



Full wwPDB NMR Structure Validation Report ⓘ

May 31, 2020 – 10:08 am BST

PDB ID : 6IF9
Title : Solution-state NMR structure of G57W human gammaS crystallin
Authors : Sharma, S.; Bari, K.J.; Chary, K.V.R.
Deposited on : 2018-09-19

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 ⓘ 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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

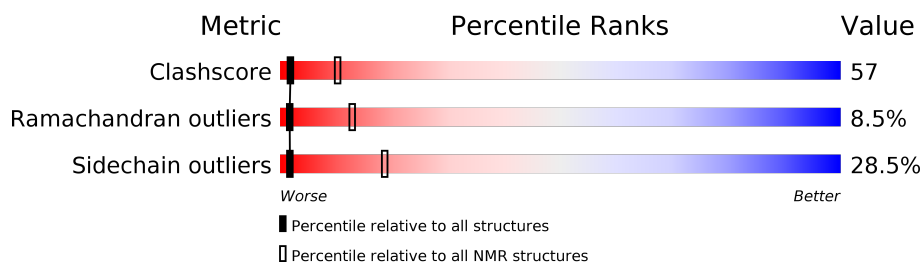
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	178	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:5-A:178 (174)	0.41	5

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2891 atoms, of which 1405 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gamma-crystallin S.

Mol	Chain	Residues	Atoms						Trace
1	A	178	Total	C	H	N	O	S	0
			2891	947	1405	254	272	13	

There is a discrepancy between the modelled and reference sequences:

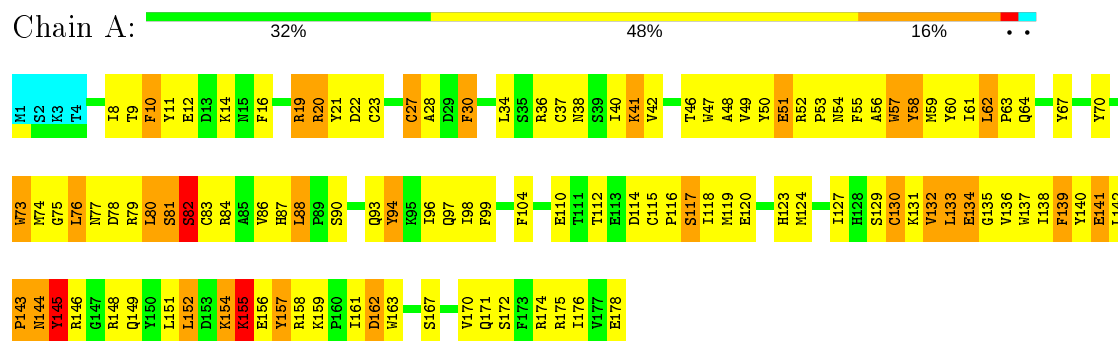
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	TRP	GLY	engineered mutation	UNP P22914

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: Gamma-crystallin S

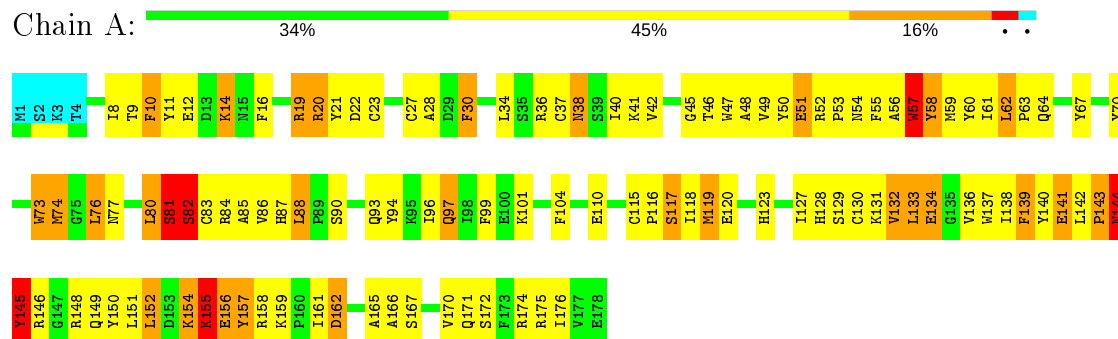


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

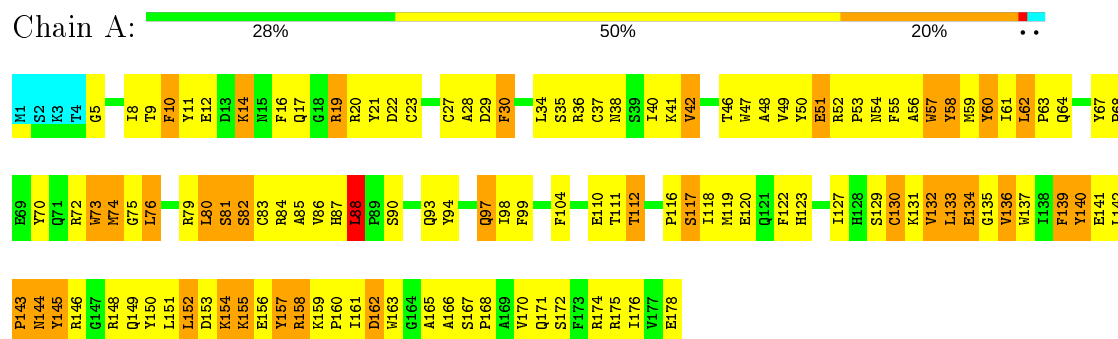
4.2.1 Score per residue for model 1

- Molecule 1: Gamma-crystallin S



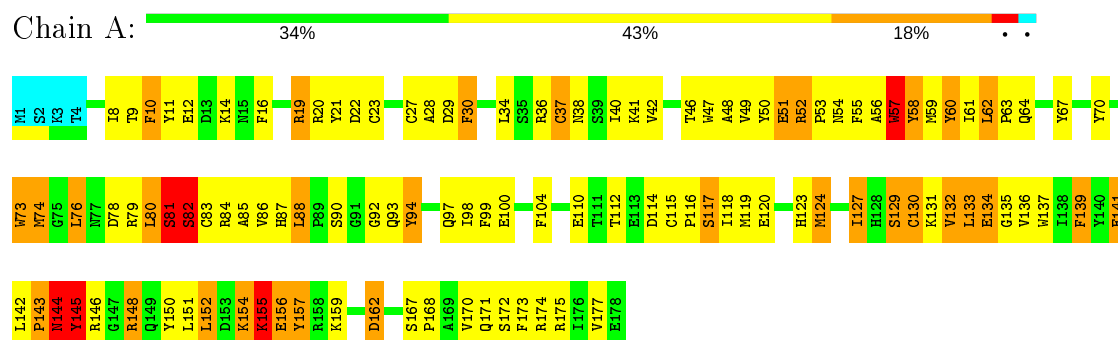
4.2.2 Score per residue for model 2

• Molecule 1: Gamma-crystallin S



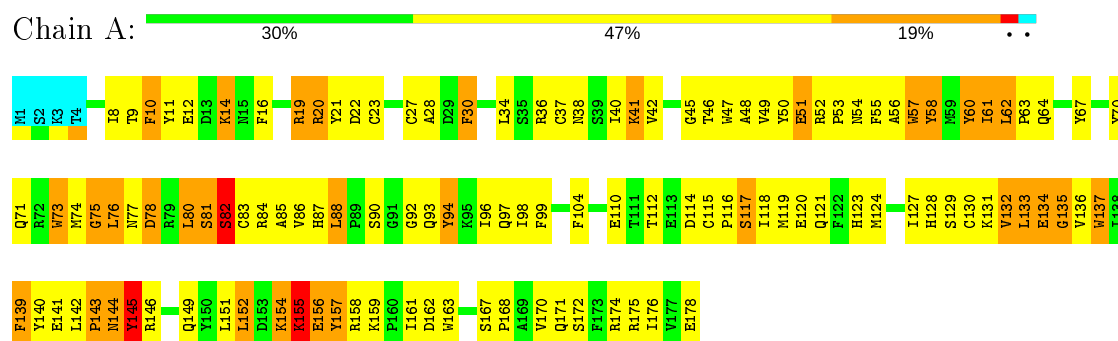
4.2.3 Score per residue for model 3

• Molecule 1: Gamma-crystallin S



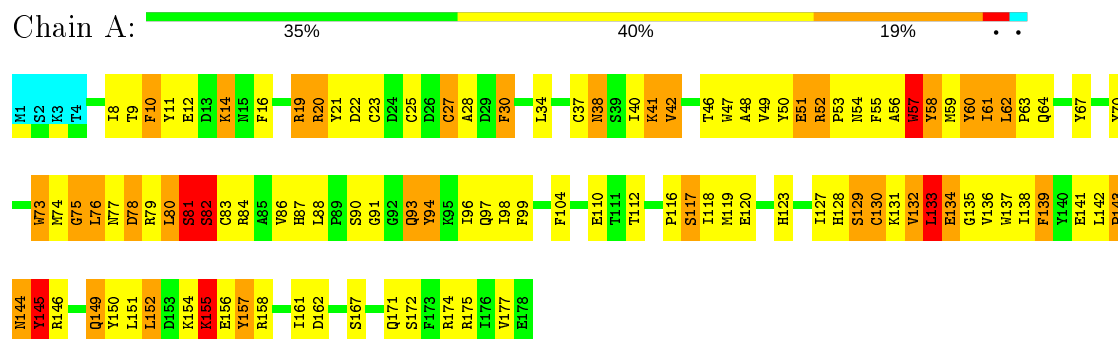
4.2.4 Score per residue for model 4

• Molecule 1: Gamma-crystallin S



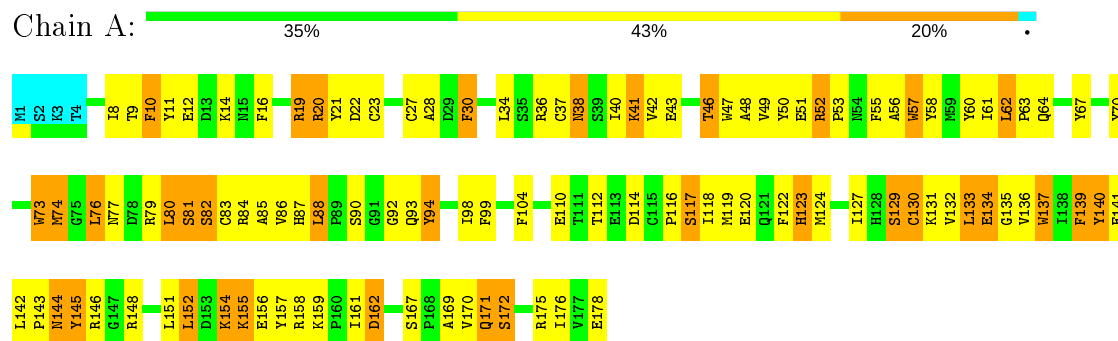
4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Gamma-crystallin S



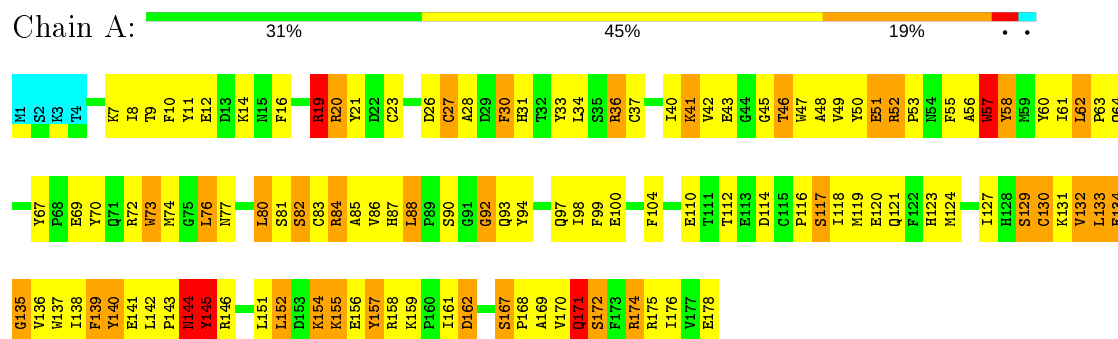
4.2.6 Score per residue for model 6

• Molecule 1: Gamma-crystallin S



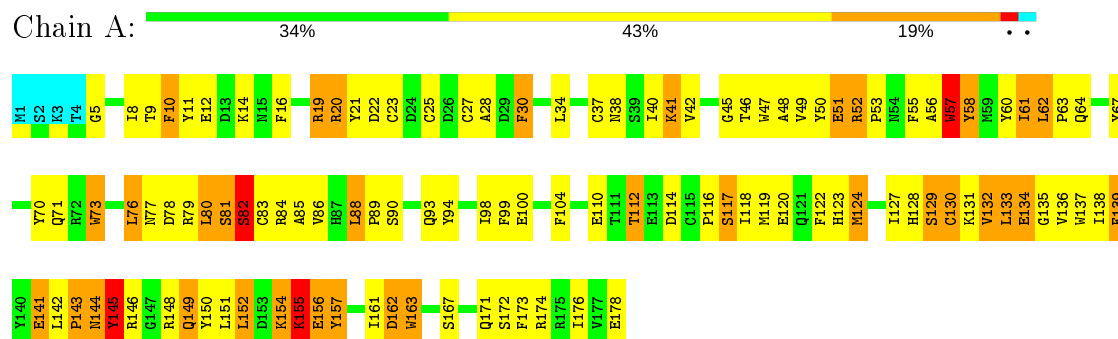
4.2.7 Score per residue for model 7

• Molecule 1: Gamma-crystallin S



4.2.8 Score per residue for model 8

• Molecule 1: Gamma-crystallin S



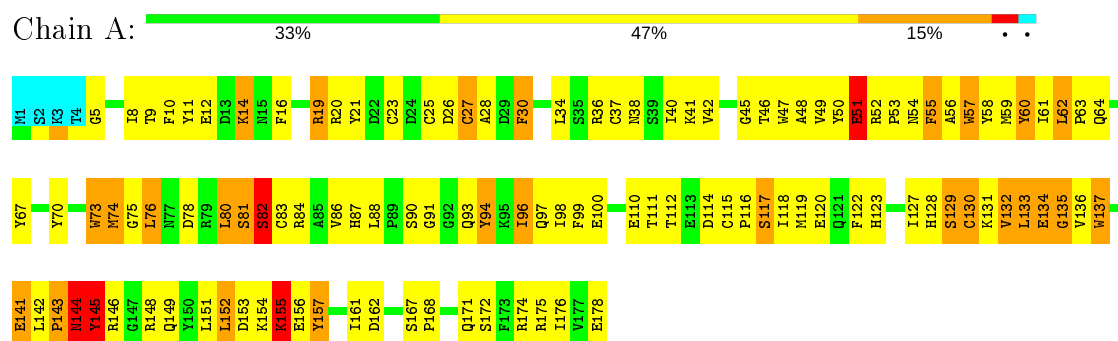
4.2.9 Score per residue for model 9

• Molecule 1: Gamma-crystallin S



4.2.10 Score per residue for model 10

• Molecule 1: Gamma-crystallin S



- Molecule 1: Gamma-crystallin S

L152	G75	M1
D153	L76	S2
K154	R79	K3
K155	L80	T4
E156	S81	T9
Y157	S82	F40
R158	S83	Y11
K159	R84	E12
P160	A85	D13
I161	V86	K14
D162	H87	H15
A165	L88	F16
A166	P89	
A167	S90	R19
P168	Q93	R20
A169	Y94	Y21
V170	F95	D22
Q171	I96	C27
S172	Q97	A28
F173	I98	D29
R174	F99	F30
R175	F104	L34
I176	E110	S35
V177	T111	R36
E178	T112	C37
	S117	I40
	I118	K41
	M119	V42
	E120	
	H123	T46
	M124	V47
	I127	A48
	H128	V49
	S129	Y50
	C130	E51
	K131	R52
	V132	P53
	E134	N54
	G135	F55
	V136	N57
	W137	Y58
	L142	N59
	F143	Y60
	Y140	L62
	E141	P63
	L142	Q64
	F143	
	N144	Y67
	Y145	Y70
	R146	Q71
		R72
		W73
		W74

- Molecule 1: Gamma-crystallin S

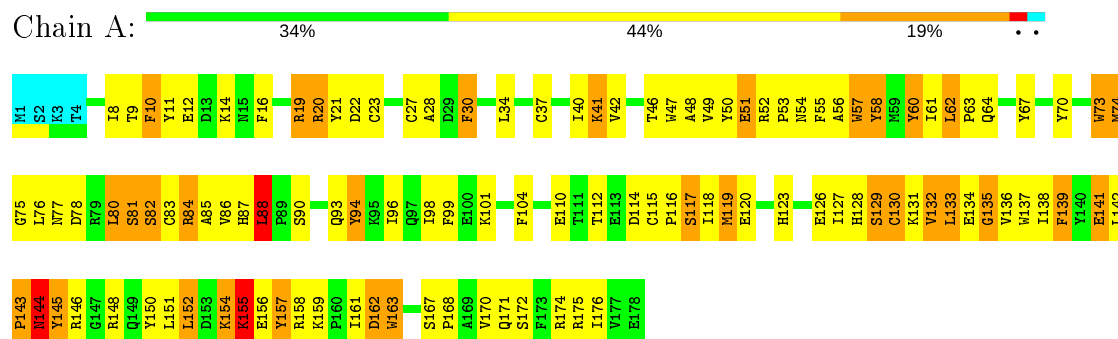
L142	Q71	M1
P143	R72	S2
N144	W73	K3
Y145	M74	T4
R146	L76	
	M77	I8
Q149	D78	T9
Y150	R79	F10
L151	L80	Y11
L152	S81	E12
D153	S82	D13
K154	C83	K14
K155	R84	M15
E156	A85	F16
Y157	V86	
R158	H87	R19
K159	L88	R20
	P89	Y21
D162	S90	D22
		C23
S167	Q93	
Q171	Y94	C27
S172	K95	A28
F173	I96	D29
R174	Q97	F30
R175	I98	
	F99	L34
E178	F104	S35
		R36
	M108	C37
	Y109	N38
	E110	T40
		K41
		V42
	D114	E43
	C115	
	P116	T46
	S117	N47
	M118	A48
	M119	V49
	E120	Y50
		E51
	H123	R52
		P53
	I127	N54
	H128	F55
	S129	A56
	C130	E57
	K131	Y58
	V132	M59
	L133	T60
	E134	L61
	G135	L62
	V136	P63
	W137	Q64
	I138	
	F139	V67
	Y140	
	R141	Y70

- Molecule 1: Gamma-crystallin S

L142	L143	L144	Y145	R146	G147	R148	L151	L152	L153	K154	K155	E156	Y157	R158	L161	D162	W163	S167	Q171	S172	F173	R174	R175	L176	V177	E178	W73	M74	G75	L76	W77	D78	R79	L80	S81	S82	C83	R84	A85	V86	H87	L88	P89	S90	G91	G92	Q93	I96	Q97	I98	F99	D103	F104	E110	T111	T112	E113	D114	C115	P116	S117	I118	M119	E120	Q121	F122	H123	I127	H128	S129	C130	K131	V132	L133	E134	G135	V136	W137	I138	F139	Y140	W141	E142
M1	S2	K3	T4	I8	T9	F10	Y11	E12	D13	K14	R15	F16	R19	R20	Y21	C27	A28	D29	F30	I34	S35	C36	C37	N38	S39	I40	K41	V42	T46	W47	A48	V49	Y50	E51	R52	P53	N54	F55	A56	R57	X58	N59	T60	I61	L62	P63	Q64	Y67	P68	D69	Y70	W71	E72																														

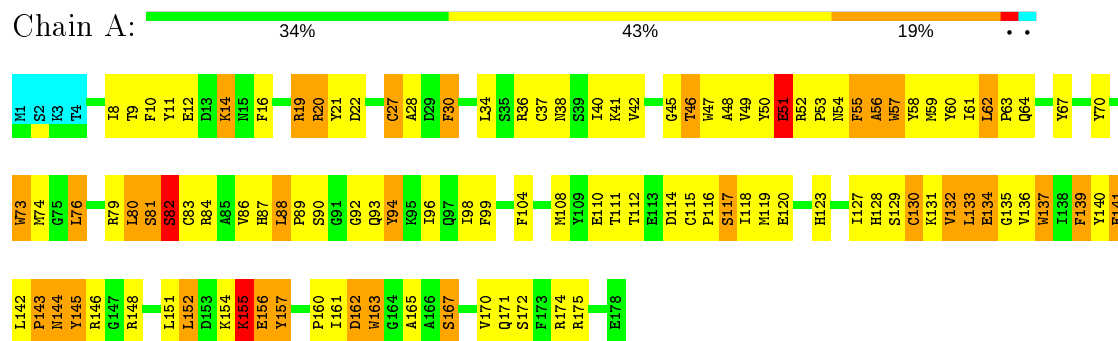
4.2.14 Score per residue for model 14

- Molecule 1: Gamma-crystallin S



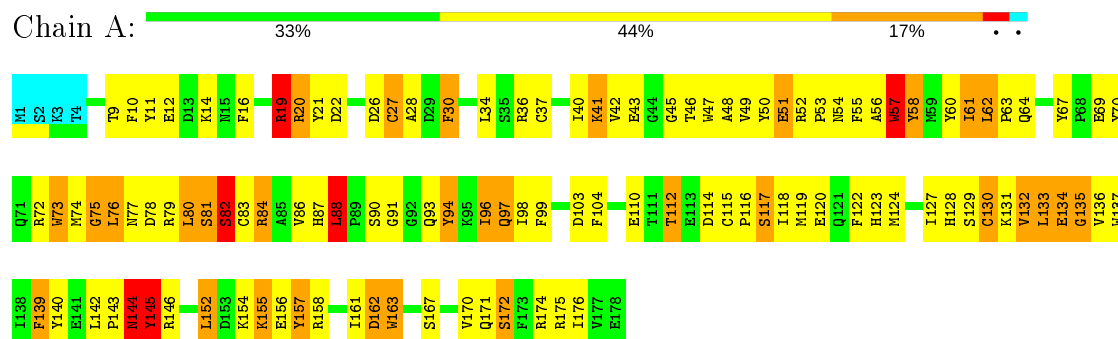
4.2.15 Score per residue for model 15

- Molecule 1: Gamma-crystallin S



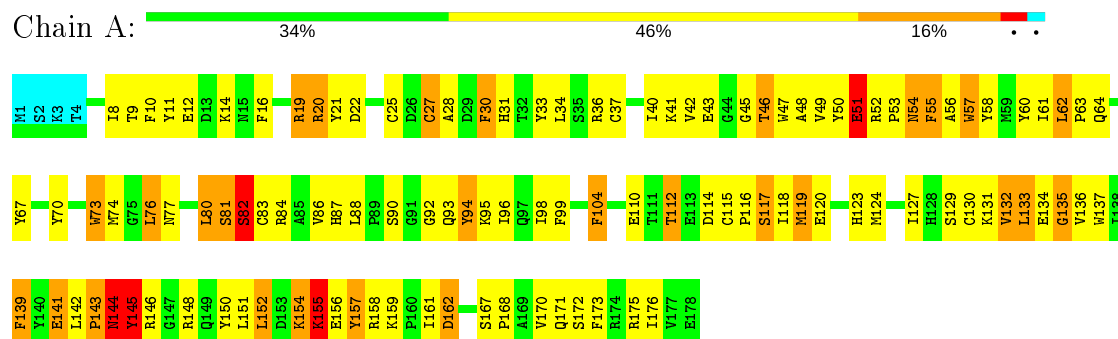
4.2.16 Score per residue for model 16

- Molecule 1: Gamma-crystallin S



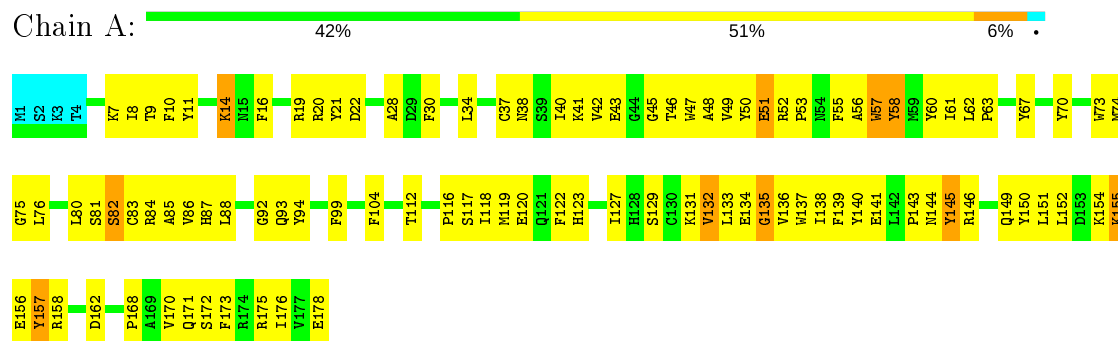
4.2.17 Score per residue for model 17

• Molecule 1: Gamma-crystallin S



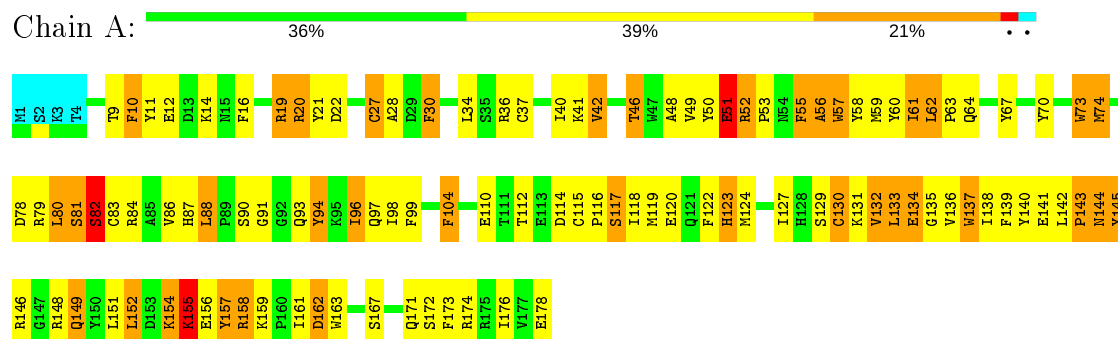
4.2.18 Score per residue for model 18

• Molecule 1: Gamma-crystallin S



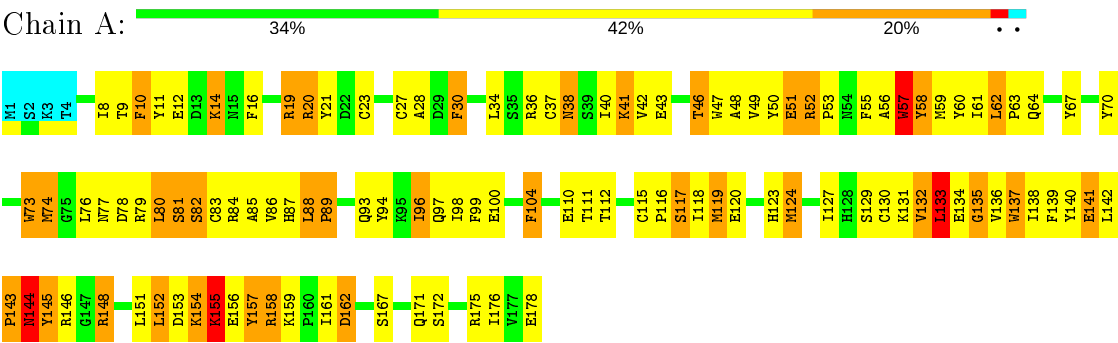
4.2.19 Score per residue for model 19

• Molecule 1: Gamma-crystallin S



4.2.20 Score per residue for model 20

● Molecule 1: Gamma-crystallin S



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 20 calculated structures, 20 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
CYANA	structure calculation	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1946
Number of shifts mapped to atoms	1946
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1456	1371	1371	161±6
All	All	29120	27420	27420	3217

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:ASN:O	1:A:146:ARG:N	1.09	1.83	6	20
1:A:152:LEU:O	1:A:152:LEU:HD13	0.99	1.56	19	10
1:A:70:TYR:O	1:A:73:TRP:CD1	0.99	2.16	4	10
1:A:152:LEU:HD13	1:A:152:LEU:O	0.98	1.57	6	10
1:A:142:LEU:O	1:A:172:SER:HB2	0.96	1.58	16	2
1:A:76:LEU:HD13	1:A:77:ASN:N	0.93	1.79	1	6
1:A:154:LYS:HB2	1:A:157:TYR:CD1	0.92	2.00	10	19
1:A:144:ASN:O	1:A:146:ARG:HG2	0.89	1.66	14	1
1:A:50:TYR:HB3	1:A:56:ALA:CB	0.85	1.99	10	6
1:A:52:ARG:O	1:A:56:ALA:HB2	0.85	1.72	15	6
1:A:48:ALA:HB2	1:A:86:VAL:CG2	0.85	2.02	12	20
1:A:153:ASP:O	1:A:154:LYS:HB2	0.84	1.73	13	1
1:A:30:PHE:O	1:A:30:PHE:CD2	0.83	2.31	10	12
1:A:30:PHE:CD2	1:A:30:PHE:O	0.82	2.32	7	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:HD23	1:A:155:LYS:HG3	0.81	1.52	14	1
1:A:143:PRO:O	1:A:172:SER:OG	0.81	1.99	13	15
1:A:40:ILE:HD12	1:A:73:TRP:CH2	0.80	2.10	18	10
1:A:86:VAL:HG11	1:A:136:VAL:HG11	0.80	1.54	2	13
1:A:60:TYR:CD2	1:A:76:LEU:HD12	0.79	2.12	11	8
1:A:61:ILE:HD12	1:A:61:ILE:N	0.79	1.93	16	7
1:A:86:VAL:CG1	1:A:136:VAL:HG11	0.79	2.08	1	18
1:A:49:VAL:O	1:A:60:TYR:O	0.79	1.99	12	17
1:A:136:VAL:HB	1:A:176:ILE:HD12	0.79	1.53	2	10
1:A:60:TYR:CD2	1:A:76:LEU:HD22	0.78	2.14	20	1
1:A:137:TRP:H	1:A:152:LEU:HD12	0.77	1.38	10	7
1:A:133:LEU:O	1:A:133:LEU:HD22	0.77	1.80	18	1
1:A:49:VAL:HG11	1:A:80:LEU:HD11	0.77	1.57	2	12
1:A:77:ASN:O	1:A:78:ASP:CB	0.77	2.32	5	6
1:A:61:ILE:N	1:A:61:ILE:HD12	0.77	1.94	5	6
1:A:137:TRP:N	1:A:152:LEU:HD12	0.77	1.95	10	1
1:A:154:LYS:O	1:A:155:LYS:HG3	0.76	1.81	18	19
1:A:73:TRP:O	1:A:74:MET:CB	0.76	2.32	11	4
1:A:133:LEU:HD13	1:A:154:LYS:O	0.75	1.82	12	16
1:A:152:LEU:C	1:A:152:LEU:HD22	0.74	2.03	8	10
1:A:73:TRP:CD1	1:A:73:TRP:N	0.74	2.55	16	7
1:A:86:VAL:HG13	1:A:136:VAL:HG11	0.73	1.60	15	7
1:A:73:TRP:N	1:A:73:TRP:CD1	0.73	2.56	15	3
1:A:154:LYS:HB3	1:A:157:TYR:CZ	0.73	2.19	13	1
1:A:163:TRP:NE1	1:A:165:ALA:HB3	0.72	1.98	15	1
1:A:60:TYR:CE2	1:A:76:LEU:HD12	0.72	2.19	4	5
1:A:152:LEU:HD22	1:A:152:LEU:C	0.72	2.05	4	10
1:A:73:TRP:O	1:A:74:MET:HB2	0.72	1.85	11	4
1:A:19:ARG:O	1:A:34:LEU:HD13	0.71	1.85	15	20
1:A:60:TYR:OH	1:A:73:TRP:O	0.71	2.08	9	9
1:A:30:PHE:O	1:A:30:PHE:CG	0.71	2.43	19	15
1:A:154:LYS:HA	1:A:157:TYR:CE1	0.71	2.20	20	19
1:A:10:PHE:HB2	1:A:34:LEU:HD22	0.71	1.61	2	19
1:A:86:VAL:HG13	1:A:136:VAL:HG21	0.71	1.62	7	15
1:A:133:LEU:HD22	1:A:155:LYS:CG	0.70	2.17	4	15
1:A:30:PHE:CG	1:A:30:PHE:O	0.70	2.43	6	5
1:A:171:GLN:N	1:A:171:GLN:CD	0.70	2.44	7	2
1:A:61:ILE:HD13	1:A:138:ILE:HG23	0.70	1.63	13	2
1:A:10:PHE:CD1	1:A:80:LEU:HD12	0.70	2.22	3	11
1:A:157:TYR:CD1	1:A:162:ASP:HB3	0.70	2.22	14	19
1:A:156:GLU:O	1:A:157:TYR:O	0.70	2.10	13	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:LEU:HB3	1:A:143:PRO:HD2	0.69	1.64	14	16
1:A:53:PRO:HA	1:A:82:SER:OG	0.69	1.88	4	20
1:A:143:PRO:O	1:A:172:SER:HB2	0.69	1.87	2	1
1:A:116:PRO:O	1:A:172:SER:HB2	0.69	1.88	7	2
1:A:133:LEU:HD22	1:A:155:LYS:HG3	0.68	1.65	12	14
1:A:87:HIS:O	1:A:136:VAL:HG23	0.68	1.87	7	18
1:A:144:ASN:O	1:A:146:ARG:CG	0.68	2.40	14	5
1:A:142:LEU:O	1:A:172:SER:HB3	0.68	1.88	7	2
1:A:52:ARG:H	1:A:56:ALA:HA	0.68	1.49	10	6
1:A:143:PRO:O	1:A:172:SER:CB	0.68	2.42	2	1
1:A:133:LEU:HD11	1:A:152:LEU:HD23	0.68	1.65	20	1
1:A:76:LEU:O	1:A:76:LEU:HD22	0.68	1.87	8	5
1:A:49:VAL:HG12	1:A:83:CYS:CB	0.68	2.19	12	18
1:A:154:LYS:C	1:A:155:LYS:HD2	0.68	2.10	11	14
1:A:76:LEU:HD22	1:A:76:LEU:O	0.68	1.89	6	1
1:A:76:LEU:N	1:A:76:LEU:HD12	0.67	2.02	2	1
1:A:163:TRP:CD1	1:A:163:TRP:N	0.67	2.62	16	2
1:A:104:PHE:CD2	1:A:104:PHE:N	0.67	2.62	13	3
1:A:144:ASN:O	1:A:145:TYR:C	0.67	2.32	16	20
1:A:49:VAL:HG12	1:A:83:CYS:HB3	0.67	1.65	9	15
1:A:94:TYR:CD2	1:A:134:GLU:HB2	0.67	2.25	20	1
1:A:62:LEU:HD23	1:A:63:PRO:HD2	0.66	1.66	11	20
1:A:130:CYS:O	1:A:155:LYS:O	0.66	2.12	16	18
1:A:130:CYS:O	1:A:157:TYR:HB2	0.66	1.91	13	1
1:A:137:TRP:CB	1:A:152:LEU:HB3	0.66	2.21	9	5
1:A:61:ILE:HD11	1:A:151:LEU:CA	0.66	2.21	9	4
1:A:139:PHE:CE2	1:A:170:VAL:HG11	0.66	2.26	2	5
1:A:40:ILE:HG21	1:A:62:LEU:HD13	0.66	1.67	18	11
1:A:70:TYR:HA	1:A:73:TRP:NE1	0.66	2.06	18	10
1:A:50:TYR:HB3	1:A:56:ALA:HB3	0.66	1.66	9	6
1:A:171:GLN:OE1	1:A:172:SER:N	0.65	2.29	7	2
1:A:160:PRO:O	1:A:163:TRP:CD1	0.65	2.49	15	1
1:A:96:ILE:HD13	1:A:97:GLN:N	0.65	2.06	19	5
1:A:119:MET:O	1:A:123:HIS:HA	0.65	1.92	20	20
1:A:133:LEU:HD22	1:A:155:LYS:HG2	0.65	1.67	20	6
1:A:50:TYR:HB3	1:A:56:ALA:HA	0.65	1.67	13	14
1:A:57:TRP:O	1:A:58:TYR:C	0.65	2.35	7	14
1:A:61:ILE:HD11	1:A:151:LEU:HA	0.64	1.67	9	4
1:A:152:LEU:HD22	1:A:153:ASP:N	0.64	2.07	10	1
1:A:52:ARG:O	1:A:56:ALA:CB	0.64	2.44	11	6
1:A:136:VAL:CB	1:A:176:ILE:HD12	0.64	2.22	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:GLU:O	1:A:156:GLU:HG2	0.64	1.92	13	12
1:A:60:TYR:HA	1:A:149:GLN:OE1	0.64	1.93	12	3
1:A:133:LEU:HD12	1:A:152:LEU:HD23	0.64	1.68	12	4
1:A:61:ILE:CD1	1:A:61:ILE:N	0.64	2.61	4	9
1:A:115:CYS:O	1:A:172:SER:HB2	0.64	1.93	20	10
1:A:48:ALA:O	1:A:84:ARG:N	0.63	2.31	16	20
1:A:152:LEU:CD1	1:A:152:LEU:O	0.63	2.44	16	11
1:A:143:PRO:HA	1:A:172:SER:HB3	0.63	1.68	20	17
1:A:73:TRP:O	1:A:74:MET:CG	0.63	2.46	11	1
1:A:137:TRP:HB3	1:A:152:LEU:CB	0.63	2.24	11	15
1:A:140:TYR:CD2	1:A:145:TYR:HA	0.63	2.29	18	2
1:A:141:GLU:O	1:A:171:GLN:NE2	0.62	2.31	7	2
1:A:137:TRP:CD1	1:A:137:TRP:C	0.62	2.73	20	1
1:A:152:LEU:O	1:A:152:LEU:CD1	0.62	2.44	18	8
1:A:74:MET:O	1:A:75:GLY:C	0.62	2.37	4	6
1:A:131:LYS:HA	1:A:156:GLU:HA	0.62	1.72	13	15
1:A:171:GLN:N	1:A:171:GLN:NE2	0.62	2.48	7	2
1:A:118:ILE:HB	1:A:171:GLN:O	0.62	1.95	2	20
1:A:140:TYR:HB2	1:A:172:SER:O	0.62	1.94	7	2
1:A:116:PRO:O	1:A:172:SER:CB	0.62	2.47	18	2
1:A:142:LEU:CB	1:A:146:ARG:HB2	0.62	2.25	14	1
1:A:118:ILE:HD13	1:A:127:ILE:HD11	0.62	1.72	7	17
1:A:134:GLU:O	1:A:135:GLY:C	0.61	2.36	7	17
1:A:86:VAL:CG1	1:A:136:VAL:HG21	0.61	2.24	7	10
1:A:76:LEU:HD13	1:A:76:LEU:C	0.61	2.15	6	2
1:A:53:PRO:O	1:A:55:PHE:CD1	0.61	2.53	16	5
1:A:48:ALA:HB2	1:A:86:VAL:HG23	0.61	1.72	12	10
1:A:173:PHE:CD1	1:A:173:PHE:N	0.61	2.68	18	1
1:A:57:TRP:O	1:A:58:TYR:CD2	0.61	2.54	19	5
1:A:96:ILE:HD11	1:A:154:LYS:NZ	0.61	2.11	12	1
1:A:143:PRO:HD3	1:A:171:GLN:CD	0.61	2.16	18	7
1:A:138:ILE:HG23	1:A:149:GLN:NE2	0.61	2.10	8	2
1:A:61:ILE:N	1:A:61:ILE:CD1	0.60	2.63	5	5
1:A:163:TRP:N	1:A:163:TRP:CD1	0.60	2.68	8	1
1:A:137:TRP:HB3	1:A:152:LEU:HB3	0.60	1.73	11	18
1:A:46:THR:HG23	1:A:63:PRO:HA	0.60	1.74	5	20
1:A:40:ILE:O	1:A:67:TYR:HB2	0.60	1.96	19	13
1:A:156:GLU:O	1:A:157:TYR:C	0.60	2.40	13	20
1:A:51:GLU:N	1:A:56:ALA:HB1	0.60	2.12	9	3
1:A:140:TYR:CE2	1:A:145:TYR:HA	0.59	2.31	6	4
1:A:88:LEU:HD13	1:A:178:GLU:HB3	0.59	1.73	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:LEU:HD13	1:A:178:GLU:HA	0.59	1.74	20	2
1:A:143:PRO:HB3	1:A:171:GLN:OE1	0.59	1.98	4	18
1:A:37:CYS:SG	1:A:80:LEU:HB2	0.59	2.37	18	13
1:A:70:TYR:O	1:A:73:TRP:NE1	0.59	2.35	2	4
1:A:104:PHE:N	1:A:104:PHE:CD2	0.59	2.69	19	2
1:A:61:ILE:HD13	1:A:138:ILE:HD13	0.59	1.74	9	1
1:A:104:PHE:CE1	1:A:131:LYS:HD2	0.59	2.33	9	5
1:A:139:PHE:CD1	1:A:170:VAL:HG11	0.59	2.32	15	4
1:A:98:ILE:HG23	1:A:127:ILE:HG13	0.59	1.75	3	1
1:A:70:TYR:HA	1:A:73:TRP:CE2	0.59	2.33	15	10
1:A:76:LEU:H	1:A:76:LEU:HD12	0.59	1.57	2	2
1:A:154:LYS:CG	1:A:155:LYS:N	0.59	2.64	19	12
1:A:56:ALA:O	1:A:57:TRP:O	0.59	2.20	13	14
1:A:152:LEU:C	1:A:152:LEU:HD13	0.59	2.18	10	2
1:A:94:TYR:CE2	1:A:137:TRP:HB2	0.59	2.33	20	1
1:A:117:SER:HB3	1:A:120:GLU:CB	0.59	2.28	16	20
1:A:116:PRO:O	1:A:172:SER:OG	0.59	2.16	16	2
1:A:99:PHE:HB2	1:A:129:SER:HB2	0.58	1.74	20	17
1:A:76:LEU:HD21	1:A:148:ARG:HA	0.58	1.73	2	4
1:A:94:TYR:CZ	1:A:175:ARG:HA	0.58	2.32	9	1
1:A:104:PHE:CZ	1:A:158:ARG:HB3	0.58	2.33	6	7
1:A:133:LEU:HD12	1:A:154:LYS:O	0.58	1.97	5	1
1:A:40:ILE:HD12	1:A:73:TRP:CZ3	0.58	2.34	19	12
1:A:141:GLU:O	1:A:171:GLN:HB2	0.58	1.99	8	17
1:A:143:PRO:CD	1:A:171:GLN:HG2	0.58	2.28	6	2
1:A:49:VAL:HG23	1:A:60:TYR:O	0.58	1.99	10	8
1:A:98:ILE:HD11	1:A:111:THR:HG22	0.58	1.74	10	3
1:A:37:CYS:SG	1:A:80:LEU:CB	0.58	2.92	11	4
1:A:76:LEU:C	1:A:76:LEU:HD13	0.57	2.20	1	4
1:A:51:GLU:OE1	1:A:58:TYR:CB	0.57	2.52	9	1
1:A:133:LEU:HD22	1:A:155:LYS:HA	0.57	1.75	13	1
1:A:139:PHE:CE1	1:A:170:VAL:HG11	0.57	2.34	4	4
1:A:127:ILE:N	1:A:127:ILE:HD13	0.57	2.14	8	10
1:A:49:VAL:HG11	1:A:80:LEU:CD1	0.57	2.30	8	12
1:A:87:HIS:O	1:A:136:VAL:CG2	0.57	2.52	2	15
1:A:60:TYR:OH	1:A:73:TRP:CG	0.57	2.55	4	3
1:A:50:TYR:N	1:A:82:SER:O	0.57	2.37	17	16
1:A:131:LYS:HA	1:A:155:LYS:O	0.57	2.00	4	15
1:A:133:LEU:HD12	1:A:152:LEU:CD2	0.57	2.29	3	5
1:A:49:VAL:CG1	1:A:80:LEU:HD11	0.57	2.28	16	7
1:A:141:GLU:C	1:A:171:GLN:NE2	0.57	2.58	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ASN:O	1:A:78:ASP:HB2	0.57	1.98	5	1
1:A:98:ILE:HD13	1:A:118:ILE:HD11	0.57	1.77	13	3
1:A:133:LEU:CD1	1:A:133:LEU:O	0.57	2.53	14	1
1:A:138:ILE:HG21	1:A:174:ARG:NE	0.56	2.14	8	1
1:A:52:ARG:O	1:A:56:ALA:N	0.56	2.38	10	6
1:A:51:GLU:OE1	1:A:57:TRP:HB3	0.56	1.99	12	12
1:A:49:VAL:CG2	1:A:60:TYR:O	0.56	2.53	9	13
1:A:50:TYR:OH	1:A:151:LEU:HD23	0.56	2.00	1	11
1:A:99:PHE:CB	1:A:129:SER:HB2	0.56	2.30	19	16
1:A:50:TYR:CD2	1:A:56:ALA:HB1	0.56	2.35	5	9
1:A:142:LEU:CB	1:A:143:PRO:HD2	0.56	2.30	14	16
1:A:46:THR:HG22	1:A:62:LEU:O	0.56	2.01	11	12
1:A:61:ILE:HD11	1:A:151:LEU:HB2	0.56	1.76	18	11
1:A:133:LEU:HD11	1:A:152:LEU:CD2	0.56	2.29	20	1
1:A:129:SER:OG	1:A:158:ARG:O	0.56	2.15	1	6
1:A:10:PHE:CE1	1:A:80:LEU:HD12	0.56	2.35	12	17
1:A:52:ARG:HB3	1:A:55:PHE:CD2	0.56	2.36	7	3
1:A:53:PRO:HB3	1:A:81:SER:HB3	0.56	1.77	16	19
1:A:52:ARG:N	1:A:56:ALA:HB2	0.56	2.16	9	1
1:A:94:TYR:O	1:A:112:THR:HA	0.56	2.01	8	12
1:A:94:TYR:O	1:A:112:THR:CA	0.56	2.53	8	4
1:A:133:LEU:HD13	1:A:155:LYS:CG	0.56	2.31	2	1
1:A:62:LEU:HD11	1:A:73:TRP:CE3	0.56	2.36	19	6
1:A:154:LYS:HB3	1:A:157:TYR:CE1	0.56	2.36	13	1
1:A:76:LEU:C	1:A:76:LEU:HD22	0.55	2.22	8	4
1:A:48:ALA:HB2	1:A:86:VAL:HG21	0.55	1.77	14	12
1:A:161:ILE:HD12	1:A:161:ILE:H	0.55	1.61	7	9
1:A:58:TYR:HB3	1:A:76:LEU:HD11	0.55	1.79	20	1
1:A:156:GLU:HG2	1:A:156:GLU:O	0.55	2.00	12	7
1:A:50:TYR:CB	1:A:56:ALA:HA	0.55	2.31	2	14
1:A:127:ILE:HG21	1:A:130:CYS:SG	0.55	2.42	16	9
1:A:138:ILE:HG21	1:A:149:GLN:CD	0.55	2.22	1	1
1:A:60:TYR:OH	1:A:75:GLY:HA3	0.55	2.01	2	1
1:A:76:LEU:HD12	1:A:149:GLN:HE21	0.55	1.61	12	1
1:A:76:LEU:HD12	1:A:149:GLN:HG3	0.55	1.77	18	1
1:A:133:LEU:HD13	1:A:155:LYS:CE	0.55	2.30	2	1
1:A:48:ALA:O	1:A:83:CYS:CA	0.55	2.55	9	15
1:A:51:GLU:CG	1:A:52:ARG:N	0.55	2.69	11	5
1:A:8:ILE:HB	1:A:47:TRP:CD1	0.55	2.37	18	15
1:A:49:VAL:HG11	1:A:80:LEU:HD13	0.55	1.78	8	5
1:A:133:LEU:N	1:A:133:LEU:CD1	0.55	2.69	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:SER:O	1:A:82:SER:C	0.55	2.45	18	9
1:A:143:PRO:HD3	1:A:171:GLN:HG2	0.55	1.78	6	2
1:A:88:LEU:HD13	1:A:178:GLU:CB	0.55	2.32	8	2
1:A:51:GLU:HG2	1:A:52:ARG:N	0.55	2.17	19	4
1:A:37:CYS:SG	1:A:78:ASP:O	0.54	2.64	14	5
1:A:157:TYR:CG	1:A:162:ASP:CG	0.54	2.81	14	8
1:A:143:PRO:N	1:A:171:GLN:HG2	0.54	2.16	7	2
1:A:112:THR:OG1	1:A:112:THR:O	0.54	2.22	9	7
1:A:94:TYR:OH	1:A:177:VAL:HG23	0.54	2.02	5	1
1:A:139:PHE:HB2	1:A:150:TYR:HB2	0.54	1.78	18	1
1:A:51:GLU:O	1:A:79:ARG:O	0.54	2.25	11	2
1:A:137:TRP:O	1:A:152:LEU:HB3	0.54	2.02	13	6
1:A:98:ILE:HD12	1:A:109:TYR:O	0.54	2.03	12	1
1:A:10:PHE:CG	1:A:30:PHE:CZ	0.54	2.95	9	8
1:A:116:PRO:O	1:A:143:PRO:C	0.54	2.46	6	16
1:A:51:GLU:HB2	1:A:58:TYR:O	0.54	2.02	14	6
1:A:154:LYS:C	1:A:155:LYS:CD	0.54	2.77	12	12
1:A:127:ILE:HG22	1:A:127:ILE:O	0.54	2.03	6	1
1:A:99:PHE:HB2	1:A:129:SER:CB	0.53	2.33	3	8
1:A:137:TRP:CB	1:A:152:LEU:CB	0.53	2.86	9	1
1:A:131:LYS:C	1:A:132:VAL:HG23	0.53	2.23	14	19
1:A:152:LEU:O	1:A:152:LEU:HD22	0.53	2.03	2	3
1:A:76:LEU:HD12	1:A:148:ARG:CG	0.53	2.33	20	1
1:A:52:ARG:HB3	1:A:55:PHE:CD1	0.53	2.38	14	9
1:A:8:ILE:HD12	1:A:42:VAL:CG2	0.53	2.33	3	9
1:A:61:ILE:HD13	1:A:138:ILE:CD1	0.53	2.33	9	1
1:A:27:CYS:HB2	1:A:30:PHE:HB3	0.53	1.80	15	12
1:A:56:ALA:O	1:A:58:TYR:N	0.53	2.41	10	6
1:A:154:LYS:O	1:A:155:LYS:CG	0.53	2.56	1	14
1:A:51:GLU:CD	1:A:58:TYR:HB2	0.53	2.24	20	7
1:A:53:PRO:C	1:A:55:PHE:H	0.53	2.07	13	14
1:A:48:ALA:CB	1:A:86:VAL:HG23	0.53	2.34	12	10
1:A:56:ALA:C	1:A:58:TYR:H	0.53	2.07	19	5
1:A:60:TYR:OH	1:A:75:GLY:CA	0.53	2.57	13	1
1:A:143:PRO:HA	1:A:172:SER:CB	0.53	2.34	20	13
1:A:67:TYR:HB3	1:A:73:TRP:CD1	0.53	2.39	19	5
1:A:48:ALA:N	1:A:86:VAL:HG23	0.53	2.18	11	8
1:A:48:ALA:O	1:A:83:CYS:HA	0.53	2.04	9	16
1:A:98:ILE:CG2	1:A:127:ILE:HD12	0.53	2.34	12	13
1:A:27:CYS:HB3	1:A:30:PHE:HB3	0.53	1.81	10	2
1:A:48:ALA:N	1:A:84:ARG:O	0.53	2.40	11	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:ILE:H	1:A:161:ILE:HD12	0.52	1.63	15	8
1:A:136:VAL:CG1	1:A:176:ILE:CD1	0.52	2.87	16	2
1:A:14:LYS:N	1:A:38:ASN:HB3	0.52	2.18	5	11
1:A:127:ILE:HD13	1:A:127:ILE:N	0.52	2.20	7	7
1:A:52:ARG:N	1:A:56:ALA:CB	0.52	2.72	9	5
1:A:94:TYR:HA	1:A:134:GLU:CG	0.52	2.34	1	2
1:A:132:VAL:O	1:A:154:LYS:CE	0.52	2.58	2	1
1:A:136:VAL:HA	1:A:152:LEU:CD1	0.52	2.35	8	8
1:A:112:THR:O	1:A:112:THR:OG1	0.52	2.27	11	7
1:A:140:TYR:O	1:A:171:GLN:OE1	0.52	2.28	6	2
1:A:76:LEU:HD22	1:A:76:LEU:C	0.52	2.24	17	2
1:A:10:PHE:N	1:A:10:PHE:CD2	0.52	2.77	11	8
1:A:152:LEU:HD22	1:A:152:LEU:O	0.52	2.05	14	7
1:A:163:TRP:CG	1:A:163:TRP:O	0.52	2.63	4	1
1:A:131:LYS:O	1:A:132:VAL:CB	0.52	2.57	19	19
1:A:60:TYR:CE2	1:A:76:LEU:HB2	0.52	2.39	3	4
1:A:51:GLU:HB2	1:A:58:TYR:HB2	0.52	1.81	20	11
1:A:93:GLN:O	1:A:134:GLU:CG	0.52	2.58	12	10
1:A:140:TYR:O	1:A:171:GLN:NE2	0.52	2.42	7	2
1:A:28:ALA:O	1:A:82:SER:HA	0.52	2.04	10	16
1:A:93:GLN:O	1:A:134:GLU:HG3	0.52	2.04	17	1
1:A:61:ILE:HD13	1:A:138:ILE:HG12	0.52	1.82	20	2
1:A:76:LEU:HD23	1:A:77:ASN:H	0.52	1.65	20	1
1:A:163:TRP:CD1	1:A:165:ALA:HB3	0.52	2.40	15	2
1:A:51:GLU:OE1	1:A:58:TYR:O	0.51	2.28	9	1
1:A:37:CYS:SG	1:A:80:LEU:HB3	0.51	2.44	9	2
1:A:142:LEU:C	1:A:171:GLN:HB3	0.51	2.25	13	15
1:A:60:TYR:CE2	1:A:76:LEU:CB	0.51	2.94	3	6
1:A:144:ASN:O	1:A:146:ARG:CB	0.51	2.58	16	4
1:A:52:ARG:N	1:A:56:ALA:HA	0.51	2.19	10	5
1:A:143:PRO:O	1:A:145:TYR:N	0.51	2.43	14	1
1:A:132:VAL:HG12	1:A:133:LEU:N	0.51	2.20	2	19
1:A:21:TYR:CD2	1:A:30:PHE:CD2	0.51	2.99	14	20
1:A:133:LEU:HG	1:A:155:LYS:HG3	0.51	1.82	18	1
1:A:142:LEU:HB3	1:A:146:ARG:HB2	0.51	1.82	14	1
1:A:133:LEU:HD13	1:A:155:LYS:HG3	0.51	1.81	2	3
1:A:96:ILE:HD11	1:A:130:CYS:SG	0.51	2.45	19	2
1:A:40:ILE:O	1:A:67:TYR:N	0.51	2.43	14	18
1:A:152:LEU:CD2	1:A:152:LEU:C	0.51	2.79	14	13
1:A:96:ILE:HD12	1:A:98:ILE:CD1	0.51	2.36	19	1
1:A:73:TRP:O	1:A:74:MET:C	0.51	2.49	2	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:PHE:CB	1:A:34:LEU:HD22	0.51	2.33	13	11
1:A:143:PRO:HD3	1:A:171:GLN:CG	0.51	2.36	18	15
1:A:127:ILE:HG22	1:A:129:SER:O	0.51	2.06	16	6
1:A:28:ALA:O	1:A:82:SER:HB3	0.51	2.05	16	6
1:A:119:MET:O	1:A:123:HIS:N	0.50	2.44	16	11
1:A:34:LEU:HD21	1:A:36:ARG:O	0.50	2.06	13	8
1:A:131:LYS:O	1:A:132:VAL:HB	0.50	2.07	4	17
1:A:98:ILE:HD11	1:A:173:PHE:CE1	0.50	2.42	3	1
1:A:52:ARG:HB2	1:A:56:ALA:HA	0.50	1.81	10	5
1:A:154:LYS:HG3	1:A:155:LYS:N	0.50	2.21	15	8
1:A:9:THR:HG22	1:A:11:TYR:CE2	0.50	2.42	20	12
1:A:97:GLN:O	1:A:130:CYS:HA	0.50	2.06	7	2
1:A:76:LEU:HD13	1:A:77:ASN:H	0.50	1.63	7	1
1:A:60:TYR:CE2	1:A:76:LEU:HG	0.50	2.41	14	2
1:A:156:GLU:O	1:A:156:GLU:CG	0.50	2.60	19	9
1:A:49:VAL:HG21	1:A:80:LEU:HD21	0.50	1.82	16	2
1:A:73:TRP:CD1	1:A:73:TRP:C	0.50	2.84	9	5
1:A:136:VAL:HG12	1:A:176:ILE:CD1	0.50	2.36	16	6
1:A:155:LYS:HD2	1:A:155:LYS:N	0.50	2.21	19	3
1:A:48:ALA:CB	1:A:86:VAL:CG2	0.50	2.88	8	12
1:A:154:LYS:CB	1:A:157:TYR:CE1	0.50	2.95	13	1
1:A:133:LEU:HD23	1:A:155:LYS:CG	0.50	2.31	14	1
1:A:10:PHE:CD2	1:A:10:PHE:N	0.49	2.79	5	11
1:A:155:LYS:N	1:A:155:LYS:HD2	0.49	2.21	12	2
1:A:48:ALA:HB3	1:A:84:ARG:O	0.49	2.07	10	2
1:A:133:LEU:HD13	1:A:152:LEU:HD23	0.49	1.83	5	1
1:A:76:LEU:HD23	1:A:77:ASN:N	0.49	2.23	20	1
1:A:143:PRO:HD3	1:A:171:GLN:HG3	0.49	1.85	19	14
1:A:137:TRP:H	1:A:152:LEU:CG	0.49	2.20	8	4
1:A:118:ILE:CG2	1:A:171:GLN:O	0.49	2.61	13	15
1:A:61:ILE:H	1:A:61:ILE:HD12	0.49	1.68	9	2
1:A:77:ASN:O	1:A:78:ASP:HB3	0.49	2.06	5	2
1:A:104:PHE:CE2	1:A:156:GLU:HG2	0.49	2.43	13	1
1:A:94:TYR:CE2	1:A:137:TRP:CB	0.49	2.95	20	1
1:A:55:PHE:N	1:A:55:PHE:CD2	0.49	2.79	1	9
1:A:53:PRO:HD3	1:A:81:SER:OG	0.49	2.08	18	12
1:A:130:CYS:O	1:A:157:TYR:CB	0.49	2.60	13	1
1:A:55:PHE:CD2	1:A:55:PHE:N	0.49	2.79	6	1
1:A:94:TYR:CE2	1:A:137:TRP:CE2	0.49	3.01	9	1
1:A:119:MET:O	1:A:123:HIS:CA	0.49	2.60	8	20
1:A:138:ILE:CG2	1:A:149:GLN:HB2	0.49	2.37	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:LEU:C	1:A:152:LEU:CD2	0.49	2.78	17	6
1:A:144:ASN:C	1:A:146:ARG:N	0.49	2.62	16	4
1:A:40:ILE:O	1:A:67:TYR:CB	0.48	2.61	20	10
1:A:156:GLU:CG	1:A:156:GLU:O	0.48	2.60	16	10
1:A:76:LEU:HD11	1:A:149:GLN:HG3	0.48	1.85	4	1
1:A:89:PRO:HA	1:A:135:GLY:HA3	0.48	1.84	20	1
1:A:161:ILE:O	1:A:161:ILE:HG22	0.48	2.08	14	5
1:A:140:TYR:CE2	1:A:174:ARG:CD	0.48	2.97	9	2
1:A:27:CYS:CB	1:A:30:PHE:HB3	0.48	2.37	11	15
1:A:142:LEU:HB3	1:A:143:PRO:CD	0.48	2.36	14	13
1:A:130:CYS:O	1:A:156:GLU:C	0.48	2.52	13	1
1:A:87:HIS:O	1:A:88:LEU:C	0.48	2.52	2	16
1:A:37:CYS:HB3	1:A:80:LEU:HB2	0.48	1.85	15	6
1:A:99:PHE:CD2	1:A:104:PHE:HA	0.48	2.44	5	3
1:A:137:TRP:N	1:A:152:LEU:HG	0.48	2.24	7	17
1:A:9:THR:CG2	1:A:11:TYR:CE2	0.48	2.96	20	12
1:A:51:GLU:OE1	1:A:58:TYR:HB2	0.48	2.08	2	8
1:A:118:ILE:O	1:A:122:PHE:HB2	0.48	2.09	16	8
1:A:138:ILE:HG23	1:A:149:GLN:HE21	0.48	1.69	5	1
1:A:116:PRO:C	1:A:172:SER:OG	0.47	2.52	2	1
1:A:40:ILE:N	1:A:67:TYR:O	0.47	2.47	11	10
1:A:139:PHE:CB	1:A:150:TYR:HB2	0.47	2.38	3	7
1:A:139:PHE:CD2	1:A:170:VAL:HG11	0.47	2.43	6	2
1:A:55:PHE:N	1:A:55:PHE:CD1	0.47	2.79	8	3
1:A:131:LYS:HA	1:A:156:GLU:CA	0.47	2.38	13	1
1:A:11:TYR:CG	1:A:16:PHE:HA	0.47	2.44	20	20
1:A:28:ALA:C	1:A:82:SER:HA	0.47	2.29	10	11
1:A:127:ILE:CD1	1:A:127:ILE:N	0.47	2.76	3	1
1:A:62:LEU:HD22	1:A:67:TYR:CE1	0.47	2.44	3	3
1:A:133:LEU:HD22	1:A:133:LEU:C	0.47	2.29	18	1
1:A:94:TYR:OH	1:A:177:VAL:HG22	0.47	2.08	3	1
1:A:94:TYR:HA	1:A:134:GLU:HG2	0.47	1.86	16	3
1:A:117:SER:HB3	1:A:120:GLU:HB3	0.47	1.86	16	6
1:A:127:ILE:HG23	1:A:129:SER:O	0.47	2.10	6	1
1:A:71:GLN:HA	1:A:75:GLY:CA	0.47	2.40	11	1
1:A:46:THR:HB	1:A:86:VAL:HG12	0.47	1.86	2	1
1:A:98:ILE:HD11	1:A:122:PHE:CD1	0.47	2.44	6	1
1:A:118:ILE:CG2	1:A:124:MET:O	0.47	2.63	6	2
1:A:49:VAL:CG2	1:A:80:LEU:HD21	0.47	2.40	16	2
1:A:138:ILE:HG23	1:A:149:GLN:CD	0.47	2.30	8	1
1:A:52:ARG:CB	1:A:56:ALA:H	0.47	2.23	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ASN:C	1:A:55:PHE:CD2	0.47	2.88	11	3
1:A:118:ILE:HG22	1:A:171:GLN:O	0.47	2.10	13	2
1:A:157:TYR:CD2	1:A:157:TYR:N	0.47	2.82	13	1
1:A:50:TYR:HB2	1:A:82:SER:O	0.47	2.10	15	5
1:A:141:GLU:C	1:A:171:GLN:HB2	0.47	2.29	18	1
1:A:133:LEU:CD1	1:A:154:LYS:O	0.47	2.61	8	4
1:A:98:ILE:HG23	1:A:127:ILE:CG2	0.47	2.39	8	1
1:A:89:PRO:CG	1:A:94:TYR:CZ	0.47	2.97	8	1
1:A:10:PHE:HD1	1:A:80:LEU:HD12	0.47	1.68	3	1
1:A:47:TRP:CZ3	1:A:85:ALA:N	0.47	2.83	8	10
1:A:87:HIS:O	1:A:88:LEU:O	0.47	2.33	14	3
1:A:70:TYR:O	1:A:73:TRP:HD1	0.47	1.89	3	2
1:A:98:ILE:HG22	1:A:124:MET:SD	0.47	2.50	4	6
1:A:98:ILE:HG23	1:A:127:ILE:HG23	0.47	1.87	8	1
1:A:74:MET:O	1:A:76:LEU:N	0.46	2.48	12	2
1:A:88:LEU:HD12	1:A:178:GLU:HB3	0.46	1.87	7	1
1:A:139:PHE:CD2	1:A:173:PHE:HB3	0.46	2.45	11	1
1:A:93:GLN:O	1:A:134:GLU:HG2	0.46	2.10	15	10
1:A:143:PRO:HB3	1:A:171:GLN:CD	0.46	2.31	16	1
1:A:134:GLU:O	1:A:136:VAL:N	0.46	2.48	14	1
1:A:86:VAL:HG13	1:A:136:VAL:CG1	0.46	2.36	1	1
1:A:116:PRO:O	1:A:143:PRO:CA	0.46	2.64	12	9
1:A:160:PRO:HA	1:A:163:TRP:NE1	0.46	2.26	2	1
1:A:28:ALA:O	1:A:82:SER:CB	0.46	2.63	18	3
1:A:99:PHE:CD1	1:A:104:PHE:HA	0.46	2.45	12	3
1:A:137:TRP:CG	1:A:138:ILE:N	0.46	2.84	20	2
1:A:19:ARG:O	1:A:34:LEU:CD1	0.46	2.62	14	5
1:A:60:TYR:C	1:A:61:ILE:HD12	0.46	2.29	16	5
1:A:53:PRO:O	1:A:55:PHE:CD2	0.46	2.69	10	1
1:A:76:LEU:HD12	1:A:149:GLN:NE2	0.46	2.25	12	1
1:A:57:TRP:O	1:A:58:TYR:CG	0.46	2.68	9	1
1:A:76:LEU:HD11	1:A:149:GLN:N	0.46	2.26	18	1
1:A:73:TRP:CD1	1:A:75:GLY:N	0.46	2.82	14	1
1:A:101:LYS:C	1:A:128:HIS:HB2	0.46	2.31	1	3
1:A:11:TYR:CE1	1:A:20:ARG:HB2	0.46	2.46	7	14
1:A:42:VAL:HG21	1:A:47:TRP:HB2	0.46	1.87	11	2
1:A:127:ILE:CG2	1:A:129:SER:O	0.46	2.64	19	1
1:A:49:VAL:HG22	1:A:60:TYR:O	0.46	2.10	9	1
1:A:42:VAL:O	1:A:42:VAL:HG12	0.46	2.11	14	8
1:A:60:TYR:CD1	1:A:60:TYR:C	0.46	2.89	18	2
1:A:94:TYR:HA	1:A:134:GLU:HG3	0.45	1.87	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:PHE:CD1	1:A:131:LYS:HD2	0.45	2.45	3	4
1:A:46:THR:HG22	1:A:47:TRP:N	0.45	2.27	2	2
1:A:52:ARG:HB3	1:A:56:ALA:H	0.45	1.71	17	4
1:A:20:ARG:CD	1:A:22:ASP:OD1	0.45	2.64	8	9
1:A:142:LEU:CB	1:A:143:PRO:CD	0.45	2.94	14	12
1:A:139:PHE:CZ	1:A:170:VAL:HG11	0.45	2.45	7	1
1:A:86:VAL:HG13	1:A:136:VAL:CG2	0.45	2.39	7	1
1:A:89:PRO:HG3	1:A:94:TYR:CZ	0.45	2.46	8	1
1:A:133:LEU:O	1:A:133:LEU:HG	0.45	2.10	2	2
1:A:140:TYR:CE1	1:A:149:GLN:HB3	0.45	2.47	12	1
1:A:133:LEU:N	1:A:133:LEU:HD13	0.45	2.25	18	1
1:A:137:TRP:HB2	1:A:152:LEU:CB	0.45	2.42	9	1
1:A:99:PHE:HB2	1:A:129:SER:O	0.45	2.12	9	3
1:A:128:HIS:CD2	1:A:168:PRO:HG3	0.45	2.46	14	2
1:A:104:PHE:CZ	1:A:156:GLU:CG	0.45	2.99	13	1
1:A:89:PRO:HB3	1:A:136:VAL:H	0.45	1.71	15	1
1:A:21:TYR:CZ	1:A:33:TYR:CD1	0.45	3.04	7	1
1:A:25:CYS:O	1:A:27:CYS:SG	0.45	2.71	17	3
1:A:42:VAL:HG12	1:A:42:VAL:O	0.45	2.12	20	9
1:A:137:TRP:CA	1:A:152:LEU:HB3	0.45	2.42	20	1
1:A:142:LEU:HB2	1:A:146:ARG:HB2	0.45	1.88	14	1
1:A:134:GLU:H	1:A:134:GLU:CD	0.45	2.16	11	1
1:A:11:TYR:CD1	1:A:16:PHE:C	0.45	2.90	19	13
1:A:161:ILE:HG22	1:A:161:ILE:O	0.45	2.12	13	2
1:A:169:ALA:C	1:A:170:VAL:CG2	0.45	2.85	7	2
1:A:118:ILE:HG23	1:A:124:MET:O	0.45	2.12	16	1
1:A:69:GLU:HB2	1:A:72:ARG:HG2	0.44	1.89	7	2
1:A:132:VAL:HG12	1:A:133:LEU:H	0.44	1.72	14	1
1:A:142:LEU:HB2	1:A:146:ARG:C	0.44	2.33	2	1
1:A:137:TRP:CZ3	1:A:175:ARG:HB3	0.44	2.47	18	1
1:A:49:VAL:CG1	1:A:80:LEU:HD13	0.44	2.42	8	1
1:A:133:LEU:HG	1:A:133:LEU:O	0.44	2.12	11	2
1:A:94:TYR:CE1	1:A:175:ARG:HD2	0.44	2.47	12	1
1:A:9:THR:HA	1:A:21:TYR:O	0.44	2.12	18	6
1:A:53:PRO:C	1:A:55:PHE:N	0.44	2.71	13	8
1:A:56:ALA:C	1:A:58:TYR:N	0.44	2.71	10	5
1:A:154:LYS:HE3	1:A:157:TYR:HB2	0.44	1.88	16	1
1:A:155:LYS:C	1:A:157:TYR:H	0.44	2.16	20	1
1:A:60:TYR:HA	1:A:149:GLN:CD	0.44	2.32	12	1
1:A:139:PHE:CE1	1:A:163:TRP:CH2	0.44	3.05	19	1
1:A:133:LEU:HD13	1:A:155:LYS:HE2	0.44	1.89	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:VAL:HB	1:A:176:ILE:CD1	0.44	2.42	8	3
1:A:47:TRP:CZ3	1:A:84:ARG:C	0.44	2.91	17	3
1:A:132:VAL:O	1:A:154:LYS:HE2	0.44	2.11	18	1
1:A:170:VAL:HG12	1:A:171:GLN:N	0.44	2.28	18	2
1:A:100:GLU:HA	1:A:124:MET:CE	0.44	2.42	20	3
1:A:88:LEU:HD13	1:A:178:GLU:CA	0.44	2.42	20	2
1:A:163:TRP:CD2	1:A:163:TRP:O	0.44	2.71	9	2
1:A:116:PRO:O	1:A:172:SER:HB3	0.44	2.12	18	1
1:A:133:LEU:CD1	1:A:152:LEU:HD23	0.44	2.38	20	1
1:A:8:ILE:HB	1:A:42:VAL:HG22	0.44	1.90	10	2
1:A:136:VAL:HG13	1:A:152:LEU:CD1	0.44	2.43	7	1
1:A:154:LYS:HB3	1:A:157:TYR:CE2	0.44	2.47	13	1
1:A:143:PRO:C	1:A:144:ASN:CG	0.44	2.75	16	1
1:A:130:CYS:HB3	1:A:154:LYS:HD2	0.43	1.89	14	4
1:A:40:ILE:CG2	1:A:41:LYS:N	0.43	2.81	4	8
1:A:31:HIS:O	1:A:34:LEU:O	0.43	2.36	7	2
1:A:160:PRO:O	1:A:163:TRP:NE1	0.43	2.51	15	1
1:A:133:LEU:O	1:A:133:LEU:HD12	0.43	2.13	14	1
1:A:118:ILE:HD13	1:A:127:ILE:CD1	0.43	2.42	6	1
1:A:60:TYR:CD2	1:A:76:LEU:CD1	0.43	3.01	13	1
1:A:133:LEU:N	1:A:133:LEU:HD12	0.43	2.29	14	1
1:A:119:MET:HA	1:A:123:HIS:CA	0.43	2.42	18	4
1:A:98:ILE:HG22	1:A:127:ILE:HD12	0.43	1.91	5	1
1:A:95:LYS:H	1:A:134:GLU:CG	0.43	2.26	17	1
1:A:50:TYR:CE2	1:A:56:ALA:HB1	0.43	2.49	3	3
1:A:118:ILE:CB	1:A:171:GLN:O	0.43	2.66	5	7
1:A:50:TYR:CE2	1:A:59:MET:HG3	0.43	2.48	9	1
1:A:73:TRP:C	1:A:73:TRP:CD1	0.43	2.91	11	2
1:A:155:LYS:O	1:A:157:TYR:CD2	0.43	2.71	13	1
1:A:130:CYS:HB2	1:A:163:TRP:CH2	0.43	2.48	2	1
1:A:154:LYS:C	1:A:155:LYS:CG	0.43	2.87	14	5
1:A:20:ARG:CD	1:A:22:ASP:OD2	0.43	2.66	18	5
1:A:37:CYS:HB2	1:A:80:LEU:HB2	0.43	1.90	9	1
1:A:61:ILE:HD11	1:A:151:LEU:N	0.43	2.29	13	1
1:A:94:TYR:CE1	1:A:137:TRP:CE3	0.43	3.07	20	1
1:A:136:VAL:C	1:A:176:ILE:HD12	0.43	2.34	10	2
1:A:133:LEU:O	1:A:133:LEU:HD13	0.43	2.13	18	1
1:A:143:PRO:HA	1:A:172:SER:OG	0.43	2.12	2	1
1:A:92:GLY:O	1:A:93:GLN:C	0.43	2.57	15	8
1:A:8:ILE:HG23	1:A:10:PHE:CZ	0.43	2.49	4	1
1:A:133:LEU:CD2	1:A:133:LEU:O	0.43	2.63	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ILE:CD1	1:A:73:TRP:CH2	0.43	3.02	8	3
1:A:36:ARG:NH2	1:A:38:ASN:HD21	0.43	2.12	3	1
1:A:54:ASN:C	1:A:55:PHE:CD1	0.43	2.92	10	1
1:A:137:TRP:CD1	1:A:138:ILE:N	0.43	2.86	20	3
1:A:136:VAL:CG1	1:A:176:ILE:HD12	0.43	2.44	14	2
1:A:127:ILE:O	1:A:168:PRO:HB3	0.43	2.14	3	8
1:A:9:THR:HG23	1:A:22:ASP:CG	0.43	2.34	19	12
1:A:10:PHE:CD1	1:A:30:PHE:CZ	0.43	3.07	11	2
1:A:140:TYR:HB2	1:A:172:SER:C	0.42	2.34	6	1
1:A:140:TYR:CE2	1:A:174:ARG:HD3	0.42	2.49	7	1
1:A:77:ASN:O	1:A:78:ASP:OD1	0.42	2.37	12	1
1:A:60:TYR:OH	1:A:75:GLY:HA2	0.42	2.13	13	1
1:A:165:ALA:O	1:A:166:ALA:C	0.42	2.57	11	3
1:A:94:TYR:CE1	1:A:137:TRP:CD1	0.42	3.08	9	2
1:A:37:CYS:SG	1:A:78:ASP:C	0.42	2.97	3	1
1:A:140:TYR:CE2	1:A:174:ARG:HG2	0.42	2.49	11	1
1:A:94:TYR:CE1	1:A:137:TRP:CE2	0.42	3.07	17	1
1:A:96:ILE:HD12	1:A:98:ILE:HD13	0.42	1.91	19	1
1:A:60:TYR:CD2	1:A:76:LEU:HD21	0.42	2.49	14	1
1:A:59:MET:HB2	1:A:149:GLN:O	0.42	2.14	2	1
1:A:50:TYR:CG	1:A:56:ALA:HA	0.42	2.49	18	4
1:A:37:CYS:SG	1:A:80:LEU:O	0.42	2.78	11	1
1:A:104:PHE:CE2	1:A:158:ARG:HB3	0.42	2.49	20	1
1:A:126:GLU:C	1:A:127:ILE:HD13	0.42	2.34	14	1
1:A:46:THR:HG22	1:A:47:TRP:H	0.42	1.74	14	2
1:A:137:TRP:H	1:A:152:LEU:CD1	0.42	2.27	19	4
1:A:94:TYR:CZ	1:A:137:TRP:CD1	0.42	3.08	9	1
1:A:68:PRO:HD2	1:A:72:ARG:HG3	0.42	1.91	13	2
1:A:37:CYS:CB	1:A:80:LEU:HB2	0.42	2.44	9	4
1:A:49:VAL:HA	1:A:83:CYS:HA	0.42	1.90	4	2
1:A:136:VAL:HG12	1:A:176:ILE:HD11	0.42	1.90	19	2
1:A:25:CYS:O	1:A:26:ASP:C	0.42	2.56	10	1
1:A:9:THR:N	1:A:41:LYS:O	0.42	2.52	16	1
1:A:76:LEU:CD1	1:A:76:LEU:N	0.42	2.72	2	1
1:A:137:TRP:HB3	1:A:152:LEU:HB2	0.42	1.92	1	1
1:A:97:GLN:HB2	1:A:131:LYS:O	0.42	2.15	12	2
1:A:96:ILE:HD13	1:A:97:GLN:H	0.42	1.74	13	2
1:A:52:ARG:HB2	1:A:56:ALA:CA	0.42	2.45	10	1
1:A:60:TYR:HE2	1:A:76:LEU:HD12	0.42	1.73	13	1
1:A:154:LYS:HB2	1:A:157:TYR:CE1	0.42	2.47	10	1
1:A:80:LEU:HD22	1:A:80:LEU:HA	0.42	1.75	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:VAL:O	1:A:154:LYS:HE3	0.41	2.15	2	1
1:A:27:CYS:HB3	1:A:30:PHE:CB	0.41	2.45	4	1
1:A:11:TYR:CE2	1:A:41:LYS:HD2	0.41	2.50	20	5
1:A:61:ILE:HB	1:A:138:ILE:CD1	0.41	2.44	18	2
1:A:62:LEU:HD11	1:A:73:TRP:CZ3	0.41	2.50	5	1
1:A:53:PRO:O	1:A:54:ASN:CB	0.41	2.68	9	1
1:A:40:ILE:HD12	1:A:73:TRP:HZ3	0.41	1.74	9	1
1:A:173:PHE:N	1:A:173:PHE:HD1	0.41	2.11	18	1
1:A:52:ARG:HB3	1:A:55:PHE:HB2	0.41	1.91	18	1
1:A:94:TYR:CD1	1:A:134:GLU:HG2	0.41	2.51	2	1
1:A:136:VAL:O	1:A:176:ILE:HD12	0.41	2.15	17	1
1:A:63:PRO:HG2	1:A:67:TYR:OH	0.41	2.14	5	1
1:A:7:LYS:O	1:A:43:GLU:N	0.41	2.54	18	2
1:A:63:PRO:C	1:A:67:TYR:HH	0.41	2.18	5	1
1:A:139:PHE:O	1:A:149:GLN:CB	0.41	2.69	19	1
1:A:98:ILE:CD1	1:A:111:THR:HG22	0.41	2.45	20	1
1:A:40:ILE:HD13	1:A:62:LEU:CD1	0.41	2.46	4	1
1:A:122:PHE:O	1:A:123:HIS:CB	0.41	2.69	6	1
1:A:170:VAL:HA	1:A:171:GLN:NE2	0.41	2.30	7	2
1:A:169:ALA:O	1:A:170:VAL:HG22	0.41	2.16	7	1
1:A:119:MET:HA	1:A:124:MET:N	0.41	2.31	20	1
1:A:146:ARG:NE	1:A:146:ARG:HA	0.41	2.30	14	1
1:A:159:LYS:O	1:A:162:ASP:HB2	0.41	2.16	14	1
1:A:96:ILE:HD11	1:A:154:LYS:HZ3	0.41	1.76	12	1
1:A:78:ASP:O	1:A:78:ASP:CG	0.41	2.58	12	1
1:A:132:VAL:O	1:A:155:LYS:O	0.41	2.39	13	1
1:A:27:CYS:C	1:A:29:ASP:N	0.41	2.74	2	2
1:A:152:LEU:CD1	1:A:152:LEU:C	0.41	2.86	10	1
1:A:103:ASP:HA	1:A:158:ARG:HB2	0.41	1.92	16	1
1:A:135:GLY:O	1:A:152:LEU:HD21	0.41	2.15	20	1
1:A:170:VAL:HG12	1:A:171:GLN:H	0.41	1.76	6	1
1:A:137:TRP:CD1	1:A:139:PHE:CE1	0.41	3.09	18	1
1:A:94:TYR:CA	1:A:134:GLU:HG2	0.41	2.46	14	1
1:A:59:MET:HB2	1:A:150:TYR:HA	0.40	1.93	1	1
1:A:139:PHE:CE1	1:A:173:PHE:HB3	0.40	2.51	13	1
1:A:130:CYS:HB2	1:A:163:TRP:CZ2	0.40	2.51	13	1
1:A:93:GLN:HG3	1:A:112:THR:OG1	0.40	2.16	20	1
1:A:97:GLN:HB2	1:A:132:VAL:HG23	0.40	1.93	1	1
1:A:11:TYR:CD1	1:A:20:ARG:CB	0.40	3.05	7	4
1:A:136:VAL:HA	1:A:152:LEU:HD11	0.40	1.91	8	1
1:A:103:ASP:C	1:A:104:PHE:CG	0.40	2.95	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:HD13	1:A:154:LYS:C	0.40	2.35	20	1
1:A:155:LYS:C	1:A:157:TYR:N	0.40	2.74	20	1
1:A:104:PHE:CE1	1:A:131:LYS:CD	0.40	3.04	5	1
1:A:60:TYR:CE2	1:A:76:LEU:HB3	0.40	2.51	9	1
1:A:60:TYR:HD1	1:A:60:TYR:C	0.40	2.18	18	1
1:A:10:PHE:O	1:A:20:ARG:HA	0.40	2.16	14	1
1:A:46:THR:CG2	1:A:62:LEU:O	0.40	2.70	1	1
1:A:27:CYS:HB2	1:A:83:CYS:SG	0.40	2.57	15	1
1:A:30:PHE:HA	1:A:33:TYR:CD1	0.40	2.51	17	1
1:A:50:TYR:CD2	1:A:56:ALA:O	0.40	2.74	18	1
1:A:60:TYR:HA	1:A:149:GLN:HB2	0.40	1.94	4	1
1:A:49:VAL:HA	1:A:82:SER:O	0.40	2.17	7	1
1:A:53:PRO:O	1:A:54:ASN:HB2	0.40	2.17	11	1
1:A:11:TYR:CD1	1:A:20:ARG:HB3	0.40	2.52	20	1
1:A:51:GLU:CD	1:A:57:TRP:HB3	0.40	2.37	14	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	173/178 (97%)	118±39 (68±23%)	25±9 (14±5%)	13±5 (8±3%)	2	15
All	All	3114/3560 (87%)	2351 (75%)	497 (16%)	266 (9%)	2	13

All 33 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	57	TRP	18
1	A	157	TYR	18
1	A	51	GLU	18
1	A	14	LYS	18
1	A	145	TYR	18
1	A	132	VAL	18
1	A	155	LYS	18

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Mol	Chain	Res	Type	Models (Total)
1	A	144	ASN	17
1	A	143	PRO	15
1	A	82	SER	14
1	A	58	TYR	13
1	A	81	SER	13
1	A	135	GLY	9
1	A	45	GLY	9
1	A	93	GLN	8
1	A	91	GLY	5
1	A	88	LEU	5
1	A	75	GLY	4
1	A	5	GLY	3
1	A	56	ALA	3
1	A	153	ASP	2
1	A	100	GLU	2
1	A	133	LEU	2
1	A	76	LEU	2
1	A	167	SER	2
1	A	78	ASP	2
1	A	74	MET	2
1	A	19	ARG	2
1	A	114	ASP	2
1	A	154	LYS	1
1	A	89	PRO	1
1	A	92	GLY	1
1	A	171	GLN	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	154/158 (97%)	105±24 (68±16%)	42±10 (27±6%)	2	21
All	All	2926/3160 (93%)	2091 (71%)	835 (29%)	2	18

All 88 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	88	LEU	19
1	A	110	GLU	19
1	A	117	SER	19
1	A	41	LYS	19
1	A	133	LEU	19
1	A	80	LEU	19
1	A	82	SER	19
1	A	167	SER	19
1	A	12	GLU	19
1	A	73	TRP	19
1	A	20	ARG	19
1	A	152	LEU	19
1	A	30	PHE	19
1	A	62	LEU	19
1	A	64	GLN	19
1	A	19	ARG	18
1	A	90	SER	17
1	A	139	PHE	17
1	A	134	GLU	16
1	A	155	LYS	16
1	A	175	ARG	16
1	A	76	LEU	15
1	A	162	ASP	15
1	A	174	ARG	15
1	A	10	PHE	14
1	A	130	CYS	14
1	A	154	LYS	13
1	A	96	ILE	13
1	A	145	TYR	13
1	A	23	CYS	12
1	A	114	ASP	12
1	A	27	CYS	11
1	A	144	ASN	11
1	A	52	ARG	11
1	A	159	LYS	11
1	A	141	GLU	11
1	A	94	TYR	11
1	A	148	ARG	10
1	A	140	TYR	10
1	A	59	MET	10
1	A	79	ARG	10
1	A	129	SER	10
1	A	57	TRP	10

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Mol	Chain	Res	Type	Models (Total)
1	A	74	MET	10
1	A	54	ASN	10
1	A	36	ARG	9
1	A	97	GLN	8
1	A	156	GLU	8
1	A	60	TYR	8
1	A	46	THR	7
1	A	137	TRP	7
1	A	81	SER	6
1	A	55	PHE	6
1	A	149	GLN	6
1	A	112	THR	6
1	A	128	HIS	5
1	A	51	GLU	5
1	A	43	GLU	5
1	A	158	ARG	5
1	A	42	VAL	5
1	A	38	ASN	5
1	A	119	MET	5
1	A	61	ILE	5
1	A	104	PHE	5
1	A	163	TRP	4
1	A	78	ASP	4
1	A	84	ARG	4
1	A	178	GLU	4
1	A	172	SER	3
1	A	124	MET	3
1	A	71	GLN	3
1	A	173	PHE	3
1	A	123	HIS	3
1	A	26	ASP	2
1	A	22	ASP	2
1	A	108	MET	2
1	A	171	GLN	2
1	A	121	GLN	2
1	A	115	CYS	2
1	A	37	CYS	1
1	A	127	ILE	1
1	A	138	ILE	1
1	A	136	VAL	1
1	A	151	LEU	1
1	A	35	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	153	ASP	1
1	A	17	GLN	1
1	A	58	TYR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1946
Number of shifts mapped to atoms	1946
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	176	-0.80 ± 0.13	Should be applied
$^{13}\text{C}_\beta$	163	-0.65 ± 0.16	Should be applied
$^{13}\text{C}'$	158	0.23 ± 0.18	None needed (< 0.5 ppm)
^{15}N	158	2.31 ± 0.45	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1763 atoms were assigned a chemical shift out of a possible 2259. 10 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	808/854 (95%)	327/340 (96%)	326/348 (94%)	155/166 (93%)
Sidechain	861/1124 (77%)	566/671 (84%)	281/391 (72%)	14/62 (23%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	94/281 (33%)	89/147 (61%)	0/125 (0%)	5/9 (56%)
Overall	1763/2259 (78%)	982/1158 (85%)	607/864 (70%)	174/237 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1798 atoms were assigned a chemical shift out of a possible 2307. 10 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	826/874 (95%)	334/348 (96%)	334/356 (94%)	158/170 (93%)
Sidechain	878/1152 (76%)	575/688 (84%)	289/401 (72%)	14/63 (22%)
Aromatic	94/281 (33%)	89/147 (61%)	0/125 (0%)	5/9 (56%)
Overall	1798/2307 (78%)	998/1183 (84%)	623/882 (71%)	177/242 (73%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	63	PRO	CD	56.99	55.31 – 45.41	6.7
1	A	149	GLN	CB	38.97	38.36 – 19.96	5.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

