



Full wwPDB NMR Structure Validation Report ⓘ

Oct 6, 2016 – 03:10 PM EDT

PDB ID : 3ZFJ
Title : N-terminal domain of pneumococcal PhtD protein with bound Zn(II)
Authors : Bersch, B.; Bougault, C.; Favier, A.; Gabel, F.; Roux, L.; Vernet, T.; Durmort, C.
Deposited on : 2012-12-11

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-20027939
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

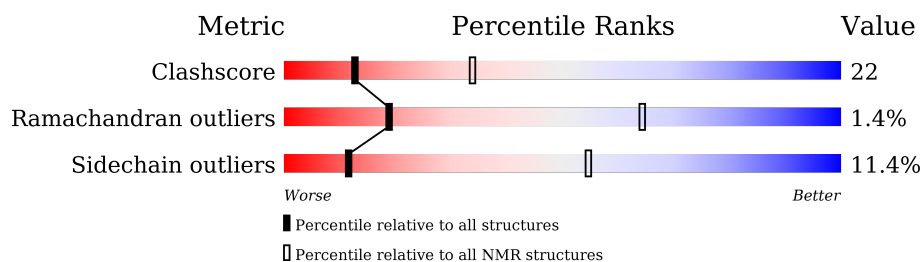
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	138	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:51-A:106, A:111-A:158 (104)	0.34	3

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	2, 3, 5, 6, 7, 9, 11, 12, 13, 15, 16, 17, 19, 20
2	1, 4, 8, 10
3	14, 18

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1897 atoms, of which 935 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D.

Mol	Chain	Residues	Atoms						Trace
1	A	120	Total	C	H	N	O	S	1
			1896	603	935	163	194	1	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	EXPRESSION TAG	UNP Q04KS8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

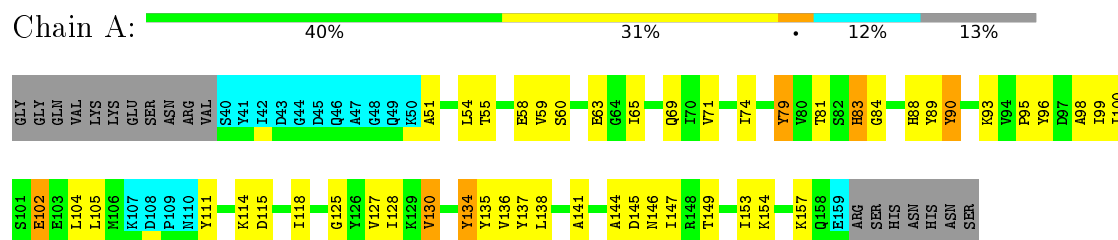
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots

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: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D

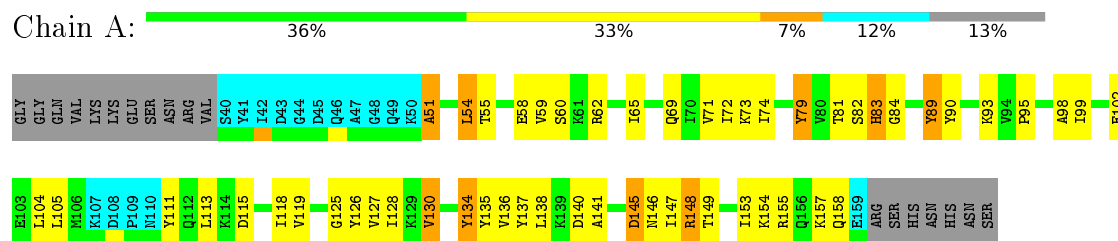


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

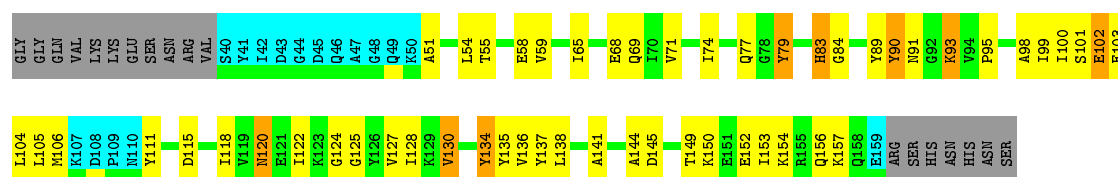
- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D



4.2.2 Score per residue for model 2

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D

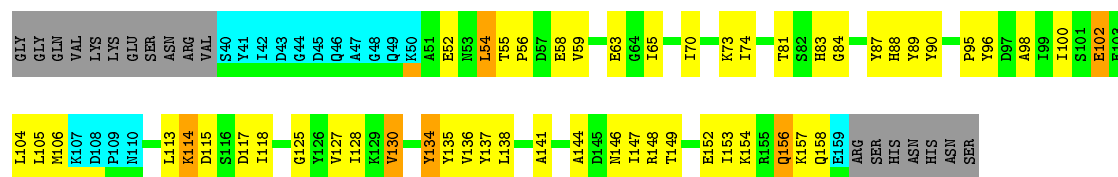




4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D

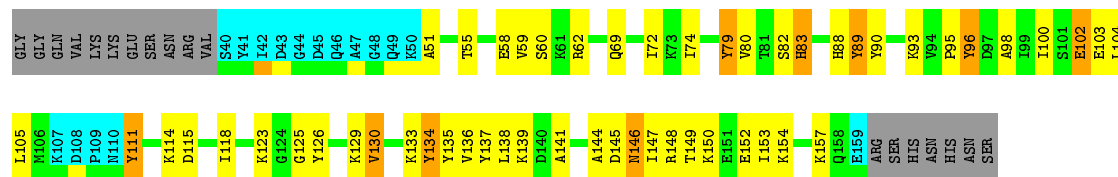
Chain A: 38% 33% 12% 13%



4.2.4 Score per residue for model 4

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D

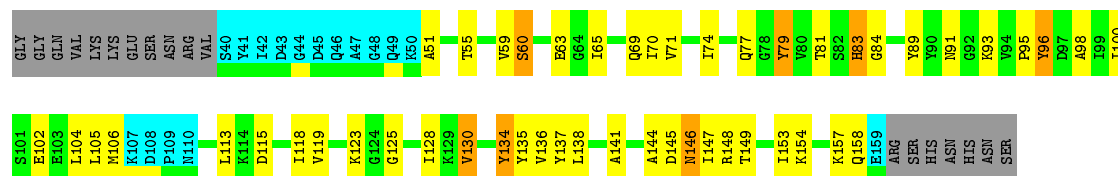
Chain A: 37% 32% 7% 12% 13%



4.2.5 Score per residue for model 5

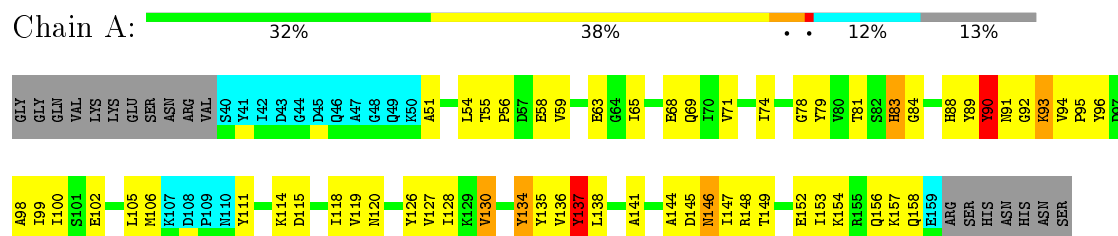
- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D

Chain A: 39% 31% 5% 12% 13%



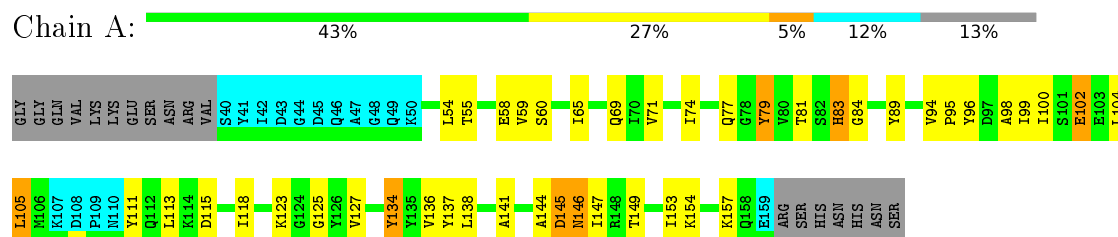
4.2.6 Score per residue for model 6

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D



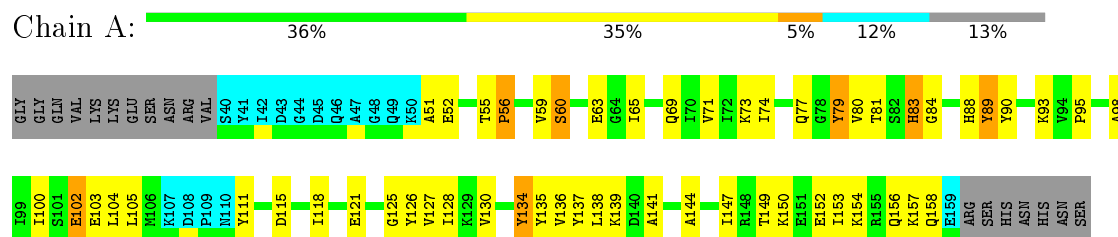
4.2.7 Score per residue for model 7

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D



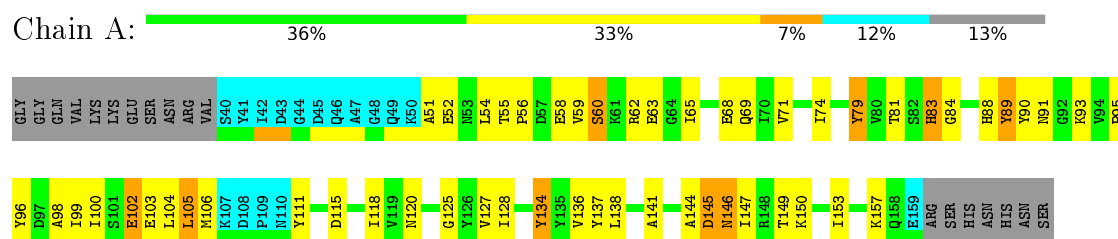
4.2.8 Score per residue for model 8

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D



4.2.9 Score per residue for model 9

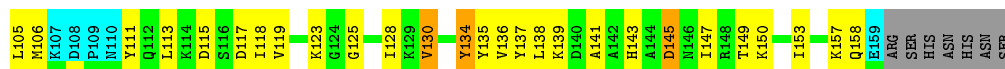
- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D





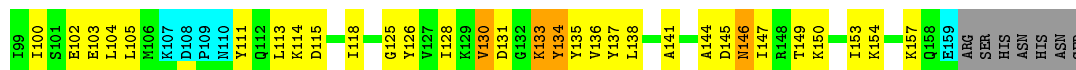
4.2.14 Score per residue for model 14

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D



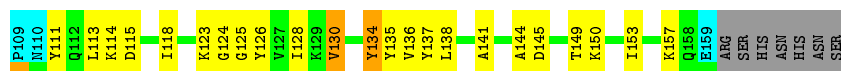
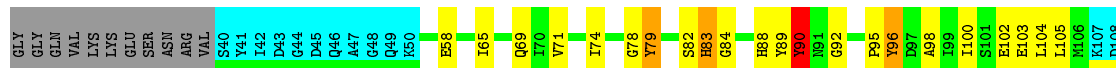
4.2.15 Score per residue for model 15

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D



4.2.16 Score per residue for model 16

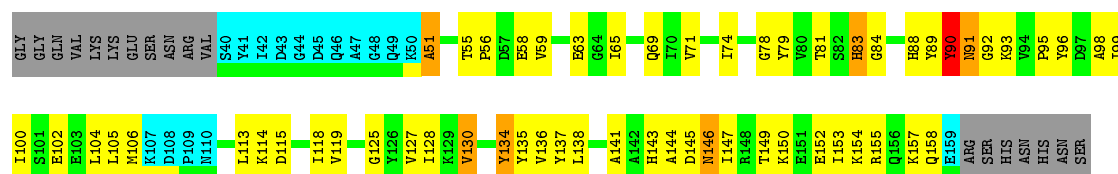
- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D



4.2.17 Score per residue for model 17

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D

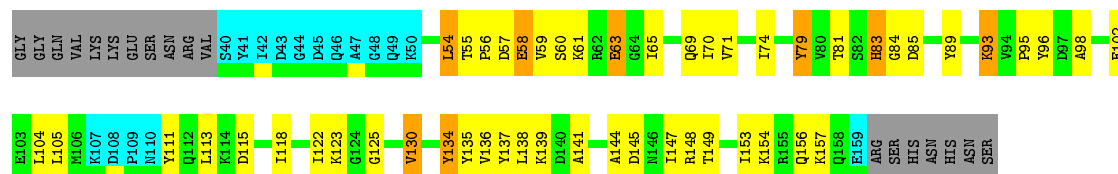




4.2.18 Score per residue for model 18

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D

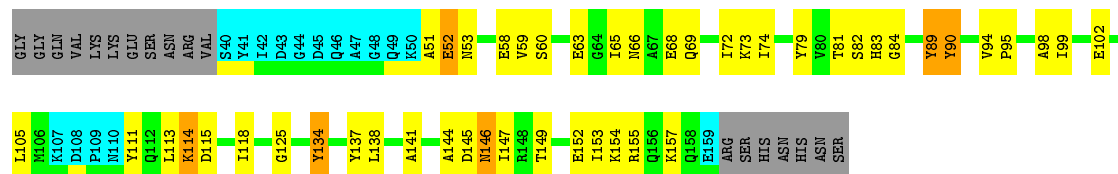
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D

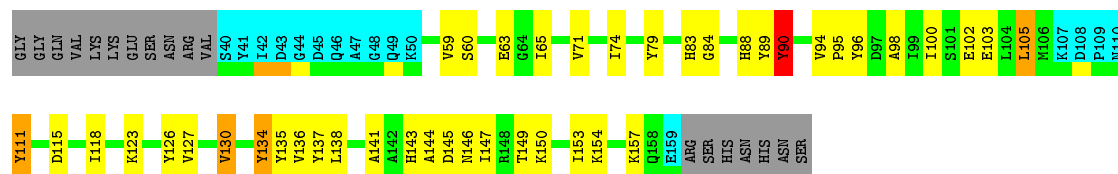
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: PNEUMOCOCCAL HISTIDINE TRIAD PROTEIN D

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *UNIO10*, *ARIA*.

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *TOTAL ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure solution	
CNS	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)	3zfj_cs.cif
Number of chemical shift lists	1
Total number of shifts	1473
Number of shifts mapped to atoms	1472
Number of unparsed shifts	1
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.58±0.20	1±2/862 (0.2±0.2%)	0.55±0.06	0±1/1163 (0.0±0.1%)
All	All	0.62	28/17240 (0.2%)	0.55	8/23260 (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±0.3
All	All	0	2

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	137	TYR	CE1-CZ	19.73	1.64	1.38	6	1
1	A	134	TYR	CE2-CZ	18.70	1.62	1.38	15	1
1	A	134	TYR	CE1-CZ	-18.65	1.14	1.38	15	1
1	A	137	TYR	CE2-CZ	-18.45	1.14	1.38	6	1
1	A	79	TYR	CE2-CZ	-11.23	1.24	1.38	11	4
1	A	79	TYR	CE1-CZ	10.48	1.52	1.38	11	4
1	A	90	TYR	CE2-CZ	-9.67	1.25	1.38	6	7
1	A	90	TYR	CE1-CZ	8.85	1.50	1.38	6	7
1	A	111	TYR	CE1-CZ	-5.40	1.31	1.38	20	1
1	A	137	TYR	CZ-OH	5.01	1.46	1.37	6	1

All unique angle 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(°)	Ideal(°)	Models	
								Worst	Total
1	A	137	TYR	CD1-CE1-CZ	-7.45	113.10	119.80	6	1
1	A	137	TYR	CE1-CZ-OH	-7.19	100.68	120.10	6	1
1	A	134	TYR	CZ-CE2-CD2	-6.87	113.62	119.80	15	1
1	A	134	TYR	CD1-CE1-CZ	6.75	125.88	119.80	15	1
1	A	134	TYR	CE1-CZ-OH	6.47	137.58	120.10	15	1
1	A	134	TYR	OH-CZ-CE2	-6.25	103.22	120.10	15	1
1	A	137	TYR	CB-CG-CD1	-5.66	117.61	121.00	6	1
1	A	137	TYR	CZ-CE2-CD2	5.12	124.41	119.80	6	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	137	TYR	Sidechain	1
1	A	111	TYR	Sidechain	1

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	846	831	830	36±5
All	All	16940	16620	16600	730

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ILE:HD12	1:A:84:GLY:HA3	0.90	1.41	13	17
1:A:60:SER:HB3	1:A:66:ASN:HA	0.82	1.48	12	4
1:A:51:ALA:H	1:A:89:TYR:HB3	0.81	1.33	12	2
1:A:138:LEU:HD23	1:A:141:ALA:HA	0.81	1.51	14	20
1:A:56:PRO:HG3	1:A:95:PRO:HG3	0.80	1.53	3	5
1:A:51:ALA:HB1	1:A:91:ASN:HB2	0.78	1.56	2	3
1:A:103:GLU:HG2	1:A:150:LYS:HE2	0.76	1.55	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:LYS:HE3	1:A:93:LYS:HA	0.73	1.59	6	1
1:A:105:LEU:HD11	1:A:147:ILE:HG13	0.73	1.60	14	2
1:A:95:PRO:HG2	1:A:98:ALA:HB2	0.72	1.59	14	20
1:A:105:LEU:HD21	1:A:147:ILE:HG13	0.71	1.61	11	9
1:A:102:GLU:HG2	1:A:149:THR:HA	0.70	1.63	9	17
1:A:115:ASP:HA	1:A:118:ILE:HD12	0.70	1.64	16	20
1:A:138:LEU:HD11	1:A:145:ASP:HB3	0.69	1.64	16	7
1:A:93:LYS:HA	1:A:93:LYS:HE3	0.69	1.64	2	2
1:A:52:GLU:HG2	1:A:90:TYR:HA	0.68	1.66	9	1
1:A:152:GLU:HA	1:A:155:ARG:HB3	0.67	1.64	19	2
1:A:79:TYR:OH	1:A:93:LYS:HA	0.67	1.90	4	8
1:A:148:ARG:HD3	1:A:156:GLN:HG3	0.66	1.65	18	1
1:A:157:LYS:HG3	1:A:158:GLN:HG3	0.65	1.69	5	1
1:A:70:ILE:HD13	1:A:148:ARG:HG2	0.65	1.68	3	1
1:A:100:ILE:HG21	1:A:136:VAL:HG21	0.65	1.67	9	13
1:A:106:MET:SD	1:A:128:ILE:HD11	0.64	2.32	9	4
1:A:120:ASN:OD1	1:A:127:VAL:HG12	0.64	1.91	2	1
1:A:74:ILE:HG13	1:A:104:LEU:HD13	0.64	1.68	15	17
1:A:94:VAL:HG21	1:A:127:VAL:HG21	0.63	1.70	20	2
1:A:103:GLU:CG	1:A:150:LYS:HD2	0.63	2.24	14	2
1:A:138:LEU:HD22	1:A:147:ILE:HG13	0.62	1.71	7	16
1:A:131:ASP:HB3	1:A:133:LYS:HE2	0.62	1.71	13	1
1:A:118:ILE:HA	1:A:128:ILE:HG22	0.62	1.72	3	10
1:A:74:ILE:HG23	1:A:79:TYR:CD1	0.61	2.30	1	7
1:A:138:LEU:CD2	1:A:141:ALA:HA	0.61	2.23	14	2
1:A:59:VAL:O	1:A:63:GLU:HG2	0.61	1.96	15	6
1:A:88:HIS:HB3	1:A:90:TYR:HE1	0.61	1.56	11	9
1:A:69:GLN:HB3	1:A:81:THR:HG21	0.61	1.71	15	6
1:A:125:GLY:HA2	1:A:137:TYR:O	0.60	1.95	19	17
1:A:148:ARG:HD2	1:A:152:GLU:HG2	0.60	1.73	3	1
1:A:69:GLN:HA	1:A:83:HIS:HB3	0.60	1.74	5	12
1:A:68:GLU:HB3	1:A:99:ILE:HG13	0.60	1.73	9	4
1:A:69:GLN:HG2	1:A:83:HIS:HD1	0.59	1.57	18	4
1:A:71:VAL:HG22	1:A:81:THR:HG22	0.59	1.74	5	7
1:A:59:VAL:HG12	1:A:63:GLU:OE2	0.59	1.96	3	4
1:A:52:GLU:HG3	1:A:90:TYR:HA	0.59	1.74	12	2
1:A:74:ILE:HG21	1:A:134:TYR:CD1	0.59	2.32	5	18
1:A:130:VAL:HG22	1:A:135:TYR:CE2	0.58	2.33	5	2
1:A:103:GLU:HG2	1:A:150:LYS:CE	0.58	2.28	12	1
1:A:79:TYR:CE1	1:A:81:THR:HG23	0.58	2.33	19	5
1:A:51:ALA:HA	1:A:90:TYR:HA	0.57	1.75	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LYS:HE2	1:A:80:VAL:HG23	0.57	1.74	15	1
1:A:149:THR:O	1:A:153:ILE:HG13	0.57	2.00	3	20
1:A:105:LEU:HD11	1:A:147:ILE:HG21	0.57	1.77	4	6
1:A:103:GLU:HG2	1:A:150:LYS:HE3	0.57	1.75	9	1
1:A:55:THR:O	1:A:59:VAL:HG23	0.56	2.00	10	15
1:A:130:VAL:HG22	1:A:135:TYR:CE1	0.56	2.35	14	13
1:A:137:TYR:CE2	1:A:139:LYS:HG2	0.56	2.35	18	5
1:A:105:LEU:HD23	1:A:147:ILE:HG13	0.56	1.76	18	1
1:A:102:GLU:OE2	1:A:150:LYS:HG2	0.56	2.01	2	1
1:A:120:ASN:OD1	1:A:122:ILE:HG23	0.56	2.00	2	1
1:A:154:LYS:O	1:A:158:GLN:HG3	0.56	2.01	12	6
1:A:127:VAL:HG22	1:A:134:TYR:HE1	0.56	1.61	7	9
1:A:138:LEU:HD13	1:A:145:ASP:CB	0.55	2.31	18	1
1:A:105:LEU:C	1:A:105:LEU:HD12	0.55	2.22	18	3
1:A:105:LEU:HD12	1:A:105:LEU:C	0.55	2.21	2	2
1:A:69:GLN:HG2	1:A:83:HIS:ND1	0.55	2.17	18	6
1:A:96:TYR:HE1	1:A:123:LYS:HA	0.55	1.60	4	8
1:A:154:LYS:HA	1:A:157:LYS:HG2	0.55	1.79	19	15
1:A:113:LEU:HD13	1:A:137:TYR:CD2	0.55	2.36	18	6
1:A:99:ILE:HG23	1:A:146:ASN:O	0.55	2.01	6	4
1:A:102:GLU:CG	1:A:149:THR:HA	0.55	2.32	20	13
1:A:100:ILE:HB	1:A:147:ILE:CD1	0.54	2.32	11	10
1:A:138:LEU:CD1	1:A:145:ASP:HB3	0.54	2.32	16	1
1:A:102:GLU:HA	1:A:105:LEU:HG	0.54	1.80	6	1
1:A:71:VAL:HG13	1:A:79:TYR:HB2	0.54	1.78	16	10
1:A:138:LEU:HD22	1:A:145:ASP:HB2	0.54	1.80	18	1
1:A:73:LYS:O	1:A:79:TYR:HB2	0.54	2.02	19	1
1:A:54:LEU:CD2	1:A:58:GLU:HB3	0.53	2.33	7	5
1:A:72:ILE:HD13	1:A:82:SER:OG	0.53	2.04	1	1
1:A:106:MET:SD	1:A:111:TYR:CD2	0.53	3.01	2	3
1:A:54:LEU:HD23	1:A:58:GLU:HB3	0.53	1.79	7	2
1:A:99:ILE:HA	1:A:146:ASN:OD1	0.52	2.05	17	3
1:A:100:ILE:HG22	1:A:101:SER:N	0.52	2.20	2	1
1:A:102:GLU:CD	1:A:102:GLU:H	0.52	2.06	2	1
1:A:96:TYR:CE1	1:A:123:LYS:HA	0.52	2.39	7	5
1:A:58:GLU:O	1:A:62:ARG:HB3	0.52	2.04	9	1
1:A:54:LEU:HD12	1:A:58:GLU:HB3	0.52	1.81	3	4
1:A:57:ASP:HB3	1:A:61:LYS:HE2	0.52	1.82	18	1
1:A:127:VAL:HG12	1:A:134:TYR:HE1	0.52	1.64	6	1
1:A:78:GLY:HA2	1:A:92:GLY:O	0.52	2.04	15	4
1:A:69:GLN:HA	1:A:83:HIS:CB	0.52	2.35	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:LEU:HD21	1:A:147:ILE:HD12	0.52	1.80	20	2
1:A:102:GLU:HA	1:A:105:LEU:CD2	0.52	2.35	7	2
1:A:93:LYS:CA	1:A:93:LYS:HE3	0.51	2.34	2	3
1:A:138:LEU:HD22	1:A:145:ASP:CB	0.51	2.35	14	1
1:A:125:GLY:HA3	1:A:145:ASP:OD2	0.51	2.05	18	1
1:A:54:LEU:HG	1:A:58:GLU:HB2	0.51	1.82	1	2
1:A:89:TYR:HD1	1:A:90:TYR:N	0.51	2.04	8	3
1:A:93:LYS:HE3	1:A:119:VAL:O	0.51	2.06	13	1
1:A:54:LEU:CD1	1:A:58:GLU:HB3	0.51	2.36	1	2
1:A:148:ARG:HD2	1:A:152:GLU:OE2	0.50	2.05	4	1
1:A:138:LEU:HD11	1:A:145:ASP:O	0.50	2.06	16	2
1:A:138:LEU:HD22	1:A:147:ILE:CG1	0.50	2.37	19	5
1:A:138:LEU:HD13	1:A:145:ASP:HA	0.50	1.82	14	1
1:A:127:VAL:HG22	1:A:134:TYR:CE1	0.50	2.41	7	7
1:A:148:ARG:HD2	1:A:156:GLN:HG3	0.50	1.82	3	2
1:A:103:GLU:CG	1:A:150:LYS:HD3	0.50	2.36	8	1
1:A:58:GLU:O	1:A:62:ARG:HB2	0.50	2.06	1	1
1:A:73:LYS:HB2	1:A:73:LYS:NZ	0.50	2.22	3	2
1:A:74:ILE:CG1	1:A:104:LEU:HD13	0.50	2.37	18	9
1:A:106:MET:SD	1:A:128:ILE:CD1	0.50	3.00	9	4
1:A:103:GLU:CG	1:A:150:LYS:HE3	0.49	2.37	9	1
1:A:60:SER:HA	1:A:63:GLU:HG2	0.49	1.82	5	4
1:A:82:SER:OG	1:A:157:LYS:HD3	0.49	2.06	16	1
1:A:105:LEU:HD23	1:A:147:ILE:HG21	0.49	1.84	8	1
1:A:117:ASP:HB2	1:A:130:VAL:HG12	0.49	1.83	14	1
1:A:102:GLU:OE2	1:A:103:GLU:HG3	0.49	2.08	2	1
1:A:148:ARG:CD	1:A:156:GLN:HG3	0.48	2.38	3	1
1:A:106:MET:HB3	1:A:137:TYR:HD1	0.48	1.69	6	1
1:A:113:LEU:HD22	1:A:137:TYR:CD2	0.48	2.44	19	4
1:A:54:LEU:HG	1:A:58:GLU:CB	0.48	2.38	1	1
1:A:126:TYR:O	1:A:136:VAL:HA	0.48	2.09	8	5
1:A:103:GLU:HG2	1:A:150:LYS:HD3	0.48	1.85	20	2
1:A:102:GLU:N	1:A:102:GLU:CD	0.48	2.67	2	1
1:A:114:LYS:O	1:A:118:ILE:HG13	0.47	2.10	19	9
1:A:106:MET:HB3	1:A:137:TYR:CD1	0.47	2.44	6	1
1:A:102:GLU:HA	1:A:105:LEU:HD23	0.47	1.85	7	1
1:A:52:GLU:HG3	1:A:90:TYR:CD2	0.47	2.44	9	1
1:A:105:LEU:HD21	1:A:147:ILE:HD11	0.47	1.86	14	1
1:A:90:TYR:N	1:A:90:TYR:CD1	0.47	2.82	20	1
1:A:99:ILE:HG21	1:A:148:ARG:HD2	0.47	1.87	1	1
1:A:90:TYR:HD1	1:A:91:ASN:N	0.47	2.08	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:GLU:OE2	1:A:83:HIS:CE1	0.47	2.68	18	2
1:A:126:TYR:HB2	1:A:137:TYR:HB3	0.46	1.86	20	2
1:A:55:THR:HB	1:A:56:PRO:HD2	0.46	1.86	18	1
1:A:70:ILE:HD13	1:A:148:ARG:HG3	0.46	1.87	18	2
1:A:106:MET:CG	1:A:137:TYR:CD1	0.46	2.98	6	1
1:A:52:GLU:HB2	1:A:90:TYR:HB3	0.46	1.87	8	1
1:A:122:ILE:HD11	1:A:136:VAL:HG13	0.46	1.87	18	1
1:A:138:LEU:HD13	1:A:145:ASP:CG	0.46	2.31	18	1
1:A:90:TYR:CD1	1:A:90:TYR:N	0.46	2.84	16	5
1:A:52:GLU:HB3	1:A:54:LEU:CD2	0.46	2.40	10	1
1:A:70:ILE:HA	1:A:99:ILE:O	0.46	2.10	10	1
1:A:117:ASP:HB3	1:A:130:VAL:HG12	0.46	1.88	3	1
1:A:100:ILE:HG13	1:A:136:VAL:HG11	0.46	1.88	2	2
1:A:73:LYS:HE2	1:A:80:VAL:CG2	0.46	2.41	15	1
1:A:106:MET:HB3	1:A:137:TYR:CB	0.45	2.41	6	1
1:A:70:ILE:HG12	1:A:99:ILE:HG21	0.45	1.87	11	1
1:A:80:VAL:HG22	1:A:89:TYR:CG	0.45	2.46	4	2
1:A:99:ILE:CG2	1:A:148:ARG:HG2	0.45	2.41	10	1
1:A:93:LYS:HE3	1:A:119:VAL:HG12	0.45	1.87	17	2
1:A:60:SER:HA	1:A:63:GLU:OE2	0.45	2.10	18	1
1:A:60:SER:HB3	1:A:65:ILE:O	0.45	2.11	18	2
1:A:60:SER:HA	1:A:63:GLU:CG	0.45	2.42	5	1
1:A:103:GLU:CG	1:A:150:LYS:HG2	0.45	2.42	4	1
1:A:100:ILE:HB	1:A:147:ILE:HD13	0.45	1.88	8	2
1:A:59:VAL:HG11	1:A:90:TYR:CE2	0.45	2.47	20	1
1:A:81:THR:O	1:A:87:TYR:HA	0.45	2.11	3	1
1:A:133:LYS:N	1:A:133:LYS:HD3	0.45	2.25	15	2
1:A:71:VAL:HB	1:A:100:ILE:HD13	0.45	1.89	9	3
1:A:103:GLU:OE1	1:A:150:LYS:HD2	0.45	2.12	16	1
1:A:155:ARG:HA	1:A:158:GLN:NE2	0.45	2.27	1	1
1:A:93:LYS:HE2	1:A:119:VAL:HG12	0.45	1.89	1	1
1:A:125:GLY:CA	1:A:137:TYR:O	0.44	2.65	4	1
1:A:113:LEU:HD22	1:A:137:TYR:CE2	0.44	2.47	15	4
1:A:74:ILE:HB	1:A:134:TYR:HB3	0.44	1.89	19	2
1:A:131:ASP:OD2	1:A:133:LYS:HE2	0.44	2.13	15	1
1:A:56:PRO:O	1:A:59:VAL:HB	0.44	2.11	8	1
1:A:99:ILE:HD13	1:A:146:ASN:HB2	0.44	1.89	11	1
1:A:103:GLU:CD	1:A:150:LYS:HD2	0.44	2.33	14	1
1:A:106:MET:HB3	1:A:137:TYR:HB2	0.44	1.88	6	1
1:A:154:LYS:O	1:A:157:LYS:HG2	0.44	2.12	12	1
1:A:124:GLY:HA3	1:A:145:ASP:CG	0.44	2.32	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:GLU:O	1:A:83:HIS:HB2	0.44	2.13	15	1
1:A:111:TYR:OH	1:A:137:TYR:CD1	0.44	2.60	20	1
1:A:138:LEU:HD22	1:A:145:ASP:HB3	0.44	1.89	14	1
1:A:105:LEU:CD2	1:A:147:ILE:HG13	0.44	2.42	18	1
1:A:124:GLY:HA3	1:A:145:ASP:OD1	0.44	2.13	10	2
1:A:145:ASP:O	1:A:146:ASN:ND2	0.44	2.51	15	7
1:A:60:SER:O	1:A:63:GLU:HG3	0.44	2.13	18	1
1:A:115:ASP:HA	1:A:118:ILE:CD1	0.44	2.42	15	1
1:A:106:MET:HG3	1:A:137:TYR:CD1	0.43	2.49	6	1
1:A:120:ASN:HB3	1:A:127:VAL:CG1	0.43	2.43	9	1
1:A:124:GLY:HA3	1:A:145:ASP:OD2	0.43	2.13	16	1
1:A:121:GLU:HB2	1:A:126:TYR:CE2	0.43	2.48	12	1
1:A:70:ILE:CD1	1:A:148:ARG:HG3	0.43	2.43	18	1
1:A:119:VAL:HG11	1:A:134:TYR:OH	0.43	2.13	6	1
1:A:70:ILE:HG12	1:A:99:ILE:CG2	0.43	2.43	11	1
1:A:74:ILE:HD13	1:A:127:VAL:HG23	0.43	1.89	13	1
1:A:84:GLY:O	1:A:157:LYS:HA	0.43	2.14	9	2
1:A:151:GLU:O	1:A:155:ARG:HG3	0.43	2.13	12	1
1:A:127:VAL:HG12	1:A:134:TYR:CE1	0.43	2.47	6	1
1:A:122:ILE:HD11	1:A:136:VAL:CG1	0.43	2.43	18	1
1:A:79:TYR:CD2	1:A:94:VAL:HG22	0.43	2.49	13	1
1:A:58:GLU:O	1:A:62:ARG:HD3	0.43	2.14	4	1
1:A:140:ASP:HB3	1:A:145:ASP:OD2	0.43	2.14	1	1
1:A:59:VAL:HG21	1:A:90:TYR:CE2	0.43	2.48	3	1
1:A:51:ALA:HA	1:A:89:TYR:O	0.43	2.14	8	1
1:A:105:LEU:O	1:A:105:LEU:HD12	0.42	2.14	18	1
1:A:119:VAL:HG21	1:A:134:TYR:OH	0.42	2.14	1	2
1:A:106:MET:SD	1:A:111:TYR:CE2	0.42	3.12	11	1
1:A:152:GLU:O	1:A:156:GLN:HG2	0.42	2.14	6	3
1:A:51:ALA:N	1:A:89:TYR:HB3	0.42	2.14	12	1
1:A:72:ILE:HD13	1:A:82:SER:HB2	0.42	1.92	19	2
1:A:105:LEU:HD12	1:A:105:LEU:O	0.41	2.15	8	3
1:A:128:ILE:O	1:A:134:TYR:HA	0.41	2.14	14	1
1:A:52:GLU:CD	1:A:59:VAL:HG11	0.41	2.35	9	1
1:A:72:ILE:HA	1:A:101:SER:CB	0.41	2.45	14	1
1:A:100:ILE:CG2	1:A:101:SER:N	0.41	2.84	2	1
1:A:73:LYS:O	1:A:79:TYR:HB3	0.41	2.15	8	1
1:A:102:GLU:CD	1:A:150:LYS:HG2	0.41	2.35	2	1
1:A:79:TYR:CE2	1:A:94:VAL:HA	0.41	2.51	6	1
1:A:95:PRO:CG	1:A:98:ALA:HB2	0.41	2.39	14	1
1:A:79:TYR:HE2	1:A:94:VAL:HA	0.41	1.76	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:GLU:OE2	1:A:83:HIS:HE1	0.41	1.99	12	1
1:A:129:LYS:HA	1:A:133:LYS:O	0.40	2.16	4	2
1:A:54:LEU:H	1:A:54:LEU:CD2	0.40	2.28	18	1
1:A:149:THR:O	1:A:153:ILE:N	0.40	2.52	16	1
1:A:120:ASN:HB3	1:A:127:VAL:HG13	0.40	1.92	10	1
1:A:75:THR:HA	1:A:134:TYR:CE2	0.40	2.51	15	1
1:A:120:ASN:HB3	1:A:127:VAL:HB	0.40	1.91	6	1
1:A:51:ALA:O	1:A:91:ASN:HB3	0.40	2.17	17	1
1:A:74:ILE:HB	1:A:134:TYR:CB	0.40	2.46	18	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	104/138 (75%)	92±1 (89±1%)	10±1 (10±1%)	2±1 (1±1%)	19	64
All	All	2080/2760 (75%)	1849 (89%)	201 (10%)	30 (1%)	19	64

All 5 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	144	ALA	18
1	A	51	ALA	8
1	A	146	ASN	2
1	A	66	ASN	1
1	A	158	GLN	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	91/120 (76%)	81±2 (89±2%)	10±2 (11±2%)	11	54
All	All	1820/2400 (76%)	1613 (89%)	207 (11%)	11	54

All 35 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	89	TYR	20
1	A	83	HIS	20
1	A	134	TYR	19
1	A	130	VAL	16
1	A	96	TYR	12
1	A	146	ASN	12
1	A	102	GLU	10
1	A	90	TYR	10
1	A	60	SER	9
1	A	145	ASP	9
1	A	58	GLU	8
1	A	79	TYR	8
1	A	77	GLN	5
1	A	143	HIS	5
1	A	54	LEU	5
1	A	91	ASN	4
1	A	105	LEU	4
1	A	88	HIS	4
1	A	93	LYS	4
1	A	148	ARG	3
1	A	114	LYS	3
1	A	52	GLU	3
1	A	133	LYS	2
1	A	65	ILE	1
1	A	56	PRO	1
1	A	156	GLN	1
1	A	150	LYS	1
1	A	85	ASP	1
1	A	157	LYS	1
1	A	53	ASN	1
1	A	63	GLU	1
1	A	68	GLU	1
1	A	73	LYS	1
1	A	120	ASN	1
1	A	121	GLU	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 90% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: 3zfj_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1473
Number of shifts mapped to atoms	1472
Number of unparsed shifts	1
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following errors were found when reading this chemical shift list.

- Entity instance (chain) must be specified. The only occurrence is reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	39	VAL	C	175.787	?	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	119	0.48 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	110	0.33 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	116	0.12 ± 0.13	None needed (< 0.5 ppm)
^{15}N	116	0.32 ± 0.37	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 90%, i.e. 1182 atoms were assigned a chemical shift out of a possible 1309. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	514/516 (100%)	206/206 (100%)	206/208 (99%)	102/102 (100%)
Sidechain	570/681 (84%)	349/396 (88%)	217/255 (85%)	4/30 (13%)
Aromatic	98/112 (88%)	48/56 (86%)	42/48 (88%)	8/8 (100%)
Overall	1182/1309 (90%)	603/658 (92%)	465/511 (91%)	114/140 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1331 atoms were assigned a chemical shift out of a possible 1493. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	585/594 (98%)	234/237 (99%)	235/240 (98%)	116/117 (99%)
Sidechain	640/779 (82%)	393/454 (87%)	243/290 (84%)	4/35 (11%)
Aromatic	106/120 (88%)	52/60 (87%)	46/52 (88%)	8/8 (100%)
Overall	1331/1493 (89%)	679/751 (90%)	524/582 (90%)	128/160 (80%)

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	129	LYS	HG2	0.02	2.67 – 0.07	-5.2

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:

