



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:28 PM BST

PDB ID : 1QJT
Title : SOLUTION STRUCTURE OF THE APO EH1 DOMAIN OF MOUSE EPI-
DERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15, EPS15
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Deposited on : 1999-07-02

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

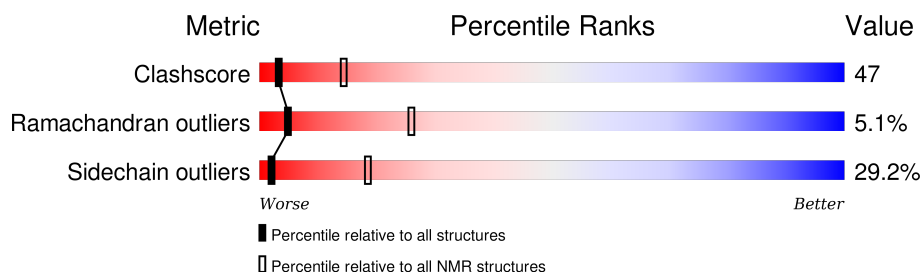
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	99	<div> <div></div> <div>28%</div> <div>56%</div> <div>14%</div> <div>.</div> </div>

2 Ensemble composition and analysis

This entry contains 30 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:9-A:105 (97)	0.38	2

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 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1509 atoms, of which 757 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15.

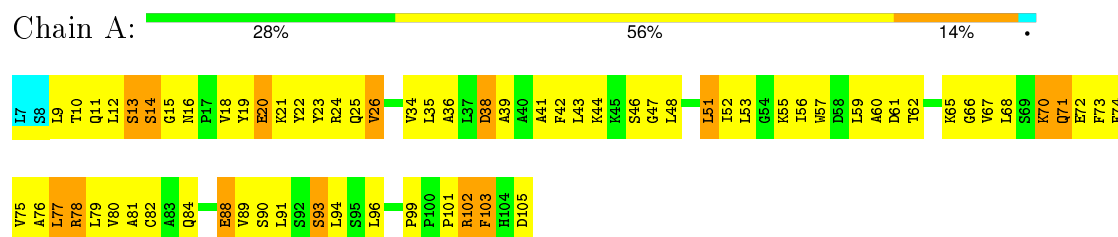
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	99	1509	483	757	127	141	1	0

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

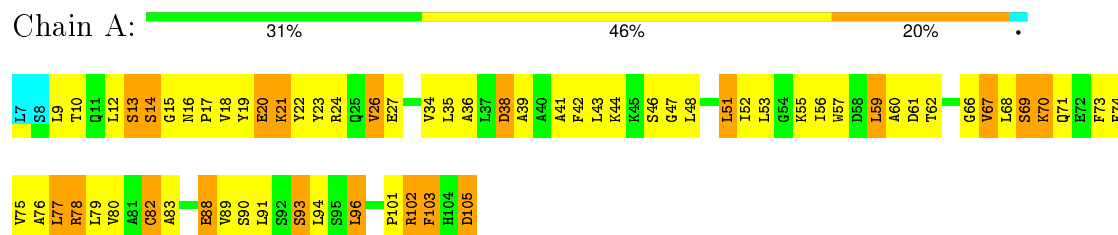


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

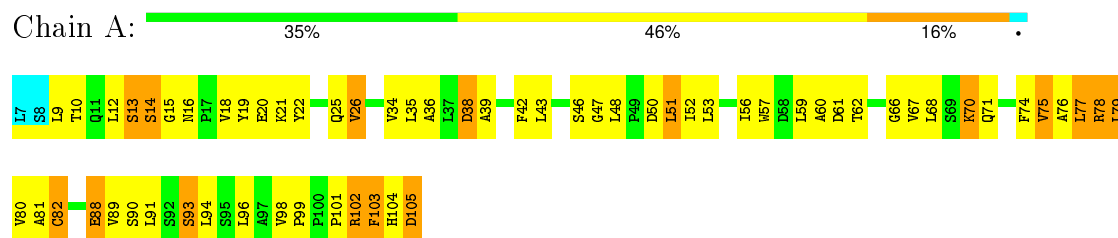
4.2.1 Score per residue for model 1

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



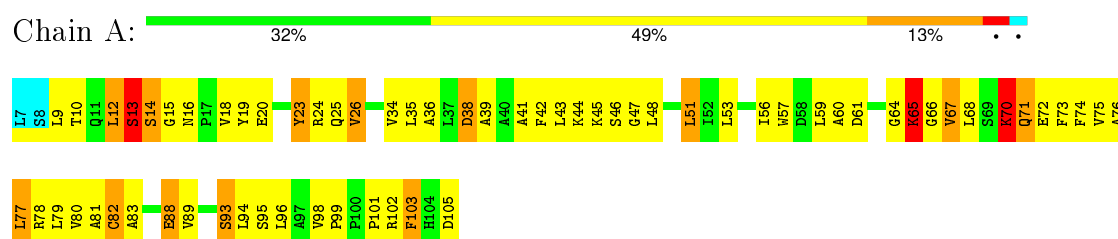
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



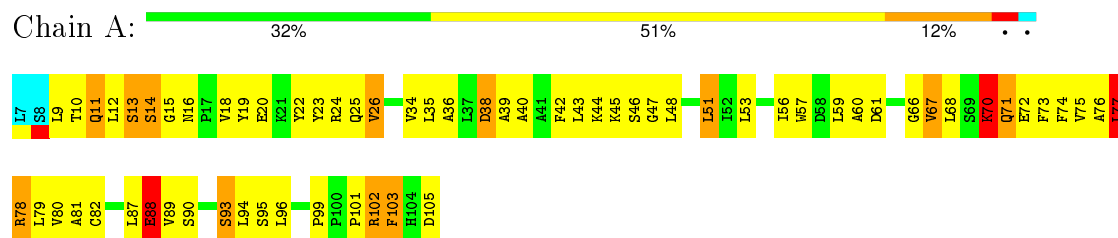
4.2.3 Score per residue for model 3

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



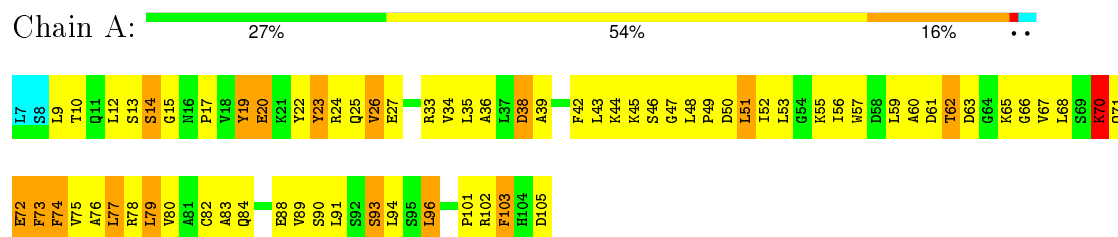
4.2.4 Score per residue for model 4

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



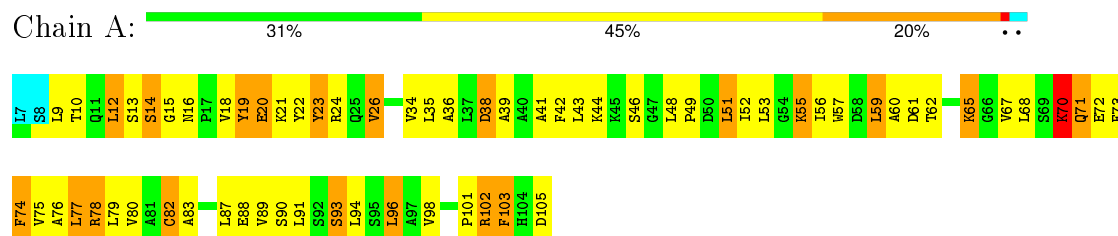
4.2.5 Score per residue for model 5

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



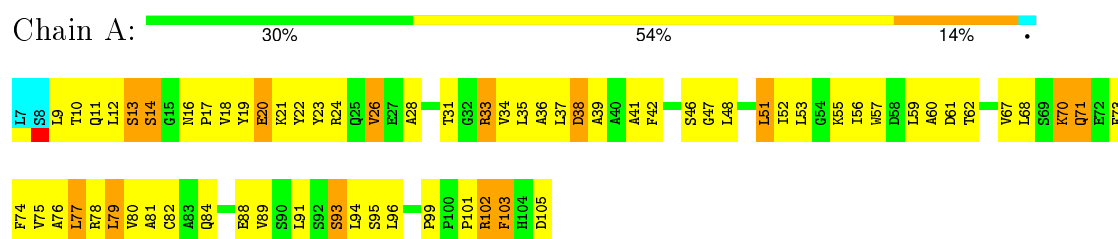
4.2.6 Score per residue for model 6

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



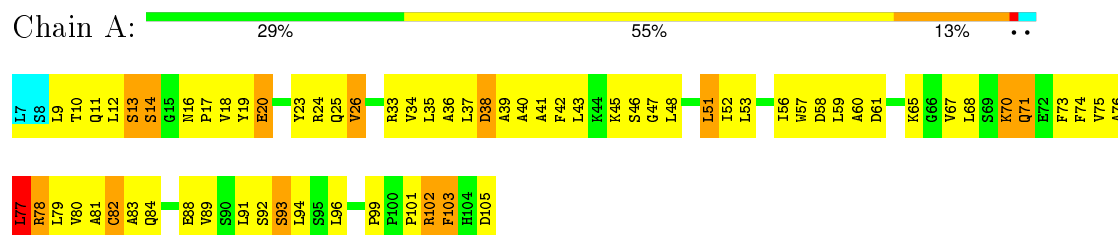
4.2.7 Score per residue for model 7

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



4.2.8 Score per residue for model 8

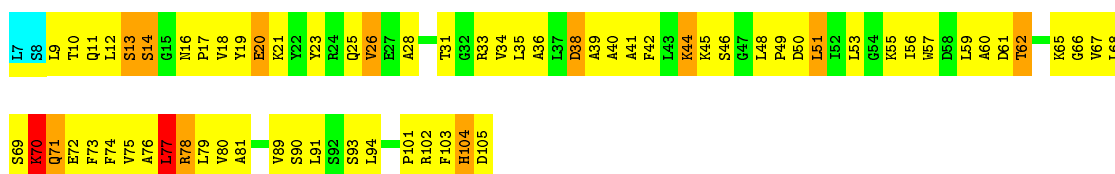
- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



4.2.9 Score per residue for model 9

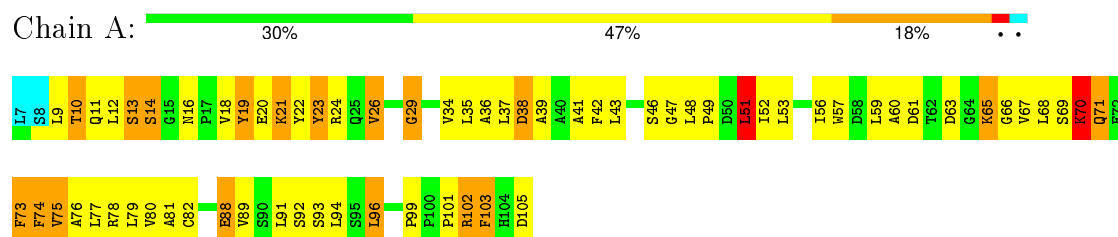
- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15





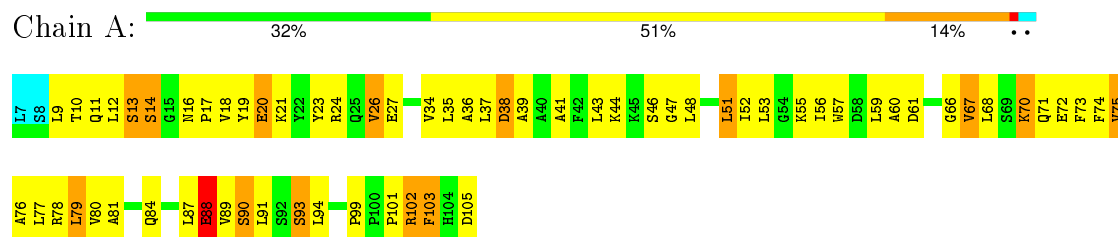
4.2.10 Score per residue for model 10

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



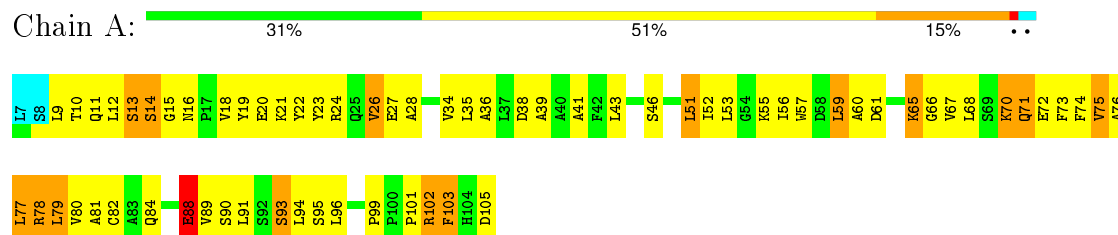
4.2.11 Score per residue for model 11

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



4.2.12 Score per residue for model 12

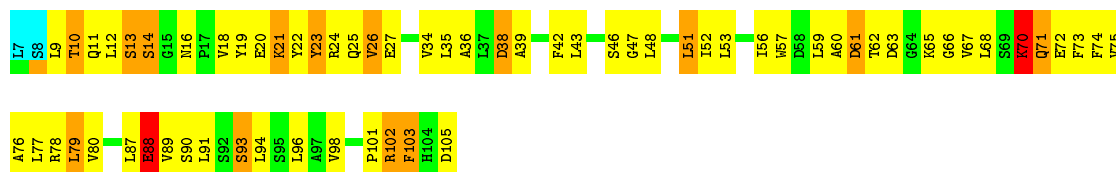
- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



4.2.13 Score per residue for model 13

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

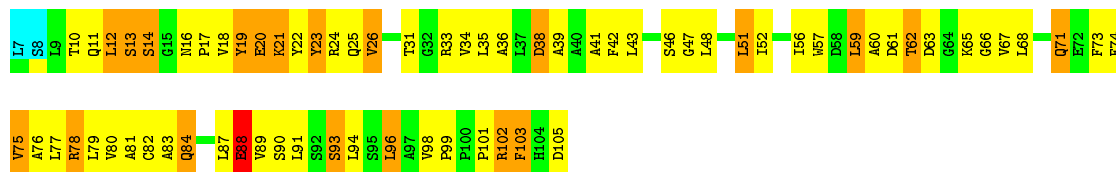
Chain A:  32% 49% 14% ..



4.2.14 Score per residue for model 14

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

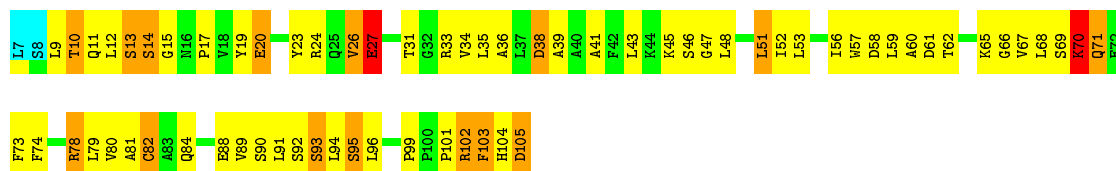
Chain A:  28% 48% 20% ..



4.2.15 Score per residue for model 15


- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

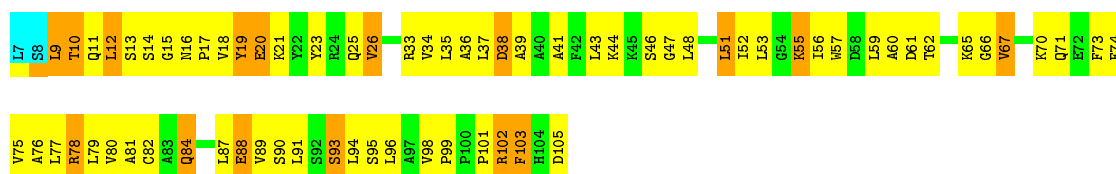
Chain A:  30% 51% 15% ..



4.2.16 Score per residue for model 16

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

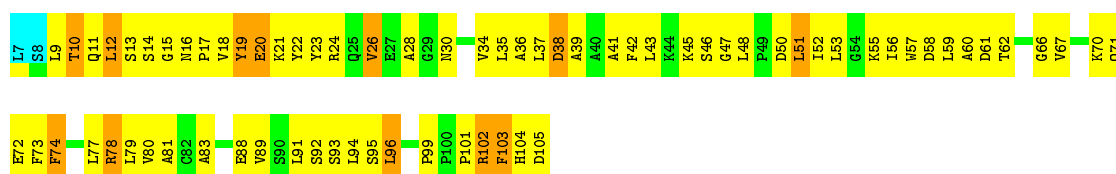
Chain A:  27% 55% 16% .



4.2.17 Score per residue for model 17

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

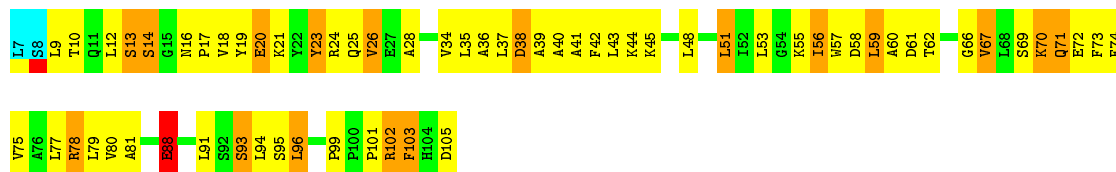
Chain A: 26% 60% 12% .



4.2.18 Score per residue for model 18

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

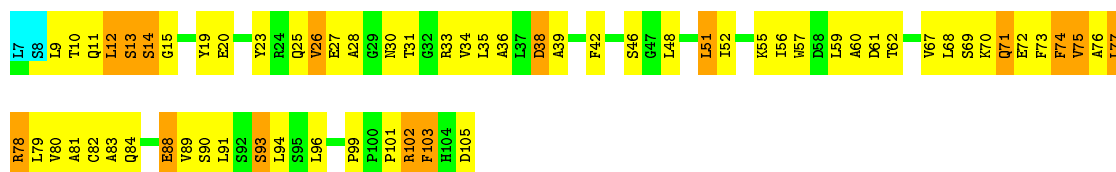
Chain A: 33% 46% 17% ..



4.2.19 Score per residue for model 19

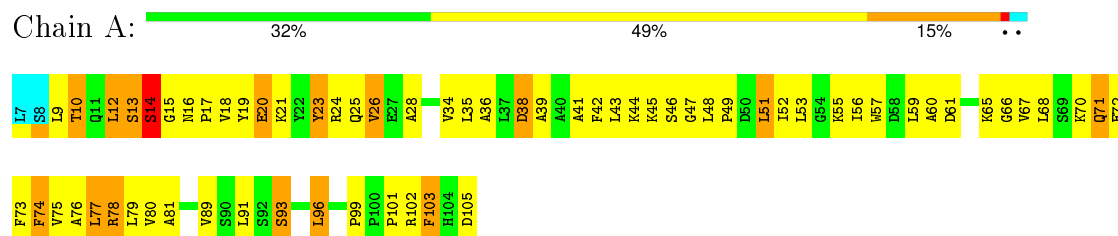
- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

Chain A: 33% 49% 15% .



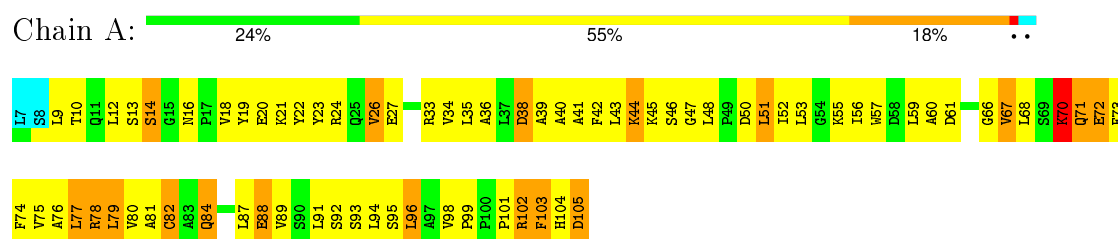
4.2.20 Score per residue for model 20

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



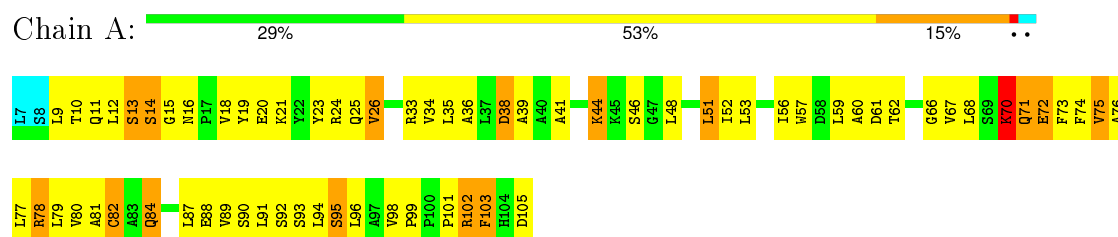
4.2.21 Score per residue for model 21

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



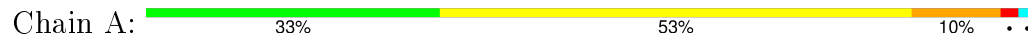
4.2.22 Score per residue for model 22

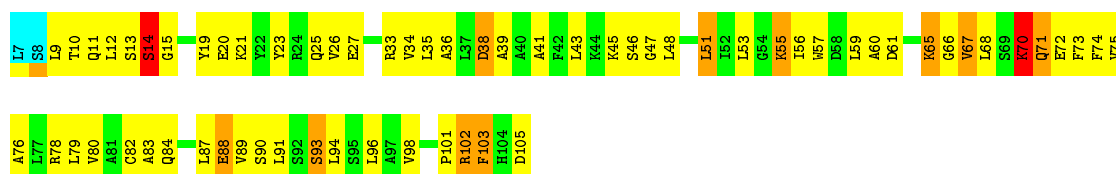
- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



4.2.23 Score per residue for model 23

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

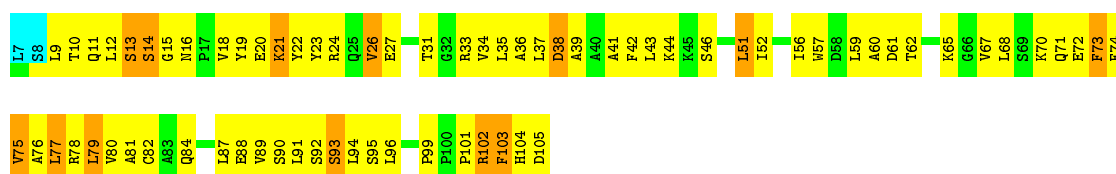




4.2.24 Score per residue for model 24

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

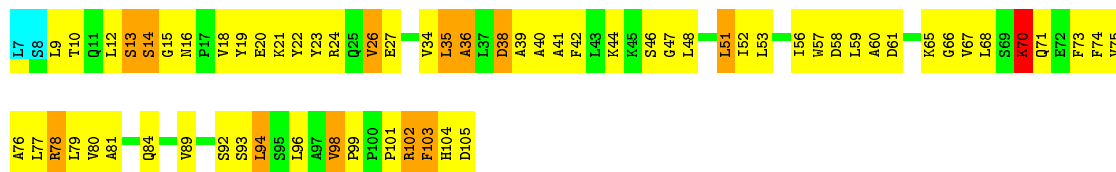
Chain A: 26% 59% 13%



4.2.25 Score per residue for model 25

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

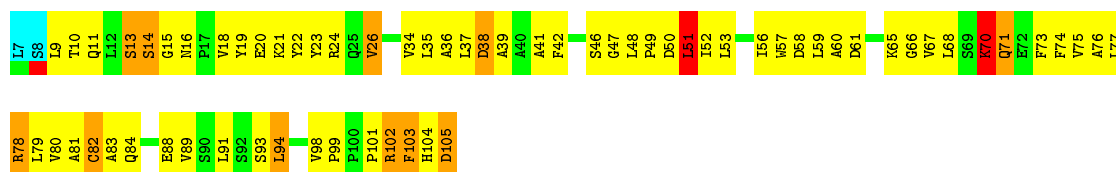
Chain A: 32% 53% 12%



4.2.26 Score per residue for model 26

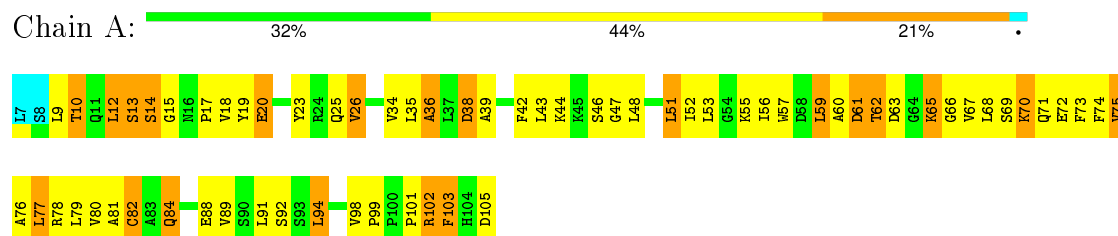
- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15

Chain A: 30% 55% 11%



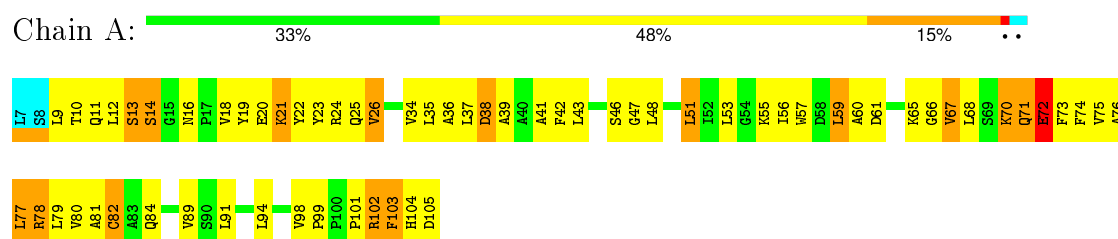
4.2.27 Score per residue for model 27

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



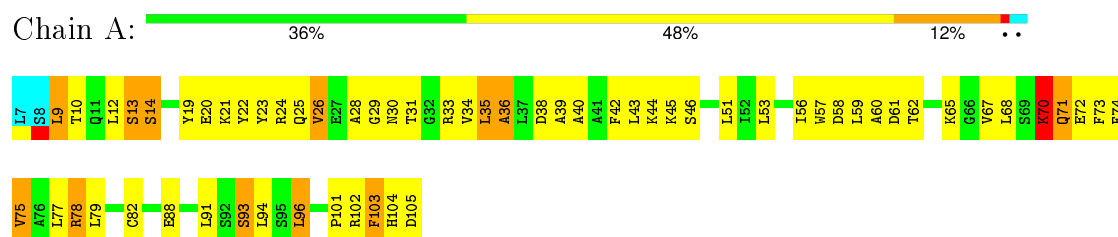
4.2.28 Score per residue for model 28

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



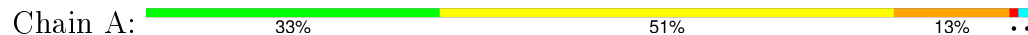
4.2.29 Score per residue for model 29

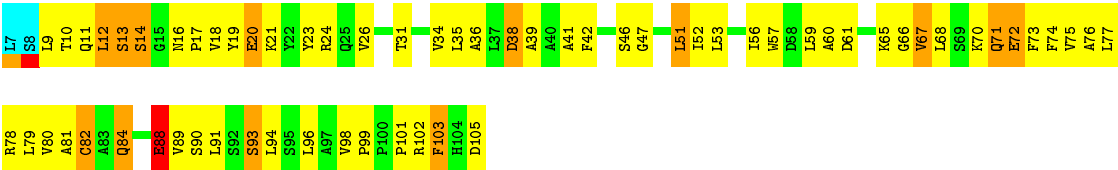
- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15



4.2.30 Score per residue for model 30

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE SUBSTRATE 15, EPS15





5 Refinement protocol and experimental data overview

The models were refined using the following method: *TAD*.

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *LOWEST OVERALL TARGET FUNCTION*.

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

Software name	Classification	Version
DYANA 1.5	refinement	
NMRPIPE	structure solution	
XEASY	structure solution	
DYANA 1.5	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 4491
Number of chemical shift lists	1
Total number of shifts	1399
Number of shifts mapped to atoms	1206
Number of unparsed shifts	0
Number of shifts with mapping errors	193
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	738	741	753	70±5
All	All	22140	22230	22590	2111

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 47.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LEU:HD13	1:A:74:PHE:CE1	0.97	1.95	20	6
1:A:48:LEU:HD12	1:A:80:VAL:HG13	0.96	1.32	17	23
1:A:28:ALA:HB3	1:A:31:THR:HG21	0.95	1.39	29	1
1:A:9:LEU:HD13	1:A:74:PHE:CZ	0.91	2.01	30	2
1:A:59:LEU:HD12	1:A:79:LEU:HD11	0.90	1.41	12	9
1:A:34:VAL:O	1:A:67:VAL:HG13	0.90	1.66	26	30
1:A:19:TYR:CE2	1:A:77:LEU:HD13	0.90	2.00	5	6
1:A:59:LEU:O	1:A:59:LEU:HD22	0.89	1.68	18	11
1:A:9:LEU:HD22	1:A:74:PHE:CG	0.89	2.02	29	21
1:A:19:TYR:CZ	1:A:77:LEU:HD13	0.89	2.03	6	5
1:A:9:LEU:HD22	1:A:74:PHE:CD2	0.89	2.03	23	11
1:A:29:GLY:O	1:A:31:THR:HG23	0.88	1.68	29	1
1:A:28:ALA:CB	1:A:35:LEU:HD12	0.88	1.97	17	2
1:A:59:LEU:HD11	1:A:91:LEU:HD12	0.87	1.41	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:ALA:O	1:A:80:VAL:HG23	0.87	1.69	4	19
1:A:77:LEU:HD23	1:A:103:PHE:CZ	0.87	2.03	9	3
1:A:56:ILE:HG23	1:A:79:LEU:HD13	0.87	1.45	21	8
1:A:49:PRO:O	1:A:53:LEU:HD12	0.82	1.75	26	5
1:A:59:LEU:HD22	1:A:59:LEU:O	0.79	1.78	12	18
1:A:81:ALA:HB1	1:A:99:PRO:O	0.79	1.78	28	23
1:A:52:ILE:HG23	1:A:89:VAL:HG21	0.78	1.52	11	3
1:A:59:LEU:HD12	1:A:79:LEU:CD1	0.78	2.08	20	16
1:A:56:ILE:HG12	1:A:79:LEU:HD22	0.78	1.55	12	13
1:A:39:ALA:CB	1:A:68:LEU:HD12	0.77	2.09	25	23
1:A:81:ALA:HB2	1:A:101:PRO:HG3	0.76	1.57	9	1
1:A:78:ARG:HB3	1:A:98:VAL:HG21	0.76	1.57	21	1
1:A:23:TYR:CE1	1:A:34:VAL:HG21	0.76	2.16	23	5
1:A:28:ALA:CB	1:A:31:THR:HG21	0.76	2.09	29	1
1:A:23:TYR:CE2	1:A:34:VAL:HG21	0.76	2.15	6	4
1:A:77:LEU:HD23	1:A:103:PHE:CE2	0.76	2.15	9	9
1:A:9:LEU:HD13	1:A:74:PHE:CE2	0.75	2.16	30	2
1:A:9:LEU:HD22	1:A:74:PHE:CD1	0.74	2.16	27	7
1:A:12:LEU:HD21	1:A:75:VAL:HG23	0.73	1.58	16	1
1:A:59:LEU:HD11	1:A:91:LEU:HG	0.73	1.58	10	13
1:A:12:LEU:O	1:A:12:LEU:HD13	0.73	1.82	27	5
1:A:48:LEU:CD1	1:A:83:ALA:HB3	0.72	2.14	23	5
1:A:90:SER:O	1:A:94:LEU:HD23	0.72	1.84	4	17
1:A:77:LEU:HD22	1:A:78:ARG:NH2	0.72	1.99	7	1
1:A:82:CYS:SG	1:A:98:VAL:HG12	0.71	2.26	28	6
1:A:51:LEU:C	1:A:51:LEU:HD12	0.71	2.07	28	3
1:A:9:LEU:HD11	1:A:70:LYS:HB2	0.70	1.61	21	6
1:A:19:TYR:CB	1:A:74:PHE:CZ	0.70	2.75	30	27
1:A:36:ALA:HB1	1:A:57:TRP:CZ2	0.70	2.22	13	19
1:A:55:LYS:HB2	1:A:89:VAL:HG11	0.70	1.64	28	9
1:A:79:LEU:HD21	1:A:89:VAL:O	0.70	1.87	11	7
1:A:77:LEU:CD2	1:A:103:PHE:CE2	0.69	2.74	9	12
1:A:51:LEU:HD12	1:A:51:LEU:C	0.69	2.06	4	8
1:A:16:ASN:CG	1:A:18:VAL:HG12	0.68	2.09	13	24
1:A:9:LEU:HD11	1:A:70:LYS:HB3	0.68	1.65	12	10
1:A:36:ALA:O	1:A:39:ALA:HB3	0.67	1.89	18	15
1:A:87:LEU:HD13	1:A:98:VAL:HG12	0.67	1.65	14	2
1:A:23:TYR:CD1	1:A:73:PHE:CG	0.67	2.83	4	3
1:A:35:LEU:O	1:A:36:ALA:HB3	0.67	1.90	29	30
1:A:9:LEU:HD23	1:A:9:LEU:N	0.66	2.05	30	5
1:A:19:TYR:CE1	1:A:78:ARG:NH2	0.66	2.64	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:PHE:CE1	1:A:77:LEU:HD12	0.66	2.25	7	6
1:A:59:LEU:CD1	1:A:91:LEU:HD12	0.66	2.19	7	1
1:A:28:ALA:HB3	1:A:35:LEU:HD12	0.66	1.67	20	5
1:A:9:LEU:CD2	1:A:74:PHE:CD1	0.66	2.79	16	4
1:A:48:LEU:CD1	1:A:80:VAL:HG13	0.66	2.21	9	1
1:A:23:TYR:CE2	1:A:34:VAL:CG2	0.65	2.79	17	5
1:A:77:LEU:CD2	1:A:103:PHE:CZ	0.65	2.80	9	5
1:A:36:ALA:HB1	1:A:57:TRP:CH2	0.65	2.27	29	15
1:A:38:ASP:O	1:A:41:ALA:HB3	0.65	1.90	23	19
1:A:19:TYR:CZ	1:A:78:ARG:NH1	0.65	2.64	11	2
1:A:9:LEU:CD2	1:A:74:PHE:CG	0.65	2.80	11	3
1:A:79:LEU:HA	1:A:94:LEU:HD11	0.64	1.67	9	1
1:A:73:PHE:CE1	1:A:77:LEU:CD1	0.64	2.80	7	1
1:A:48:LEU:HD11	1:A:84:GLN:HG2	0.64	1.69	19	2
1:A:78:ARG:CB	1:A:98:VAL:HG21	0.63	2.23	21	1
1:A:51:LEU:HD12	1:A:52:ILE:HG12	0.63	1.70	26	2
1:A:23:TYR:CZ	1:A:34:VAL:CG2	0.63	2.81	6	4
1:A:26:VAL:HG23	1:A:34:VAL:HG13	0.63	1.69	20	14
1:A:59:LEU:HD11	1:A:91:LEU:CD1	0.63	2.22	7	3
1:A:12:LEU:HD11	1:A:74:PHE:O	0.63	1.93	19	1
1:A:78:ARG:HH21	1:A:101:PRO:CG	0.62	2.06	12	2
1:A:46:SER:HB2	1:A:80:VAL:HG11	0.62	1.71	14	3
1:A:28:ALA:HB1	1:A:35:LEU:HD12	0.62	1.69	17	1
1:A:79:LEU:O	1:A:79:LEU:HD23	0.62	1.94	9	3
1:A:19:TYR:HB2	1:A:74:PHE:CZ	0.62	2.30	30	24
1:A:81:ALA:HB2	1:A:101:PRO:CG	0.62	2.24	9	2
1:A:40:ALA:HB2	1:A:57:TRP:CZ3	0.62	2.30	4	7
1:A:56:ILE:HG13	1:A:89:VAL:HG13	0.62	1.71	16	5
1:A:19:TYR:CB	1:A:74:PHE:CE2	0.62	2.83	18	19
1:A:102:ARG:O	1:A:103:PHE:CD2	0.61	2.53	9	1
1:A:19:TYR:CE1	1:A:78:ARG:CZ	0.61	2.83	7	1
1:A:16:ASN:OD1	1:A:18:VAL:HG12	0.61	1.96	8	11
1:A:53:LEU:HD23	1:A:56:ILE:HD12	0.60	1.71	1	8
1:A:81:ALA:HB2	1:A:101:PRO:HB3	0.60	1.73	22	2
1:A:23:TYR:CZ	1:A:34:VAL:HG23	0.60	2.31	18	2
1:A:23:TYR:CD1	1:A:73:PHE:CD1	0.60	2.89	4	1
1:A:48:LEU:HD13	1:A:83:ALA:HB3	0.60	1.72	23	3
1:A:9:LEU:HD21	1:A:70:LYS:C	0.60	2.17	17	3
1:A:26:VAL:CG2	1:A:34:VAL:HG13	0.60	2.26	14	6
1:A:19:TYR:CZ	1:A:78:ARG:CZ	0.60	2.85	7	2
1:A:19:TYR:CD2	1:A:77:LEU:HD13	0.59	2.32	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TYR:CE1	1:A:34:VAL:CG2	0.59	2.85	23	2
1:A:39:ALA:CB	1:A:68:LEU:CD1	0.59	2.80	12	21
1:A:23:TYR:CE2	1:A:34:VAL:HG23	0.59	2.31	10	1
1:A:9:LEU:HD11	1:A:70:LYS:CB	0.59	2.27	23	4
1:A:19:TYR:HB3	1:A:74:PHE:CZ	0.59	2.32	10	30
1:A:26:VAL:CG2	1:A:34:VAL:CG2	0.59	2.80	8	3
1:A:26:VAL:HG12	1:A:42:PHE:HB2	0.58	1.75	24	18
1:A:102:ARG:O	1:A:103:PHE:CG	0.58	2.57	9	1
1:A:91:LEU:HA	1:A:94:LEU:HD23	0.58	1.74	13	12
1:A:93:SER:O	1:A:96:LEU:HD11	0.58	1.99	17	6
1:A:77:LEU:HD22	1:A:78:ARG:HH21	0.58	1.56	7	1
1:A:81:ALA:HB2	1:A:101:PRO:CB	0.58	2.29	22	2
1:A:13:SER:OG	1:A:19:TYR:CE1	0.58	2.56	15	1
1:A:35:LEU:O	1:A:36:ALA:CB	0.57	2.52	25	29
1:A:31:THR:HG23	1:A:33:ARG:H	0.57	1.58	15	4
1:A:9:LEU:HD23	1:A:74:PHE:CD1	0.57	2.34	16	1
1:A:91:LEU:HD23	1:A:94:LEU:CB	0.57	2.30	29	12
1:A:23:TYR:C	1:A:23:TYR:CD1	0.56	2.79	18	8
1:A:56:ILE:CG1	1:A:79:LEU:HD22	0.56	2.30	18	2
1:A:73:PHE:CD1	1:A:73:PHE:C	0.56	2.79	10	5
1:A:73:PHE:C	1:A:73:PHE:CD1	0.56	2.78	5	9
1:A:46:SER:CB	1:A:80:VAL:HG11	0.56	2.31	14	2
1:A:26:VAL:HG23	1:A:34:VAL:CG2	0.56	2.30	8	3
1:A:75:VAL:HG12	1:A:76:ALA:N	0.55	2.16	24	13
1:A:78:ARG:NH2	1:A:101:PRO:CG	0.55	2.69	12	21
1:A:55:LYS:CB	1:A:89:VAL:HG11	0.55	2.32	28	1
1:A:39:ALA:HB1	1:A:68:LEU:HD12	0.55	1.78	21	5
1:A:65:LYS:O	1:A:67:VAL:HG23	0.55	2.01	10	1
1:A:88:GLU:CB	1:A:93:SER:CB	0.54	2.85	16	15
1:A:20:GLU:OE1	1:A:23:TYR:CD1	0.54	2.60	6	1
1:A:19:TYR:HB2	1:A:74:PHE:CE2	0.54	2.37	28	17
1:A:78:ARG:HH21	1:A:101:PRO:HG3	0.54	1.61	12	2
1:A:91:LEU:HD23	1:A:94:LEU:HB2	0.54	1.78	21	6
1:A:56:ILE:CG1	1:A:89:VAL:CG1	0.54	2.86	24	13
1:A:82:CYS:SG	1:A:87:LEU:HD13	0.53	2.43	22	1
1:A:12:LEU:HD13	1:A:12:LEU:O	0.53	2.03	10	4
1:A:34:VAL:O	1:A:67:VAL:CG1	0.53	2.57	20	27
1:A:36:ALA:HB2	1:A:66:GLY:O	0.53	2.05	21	10
1:A:21:LYS:CG	1:A:22:TYR:CD1	0.53	2.93	2	1
1:A:78:ARG:NH2	1:A:101:PRO:CD	0.52	2.72	12	3
1:A:67:VAL:CG1	1:A:68:LEU:N	0.52	2.72	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TYR:CA	1:A:73:PHE:CE2	0.52	2.92	23	1
1:A:57:TRP:HA	1:A:60:ALA:HB3	0.52	1.81	14	3
1:A:56:ILE:CD1	1:A:80:VAL:HG22	0.52	2.33	12	1
1:A:10:THR:O	1:A:14:SER:N	0.52	2.43	6	25
1:A:12:LEU:HD23	1:A:71:GLN:OE1	0.52	2.04	1	2
1:A:34:VAL:HG12	1:A:36:ALA:H	0.52	1.65	7	9
1:A:19:TYR:CE2	1:A:78:ARG:NH1	0.52	2.77	11	2
1:A:82:CYS:SG	1:A:98:VAL:HG11	0.52	2.45	2	1
1:A:26:VAL:CG2	1:A:34:VAL:CG1	0.52	2.87	5	2
1:A:26:VAL:O	1:A:38:ASP:CB	0.52	2.58	14	29
1:A:94:LEU:O	1:A:95:SER:CB	0.52	2.58	17	11
1:A:21:LYS:HD3	1:A:22:TYR:CE1	0.52	2.40	2	1
1:A:94:LEU:HD22	1:A:98:VAL:HG11	0.51	1.82	25	1
1:A:91:LEU:CD2	1:A:94:LEU:HD12	0.51	2.36	8	2
1:A:93:SER:O	1:A:96:LEU:CD1	0.51	2.58	17	6
1:A:9:LEU:N	1:A:9:LEU:HD23	0.51	2.20	23	3
1:A:46:SER:HB3	1:A:103:PHE:CE1	0.51	2.41	28	21
1:A:23:TYR:HA	1:A:73:PHE:CE2	0.51	2.41	23	5
1:A:34:VAL:O	1:A:34:VAL:HG13	0.51	2.05	8	1
1:A:10:THR:O	1:A:15:GLY:N	0.51	2.43	5	16
1:A:80:VAL:O	1:A:84:GLN:CG	0.51	2.59	30	8
1:A:42:PHE:O	1:A:45:LYS:CG	0.51	2.58	18	1
1:A:48:LEU:HD11	1:A:83:ALA:HB3	0.51	1.81	23	6
1:A:46:SER:HB3	1:A:103:PHE:CZ	0.50	2.41	7	7
1:A:42:PHE:CE2	1:A:77:LEU:HD21	0.50	2.41	10	1
1:A:19:TYR:OH	1:A:78:ARG:CZ	0.50	2.59	8	16
1:A:56:ILE:HG12	1:A:89:VAL:HG12	0.50	1.82	24	5
1:A:23:TYR:HB2	1:A:73:PHE:CE2	0.50	2.41	23	3
1:A:101:PRO:HB2	1:A:103:PHE:CD2	0.50	2.42	7	27
1:A:26:VAL:HG23	1:A:34:VAL:HG23	0.50	1.82	29	3
1:A:9:LEU:HD21	1:A:71:GLN:N	0.50	2.21	26	7
1:A:56:ILE:CG1	1:A:89:VAL:HG12	0.50	2.37	4	2
1:A:10:THR:O	1:A:14:SER:CA	0.50	2.59	23	16
1:A:57:TRP:CZ2	1:A:68:LEU:HD21	0.50	2.41	26	1
1:A:77:LEU:HD22	1:A:103:PHE:CE2	0.50	2.42	17	2
1:A:16:ASN:CG	1:A:18:VAL:CG1	0.49	2.80	13	11
1:A:71:GLN:CG	1:A:72:GLU:N	0.49	2.75	30	1
1:A:36:ALA:CB	1:A:66:GLY:O	0.49	2.60	21	11
1:A:46:SER:O	1:A:102:ARG:CB	0.49	2.60	29	8
1:A:71:GLN:O	1:A:75:VAL:N	0.49	2.45	13	24
1:A:19:TYR:CE2	1:A:77:LEU:CD1	0.49	2.86	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:GLY:O	1:A:67:VAL:CG2	0.49	2.61	13	2
1:A:56:ILE:O	1:A:60:ALA:N	0.49	2.46	11	28
1:A:51:LEU:HD23	1:A:52:ILE:H	0.49	1.67	20	4
1:A:40:ALA:HA	1:A:43:LEU:HD12	0.49	1.83	18	1
1:A:66:GLY:C	1:A:67:VAL:CG2	0.49	2.80	30	4
1:A:23:TYR:HB2	1:A:73:PHE:CE1	0.49	2.42	7	19
1:A:43:LEU:HD22	1:A:80:VAL:HG21	0.49	1.84	28	1
1:A:23:TYR:HA	1:A:73:PHE:CZ	0.49	2.43	6	24
1:A:49:PRO:O	1:A:53:LEU:CD1	0.49	2.60	9	2
1:A:21:LYS:CD	1:A:22:TYR:CE1	0.49	2.96	2	1
1:A:19:TYR:HB3	1:A:74:PHE:CE1	0.49	2.43	13	4
1:A:56:ILE:HG12	1:A:79:LEU:HD13	0.49	1.84	18	1
1:A:104:HIS:CG	1:A:105:ASP:N	0.49	2.81	15	2
1:A:90:SER:O	1:A:94:LEU:CD2	0.49	2.61	1	9
1:A:21:LYS:HG2	1:A:22:TYR:CD1	0.48	2.43	10	5
1:A:72:GLU:OE1	1:A:73:PHE:N	0.48	2.46	30	1
1:A:19:TYR:CD2	1:A:77:LEU:CD1	0.48	2.96	5	1
1:A:93:SER:HA	1:A:96:LEU:HD12	0.48	1.85	25	1
1:A:59:LEU:HD21	1:A:91:LEU:HD12	0.48	1.86	12	1
1:A:26:VAL:HG23	1:A:34:VAL:CG1	0.48	2.38	6	4
1:A:9:LEU:HD23	1:A:74:PHE:CG	0.48	2.43	16	1
1:A:51:LEU:HG	1:A:52:ILE:N	0.48	2.23	16	19
1:A:26:VAL:HG12	1:A:42:PHE:CB	0.48	2.39	14	7
1:A:9:LEU:N	1:A:9:LEU:CD2	0.48	2.76	30	1
1:A:79:LEU:O	1:A:82:CYS:CB	0.48	2.62	23	7
1:A:91:LEU:HD23	1:A:94:LEU:HG	0.48	1.86	11	1
1:A:94:LEU:CD2	1:A:98:VAL:HG11	0.48	2.38	25	1
1:A:59:LEU:HD12	1:A:79:LEU:HD12	0.48	1.84	15	2
1:A:57:TRP:O	1:A:61:ASP:N	0.48	2.47	4	16
1:A:19:TYR:OH	1:A:78:ARG:CD	0.48	2.62	26	2
1:A:43:LEU:O	1:A:46:SER:N	0.48	2.47	2	20
1:A:12:LEU:HG	1:A:74:PHE:CD2	0.48	2.44	6	1
1:A:26:VAL:HG12	1:A:42:PHE:CD2	0.47	2.44	14	1
1:A:49:PRO:O	1:A:53:LEU:CG	0.47	2.62	9	1
1:A:59:LEU:HD13	1:A:59:LEU:C	0.47	2.28	27	4
1:A:22:TYR:HB3	1:A:42:PHE:CZ	0.47	2.44	7	9
1:A:59:LEU:C	1:A:59:LEU:HD13	0.47	2.29	1	3
1:A:12:LEU:C	1:A:12:LEU:HD13	0.47	2.30	11	2
1:A:19:TYR:CE1	1:A:77:LEU:HD13	0.47	2.45	21	2
1:A:87:LEU:CD1	1:A:98:VAL:HG12	0.47	2.39	16	3
1:A:36:ALA:O	1:A:39:ALA:N	0.47	2.47	26	27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD12	1:A:80:VAL:CG1	0.47	2.39	1	4
1:A:9:LEU:HB3	1:A:74:PHE:CE2	0.47	2.45	27	4
1:A:23:TYR:CD1	1:A:23:TYR:C	0.47	2.88	13	5
1:A:22:TYR:HB3	1:A:42:PHE:CE2	0.47	2.45	17	2
1:A:42:PHE:O	1:A:45:LYS:CB	0.47	2.62	18	1
1:A:57:TRP:O	1:A:60:ALA:N	0.47	2.47	16	30
1:A:34:VAL:HG22	1:A:36:ALA:H	0.47	1.68	27	2
1:A:34:VAL:HG11	1:A:68:LEU:HB2	0.47	1.87	8	3
1:A:19:TYR:OH	1:A:78:ARG:NE	0.47	2.49	10	8
1:A:53:LEU:O	1:A:56:ILE:N	0.46	2.48	9	25
1:A:56:ILE:CG1	1:A:89:VAL:HG13	0.46	2.40	21	5
1:A:39:ALA:HB3	1:A:68:LEU:CD1	0.46	2.40	25	1
1:A:34:VAL:O	1:A:67:VAL:HG22	0.46	2.10	24	1
1:A:19:TYR:OH	1:A:78:ARG:NH1	0.46	2.49	30	6
1:A:13:SER:O	1:A:15:GLY:N	0.46	2.49	20	5
1:A:17:PRO:O	1:A:20:GLU:N	0.46	2.48	18	14
1:A:23:TYR:HB2	1:A:73:PHE:CD1	0.46	2.46	8	2
1:A:75:VAL:HG11	1:A:91:LEU:HD11	0.46	1.88	14	4
1:A:88:GLU:N	1:A:93:SER:OG	0.46	2.49	3	2
1:A:19:TYR:OH	1:A:78:ARG:NH2	0.46	2.48	10	4
1:A:9:LEU:HB3	1:A:74:PHE:CZ	0.46	2.46	27	1
1:A:40:ALA:HB2	1:A:57:TRP:HZ3	0.46	1.69	18	2
1:A:21:LYS:HG2	1:A:22:TYR:CD2	0.46	2.45	13	1
1:A:46:SER:OG	1:A:47:GLY:N	0.46	2.49	7	22
1:A:23:TYR:CE1	1:A:69:SER:O	0.46	2.69	19	1
1:A:49:PRO:HG2	1:A:51:LEU:HD23	0.46	1.88	6	2
1:A:38:ASP:O	1:A:41:ALA:N	0.45	2.49	28	12
1:A:13:SER:C	1:A:15:GLY:N	0.45	2.69	27	12
1:A:59:LEU:HD11	1:A:91:LEU:CG	0.45	2.42	22	1
1:A:19:TYR:HA	1:A:22:TYR:CD2	0.45	2.46	14	1
1:A:18:VAL:HG13	1:A:19:TYR:HD1	0.45	1.71	27	1
1:A:9:LEU:HD21	1:A:70:LYS:HB3	0.45	1.88	13	1
1:A:41:ALA:O	1:A:44:LYS:CG	0.45	2.64	22	2
1:A:34:VAL:C	1:A:36:ALA:N	0.45	2.69	24	2
1:A:19:TYR:CD1	1:A:77:LEU:HD13	0.45	2.45	2	2
1:A:23:TYR:O	1:A:23:TYR:CD1	0.45	2.70	26	1
1:A:39:ALA:CB	1:A:68:LEU:HD11	0.45	2.41	24	3
1:A:36:ALA:O	1:A:39:ALA:CB	0.45	2.61	18	2
1:A:80:VAL:O	1:A:84:GLN:N	0.45	2.50	11	1
1:A:102:ARG:O	1:A:103:PHE:O	0.45	2.35	22	29
1:A:82:CYS:SG	1:A:94:LEU:HD13	0.45	2.52	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:GLN:OE1	1:A:72:GLU:N	0.45	2.50	28	1
1:A:94:LEU:HD23	1:A:98:VAL:HG11	0.45	1.88	27	1
1:A:56:ILE:HG13	1:A:89:VAL:CG1	0.45	2.42	24	23
1:A:56:ILE:HG12	1:A:89:VAL:CG1	0.45	2.42	2	10
1:A:26:VAL:CG2	1:A:27:GLU:N	0.45	2.80	23	3
1:A:19:TYR:CE2	1:A:77:LEU:HB3	0.45	2.46	16	3
1:A:66:GLY:C	1:A:67:VAL:HG23	0.45	2.32	13	2
1:A:39:ALA:HB3	1:A:68:LEU:HD12	0.45	1.86	25	1
1:A:78:ARG:O	1:A:81:ALA:N	0.45	2.50	25	4
1:A:73:PHE:HE1	1:A:77:LEU:HD12	0.45	1.70	6	1
1:A:59:LEU:CD1	1:A:79:LEU:HD11	0.45	2.39	18	2
1:A:42:PHE:HE2	1:A:77:LEU:HD21	0.45	1.70	27	1
1:A:73:PHE:CE2	1:A:77:LEU:HD12	0.45	2.47	9	1
1:A:88:GLU:HB2	1:A:93:SER:CB	0.44	2.42	16	7
1:A:60:ALA:O	1:A:61:ASP:C	0.44	2.55	16	30
1:A:27:GLU:CG	1:A:33:ARG:O	0.44	2.65	21	1
1:A:91:LEU:HD23	1:A:94:LEU:HD12	0.44	1.90	8	2
1:A:26:VAL:CG2	1:A:34:VAL:HG21	0.44	2.41	8	1
1:A:13:SER:O	1:A:16:ASN:N	0.44	2.51	3	2
1:A:45:LYS:HD3	1:A:104:HIS:CG	0.44	2.47	9	1
1:A:34:VAL:O	1:A:34:VAL:CG1	0.44	2.64	8	1
1:A:52:ILE:HG21	1:A:83:ALA:HB1	0.44	1.89	1	3
1:A:42:PHE:CD1	1:A:42:PHE:C	0.44	2.90	18	2
1:A:16:ASN:OD1	1:A:18:VAL:CG1	0.44	2.65	8	2
1:A:9:LEU:HD21	1:A:70:LYS:HB2	0.44	1.88	23	2
1:A:77:LEU:CD2	1:A:103:PHE:CD2	0.44	3.01	22	1
1:A:19:TYR:O	1:A:22:TYR:N	0.44	2.51	17	1
1:A:59:LEU:CD1	1:A:79:LEU:CD1	0.44	2.95	18	1
1:A:42:PHE:O	1:A:45:LYS:N	0.44	2.49	9	2
1:A:28:ALA:O	1:A:31:THR:OG1	0.43	2.36	19	2
1:A:78:ARG:CZ	1:A:101:PRO:CG	0.43	2.96	25	1
1:A:46:SER:CB	1:A:103:PHE:CE1	0.43	3.00	28	1
1:A:48:LEU:HD11	1:A:80:VAL:O	0.43	2.12	13	1
1:A:82:CYS:SG	1:A:98:VAL:CG1	0.43	3.04	21	4
1:A:93:SER:O	1:A:96:LEU:HD12	0.43	2.13	8	2
1:A:87:LEU:HD12	1:A:98:VAL:HG12	0.43	1.89	23	2
1:A:12:LEU:HD12	1:A:74:PHE:HB3	0.43	1.90	16	1
1:A:23:TYR:CE1	1:A:34:VAL:HG11	0.43	2.48	29	1
1:A:66:GLY:O	1:A:67:VAL:HG22	0.43	2.13	30	1
1:A:82:CYS:HA	1:A:98:VAL:HG23	0.43	1.89	30	1
1:A:88:GLU:CB	1:A:93:SER:OG	0.43	2.66	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TYR:CD1	1:A:73:PHE:CD2	0.43	3.06	29	1
1:A:78:ARG:CZ	1:A:101:PRO:HG3	0.43	2.44	25	4
1:A:75:VAL:CG1	1:A:76:ALA:N	0.43	2.81	24	2
1:A:51:LEU:C	1:A:51:LEU:CD1	0.43	2.80	9	2
1:A:22:TYR:O	1:A:26:VAL:HG13	0.43	2.12	17	1
1:A:36:ALA:O	1:A:37:LEU:C	0.43	2.57	8	5
1:A:36:ALA:HB1	1:A:57:TRP:HZ2	0.43	1.70	13	1
1:A:43:LEU:C	1:A:45:LYS:N	0.43	2.72	15	8
1:A:18:VAL:HG13	1:A:19:TYR:N	0.43	2.29	11	2
1:A:88:GLU:CB	1:A:93:SER:HB2	0.43	2.44	16	6
1:A:22:TYR:OH	1:A:105:ASP:CB	0.43	2.67	12	1
1:A:64:GLY:O	1:A:65:LYS:CB	0.43	2.65	3	1
1:A:48:LEU:HD22	1:A:52:ILE:HG21	0.43	1.91	20	1
1:A:29:GLY:O	1:A:30:ASN:C	0.42	2.56	29	1
1:A:23:TYR:CZ	1:A:69:SER:O	0.42	2.72	1	1
1:A:39:ALA:HB2	1:A:68:LEU:HD12	0.42	1.91	24	3
1:A:12:LEU:HD21	1:A:74:PHE:O	0.42	2.14	6	1
1:A:75:VAL:CG1	1:A:91:LEU:HD11	0.42	2.44	7	1
1:A:34:VAL:CG1	1:A:68:LEU:HB2	0.42	2.45	28	3
1:A:23:TYR:HB2	1:A:73:PHE:CD2	0.42	2.50	23	2
1:A:51:LEU:CD1	1:A:51:LEU:C	0.42	2.80	23	1
1:A:78:ARG:HH21	1:A:101:PRO:CD	0.42	2.27	22	1
1:A:35:LEU:O	1:A:66:GLY:O	0.42	2.37	27	5
1:A:66:GLY:O	1:A:67:VAL:C	0.42	2.58	16	11
1:A:45:LYS:HB3	1:A:104:HIS:CD2	0.42	2.50	9	1
1:A:72:GLU:O	1:A:75:VAL:N	0.42	2.52	27	1
1:A:26:VAL:HG21	1:A:39:ALA:HB2	0.41	1.92	28	2
1:A:22:TYR:O	1:A:25:GLN:N	0.41	2.53	13	1
1:A:48:LEU:CD1	1:A:80:VAL:O	0.41	2.68	4	1
1:A:79:LEU:O	1:A:82:CYS:N	0.41	2.53	14	1
1:A:23:TYR:CE1	1:A:73:PHE:CG	0.41	3.07	4	1
1:A:26:VAL:CG1	1:A:42:PHE:CB	0.41	2.99	29	1
1:A:81:ALA:CB	1:A:99:PRO:O	0.41	2.66	26	1
1:A:82:CYS:CA	1:A:98:VAL:HG23	0.41	2.46	30	1
1:A:17:PRO:C	1:A:19:TYR:N	0.41	2.72	15	1
1:A:46:SER:CB	1:A:103:PHE:CZ	0.41	3.03	28	1
1:A:9:LEU:HD22	1:A:74:PHE:CB	0.41	2.45	5	2
1:A:70:LYS:O	1:A:71:GLN:C	0.41	2.59	29	11
1:A:24:ARG:NH2	1:A:29:GLY:O	0.41	2.54	10	1
1:A:75:VAL:C	1:A:77:LEU:N	0.41	2.72	4	3
1:A:60:ALA:O	1:A:72:GLU:OE1	0.41	2.39	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:LEU:O	1:A:79:LEU:CD2	0.41	2.68	9	1
1:A:82:CYS:SG	1:A:87:LEU:CB	0.41	3.08	24	3
1:A:57:TRP:O	1:A:60:ALA:HB3	0.41	2.14	22	1
1:A:26:VAL:O	1:A:38:ASP:CG	0.41	2.59	15	4
1:A:9:LEU:CD2	1:A:71:GLN:HA	0.41	2.46	30	1
1:A:52:ILE:CG2	1:A:89:VAL:HG21	0.41	2.36	11	1
1:A:82:CYS:C	1:A:84:GLN:N	0.41	2.74	24	2
1:A:21:LYS:HG3	1:A:22:TYR:CD1	0.41	2.50	14	2
1:A:59:LEU:C	1:A:59:LEU:HD22	0.41	2.32	18	1
1:A:65:LYS:O	1:A:66:GLY:C	0.41	2.60	26	1
1:A:13:SER:O	1:A:14:SER:C	0.41	2.59	23	2
1:A:26:VAL:O	1:A:27:GLU:C	0.41	2.59	15	3
1:A:88:GLU:O	1:A:93:SER:OG	0.41	2.39	21	1
1:A:12:LEU:CD1	1:A:12:LEU:O	0.41	2.68	16	1
1:A:30:ASN:O	1:A:31:THR:CG2	0.41	2.69	19	1
1:A:34:VAL:HG13	1:A:34:VAL:O	0.41	2.15	28	1
1:A:61:ASP:OD2	1:A:65:LYS:CE	0.41	2.69	27	1
1:A:78:ARG:NH2	1:A:101:PRO:HD3	0.41	2.31	15	1
1:A:40:ALA:O	1:A:44:LYS:CG	0.41	2.69	9	1
1:A:88:GLU:HB3	1:A:93:SER:CB	0.40	2.47	1	5
1:A:88:GLU:CB	1:A:93:SER:HB3	0.40	2.45	4	1
1:A:73:PHE:CE1	1:A:77:LEU:HD11	0.40	2.51	7	1
1:A:12:LEU:O	1:A:12:LEU:CD1	0.40	2.62	27	1
1:A:22:TYR:OH	1:A:105:ASP:C	0.40	2.60	1	3
1:A:87:LEU:O	1:A:88:GLU:O	0.40	2.39	21	1
1:A:26:VAL:HG12	1:A:42:PHE:CG	0.40	2.52	21	1
1:A:78:ARG:NH2	1:A:101:PRO:HG3	0.40	2.31	5	2
1:A:51:LEU:CG	1:A:52:ILE:N	0.40	2.85	2	3
1:A:91:LEU:CA	1:A:94:LEU:HD23	0.40	2.43	13	1
1:A:9:LEU:CD1	1:A:74:PHE:CZ	0.40	2.90	30	1
1:A:9:LEU:CD1	1:A:70:LYS:HB3	0.40	2.46	16	1
1:A:104:HIS:O	1:A:105:ASP:C	0.40	2.60	17	1
1:A:82:CYS:SG	1:A:93:SER:O	0.40	2.80	8	2
1:A:39:ALA:HB1	1:A:68:LEU:CD1	0.40	2.45	13	1
1:A:60:ALA:C	1:A:72:GLU:OE1	0.40	2.59	13	1
1:A:79:LEU:CD2	1:A:89:VAL:O	0.40	2.67	2	1
1:A:72:GLU:N	1:A:72:GLU:CD	0.40	2.75	4	1
1:A:27:GLU:HB2	1:A:34:VAL:HG22	0.40	1.93	19	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	96/99 (97%)	69±3 (72±3%)	22±3 (23±3%)	5±1 (5±1%)	5	26
All	All	2880/2970 (97%)	2076 (72%)	657 (23%)	147 (5%)	5	26

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	103	PHE	29
1	A	70	LYS	20
1	A	62	THR	16
1	A	88	GLU	15
1	A	13	SER	13
1	A	72	GLU	11
1	A	77	LEU	9
1	A	67	VAL	9
1	A	65	LYS	8
1	A	10	THR	5
1	A	14	SER	4
1	A	36	ALA	3
1	A	51	LEU	2
1	A	29	GLY	1
1	A	28	ALA	1
1	A	27	GLU	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	79/81 (98%)	56±3 (71±3%)	23±3 (29±3%)	2	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2370/2430 (98%)	1679 (71%)	691 (29%)	2 18

All 57 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	20	GLU	30
1	A	14	SER	30
1	A	51	LEU	30
1	A	13	SER	29
1	A	38	ASP	28
1	A	105	ASP	28
1	A	26	VAL	28
1	A	12	LEU	26
1	A	93	SER	24
1	A	102	ARG	24
1	A	96	LEU	23
1	A	24	ARG	23
1	A	71	GLN	23
1	A	70	LYS	22
1	A	21	LYS	21
1	A	78	ARG	20
1	A	82	CYS	17
1	A	77	LEU	17
1	A	11	GLN	17
1	A	44	LYS	16
1	A	25	GLN	16
1	A	65	LYS	15
1	A	88	GLU	14
1	A	84	GLN	12
1	A	55	LYS	10
1	A	75	VAL	10
1	A	72	GLU	10
1	A	92	SER	9
1	A	79	LEU	9
1	A	33	ARG	9
1	A	23	TYR	8
1	A	104	HIS	7
1	A	58	ASP	7
1	A	59	LEU	7
1	A	19	TYR	6
1	A	74	PHE	6

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Mol	Chain	Res	Type	Models (Total)
1	A	50	ASP	6
1	A	27	GLU	6
1	A	69	SER	6
1	A	37	LEU	5
1	A	63	ASP	5
1	A	62	THR	5
1	A	94	LEU	4
1	A	73	PHE	3
1	A	35	LEU	2
1	A	10	THR	2
1	A	61	ASP	2
1	A	31	THR	2
1	A	95	SER	2
1	A	9	LEU	2
1	A	45	LYS	2
1	A	67	VAL	1
1	A	90	SER	1
1	A	56	ILE	1
1	A	98	VAL	1
1	A	87	LEU	1
1	A	30	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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4491

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1399
Number of shifts mapped to atoms	1206
Number of unparsed shifts	0
Number of shifts with mapping errors	193
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 193 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	118	ALA	HB1	1.37	-1.0	1
A	109	PRO	HD3	3.8	-1.0	2
A	119	GLU	CA	55.6	-1.0	1
A	110	LEU	HD23	0.86	-1.0	1
A	110	LEU	CA	55.2	-1.0	1
A	4	ALA	HB3	1.39	-1.0	1
A	111	LEU	HD21	0.84	-1.0	1
A	118	ALA	H	8.27	-1.0	1
A	109	PRO	HG2	1.99	-1.0	2
A	120	LEU	H	7.85	-1.0	1
A	119	GLU	C	175.3	-1.0	1
A	3	ALA	N	123.2	-1.0	1
A	109	PRO	C	176.8	-1.0	1
A	114	GLY	HA3	4.1	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	119	GLU	N	120.6	-1.0	1
A	109	PRO	CA	62.9	-1.0	1
A	110	LEU	HD12	0.88	-1.0	1
A	111	LEU	H	8.2	-1.0	1
A	106	SER	CA	58.4	-1.0	1
A	2	ALA	CB	18.7	-1.0	1
A	3	ALA	HA	4.18	-1.0	1
A	119	GLU	HB2	1.95	-1.0	2
A	114	GLY	N	110.6	-1.0	1
A	106	SER	N	116.3	-1.0	1
A	2	ALA	C	177.8	-1.0	1
A	111	LEU	HD11	0.91	-1.0	1
A	2	ALA	HB3	1.38	-1.0	1
A	117	VAL	HG21	0.9	-1.0	1
A	117	VAL	HG11	0.91	-1.0	1
A	3	ALA	HB3	1.39	-1.0	1
A	6	GLN	HE21	6.81	-1.0	2
A	114	GLY	CA	44.1	-1.0	1
A	116	SER	C	176.6	-1.0	1
A	111	LEU	HB3	1.66	-1.0	2
A	6	GLN	NE2	112.4	-1.0	1
A	113	SER	C	174.5	-1.0	1
A	115	PRO	HD2	3.61	-1.0	2
A	108	SER	H	8.18	-1.0	1
A	116	SER	N	116.3	-1.0	1
A	112	THR	CB	69.6	-1.0	1
A	6	GLN	CA	55.4	-1.0	1
A	112	THR	HG22	1.17	-1.0	1
A	109	PRO	CB	31.7	-1.0	1
A	115	PRO	HB2	2.0	-1.0	2
A	106	SER	CB	63.7	-1.0	1
A	113	SER	CB	63.8	-1.0	1
A	118	ALA	C	178.2	-1.0	1
A	6	GLN	C	175.9	-1.0	1
A	115	PRO	CD	49.6	-1.0	1
A	112	THR	H	8.07	-1.0	1
A	107	SER	HA	4.49	-1.0	1
A	6	GLN	N	117.6	-1.0	1
A	107	SER	N	117.6	-1.0	1
A	111	LEU	HD12	0.91	-1.0	1
A	3	ALA	C	178.3	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	6	GLN	HE22	7.47	-1.0	2
A	4	ALA	HB1	1.39	-1.0	1
A	110	LEU	CD2	23.3	-1.0	1
A	111	LEU	CD2	23.2	-1.0	1
A	112	THR	N	114.1	-1.0	1
A	107	SER	CA	58.3	-1.0	1
A	6	GLN	H	8.01	-1.0	1
A	118	ALA	HA	4.32	-1.0	1
A	112	THR	C	174.5	-1.0	1
A	6	GLN	HB3	2.12	-1.0	2
A	5	ALA	CA	52.8	-1.0	1
A	111	LEU	HA	4.43	-1.0	1
A	112	THR	CA	61.3	-1.0	1
A	6	GLN	CB	28.8	-1.0	1
A	109	PRO	CG	27.0	-1.0	1
A	120	LEU	N	128.8	-1.0	1
A	3	ALA	H	8.22	-1.0	1
A	107	SER	C	174.2	-1.0	1
A	113	SER	HA	4.51	-1.0	1
A	5	ALA	N	120.4	-1.0	1
A	110	LEU	HD11	0.88	-1.0	1
A	6	GLN	HG2	2.34	-1.0	2
A	5	ALA	HA	4.22	-1.0	1
A	117	VAL	N	121.5	-1.0	1
A	2	ALA	CA	52.6	-1.0	1
A	115	PRO	HB3	2.26	-1.0	2
A	110	LEU	HA	4.28	-1.0	1
A	4	ALA	HA	4.18	-1.0	1
A	119	GLU	HB3	2.11	-1.0	2
A	111	LEU	CD1	24.7	-1.0	1
A	117	VAL	CG2	19.9	-1.0	1
A	109	PRO	HB2	1.89	-1.0	2
A	106	SER	HA	4.47	-1.0	1
A	2	ALA	HB2	1.38	-1.0	1
A	108	SER	CA	56.3	-1.0	1
A	117	VAL	HG12	0.91	-1.0	1
A	118	ALA	HB3	1.37	-1.0	1
A	116	SER	CB	63.7	-1.0	1
A	6	GLN	CG	33.5	-1.0	1
A	111	LEU	HD23	0.84	-1.0	1
A	117	VAL	CB	32.8	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	107	SER	H	8.46	-1.0	1
A	120	LEU	HA	4.19	-1.0	1
A	110	LEU	HB2	1.58	-1.0	2
A	6	GLN	HA	4.26	-1.0	1
A	4	ALA	CB	18.6	-1.0	1
A	117	VAL	H	8.11	-1.0	1
A	112	THR	HG21	1.17	-1.0	1
A	106	SER	C	174.6	-1.0	1
A	118	ALA	CB	18.8	-1.0	1
A	115	PRO	CG	26.7	-1.0	1
A	117	VAL	CG1	20.7	-1.0	1
A	5	ALA	HB1	1.39	-1.0	1
A	110	LEU	H	8.22	-1.0	1
A	111	LEU	CA	54.7	-1.0	1
A	108	SER	HB2	3.85	-1.0	2
A	2	ALA	HA	4.24	-1.0	1
A	115	PRO	HG2	2.0	-1.0	2
A	111	LEU	HD13	0.91	-1.0	1
A	2	ALA	HB1	1.38	-1.0	1
A	3	ALA	HB1	1.39	-1.0	1
A	2	ALA	H	8.33	-1.0	1
A	4	ALA	N	122.2	-1.0	1
A	111	LEU	HG	1.6	-1.0	1
A	116	SER	CA	58.1	-1.0	1
A	111	LEU	N	123.0	-1.0	1
A	118	ALA	N	127.2	-1.0	1
A	4	ALA	CA	52.9	-1.0	1
A	5	ALA	CB	18.7	-1.0	1
A	110	LEU	HD21	0.86	-1.0	1
A	110	LEU	CG	27.1	-1.0	1
A	109	PRO	CD	50.5	-1.0	1
A	117	VAL	HG23	0.9	-1.0	1
A	118	ALA	CA	52.2	-1.0	1
A	119	GLU	H	8.25	-1.0	1
A	5	ALA	H	7.98	-1.0	1
A	115	PRO	CB	31.9	-1.0	1
A	5	ALA	HB2	1.39	-1.0	1
A	111	LEU	CB	42.1	-1.0	1
A	106	SER	HB2	3.89	-1.0	2
A	106	SER	H	8.45	-1.0	1
A	3	ALA	CA	52.6	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	112	THR	HA	4.39	-1.0	1
A	116	SER	HA	4.48	-1.0	1
A	109	PRO	HB3	2.27	-1.0	2
A	108	SER	CB	63.2	-1.0	1
A	117	VAL	HG13	0.91	-1.0	1
A	118	ALA	HB2	1.37	-1.0	1
A	109	PRO	HD2	3.72	-1.0	2
A	110	LEU	HD22	0.86	-1.0	1
A	6	GLN	CD	180.5	-1.0	1
A	110	LEU	CB	42.0	-1.0	1
A	111	LEU	HD22	0.84	-1.0	1
A	115	PRO	C	176.2	-1.0	1
A	113	SER	H	8.26	-1.0	1
A	117	VAL	CA	61.8	-1.0	1
A	117	VAL	HA	4.16	-1.0	1
A	113	SER	HB2	3.88	-1.0	2
A	115	PRO	CA	63.0	-1.0	1
A	107	SER	HB2	3.9	-1.0	2
A	114	GLY	HA2	4.14	-1.0	2
A	111	LEU	CG	26.8	-1.0	1
A	110	LEU	HD13	0.88	-1.0	1
A	116	SER	HB2	3.88	-1.0	2
A	119	GLU	HA	4.28	-1.0	1
A	3	ALA	CB	18.9	-1.0	1
A	108	SER	N	118.5	-1.0	1
A	114	GLY	H	8.23	-1.0	1
A	115	PRO	HA	4.47	-1.0	1
A	111	LEU	C	177.5	-1.0	1
A	3	ALA	HB2	1.39	-1.0	1
A	109	PRO	HA	4.42	-1.0	1
A	117	VAL	HB	2.08	-1.0	1
A	111	LEU	HB2	1.6	-1.0	2
A	5	ALA	C	178.0	-1.0	1
A	112	THR	HG23	1.17	-1.0	1
A	119	GLU	HG3	2.34	-1.0	2
A	117	VAL	HG22	0.9	-1.0	1
A	108	SER	HA	4.78	-1.0	1
A	113	SER	CA	58.0	-1.0	1
A	6	GLN	HB2	1.95	-1.0	2
A	5	ALA	HB3	1.39	-1.0	1
A	4	ALA	H	8.27	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1	MET	C	176.1	-1.0	1
A	120	LEU	CA	56.1	-1.0	1
A	113	SER	N	117.5	-1.0	1
A	112	THR	CG2	21.1	-1.0	1
A	116	SER	H	8.45	-1.0	1
A	112	THR	HB	4.26	-1.0	1
A	110	LEU	HG	1.58	-1.0	1
A	4	ALA	HB2	1.39	-1.0	1
A	110	LEU	CD1	24.7	-1.0	1
A	110	LEU	N	121.7	-1.0	1
A	107	SER	CB	63.8	-1.0	1
A	110	LEU	C	177.3	-1.0	1
A	2	ALA	N	125.6	-1.0	1
A	117	VAL	C	175.8	-1.0	1
A	4	ALA	C	178.0	-1.0	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	119	0.11 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	108	0.47 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	111	-0.26 ± 0.12	None needed (< 0.5 ppm)
^{15}N	111	0.34 ± 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 1061 atoms were assigned a chemical shift out of a possible 1158. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	467/475 (98%)	188/189 (99%)	188/194 (97%)	91/92 (99%)
Sidechain	547/604 (91%)	329/352 (93%)	207/227 (91%)	11/25 (44%)
Aromatic	47/79 (59%)	25/42 (60%)	21/35 (60%)	1/2 (50%)
Overall	1061/1158 (92%)	542/583 (93%)	416/456 (91%)	103/119 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1083 atoms were assigned a chemical shift out of a possible

1180. 25 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	477/485 (98%)	192/193 (99%)	192/198 (97%)	93/94 (99%)
Sidechain	559/616 (91%)	336/359 (94%)	212/232 (91%)	11/25 (44%)
Aromatic	47/79 (59%)	25/42 (60%)	21/35 (60%)	1/2 (50%)
Overall	1083/1180 (92%)	553/594 (93%)	425/465 (91%)	105/121 (87%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	70	LYS	HG2	-0.45	2.67 – 0.07	-7.0

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

