Full wwPDB NMR Structure Validation Report (i)

Feb 17, 2022 – 10:02 AM EST

PDB ID	:	1OV2
Title	:	Ensemble of the solution structures of domain one of receptor associated protein
Authors	:	Wu, Y.; Migliorini, M.; Yu, P.; Strickland, D.K.; Wang, Y.X.
Deposited on	:	2003-03-25

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:

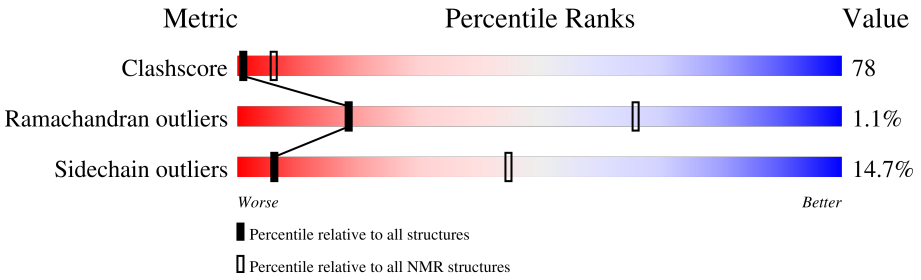
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	99	18% 49% 5% 10% 17%

2 Ensemble composition and analysis (i)

This entry contains 39 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average,minimized average structure*.

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:19-A:90 (72)	0.16	2

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1379 atoms, of which 700 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-2-macroglobulin receptor-associated protein precursor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	82	1379	428	700	126	124	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: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 18% 49% 5% 10% 17%

TYR SER ARG GLU LYS ASN GLN PRO LYS PRO SER PRO LYS ARG GLU SER G17 E18 E19 F20 R21 M22 E23 K24 L25 N26 W29 E30 K31 A32 Q33 R34 L35 H36 L37 P38 P39 V40 R41 L42 A43 E44 L45 H46 A47 K50 I51 Q52 E53 R54 D55 E56 L57 A58 W59 K60 K61 L62

K63 L64 L67 D68 E72 K73 E74 A75 R76 L77 I78 R79 N80 L81 N82 V83 I84 L85 Y88 G89 L90 D91 G92 K93 K94 D95 A96 R97 Q98 VAL

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: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 21% 45% 5% • 10% 17%

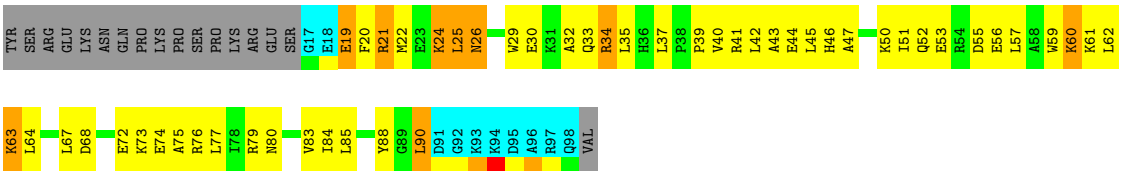
TYR SER ARG GLU LYS ASN GLN PRO LYS PRO SER PRO LYS ARG GLU SER G17 E18 E19 F20 R21 M22 E23 K24 L25 N26 W29 E30 K31 A32 Q33 R34 L35 H36 L37 P38 P39 V40 R41 L42 A43 E44 L45 H46 A47 K50 I51 Q52 E53 R54 D55 E56 L57 A58 W59 K60 K61 L62

K63 L64 L67 D68 E72 K73 E74 A75 R76 L77 I78 R79 N80 L81 N82 V83 I84 L85 Y88 G89 L90 D91 G92 K93 K94 D95 A96 R97 Q98 VAL

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

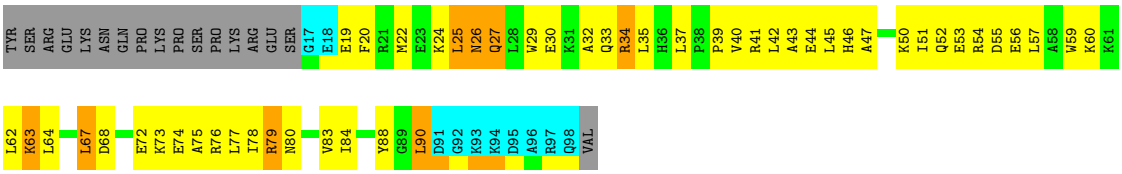
Chain A: 21% 42% 9% 10% 17%



4.2.3 Score per residue for model 3

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

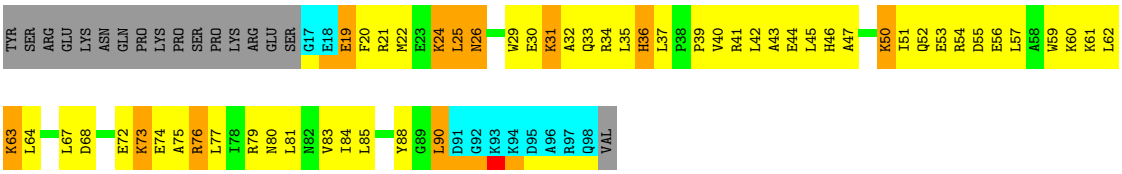
Chain A: 21% 43% 8% 10% 17%



4.2.4 Score per residue for model 4

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

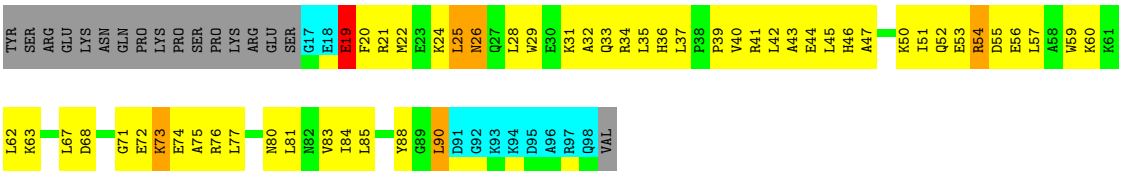
Chain A: 17% 44% 11% 10% 17%



4.2.5 Score per residue for model 5

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 19% 47% 5% • 10% 17%



4.2.6 Score per residue for model 6

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 18% 41% 13% 10% 17%

TYR SER ARG GLU LYS ASN GLN PRO LYS PRO SER PRO LYS ARG GLU SER G17 E18 E19 F20 R21 M22 E23 K24 L25 N26 W29 E30 K31 A32 Q33 R34 L35 H36 L37 P38 P39 V40 R41 L42 A43 E44 L45 H46 A47 K50 I51 Q52 E53 R54 D55 E56 L57 A58 W59 K60 K61 L62

K63 L64 L67 D68 E69 D70 G71 E72 K73 E74 A75 R76 L77 I78 R79 N80 V83 I84 L85 Y88 G89 L90 D91 G92 K93 K94 D95 A96 R97 Q98 VAL

4.2.7 Score per residue for model 7

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 18% 47% 7% 10% 17%

TYR SER ARG GLU LYS ASN GLN PRO LYS PRO SER PRO LYS ARG GLU SER G17 E18 E19 F20 R21 M22 E23 K24 L25 N26 W29 E30 K31 A32 Q33 R34 L35 H36 L37 P38 P39 V40 R41 L42 A43 E44 L45 H46 A47 K50 I51 Q52 E53 R54 D55 E56 L57 A58 W59 K60 K61 L62

K63 L64 L67 D68 E69 D70 G71 E72 K73 E74 A75 R76 L77 I78 R79 N80 V83 I84 L85 Y88 G89 L90 D91 G92 K93 K94 D95 A96 R97 Q98 VAL

4.2.8 Score per residue for model 8

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 17% 44% 10% • 10% 17%

TYR SER ARG GLU LYS ASN GLN PRO LYS PRO SER PRO LYS ARG GLU SER G17 E18 E19 F20 R21 M22 E23 K24 L25 N26 Q27 L28 W29 E30 K31 A32 Q33 R34 L35 H36 L37 P38 P39 V40 R41 L42 A43 E44 L45 H46 A47 K50 I51 Q52 E53 R54 D55 E56 L57 A58 W59 K60 K61

L62 K63 L67 D68 E69 D70 G71 E72 K73 E74 A75 R76 L77 I78 R79 N80 V83 I84 L85 A86 K87 Y88 G89 L90 D91 G92 K93 K94 D95 A96 R97 Q98 VAL

4.2.9 Score per residue for model 9

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 21% 43% 8% 10% 17%

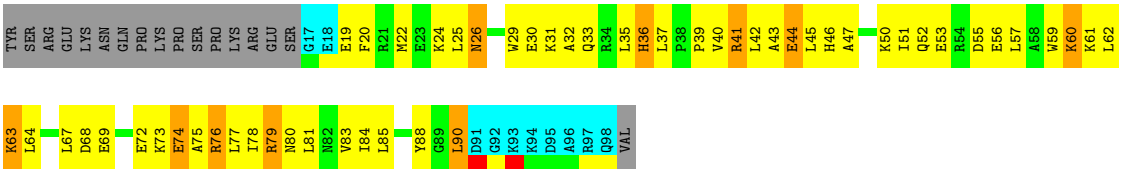
TYR SER ARG GLU LYS ASN GLN PRO LYS PRO SER PRO LYS ARG GLU SER G17 E18 E19 F20 R21 M22 E23 K24 L25 N26 W29 E30 K31 A32 Q33 R34 L35 H36 L37 P38 P39 V40 R41 L42 A43 E44 L45 H46 A47 K50 I51 Q52 E53 R54 D55 E56 L57 A58 W59 K60 K61 L62

K63 L64 L67 D68 E72 K73 E74 A75 R76 L77 N80 V83 I84 L85 Y88 G89 L90 D91 G92 K93 K94 D95 A96 R97 Q98 VAL

4.2.10 Score per residue for model 10

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

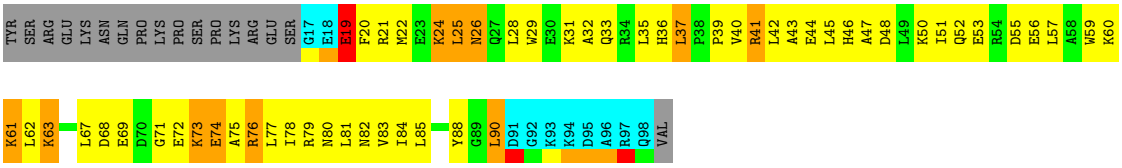
Chain A: 18% 44% 10% 10% 17%



4.2.11 Score per residue for model 11

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

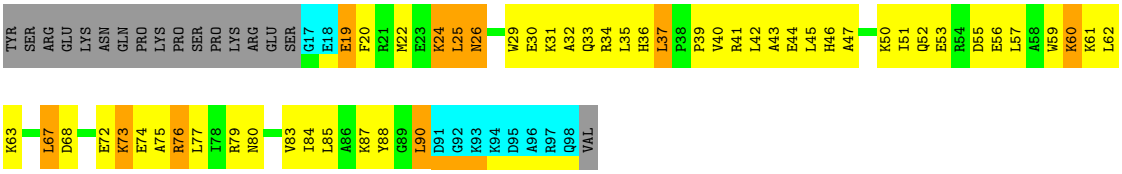
Chain A: 15% 45% 11% • 10% 17%



4.2.12 Score per residue for model 12

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

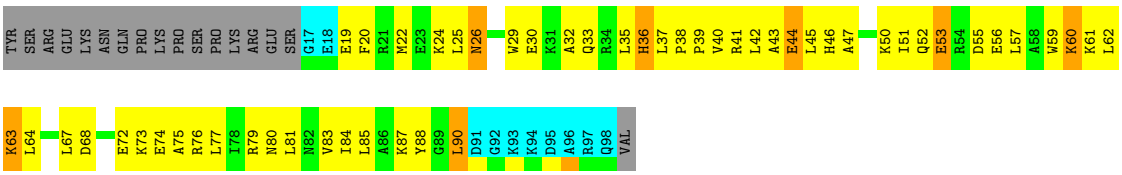
Chain A: 20% 42% 10% 10% 17%



4.2.13 Score per residue for model 13

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

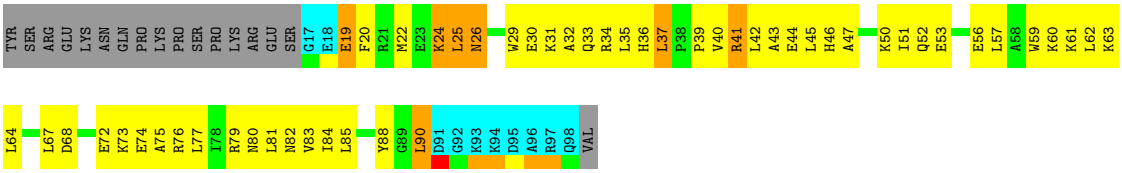
Chain A: 19% 46% 7% 10% 17%



4.2.14 Score per residue for model 14

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

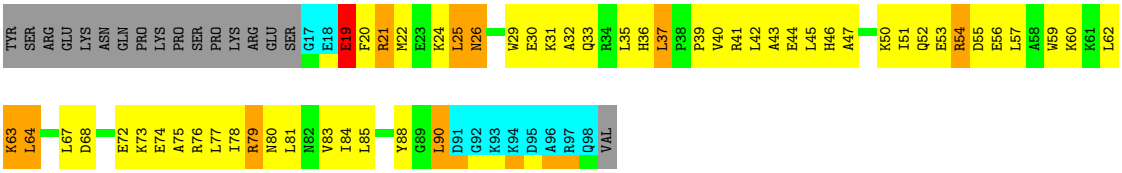
Chain A: 19% 46% 7% 10% 17%



4.2.15 Score per residue for model 15

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

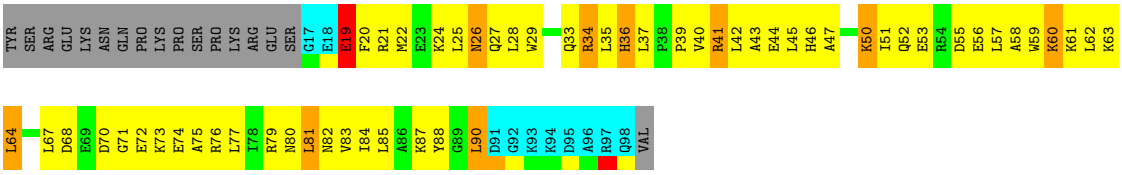
Chain A: 18% 44% 9% • 10% 17%



4.2.16 Score per residue for model 16

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

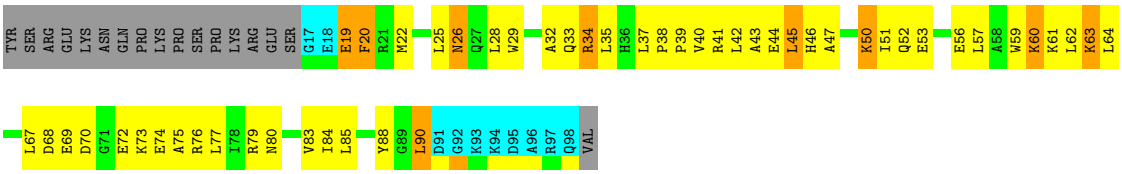
Chain A: 14% 48% 9% • 10% 17%



4.2.17 Score per residue for model 17

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

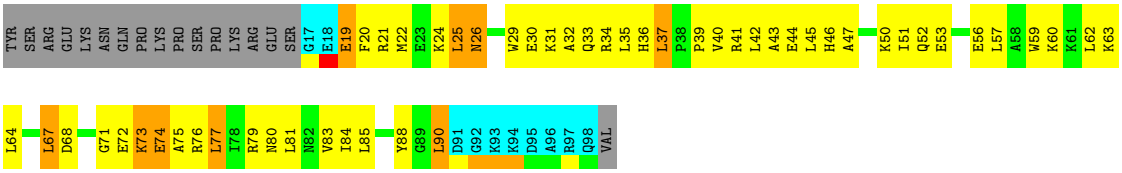
Chain A: 21% 42% 9% 10% 17%



4.2.18 Score per residue for model 18

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

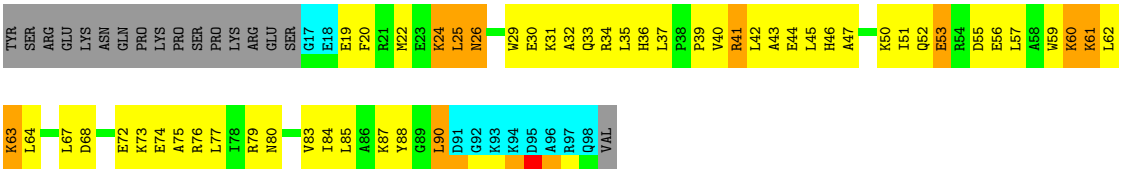
Chain A: 19% 44% 9% 10% 17%



4.2.19 Score per residue for model 19

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 19% 44% 9% 10% 17%



4.2.20 Score per residue for model 20

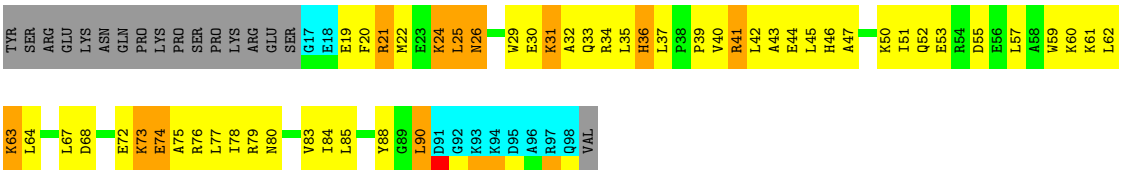
• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 17% 51% 5% 10% 17%

4.2.21 Score per residue for model 21

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

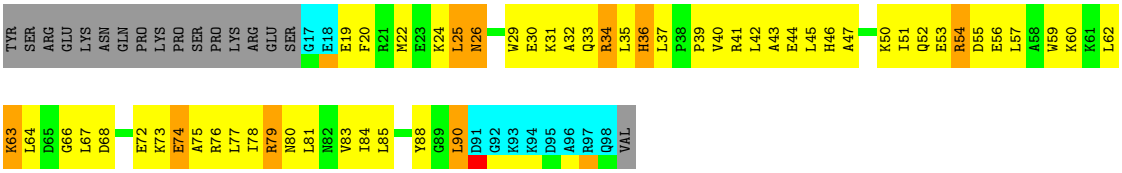
Chain A: 19% 42% 11% 10% 17%



4.2.22 Score per residue for model 22

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

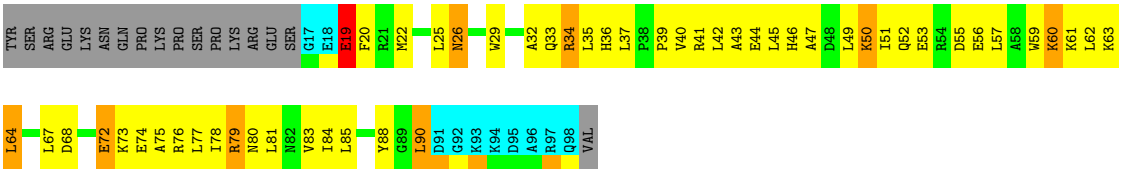
Chain A: 17% 46% 9% 10% 17%



4.2.23 Score per residue for model 23

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

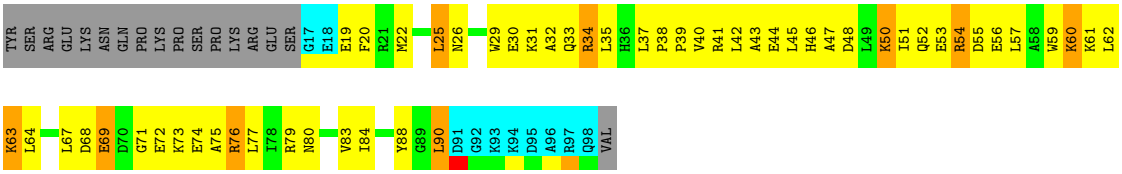
Chain A: 20% 43% 8% • 10% 17%



4.2.24 Score per residue for model 24

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

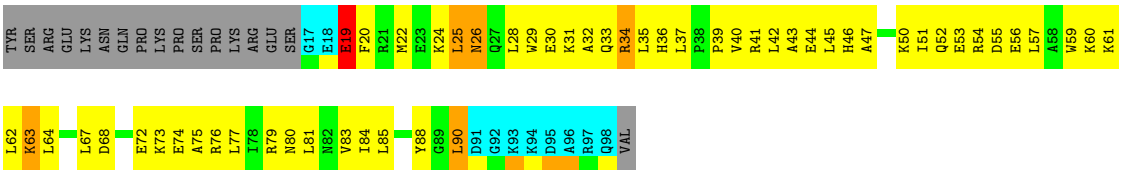
Chain A: 18% 45% 9% 10% 17%



4.2.25 Score per residue for model 25

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

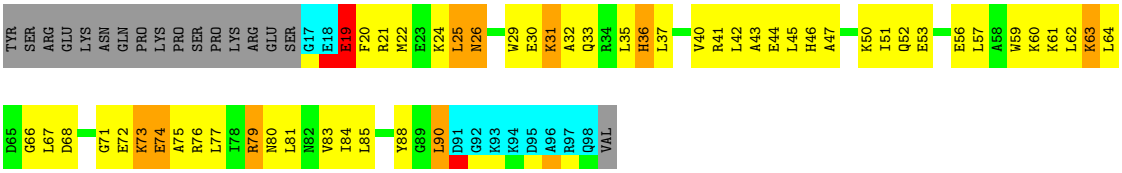
Chain A: 17% 49% 5% • 10% 17%



4.2.26 Score per residue for model 26

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

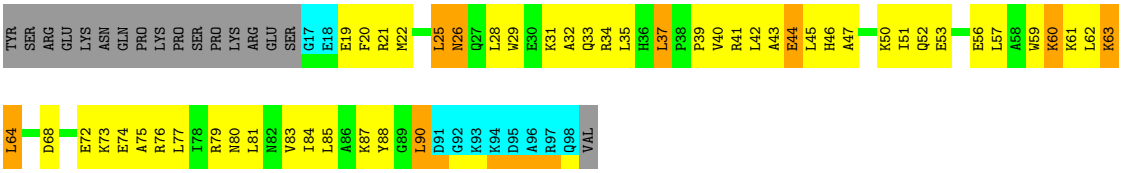
Chain A: 19% 43% 9% • 10% 17%



4.2.27 Score per residue for model 27

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 21% 43% 8% 10% 17%



4.2.28 Score per residue for model 28

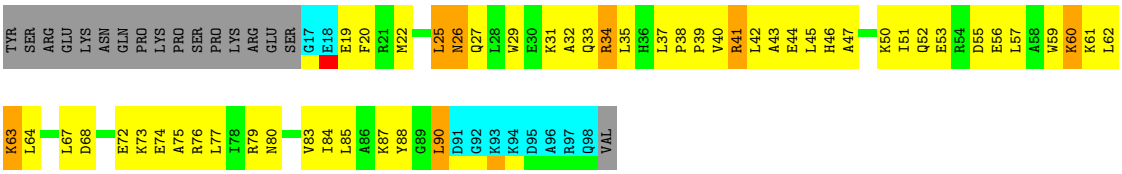
• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 22% 41% 9% 10% 17%

4.2.29 Score per residue for model 29

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 20% 45% 7% 10% 17%



4.2.30 Score per residue for model 30

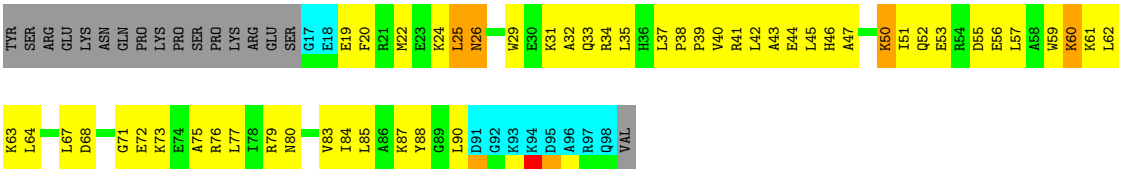
- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 15% 47% 10% 10% 17%

4.2.31 Score per residue for model 31

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

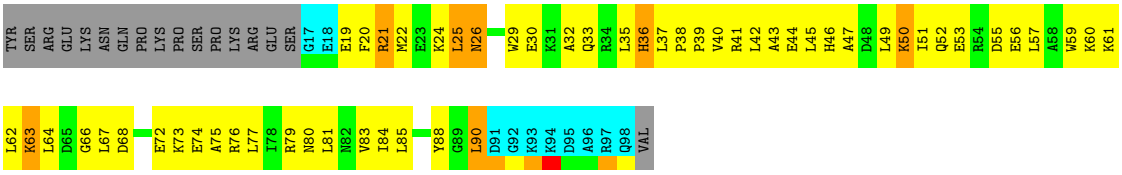
Chain A: 20% 48% • 10% 17%



4.2.32 Score per residue for model 32

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

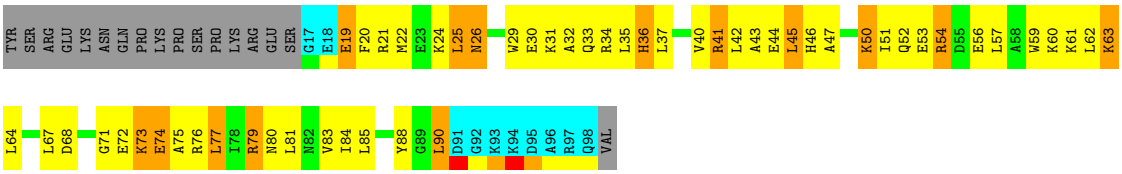
Chain A: 17% 48% 7% 10% 17%



4.2.33 Score per residue for model 33

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

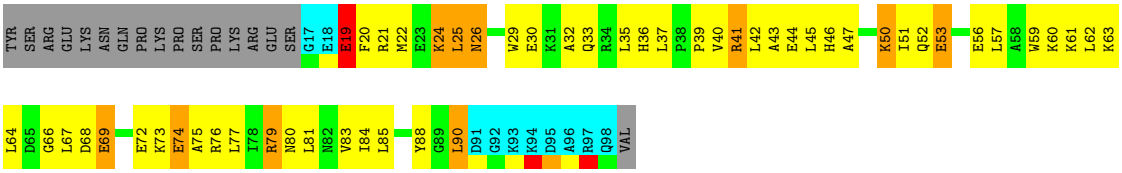
Chain A: 18% 40% 14% 10% 17%



4.2.34 Score per residue for model 34

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

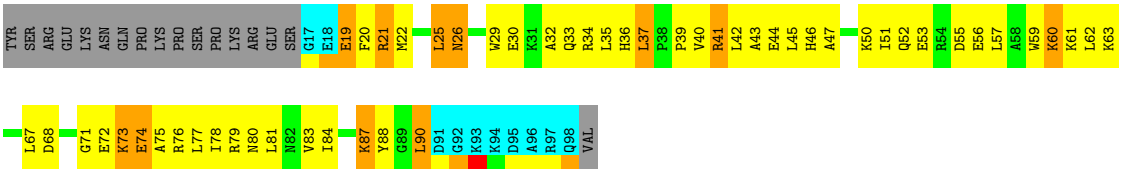
Chain A: 19% 42% 10% • 10% 17%



4.2.35 Score per residue for model 35

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

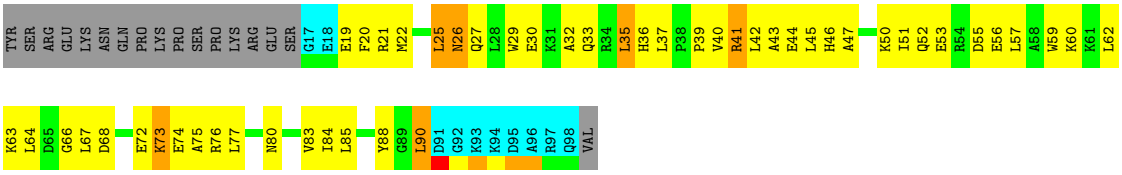
Chain A: 19% 42% 11% 10% 17%



4.2.36 Score per residue for model 36

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

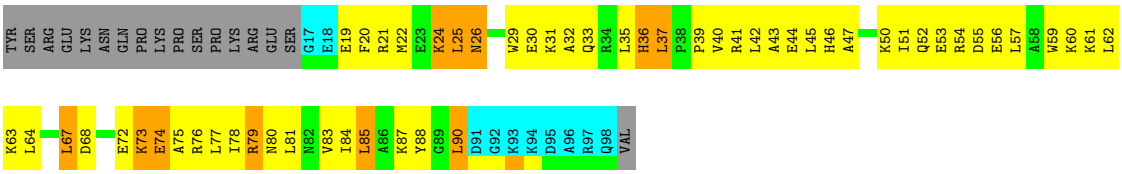
Chain A: 22% 44% 6% 10% 17%



4.2.37 Score per residue for model 37

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

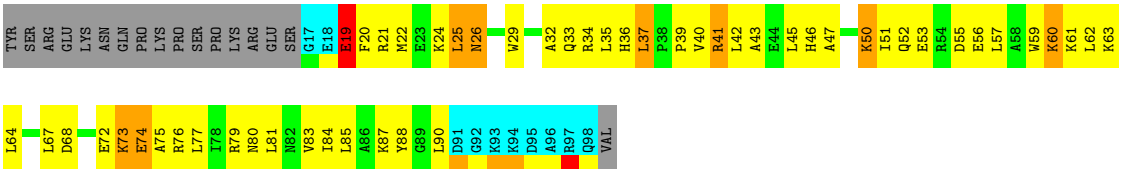
Chain A: 16% 45% 11% 10% 17%



4.2.38 Score per residue for model 38

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

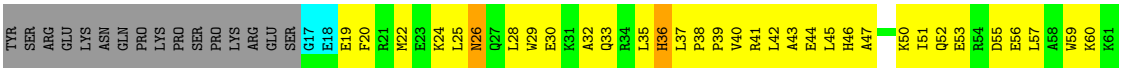
Chain A: 20% 43% 8% • 10% 17%

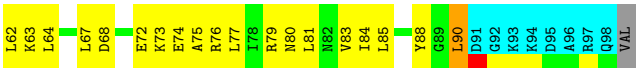


4.2.39 Score per residue for model 39

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein precursor

Chain A: 20% 49% • 10% 17%





5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsiona angle dynamics and simulated anealing*.

Of the 60 calculated structures, 39 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
xplor-nih	structure solution	1
interhlx	structure solution	1
interhlx	refinement	1

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	603	628	628	96±10
All	All	23517	24492	24492	3763

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 78.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:N	1:A:37:LEU:HD12	0.97	1.74	6	13
1:A:90:LEU:HD12	1:A:90:LEU:O	0.96	1.60	32	5
1:A:25:LEU:HD22	1:A:53:GLU:CD	0.96	1.80	13	1
1:A:52:GLN:HE21	1:A:77:LEU:HD23	0.95	1.22	24	24
1:A:79:ARG:O	1:A:83:VAL:HG23	0.93	1.63	35	35
1:A:37:LEU:HD12	1:A:37:LEU:H	0.93	1.24	18	29
1:A:20:PHE:CD2	1:A:25:LEU:HD22	0.91	2.01	17	3
1:A:37:LEU:HD12	1:A:37:LEU:N	0.90	1.81	7	9
1:A:20:PHE:CG	1:A:53:GLU:CD	0.90	2.45	13	1
1:A:29:TRP:CH2	1:A:46:HIS:CD2	0.90	2.59	16	38
1:A:25:LEU:HD13	1:A:53:GLU:OE2	0.87	1.68	13	1
1:A:56:GLU:OE2	1:A:81:LEU:HD11	0.86	1.70	34	11
1:A:68:ASP:OD2	1:A:72:GLU:N	0.85	2.09	5	34
1:A:52:GLN:NE2	1:A:77:LEU:HD23	0.85	1.87	15	26

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:GLU:N	1:A:19:GLU:OE1	0.85	2.09	32	28
1:A:19:GLU:OE1	1:A:20:PHE:CE2	0.85	2.30	22	5
1:A:85:LEU:HD12	1:A:90:LEU:O	0.84	1.72	1	5
1:A:35:LEU:HD11	1:A:90:LEU:HD21	0.83	1.45	25	6
1:A:20:PHE:CE2	1:A:25:LEU:HD22	0.83	2.09	17	3
1:A:72:GLU:O	1:A:75:ALA:N	0.82	2.13	9	39
1:A:19:GLU:H	1:A:19:GLU:CD	0.79	1.81	29	12
1:A:90:LEU:O	1:A:90:LEU:CD1	0.78	2.32	3	6
1:A:62:LEU:HD23	1:A:67:LEU:CB	0.77	2.08	10	37
1:A:33:GLN:O	1:A:36:HIS:CD2	0.77	2.38	16	29
1:A:68:ASP:OD2	1:A:73:LYS:N	0.77	2.17	9	23
1:A:90:LEU:O	1:A:90:LEU:CG	0.77	2.32	23	5
1:A:53:GLU:OE2	1:A:57:LEU:HD11	0.76	1.80	26	2
1:A:73:LYS:H	1:A:73:LYS:CD	0.76	1.93	31	3
1:A:19:GLU:OE1	1:A:29:TRP:CG	0.76	2.39	17	4
1:A:33:GLN:O	1:A:36:HIS:N	0.76	2.19	4	17
1:A:59:TRP:O	1:A:62:LEU:N	0.75	2.19	27	37
1:A:19:GLU:N	1:A:19:GLU:CD	0.75	2.40	38	18
1:A:40:VAL:CG1	1:A:41:ARG:N	0.75	2.50	4	39
1:A:50:LYS:O	1:A:53:GLU:N	0.75	2.20	15	39
1:A:22:MET:SD	1:A:24:LYS:NZ	0.75	2.59	25	2
1:A:35:LEU:HD13	1:A:90:LEU:HD21	0.75	1.58	29	2
1:A:79:ARG:HH11	1:A:79:ARG:CB	0.74	1.96	33	1
1:A:90:LEU:O	1:A:90:LEU:HD12	0.74	1.83	23	3
1:A:19:GLU:CD	1:A:29:TRP:CD1	0.74	2.60	21	5
1:A:42:LEU:O	1:A:46:HIS:CB	0.74	2.36	27	39
1:A:19:GLU:CD	1:A:19:GLU:N	0.74	2.41	24	12
1:A:53:GLU:OE2	1:A:57:LEU:HD12	0.74	1.83	28	10
1:A:56:GLU:OE2	1:A:81:LEU:HD21	0.73	1.81	4	2
1:A:37:LEU:N	1:A:37:LEU:CD1	0.73	2.50	6	12
1:A:59:TRP:CD2	1:A:74:GLU:OE1	0.73	2.41	17	1
1:A:19:GLU:OE2	1:A:29:TRP:CB	0.73	2.37	22	4
1:A:59:TRP:HA	1:A:62:LEU:HD12	0.73	1.59	34	37
1:A:21:ARG:CG	1:A:21:ARG:HH11	0.73	1.97	28	9
1:A:59:TRP:CE2	1:A:74:GLU:HB2	0.72	2.20	6	38
1:A:45:LEU:HD12	1:A:88:TYR:CD2	0.72	2.20	33	19
1:A:34:ARG:CG	1:A:34:ARG:HH11	0.72	1.98	7	11
1:A:41:ARG:CG	1:A:41:ARG:HH11	0.72	1.98	21	13
1:A:74:GLU:OE1	1:A:78:ILE:HD11	0.71	1.85	1	6
1:A:54:ARG:HH11	1:A:54:ARG:CG	0.71	1.98	30	8
1:A:19:GLU:CD	1:A:20:PHE:CE2	0.71	2.63	21	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:TRP:CE3	1:A:74:GLU:OE2	0.71	2.43	17	1
1:A:79:ARG:HH11	1:A:79:ARG:CG	0.71	1.98	22	8
1:A:20:PHE:CG	1:A:53:GLU:OE2	0.71	2.43	13	1
1:A:59:TRP:CZ3	1:A:74:GLU:OE2	0.71	2.44	17	1
1:A:45:LEU:N	1:A:88:TYR:OH	0.70	2.24	21	36
1:A:55:ASP:CB	1:A:77:LEU:HD21	0.70	2.16	23	31
1:A:68:ASP:OD2	1:A:71:GLY:C	0.70	2.29	16	8
1:A:22:MET:HB2	1:A:25:LEU:HD12	0.70	1.61	13	6
1:A:90:LEU:O	1:A:90:LEU:HG	0.70	1.85	23	4
1:A:20:PHE:CD2	1:A:53:GLU:OE1	0.70	2.45	16	3
1:A:19:GLU:OE1	1:A:20:PHE:CD2	0.70	2.45	11	2
1:A:19:GLU:CD	1:A:19:GLU:H	0.69	1.90	36	5
1:A:20:PHE:CG	1:A:53:GLU:OE1	0.69	2.46	16	3
1:A:76:ARG:CG	1:A:76:ARG:HH11	0.69	1.98	24	3
1:A:37:LEU:H	1:A:37:LEU:CD1	0.69	2.00	14	13
1:A:20:PHE:CD1	1:A:53:GLU:OE1	0.69	2.45	13	3
1:A:53:GLU:OE2	1:A:57:LEU:HD22	0.69	1.88	34	5
1:A:19:GLU:OE1	1:A:29:TRP:CD1	0.69	2.45	16	7
1:A:20:PHE:CD1	1:A:53:GLU:CD	0.69	2.65	13	2
1:A:76:ARG:CG	1:A:76:ARG:NH1	0.68	2.56	24	4
1:A:52:GLN:OE1	1:A:77:LEU:HD22	0.68	1.89	17	1
1:A:22:MET:O	1:A:26:ASN:OD1	0.68	2.12	33	39
1:A:21:ARG:NH1	1:A:53:GLU:OE2	0.68	2.27	15	4
1:A:21:ARG:CG	1:A:21:ARG:NH1	0.68	2.57	36	9
1:A:62:LEU:HD23	1:A:67:LEU:HB2	0.68	1.66	30	35
1:A:44:GLU:OE1	1:A:44:GLU:N	0.68	2.27	27	3
1:A:54:ARG:HH11	1:A:54:ARG:CB	0.68	2.02	33	2
1:A:27:GLN:N	1:A:27:GLN:OE1	0.67	2.28	3	1
1:A:76:ARG:O	1:A:80:ASN:ND2	0.67	2.27	18	8
1:A:90:LEU:HD12	1:A:90:LEU:C	0.67	2.10	39	5
1:A:54:ARG:CG	1:A:54:ARG:NH1	0.67	2.56	4	8
1:A:63:LYS:HZ2	1:A:64:LEU:N	0.67	1.88	30	3
1:A:41:ARG:CG	1:A:41:ARG:NH1	0.67	2.57	28	15
1:A:34:ARG:CG	1:A:34:ARG:NH1	0.67	2.56	22	12
1:A:43:ALA:O	1:A:47:ALA:CB	0.67	2.43	27	39
1:A:79:ARG:CG	1:A:79:ARG:NH1	0.67	2.56	3	7
1:A:25:LEU:CD1	1:A:53:GLU:OE2	0.67	2.42	13	1
1:A:24:LYS:CG	1:A:25:LEU:N	0.67	2.57	2	20
1:A:52:GLN:HE21	1:A:77:LEU:CD2	0.67	2.02	30	16
1:A:73:LYS:CD	1:A:73:LYS:N	0.67	2.57	31	1
1:A:29:TRP:CZ2	1:A:46:HIS:CD2	0.67	2.82	16	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:TRP:CE2	1:A:74:GLU:CD	0.67	2.68	17	1
1:A:19:GLU:CD	1:A:20:PHE:H	0.66	1.94	16	5
1:A:40:VAL:HG13	1:A:41:ARG:N	0.66	2.03	2	39
1:A:35:LEU:CD2	1:A:90:LEU:HD21	0.66	2.20	6	19
1:A:20:PHE:CB	1:A:53:GLU:OE2	0.66	2.43	13	1
1:A:19:GLU:CD	1:A:20:PHE:CD1	0.66	2.69	17	1
1:A:59:TRP:CD2	1:A:74:GLU:CD	0.66	2.68	17	1
1:A:41:ARG:HH11	1:A:41:ARG:HG3	0.66	1.50	6	2
1:A:34:ARG:HG3	1:A:34:ARG:HH11	0.66	1.50	16	2
1:A:79:ARG:HH12	1:A:83:VAL:HG21	0.65	1.51	34	4
1:A:60:LYS:O	1:A:64:LEU:HD23	0.65	1.91	16	6
1:A:79:ARG:HH11	1:A:79:ARG:HG3	0.65	1.51	8	1
1:A:20:PHE:CE1	1:A:53:GLU:OE1	0.65	2.50	13	3
1:A:72:GLU:CG	1:A:73:LYS:N	0.65	2.59	20	1
1:A:21:ARG:HH11	1:A:21:ARG:CB	0.65	2.04	35	1
1:A:76:ARG:CZ	1:A:79:ARG:HH21	0.65	2.05	11	1
1:A:19:GLU:HG3	1:A:20:PHE:H	0.65	1.51	17	5
1:A:21:ARG:HH11	1:A:21:ARG:HG3	0.65	1.51	37	1
1:A:26:ASN:OD1	1:A:26:ASN:N	0.64	2.30	33	37
1:A:35:LEU:HD11	1:A:90:LEU:CD2	0.64	2.22	25	3
1:A:24:LYS:NZ	1:A:56:GLU:CD	0.64	2.51	31	2
1:A:76:ARG:NH1	1:A:79:ARG:NH2	0.64	2.45	16	1
1:A:24:LYS:NZ	1:A:56:GLU:OE1	0.64	2.28	3	5
1:A:76:ARG:NH2	1:A:79:ARG:NH2	0.64	2.45	11	1
1:A:20:PHE:CD1	1:A:20:PHE:N	0.64	2.63	17	2
1:A:59:TRP:CG	1:A:74:GLU:OE1	0.64	2.49	17	1
1:A:44:GLU:OE2	1:A:88:TYR:CZ	0.64	2.50	14	4
1:A:79:ARG:CZ	1:A:79:ARG:CB	0.64	2.75	8	1
1:A:68:ASP:OD2	1:A:71:GLY:CA	0.64	2.46	33	8
1:A:19:GLU:OE1	1:A:20:PHE:CD1	0.64	2.50	16	1
1:A:24:LYS:HZ3	1:A:56:GLU:CD	0.64	1.96	31	1
1:A:80:ASN:O	1:A:84:ILE:HD12	0.64	1.93	33	32
1:A:79:ARG:NH1	1:A:83:VAL:HG21	0.63	2.07	34	4
1:A:76:ARG:HH11	1:A:76:ARG:HG3	0.63	1.52	8	2
1:A:79:ARG:HG3	1:A:79:ARG:HH11	0.63	1.52	37	2
1:A:55:ASP:HB3	1:A:77:LEU:HD21	0.63	1.69	35	29
1:A:76:ARG:CZ	1:A:76:ARG:CB	0.63	2.74	28	1
1:A:44:GLU:CG	1:A:88:TYR:OH	0.63	2.46	24	13
1:A:19:GLU:OE1	1:A:20:PHE:CE1	0.63	2.52	17	1
1:A:76:ARG:HH11	1:A:80:ASN:HD21	0.62	1.36	24	1
1:A:44:GLU:C	1:A:88:TYR:OH	0.62	2.38	39	33

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:GLU:CD	1:A:78:ILE:HD11	0.62	2.15	6	10
1:A:25:LEU:HD11	1:A:56:GLU:CD	0.62	2.15	11	2
1:A:35:LEU:HD22	1:A:90:LEU:HD11	0.62	1.69	8	13
1:A:35:LEU:HD22	1:A:90:LEU:HD21	0.62	1.70	5	9
1:A:19:GLU:CG	1:A:20:PHE:H	0.62	2.07	38	7
1:A:50:LYS:O	1:A:53:GLU:HB3	0.62	1.95	33	36
1:A:56:GLU:HG2	1:A:77:LEU:HD22	0.62	1.72	29	20
1:A:29:TRP:NE1	1:A:33:GLN:OE1	0.61	2.33	18	4
1:A:44:GLU:OE1	1:A:44:GLU:CA	0.61	2.48	27	3
1:A:35:LEU:HD21	1:A:90:LEU:HD21	0.61	1.72	35	10
1:A:50:LYS:CB	1:A:50:LYS:NZ	0.61	2.63	4	7
1:A:26:ASN:N	1:A:26:ASN:OD1	0.61	2.30	26	2
1:A:68:ASP:OD2	1:A:73:LYS:CD	0.61	2.49	36	1
1:A:76:ARG:HH11	1:A:76:ARG:CG	0.61	2.07	28	2
1:A:20:PHE:N	1:A:20:PHE:HD1	0.61	1.92	17	2
1:A:56:GLU:HG3	1:A:77:LEU:HD22	0.61	1.72	16	3
1:A:71:GLY:O	1:A:74:GLU:N	0.61	2.34	16	1
1:A:45:LEU:HD12	1:A:88:TYR:CE2	0.61	2.31	6	19
1:A:22:MET:CB	1:A:25:LEU:HD12	0.61	2.25	13	1
1:A:76:ARG:HH11	1:A:76:ARG:CB	0.60	2.08	12	2
1:A:34:ARG:HH11	1:A:34:ARG:CB	0.60	2.08	3	1
1:A:76:ARG:CG	1:A:77:LEU:N	0.60	2.64	13	1
1:A:73:LYS:N	1:A:73:LYS:HD2	0.60	2.10	31	1
1:A:19:GLU:HG2	1:A:20:PHE:CD2	0.60	2.31	29	19
1:A:25:LEU:HD22	1:A:53:GLU:OE2	0.60	1.96	13	1
1:A:20:PHE:CE2	1:A:53:GLU:OE1	0.60	2.55	16	2
1:A:45:LEU:HD12	1:A:88:TYR:CD1	0.60	2.32	16	4
1:A:34:ARG:NH1	1:A:34:ARG:CG	0.60	2.65	16	1
1:A:29:TRP:CD1	1:A:33:GLN:OE1	0.60	2.54	7	3
1:A:76:ARG:NH1	1:A:79:ARG:HH21	0.60	1.95	11	2
1:A:66:GLY:C	1:A:67:LEU:HD22	0.60	2.18	26	6
1:A:63:LYS:C	1:A:63:LYS:NZ	0.59	2.54	3	3
1:A:52:GLN:O	1:A:56:GLU:CG	0.59	2.50	34	9
1:A:32:ALA:O	1:A:37:LEU:CD1	0.59	2.49	8	15
1:A:21:ARG:N	1:A:21:ARG:CD	0.59	2.66	8	3
1:A:19:GLU:CD	1:A:20:PHE:CD2	0.59	2.76	21	5
1:A:29:TRP:CH2	1:A:46:HIS:CG	0.59	2.91	16	1
1:A:85:LEU:HD13	1:A:90:LEU:HG	0.59	1.73	32	1
1:A:19:GLU:CG	1:A:20:PHE:N	0.59	2.65	38	9
1:A:20:PHE:CZ	1:A:53:GLU:OE1	0.59	2.55	13	2
1:A:63:LYS:HZ2	1:A:63:LYS:C	0.59	2.00	30	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLU:OE2	1:A:57:LEU:CD1	0.59	2.51	15	15
1:A:34:ARG:HH11	1:A:34:ARG:CG	0.59	2.09	16	2
1:A:76:ARG:NH1	1:A:76:ARG:HG2	0.59	2.12	12	2
1:A:68:ASP:OD1	1:A:71:GLY:N	0.59	2.36	31	1
1:A:32:ALA:O	1:A:35:LEU:N	0.59	2.36	5	28
1:A:35:LEU:CD1	1:A:90:LEU:HD21	0.59	2.27	13	7
1:A:76:ARG:CD	1:A:80:ASN:ND2	0.58	2.66	12	1
1:A:22:MET:CB	1:A:24:LYS:NZ	0.58	2.66	16	2
1:A:31:LYS:O	1:A:35:LEU:HD12	0.58	1.98	33	5
1:A:34:ARG:NH1	1:A:34:ARG:HG2	0.58	2.13	3	1
1:A:63:LYS:NZ	1:A:64:LEU:CD2	0.58	2.67	27	2
1:A:25:LEU:HD22	1:A:53:GLU:OE1	0.58	1.98	13	1
1:A:52:GLN:O	1:A:56:GLU:OE1	0.58	2.21	18	5
1:A:76:ARG:O	1:A:80:ASN:OD1	0.58	2.22	24	11
1:A:32:ALA:HB1	1:A:37:LEU:HD13	0.58	1.76	24	14
1:A:40:VAL:O	1:A:44:GLU:OE2	0.58	2.22	10	3
1:A:69:GLU:OE2	1:A:70:ASP:OD1	0.58	2.22	7	1
1:A:52:GLN:HE22	1:A:80:ASN:HD22	0.57	1.41	24	2
1:A:41:ARG:HH11	1:A:41:ARG:CG	0.57	2.12	6	2
1:A:42:LEU:O	1:A:46:HIS:HB2	0.57	1.99	7	36
1:A:25:LEU:CB	1:A:53:GLU:OE2	0.57	2.52	13	1
1:A:45:LEU:HD12	1:A:88:TYR:CE1	0.57	2.34	8	7
1:A:40:VAL:CG1	1:A:41:ARG:H	0.57	2.13	2	35
1:A:44:GLU:OE2	1:A:88:TYR:OH	0.57	2.23	4	3
1:A:32:ALA:HB1	1:A:37:LEU:CD1	0.57	2.29	36	23
1:A:32:ALA:O	1:A:37:LEU:HD11	0.57	2.00	6	14
1:A:76:ARG:CD	1:A:76:ARG:C	0.57	2.73	12	1
1:A:73:LYS:O	1:A:77:LEU:HD13	0.57	1.99	18	7
1:A:31:LYS:CB	1:A:31:LYS:NZ	0.57	2.66	26	1
1:A:34:ARG:CA	1:A:34:ARG:HE	0.57	2.12	2	1
1:A:52:GLN:C	1:A:56:GLU:OE1	0.57	2.44	14	7
1:A:25:LEU:HD21	1:A:56:GLU:OE1	0.56	2.00	13	1
1:A:59:TRP:O	1:A:60:LYS:C	0.56	2.44	22	39
1:A:45:LEU:HD13	1:A:88:TYR:CD2	0.56	2.35	4	6
1:A:35:LEU:HD12	1:A:90:LEU:HD11	0.56	1.77	16	2
1:A:54:ARG:NH1	1:A:54:ARG:HG2	0.56	2.15	22	2
1:A:52:GLN:NE2	1:A:80:ASN:CB	0.56	2.69	33	5
1:A:52:GLN:NE2	1:A:77:LEU:CD2	0.56	2.66	38	2
1:A:53:GLU:CD	1:A:57:LEU:HD12	0.56	2.21	18	14
1:A:35:LEU:O	1:A:36:HIS:O	0.56	2.23	26	11
1:A:79:ARG:CB	1:A:79:ARG:NH1	0.56	2.69	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ALA:HB2	1:A:45:LEU:CD2	0.56	2.31	38	2
1:A:19:GLU:HG2	1:A:20:PHE:N	0.56	2.16	29	20
1:A:45:LEU:CD1	1:A:88:TYR:CD2	0.56	2.88	32	23
1:A:76:ARG:O	1:A:80:ASN:CG	0.56	2.45	38	24
1:A:77:LEU:O	1:A:81:LEU:HD23	0.56	2.01	32	6
1:A:53:GLU:OE2	1:A:57:LEU:CD2	0.55	2.54	14	7
1:A:69:GLU:OE1	1:A:69:GLU:O	0.55	2.24	20	2
1:A:21:ARG:NH1	1:A:21:ARG:HG2	0.55	2.14	35	1
1:A:44:GLU:CD	1:A:88:TYR:OH	0.55	2.45	17	5
1:A:60:LYS:HG3	1:A:61:LYS:N	0.55	2.16	2	11
1:A:73:LYS:H	1:A:73:LYS:HD3	0.55	1.62	31	1
1:A:52:GLN:OE1	1:A:52:GLN:O	0.55	2.25	17	1
1:A:50:LYS:O	1:A:51:ILE:C	0.55	2.45	37	39
1:A:61:LYS:CB	1:A:61:LYS:NZ	0.55	2.70	37	1
1:A:37:LEU:HD13	1:A:42:LEU:CD1	0.55	2.32	3	17
1:A:45:LEU:HA	1:A:88:TYR:CZ	0.54	2.37	37	12
1:A:57:LEU:O	1:A:60:LYS:HG2	0.54	2.02	1	30
1:A:85:LEU:HD13	1:A:90:LEU:CB	0.54	2.33	37	1
1:A:34:ARG:CZ	1:A:34:ARG:CB	0.54	2.85	16	1
1:A:22:MET:O	1:A:26:ASN:CG	0.54	2.46	13	10
1:A:67:LEU:N	1:A:67:LEU:CD2	0.54	2.70	32	3
1:A:69:GLU:OE1	1:A:69:GLU:C	0.54	2.46	7	3
1:A:62:LEU:HD13	1:A:73:LYS:HD3	0.54	1.79	27	7
1:A:22:MET:HB3	1:A:24:LYS:HZ2	0.54	1.63	16	1
1:A:90:LEU:C	1:A:90:LEU:CD1	0.54	2.75	39	2
1:A:58:ALA:O	1:A:62:LEU:HG	0.54	2.02	16	1
1:A:19:GLU:CD	1:A:29:TRP:CG	0.54	2.80	17	4
1:A:40:VAL:O	1:A:44:GLU:CD	0.54	2.46	27	1
1:A:45:LEU:CA	1:A:88:TYR:CZ	0.53	2.91	37	18
1:A:78:ILE:HA	1:A:81:LEU:HD12	0.53	1.78	37	3
1:A:19:GLU:OE2	1:A:20:PHE:N	0.53	2.36	23	2
1:A:59:TRP:CH2	1:A:63:LYS:HD2	0.53	2.39	27	39
1:A:79:ARG:NH1	1:A:79:ARG:HG2	0.53	2.19	33	1
1:A:42:LEU:O	1:A:46:HIS:HB3	0.53	2.02	29	34
1:A:79:ARG:HH11	1:A:79:ARG:CA	0.53	2.17	33	1
1:A:38:PRO:O	1:A:42:LEU:CB	0.53	2.56	24	1
1:A:19:GLU:HG2	1:A:20:PHE:H	0.53	1.64	27	27
1:A:59:TRP:CZ3	1:A:63:LYS:CD	0.53	2.92	19	34
1:A:74:GLU:OE2	1:A:78:ILE:HD11	0.53	2.04	21	4
1:A:76:ARG:CB	1:A:76:ARG:NH1	0.53	2.72	28	1
1:A:72:GLU:C	1:A:74:GLU:N	0.53	2.59	37	33

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:GLU:HG3	1:A:20:PHE:N	0.53	2.18	22	4
1:A:72:GLU:O	1:A:74:GLU:N	0.52	2.42	6	30
1:A:79:ARG:NH1	1:A:83:VAL:CG2	0.52	2.71	34	4
1:A:21:ARG:HH11	1:A:21:ARG:HG2	0.52	1.64	9	8
1:A:71:GLY:O	1:A:74:GLU:CB	0.52	2.57	16	1
1:A:19:GLU:OE2	1:A:20:PHE:CD2	0.52	2.62	21	2
1:A:34:ARG:NH1	1:A:34:ARG:HG3	0.52	2.19	30	10
1:A:46:HIS:CE1	1:A:50:LYS:HZ3	0.52	2.21	2	1
1:A:24:LYS:NZ	1:A:56:GLU:CG	0.52	2.73	31	1
1:A:21:ARG:HG3	1:A:21:ARG:NH1	0.52	2.19	37	1
1:A:41:ARG:NH1	1:A:41:ARG:HG3	0.52	2.20	10	13
1:A:85:LEU:HD12	1:A:90:LEU:C	0.52	2.25	29	8
1:A:19:GLU:OE2	1:A:29:TRP:HB2	0.52	2.05	22	2
1:A:79:ARG:HG3	1:A:79:ARG:NH1	0.52	2.20	37	2
1:A:44:GLU:CB	1:A:88:TYR:OH	0.52	2.58	34	7
1:A:62:LEU:HD23	1:A:67:LEU:HB3	0.52	1.79	10	12
1:A:22:MET:CE	1:A:60:LYS:NZ	0.52	2.73	19	1
1:A:63:LYS:HG3	1:A:64:LEU:N	0.52	2.20	13	12
1:A:54:ARG:NH1	1:A:54:ARG:HG3	0.52	2.19	15	6
1:A:21:ARG:NH1	1:A:21:ARG:HG3	0.52	2.20	36	8
1:A:77:LEU:O	1:A:80:ASN:N	0.51	2.43	16	17
1:A:25:LEU:CG	1:A:53:GLU:OE2	0.51	2.57	13	1
1:A:21:ARG:HH11	1:A:21:ARG:CG	0.51	2.18	37	1
1:A:35:LEU:CD1	1:A:90:LEU:HD22	0.51	2.36	23	1
1:A:20:PHE:CD2	1:A:25:LEU:HB3	0.51	2.40	28	30
1:A:29:TRP:CH2	1:A:42:LEU:HD21	0.51	2.40	24	11
1:A:57:LEU:HD23	1:A:60:LYS:HD2	0.51	1.81	18	5
1:A:37:LEU:HB2	1:A:42:LEU:HD13	0.51	1.81	24	1
1:A:76:ARG:NH1	1:A:80:ASN:HD21	0.51	2.01	24	1
1:A:35:LEU:HG	1:A:90:LEU:HD21	0.51	1.81	38	1
1:A:69:GLU:H	1:A:69:GLU:CD	0.51	2.08	8	2
1:A:45:LEU:CD1	1:A:88:TYR:CD1	0.51	2.94	8	6
1:A:76:ARG:NH1	1:A:76:ARG:HG3	0.51	2.20	24	1
1:A:79:ARG:NH1	1:A:79:ARG:HG3	0.51	2.20	23	5
1:A:79:ARG:NH1	1:A:79:ARG:CG	0.51	2.71	37	2
1:A:72:GLU:OE1	1:A:73:LYS:N	0.51	2.44	34	1
1:A:29:TRP:CE2	1:A:33:GLN:OE1	0.51	2.64	18	3
1:A:43:ALA:O	1:A:47:ALA:HB3	0.51	2.04	16	32
1:A:25:LEU:HD11	1:A:56:GLU:OE1	0.50	2.06	11	1
1:A:60:LYS:CG	1:A:61:LYS:N	0.50	2.74	33	15
1:A:46:HIS:CE1	1:A:50:LYS:NZ	0.50	2.79	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LYS:NZ	1:A:64:LEU:HD21	0.50	2.21	27	2
1:A:32:ALA:O	1:A:33:GLN:C	0.50	2.48	24	27
1:A:19:GLU:OE2	1:A:29:TRP:CG	0.50	2.64	22	1
1:A:33:GLN:C	1:A:36:HIS:H	0.50	2.08	4	11
1:A:57:LEU:HD23	1:A:60:LYS:HD3	0.50	1.83	30	2
1:A:22:MET:CE	1:A:60:LYS:HZ3	0.50	2.19	19	2
1:A:53:GLU:HG2	1:A:57:LEU:HD22	0.50	1.81	29	3
1:A:38:PRO:O	1:A:42:LEU:HB2	0.50	2.07	24	4
1:A:76:ARG:HG3	1:A:76:ARG:NH1	0.50	2.20	8	1
1:A:80:ASN:ND2	1:A:80:ASN:N	0.50	2.60	14	2
1:A:62:LEU:HD13	1:A:73:LYS:HD2	0.50	1.84	16	1
1:A:21:ARG:HE	1:A:57:LEU:HD13	0.50	1.66	26	1
1:A:85:LEU:CD2	1:A:85:LEU:N	0.50	2.74	10	8
1:A:26:ASN:O	1:A:29:TRP:N	0.50	2.44	16	1
1:A:45:LEU:O	1:A:49:LEU:HD13	0.50	2.07	23	1
1:A:51:ILE:N	1:A:51:ILE:HD12	0.49	2.22	27	18
1:A:54:ARG:HH11	1:A:54:ARG:HG2	0.49	1.67	25	6
1:A:76:ARG:NH1	1:A:76:ARG:CG	0.49	2.72	8	1
1:A:39:PRO:O	1:A:43:ALA:N	0.49	2.45	24	37
1:A:53:GLU:HG2	1:A:57:LEU:HD12	0.49	1.83	15	9
1:A:41:ARG:HH11	1:A:41:ARG:HG2	0.49	1.67	29	13
1:A:72:GLU:HG3	1:A:73:LYS:N	0.49	2.22	20	1
1:A:34:ARG:HH11	1:A:34:ARG:HG2	0.49	1.66	29	10
1:A:41:ARG:HG3	1:A:41:ARG:NH1	0.49	2.22	32	2
1:A:34:ARG:HG3	1:A:34:ARG:NH1	0.49	2.19	8	1
1:A:80:ASN:HD22	1:A:80:ASN:N	0.49	2.05	33	1
1:A:68:ASP:OD2	1:A:73:LYS:HG2	0.49	2.06	36	6
1:A:56:GLU:O	1:A:59:TRP:N	0.49	2.44	17	3
1:A:31:LYS:NZ	1:A:31:LYS:HB3	0.49	2.22	26	1
1:A:69:GLU:C	1:A:69:GLU:CD	0.49	2.71	7	1
1:A:69:GLU:CG	1:A:70:ASP:N	0.49	2.74	7	2
1:A:48:ASP:N	1:A:48:ASP:OD1	0.49	2.44	11	2
1:A:59:TRP:CZ3	1:A:63:LYS:HD3	0.48	2.43	39	27
1:A:20:PHE:CG	1:A:25:LEU:HB3	0.48	2.43	33	1
1:A:35:LEU:HD22	1:A:90:LEU:CD1	0.48	2.37	1	3
1:A:52:GLN:OE1	1:A:80:ASN:CB	0.48	2.61	21	19
1:A:67:LEU:HD22	1:A:67:LEU:N	0.48	2.23	26	4
1:A:21:ARG:NH1	1:A:21:ARG:CG	0.48	2.71	37	1
1:A:27:GLN:OE1	1:A:27:GLN:CA	0.48	2.61	3	1
1:A:52:GLN:HE22	1:A:80:ASN:CB	0.48	2.20	31	3
1:A:68:ASP:OD2	1:A:72:GLU:CG	0.48	2.61	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:ASP:OD2	1:A:71:GLY:N	0.48	2.46	33	1
1:A:60:LYS:O	1:A:63:LYS:HG2	0.48	2.08	14	7
1:A:76:ARG:HG2	1:A:77:LEU:N	0.48	2.23	13	1
1:A:21:ARG:CG	1:A:57:LEU:HD21	0.48	2.38	16	1
1:A:76:ARG:HH11	1:A:79:ARG:HH21	0.48	1.51	16	1
1:A:85:LEU:C	1:A:87:LYS:N	0.48	2.67	19	10
1:A:85:LEU:CD1	1:A:90:LEU:CB	0.48	2.91	36	2
1:A:72:GLU:O	1:A:73:LYS:C	0.48	2.50	12	37
1:A:53:GLU:CG	1:A:57:LEU:HD12	0.48	2.39	35	8
1:A:22:MET:CE	1:A:56:GLU:OE1	0.48	2.62	23	1
1:A:29:TRP:O	1:A:30:GLU:C	0.47	2.51	26	29
1:A:40:VAL:HG12	1:A:41:ARG:H	0.47	1.69	4	35
1:A:24:LYS:HG3	1:A:25:LEU:N	0.47	2.24	16	23
1:A:35:LEU:HD22	1:A:90:LEU:CG	0.47	2.39	18	2
1:A:85:LEU:O	1:A:87:LYS:N	0.47	2.47	30	3
1:A:68:ASP:CG	1:A:73:LYS:HG3	0.47	2.30	24	2
1:A:56:GLU:O	1:A:59:TRP:HB3	0.47	2.09	17	21
1:A:55:ASP:HB2	1:A:77:LEU:HD21	0.47	1.84	39	11
1:A:79:ARG:HH11	1:A:79:ARG:HG2	0.47	1.68	22	5
1:A:21:ARG:HB2	1:A:57:LEU:HD21	0.47	1.85	18	5
1:A:19:GLU:OE2	1:A:29:TRP:CD1	0.47	2.68	22	1
1:A:69:GLU:CD	1:A:70:ASP:OD2	0.47	2.53	6	1
1:A:85:LEU:HD13	1:A:90:LEU:HB2	0.47	1.87	36	2
1:A:83:VAL:O	1:A:84:ILE:C	0.47	2.53	11	28
1:A:31:LYS:O	1:A:35:LEU:CD1	0.47	2.63	4	6
1:A:63:LYS:CG	1:A:64:LEU:N	0.47	2.77	7	17
1:A:25:LEU:HD21	1:A:56:GLU:CD	0.47	2.30	13	1
1:A:60:LYS:HG2	1:A:61:LYS:N	0.47	2.25	14	9
1:A:80:ASN:O	1:A:84:ILE:CD1	0.47	2.62	33	5
1:A:70:ASP:C	1:A:72:GLU:N	0.47	2.67	16	1
1:A:76:ARG:NH1	1:A:76:ARG:HB2	0.47	2.23	28	1
1:A:35:LEU:N	1:A:35:LEU:HD12	0.47	2.24	27	1
1:A:73:LYS:CD	1:A:73:LYS:H	0.47	2.22	36	6
1:A:19:GLU:HB2	1:A:20:PHE:CE1	0.47	2.45	33	1
1:A:24:LYS:HG2	1:A:25:LEU:H	0.47	1.70	38	11
1:A:75:ALA:O	1:A:76:ARG:C	0.47	2.51	24	37
1:A:25:LEU:CD2	1:A:53:GLU:OE2	0.47	2.62	13	1
1:A:29:TRP:CH2	1:A:42:LEU:CD2	0.46	2.98	36	9
1:A:31:LYS:O	1:A:35:LEU:HD13	0.46	2.10	4	1
1:A:69:GLU:CD	1:A:70:ASP:N	0.46	2.69	7	1
1:A:84:ILE:O	1:A:87:LYS:CB	0.46	2.63	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ILE:N	1:A:51:ILE:CD1	0.46	2.79	24	6
1:A:90:LEU:HD23	1:A:90:LEU:O	0.46	2.11	13	1
1:A:56:GLU:OE2	1:A:81:LEU:CD1	0.46	2.64	39	2
1:A:19:GLU:HG3	1:A:29:TRP:CD1	0.46	2.46	27	16
1:A:59:TRP:NE1	1:A:74:GLU:HB2	0.46	2.26	17	8
1:A:22:MET:SD	1:A:24:LYS:CE	0.46	3.04	7	1
1:A:85:LEU:HD12	1:A:90:LEU:HB3	0.46	1.87	12	1
1:A:63:LYS:CE	1:A:64:LEU:CD2	0.46	2.92	15	1
1:A:24:LYS:HG2	1:A:25:LEU:N	0.46	2.26	2	6
1:A:57:LEU:O	1:A:60:LYS:HG3	0.46	2.11	9	7
1:A:79:ARG:NH1	1:A:79:ARG:HB2	0.46	2.25	8	1
1:A:76:ARG:HH11	1:A:79:ARG:NH2	0.46	2.06	16	1
1:A:74:GLU:OE1	1:A:74:GLU:HA	0.46	2.10	17	1
1:A:35:LEU:HD22	1:A:90:LEU:CD2	0.46	2.41	33	2
1:A:74:GLU:O	1:A:75:ALA:C	0.46	2.53	21	4
1:A:35:LEU:HD22	1:A:90:LEU:HD13	0.46	1.86	21	2
1:A:79:ARG:HH12	1:A:83:VAL:CG2	0.46	2.24	23	2
1:A:50:LYS:NZ	1:A:50:LYS:HB2	0.46	2.26	10	2
1:A:41:ARG:CB	1:A:41:ARG:CZ	0.46	2.94	6	1
1:A:21:ARG:HH11	1:A:21:ARG:HB2	0.46	1.70	35	1
1:A:62:LEU:HD22	1:A:73:LYS:HD3	0.46	1.88	30	2
1:A:69:GLU:OE1	1:A:70:ASP:OD1	0.45	2.33	20	2
1:A:52:GLN:NE2	1:A:80:ASN:HB2	0.45	2.26	33	11
1:A:44:GLU:N	1:A:44:GLU:CD	0.45	2.69	10	2
1:A:76:ARG:HH11	1:A:76:ARG:HB2	0.45	1.71	12	1
1:A:62:LEU:HD23	1:A:67:LEU:HD12	0.45	1.87	16	1
1:A:67:LEU:N	1:A:67:LEU:HD22	0.45	2.24	22	1
1:A:41:ARG:CZ	1:A:41:ARG:HB2	0.45	2.42	6	2
1:A:76:ARG:HH11	1:A:76:ARG:HB3	0.45	1.72	11	1
1:A:59:TRP:C	1:A:61:LYS:N	0.45	2.69	7	12
1:A:56:GLU:HA	1:A:77:LEU:HD13	0.45	1.89	16	8
1:A:75:ALA:O	1:A:79:ARG:HG3	0.45	2.10	33	2
1:A:45:LEU:HB2	1:A:88:TYR:CZ	0.45	2.47	17	13
1:A:59:TRP:HB2	1:A:77:LEU:CD1	0.45	2.42	13	14
1:A:59:TRP:O	1:A:61:LYS:N	0.45	2.50	17	5
1:A:29:TRP:NE1	1:A:33:GLN:NE2	0.45	2.65	12	1
1:A:45:LEU:CA	1:A:88:TYR:OH	0.45	2.64	15	6
1:A:35:LEU:CD2	1:A:90:LEU:HD13	0.45	2.42	3	1
1:A:73:LYS:H	1:A:73:LYS:HD2	0.45	1.71	36	3
1:A:43:ALA:O	1:A:47:ALA:HB2	0.45	2.11	29	7
1:A:52:GLN:CG	1:A:56:GLU:OE1	0.45	2.64	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LYS:CB	1:A:63:LYS:HZ3	0.45	2.25	3	1
1:A:68:ASP:OD2	1:A:73:LYS:HG3	0.45	2.12	29	3
1:A:76:ARG:HD3	1:A:80:ASN:ND2	0.45	2.26	12	1
1:A:53:GLU:HG2	1:A:57:LEU:HD13	0.45	1.89	14	1
1:A:24:LYS:HB3	1:A:24:LYS:HZ2	0.45	1.71	19	2
1:A:60:LYS:CD	1:A:64:LEU:HD12	0.45	2.41	38	1
1:A:76:ARG:CD	1:A:80:ASN:HD21	0.45	2.25	12	1
1:A:46:HIS:O	1:A:50:LYS:CG	0.44	2.66	11	2
1:A:76:ARG:HH11	1:A:76:ARG:HG2	0.44	1.68	24	1
1:A:61:LYS:O	1:A:62:LEU:C	0.44	2.53	13	11
1:A:29:TRP:CZ3	1:A:46:HIS:CD2	0.44	3.04	16	1
1:A:62:LEU:HD13	1:A:73:LYS:CD	0.44	2.42	16	1
1:A:79:ARG:CZ	1:A:79:ARG:HB2	0.44	2.42	37	2
1:A:59:TRP:CZ2	1:A:63:LYS:HB3	0.44	2.48	10	4
1:A:77:LEU:O	1:A:81:LEU:HD12	0.44	2.12	11	1
1:A:79:ARG:NH1	1:A:79:ARG:HA	0.44	2.26	33	1
1:A:50:LYS:O	1:A:53:GLU:CB	0.44	2.66	13	5
1:A:85:LEU:CD1	1:A:90:LEU:HB3	0.44	2.43	27	8
1:A:36:HIS:C	1:A:37:LEU:HD12	0.44	2.30	37	2
1:A:68:ASP:OD2	1:A:73:LYS:CG	0.44	2.66	36	1
1:A:85:LEU:N	1:A:85:LEU:CD2	0.44	2.81	32	14
1:A:20:PHE:CD2	1:A:53:GLU:CD	0.44	2.90	13	1
1:A:83:VAL:HG12	1:A:87:LYS:NZ	0.44	2.28	35	1
1:A:32:ALA:HB1	1:A:37:LEU:HD11	0.44	1.88	4	4
1:A:60:LYS:O	1:A:64:LEU:CD2	0.44	2.65	16	1
1:A:31:LYS:HB3	1:A:31:LYS:HZ2	0.44	1.73	26	1
1:A:35:LEU:O	1:A:36:HIS:C	0.44	2.56	26	2
1:A:80:ASN:N	1:A:80:ASN:HD22	0.44	2.08	14	1
1:A:77:LEU:O	1:A:81:LEU:CD1	0.44	2.66	4	2
1:A:79:ARG:O	1:A:83:VAL:CG2	0.44	2.57	24	3
1:A:69:GLU:OE2	1:A:70:ASP:OD2	0.44	2.36	6	1
1:A:24:LYS:O	1:A:28:LEU:HD12	0.44	2.13	8	1
1:A:59:TRP:CH2	1:A:74:GLU:OE2	0.44	2.70	17	1
1:A:24:LYS:HZ1	1:A:56:GLU:CD	0.43	2.12	3	1
1:A:28:LEU:CD2	1:A:85:LEU:HD11	0.43	2.43	5	1
1:A:84:ILE:O	1:A:87:LYS:HB3	0.43	2.12	16	1
1:A:52:GLN:O	1:A:56:GLU:HG2	0.43	2.13	26	2
1:A:80:ASN:N	1:A:80:ASN:ND2	0.43	2.66	33	2
1:A:53:GLU:O	1:A:54:ARG:C	0.43	2.56	33	1
1:A:21:ARG:N	1:A:21:ARG:HD3	0.43	2.28	2	3
1:A:22:MET:HB3	1:A:24:LYS:NZ	0.43	2.27	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:GLU:CG	1:A:77:LEU:HD22	0.43	2.42	24	1
1:A:44:GLU:O	1:A:48:ASP:CG	0.43	2.57	24	2
1:A:37:LEU:HD13	1:A:42:LEU:HD12	0.43	1.90	26	6
1:A:25:LEU:O	1:A:26:ASN:C	0.43	2.54	20	5
1:A:72:GLU:O	1:A:75:ALA:HB3	0.43	2.13	29	5
1:A:79:ARG:CZ	1:A:79:ARG:HB3	0.43	2.43	8	1
1:A:52:GLN:HE21	1:A:80:ASN:HB3	0.43	1.73	34	2
1:A:22:MET:HB3	1:A:24:LYS:HZ3	0.43	1.72	9	1
1:A:53:GLU:CG	1:A:57:LEU:HD22	0.43	2.43	23	2
1:A:35:LEU:CG	1:A:90:LEU:HD21	0.43	2.44	38	1
1:A:22:MET:CB	1:A:24:LYS:HZ3	0.43	2.26	9	1
1:A:76:ARG:HH22	1:A:79:ARG:NH2	0.43	2.10	11	1
1:A:76:ARG:HG3	1:A:77:LEU:N	0.43	2.28	12	1
1:A:20:PHE:HB3	1:A:53:GLU:OE2	0.43	2.12	13	1
1:A:52:GLN:O	1:A:56:GLU:HG3	0.43	2.13	18	1
1:A:25:LEU:CD2	1:A:53:GLU:CD	0.43	2.72	13	1
1:A:22:MET:SD	1:A:24:LYS:HE2	0.43	2.54	7	1
1:A:44:GLU:CD	1:A:88:TYR:CE1	0.43	2.92	31	2
1:A:44:GLU:O	1:A:48:ASP:OD1	0.43	2.36	24	1
1:A:37:LEU:HB2	1:A:42:LEU:CD1	0.42	2.44	24	8
1:A:20:PHE:CD1	1:A:53:GLU:HG3	0.42	2.49	4	7
1:A:19:GLU:CD	1:A:20:PHE:N	0.42	2.69	16	1
1:A:31:LYS:CB	1:A:31:LYS:HZ2	0.42	2.26	26	1
1:A:62:LEU:CD2	1:A:67:LEU:CB	0.42	2.96	3	8
1:A:22:MET:CG	1:A:24:LYS:NZ	0.42	2.82	25	2
1:A:24:LYS:CD	1:A:56:GLU:OE2	0.42	2.67	22	1
1:A:24:LYS:CE	1:A:56:GLU:CD	0.42	2.88	25	1
1:A:52:GLN:HE21	1:A:80:ASN:CB	0.42	2.26	33	1
1:A:19:GLU:OE2	1:A:29:TRP:HB3	0.42	2.14	35	1
1:A:59:TRP:CD2	1:A:74:GLU:HG3	0.42	2.50	6	3
1:A:69:GLU:CD	1:A:70:ASP:OD1	0.42	2.57	20	1
1:A:72:GLU:HG2	1:A:73:LYS:H	0.42	1.74	20	1
1:A:76:ARG:NH2	1:A:79:ARG:HH21	0.42	2.08	11	1
1:A:54:ARG:HH11	1:A:54:ARG:HB3	0.42	1.72	33	2
1:A:69:GLU:CD	1:A:69:GLU:H	0.42	2.17	11	1
1:A:52:GLN:OE1	1:A:77:LEU:CD2	0.42	2.65	17	1
1:A:60:LYS:C	1:A:60:LYS:CD	0.42	2.88	38	1
1:A:41:ARG:NH1	1:A:88:TYR:CD1	0.42	2.87	36	1
1:A:50:LYS:CB	1:A:50:LYS:HZ3	0.42	2.28	4	1
1:A:31:LYS:HA	1:A:34:ARG:NH2	0.42	2.30	8	1
1:A:25:LEU:HB3	1:A:53:GLU:OE2	0.42	2.15	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:HD23	1:A:85:LEU:HD21	0.42	1.90	16	1
1:A:34:ARG:NH1	1:A:34:ARG:HB2	0.42	2.30	16	1
1:A:63:LYS:HZ3	1:A:63:LYS:HB2	0.42	1.74	3	1
1:A:69:GLU:CD	1:A:70:ASP:CG	0.42	2.79	6	1
1:A:29:TRP:CZ3	1:A:46:HIS:HB2	0.42	2.50	7	2
1:A:19:GLU:OE2	1:A:26:ASN:OD1	0.42	2.38	8	1
1:A:45:LEU:HB2	1:A:88:TYR:CE1	0.42	2.50	36	4
1:A:85:LEU:CD1	1:A:90:LEU:HG	0.42	2.45	10	2
1:A:59:TRP:HB2	1:A:77:LEU:CD2	0.42	2.44	28	2
1:A:59:TRP:CD2	1:A:74:GLU:OE2	0.42	2.69	17	1
1:A:45:LEU:HD13	1:A:88:TYR:CD1	0.42	2.50	23	1
1:A:49:LEU:HD23	1:A:49:LEU:HA	0.42	1.76	32	1
1:A:76:ARG:HB3	1:A:76:ARG:CZ	0.42	2.44	8	1
1:A:83:VAL:O	1:A:87:LYS:N	0.42	2.52	16	1
1:A:20:PHE:CE2	1:A:53:GLU:HB2	0.42	2.49	17	1
1:A:51:ILE:CD1	1:A:51:ILE:H	0.42	2.28	24	2
1:A:81:LEU:HA	1:A:84:ILE:HD12	0.42	1.92	27	2
1:A:52:GLN:NE2	1:A:80:ASN:HB3	0.42	2.29	34	1
1:A:81:LEU:HD13	1:A:81:LEU:HA	0.41	1.76	5	1
1:A:22:MET:HG3	1:A:24:LYS:HZ1	0.41	1.75	16	1
1:A:35:LEU:N	1:A:35:LEU:HD23	0.41	2.28	23	1
1:A:56:GLU:OE2	1:A:81:LEU:CD2	0.41	2.67	32	1
1:A:35:LEU:HD21	1:A:90:LEU:HD13	0.41	1.90	3	1
1:A:22:MET:HG3	1:A:24:LYS:NZ	0.41	2.31	16	1
1:A:77:LEU:O	1:A:81:LEU:CD2	0.41	2.69	32	1
1:A:34:ARG:HH11	1:A:34:ARG:HB3	0.41	1.72	3	1
1:A:52:GLN:OE1	1:A:84:ILE:CD1	0.41	2.68	5	1
1:A:68:ASP:OD1	1:A:72:GLU:CG	0.41	2.68	28	1
1:A:57:LEU:N	1:A:57:LEU:CD1	0.41	2.83	33	5
1:A:34:ARG:CZ	1:A:34:ARG:HB2	0.41	2.46	8	2
1:A:35:LEU:HD12	1:A:90:LEU:HD21	0.41	1.92	37	1
1:A:50:LYS:NZ	1:A:50:LYS:HB3	0.41	2.31	17	1
1:A:31:LYS:O	1:A:34:ARG:CB	0.41	2.68	24	1
1:A:34:ARG:CA	1:A:34:ARG:NE	0.41	2.82	2	1
1:A:28:LEU:N	1:A:28:LEU:CD1	0.41	2.82	11	1
1:A:32:ALA:CB	1:A:45:LEU:CD2	0.41	2.99	38	1
1:A:80:ASN:OD1	1:A:80:ASN:N	0.41	2.54	19	1
1:A:24:LYS:HZ3	1:A:56:GLU:CG	0.41	2.28	31	1
1:A:57:LEU:CD1	1:A:57:LEU:N	0.41	2.83	34	1
1:A:46:HIS:CE1	1:A:50:LYS:HD2	0.41	2.51	10	1
1:A:45:LEU:HD13	1:A:88:TYR:CG	0.41	2.50	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:ARG:HD3	1:A:77:LEU:N	0.41	2.30	10	1
1:A:21:ARG:CZ	1:A:21:ARG:HB3	0.40	2.45	37	1
1:A:19:GLU:OE2	1:A:26:ASN:CG	0.40	2.60	8	1
1:A:39:PRO:O	1:A:42:LEU:N	0.40	2.54	10	1
1:A:38:PRO:O	1:A:42:LEU:N	0.40	2.53	39	3
1:A:69:GLU:C	1:A:71:GLY:N	0.40	2.73	24	1
1:A:22:MET:CE	1:A:24:LYS:NZ	0.40	2.84	28	1
1:A:60:LYS:NZ	1:A:61:LYS:HE2	0.40	2.31	33	1
1:A:52:GLN:NE2	1:A:80:ASN:HD22	0.40	2.14	16	1
1:A:76:ARG:HD3	1:A:80:ASN:HD21	0.40	1.77	12	1
1:A:70:ASP:O	1:A:72:GLU:N	0.40	2.55	16	1
1:A:45:LEU:O	1:A:46:HIS:C	0.40	2.59	17	1
1:A:52:GLN:OE1	1:A:52:GLN:CA	0.40	2.70	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	72/99 (73%)	61±2 (84±3%)	10±2 (14±3%)	1±1 (1±1%)	18	66
All	All	2808/3861 (73%)	2372 (84%)	406 (14%)	30 (1%)	18	66

All 2 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	19	GLU	18
1	A	36	HIS	12

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	63/87 (72%)	54±2 (85±4%)	9±2 (15±4%)	6 45
All	All	2457/3393 (72%)	2097 (85%)	360 (15%)	6 45

All 35 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	90	LEU	37
1	A	26	ASN	36
1	A	25	LEU	34
1	A	34	ARG	26
1	A	63	LYS	23
1	A	31	LYS	18
1	A	60	LYS	17
1	A	37	LEU	15
1	A	73	LYS	14
1	A	41	ARG	14
1	A	19	GLU	13
1	A	74	GLU	13
1	A	79	ARG	11
1	A	50	LYS	11
1	A	24	LYS	10
1	A	21	ARG	9
1	A	54	ARG	8
1	A	67	LEU	6
1	A	76	ARG	6
1	A	64	LEU	5
1	A	53	GLU	4
1	A	27	GLN	4
1	A	69	GLU	4
1	A	61	LYS	4
1	A	44	GLU	3
1	A	72	GLU	2
1	A	87	LYS	2
1	A	82	ASN	2
1	A	45	LEU	2
1	A	77	LEU	2
1	A	81	LEU	1
1	A	20	PHE	1
1	A	28	LEU	1
1	A	35	LEU	1
1	A	85	LEU	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