1:A:27:ASN:C	0.46	2.53	19	1
1:A:41:CYS:O	1:A:42:PHE:CD1	0.46	2.69	5	1
1:A:14:LYS:CG	1:A:14:LYS:O	0.46	2.63	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:VAL:HG12	1:A:44:GLN:CA	0.46	2.41	7	2
1:A:10:CYS:HB2	1:A:32:HIS:CE1	0.46	2.45	4	1
1:A:12:ARG:NE	1:A:31:TYR:CE2	0.46	2.82	5	1
1:A:13:CYS:HB3	1:A:35:CYS:SG	0.46	2.50	22	2
1:A:50:PHE:N	1:A:50:PHE:HD1	0.46	2.06	10	3
1:A:12:ARG:NH1	1:A:12:ARG:HG2	0.46	2.26	9	2
1:A:49:LEU:HD22	1:A:50:PHE:N	0.46	2.26	7	1
1:A:35:CYS:O	1:A:36:PHE:C	0.46	2.55	3	4
1:A:36:PHE:CD1	1:A:48:GLY:HA2	0.46	2.46	9	2
1:A:12:ARG:CD	1:A:12:ARG:H	0.45	2.24	4	2
1:A:41:CYS:SG	1:A:43:GLN:HG2	0.45	2.51	20	2
1:A:37:VAL:HG23	1:A:57:LYS:HZ1	0.45	1.70	6	1
1:A:52:GLU:N	1:A:52:GLU:CD	0.45	2.70	24	1
1:A:49:LEU:C	1:A:49:LEU:HD23	0.45	2.32	8	2
1:A:29:GLU:C	1:A:30:LEU:HD22	0.45	2.32	14	3
1:A:49:LEU:HD13	1:A:49:LEU:O	0.45	2.11	7	1
1:A:36:PHE:CD1	1:A:36:PHE:N	0.45	2.85	10	1
1:A:36:PHE:CE2	1:A:48:GLY:C	0.45	2.91	16	1
1:A:27:ASN:C	1:A:29:GLU:N	0.45	2.70	3	1
1:A:31:TYR:CE2	1:A:52:GLU:CD	0.44	2.91	19	1
1:A:38:CYS:C	1:A:40:GLN:N	0.44	2.70	7	3
1:A:12:ARG:CB	1:A:37:VAL:HG21	0.44	2.42	10	3
1:A:36:PHE:HB3	1:A:50:PHE:CE1	0.44	2.47	10	1
1:A:32:HIS:H	1:A:35:CYS:HB2	0.44	1.73	7	3
1:A:37:VAL:CG2	1:A:57:LYS:HE3	0.44	2.42	10	1
1:A:30:LEU:HD23	1:A:30:LEU:N	0.44	2.24	13	1
1:A:62:ASP:O	1:A:66:LEU:HG	0.44	2.13	22	1
1:A:36:PHE:CZ	1:A:48:GLY:O	0.44	2.70	24	1
1:A:17:PHE:O	1:A:18:ALA:HB2	0.43	2.13	11	2
1:A:23:ILE:CD1	1:A:30:LEU:HD12	0.43	2.43	11	2
1:A:31:TYR:OH	1:A:52:GLU:CD	0.43	2.56	18	1
1:A:36:PHE:CE2	1:A:49:LEU:HA	0.43	2.48	24	1
1:A:51:TYR:CE1	1:A:63:PHE:CE2	0.43	3.06	17	3
1:A:12:ARG:NH2	1:A:31:TYR:CD2	0.43	2.87	11	2
1:A:38:CYS:SG	1:A:62:ASP:OD2	0.43	2.76	12	2
1:A:23:ILE:HD11	1:A:30:LEU:CD1	0.43	2.39	17	1
1:A:46:PRO:O	1:A:47:GLU:CB	0.43	2.66	16	3
1:A:59:CYS:C	1:A:61:HIS:H	0.43	2.17	11	3
1:A:45:PHE:C	1:A:47:GLU:H	0.43	2.17	12	1
1:A:27:ASN:ND2	1:A:54:GLU:HA	0.43	2.29	23	2
1:A:60:GLU:O	1:A:64:GLN:HB3	0.43	2.13	21	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ARG:NE	1:A:37:VAL:CG2	0.43	2.81	4	1
1:A:36:PHE:O	1:A:44:GLN:HA	0.43	2.14	5	1
1:A:10:CYS:SG	1:A:12:ARG:CG	0.43	3.06	11	2
1:A:17:PHE:CE2	1:A:23:ILE:HG13	0.43	2.49	17	1
1:A:50:PHE:CD1	1:A:50:PHE:C	0.43	2.91	12	4
1:A:29:GLU:N	1:A:31:TYR:OH	0.43	2.49	19	1
1:A:41:CYS:O	1:A:43:GLN:N	0.43	2.52	5	1
1:A:26:SER:C	1:A:28:GLY:H	0.42	2.17	12	2
1:A:11:GLU:HG3	1:A:12:ARG:NH2	0.42	2.29	13	1
1:A:52:GLU:CD	1:A:52:GLU:N	0.42	2.72	22	1
1:A:25:ASN:ND2	1:A:25:ASN:C	0.42	2.71	25	1
1:A:56:ARG:HB3	1:A:58:TYR:CZ	0.42	2.50	3	1
1:A:49:LEU:C	1:A:49:LEU:CD2	0.42	2.87	8	1
1:A:37:VAL:O	1:A:57:LYS:HG2	0.42	2.15	25	2
1:A:52:GLU:CD	1:A:52:GLU:C	0.42	2.78	17	1
1:A:36:PHE:CE2	1:A:52:GLU:CD	0.42	2.93	13	1
1:A:47:GLU:HG3	1:A:49:LEU:H	0.42	1.74	18	1
1:A:29:GLU:C	1:A:30:LEU:HD12	0.42	2.35	23	1
1:A:23:ILE:O	1:A:23:ILE:HG22	0.42	2.14	24	7
1:A:29:GLU:HB2	1:A:31:TYR:OH	0.42	2.15	8	1
1:A:56:ARG:NH1	1:A:56:ARG:HG3	0.42	2.30	1	3
1:A:14:LYS:N	1:A:14:LYS:CD	0.42	2.83	11	1
1:A:37:VAL:O	1:A:57:LYS:HE3	0.42	2.15	21	1
1:A:38:CYS:O	1:A:42:PHE:HA	0.41	2.14	4	1
1:A:14:LYS:O	1:A:14:LYS:CD	0.41	2.68	23	1
1:A:12:ARG:NH1	1:A:12:ARG:HG3	0.41	2.29	5	1
1:A:12:ARG:CZ	1:A:57:LYS:HD3	0.41	2.46	9	1
1:A:11:GLU:HB3	1:A:12:ARG:CZ	0.41	2.45	4	1
1:A:12:ARG:HB2	1:A:37:VAL:CG2	0.41	2.46	22	2
1:A:12:ARG:CD	1:A:35:CYS:HB3	0.41	2.45	12	1
1:A:52:GLU:CD	1:A:53:PHE:N	0.41	2.74	1	2
1:A:37:VAL:HA	1:A:44:GLN:HA	0.41	1.91	7	1
1:A:17:PHE:HB3	1:A:32:HIS:NE2	0.41	2.31	4	1
1:A:44:GLN:NE2	1:A:44:GLN:H	0.41	2.13	3	1
1:A:52:GLU:HG3	1:A:53:PHE:N	0.41	2.31	8	1
1:A:36:PHE:O	1:A:45:PHE:N	0.41	2.52	10	1
1:A:12:ARG:HD3	1:A:35:CYS:HB3	0.41	1.93	12	1
1:A:61:HIS:CD2	1:A:61:HIS:C	0.41	2.94	18	1
1:A:27:ASN:ND2	1:A:55:GLY:H	0.41	2.12	21	1
1:A:12:ARG:CG	1:A:12:ARG:NH1	0.41	2.82	24	1
1:A:18:ALA:CB	1:A:19:PRO:CD	0.41	2.99	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:CYS:C	1:A:40:GLN:H	0.41	2.18	7	1
1:A:33:GLU:O	1:A:47:GLU:N	0.40	2.55	2	2
1:A:50:PHE:CD2	1:A:59:CYS:CA	0.40	3.04	2	1
1:A:36:PHE:CE1	1:A:48:GLY:O	0.40	2.74	8	1
1:A:46:PRO:C	1:A:48:GLY:H	0.40	2.19	17	1
1:A:60:GLU:O	1:A:64:GLN:CG	0.40	2.70	5	2
1:A:66:LEU:O	1:A:67:PHE:CB	0.40	2.69	5	1
1:A:56:ARG:HB3	1:A:58:TYR:CE2	0.40	2.51	3	1
1:A:46:PRO:O	1:A:48:GLY:N	0.40	2.55	2	1
1:A:51:TYR:CD1	1:A:51:TYR:C	0.40	2.94	8	1
1:A:45:PHE:CE2	1:A:59:CYS:HB3	0.40	2.51	18	1
1:A:66:LEU:C	1:A:67:PHE:CD1	0.40	2.95	22	1
1:A:37:VAL:O	1:A:57:LYS:CG	0.40	2.69	25	1
1:A:37:VAL:HA	1:A:43:GLN:O	0.40	2.17	20	1
1:A:66:LEU:O	1:A:67:PHE:CD2	0.40	2.74	22	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	60/77 (78%)	43±2 (71±3%)	13±2 (22±3%)	4±2 (7±3%)	2 18
All	All	1500/1925 (78%)	1072 (71%)	327 (22%)	101 (7%)	2 18

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	18	ALA	25
1	A	36	PHE	14
1	A	50	PHE	9
1	A	49	LEU	9
1	A	46	PRO	8
1	A	27	ASN	7
1	A	28	GLY	7

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Mol	Chain	Res	Type	Models (Total)
1	A	16	GLY	5
1	A	67	PHE	5
1	A	8	ALA	4
1	A	19	PRO	2
1	A	20	ALA	2
1	A	47	GLU	1
1	A	26	SER	1
1	A	42	PHE	1
1	A	39	ALA	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	51/64 (80%)	33±3 (65±5%)	18±3 (35±5%)	1 9
All	All	1275/1600 (80%)	823 (65%)	452 (35%)	1 9

All 38 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	13	CYS	25
1	A	17	PHE	25
1	A	31	TYR	25
1	A	50	PHE	25
1	A	61	HIS	25
1	A	62	ASP	24
1	A	37	VAL	23
1	A	44	GLN	22
1	A	53	PHE	22
1	A	23	ILE	21
1	A	12	ARG	20
1	A	51	TYR	20
1	A	63	PHE	16
1	A	52	GLU	15
1	A	57	LYS	15
1	A	33	GLU	14

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Mol	Chain	Res	Type	Models (Total)
1	A	27	ASN	11
1	A	64	GLN	10
1	A	65	MET	10
1	A	54	GLU	10
1	A	67	PHE	9
1	A	34	GLN	8
1	A	56	ARG	8
1	A	14	LYS	7
1	A	45	PHE	6
1	A	21	GLU	6
1	A	26	SER	6
1	A	25	ASN	5
1	A	29	GLU	5
1	A	47	GLU	3
1	A	60	GLU	3
1	A	49	LEU	2
1	A	42	PHE	1
1	A	30	LEU	1
1	A	43	GLN	1
1	A	11	GLU	1
1	A	46	PRO	1
1	A	10	CYS	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)

Of 2 ligands modelled in this entry, 2 are 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 (i)

No chemical shift data were provided