



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:01 AM BST

PDB ID : 2KUM
Title : Solution structure of the human chemokine CCL27
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Deposited on : 2010-02-22

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

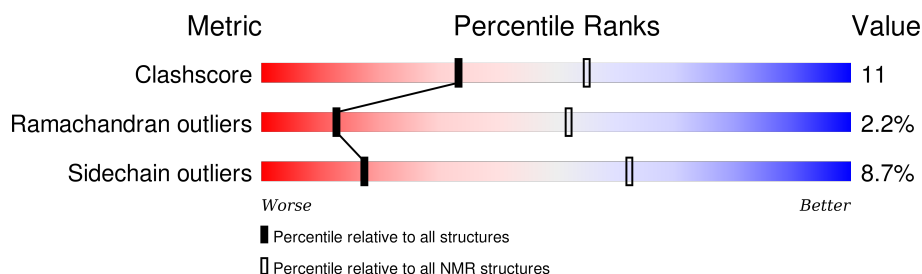
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	88	<div> <div></div> <div>49%</div> <div>24%</div> <div>27%</div> </div>

2 Ensemble composition and analysis

This entry contains 30 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:9-A:72 (64)	0.39	1

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1443 atoms, of which 731 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called C-C motif chemokine 27.

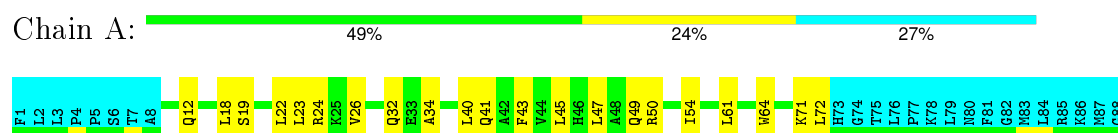
Mol	Chain	Residues	Atoms						Trace
1	A	88	Total	C	H	N	O	S	0
			1443	454	731	130	122	6	

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: C-C motif chemokine 27

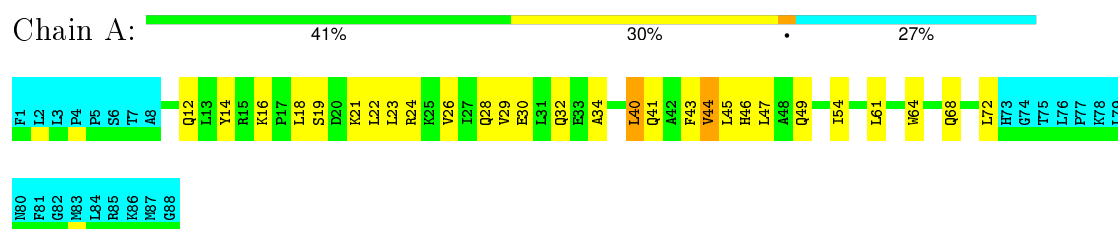


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

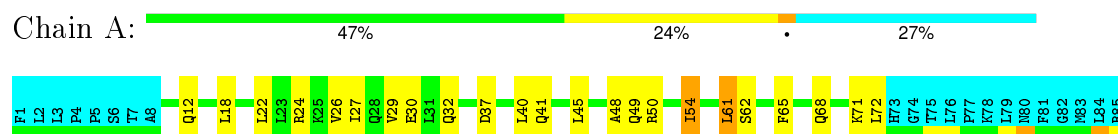
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: C-C motif chemokine 27



4.2.2 Score per residue for model 2

- Molecule 1: C-C motif chemokine 27



K86
K87
G88

4.2.3 Score per residue for model 3

- Molecule 1: C-C motif chemokine 27

Chain A: 51% 22% 27%

F1 L2 L3 P4 P5 S6 T7 A8 Q12 L18 S19 L22 L23 V26 E30 L31 Q32 D37 L40 Q41 L45 H46 L47 R50 L61 S62 Q63 R64 Q68 L72 H73 G74 T75 L76 L77 P77 K78 L79 N80 F81 G82 N83 L84 R85 K86 N87 G88

4.2.4 Score per residue for model 4

- Molecule 1: C-C motif chemokine 27

Chain A: 41% 31% 27%

F1 L2 L3 P4 P5 S6 T7 A8 C9 C10 T11 Q12 L13 Y14 R15 K16 P17 L18 L19 S19 L22 L23 V26 A34 Q41 A42 F43 H46 L47 A48 Q49 C53 I54 R55 P56 Q57 S60 L61 W64 F65 E66 H67 Q68 K71 L72 H73 G74 T75 L76 L77 P77 K78 L79

N80 F81 G82 N83 L84 R85 K86 N87 G88

4.2.5 Score per residue for model 5

- Molecule 1: C-C motif chemokine 27

Chain A: 41% 28% 27%

F1 L2 L3 P4 P5 S6 T7 A8 C9 C10 T11 Q12 L13 Y14 R15 K16 P17 L18 L19 S19 D20 K21 L22 L23 R24 V26 Q32 D35 F43 V44 L45 H46 L47 A48 Q49 R50 I54 S60 L61 W64 F65 E66 H67 K71 L72 H73 G74 T75 L76 L77 P77 K78 N80

F81 G82 N83 L84 R85 K86 N87 G88

4.2.6 Score per residue for model 6

- Molecule 1: C-C motif chemokine 27

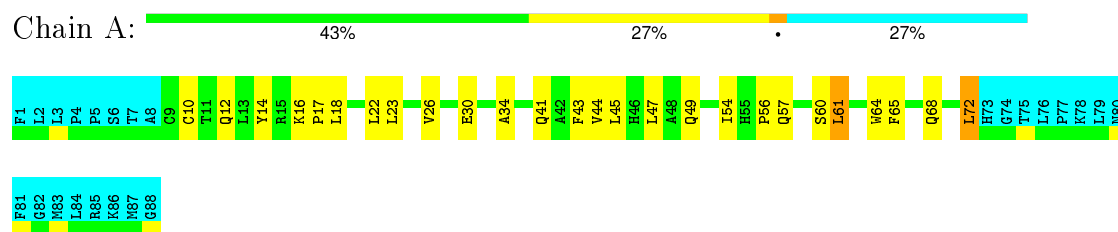
Chain A: 45% 24% 27%

F1 L2 L3 P4 P5 S6 T7 A8 Q12 R15 L18 S19 D20 K21 L22 L23 R24 V26 E30 L31 Q32 E33 A34 D35 Q41 V44 L45 H46 L47 A48 Q49 I54 H55 N58 L61 H67 K71 L72 H73 G74 T75 L76 L77 P77 K78 L79 N80 F81 G82

N83 L84 R85 K86 N87 G88

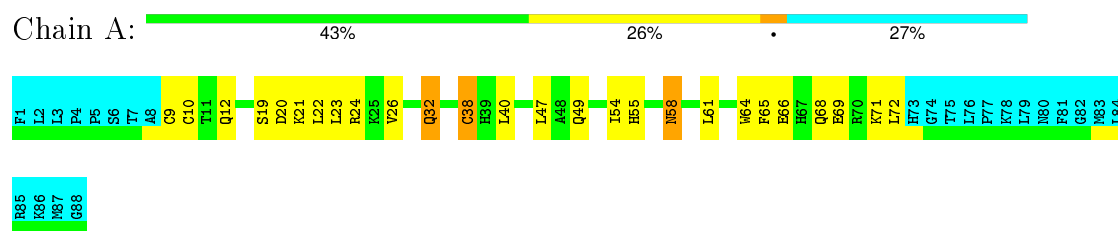
4.2.7 Score per residue for model 7

- Molecule 1: C-C motif chemokine 27



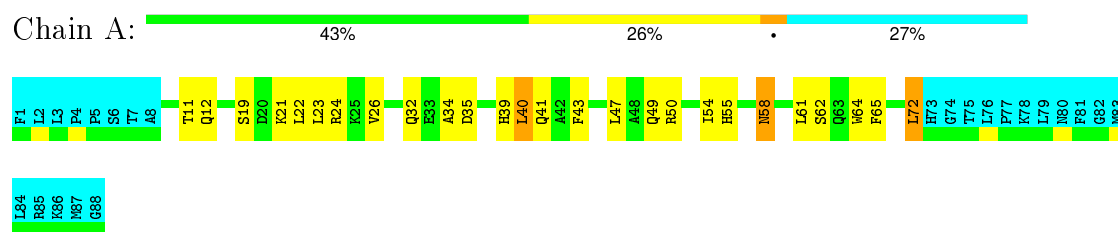
4.2.8 Score per residue for model 8

- Molecule 1: C-C motif chemokine 27



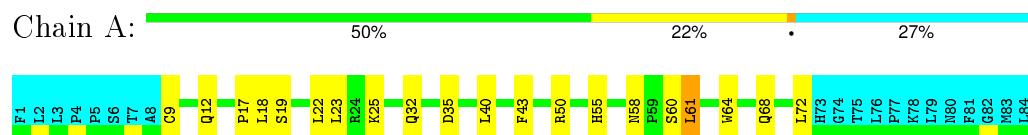
4.2.9 Score per residue for model 9

- Molecule 1: C-C motif chemokine 27



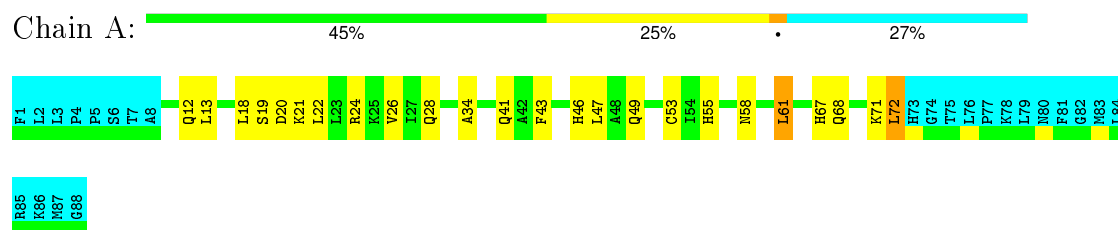
4.2.10 Score per residue for model 10

- Molecule 1: C-C motif chemokine 27



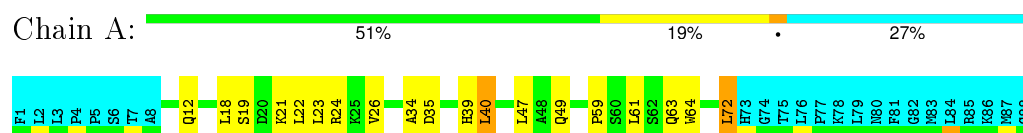
4.2.11 Score per residue for model 11

- Molecule 1: C-C motif chemokine 27



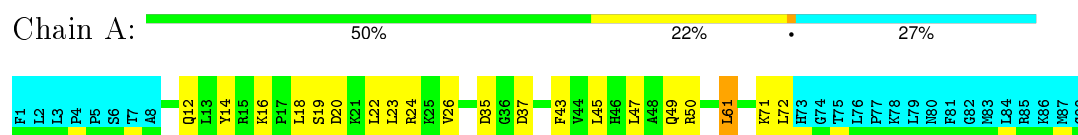
4.2.12 Score per residue for model 12

- Molecule 1: C-C motif chemokine 27



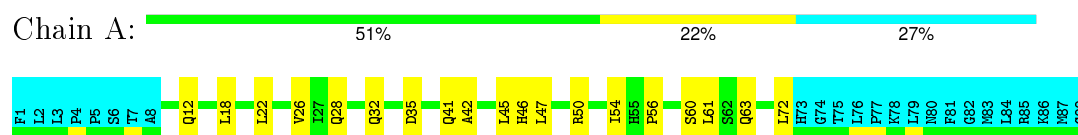
4.2.13 Score per residue for model 13

- Molecule 1: C-C motif chemokine 27



4.2.14 Score per residue for model 14

- Molecule 1: C-C motif chemokine 27



4.2.15 Score per residue for model 15

- Molecule 1: C-C motif chemokine 27

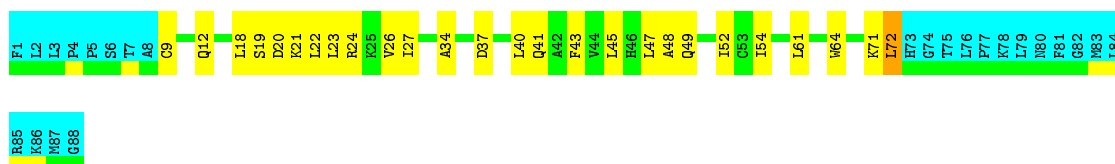




4.2.16 Score per residue for model 16

- Molecule 1: C-C motif chemokine 27

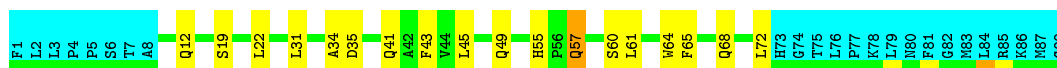
Chain A: 43% 28% 27%



4.2.17 Score per residue for model 17

- Molecule 1: C-C motif chemokine 27

Chain A: 52% 19% 27%



4.2.18 Score per residue for model 18

- Molecule 1: C-C motif chemokine 27

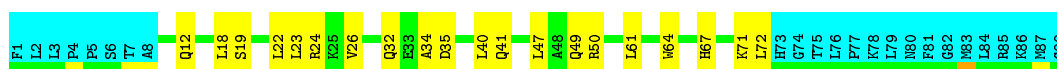
Chain A: 56% 16% 27%



4.2.19 Score per residue for model 19

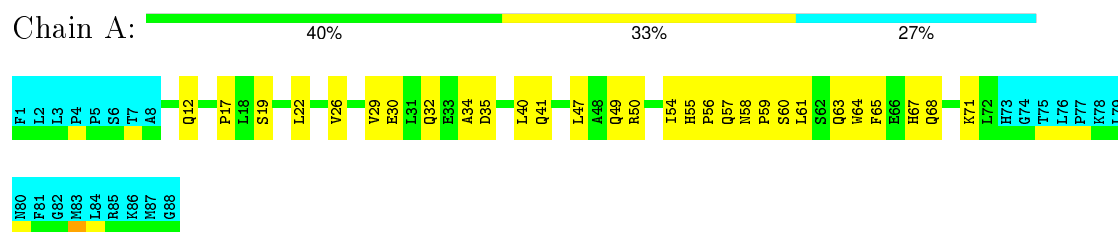
- Molecule 1: C-C motif chemokine 27

Chain A: 50% 23% 27%



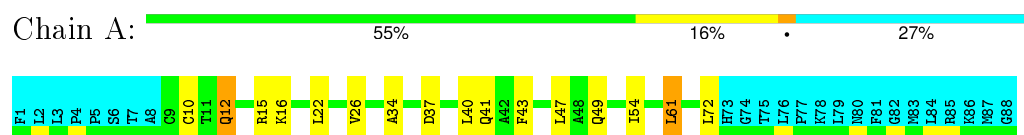
4.2.20 Score per residue for model 20

- Molecule 1: C-C motif chemokine 27



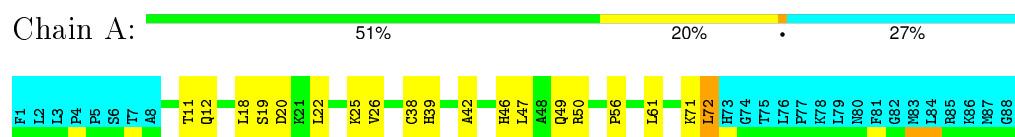
4.2.21 Score per residue for model 21

- Molecule 1: C-C motif chemokine 27



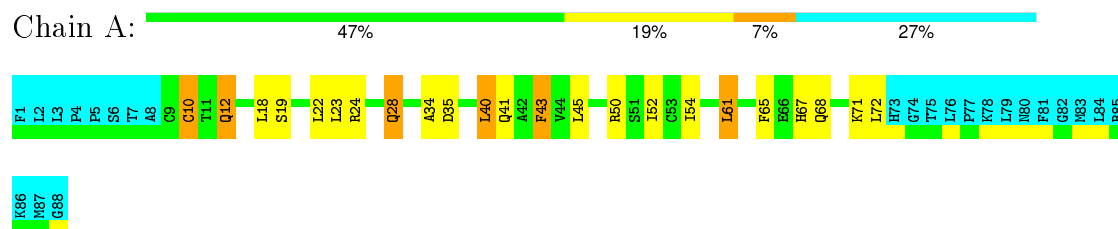
4.2.22 Score per residue for model 22

- Molecule 1: C-C motif chemokine 27



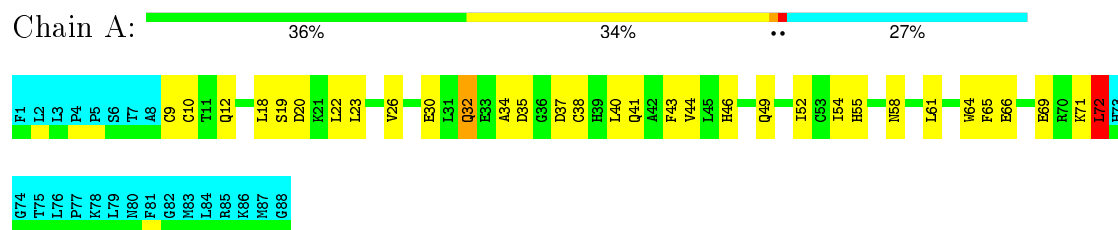
4.2.23 Score per residue for model 23

- Molecule 1: C-C motif chemokine 27



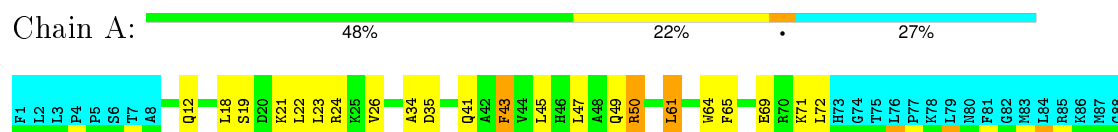
4.2.24 Score per residue for model 24

- Molecule 1: C-C motif chemokine 27



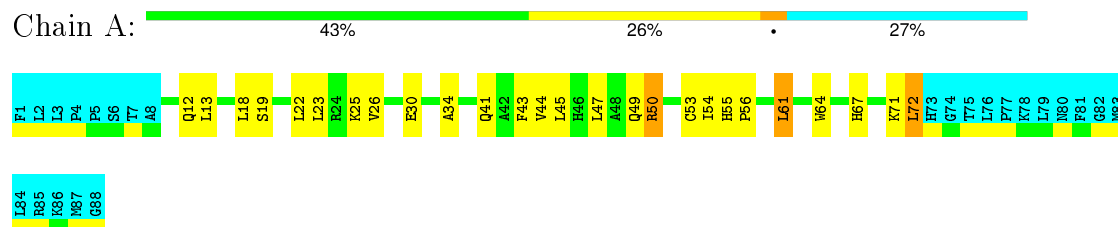
4.2.25 Score per residue for model 25

- Molecule 1: C-C motif chemokine 27



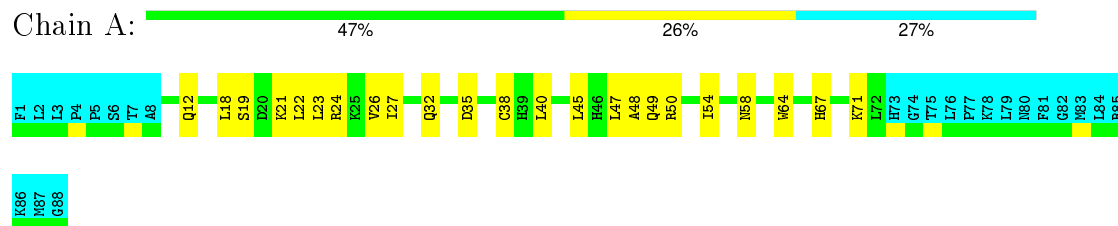
4.2.26 Score per residue for model 26

- Molecule 1: C-C motif chemokine 27



4.2.27 Score per residue for model 27

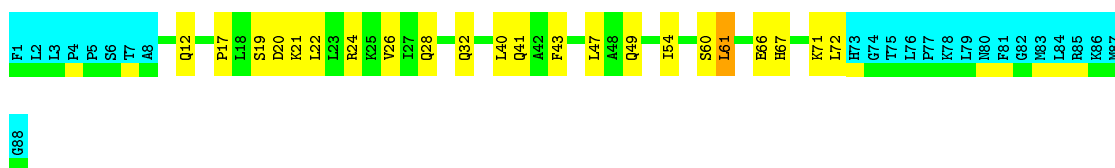
- Molecule 1: C-C motif chemokine 27



4.2.28 Score per residue for model 28

- Molecule 1: C-C motif chemokine 27

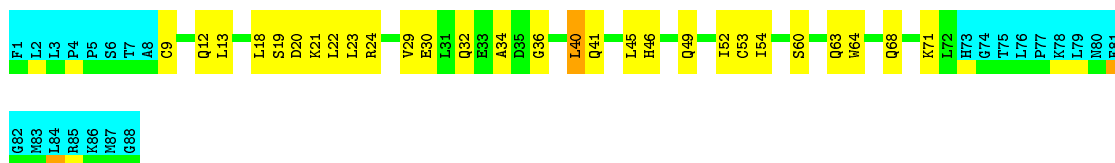




4.2.29 Score per residue for model 29

- Molecule 1: C-C motif chemokine 27

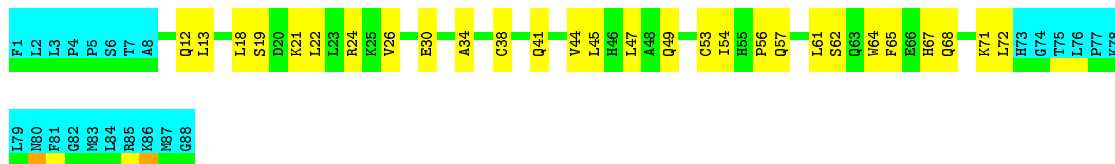
Chain A: 41% 31% 27%



4.2.30 Score per residue for model 30

- Molecule 1: C-C motif chemokine 27

Chain A: 41% 32% 27%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics, molecular dynamics*.

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	1.2
CNS	structure solution	1.1
CNS	refinement	1.1

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 16839
Number of chemical shift lists	1
Total number of shifts	1167
Number of shifts mapped to atoms	1167
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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

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	528	531	527	12±3
All	All	15840	15930	15810	345

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:VAL:HG22	1:A:47:LEU:HG	0.84	1.49	1	15
1:A:30:GLU:HB2	1:A:44:VAL:HB	0.76	1.54	26	1
1:A:18:LEU:HB3	1:A:22:LEU:HD11	0.73	1.60	5	13
1:A:26:VAL:HA	1:A:47:LEU:HA	0.72	1.61	30	14
1:A:17:PRO:HA	1:A:60:SER:HB2	0.71	1.62	4	3
1:A:43:PHE:HB3	1:A:61:LEU:HG	0.71	1.59	10	8
1:A:47:LEU:HB2	1:A:50:ARG:HB2	0.70	1.61	27	2
1:A:9:CYS:HA	1:A:32:GLN:OE1	0.69	1.87	18	2
1:A:18:LEU:HD12	1:A:45:LEU:HD12	0.63	1.67	23	14
1:A:17:PRO:HA	1:A:60:SER:OG	0.62	1.94	20	2
1:A:67:HIS:O	1:A:71:LYS:HB2	0.62	1.95	6	11
1:A:28:GLN:HE21	1:A:28:GLN:HA	0.61	1.56	23	1
1:A:23:LEU:HB3	1:A:64:TRP:CH2	0.60	2.31	3	2
1:A:32:GLN:O	1:A:41:GLN:HA	0.59	1.97	3	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:TRP:O	1:A:68:GLN:HG2	0.58	1.98	15	4
1:A:26:VAL:HB	1:A:64:TRP:CZ2	0.58	2.33	27	2
1:A:19:SER:O	1:A:22:LEU:HG	0.58	1.97	6	24
1:A:55:HIS:O	1:A:58:ASN:HB2	0.58	1.98	24	7
1:A:17:PRO:HA	1:A:60:SER:HB3	0.58	1.74	10	1
1:A:21:LYS:O	1:A:24:ARG:HG2	0.57	1.99	28	13
1:A:9:CYS:HA	1:A:38:CYS:HB2	0.57	1.77	24	1
1:A:15:ARG:HG3	1:A:16:LYS:H	0.57	1.60	21	1
1:A:65:PHE:HA	1:A:68:GLN:HE21	0.57	1.58	23	4
1:A:13:LEU:HD23	1:A:53:CYS:SG	0.57	2.40	30	4
1:A:72:LEU:H	1:A:72:LEU:HD13	0.56	1.59	6	2
1:A:23:LEU:HB3	1:A:64:TRP:CZ3	0.56	2.35	5	14
1:A:24:ARG:HB3	1:A:71:LYS:HD3	0.56	1.77	25	6
1:A:14:TYR:CE2	1:A:16:LYS:HB2	0.56	2.35	13	5
1:A:43:PHE:CB	1:A:61:LEU:HG	0.55	2.31	7	9
1:A:64:TRP:CH2	1:A:72:LEU:HD11	0.55	2.37	19	2
1:A:23:LEU:HG	1:A:64:TRP:CZ3	0.54	2.37	9	2
1:A:30:GLU:HG3	1:A:44:VAL:HB	0.53	1.78	7	3
1:A:28:GLN:HB2	1:A:46:HIS:HB3	0.53	1.80	11	4
1:A:20:ASP:OD1	1:A:71:LYS:HE3	0.53	2.03	13	7
1:A:64:TRP:CH2	1:A:72:LEU:HD21	0.53	2.39	1	1
1:A:64:TRP:CZ2	1:A:72:LEU:HD21	0.53	2.39	16	4
1:A:42:ALA:HA	1:A:56:PRO:HG3	0.53	1.80	14	1
1:A:9:CYS:HA	1:A:32:GLN:NE2	0.52	2.18	10	1
1:A:10:CYS:O	1:A:40:LEU:HD21	0.52	2.04	24	1
1:A:65:PHE:HA	1:A:68:GLN:OE1	0.52	2.05	20	1
1:A:29:VAL:HG21	1:A:68:GLN:HE22	0.52	1.64	29	3
1:A:64:TRP:CE2	1:A:68:GLN:HB3	0.51	2.41	15	4
1:A:12:GLN:O	1:A:53:CYS:HB2	0.50	2.06	4	1
1:A:34:ALA:HB2	1:A:41:GLN:HB2	0.50	1.84	30	16
1:A:22:LEU:HA	1:A:25:LYS:NZ	0.50	2.21	22	1
1:A:72:LEU:N	1:A:72:LEU:HD13	0.50	2.20	15	2
1:A:32:GLN:NE2	1:A:40:LEU:HB3	0.49	2.23	10	1
1:A:42:ALA:HA	1:A:56:PRO:HD3	0.49	1.83	22	1
1:A:45:LEU:HD21	1:A:61:LEU:HD13	0.49	1.85	17	1
1:A:43:PHE:O	1:A:54:ILE:HB	0.49	2.07	24	7
1:A:30:GLU:HG3	1:A:44:VAL:HG22	0.49	1.85	1	1
1:A:59:PRO:O	1:A:63:GLN:HG3	0.48	2.08	12	1
1:A:67:HIS:O	1:A:71:LYS:HG3	0.48	2.07	23	2
1:A:32:GLN:OE1	1:A:38:CYS:HB2	0.48	2.08	27	1
1:A:9:CYS:HA	1:A:38:CYS:CB	0.47	2.39	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:HD13	1:A:40:LEU:H	0.47	1.69	23	1
1:A:54:ILE:HD11	1:A:58:ASN:HD22	0.47	1.68	27	1
1:A:62:SER:O	1:A:65:PHE:HB2	0.47	2.09	30	1
1:A:68:GLN:HB2	1:A:72:LEU:HD22	0.47	1.85	3	1
1:A:47:LEU:HB2	1:A:50:ARG:O	0.47	2.10	25	2
1:A:32:GLN:NE2	1:A:40:LEU:HG	0.47	2.25	1	1
1:A:32:GLN:HG2	1:A:40:LEU:O	0.46	2.11	10	3
1:A:10:CYS:SG	1:A:12:GLN:NE2	0.45	2.89	5	4
1:A:56:PRO:O	1:A:57:GLN:HB2	0.45	2.11	30	4
1:A:30:GLU:CG	1:A:44:VAL:HB	0.44	2.42	24	1
1:A:14:TYR:CE2	1:A:16:LYS:HE2	0.44	2.47	4	1
1:A:32:GLN:NE2	1:A:38:CYS:HB3	0.44	2.28	8	2
1:A:18:LEU:HD21	1:A:52:ILE:HG21	0.44	1.89	24	5
1:A:17:PRO:HA	1:A:60:SER:CB	0.44	2.40	28	1
1:A:71:LYS:O	1:A:72:LEU:HD22	0.44	2.12	15	1
1:A:26:VAL:O	1:A:72:LEU:HG	0.44	2.12	3	4
1:A:31:LEU:HD13	1:A:43:PHE:CZ	0.44	2.48	17	1
1:A:24:ARG:HB3	1:A:71:LYS:HD2	0.43	1.90	6	1
1:A:26:VAL:O	1:A:72:LEU:HD12	0.43	2.13	2	1
1:A:45:LEU:HD22	1:A:45:LEU:N	0.43	2.28	29	1
1:A:71:LYS:HB3	1:A:72:LEU:HD13	0.43	1.89	15	1
1:A:65:PHE:O	1:A:68:GLN:HG2	0.43	2.13	2	1
1:A:26:VAL:HA	1:A:47:LEU:HG	0.43	1.91	4	1
1:A:60:SER:HA	1:A:63:GLN:OE1	0.43	2.14	14	2
1:A:15:ARG:HG3	1:A:16:LYS:N	0.43	2.28	21	1
1:A:15:ARG:HA	1:A:58:ASN:OD1	0.43	2.13	6	1
1:A:64:TRP:HZ2	1:A:72:LEU:HD11	0.43	1.72	3	1
1:A:54:ILE:HD13	1:A:60:SER:HB2	0.43	1.88	5	1
1:A:22:LEU:HA	1:A:25:LYS:HD3	0.43	1.90	26	2
1:A:27:ILE:HD13	1:A:48:ALA:HA	0.42	1.90	2	2
1:A:19:SER:O	1:A:23:LEU:HG	0.42	2.13	25	4
1:A:64:TRP:CZ2	1:A:68:GLN:HB3	0.42	2.50	8	1
1:A:24:ARG:CB	1:A:71:LYS:HD3	0.42	2.43	25	1
1:A:60:SER:O	1:A:64:TRP:HB2	0.42	2.14	20	1
1:A:72:LEU:N	1:A:72:LEU:HD22	0.42	2.28	22	1
1:A:39:HIS:O	1:A:40:LEU:HB3	0.42	2.15	12	1
1:A:62:SER:HA	1:A:65:PHE:CD2	0.42	2.49	2	2
1:A:39:HIS:O	1:A:40:LEU:HB2	0.42	2.15	9	1
1:A:61:LEU:O	1:A:64:TRP:HB3	0.41	2.15	10	2
1:A:28:GLN:OE1	1:A:28:GLN:HA	0.41	2.15	28	1
1:A:9:CYS:HB2	1:A:37:ASP:OD1	0.41	2.15	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ILE:HD13	1:A:48:ALA:HB2	0.41	1.91	27	1
1:A:54:ILE:HG21	1:A:61:LEU:HD23	0.41	1.93	2	1
1:A:26:VAL:O	1:A:72:LEU:HD21	0.41	2.16	11	1
1:A:23:LEU:HA	1:A:26:VAL:HG23	0.41	1.93	27	1
1:A:60:SER:HA	1:A:63:GLN:CG	0.41	2.46	20	1
1:A:18:LEU:CD1	1:A:54:ILE:HD11	0.40	2.46	24	1
1:A:34:ALA:HA	1:A:40:LEU:O	0.40	2.16	20	1
1:A:66:GLU:O	1:A:69:GLU:HB3	0.40	2.16	24	2
1:A:54:ILE:HG23	1:A:58:ASN:CB	0.40	2.46	24	1
1:A:55:HIS:HB3	1:A:57:GLN:HE22	0.40	1.75	17	1
1:A:59:PRO:O	1:A:63:GLN:HG2	0.40	2.17	20	1
1:A:38:CYS:SG	1:A:39:HIS:N	0.40	2.94	22	1
1:A:68:GLN:HA	1:A:72:LEU:CD2	0.40	2.47	1	1
1:A:55:HIS:CD2	1:A:56:PRO:HD2	0.40	2.51	26	1

6.3 Torsion angles

6.3.1 Protein backbone

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	64/88 (73%)	57±2 (89±3%)	6±2 (9±3%)	1±1 (2±1%)	13	52
All	All	1920/2640 (73%)	1705 (89%)	172 (9%)	43 (2%)	13	52

All 6 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	72	LEU	19
1	A	35	ASP	14
1	A	37	ASP	5
1	A	40	LEU	3
1	A	36	GLY	1
1	A	34	ALA	1

6.3.2 Protein sidechains ⓘ

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	60/80 (75%)	55±2 (91±3%)	5±2 (9±3%)	17 62
All	All	1800/2400 (75%)	1643 (91%)	157 (9%)	17 62

All 27 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	12	GLN	30
1	A	61	LEU	26
1	A	49	GLN	26
1	A	50	ARG	12
1	A	40	LEU	10
1	A	54	ILE	10
1	A	72	LEU	6
1	A	22	LEU	5
1	A	30	GLU	3
1	A	46	HIS	3
1	A	58	ASN	3
1	A	43	PHE	2
1	A	10	CYS	2
1	A	11	THR	2
1	A	38	CYS	2
1	A	60	SER	2
1	A	9	CYS	2
1	A	32	GLN	2
1	A	62	SER	1
1	A	44	VAL	1
1	A	68	GLN	1
1	A	20	ASP	1
1	A	28	GLN	1
1	A	70	ARG	1
1	A	29	VAL	1
1	A	57	GLN	1
1	A	71	LYS	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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16839

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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	1167
Number of shifts mapped to atoms	1167
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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
$^{13}\text{C}_\alpha$	88	0.07 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	84	0.19 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	80	0.15 ± 0.16	None needed (< 0.5 ppm)
^{15}N	79	-0.03 ± 0.52	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 91%, i.e. 777 atoms were assigned a chemical shift out of a possible 855. 1 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	306/314 (97%)	123/125 (98%)	124/128 (97%)	59/61 (97%)
Sidechain	425/471 (90%)	262/279 (94%)	150/167 (90%)	13/25 (52%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	46/70 (66%)	24/36 (67%)	21/25 (84%)	1/9 (11%)
Overall	777/855 (91%)	409/440 (93%)	295/320 (92%)	73/95 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1052 atoms were assigned a chemical shift out of a possible 1156. 1 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	414/428 (97%)	167/170 (98%)	168/176 (95%)	79/82 (96%)
Sidechain	573/632 (91%)	353/376 (94%)	205/225 (91%)	15/31 (48%)
Aromatic	65/96 (68%)	34/50 (68%)	30/35 (86%)	1/11 (9%)
Overall	1052/1156 (91%)	554/596 (93%)	403/436 (92%)	95/124 (77%)

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	24	ARG	NE	109.13	92.63 – 76.73	15.4
1	A	85	ARG	NE	108.72	92.63 – 76.73	15.1
1	A	70	ARG	NE	108.62	92.63 – 76.73	15.1
1	A	50	ARG	NE	108.54	92.63 – 76.73	15.0
1	A	15	ARG	NE	108.52	92.63 – 76.73	15.0

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:

