Full wwPDB NMR Structure Validation Report (i)

Feb 14, 2022 – 07:44 AM EST

PDB ID	:	1JH4
Title	:	Solution structure of the C-terminal PABC domain of human poly(A)-binding protein in complex with the peptide from Paip1
Authors	:	Kozlov, G.; Siddiqui, N.; Coillet-Matillon, S.; Ekiel, I.; Gehring, K.
Deposited on	:	2001-06-27

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

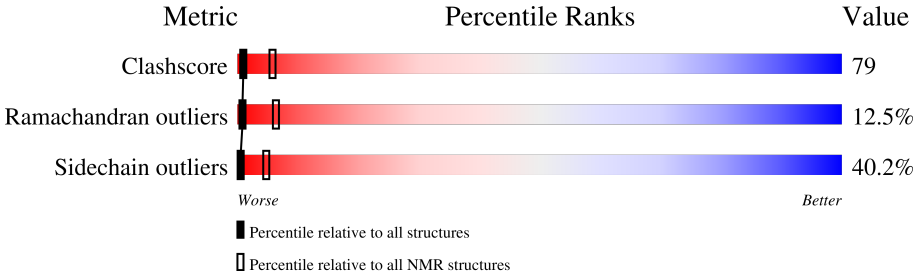
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	98	11% 41% 17% • 27%
2	B	22	9% 41% 14% 36%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 6 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:8-A:79, B:5-B:18 (86)	0.26	6

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 4 clusters and 6 single-model clusters were found.

Cluster number	Models
1	2, 5, 8, 9, 16, 17, 19, 25, 29
2	1, 4, 6, 7, 21, 26, 27
3	14, 18, 20, 24, 28, 30
4	11, 13
Single-model clusters	3; 10; 12; 15; 22; 23

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1804 atoms, of which 911 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called polyadenylate-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	98	1469	452	747	124	141	5	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P11940
A	2	PRO	-	cloning artifact	UNP P11940
A	3	LEU	-	cloning artifact	UNP P11940
A	4	GLY	-	cloning artifact	UNP P11940
A	5	SER	-	cloning artifact	UNP P11940

- Molecule 2 is a protein called polyadenylate-binding protein-interacting protein-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	22	335	111	164	24	35	1	0

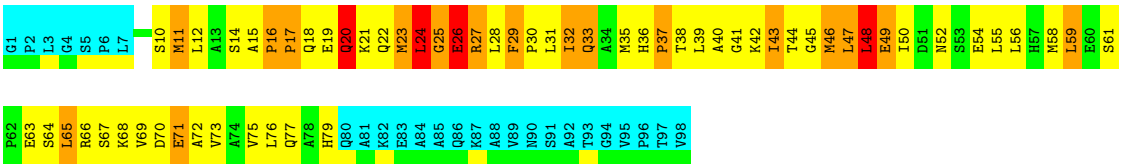
4 Residue-property plots (i)

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: polyadenylate-binding protein 1

Chain A: 11% 41% 17% • 27%



• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 9% 41% 14% 36%

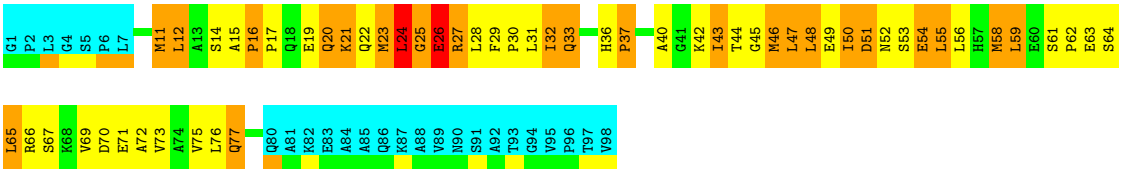
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: polyadenylate-binding protein 1

Chain A: 16% 32% 23% • 27%



• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 14% 32% 18% 36%

V1 L2 M3 S4 K5 L6 S7 V8 N9 A10 P11 E12 F13 Y14 P15 S16 G17 Y18 S19 S20 S21 Y22

4.2.2 Score per residue for model 2

- Molecule 1: polyadenylate-binding protein 1

Chain A: 15% 37% 17% • 27%

G1 P2 L3 G4 S5 P6 L7 M11 L12 A15 P16 P17 Q18 E19 Q20 K21 Q22 M23 L24 G25 E26 R27 L28 F29 P30 L31 I32 Q33 A34 M35 H36 P37 T38 L39 A40 G41 K42 I43 T44 G45 M46 L47 L48 E49 I50 D51 N52 L55 L56 H57 M58 L59 E60 S61 P62 E63 S64

L65 R66 S67 K68 V69 D70 E71 A72 V73 A74 V75 L76 Q77 A78 H79 Q80 A81 K82 E83 A84 A85 Q86 K87 A88 V89 N90 S91 A92 T93 G94 V95 P96 T97 V98

- Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 9% 32% 23% 36%

V1 L2 M3 S4 K5 L6 S7 V8 N9 A10 P11 E12 F13 Y14 P15 S16 G17 Y18 S19 S20 S21 Y22

4.2.3 Score per residue for model 3

- Molecule 1: polyadenylate-binding protein 1

Chain A: 14% 39% 17% • 27%

G1 P2 L3 G4 S5 P6 L7 S10 M11 L12 A13 S14 A15 P16 P17 Q18 E19 Q20 K21 Q22 M23 L24 G25 E26 R27 L28 F29 P30 L31 I32 Q33 A34 M35 H36 P37 T38 L39 A40 G41 K42 I43 T44 G45 M46 L47 L48 E49 I50 D51 N52 S53 E54 L55 L56 H57 M58 L59 E60 S61

P62 E63 S64 L65 K68 V69 D70 E71 A72 V73 A74 V75 L76 Q77 A78 H79 Q80 A81 K82 E83 A84 A85 Q86 K87 A88 V89 N90 S91 A92 T93 G94 V95 P96 T97 V98

- Molecule 2: polyadenylate-binding protein-interacting protein-1

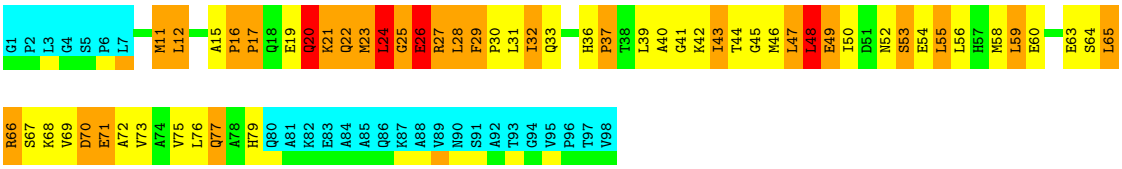
Chain B: 14% 36% 14% 36%

V1 L2 M3 S4 K5 L6 S7 V8 N9 A10 P11 E12 F13 Y14 P15 S16 G17 Y18 S19 S20 S21 Y22

4.2.4 Score per residue for model 4

- Molecule 1: polyadenylate-binding protein 1

Chain A: 15% 30% 24% • 27%



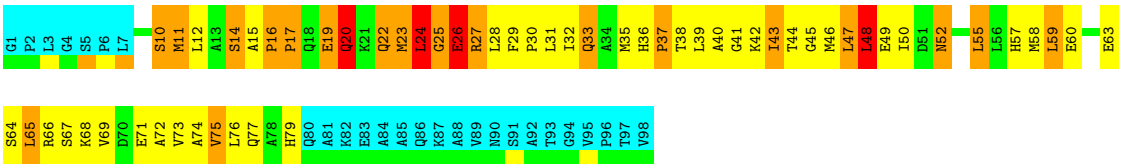
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 9% 23% 32% 36%

4.2.5 Score per residue for model 5

• Molecule 1: polyadenylate-binding protein 1

Chain A: 14% 36% 19% • 27%



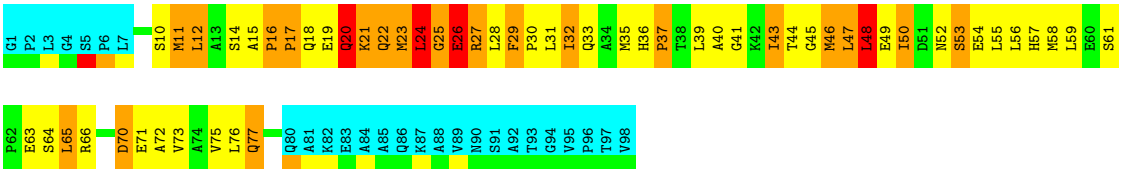
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 14% 32% 18% 36%

4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: polyadenylate-binding protein 1

Chain A: 15% 34% 20% • 27%



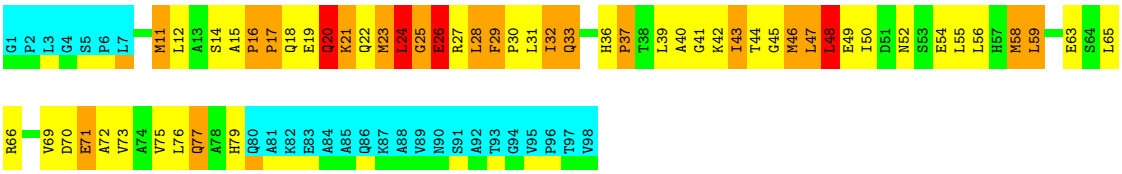
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 5% 41% 18% 36%

4.2.7 Score per residue for model 7

- Molecule 1: polyadenylate-binding protein 1

Chain A: 18% 33% 18% • 27%



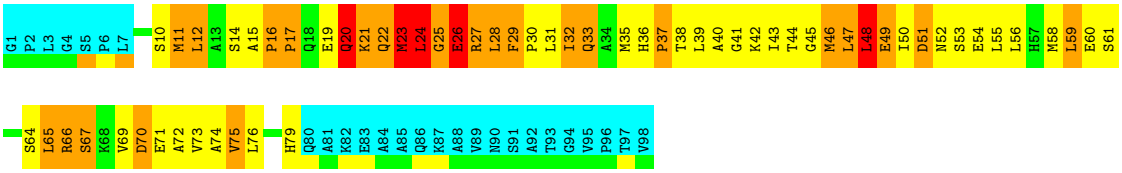
- Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 14% 32% 18% 36%

4.2.8 Score per residue for model 8

- Molecule 1: polyadenylate-binding protein 1

Chain A: 11% 34% 23% 5% 27%



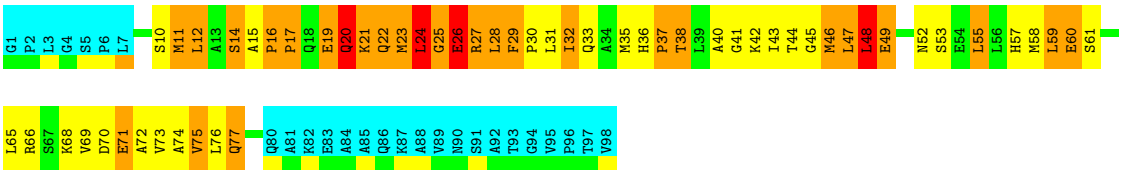
- Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 9% 32% 23% 36%

4.2.9 Score per residue for model 9

- Molecule 1: polyadenylate-binding protein 1

Chain A: 16% 28% 26% • 27%



• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 14% 41% 9% 36%

V1 L2 M3 S4 K5 L6 S7 A10 P11 E12 F13 Y14 P15 S16 G17 Y18 S19 S20 S21 Y22

4.2.10 Score per residue for model 10

• Molecule 1: polyadenylate-binding protein 1

Chain A: 14% 33% 22% • 27%

G1 P2 L3 G4 S5 P6 L7 M11 L12 A13 S14 A15 P16 P17 Q18 E19 Q20 K21 Q22 M23 L24 G25 E26 R27 L28 F29 P30 L31 I32 Q33 H36 P37 T38 L39 A40 G41 K42 I43 T44 G45 M46 L47 L48 E49 I50 D51 N52 S53 E54 L55 L56 H57 M58 L59 S64 L65 R66

S67 K68 V69 D70 E71 A72 V73 A74 V75 L76 Q77 Q80 A81 K82 E83 A84 A85 Q86 K87 A88 V89 N90 S91 A92 T93 G94 V95 P96 T97 V98

• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 14% 32% 18% 36%

V1 L2 M3 S4 K5 L6 S7 V8 N9 A10 P11 E12 F13 Y14 P15 S16 G17 Y18 S19 S20 S21 Y22

4.2.11 Score per residue for model 11

• Molecule 1: polyadenylate-binding protein 1

Chain A: 20% 32% 17% • 27%

G1 P2 L3 G4 S5 P6 L7 T8 M11 L12 A15 P16 P17 Q18 E19 Q20 K21 Q22 M23 L24 G25 E26 R27 L28 F29 P30 L31 I32 Q33 H36 P37 T38 L39 A40 G41 K42 I43 T44 G45 M46 L47 L48 E49 I50 D51 N52 S53 E54 L55 L56 H57 M58 L59 L65 R66 S67

K68 V69 D70 E71 A72 V73 A74 V75 L76 Q77 Q80 A81 K82 E83 A84 A85 Q86 K87 A88 V89 N90 S91 A92 T93 G94 V95 P96 T97 V98

• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 5% 50% 9% 36%

V1 L2 M3 S4 K5 L6 S7 V8 N9 A10 P11 E12 F13 Y14 P15 S16 G17 Y18 S19 S20 S21 Y22

4.2.12 Score per residue for model 12

• Molecule 1: polyadenylate-binding protein 1

Chain A: 15% 37% 18% • 27%

G1 P2 L3 G4 S5 P6 L7 T8 M11 L12 A13 S14 A15 P16 P17 Q18 E19 Q20 K21 Q22 M23 L24 G25 E26 R27 L28 F29 P30 L31 I32 Q33 A34 M35 H36 P37 T38 L39 A40 G41 K42 I43 T44 G45 M46 L47 L48 E49 N52 S53 E54 L55 M58 L59 E60 S61 P62 E63

S64 L65 R66 S67 K68 V69 D70 E71 A72 V73 A74 V75 L76 Q77 Q80 A81 K82 E83 A84 A85 Q86 K87 A88 V89 N90 S91 A92 T93 G94 V95 P96 T97 V98

• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 14% 32% 18% 36%

V1 L2 M3 S4 K5 L6 S7 V8 N9 A10 P11 E12 F13 Y14 P15 S16 G17 Y18 S19 S20 S21 Y22

4.2.13 Score per residue for model 13

• Molecule 1: polyadenylate-binding protein 1

Chain A: 12% 38% 19% • 27%

G1 P2 L3 G4 S5 P6 L7 T8 M11 L12 A13 S14 A15 P16 P17 Q18 E19 Q20 K21 Q22 M23 L24 G25 E26 R27 L28 F29 P30 L31 I32 Q33 A34 M35 H36 P37 T38 L39 A40 G41 K42 I43 T44 G45 M46 L47 L48 E49 I50 D51 N52 L55 L56 H57 M58 L59 E60 E63

S64 L65 R66 S67 K68 V69 D70 E71 A72 V73 A74 V75 L76 Q77 A78 H79 Q80 A81 K82 E83 A84 A85 Q86 K87 A88 V89 N90 S91 A92 T93 G94 V95 P96 T97 V98

• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 5% 36% 23% 36%

V1 L2 M3 S4 K5 L6 S7 V8 N9 A10 P11 E12 F13 Y14 P15 S16 G17 Y18 S19 S20 S21 Y22

4.2.14 Score per residue for model 14

• Molecule 1: polyadenylate-binding protein 1

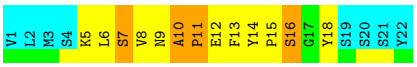
Chain A: 18% 34% 17% • 27%

G1 P2 L3 G4 S5 P6 L7 T8 M11 L12 A15 P16 P17 Q18 E19 Q20 K21 Q22 M23 L24 G25 E26 R27 L28 F29 P30 L31 I32 Q33 A34 M35 H36 P37 T38 L39 A40 G41 K42 I43 T44 G45 M46 L47 L48 E49 I50 D51 N52 S53 E54 L55 L59 E60 S61 L65 R66

S67 K68 V69 D70 E71 A72 V73 A74 V75 L76 Q77 Q80 A81 K82 E83 A84 A85 Q86 K87 A88 V89 N90 S91 A92 T93 G94 V95 P96 T97 V98

• Molecule 2: polyadenylate-binding protein-interacting protein-1

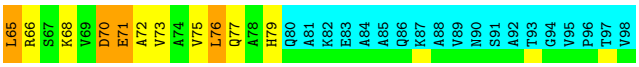
Chain B: 5% 41% 18% 36%



4.2.15 Score per residue for model 15

- Molecule 1: polyadenylate-binding protein 1

Chain A:



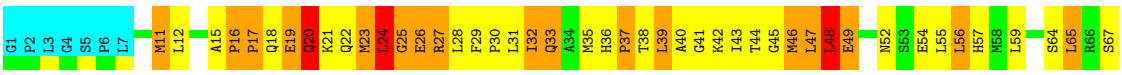
- Molecule 2: polyadenylate-binding protein-interacting protein-1

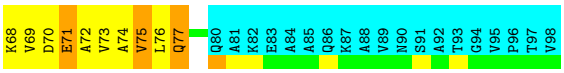
Chain B:

4.2.16 Score per residue for model 16

- Molecule 1: polyadenylate-binding protein 1

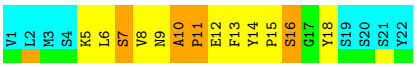
Chain A:





- Molecule 2: polyadenylate-binding protein-interacting protein-1

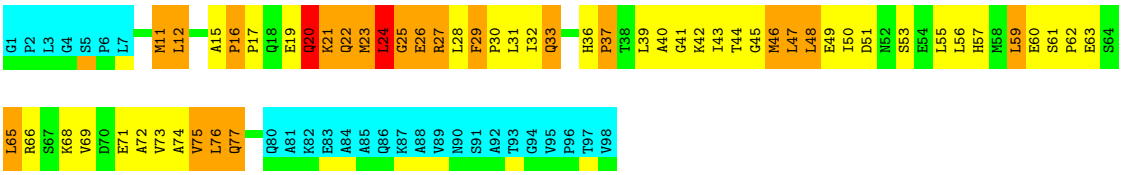
Chain B:



4.2.17 Score per residue for model 17

- Molecule 1: polyadenylate-binding protein 1

Chain A:



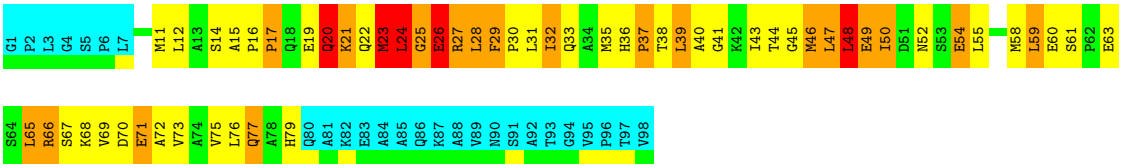
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 14% 27% 23% 36%

4.2.18 Score per residue for model 18

• Molecule 1: polyadenylate-binding protein 1

Chain A: 15% 34% 19% 5% 27%



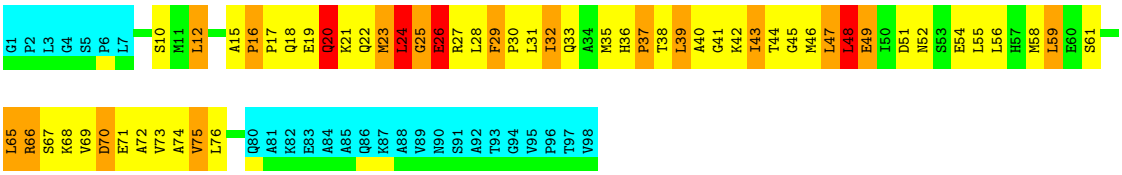
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 5% 36% 23% 36%

4.2.19 Score per residue for model 19

• Molecule 1: polyadenylate-binding protein 1

Chain A: 16% 37% 16% • 27%



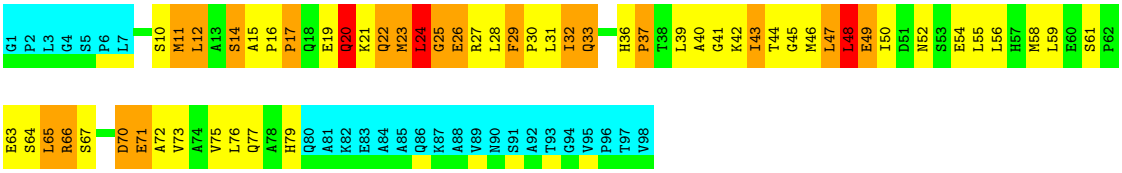
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 9% 41% 14% 36%

4.2.20 Score per residue for model 20

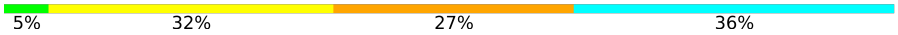
- Molecule 1: polyadenylate-binding protein 1

Chain A:



- Molecule 2: polyadenylate-binding protein-interacting protein-1

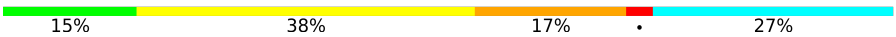
Chain B:

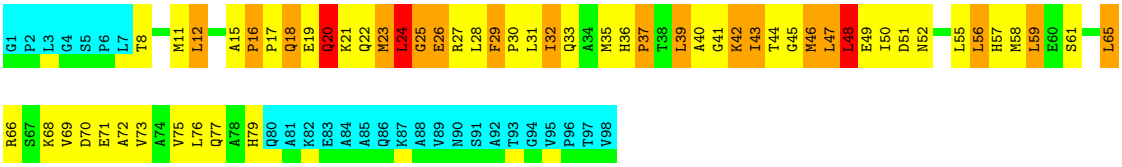


4.2.21 Score per residue for model 21

- Molecule 1: polyadenylate-binding protein 1

Chain A:





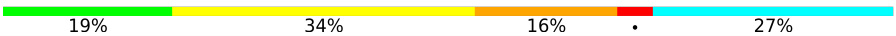
- Molecule 2: polyadenylate-binding protein-interacting protein-1

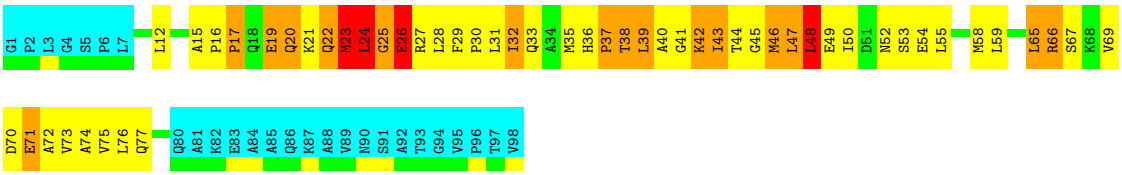
Chain B:

4.2.22 Score per residue for model 22

- Molecule 1: polyadenylate-binding protein 1

Chain A:





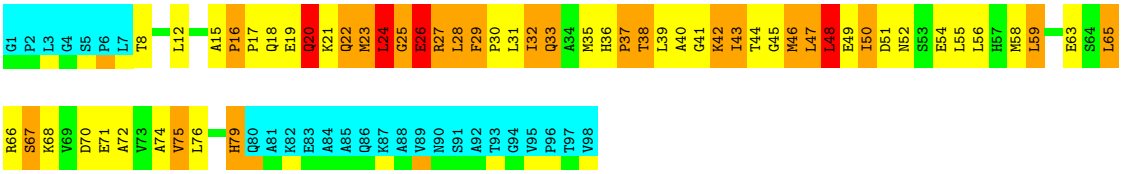
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 9% 36% 18% 36%

4.2.23 Score per residue for model 23

• Molecule 1: polyadenylate-binding protein 1

Chain A: 16% 32% 21% • 27%



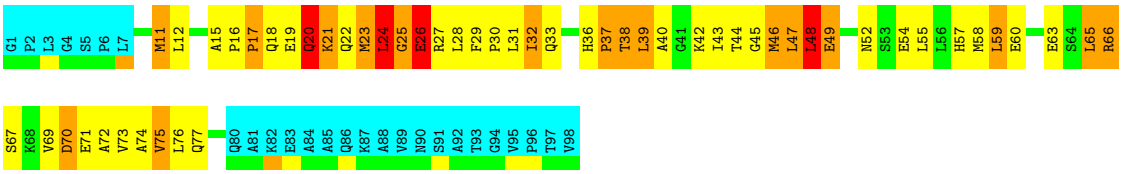
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 5% 50% 9% 36%

4.2.24 Score per residue for model 24

• Molecule 1: polyadenylate-binding protein 1

Chain A: 18% 34% 17% • 27%



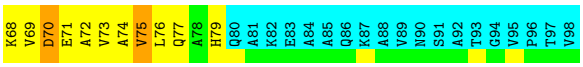
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 9% 32% 23% 36%

4.2.25 Score per residue for model 25

- Molecule 1: polyadenylate-binding protein 1

Chain A:



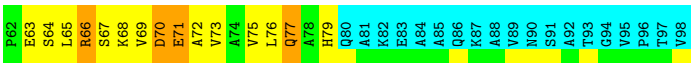
- Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B:

4.2.26 Score per residue for model 26

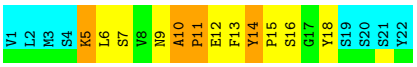
- Molecule 1: polyadenylate-binding protein 1

Chain A:



- Molecule 2: polyadenylate-binding protein-interacting protein-1

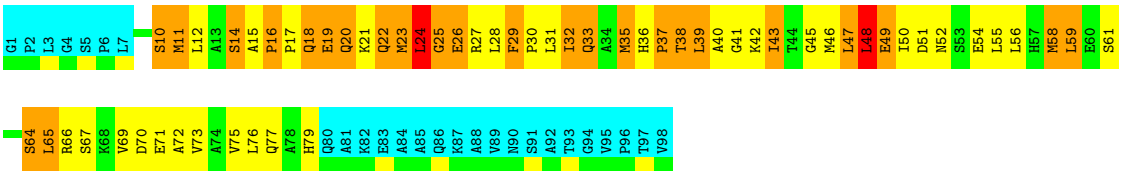
Chain B:



4.2.27 Score per residue for model 27

- Molecule 1: polyadenylate-binding protein 1

Chain A:



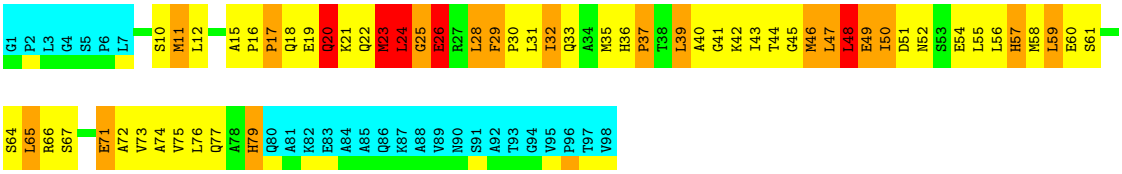
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 14% 23% 27% 36%

4.2.28 Score per residue for model 28

• Molecule 1: polyadenylate-binding protein 1

Chain A: 14% 37% 17% 5% 27%



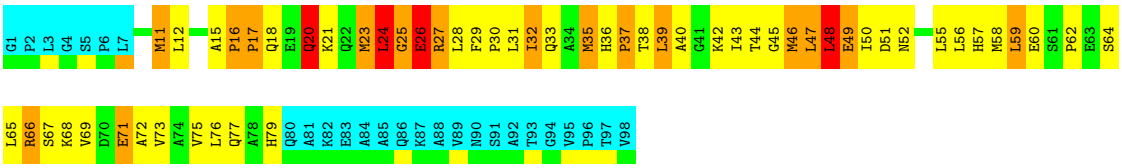
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 9% 36% 18% 36%

4.2.29 Score per residue for model 29

• Molecule 1: polyadenylate-binding protein 1

Chain A: 16% 37% 16% • 27%



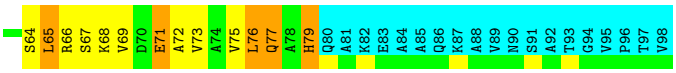
• Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B: 14% 36% 14% 36%

4.2.30 Score per residue for model 30

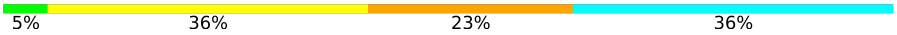
- Molecule 1: polyadenylate-binding protein 1

Chain A:



- Molecule 2: polyadenylate-binding protein-interacting protein-1

Chain B:



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	0.9
CNS	refinement	0.9

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	547	563	563	96±9
2	B	111	104	104	28±5
All	All	19740	20010	20010	3146

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 79.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD21	1:A:72:ALA:HB2	1.05	1.28	28	15
1:A:32:ILE:HG13	1:A:43:ILE:HG21	1.02	1.30	6	24
1:A:28:LEU:HD11	1:A:47:LEU:HB2	1.00	1.28	10	10
1:A:32:ILE:HD13	1:A:43:ILE:HD13	0.96	1.38	17	3
1:A:28:LEU:HB2	1:A:44:THR:HG23	0.95	1.38	23	24
1:A:74:ALA:HB3	2:B:5:LYS:HG3	0.92	1.41	16	12
1:A:28:LEU:HD12	1:A:48:LEU:HD12	0.92	1.42	25	26
1:A:47:LEU:HD21	1:A:72:ALA:CB	0.92	1.95	20	30
1:A:31:LEU:HB3	1:A:65:LEU:HD21	0.91	1.41	6	26
1:A:69:VAL:O	1:A:73:VAL:HG23	0.90	1.66	13	14
1:A:28:LEU:HD21	1:A:47:LEU:HG	0.90	1.44	10	5
1:A:28:LEU:HD13	1:A:47:LEU:HB2	0.89	1.42	3	20
1:A:46:MET:HG2	1:A:76:LEU:HD13	0.87	1.42	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:MET:HG2	1:A:76:LEU:HD12	0.84	1.49	22	2
1:A:31:LEU:HD13	1:A:65:LEU:HD23	0.84	1.47	29	20
1:A:32:ILE:HD12	1:A:40:ALA:HA	0.84	1.49	25	26
1:A:48:LEU:HD22	2:B:13:PHE:HA	0.84	1.49	14	29
1:A:28:LEU:HD12	1:A:55:LEU:HD21	0.84	1.49	9	7
1:A:32:ILE:CD1	1:A:43:ILE:HD13	0.82	2.05	17	3
1:A:26:GLU:HG3	1:A:55:LEU:HD13	0.81	1.51	9	8
1:A:75:VAL:HG11	2:B:8:VAL:HG12	0.81	1.53	11	9
1:A:70:ASP:O	1:A:73:VAL:HG22	0.81	1.76	1	2
1:A:73:VAL:O	1:A:77:GLN:HB2	0.80	1.76	16	19
1:A:32:ILE:CG1	1:A:43:ILE:HG21	0.80	2.07	6	29
1:A:46:MET:O	2:B:10:ALA:HB3	0.79	1.75	5	24
1:A:46:MET:HG3	1:A:76:LEU:HD13	0.79	1.54	14	5
1:A:71:GLU:HG2	2:B:6:LEU:HD12	0.79	1.54	26	12
1:A:32:ILE:HD11	1:A:37:PRO:HD2	0.78	1.53	12	25
2:B:10:ALA:HB1	2:B:11:PRO:HD2	0.78	1.54	22	30
2:B:10:ALA:HB1	2:B:11:PRO:CD	0.78	2.07	22	30
1:A:11:MET:HG2	1:A:24:LEU:HD21	0.78	1.55	6	6
1:A:58:MET:HB2	1:A:65:LEU:HA	0.78	1.55	26	10
1:A:26:GLU:HG2	1:A:55:LEU:HD13	0.78	1.52	5	5
1:A:47:LEU:HD22	2:B:7:SER:HB2	0.78	1.56	7	6
1:A:52:ASN:HA	1:A:55:LEU:HD12	0.76	1.56	15	5
1:A:32:ILE:HD12	1:A:40:ALA:CA	0.76	2.11	22	26
1:A:47:LEU:CD2	1:A:76:LEU:HD11	0.76	2.10	25	1
1:A:32:ILE:HG12	1:A:40:ALA:HA	0.76	1.57	13	4
1:A:72:ALA:HB2	2:B:7:SER:HB3	0.76	1.56	3	5
1:A:24:LEU:HB3	1:A:29:PHE:HD2	0.76	1.39	11	27
1:A:31:LEU:HD13	1:A:65:LEU:CD2	0.76	2.09	29	13
1:A:28:LEU:HG	1:A:55:LEU:HD23	0.75	1.56	24	9
1:A:47:LEU:HD22	2:B:7:SER:HB3	0.75	1.58	23	7
1:A:31:LEU:HD22	1:A:65:LEU:CD2	0.75	2.10	10	2
1:A:71:GLU:HG3	2:B:6:LEU:HD12	0.75	1.56	1	8
1:A:71:GLU:HB3	2:B:5:LYS:HB3	0.75	1.58	10	14
1:A:15:ALA:HB1	1:A:19:GLU:HB2	0.75	1.59	15	8
1:A:65:LEU:HD13	1:A:66:ARG:N	0.74	1.98	17	18
1:A:28:LEU:CD1	1:A:47:LEU:HB2	0.73	2.13	6	23
1:A:28:LEU:CB	1:A:44:THR:HG23	0.73	2.12	30	8
1:A:26:GLU:HA	2:B:16:SER:OG	0.73	1.84	17	3
1:A:27:ARG:CG	1:A:59:LEU:HD13	0.73	2.13	1	2
1:A:46:MET:HG2	2:B:9:ASN:HA	0.73	1.59	19	3
1:A:28:LEU:HD11	1:A:47:LEU:CB	0.73	2.12	8	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:14:TYR:HB3	2:B:15:PRO:HD2	0.73	1.60	30	20
1:A:27:ARG:HG3	1:A:59:LEU:HD13	0.72	1.59	1	2
1:A:38:THR:HG22	1:A:39:LEU:HG	0.72	1.58	15	1
1:A:47:LEU:HD13	2:B:7:SER:CB	0.72	2.15	6	22
1:A:27:ARG:NE	1:A:59:LEU:HD13	0.72	2.00	26	6
1:A:12:LEU:HD21	1:A:21:LYS:CE	0.72	2.14	20	1
1:A:52:ASN:ND2	2:B:16:SER:OG	0.72	2.23	21	3
1:A:12:LEU:HD23	1:A:24:LEU:HD11	0.72	1.60	25	4
1:A:28:LEU:HD13	1:A:44:THR:O	0.71	1.83	10	6
1:A:75:VAL:HG21	2:B:8:VAL:HA	0.71	1.61	30	9
1:A:26:GLU:OE1	1:A:55:LEU:HD22	0.71	1.85	11	3
1:A:17:PRO:O	1:A:20:GLN:HG3	0.71	1.84	13	1
1:A:31:LEU:HD21	1:A:59:LEU:HA	0.71	1.62	7	11
1:A:72:ALA:HB2	2:B:7:SER:HB2	0.71	1.63	13	9
1:A:31:LEU:HD22	1:A:65:LEU:HD21	0.71	1.61	26	2
1:A:53:SER:HA	1:A:56:LEU:HD12	0.71	1.61	6	3
1:A:36:HIS:CD2	1:A:40:ALA:HB2	0.71	2.21	30	25
1:A:52:ASN:HA	1:A:55:LEU:CD1	0.70	2.15	15	7
1:A:33:GLN:HA	1:A:36:HIS:CD2	0.70	2.21	28	29
1:A:46:MET:CB	1:A:76:LEU:HD12	0.70	2.17	29	1
1:A:47:LEU:HD21	1:A:76:LEU:HD11	0.70	1.62	25	1
1:A:28:LEU:HG	1:A:55:LEU:CD2	0.70	2.16	3	10
1:A:32:ILE:O	1:A:32:ILE:HD13	0.70	1.86	1	21
1:A:46:MET:HG3	2:B:9:ASN:HA	0.70	1.62	30	8
1:A:26:GLU:OE1	1:A:48:LEU:HD21	0.69	1.87	18	11
1:A:8:THR:HG21	1:A:30:PRO:HB3	0.69	1.62	13	5
1:A:27:ARG:CZ	1:A:59:LEU:HD12	0.69	2.17	18	1
1:A:71:GLU:CG	2:B:6:LEU:HD12	0.69	2.17	27	9
1:A:26:GLU:OE2	1:A:55:LEU:HD22	0.69	1.87	5	1
1:A:66:ARG:O	1:A:70:ASP:HB2	0.69	1.88	1	16
1:A:75:VAL:HG11	2:B:7:SER:O	0.68	1.88	21	5
1:A:17:PRO:O	1:A:20:GLN:HG2	0.68	1.89	4	20
1:A:74:ALA:HB3	2:B:5:LYS:HG2	0.68	1.65	24	1
1:A:46:MET:HE1	1:A:76:LEU:N	0.68	2.03	23	1
1:A:47:LEU:HD13	2:B:7:SER:HB3	0.68	1.65	7	4
1:A:28:LEU:HG	1:A:55:LEU:HD11	0.68	1.66	25	1
2:B:5:LYS:N	2:B:5:LYS:HD2	0.68	2.04	24	5
1:A:21:LYS:HB3	1:A:26:GLU:HA	0.68	1.66	15	1
1:A:38:THR:HG21	1:A:76:LEU:HD22	0.67	1.66	18	2
1:A:28:LEU:HD13	1:A:47:LEU:CB	0.67	2.17	3	3
1:A:71:GLU:O	1:A:75:VAL:HG12	0.67	1.88	1	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ARG:O	1:A:31:LEU:HG	0.67	1.90	12	15
1:A:75:VAL:HB	2:B:5:LYS:HB2	0.67	1.67	7	10
1:A:52:ASN:O	1:A:56:LEU:HD12	0.67	1.90	15	5
1:A:50:ILE:CG2	1:A:55:LEU:HG	0.67	2.19	5	4
2:B:14:TYR:HB2	2:B:15:PRO:HD2	0.67	1.67	15	3
1:A:27:ARG:H	1:A:55:LEU:HD23	0.67	1.50	20	2
1:A:28:LEU:HD11	1:A:55:LEU:CD2	0.67	2.20	1	4
1:A:58:MET:HB3	1:A:65:LEU:HD23	0.66	1.66	8	3
1:A:19:GLU:HG2	1:A:22:GLN:NE2	0.66	2.05	9	1
1:A:47:LEU:HD13	2:B:7:SER:OG	0.66	1.90	6	9
1:A:32:ILE:CD1	1:A:37:PRO:HD2	0.66	2.19	5	25
1:A:26:GLU:HB2	1:A:55:LEU:HD22	0.66	1.66	27	5
1:A:31:LEU:CB	1:A:65:LEU:HD21	0.66	2.18	6	6
1:A:24:LEU:HB3	1:A:29:PHE:CD2	0.66	2.26	6	18
1:A:35:MET:SD	1:A:69:VAL:HG11	0.66	2.31	13	1
1:A:32:ILE:HG23	1:A:40:ALA:HB1	0.65	1.69	13	11
1:A:49:GLU:HB3	2:B:10:ALA:HB2	0.65	1.68	10	9
1:A:52:ASN:ND2	2:B:16:SER:HB3	0.65	2.07	6	13
1:A:40:ALA:O	1:A:43:ILE:HG22	0.65	1.92	16	17
1:A:46:MET:HG2	1:A:76:LEU:HG	0.65	1.68	8	9
1:A:26:GLU:HG2	1:A:48:LEU:HD11	0.64	1.68	6	9
1:A:29:PHE:O	1:A:33:GLN:HB2	0.64	1.91	19	18
1:A:39:LEU:HD13	1:A:42:LYS:HB2	0.63	1.69	15	2
1:A:52:ASN:O	1:A:56:LEU:HG	0.63	1.92	1	2
1:A:44:THR:HG22	1:A:48:LEU:HD13	0.62	1.71	26	14
1:A:75:VAL:CG2	2:B:5:LYS:HB2	0.62	2.24	24	12
1:A:32:ILE:HG13	1:A:43:ILE:CG2	0.62	2.23	10	10
2:B:15:PRO:HB2	2:B:18:TYR:CD1	0.62	2.30	2	21
1:A:71:GLU:HG2	2:B:6:LEU:HG	0.62	1.71	20	1
1:A:31:LEU:HD22	1:A:65:LEU:HG	0.62	1.71	16	12
1:A:72:ALA:HB2	2:B:7:SER:CB	0.62	2.25	8	7
1:A:46:MET:HE1	1:A:76:LEU:CA	0.62	2.24	23	1
1:A:26:GLU:OE1	1:A:48:LEU:HD11	0.62	1.94	21	3
1:A:26:GLU:HB3	2:B:16:SER:CB	0.62	2.25	4	18
1:A:28:LEU:CD1	1:A:48:LEU:HD12	0.62	2.24	13	7
1:A:46:MET:HE1	1:A:76:LEU:HA	0.62	1.72	23	1
1:A:21:LYS:HB2	2:B:15:PRO:HA	0.61	1.72	12	1
1:A:37:PRO:HG3	1:A:73:VAL:HG22	0.61	1.72	27	6
1:A:37:PRO:HG3	1:A:73:VAL:HG12	0.61	1.71	1	1
1:A:43:ILE:HG13	1:A:76:LEU:HD13	0.61	1.71	20	4
1:A:65:LEU:C	1:A:65:LEU:HD22	0.61	2.16	20	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LEU:HD23	1:A:60:GLU:HG2	0.61	1.71	12	5
1:A:28:LEU:HD12	1:A:55:LEU:CD2	0.61	2.25	30	2
1:A:15:ALA:HB1	1:A:19:GLU:HB3	0.61	1.72	7	11
1:A:46:MET:CG	1:A:76:LEU:HD13	0.61	2.22	11	4
1:A:45:GLY:N	2:B:13:PHE:HB3	0.61	2.11	29	24
1:A:39:LEU:O	1:A:43:ILE:HG22	0.60	1.95	28	4
1:A:10:SER:O	1:A:14:SER:HB2	0.60	1.96	30	10
1:A:26:GLU:CD	2:B:16:SER:HB3	0.60	2.17	21	2
1:A:21:LYS:O	2:B:15:PRO:HA	0.60	1.97	15	18
1:A:26:GLU:CG	1:A:55:LEU:HD13	0.60	2.27	2	5
1:A:52:ASN:HA	1:A:55:LEU:HD13	0.60	1.72	3	6
1:A:47:LEU:HD23	1:A:47:LEU:N	0.60	2.11	10	1
1:A:58:MET:HB3	1:A:65:LEU:HA	0.60	1.72	10	6
1:A:28:LEU:HD21	1:A:47:LEU:CG	0.60	2.23	10	4
1:A:46:MET:CG	1:A:76:LEU:HD12	0.60	2.25	22	2
1:A:28:LEU:HG	1:A:55:LEU:HD21	0.59	1.71	25	6
1:A:69:VAL:O	1:A:72:ALA:HB3	0.59	1.97	7	10
1:A:75:VAL:HG13	1:A:76:LEU:H	0.59	1.57	22	17
1:A:74:ALA:HB3	2:B:5:LYS:CG	0.59	2.25	8	9
1:A:75:VAL:HG22	2:B:5:LYS:CG	0.59	2.26	2	10
1:A:72:ALA:HA	2:B:7:SER:O	0.59	1.98	8	6
1:A:72:ALA:O	1:A:76:LEU:HG	0.59	1.98	25	2
1:A:11:MET:CB	1:A:24:LEU:HD21	0.59	2.28	21	6
1:A:75:VAL:HG21	2:B:7:SER:O	0.59	1.96	19	3
1:A:55:LEU:HA	1:A:58:MET:HE3	0.59	1.74	2	2
1:A:31:LEU:HD22	1:A:65:LEU:HD11	0.59	1.73	9	3
1:A:71:GLU:N	1:A:71:GLU:OE1	0.59	2.36	28	6
1:A:26:GLU:CG	1:A:55:LEU:HD22	0.58	2.28	30	5
1:A:15:ALA:HB3	1:A:19:GLU:O	0.58	1.98	11	17
1:A:31:LEU:HD21	1:A:59:LEU:CA	0.58	2.28	14	8
1:A:19:GLU:CA	1:A:22:GLN:HG2	0.58	2.28	20	3
1:A:26:GLU:CG	1:A:48:LEU:HD11	0.58	2.28	6	9
1:A:28:LEU:O	1:A:32:ILE:HG22	0.58	1.99	17	6
1:A:58:MET:O	1:A:65:LEU:HB2	0.58	1.99	1	8
1:A:32:ILE:HG12	1:A:43:ILE:HG21	0.58	1.75	2	2
1:A:50:ILE:HG22	1:A:55:LEU:CD1	0.58	2.28	28	2
1:A:12:LEU:CD2	1:A:24:LEU:HD11	0.58	2.28	26	2
1:A:72:ALA:CB	2:B:7:SER:HB3	0.58	2.28	3	1
1:A:28:LEU:CD1	1:A:55:LEU:HD11	0.58	2.29	25	1
2:B:14:TYR:CD2	2:B:15:PRO:HD2	0.58	2.32	6	6
1:A:26:GLU:HG3	1:A:55:LEU:HD22	0.58	1.76	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:PHE:CD1	1:A:40:ALA:HB1	0.58	2.33	9	29
1:A:51:ASP:O	1:A:55:LEU:HD12	0.57	1.98	14	5
1:A:31:LEU:CD2	1:A:59:LEU:HA	0.57	2.28	14	9
1:A:72:ALA:O	1:A:76:LEU:HB3	0.57	1.99	15	4
1:A:46:MET:SD	2:B:9:ASN:HA	0.57	2.39	10	1
2:B:6:LEU:C	2:B:6:LEU:HD13	0.57	2.20	11	2
1:A:28:LEU:CG	1:A:55:LEU:HD11	0.57	2.29	25	1
1:A:39:LEU:O	1:A:43:ILE:HB	0.57	1.99	29	15
1:A:24:LEU:O	1:A:25:GLY:C	0.57	2.43	8	29
1:A:47:LEU:CD2	1:A:72:ALA:HB2	0.57	2.20	28	9
1:A:65:LEU:HD22	1:A:65:LEU:O	0.57	1.98	20	10
1:A:65:LEU:O	1:A:69:VAL:HG23	0.57	2.00	3	4
1:A:19:GLU:HA	1:A:22:GLN:HG2	0.57	1.77	20	2
1:A:73:VAL:O	1:A:77:GLN:HB3	0.57	1.99	17	4
1:A:26:GLU:OE1	1:A:28:LEU:HG	0.57	1.99	15	2
1:A:20:GLN:NE2	2:B:17:GLY:O	0.57	2.38	13	1
1:A:27:ARG:HG2	1:A:59:LEU:HD13	0.57	1.75	11	3
1:A:47:LEU:O	1:A:49:GLU:N	0.57	2.38	4	28
1:A:46:MET:HB3	1:A:76:LEU:HD22	0.57	1.77	25	1
1:A:76:LEU:HD13	1:A:77:GLN:N	0.56	2.15	3	1
1:A:11:MET:HB3	1:A:24:LEU:HD21	0.56	1.75	11	5
1:A:52:ASN:OD1	1:A:56:LEU:HD13	0.56	2.00	13	1
1:A:58:MET:HG2	1:A:65:LEU:HA	0.56	1.77	11	2
1:A:69:VAL:O	1:A:73:VAL:HG13	0.56	2.01	9	1
1:A:26:GLU:OE1	1:A:52:ASN:HA	0.56	2.01	14	3
1:A:19:GLU:HA	1:A:22:GLN:HG3	0.56	1.76	12	1
1:A:26:GLU:OE2	1:A:48:LEU:HG	0.56	2.00	14	4
1:A:75:VAL:HG11	2:B:8:VAL:HA	0.56	1.75	23	1
1:A:18:GLN:HB2	2:B:18:TYR:CZ	0.56	2.35	30	4
2:B:6:LEU:HD22	2:B:6:LEU:O	0.56	2.01	5	1
1:A:52:ASN:HB2	2:B:16:SER:HB2	0.56	1.78	29	2
1:A:29:PHE:HA	1:A:32:ILE:HG22	0.56	1.78	3	9
1:A:29:PHE:CE1	1:A:41:GLY:N	0.56	2.74	13	23
2:B:10:ALA:CB	2:B:11:PRO:CD	0.56	2.82	22	18
1:A:12:LEU:HD21	1:A:21:LYS:HE2	0.56	1.78	20	1
1:A:50:ILE:CG2	1:A:55:LEU:CD1	0.56	2.84	26	4
1:A:74:ALA:HB3	2:B:5:LYS:HD2	0.56	1.78	22	1
1:A:32:ILE:HD13	1:A:32:ILE:C	0.56	2.19	1	18
1:A:75:VAL:HG13	1:A:76:LEU:N	0.56	2.16	15	17
1:A:26:GLU:HG3	1:A:55:LEU:CD1	0.56	2.28	13	6
1:A:47:LEU:HD22	2:B:7:SER:CB	0.55	2.30	23	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:MET:HE3	1:A:72:ALA:HA	0.55	1.77	10	1
1:A:52:ASN:HB2	2:B:16:SER:OG	0.55	2.01	24	9
1:A:46:MET:CE	1:A:72:ALA:HA	0.55	2.31	10	1
1:A:47:LEU:N	1:A:47:LEU:CD2	0.55	2.70	23	19
1:A:46:MET:HG3	1:A:76:LEU:CD1	0.55	2.31	10	3
1:A:26:GLU:CD	1:A:48:LEU:HD11	0.55	2.22	21	5
1:A:47:LEU:C	1:A:49:GLU:H	0.55	2.05	6	29
2:B:10:ALA:O	2:B:11:PRO:O	0.55	2.25	7	30
1:A:22:GLN:HG2	2:B:15:PRO:HB3	0.55	1.78	23	7
1:A:21:LYS:HG3	2:B:17:GLY:H	0.55	1.61	18	3
1:A:75:VAL:HG22	2:B:5:LYS:CD	0.55	2.32	24	1
1:A:28:LEU:HD21	1:A:55:LEU:HD23	0.55	1.78	1	1
1:A:45:GLY:O	2:B:11:PRO:O	0.55	2.25	5	16
1:A:27:ARG:NH1	1:A:56:LEU:HD11	0.55	2.17	21	1
1:A:47:LEU:HD21	1:A:72:ALA:HB1	0.55	1.79	29	9
1:A:27:ARG:HB2	1:A:55:LEU:HB3	0.55	1.79	27	5
1:A:47:LEU:HA	2:B:7:SER:HB3	0.55	1.79	15	2
1:A:26:GLU:N	1:A:26:GLU:OE1	0.55	2.39	16	2
1:A:37:PRO:HG3	1:A:73:VAL:HG21	0.55	1.78	3	1
1:A:58:MET:HB2	1:A:65:LEU:CA	0.55	2.32	12	2
1:A:32:ILE:HG23	1:A:40:ALA:CB	0.54	2.32	30	19
1:A:28:LEU:CD1	1:A:55:LEU:HD21	0.54	2.32	28	6
1:A:29:PHE:N	1:A:30:PRO:CD	0.54	2.70	26	30
1:A:26:GLU:OE1	1:A:55:LEU:CB	0.54	2.55	2	1
1:A:38:THR:OG1	1:A:43:ILE:HD12	0.54	2.02	9	2
1:A:28:LEU:CD1	1:A:55:LEU:HD22	0.54	2.32	2	2
1:A:47:LEU:CD2	1:A:72:ALA:CB	0.54	2.85	17	14
1:A:67:SER:O	1:A:71:GLU:HG2	0.54	2.03	2	6
2:B:16:SER:OG	2:B:17:GLY:N	0.54	2.41	21	2
1:A:43:ILE:HA	1:A:76:LEU:HD22	0.54	1.78	23	1
1:A:43:ILE:HG13	1:A:76:LEU:HD22	0.53	1.80	19	4
1:A:75:VAL:HB	2:B:5:LYS:CG	0.53	2.33	18	5
1:A:27:ARG:H	1:A:55:LEU:HD22	0.53	1.63	22	5
1:A:29:PHE:CE1	1:A:40:ALA:CB	0.53	2.91	6	24
1:A:27:ARG:C	1:A:30:PRO:HD2	0.53	2.24	11	26
1:A:26:GLU:OE1	1:A:55:LEU:HD13	0.53	2.04	2	5
1:A:36:HIS:HD2	1:A:40:ALA:HB2	0.53	1.63	25	11
1:A:47:LEU:HD11	1:A:68:LYS:O	0.53	2.03	23	4
1:A:32:ILE:HD12	1:A:40:ALA:CB	0.53	2.33	22	7
1:A:55:LEU:H	1:A:55:LEU:HD12	0.53	1.63	19	3
1:A:15:ALA:O	1:A:16:PRO:O	0.53	2.27	17	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ALA:HA	1:A:43:ILE:CG2	0.53	2.34	3	5
1:A:47:LEU:N	1:A:47:LEU:HD23	0.53	2.19	23	12
1:A:26:GLU:HA	2:B:16:SER:HG	0.53	1.63	17	1
2:B:15:PRO:HB2	2:B:18:TYR:HD1	0.53	1.64	11	19
1:A:29:PHE:HA	1:A:32:ILE:CG2	0.53	2.33	5	4
1:A:50:ILE:HG12	1:A:54:GLU:CB	0.53	2.34	25	2
1:A:11:MET:CG	1:A:24:LEU:HD21	0.53	2.34	28	4
1:A:8:THR:HG23	1:A:33:GLN:OE1	0.53	2.03	26	2
1:A:52:ASN:HB2	2:B:16:SER:HB3	0.53	1.80	5	3
1:A:46:MET:CG	2:B:9:ASN:HA	0.52	2.34	30	8
1:A:29:PHE:CE1	1:A:40:ALA:HB1	0.52	2.39	3	1
1:A:26:GLU:OE1	1:A:26:GLU:N	0.52	2.42	22	8
1:A:54:GLU:O	1:A:58:MET:HG2	0.52	2.04	28	1
1:A:47:LEU:HD23	1:A:47:LEU:H	0.52	1.65	23	3
1:A:50:ILE:CG2	1:A:55:LEU:HD12	0.52	2.34	28	1
1:A:71:GLU:CB	2:B:5:LYS:HB3	0.52	2.33	24	10
1:A:23:MET:O	1:A:25:GLY:N	0.52	2.43	17	29
1:A:29:PHE:HB3	1:A:30:PRO:HD3	0.52	1.81	15	8
1:A:45:GLY:CA	2:B:13:PHE:HB3	0.52	2.34	24	13
1:A:16:PRO:O	1:A:17:PRO:O	0.52	2.27	28	9
1:A:23:MET:O	2:B:13:PHE:CE2	0.52	2.62	18	23
1:A:71:GLU:HG3	2:B:5:LYS:HD3	0.52	1.81	22	1
1:A:12:LEU:HD11	1:A:20:GLN:HB3	0.52	1.81	12	1
2:B:15:PRO:CG	2:B:18:TYR:CD1	0.52	2.92	25	15
1:A:46:MET:HB2	1:A:76:LEU:HD13	0.52	1.81	7	1
1:A:26:GLU:HB2	1:A:55:LEU:CD2	0.52	2.36	20	1
1:A:57:HIS:O	1:A:60:GLU:HG2	0.52	2.05	28	1
1:A:28:LEU:HG	1:A:55:LEU:HD22	0.51	1.81	2	3
2:B:15:PRO:CB	2:B:18:TYR:CD1	0.51	2.92	2	15
1:A:37:PRO:CG	1:A:73:VAL:HG22	0.51	2.35	4	2
1:A:65:LEU:HD13	1:A:65:LEU:C	0.51	2.26	29	8
1:A:26:GLU:CD	1:A:27:ARG:H	0.51	2.09	15	4
1:A:56:LEU:HD23	1:A:59:LEU:HD11	0.51	1.82	23	1
1:A:72:ALA:O	1:A:76:LEU:N	0.51	2.44	28	14
1:A:58:MET:SD	1:A:68:LYS:HG3	0.51	2.46	30	2
1:A:58:MET:HE2	1:A:65:LEU:HD23	0.51	1.83	6	2
1:A:26:GLU:CB	1:A:55:LEU:HD13	0.51	2.36	15	1
1:A:28:LEU:CD1	1:A:55:LEU:CD2	0.51	2.89	21	3
1:A:47:LEU:CD2	1:A:47:LEU:N	0.51	2.74	25	11
1:A:44:THR:HG22	1:A:48:LEU:CD1	0.51	2.35	22	4
1:A:32:ILE:O	1:A:36:HIS:N	0.51	2.40	13	30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:MET:HG2	1:A:24:LEU:CD2	0.50	2.36	7	6
1:A:46:MET:HB2	1:A:76:LEU:CD1	0.50	2.35	7	1
1:A:28:LEU:CG	1:A:55:LEU:HD22	0.50	2.36	2	1
1:A:38:THR:HG22	1:A:43:ILE:HD12	0.50	1.83	18	1
1:A:46:MET:CB	1:A:76:LEU:HD13	0.50	2.36	7	1
1:A:26:GLU:CD	2:B:16:SER:HB2	0.50	2.26	12	4
1:A:36:HIS:N	1:A:37:PRO:CD	0.50	2.75	13	23
1:A:32:ILE:CG2	1:A:40:ALA:HA	0.50	2.36	30	12
1:A:73:VAL:O	1:A:77:GLN:CB	0.50	2.59	17	12
1:A:32:ILE:O	1:A:35:MET:N	0.50	2.44	27	10
1:A:31:LEU:HD22	1:A:65:LEU:CD1	0.50	2.36	9	1
1:A:26:GLU:OE2	1:A:28:LEU:HB2	0.50	2.07	4	1
1:A:28:LEU:HD13	1:A:44:THR:HA	0.50	1.84	10	1
1:A:23:MET:O	2:B:13:PHE:HE2	0.49	1.90	26	10
1:A:27:ARG:HG3	1:A:56:LEU:HD23	0.49	1.83	7	2
1:A:28:LEU:HD21	1:A:47:LEU:HB2	0.49	1.83	23	3
1:A:71:GLU:O	2:B:5:LYS:HG2	0.49	2.07	4	2
1:A:18:GLN:O	2:B:18:TYR:CD1	0.49	2.65	7	6
1:A:26:GLU:HG3	1:A:48:LEU:CD1	0.49	2.38	14	2
1:A:32:ILE:HD11	1:A:37:PRO:CD	0.49	2.36	2	1
1:A:43:ILE:O	1:A:47:LEU:HD23	0.49	2.07	12	4
1:A:43:ILE:HG22	1:A:44:THR:N	0.49	2.23	10	2
1:A:46:MET:SD	1:A:72:ALA:HB1	0.49	2.48	19	1
1:A:32:ILE:HG12	1:A:40:ALA:CA	0.49	2.33	17	1
1:A:32:ILE:CD1	1:A:40:ALA:HA	0.49	2.36	23	7
1:A:32:ILE:CG2	1:A:40:ALA:HB1	0.49	2.37	13	2
1:A:72:ALA:HA	1:A:75:VAL:CG1	0.49	2.38	14	3
1:A:24:LEU:O	1:A:25:GLY:O	0.49	2.31	12	20
1:A:27:ARG:HE	1:A:56:LEU:HD23	0.49	1.68	6	1
1:A:46:MET:HE1	2:B:8:VAL:C	0.49	2.28	19	1
1:A:55:LEU:HA	1:A:58:MET:CE	0.49	2.36	2	4
1:A:43:ILE:CG2	1:A:44:THR:N	0.49	2.76	13	15
1:A:47:LEU:HD11	1:A:72:ALA:CB	0.49	2.38	3	2
1:A:38:THR:O	1:A:39:LEU:HD12	0.49	2.07	10	1
1:A:38:THR:HG23	1:A:43:ILE:HD12	0.49	1.84	13	1
1:A:44:THR:O	1:A:48:LEU:HD13	0.49	2.07	13	3
1:A:55:LEU:O	1:A:58:MET:HG3	0.49	2.07	1	2
1:A:75:VAL:HG13	1:A:76:LEU:HD12	0.49	1.84	1	1
1:A:26:GLU:CB	1:A:55:LEU:HD22	0.49	2.35	27	2
1:A:25:GLY:N	2:B:13:PHE:HD2	0.48	2.06	15	1
1:A:46:MET:HG2	2:B:9:ASN:ND2	0.48	2.23	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:GLU:HA	1:A:71:GLU:OE1	0.48	2.06	30	1
1:A:71:GLU:HG3	2:B:6:LEU:CD1	0.48	2.37	24	2
1:A:41:GLY:O	2:B:13:PHE:CE1	0.48	2.65	5	2
1:A:11:MET:SD	1:A:23:MET:HB2	0.48	2.48	26	5
1:A:27:ARG:NH2	1:A:59:LEU:HD22	0.48	2.23	19	1
1:A:46:MET:SD	1:A:47:LEU:HD22	0.48	2.48	19	1
2:B:15:PRO:CB	2:B:18:TYR:HD1	0.48	2.21	17	6
1:A:22:GLN:HG3	1:A:23:MET:H	0.48	1.67	20	1
1:A:47:LEU:CD2	1:A:72:ALA:HB1	0.48	2.38	3	5
1:A:26:GLU:CD	1:A:48:LEU:HG	0.48	2.28	1	3
1:A:26:GLU:OE2	2:B:16:SER:OG	0.48	2.31	18	4
1:A:72:ALA:HB1	1:A:76:LEU:HD11	0.48	1.85	25	1
1:A:18:GLN:HB2	2:B:18:TYR:CE1	0.48	2.43	29	3
1:A:62:PRO:HA	1:A:65:LEU:HB3	0.48	1.85	1	3
1:A:75:VAL:HG22	2:B:5:LYS:HG2	0.48	1.85	2	2
1:A:38:THR:OG1	1:A:39:LEU:N	0.48	2.47	27	13
1:A:58:MET:HB3	1:A:65:LEU:HG	0.48	1.86	9	2
1:A:28:LEU:CD1	1:A:44:THR:O	0.48	2.62	19	2
1:A:31:LEU:HD21	1:A:59:LEU:HB2	0.48	1.85	30	3
1:A:18:GLN:O	2:B:18:TYR:CE1	0.48	2.67	13	3
1:A:28:LEU:HD21	1:A:47:LEU:CB	0.48	2.38	23	6
1:A:49:GLU:HB2	2:B:10:ALA:HB2	0.47	1.85	8	1
1:A:40:ALA:HA	1:A:43:ILE:HG22	0.47	1.86	3	2
1:A:21:LYS:N	1:A:21:LYS:HD2	0.47	2.25	11	2
1:A:75:VAL:HG22	2:B:5:LYS:HB2	0.47	1.85	24	1
1:A:28:LEU:HD12	1:A:44:THR:O	0.47	2.09	19	1
1:A:75:VAL:HG22	2:B:5:LYS:HD2	0.47	1.86	24	1
1:A:11:MET:HG2	1:A:24:LEU:HD23	0.47	1.87	26	1
1:A:52:ASN:O	1:A:56:LEU:HD13	0.47	2.09	3	3
1:A:47:LEU:HD22	2:B:7:SER:OG	0.47	2.10	22	1
1:A:28:LEU:CD2	1:A:47:LEU:HG	0.47	2.40	23	1
1:A:32:ILE:HG21	1:A:40:ALA:HA	0.47	1.85	27	7
1:A:32:ILE:HD13	1:A:43:ILE:HG21	0.47	1.86	17	1
1:A:38:THR:CG2	1:A:43:ILE:HD12	0.47	2.40	29	2
1:A:43:ILE:HA	1:A:76:LEU:HD11	0.47	1.86	18	2
1:A:31:LEU:CD2	1:A:65:LEU:HD21	0.47	2.37	26	1
1:A:26:GLU:CG	1:A:48:LEU:CD1	0.47	2.93	27	2
1:A:46:MET:CE	1:A:76:LEU:HB2	0.47	2.40	10	1
1:A:15:ALA:HB1	1:A:19:GLU:CB	0.47	2.40	14	2
1:A:28:LEU:HD22	1:A:47:LEU:CB	0.47	2.40	20	8
1:A:39:LEU:HD13	1:A:42:LYS:CB	0.47	2.40	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:14:TYR:HB3	2:B:15:PRO:CD	0.47	2.38	30	1
1:A:22:GLN:HA	2:B:15:PRO:HB3	0.46	1.87	11	7
1:A:16:PRO:HG2	1:A:19:GLU:HG3	0.46	1.86	23	1
2:B:14:TYR:CB	2:B:15:PRO:HD2	0.46	2.40	23	19
1:A:47:LEU:CD1	1:A:72:ALA:CB	0.46	2.94	3	1
1:A:74:ALA:HB1	2:B:5:LYS:HE3	0.46	1.86	11	1
1:A:26:GLU:HG3	1:A:48:LEU:HD11	0.46	1.85	14	2
1:A:39:LEU:O	1:A:43:ILE:CG2	0.46	2.62	28	3
1:A:58:MET:HB3	1:A:65:LEU:CA	0.46	2.40	24	1
1:A:29:PHE:CE1	1:A:40:ALA:HB3	0.46	2.46	6	6
1:A:26:GLU:OE2	1:A:55:LEU:HD13	0.46	2.11	5	1
1:A:54:GLU:O	1:A:58:MET:CE	0.46	2.63	11	1
1:A:18:GLN:O	1:A:20:GLN:OE1	0.46	2.33	13	1
1:A:26:GLU:OE1	1:A:52:ASN:CA	0.46	2.63	14	1
1:A:31:LEU:HB3	1:A:65:LEU:CD2	0.46	2.38	25	3
1:A:58:MET:HB3	1:A:65:LEU:HB2	0.46	1.86	29	1
1:A:27:ARG:NH2	1:A:59:LEU:HD12	0.46	2.24	18	1
1:A:79:HIS:CG	2:B:9:ASN:ND2	0.46	2.84	20	1
1:A:26:GLU:OE1	1:A:55:LEU:CD2	0.46	2.63	2	2
1:A:28:LEU:CD2	1:A:47:LEU:CB	0.46	2.94	17	4
1:A:76:LEU:C	1:A:76:LEU:HD23	0.46	2.31	28	1
1:A:29:PHE:CE1	1:A:33:GLN:CG	0.46	2.98	3	1
1:A:37:PRO:HG3	1:A:73:VAL:CG2	0.46	2.40	4	2
1:A:56:LEU:O	1:A:60:GLU:HG3	0.46	2.11	8	1
1:A:11:MET:HE1	1:A:23:MET:HG3	0.46	1.88	20	1
1:A:47:LEU:HD11	1:A:72:ALA:HB3	0.46	1.88	3	1
1:A:43:ILE:HG13	1:A:76:LEU:CD1	0.46	2.40	4	1
1:A:50:ILE:HG21	1:A:54:GLU:HB3	0.46	1.86	23	3
1:A:31:LEU:HD21	1:A:59:LEU:CB	0.46	2.41	28	1
1:A:71:GLU:HB3	2:B:5:LYS:CB	0.46	2.41	17	4
1:A:47:LEU:HA	2:B:7:SER:OG	0.46	2.10	3	1
1:A:75:VAL:O	1:A:78:ALA:HB3	0.46	2.11	3	1
1:A:66:ARG:O	1:A:70:ASP:CB	0.46	2.63	22	5
1:A:12:LEU:HD22	1:A:20:GLN:O	0.46	2.11	26	5
1:A:28:LEU:HD12	1:A:48:LEU:CD1	0.46	2.41	19	2
1:A:26:GLU:OE1	1:A:55:LEU:HD12	0.46	2.11	29	1
1:A:76:LEU:HD13	1:A:76:LEU:C	0.45	2.32	3	1
1:A:52:ASN:HB2	2:B:16:SER:CB	0.45	2.41	5	1
1:A:26:GLU:HG2	1:A:55:LEU:CD1	0.45	2.41	15	1
1:A:24:LEU:O	1:A:24:LEU:CD1	0.45	2.64	16	1
2:B:7:SER:O	2:B:8:VAL:HB	0.45	2.11	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:GLU:HG3	2:B:5:LYS:HG3	0.45	1.89	20	1
1:A:46:MET:CE	1:A:76:LEU:HA	0.45	2.41	23	1
1:A:46:MET:HG2	1:A:76:LEU:CD2	0.45	2.42	3	2
1:A:65:LEU:HD12	1:A:66:ARG:HE	0.45	1.71	8	1
1:A:32:ILE:HD12	1:A:40:ALA:HB2	0.45	1.88	1	4
1:A:32:ILE:C	1:A:32:ILE:CD1	0.45	2.85	20	4
1:A:55:LEU:HD23	1:A:58:MET:HE1	0.45	1.89	4	1
1:A:71:GLU:OE2	2:B:6:LEU:HD12	0.45	2.11	9	1
1:A:32:ILE:HG12	1:A:43:ILE:CG2	0.45	2.41	5	1
1:A:43:ILE:HG23	1:A:44:THR:N	0.45	2.26	24	5
1:A:35:MET:HB2	1:A:37:PRO:HD3	0.45	1.89	2	2
1:A:24:LEU:HB3	1:A:29:PHE:CB	0.45	2.42	4	1
1:A:32:ILE:CD1	1:A:36:HIS:HA	0.45	2.42	27	2
1:A:79:HIS:ND1	2:B:9:ASN:ND2	0.45	2.65	30	1
1:A:71:GLU:HG3	2:B:5:LYS:HB3	0.45	1.89	12	3
1:A:26:GLU:OE2	1:A:48:LEU:HD11	0.45	2.11	4	1
2:B:5:LYS:N	2:B:5:LYS:CD	0.45	2.78	24	1
1:A:28:LEU:CG	1:A:55:LEU:HD21	0.45	2.41	28	1
1:A:55:LEU:HA	1:A:58:MET:CG	0.45	2.42	27	4
1:A:64:SER:O	1:A:67:SER:HB2	0.45	2.12	27	3
1:A:40:ALA:C	1:A:43:ILE:HG22	0.45	2.32	12	5
1:A:46:MET:CB	1:A:76:LEU:CD1	0.44	2.95	7	1
1:A:26:GLU:CB	2:B:16:SER:HB3	0.44	2.42	10	1
1:A:71:GLU:OE1	1:A:71:GLU:CA	0.44	2.65	30	3
1:A:27:ARG:HG2	1:A:59:LEU:CD1	0.44	2.42	23	1
1:A:72:ALA:O	1:A:76:LEU:HB2	0.44	2.12	1	2
1:A:26:GLU:CG	2:B:16:SER:HB3	0.44	2.42	17	3
2:B:14:TYR:CG	2:B:15:PRO:HD2	0.44	2.47	20	1
2:B:14:TYR:CD1	2:B:14:TYR:N	0.44	2.85	26	1
1:A:47:LEU:C	1:A:49:GLU:N	0.44	2.71	10	7
1:A:64:SER:O	1:A:68:LYS:HG2	0.44	2.12	10	1
1:A:72:ALA:O	1:A:76:LEU:CB	0.44	2.66	4	3
1:A:16:PRO:CB	1:A:17:PRO:HD3	0.44	2.43	15	1
1:A:59:LEU:HD23	1:A:60:GLU:HG3	0.44	1.88	29	1
1:A:16:PRO:CG	1:A:17:PRO:HD3	0.44	2.42	15	1
1:A:42:LYS:O	1:A:46:MET:SD	0.44	2.76	21	2
1:A:71:GLU:HB3	2:B:6:LEU:H	0.44	1.72	11	1
1:A:38:THR:HG22	1:A:39:LEU:CG	0.44	2.37	15	1
1:A:15:ALA:CB	1:A:19:GLU:O	0.44	2.65	19	1
1:A:46:MET:CE	1:A:76:LEU:HD21	0.44	2.42	24	1
1:A:28:LEU:HD11	1:A:55:LEU:HD22	0.44	1.88	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:GLU:HG2	1:A:55:LEU:HD22	0.44	1.89	30	1
1:A:55:LEU:HA	1:A:58:MET:SD	0.44	2.52	5	1
1:A:20:GLN:HB2	1:A:21:LYS:HD2	0.44	1.89	11	1
1:A:46:MET:SD	1:A:76:LEU:CD1	0.44	3.06	15	1
1:A:22:GLN:CA	2:B:15:PRO:HB3	0.44	2.43	20	2
1:A:55:LEU:HG	1:A:58:MET:HE3	0.44	1.89	3	1
2:B:5:LYS:HD2	2:B:5:LYS:H	0.44	1.70	24	1
1:A:79:HIS:CG	2:B:9:ASN:OD1	0.43	2.71	2	2
1:A:46:MET:SD	1:A:46:MET:N	0.43	2.91	6	2
1:A:28:LEU:HB3	1:A:44:THR:HG23	0.43	1.88	8	1
1:A:52:ASN:CB	2:B:16:SER:OG	0.43	2.66	24	2
2:B:9:ASN:ND2	2:B:9:ASN:O	0.43	2.51	14	1
1:A:26:GLU:HB2	1:A:55:LEU:HD13	0.43	1.89	15	1
1:A:31:LEU:HD13	1:A:58:MET:HE2	0.43	1.90	21	1
1:A:26:GLU:OE2	1:A:55:LEU:CD2	0.43	2.63	5	1
1:A:32:ILE:HG21	1:A:43:ILE:CG2	0.43	2.44	19	2
1:A:27:ARG:HB3	1:A:55:LEU:HD22	0.43	1.89	25	1
1:A:75:VAL:CG2	2:B:7:SER:O	0.43	2.66	17	1
1:A:49:GLU:O	1:A:49:GLU:HG3	0.43	2.14	8	2
1:A:71:GLU:HG3	2:B:6:LEU:HB2	0.43	1.90	1	1
1:A:75:VAL:CG1	1:A:76:LEU:N	0.43	2.82	4	2
1:A:46:MET:HB3	1:A:76:LEU:CD2	0.43	2.44	25	1
1:A:76:LEU:HD23	1:A:77:GLN:N	0.43	2.29	29	1
1:A:27:ARG:HD2	1:A:30:PRO:HG2	0.43	1.89	18	1
1:A:43:ILE:HA	1:A:76:LEU:CD2	0.43	2.44	1	1
1:A:26:GLU:OE2	1:A:48:LEU:CD1	0.43	2.66	4	1
1:A:44:THR:HG22	2:B:13:PHE:HB2	0.43	1.89	20	1
1:A:26:GLU:HG3	1:A:55:LEU:CD2	0.43	2.44	26	2
1:A:28:LEU:CD2	1:A:47:LEU:HB2	0.43	2.44	23	4
1:A:32:ILE:HG23	1:A:33:GLN:N	0.43	2.28	10	5
1:A:65:LEU:HD22	1:A:65:LEU:C	0.43	2.34	23	2
2:B:12:GLU:HG3	2:B:13:PHE:H	0.43	1.74	20	1
1:A:55:LEU:O	1:A:58:MET:HG2	0.43	2.14	21	1
1:A:42:LYS:NZ	2:B:12:GLU:OE2	0.43	2.52	23	1
1:A:27:ARG:H	1:A:55:LEU:CD2	0.43	2.26	27	1
1:A:32:ILE:CD1	1:A:43:ILE:HG21	0.42	2.43	17	1
1:A:55:LEU:CA	1:A:58:MET:HE3	0.42	2.43	2	1
1:A:26:GLU:OE2	1:A:55:LEU:CB	0.42	2.67	5	1
1:A:28:LEU:HD22	1:A:47:LEU:HB3	0.42	1.91	14	1
1:A:21:LYS:C	2:B:15:PRO:HA	0.42	2.35	15	1
1:A:79:HIS:CB	2:B:9:ASN:ND2	0.42	2.82	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:MET:HE1	1:A:23:MET:HB2	0.42	1.91	2	1
1:A:44:THR:O	1:A:48:LEU:CD1	0.42	2.68	5	2
1:A:16:PRO:N	1:A:17:PRO:CD	0.42	2.82	22	5
1:A:26:GLU:HB3	2:B:16:SER:HB2	0.42	1.90	11	1
1:A:27:ARG:HB2	1:A:55:LEU:CB	0.42	2.44	14	2
1:A:27:ARG:C	1:A:55:LEU:HD22	0.42	2.34	25	1
1:A:29:PHE:HE1	1:A:41:GLY:N	0.42	2.12	6	1
1:A:19:GLU:C	1:A:22:GLN:HG2	0.42	2.35	20	1
1:A:46:MET:CG	1:A:76:LEU:HD21	0.42	2.45	1	1
1:A:31:LEU:HD22	1:A:65:LEU:CG	0.42	2.44	10	1
1:A:32:ILE:HD11	1:A:43:ILE:HD13	0.42	1.86	13	1
1:A:26:GLU:CG	2:B:16:SER:HB2	0.42	2.44	20	1
1:A:39:LEU:HD23	1:A:42:LYS:HB2	0.42	1.92	20	1
1:A:41:GLY:O	2:B:13:PHE:CD1	0.42	2.73	23	1
1:A:75:VAL:N	2:B:5:LYS:HD3	0.42	2.30	7	1
2:B:13:PHE:O	2:B:13:PHE:CG	0.42	2.73	20	2
1:A:75:VAL:HG22	2:B:5:LYS:CB	0.42	2.45	11	2
1:A:31:LEU:HD13	1:A:65:LEU:HG	0.42	1.90	13	1
2:B:15:PRO:HG3	2:B:18:TYR:CE1	0.42	2.49	22	1
1:A:43:ILE:HA	1:A:76:LEU:CD1	0.42	2.45	20	1
1:A:57:HIS:O	1:A:60:GLU:CG	0.42	2.68	26	1
1:A:32:ILE:CG2	1:A:33:GLN:N	0.42	2.83	3	3
1:A:46:MET:HE2	1:A:76:LEU:HD11	0.42	1.90	5	1
1:A:46:MET:HE1	1:A:76:LEU:HB2	0.42	1.90	10	1
1:A:27:ARG:HB3	1:A:55:LEU:HB3	0.42	1.92	16	1
1:A:22:GLN:HG3	1:A:23:MET:N	0.42	2.30	20	1
1:A:45:GLY:HA2	2:B:13:PHE:CA	0.42	2.45	20	1
1:A:49:GLU:OE1	2:B:8:VAL:HG22	0.42	2.14	20	1
1:A:71:GLU:HG2	2:B:6:LEU:CG	0.42	2.41	20	1
1:A:26:GLU:OE1	1:A:55:LEU:CG	0.42	2.67	2	1
1:A:37:PRO:HB2	1:A:73:VAL:HG13	0.42	1.92	4	1
1:A:38:THR:HG21	1:A:76:LEU:HD23	0.42	1.92	30	1
1:A:35:MET:CE	1:A:69:VAL:HB	0.41	2.45	5	1
1:A:16:PRO:HG2	1:A:17:PRO:HD3	0.41	1.91	15	1
1:A:65:LEU:CD1	1:A:66:ARG:N	0.41	2.79	18	1
1:A:11:MET:HG3	1:A:12:LEU:N	0.41	2.30	8	2
1:A:52:ASN:OD1	1:A:52:ASN:O	0.41	2.37	13	1
1:A:12:LEU:HD22	1:A:12:LEU:HA	0.41	1.79	8	3
1:A:32:ILE:CG2	1:A:40:ALA:CB	0.41	2.98	27	2
1:A:52:ASN:CA	1:A:55:LEU:HD12	0.41	2.45	13	1
1:A:71:GLU:CA	1:A:71:GLU:OE1	0.41	2.68	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:VAL:O	1:A:79:HIS:N	0.41	2.50	23	1
1:A:29:PHE:CD1	1:A:40:ALA:CB	0.41	3.03	6	2
1:A:65:LEU:HD22	1:A:69:VAL:HG23	0.41	1.91	7	3
2:B:15:PRO:CG	2:B:18:TYR:CE1	0.41	3.03	18	1
1:A:76:LEU:HD23	1:A:76:LEU:C	0.41	2.36	29	1
1:A:55:LEU:HA	1:A:58:MET:HG2	0.41	1.92	1	1
1:A:11:MET:HE2	1:A:12:LEU:HA	0.41	1.93	4	1
1:A:46:MET:HB2	1:A:76:LEU:HD12	0.41	1.91	29	1
1:A:19:GLU:HG2	1:A:22:GLN:HG3	0.41	1.92	5	1
1:A:50:ILE:CG2	1:A:55:LEU:CG	0.41	2.95	5	1
1:A:26:GLU:CD	1:A:48:LEU:HD21	0.41	2.36	16	1
1:A:40:ALA:CA	1:A:43:ILE:HG22	0.41	2.46	18	1
1:A:55:LEU:HD12	1:A:55:LEU:H	0.41	1.75	8	1
1:A:57:HIS:O	1:A:60:GLU:HG3	0.41	2.16	9	1
1:A:52:ASN:HD22	2:B:17:GLY:N	0.41	2.14	13	1
1:A:54:GLU:O	1:A:58:MET:HG3	0.41	2.16	30	1
1:A:74:ALA:CB	2:B:5:LYS:HD2	0.41	2.46	5	2
1:A:46:MET:CG	2:B:9:ASN:ND2	0.41	2.84	6	1
1:A:67:SER:O	1:A:71:GLU:OE2	0.41	2.39	16	1
1:A:52:ASN:O	1:A:52:ASN:OD1	0.41	2.38	18	1
1:A:71:GLU:OE1	1:A:71:GLU:N	0.41	2.54	18	1
2:B:12:GLU:HB3	2:B:14:TYR:CE1	0.41	2.51	18	1
1:A:26:GLU:OE2	2:B:16:SER:CB	0.41	2.69	26	1
1:A:43:ILE:CG1	1:A:76:LEU:HD12	0.41	2.46	27	1
1:A:39:LEU:O	1:A:43:ILE:CB	0.41	2.69	15	1
1:A:47:LEU:HD13	2:B:7:SER:HB2	0.41	1.93	19	1
1:A:35:MET:HE3	1:A:69:VAL:CG1	0.40	2.47	5	1
1:A:55:LEU:HG	1:A:58:MET:CE	0.40	2.46	23	1
1:A:46:MET:SD	2:B:9:ASN:ND2	0.40	2.95	25	1
1:A:50:ILE:HG22	1:A:55:LEU:HD11	0.40	1.93	26	1
1:A:74:ALA:CB	2:B:5:LYS:HE3	0.40	2.46	28	1
1:A:76:LEU:N	1:A:76:LEU:HD23	0.40	2.31	7	1
1:A:46:MET:CE	1:A:75:VAL:HG13	0.40	2.47	10	1
1:A:28:LEU:CD1	1:A:47:LEU:CB	0.40	2.99	15	2
1:A:29:PHE:CE1	1:A:40:ALA:C	0.40	2.95	12	1
1:A:11:MET:SD	1:A:24:LEU:HG	0.40	2.56	14	1
2:B:9:ASN:O	2:B:10:ALA:O	0.40	2.40	24	1
1:A:27:ARG:O	1:A:30:PRO:HD2	0.40	2.15	26	1
1:A:65:LEU:C	1:A:65:LEU:HD23	0.40	2.37	9	1
1:A:26:GLU:HG2	1:A:48:LEU:CD1	0.40	2.46	19	1
1:A:71:GLU:OE1	2:B:5:LYS:HB3	0.40	2.16	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LEU:O	1:A:58:MET:CG	0.40	2.69	26	1
1:A:71:GLU:CG	2:B:5:LYS:HB3	0.40	2.47	12	1
1:A:24:LEU:CB	1:A:29:PHE:HD2	0.40	2.30	15	1
1:A:38:THR:C	1:A:39:LEU:HG	0.40	2.36	29	1
1:A:51:ASP:O	1:A:55:LEU:CD1	0.40	2.70	1	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	72/98 (73%)	52±2 (73±3%)	11±2 (16±3%)	8±1 (11±1%)	1	7
2	B	14/22 (64%)	7±1 (53±8%)	4±1 (30±7%)	2±1 (18±5%)	0	3
All	All	2580/3600 (72%)	1793 (69%)	465 (18%)	322 (12%)	1	6

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	23	MET	30
1	A	24	LEU	30
1	A	37	PRO	30
2	B	11	PRO	30
1	A	25	GLY	29
1	A	48	LEU	29
1	A	17	PRO	28
2	B	10	ALA	28
1	A	20	GLN	27
1	A	26	GLU	22
1	A	16	PRO	21
2	B	8	VAL	12
2	B	15	PRO	3
1	A	40	ALA	1
1	A	41	GLY	1
2	B	18	TYR	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	61/79 (77%)	34±3 (56±4%)	27±3 (44±4%)	0 2
2	B	12/20 (60%)	10±1 (82±9%)	2±1 (18±9%)	4 37
All	All	2190/2970 (74%)	1310 (60%)	880 (40%)	0 5

All 60 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	12	LEU	30
1	A	24	LEU	30
1	A	26	GLU	30
1	A	47	LEU	30
1	A	20	GLN	29
1	A	59	LEU	29
1	A	48	LEU	28
1	A	21	LYS	26
1	A	32	ILE	26
1	A	22	GLN	24
1	A	42	LYS	24
1	A	65	LEU	24
1	A	11	MET	22
1	A	46	MET	20
1	A	29	PHE	20
1	A	39	LEU	19
1	A	49	GLU	19
1	A	50	ILE	18
2	B	16	SER	18
1	A	33	GLN	17
1	A	61	SER	17
1	A	27	ARG	16
1	A	54	GLU	16
1	A	63	GLU	16
1	A	79	HIS	16
1	A	68	LYS	16
1	A	43	ILE	15
1	A	64	SER	15

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Mol	Chain	Res	Type	Models (Total)
1	A	67	SER	15
1	A	18	GLN	15
1	A	71	GLU	15
1	A	70	ASP	13
1	A	75	VAL	13
1	A	66	ARG	13
2	B	5	LYS	13
1	A	14	SER	12
1	A	77	GLN	12
2	B	12	GLU	12
1	A	53	SER	11
1	A	56	LEU	11
1	A	55	LEU	9
1	A	35	MET	9
1	A	38	THR	9
2	B	7	SER	9
1	A	28	LEU	9
1	A	57	HIS	9
1	A	51	ASP	8
1	A	23	MET	8
2	B	18	TYR	7
1	A	19	GLU	7
1	A	58	MET	6
1	A	76	LEU	6
1	A	10	SER	6
1	A	60	GLU	3
2	B	14	TYR	3
2	B	6	LEU	2
1	A	8	THR	2
2	B	8	VAL	1
1	A	52	ASN	1
2	B	9	ASN	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