Full wwPDB NMR Structure Validation Report (i)

May 7, 2024 – 01:52 pm BST

PDB ID	:	2BL5
Title	:	Solution structure of the KH-QUA2 region of the Xenopus STAR-GSG Quaking protein.
Authors	:	Maguire, M.L.; Guler-Gane, G.; Nietlispach, D.; Raine, A.R.C.; Zorn, A.M.; Standart, N.; Broadhurst, R.W.
Deposited on	:	2005-03-01

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

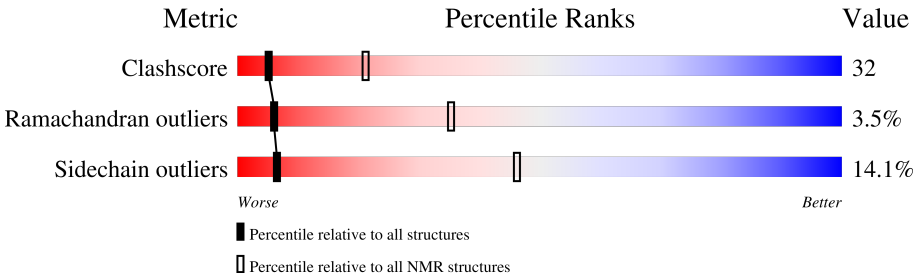
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	140	29% 49% • • 14% •

2 Ensemble composition and analysis (i)

This entry contains 17 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:1-A:101 (101)	0.64	1
2	A:107-A:121 (15)	1.78	16

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 6, 7, 8, 9, 10, 11, 12, 14, 16, 17
2	2, 15
3	5, 13

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2189 atoms, of which 1120 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MGC83862 PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	135	2189	673	1120	193	198	5	1

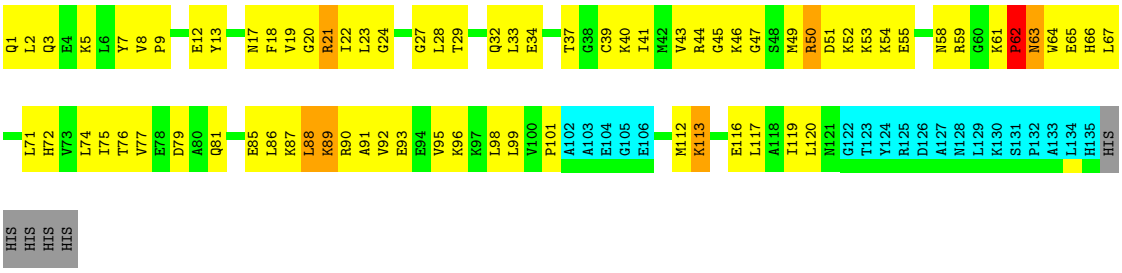
4 Residue-property plots (i)

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: MGC83862 PROTEIN

Chain A: 29% 49% • • 14% •



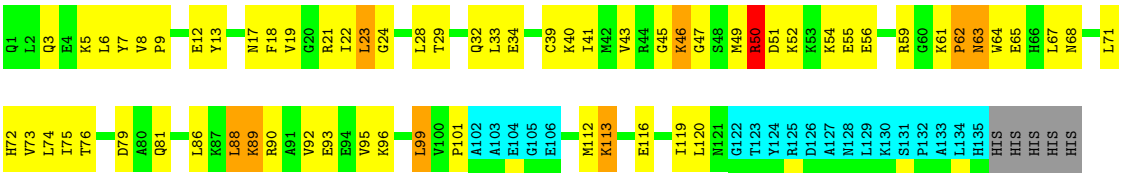
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: MGC83862 PROTEIN

Chain A: 36% 40% 6% • 14% •



4.2.2 Score per residue for model 2

• Molecule 1: MGC83862 PROTEIN

Chain A: 31% 46% 6% 14% •

Q1 L2 Q3 E4 K5 L6 Y7 V8 P9 E12 N17 F18 V19 G20 R21 I22 L23 G24 P25 R26 G27 L28 T29 Q32 L33 E34 T37 G38 C39 K40 I41 M42 V43 R44 G45 K46 G47 S48 M49 R50 D51 K52 K53 K54 E55 E56 Q57 N58 R59 G60 K61 P62 N63 W64 E65 H66

L67 N68 L71 H72 V73 L74 I75 T76 V77 N82 R83 A84 E85 L86 K87 L88 K89 R90 A91 V92 E93 E94 V95 K96 L99 A102 A103 E104 G105 E106 K110 K111 M112 K113 E116 L117 A118 I119 L120 N121 G122 T123 Y124 R125 D126 A127 N128 L129 K130 S131 P132 A133 L134 H135

HIS HIS HIS HIS HIS

4.2.3 Score per residue for model 3

- Molecule 1: MGC83862 PROTEIN

Chain A: 30% 42% 11% 14% •

Q1 L2 Q3 E4 K5 L6 Y7 V8 Y13 N17 F18 V19 G20 R21 I22 L23 G24 P25 R26 G27 L28 T29 Q32 L33 E34 T37 G38 C39 K40 I41 M42 V43 R44 G45 K46 G47 S48 M49 R50 D51 K52 K53 K54 E55 E56 Q57 N58 R59 G60 K61 P62 N63 W64 E65 H66 L67

N68 L71 H72 V73 L74 I75 T76 V77 E78 D79 E85 L86 K87 L88 K89 R90 A91 V95 L98 L99 V100 P101 A102 A103 E104 G105 E106 L109 M112 K113 E116 L117 A118 I119 L120 N121 G122 T123 Y124 R125 D126 A127 N128 L129 K130 S131 P132 A133 L134 H135 HIS HIS HIS

HIS HIS

4.2.4 Score per residue for model 4

- Molecule 1: MGC83862 PROTEIN

Chain A: 41% 41% • 14% •

Q1 L2 Q3 E4 K5 L6 Y7 V8 P9 E12 Y13 F18 R21 I22 L23 R26 G27 L28 T29 Q32 L33 E34 T37 G38 C39 K40 V43 R44 G45 M49 R50 D51 K52 K53 K54 E55 R59 P62 N63 W64 E65 H66 L71 H72 V73 L74 I75 D79

A80 Q81 E85 L86 K87 L88 K89 R90 A91 V92 V95 L98 L99 V100 P101 A102 A103 E104 G105 E106 K110 K111 M112 K113 E116 G122 T123 Y124 R125 D126 A127 N128 L129 K130 S131 P132 A133 L134 H135 HIS HIS HIS HIS HIS

4.2.5 Score per residue for model 5

- Molecule 1: MGC83862 PROTEIN

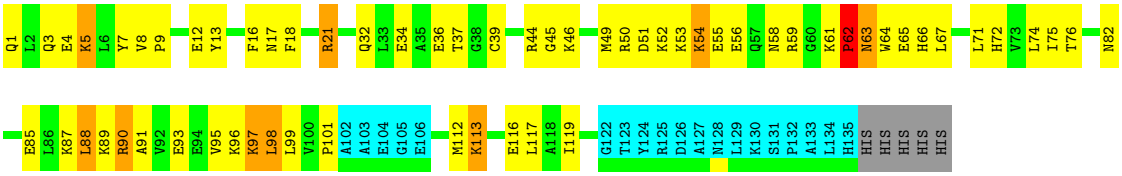
Chain A: 36% 39% 7% • 14% •

Q1 L2 Q3 E4 K5 V8 P9 E12 N17 F18 V19 G20 R21 I22 L23 G24 G27 L28 T29 Q32 L33 E34 A35 E36 T37 G38 C39 K40 I41 R44 G45 K46 G47 S48 M49 R50 D51 K52 K53 K54 E55 R59 G60 K61 P62 N63 W64 E65 H66 L67 L71

4.2.6 Score per residue for model 6

- Molecule 1: MGC83862 PROTEIN

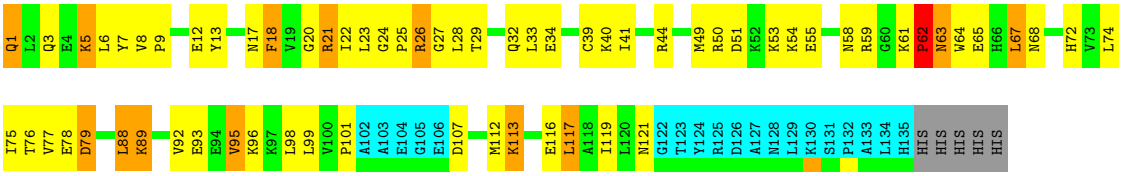
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: MGC83862 PROTEIN

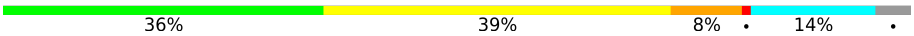
Chain A:

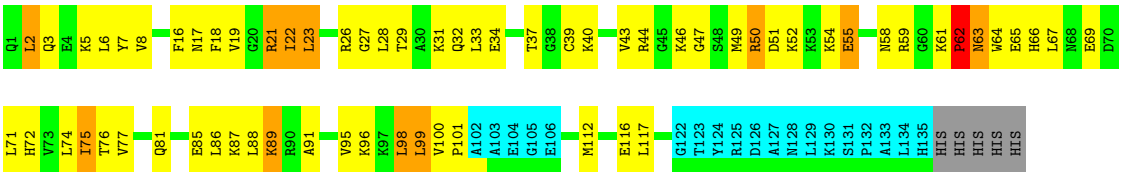


4.2.8 Score per residue for model 8

- Molecule 1: MGC83862 PROTEIN

Chain A:

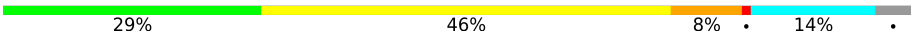


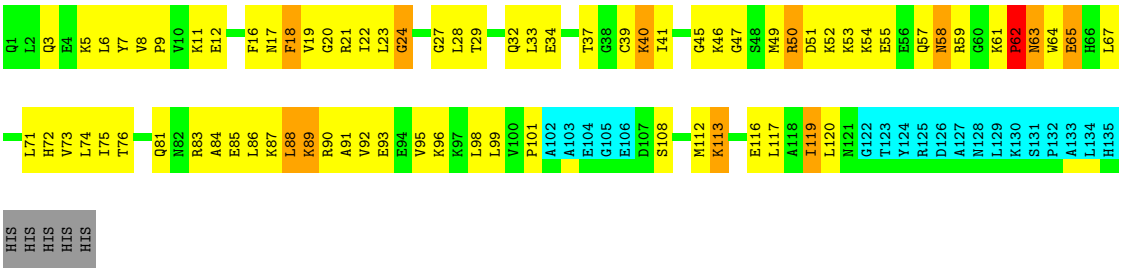


4.2.9 Score per residue for model 9

- Molecule 1: MGC83862 PROTEIN

Chain A:

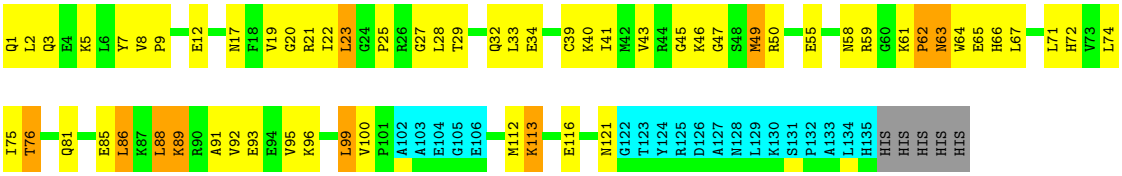




4.2.10 Score per residue for model 10

- Molecule 1: MGC83862 PROTEIN

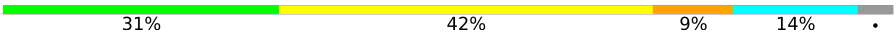
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: MGC83862 PROTEIN

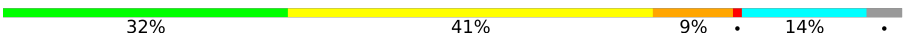
Chain A:

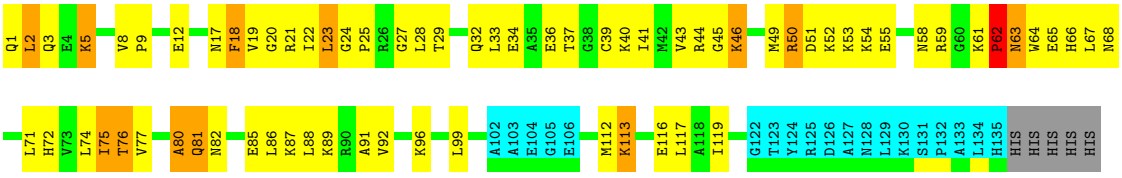


4.2.12 Score per residue for model 12

- Molecule 1: MGC83862 PROTEIN

Chain A:

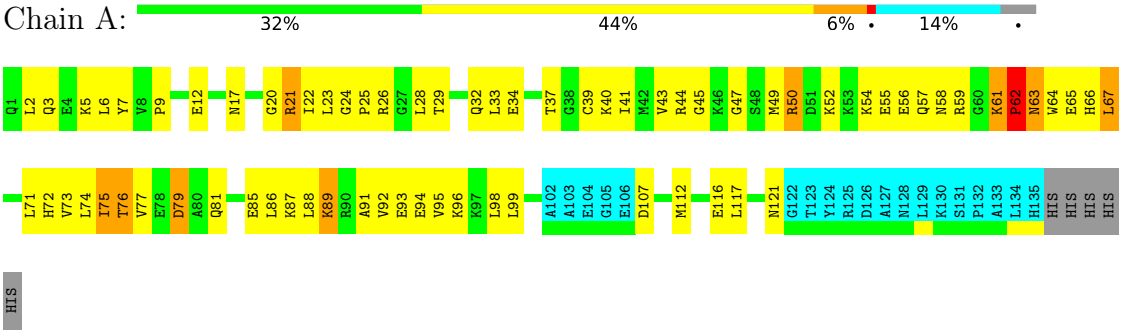




4.2.13 Score per residue for model 13

- Molecule 1: MGC83862 PROTEIN

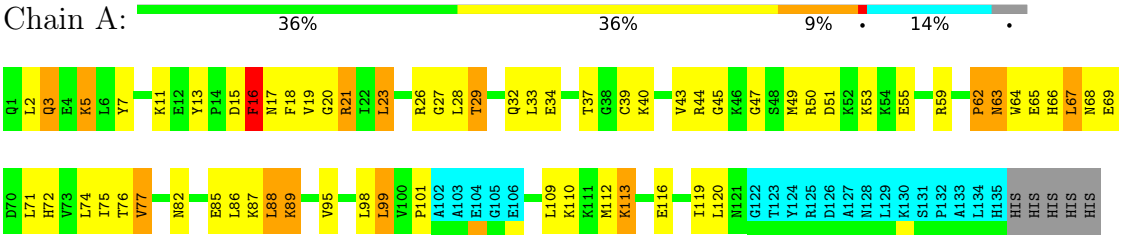
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: MGC83862 PROTEIN

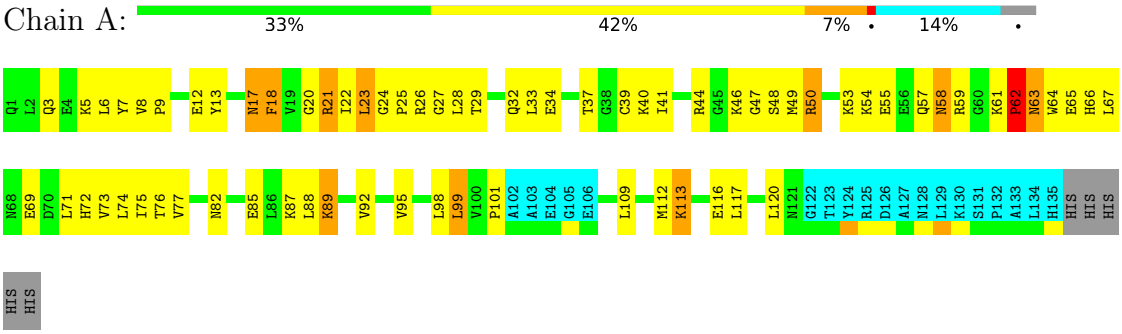
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: MGC83862 PROTEIN

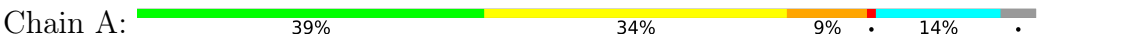
Chain A:

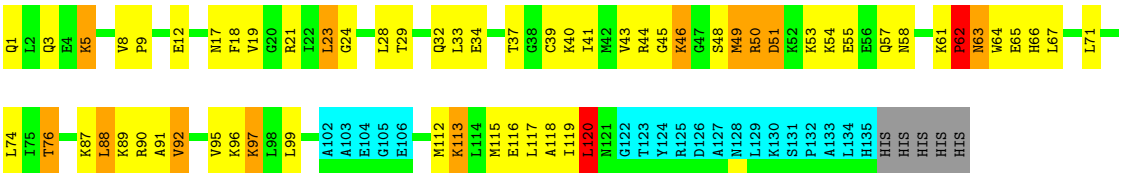


4.2.16 Score per residue for model 16

- Molecule 1: MGC83862 PROTEIN

Chain A:

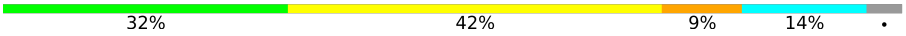


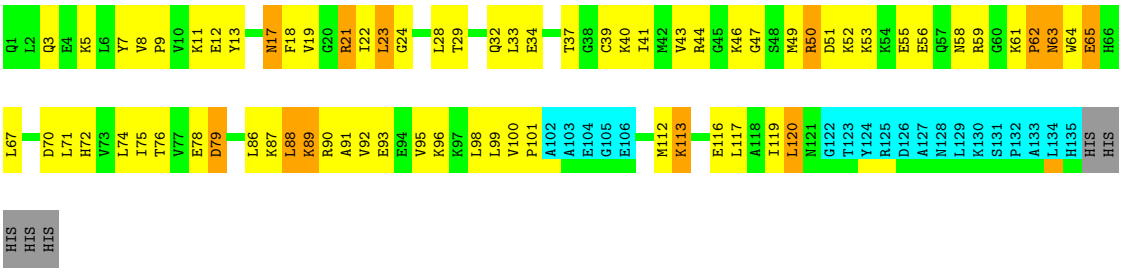


4.2.17 Score per residue for model 17

- Molecule 1: MGC83862 PROTEIN

Chain A:





5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 17 were deposited, based on the following criterion: *NO DISTANCE RESTRAINT VIOLATIONS GREATER THAN 0.5 ANGSTROMS AND NO DIHEDRAL ANGLE RESTRAINT VIOLATIONS GREATER THAN 5 DEGREES*.

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

Software name	Classification	Version
ARIA	refinement	1.2
ANSIG	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.46±0.05	1±1/951 (0.1± 0.1%)	0.50±0.02	0±0/1273 (0.0± 0.0%)
All	All	0.46	13/16167 (0.1%)	0.50	2/21641 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	18	PHE	CE2-CZ	8.94	1.54	1.37	12	8
1	A	18	PHE	CE1-CZ	-7.77	1.22	1.37	12	4
1	A	16	PHE	CE2-CZ	5.08	1.47	1.37	14	1

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	62	PRO	N-CA-CB	-5.22	96.86	102.60	8	2

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	16	PHE	Sidechain	1

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	938	996	994	62±7
All	All	15946	16932	16898	1059

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:MET:HA	1:A:116:GLU:HB2	1.01	1.29	10	16
1:A:62:PRO:HA	1:A:65:GLU:HB3	1.00	1.32	2	17
1:A:39:CYS:HB2	1:A:88:LEU:HD22	0.98	1.34	1	5
1:A:49:MET:HB2	1:A:63:ASN:HB3	0.95	1.39	11	12
1:A:3:GLN:HB3	1:A:74:LEU:HD11	0.94	1.39	9	4
1:A:49:MET:HA	1:A:64:TRP:CZ3	0.94	1.97	15	2
1:A:108:SER:HA	1:A:112:MET:HB3	0.93	1.41	5	1
1:A:5:LYS:HG3	1:A:74:LEU:HD12	0.90	1.43	13	4
1:A:49:MET:HG2	1:A:63:ASN:HB3	0.90	1.43	10	2
1:A:64:TRP:HA	1:A:67:LEU:HB2	0.86	1.47	7	9
1:A:34:GLU:HB3	1:A:40:LYS:HA	0.83	1.49	10	16
1:A:3:GLN:HB3	1:A:74:LEU:HD21	0.83	1.51	10	10
1:A:21:ARG:HH12	1:A:22:ILE:HG12	0.83	1.33	9	1
1:A:6:LEU:HD13	1:A:96:LYS:HD3	0.83	1.49	8	1
1:A:39:CYS:HB3	1:A:88:LEU:HD22	0.82	1.48	10	3
1:A:37:THR:HA	1:A:87:LYS:HD3	0.81	1.52	15	6
1:A:49:MET:HB3	1:A:54:LYS:HD3	0.80	1.54	1	5
1:A:54:LYS:HA	1:A:58:ASN:HB2	0.79	1.52	16	1
1:A:23:LEU:HD21	1:A:43:VAL:HG21	0.78	1.55	4	1
1:A:37:THR:HA	1:A:87:LYS:HD2	0.77	1.56	17	5
1:A:21:ARG:NH1	1:A:22:ILE:HG12	0.77	1.93	9	1
1:A:21:ARG:CZ	1:A:99:LEU:HA	0.76	2.09	9	3
1:A:2:LEU:HG	1:A:77:VAL:HG12	0.76	1.55	5	1
1:A:112:MET:HA	1:A:116:GLU:HG3	0.76	1.58	5	1
1:A:50:ARG:HD3	1:A:67:LEU:HD11	0.75	1.58	3	1
1:A:61:LYS:HB2	1:A:62:PRO:HD2	0.74	1.59	2	4
1:A:45:GLY:HA3	1:A:71:LEU:HA	0.74	1.58	6	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ASP:HB2	1:A:54:LYS:HD3	0.74	1.56	9	1
1:A:52:LYS:HA	1:A:55:GLU:HG2	0.74	1.60	3	1
1:A:39:CYS:SG	1:A:88:LEU:HD23	0.74	2.23	12	1
1:A:39:CYS:HB2	1:A:77:VAL:HG13	0.74	1.59	14	1
1:A:63:ASN:ND2	1:A:63:ASN:H	0.73	1.80	11	7
1:A:33:LEU:HD22	1:A:91:ALA:HB1	0.72	1.61	13	9
1:A:51:ASP:HB3	1:A:54:LYS:HD2	0.71	1.62	4	1
1:A:64:TRP:HE3	1:A:67:LEU:HD22	0.70	1.45	17	7
1:A:2:LEU:HD23	1:A:81:GLN:HG3	0.70	1.63	8	1
1:A:23:LEU:HD11	1:A:43:VAL:HG21	0.70	1.63	3	3
1:A:6:LEU:HD13	1:A:96:LYS:HE3	0.69	1.63	7	1
1:A:113:LYS:HE2	1:A:113:LYS:O	0.69	1.87	9	9
1:A:58:ASN:HB3	1:A:61:LYS:HE3	0.69	1.63	8	1
1:A:23:LEU:HD12	1:A:43:VAL:HG21	0.68	1.65	1	7
1:A:37:THR:HG22	1:A:87:LYS:HG3	0.68	1.66	11	1
1:A:23:LEU:HA	1:A:27:GLY:HA2	0.68	1.64	9	9
1:A:8:VAL:HG11	1:A:99:LEU:HD22	0.68	1.66	12	1
1:A:62:PRO:CA	1:A:65:GLU:HB3	0.68	2.16	2	14
1:A:63:ASN:H	1:A:63:ASN:HD22	0.68	1.32	17	7
1:A:33:LEU:HG	1:A:91:ALA:HB1	0.68	1.66	4	2
1:A:85:GLU:HA	1:A:88:LEU:HD13	0.68	1.66	14	1
1:A:19:VAL:HG13	1:A:23:LEU:HD22	0.67	1.63	2	3
1:A:51:ASP:HB3	1:A:53:LYS:HG2	0.67	1.66	3	1
1:A:26:ARG:O	1:A:29:THR:HB	0.67	1.90	14	2
1:A:85:GLU:HA	1:A:88:LEU:HG	0.67	1.67	8	5
1:A:5:LYS:HG3	1:A:74:LEU:HD13	0.67	1.67	9	1
1:A:34:GLU:HA	1:A:39:CYS:O	0.66	1.89	2	17
1:A:54:LYS:HA	1:A:57:GLN:NE2	0.66	2.05	11	1
1:A:61:LYS:HB3	1:A:62:PRO:HD2	0.66	1.67	16	9
1:A:93:GLU:HG2	1:A:96:LYS:HD3	0.66	1.68	1	1
1:A:2:LEU:HD21	1:A:85:GLU:HB3	0.66	1.68	2	1
1:A:112:MET:HA	1:A:116:GLU:CB	0.65	2.21	15	14
1:A:5:LYS:HB3	1:A:72:HIS:CD2	0.65	2.26	14	6
1:A:75:ILE:HD12	1:A:88:LEU:HD12	0.65	1.67	7	7
1:A:50:ARG:H	1:A:50:ARG:CD	0.65	2.04	15	2
1:A:33:LEU:HD12	1:A:41:ILE:HG21	0.64	1.66	5	6
1:A:20:GLY:O	1:A:25:PRO:HD3	0.64	1.92	15	7
1:A:46:LYS:HA	1:A:67:LEU:HD22	0.64	1.70	12	1
1:A:55:GLU:O	1:A:59:ARG:HB3	0.64	1.93	8	15
1:A:92:VAL:O	1:A:95:VAL:HG12	0.64	1.92	7	1
1:A:21:ARG:HD3	1:A:98:LEU:O	0.64	1.92	14	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:GLU:O	1:A:88:LEU:HD22	0.64	1.93	3	2
1:A:113:LYS:O	1:A:113:LYS:HE3	0.64	1.93	7	4
1:A:21:ARG:NH1	1:A:99:LEU:HA	0.64	2.08	8	1
1:A:19:VAL:HA	1:A:23:LEU:HD13	0.63	1.68	3	1
1:A:85:GLU:HA	1:A:88:LEU:CG	0.63	2.23	8	6
1:A:46:LYS:HA	1:A:67:LEU:HG	0.63	1.69	6	1
1:A:85:GLU:O	1:A:89:LYS:HG2	0.63	1.93	2	1
1:A:8:VAL:HG11	1:A:99:LEU:HB2	0.63	1.69	10	8
1:A:23:LEU:H	1:A:23:LEU:HD13	0.62	1.53	12	8
1:A:4:GLU:HB2	1:A:75:ILE:HG13	0.62	1.69	6	1
1:A:85:GLU:HA	1:A:88:LEU:CD1	0.62	2.24	14	3
1:A:54:LYS:HA	1:A:58:ASN:HB3	0.62	1.72	2	1
1:A:75:ILE:HD12	1:A:88:LEU:HD23	0.62	1.69	2	2
1:A:75:ILE:HD12	1:A:88:LEU:HD13	0.62	1.69	5	6
1:A:2:LEU:HG	1:A:77:VAL:CG1	0.62	2.25	12	1
1:A:37:THR:HG22	1:A:87:LYS:HG2	0.62	1.72	12	8
1:A:1:GLN:HB2	1:A:77:VAL:O	0.62	1.95	7	1
1:A:19:VAL:HG13	1:A:23:LEU:HD21	0.61	1.73	8	5
1:A:49:MET:HA	1:A:64:TRP:HZ3	0.61	1.55	8	2
1:A:16:PHE:CE2	1:A:101:PRO:HA	0.61	2.30	9	3
1:A:112:MET:HG3	1:A:116:GLU:HB2	0.61	1.73	5	1
1:A:17:ASN:ND2	1:A:20:GLY:H	0.61	1.93	14	1
1:A:9:PRO:HB2	1:A:12:GLU:HG2	0.61	1.72	2	13
1:A:29:THR:O	1:A:33:LEU:HD13	0.60	1.96	8	5
1:A:88:LEU:H	1:A:88:LEU:HD13	0.60	1.55	2	1
1:A:21:ARG:HD2	1:A:98:LEU:O	0.60	1.95	9	3
1:A:46:LYS:HA	1:A:67:LEU:HD12	0.60	1.73	8	5
1:A:88:LEU:HD12	1:A:89:LYS:N	0.60	2.11	12	4
1:A:49:MET:HB2	1:A:63:ASN:CB	0.60	2.26	1	10
1:A:93:GLU:O	1:A:96:LYS:HB2	0.60	1.96	7	6
1:A:29:THR:O	1:A:33:LEU:HG	0.60	1.96	9	10
1:A:44:ARG:O	1:A:71:LEU:HA	0.60	1.97	15	2
1:A:39:CYS:CB	1:A:88:LEU:HG	0.59	2.27	2	1
1:A:108:SER:HA	1:A:112:MET:CB	0.59	2.25	5	1
1:A:44:ARG:HD2	1:A:66:HIS:ND1	0.59	2.12	12	1
1:A:3:GLN:HB3	1:A:74:LEU:CD1	0.59	2.24	1	2
1:A:89:LYS:HA	1:A:92:VAL:HG12	0.59	1.74	9	12
1:A:39:CYS:SG	1:A:88:LEU:HG	0.59	2.38	2	1
1:A:17:ASN:OD1	1:A:20:GLY:HA3	0.58	1.98	15	1
1:A:55:GLU:HB3	1:A:64:TRP:CH2	0.58	2.33	10	7
1:A:49:MET:HA	1:A:64:TRP:CH2	0.58	2.33	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:HA	1:A:27:GLY:CA	0.58	2.28	9	6
1:A:18:PHE:O	1:A:22:ILE:HG13	0.58	1.98	9	1
1:A:16:PHE:CZ	1:A:21:ARG:HD3	0.58	2.34	9	2
1:A:97:LYS:HE3	1:A:97:LYS:HA	0.58	1.73	6	1
1:A:16:PHE:HE2	1:A:21:ARG:NH1	0.57	1.96	8	1
1:A:1:GLN:HE21	1:A:76:THR:HG22	0.57	1.58	3	6
1:A:28:LEU:O	1:A:32:GLN:HG2	0.57	1.98	8	16
1:A:109:LEU:O	1:A:113:LYS:HB2	0.57	2.00	5	1
1:A:119:ILE:HG22	1:A:120:LEU:H	0.57	1.58	14	1
1:A:59:ARG:HA	1:A:64:TRP:NE1	0.57	2.14	2	6
1:A:52:LYS:O	1:A:55:GLU:HG3	0.57	1.99	17	8
1:A:39:CYS:SG	1:A:88:LEU:HD13	0.57	2.40	6	4
1:A:3:GLN:NE2	1:A:74:LEU:HD11	0.56	2.15	3	11
1:A:47:GLY:HA2	1:A:50:ARG:HG2	0.56	1.76	10	2
1:A:95:VAL:HG13	1:A:98:LEU:HD11	0.56	1.77	17	1
1:A:64:TRP:CE3	1:A:67:LEU:HD22	0.56	2.35	11	7
1:A:9:PRO:HB2	1:A:12:GLU:CG	0.56	2.30	7	10
1:A:82:ASN:HA	1:A:85:GLU:HG2	0.56	1.78	6	2
1:A:39:CYS:CB	1:A:88:LEU:HD22	0.56	2.27	17	4
1:A:44:ARG:HA	1:A:66:HIS:CD2	0.56	2.36	15	8
1:A:50:ARG:H	1:A:50:ARG:HD3	0.56	1.59	15	1
1:A:62:PRO:HA	1:A:65:GLU:CB	0.55	2.20	2	7
1:A:117:LEU:HB3	1:A:119:ILE:HG12	0.55	1.77	7	1
1:A:37:THR:HA	1:A:87:LYS:HG2	0.55	1.77	14	1
1:A:37:THR:HA	1:A:87:LYS:CG	0.55	2.32	14	1
1:A:112:MET:HG2	1:A:116:GLU:HG3	0.55	1.79	16	4
1:A:90:ARG:O	1:A:93:GLU:HG2	0.55	2.02	17	1
1:A:33:LEU:HG	1:A:91:ALA:CB	0.55	2.31	4	3
1:A:51:ASP:OD1	1:A:53:LYS:HG2	0.55	2.02	14	5
1:A:95:VAL:O	1:A:99:LEU:HD13	0.54	2.01	15	5
1:A:64:TRP:HA	1:A:67:LEU:CB	0.54	2.32	17	10
1:A:87:LYS:O	1:A:90:ARG:HG2	0.54	2.01	4	2
1:A:97:LYS:HA	1:A:97:LYS:HE2	0.54	1.78	16	1
1:A:32:GLN:O	1:A:36:GLU:HB2	0.54	2.02	5	2
1:A:115:MET:HA	1:A:119:ILE:HG12	0.54	1.79	16	1
1:A:7:TYR:HA	1:A:72:HIS:CB	0.54	2.33	14	14
1:A:49:MET:HB3	1:A:54:LYS:CD	0.54	2.31	1	3
1:A:93:GLU:HA	1:A:96:LYS:CG	0.54	2.31	17	1
1:A:21:ARG:NH2	1:A:99:LEU:HA	0.54	2.17	9	3
1:A:58:ASN:O	1:A:61:LYS:HB2	0.54	2.03	3	3
1:A:112:MET:CA	1:A:116:GLU:HB2	0.53	2.23	12	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:GLU:HA	1:A:88:LEU:HD21	0.53	1.79	15	2
1:A:96:LYS:HD2	1:A:99:LEU:HD11	0.53	1.78	10	2
1:A:47:GLY:H	1:A:67:LEU:HD12	0.53	1.64	2	1
1:A:52:LYS:O	1:A:56:GLU:HG3	0.53	2.03	3	4
1:A:5:LYS:HG3	1:A:74:LEU:HG	0.53	1.81	6	2
1:A:54:LYS:HG3	1:A:58:ASN:HB3	0.53	1.79	6	2
1:A:3:GLN:CB	1:A:74:LEU:HD11	0.53	2.30	14	4
1:A:39:CYS:HB2	1:A:88:LEU:HD12	0.53	1.81	3	2
1:A:95:VAL:O	1:A:99:LEU:HG	0.52	2.03	6	11
1:A:87:LYS:O	1:A:90:ARG:HG3	0.52	2.04	16	2
1:A:53:LYS:O	1:A:57:GLN:HG3	0.52	2.04	11	2
1:A:49:MET:CG	1:A:63:ASN:HB3	0.52	2.34	3	2
1:A:47:GLY:HA2	1:A:50:ARG:HB2	0.52	1.81	1	2
1:A:44:ARG:HD3	1:A:74:LEU:HD13	0.52	1.80	13	1
1:A:63:ASN:ND2	1:A:63:ASN:N	0.52	2.55	11	7
1:A:22:ILE:HD11	1:A:98:LEU:HB3	0.52	1.82	8	1
1:A:74:LEU:HD21	1:A:76:THR:HG23	0.52	1.82	13	1
1:A:54:LYS:HB3	1:A:64:TRP:HZ2	0.52	1.65	15	2
1:A:86:LEU:O	1:A:89:LYS:HG2	0.52	2.05	12	1
1:A:58:ASN:ND2	1:A:61:LYS:HE3	0.52	2.20	2	1
1:A:85:GLU:HA	1:A:88:LEU:CD2	0.52	2.34	15	4
1:A:77:VAL:HB	1:A:88:LEU:CD2	0.52	2.35	15	3
1:A:59:ARG:HA	1:A:64:TRP:CD1	0.52	2.40	1	1
1:A:93:GLU:HA	1:A:96:LYS:HG3	0.51	1.82	17	1
1:A:61:LYS:HE3	1:A:62:PRO:HD2	0.51	1.80	1	1
1:A:49:MET:SD	1:A:50:ARG:HD2	0.51	2.45	16	1
1:A:22:ILE:HB	1:A:23:LEU:HD12	0.51	1.82	3	1
1:A:21:ARG:HH22	1:A:22:ILE:HG12	0.51	1.66	11	1
1:A:112:MET:HG2	1:A:117:LEU:HD23	0.51	1.83	5	1
1:A:50:ARG:HA	1:A:64:TRP:CH2	0.51	2.41	13	2
1:A:61:LYS:CB	1:A:62:PRO:HD2	0.51	2.34	2	3
1:A:63:ASN:HD22	1:A:63:ASN:N	0.51	2.03	11	5
1:A:77:VAL:HB	1:A:88:LEU:HD12	0.51	1.83	3	1
1:A:26:ARG:HB3	1:A:29:THR:HB	0.51	1.82	4	1
1:A:21:ARG:NH2	1:A:22:ILE:HG12	0.51	2.21	11	1
1:A:18:PHE:HB2	1:A:71:LEU:HD13	0.51	1.82	3	1
1:A:47:GLY:HA2	1:A:50:ARG:HG3	0.51	1.81	14	2
1:A:93:GLU:O	1:A:96:LYS:HB3	0.51	2.06	2	2
1:A:55:GLU:HB3	1:A:64:TRP:CZ2	0.51	2.41	10	3
1:A:6:LEU:HB2	1:A:73:VAL:CG2	0.51	2.36	9	2
1:A:39:CYS:SG	1:A:75:ILE:HB	0.50	2.46	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:CYS:HB2	1:A:88:LEU:HG	0.50	1.84	2	1
1:A:108:SER:O	1:A:112:MET:HB2	0.50	2.06	9	2
1:A:3:GLN:HE21	1:A:5:LYS:HE3	0.50	1.67	14	1
1:A:116:GLU:HA	1:A:119:ILE:HG12	0.50	1.84	1	1
1:A:4:GLU:HB2	1:A:75:ILE:CG1	0.50	2.37	6	1
1:A:55:GLU:HG2	1:A:64:TRP:CH2	0.50	2.42	12	2
1:A:23:LEU:HD12	1:A:23:LEU:N	0.50	2.21	3	2
1:A:20:GLY:O	1:A:24:GLY:HA3	0.50	2.07	9	2
1:A:13:TYR:CE2	1:A:101:PRO:HG3	0.50	2.42	3	7
1:A:96:LYS:O	1:A:99:LEU:HB2	0.50	2.07	12	1
1:A:53:LYS:HB2	1:A:57:GLN:NE2	0.50	2.22	2	2
1:A:32:GLN:O	1:A:36:GLU:HB3	0.50	2.06	6	1
1:A:18:PHE:HD1	1:A:21:ARG:NH1	0.50	2.04	8	1
1:A:61:LYS:HB2	1:A:62:PRO:CD	0.49	2.34	2	1
1:A:16:PHE:CE2	1:A:21:ARG:HD3	0.49	2.42	11	2
1:A:44:ARG:HG2	1:A:66:HIS:ND1	0.49	2.22	13	1
1:A:79:ASP:OD1	1:A:81:GLN:HG3	0.49	2.08	1	1
1:A:2:LEU:CD2	1:A:81:GLN:HG3	0.49	2.36	8	1
1:A:58:ASN:O	1:A:61:LYS:HG2	0.49	2.08	9	3
1:A:37:THR:HA	1:A:87:LYS:CD	0.49	2.37	16	3
1:A:93:GLU:HA	1:A:96:LYS:HB2	0.49	1.84	9	1
1:A:41:ILE:HD12	1:A:92:VAL:HG23	0.48	1.83	12	8
1:A:34:GLU:CB	1:A:40:LYS:HA	0.48	2.33	10	6
1:A:18:PHE:O	1:A:22:ILE:HG12	0.48	2.08	12	3
1:A:39:CYS:HB2	1:A:77:VAL:HB	0.48	1.84	2	1
1:A:78:GLU:O	1:A:79:ASP:HB2	0.48	2.08	17	4
1:A:39:CYS:SG	1:A:88:LEU:HD22	0.48	2.48	4	2
1:A:86:LEU:O	1:A:89:LYS:HG3	0.48	2.09	13	6
1:A:53:LYS:O	1:A:57:GLN:HG2	0.48	2.09	16	2
1:A:19:VAL:HG13	1:A:71:LEU:HD11	0.48	1.86	5	2
1:A:54:LYS:HG2	1:A:58:ASN:HB2	0.48	1.85	12	1
1:A:18:PHE:HD1	1:A:21:ARG:HH12	0.48	1.52	8	1
1:A:47:GLY:H	1:A:49:MET:HG2	0.48	1.69	15	1
1:A:84:ALA:O	1:A:88:LEU:HD13	0.48	2.08	2	1
1:A:26:ARG:O	1:A:29:THR:HG22	0.48	2.09	7	4
1:A:95:VAL:HG12	1:A:99:LEU:HD23	0.48	1.84	13	1
1:A:119:ILE:HG13	1:A:120:LEU:H	0.47	1.68	3	2
1:A:18:PHE:HB2	1:A:71:LEU:HD21	0.47	1.84	4	2
1:A:49:MET:HA	1:A:63:ASN:CB	0.47	2.39	16	1
1:A:58:ASN:OD1	1:A:61:LYS:HD2	0.47	2.09	15	1
1:A:41:ILE:CD1	1:A:92:VAL:HG23	0.47	2.40	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:VAL:HG22	1:A:18:PHE:CZ	0.47	2.44	3	5
1:A:11:LYS:HG3	1:A:70:ASP:OD1	0.47	2.10	17	1
1:A:40:LYS:HB2	1:A:40:LYS:NZ	0.47	2.24	3	1
1:A:54:LYS:HG3	1:A:58:ASN:HB2	0.47	1.85	7	1
1:A:44:ARG:HD3	1:A:69:GLU:OE1	0.47	2.10	14	2
1:A:22:ILE:HG12	1:A:98:LEU:CD1	0.47	2.40	17	1
1:A:95:VAL:HA	1:A:98:LEU:HG	0.47	1.86	17	1
1:A:92:VAL:O	1:A:95:VAL:HB	0.47	2.08	17	5
1:A:39:CYS:SG	1:A:88:LEU:HB3	0.47	2.49	10	1
1:A:39:CYS:O	1:A:39:CYS:SG	0.47	2.73	10	1
1:A:83:ARG:HG3	1:A:84:ALA:N	0.47	2.24	9	1
1:A:6:LEU:HB2	1:A:73:VAL:HG23	0.47	1.86	1	3
1:A:1:GLN:NE2	1:A:76:THR:HG22	0.47	2.25	12	1
1:A:65:GLU:HG2	1:A:66:HIS:N	0.46	2.25	3	2
1:A:86:LEU:HA	1:A:89:LYS:CD	0.46	2.40	3	1
1:A:75:ILE:CD1	1:A:88:LEU:HD13	0.46	2.40	12	1
1:A:16:PHE:CD2	1:A:101:PRO:HA	0.46	2.45	8	3
1:A:51:ASP:CB	1:A:54:LYS:HB2	0.46	2.40	8	1
1:A:63:ASN:HA	1:A:66:HIS:NE2	0.46	2.25	15	3
1:A:44:ARG:HD2	1:A:74:LEU:HD13	0.46	1.88	7	3
1:A:47:GLY:HA2	1:A:50:ARG:CG	0.46	2.40	14	2
1:A:75:ILE:HD12	1:A:88:LEU:CD2	0.46	2.40	14	1
1:A:49:MET:CA	1:A:64:TRP:CZ3	0.46	2.87	15	1
1:A:40:LYS:O	1:A:40:LYS:HG3	0.46	2.10	3	4
1:A:33:LEU:CG	1:A:91:ALA:HB1	0.46	2.36	4	2
1:A:46:LYS:HB3	1:A:46:LYS:NZ	0.46	2.25	12	2
1:A:93:GLU:HA	1:A:96:LYS:HD3	0.46	1.88	1	1
1:A:48:SER:HB2	1:A:49:MET:SD	0.46	2.50	3	1
1:A:49:MET:SD	1:A:50:ARG:N	0.46	2.88	16	1
1:A:39:CYS:SG	1:A:88:LEU:CB	0.46	3.04	10	1
1:A:91:ALA:O	1:A:94:GLU:HG2	0.46	2.10	13	1
1:A:13:TYR:CZ	1:A:101:PRO:HG3	0.46	2.47	4	2
1:A:47:GLY:O	1:A:50:ARG:HD2	0.46	2.10	8	1
1:A:80:ALA:O	1:A:81:GLN:HB3	0.46	2.11	12	1
1:A:11:LYS:HE2	1:A:11:LYS:HA	0.46	1.87	14	1
1:A:49:MET:HB3	1:A:63:ASN:HB2	0.46	1.88	16	1
1:A:66:HIS:HB2	1:A:69:GLU:OE1	0.45	2.11	15	2
1:A:77:VAL:HB	1:A:88:LEU:HD22	0.45	1.86	15	1
1:A:5:LYS:N	1:A:5:LYS:HD2	0.45	2.27	4	5
1:A:90:ARG:HG3	1:A:91:ALA:N	0.45	2.26	4	2
1:A:61:LYS:O	1:A:63:ASN:N	0.45	2.49	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:LEU:C	1:A:2:LEU:HD12	0.45	2.32	8	1
1:A:80:ALA:O	1:A:81:GLN:HB2	0.45	2.12	11	1
1:A:67:LEU:HD23	1:A:67:LEU:O	0.45	2.11	15	1
1:A:96:LYS:HA	1:A:99:LEU:CD1	0.45	2.42	1	1
1:A:49:MET:SD	1:A:63:ASN:HB3	0.45	2.52	3	1
1:A:53:LYS:HG3	1:A:54:LYS:HD2	0.45	1.88	9	1
1:A:55:GLU:HA	1:A:64:TRP:CZ2	0.45	2.47	2	2
1:A:18:PHE:HB2	1:A:71:LEU:CD2	0.45	2.42	17	2
1:A:49:MET:HB2	1:A:64:TRP:CE2	0.45	2.46	16	1
1:A:39:CYS:CB	1:A:88:LEU:HB3	0.45	2.42	4	3
1:A:44:ARG:O	1:A:71:LEU:HD12	0.45	2.12	8	3
1:A:21:ARG:HD3	1:A:98:LEU:HG	0.45	1.89	3	1
1:A:23:LEU:HD13	1:A:23:LEU:N	0.45	2.27	10	4
1:A:89:LYS:HD3	1:A:90:ARG:N	0.44	2.27	1	2
1:A:39:CYS:SG	1:A:75:ILE:HG22	0.44	2.52	10	1
1:A:117:LEU:O	1:A:117:LEU:HD13	0.44	2.13	9	1
1:A:50:ARG:HA	1:A:64:TRP:HH2	0.44	1.72	14	1
1:A:49:MET:O	1:A:51:ASP:N	0.44	2.46	14	6
1:A:22:ILE:HG22	1:A:23:LEU:HD13	0.44	1.89	4	1
1:A:79:ASP:OD1	1:A:81:GLN:HG2	0.44	2.12	4	1
1:A:1:GLN:CB	1:A:78:GLU:HA	0.44	2.43	7	1
1:A:7:TYR:HA	1:A:72:HIS:HB2	0.44	1.90	1	3
1:A:21:ARG:HH12	1:A:22:ILE:HD13	0.44	1.73	11	1
1:A:85:GLU:HA	1:A:88:LEU:HD11	0.44	1.90	2	1
1:A:44:ARG:NH1	1:A:66:HIS:HB3	0.44	2.28	6	1
1:A:93:GLU:OE2	1:A:96:LYS:HG3	0.44	2.13	13	2
1:A:1:GLN:HB2	1:A:78:GLU:HA	0.43	1.88	7	1
1:A:48:SER:HA	1:A:50:ARG:NH1	0.43	2.28	15	1
1:A:22:ILE:HD12	1:A:95:VAL:HG13	0.43	1.89	1	5
1:A:96:LYS:HA	1:A:99:LEU:CD2	0.43	2.43	10	1
1:A:64:TRP:CA	1:A:67:LEU:HB2	0.43	2.32	7	2
1:A:77:VAL:HB	1:A:88:LEU:CD1	0.43	2.43	3	1
1:A:31:LYS:HB2	1:A:31:LYS:NZ	0.43	2.27	8	1
1:A:43:VAL:CG1	1:A:71:LEU:HD11	0.43	2.44	13	1
1:A:63:ASN:O	1:A:67:LEU:HB2	0.43	2.13	3	6
1:A:3:GLN:NE2	1:A:74:LEU:HD21	0.43	2.29	4	1
1:A:16:PHE:CZ	1:A:101:PRO:HA	0.43	2.49	9	1
1:A:75:ILE:HD12	1:A:88:LEU:CD1	0.43	2.44	15	2
1:A:44:ARG:HD2	1:A:66:HIS:HD1	0.43	1.72	12	1
1:A:51:ASP:O	1:A:55:GLU:HG2	0.43	2.14	16	2
1:A:4:GLU:O	1:A:74:LEU:HA	0.43	2.13	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:PHE:CD1	1:A:21:ARG:NH1	0.43	2.86	8	1
1:A:5:LYS:HD3	1:A:74:LEU:HD13	0.43	1.91	14	1
1:A:82:ASN:HA	1:A:85:GLU:HG3	0.43	1.89	2	1
1:A:96:LYS:HA	1:A:99:LEU:HG	0.43	1.91	16	3
1:A:3:GLN:NE2	1:A:5:LYS:HE3	0.42	2.28	14	1
1:A:50:ARG:HD3	1:A:50:ARG:N	0.42	2.26	15	1
1:A:1:GLN:HB3	1:A:78:GLU:OE1	0.42	2.13	7	1
1:A:8:VAL:HG13	1:A:8:VAL:O	0.42	2.14	11	2
1:A:49:MET:C	1:A:51:ASP:H	0.42	2.17	9	3
1:A:44:ARG:HB2	1:A:72:HIS:CE1	0.42	2.50	3	1
1:A:74:LEU:C	1:A:74:LEU:HD23	0.42	2.35	3	2
1:A:19:VAL:HG12	1:A:23:LEU:HD11	0.42	1.91	16	1
1:A:85:GLU:HG3	1:A:86:LEU:N	0.42	2.28	9	1
1:A:48:SER:O	1:A:63:ASN:HB3	0.42	2.15	16	1
1:A:79:ASP:OD1	1:A:81:GLN:HB2	0.42	2.15	13	1
1:A:82:ASN:O	1:A:85:GLU:HG2	0.42	2.15	14	1
1:A:17:ASN:O	1:A:21:ARG:HB3	0.42	2.15	17	1
1:A:13:TYR:CE1	1:A:101:PRO:HG3	0.42	2.50	4	1
1:A:54:LYS:CA	1:A:58:ASN:HB3	0.41	2.43	2	1
1:A:51:ASP:OD2	1:A:53:LYS:HG2	0.41	2.15	5	1
1:A:18:PHE:O	1:A:22:ILE:HB	0.41	2.15	8	1
1:A:49:MET:HG2	1:A:67:LEU:HD13	0.41	1.92	16	1
1:A:73:VAL:HG21	1:A:99:LEU:HD12	0.41	1.91	1	1
1:A:5:LYS:N	1:A:5:LYS:CD	0.41	2.83	4	1
1:A:64:TRP:CE3	1:A:67:LEU:HD13	0.41	2.50	6	1
1:A:16:PHE:HZ	1:A:21:ARG:HH11	0.41	1.57	14	1
1:A:95:VAL:HG12	1:A:99:LEU:CD1	0.41	2.45	1	1
1:A:1:GLN:HE21	1:A:76:THR:CG2	0.41	2.28	3	1
1:A:50:ARG:HB2	1:A:64:TRP:CH2	0.41	2.50	10	1
1:A:23:LEU:HB2	1:A:27:GLY:HA2	0.41	1.93	14	1
1:A:52:LYS:HA	1:A:55:GLU:OE1	0.41	2.15	12	1
1:A:81:GLN:HG3	1:A:82:ASN:N	0.41	2.31	12	1
1:A:17:ASN:ND2	1:A:20:GLY:N	0.41	2.66	14	1
1:A:75:ILE:HD13	1:A:92:VAL:HG11	0.41	1.91	15	1
1:A:85:GLU:CA	1:A:88:LEU:HG	0.41	2.42	8	1
1:A:64:TRP:O	1:A:68:ASN:ND2	0.41	2.54	12	1
1:A:8:VAL:HG22	1:A:18:PHE:CE2	0.41	2.50	17	1
1:A:52:LYS:O	1:A:56:GLU:HG2	0.41	2.15	17	1
1:A:89:LYS:O	1:A:92:VAL:HG12	0.41	2.16	17	1
1:A:46:LYS:HA	1:A:67:LEU:CD2	0.41	2.42	12	1
1:A:44:ARG:HB2	1:A:72:HIS:NE2	0.41	2.31	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:MET:HA	1:A:116:GLU:CG	0.41	2.46	13	1
1:A:39:CYS:CB	1:A:88:LEU:HD12	0.41	2.46	14	1
1:A:88:LEU:CD2	1:A:89:LYS:N	0.41	2.84	14	1
1:A:33:LEU:HD13	1:A:41:ILE:HG21	0.41	1.93	15	1
1:A:95:VAL:HG12	1:A:99:LEU:HD13	0.41	1.91	14	2
1:A:53:LYS:HG3	1:A:54:LYS:N	0.41	2.31	7	1
1:A:19:VAL:HG13	1:A:71:LEU:HD21	0.41	1.93	10	1
1:A:43:VAL:HG23	1:A:48:SER:HB3	0.41	1.92	11	1
1:A:46:LYS:HD3	1:A:67:LEU:HD12	0.41	1.93	16	1
1:A:19:VAL:HG23	1:A:71:LEU:HD11	0.40	1.91	3	1
1:A:64:TRP:HA	1:A:67:LEU:HB3	0.40	1.93	6	1
1:A:62:PRO:O	1:A:65:GLU:HB3	0.40	2.15	8	1
1:A:89:LYS:NZ	1:A:89:LYS:HB2	0.40	2.32	9	1
1:A:19:VAL:O	1:A:23:LEU:HD13	0.40	2.17	14	1
1:A:23:LEU:N	1:A:23:LEU:CD1	0.40	2.85	3	1
1:A:50:ARG:CD	1:A:50:ARG:N	0.40	2.83	8	1
1:A:39:CYS:HB3	1:A:88:LEU:HB3	0.40	1.92	17	1
1:A:9:PRO:O	1:A:12:GLU:HB2	0.40	2.16	9	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	115/140 (82%)	90±33 (78±29%)	8±3 (7±3%)	4±2 (3±2%)	7	39
All	All	1725/2380 (72%)	1530 (89%)	134 (8%)	61 (4%)	6	35

All 12 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	62	PRO	15
1	A	24	GLY	12
1	A	50	ARG	11
1	A	119	ILE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	79	ASP	5
1	A	81	GLN	4
1	A	118	ALA	3
1	A	107	ASP	2
1	A	25	PRO	1
1	A	46	LYS	1
1	A	80	ALA	1
1	A	120	LEU	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	103/121 (85%)	83±21 (81±20%)	14±4 (13±4%)	7 48
All	All	1648/2057 (80%)	1415 (86%)	233 (14%)	6 46

All 50 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	63	ASN	16
1	A	76	THR	16
1	A	17	ASN	15
1	A	21	ARG	14
1	A	89	LYS	14
1	A	113	LYS	14
1	A	117	LEU	12
1	A	88	LEU	11
1	A	5	LYS	10
1	A	62	PRO	10
1	A	23	LEU	8
1	A	2	LEU	6
1	A	50	ARG	5
1	A	68	ASN	5
1	A	99	LEU	5
1	A	65	GLU	5
1	A	46	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	67	LEU	4
1	A	75	ILE	4
1	A	120	LEU	3
1	A	49	MET	3
1	A	86	LEU	3
1	A	77	VAL	3
1	A	90	ARG	3
1	A	121	ASN	3
1	A	58	ASN	3
1	A	40	LYS	2
1	A	48	SER	2
1	A	71	LEU	2
1	A	1	GLN	2
1	A	97	LYS	2
1	A	98	LEU	2
1	A	26	ARG	2
1	A	57	GLN	2
1	A	85	GLU	2
1	A	51	ASP	2
1	A	59	ARG	1
1	A	116	GLU	1
1	A	54	LYS	1
1	A	95	VAL	1
1	A	22	ILE	1
1	A	55	GLU	1
1	A	11	LYS	1
1	A	111	LYS	1
1	A	119	ILE	1
1	A	61	LYS	1
1	A	3	GLN	1
1	A	15	ASP	1
1	A	29	THR	1
1	A	92	VAL	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