WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 12:14 am GMT

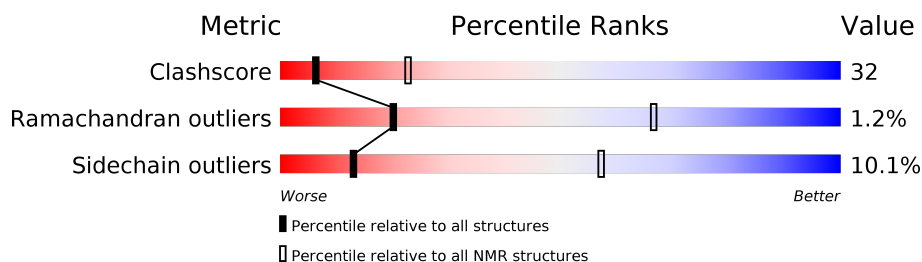|		
PDB ID	:	2LKD
Title	:	IF2-G2 GDP complex
Authors	:	Wienk, H.; Tishchenko, E.; Belardinelli, R.; Tomaselli, S.; Dongre, R.; Spurio, R.; Folkers, G.E.; Gualerzi, C.O.; Boelens, R.
Deposited on	:	2011-10-10

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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	Percentile Ranks	Value
Clashscore		32
Ramachandran outliers		1.2%
Sidechain outliers		10.1%

Worse · · · *Better*

▌Percentile relative to all structures
▯Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	178	22%　　36%　·　41%

2 Ensemble composition and analysis ⓘ

This entry contains 18 models. Model 11 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:12-A:28,　　　A:81-A:168 (105)	0.27	11

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

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

The models can be grouped into 4 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 4, 6, 10, 11, 14
2	3, 5, 8
3	9, 16
4	15, 17
Single-model clusters	2; 7; 12; 13; 18

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3 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 2786 atoms, of which 1394 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	178	2746	856	1382	234	264	10	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P04766
A	2	SER	-	EXPRESSION TAG	UNP P04766
A	3	HIS	-	EXPRESSION TAG	UNP P04766
A	4	MET	-	EXPRESSION TAG	UNP P04766
A	76	ALA	ARG	SEE REMARK 999	UNP P04766

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
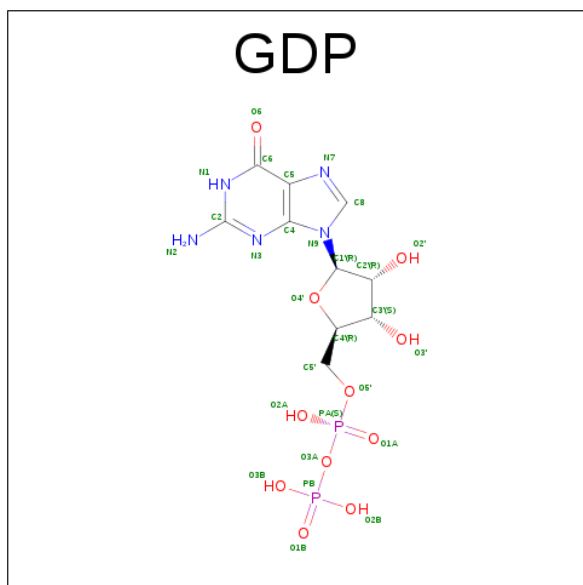

Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
2	A	1	40	10	12	5	11	2

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: Translation initiation factor IF-2
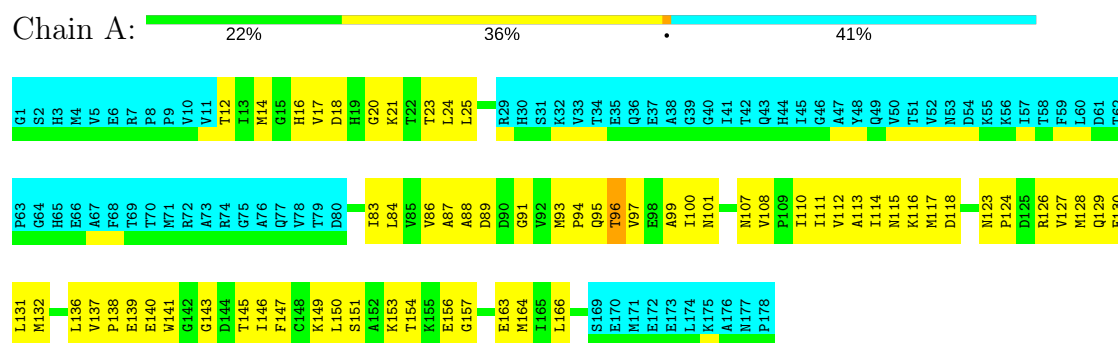
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Translation initiation factor IF-2

4.2.2 Score per residue for model 2

• Molecule 1: Translation initiation factor IF-2

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Translation initiation factor IF-2

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Translation initiation factor IF-2

Chain A:

4.2.5 Score per residue for model 5

• Molecule 1: Translation initiation factor IF-2

Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: Translation initiation factor IF-2

Chain A:

4.2.7 Score per residue for model 7

• Molecule 1: Translation initiation factor IF-2

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: Translation initiation factor IF-2

Chain A:

4.2.9 Score per residue for model 9

• Molecule 1: Translation initiation factor IF-2

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: Translation initiation factor IF-2

Chain A:
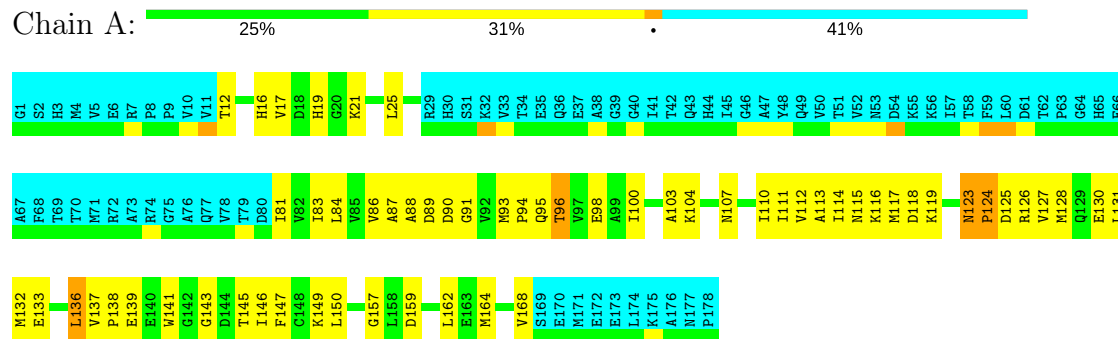
4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: Translation initiation factor IF-2

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Translation initiation factor IF-2

Chain A:
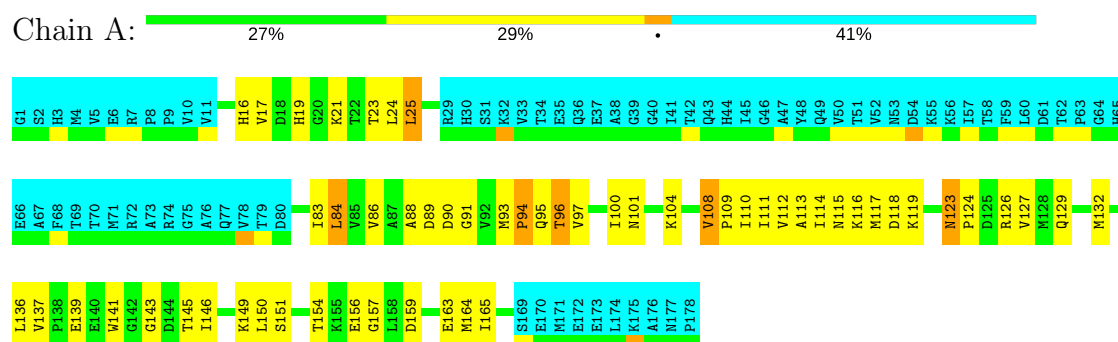
4.2.13 Score per residue for model 13

• Molecule 1: Translation initiation factor IF-2
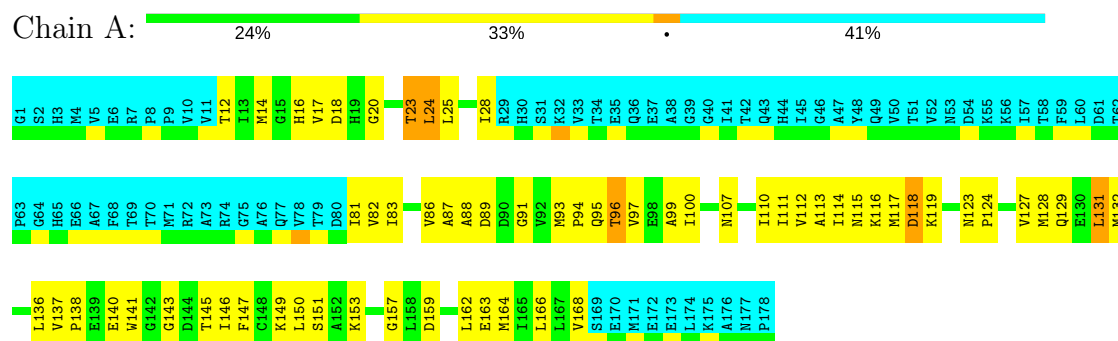
Chain A:
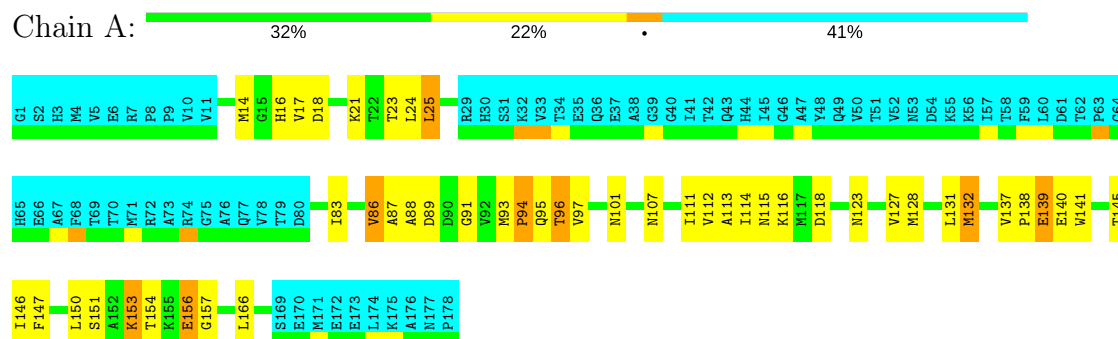
4.2.14 Score per residue for model 14

• Molecule 1: Translation initiation factor IF-2
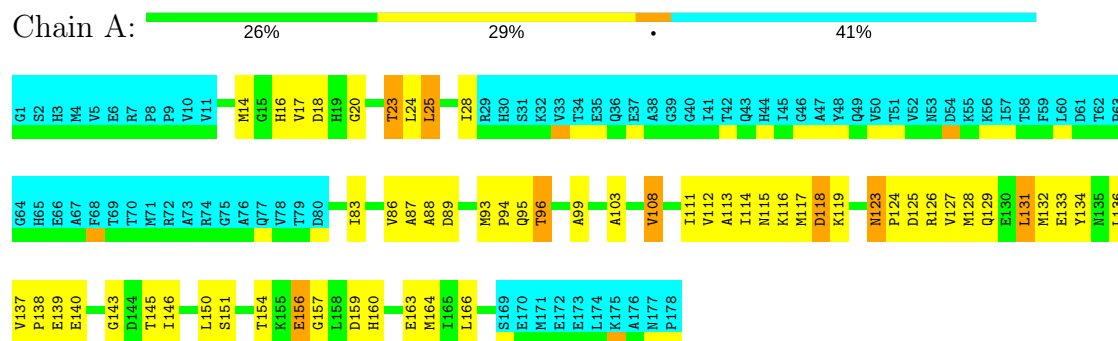
4.2.15 Score per residue for model 15

• Molecule 1: Translation initiation factor IF-2
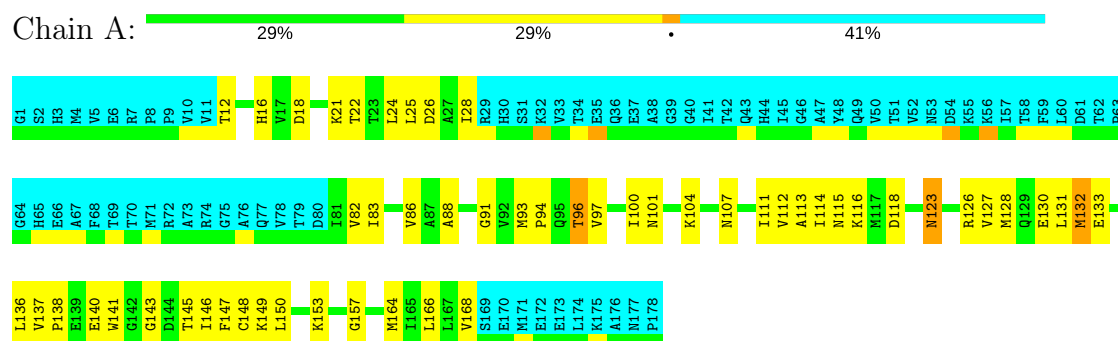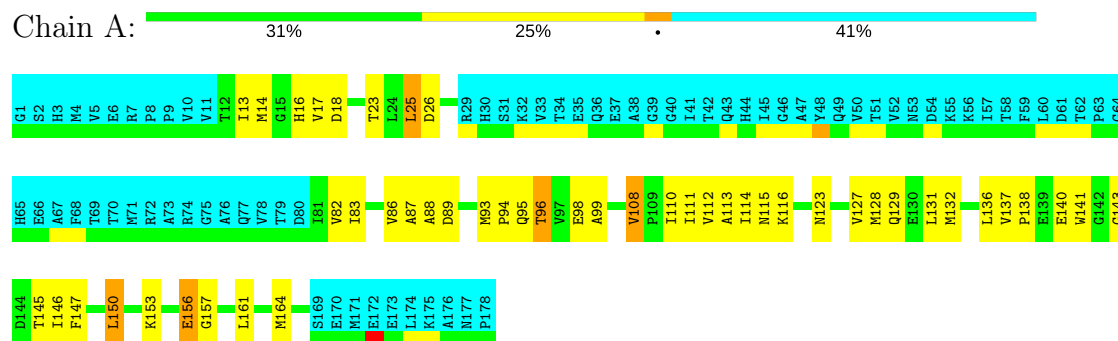

4.2.16 Score per residue for model 16

• Molecule 1: Translation initiation factor IF-2
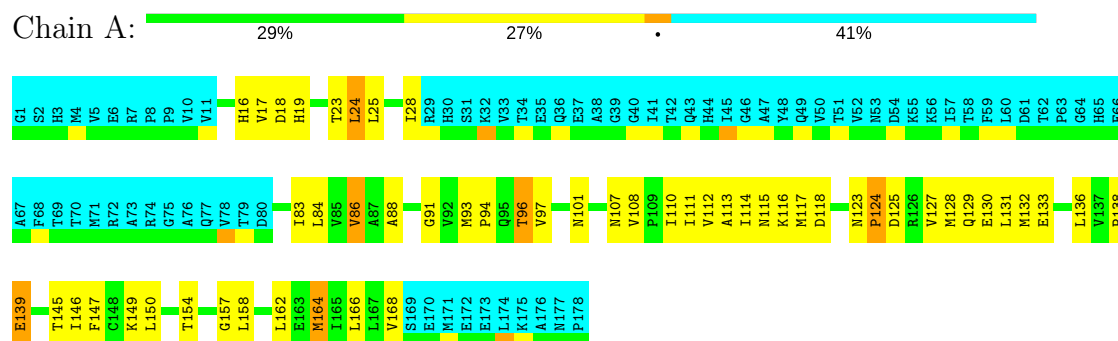
4.2.17 Score per residue for model 17

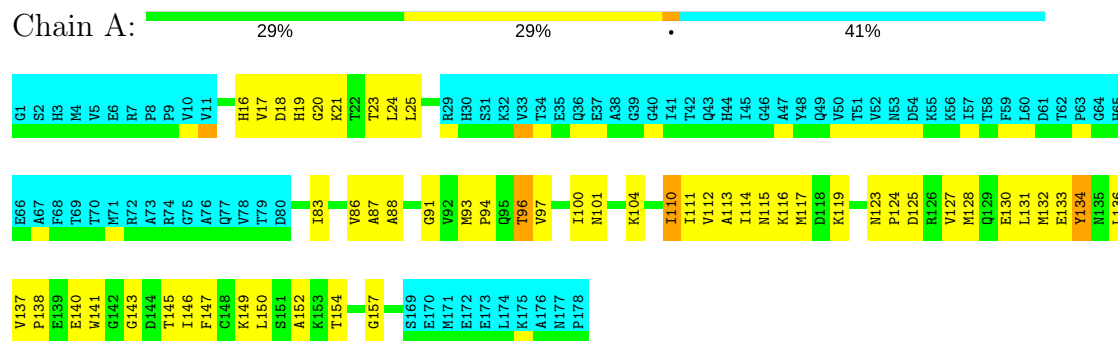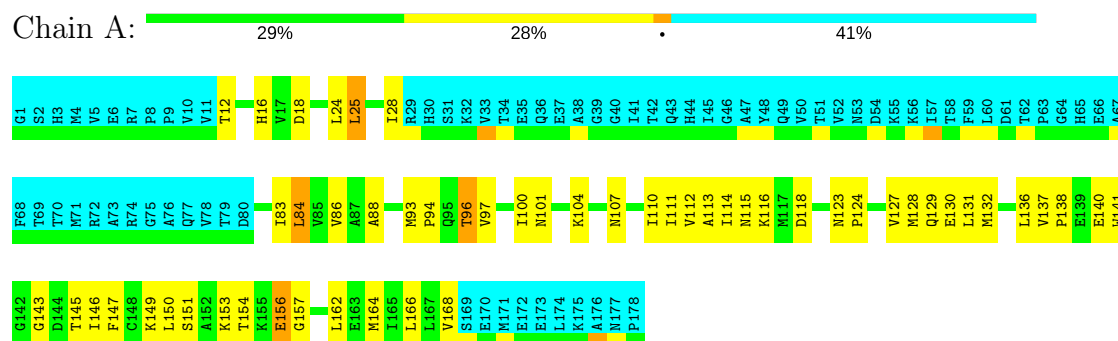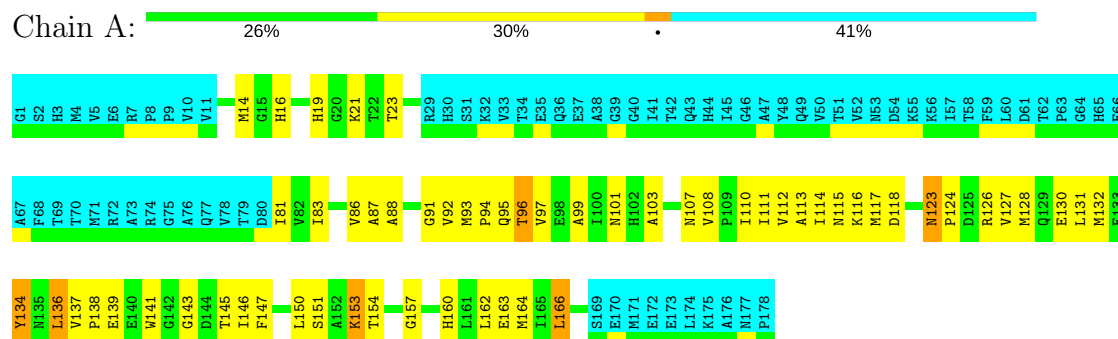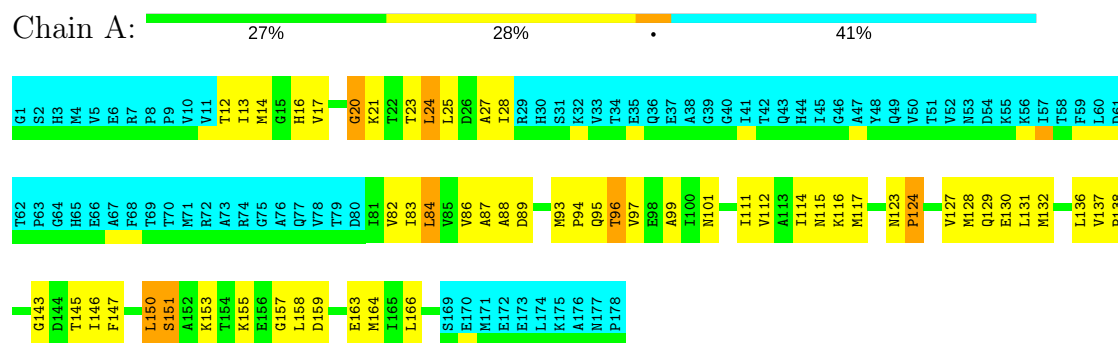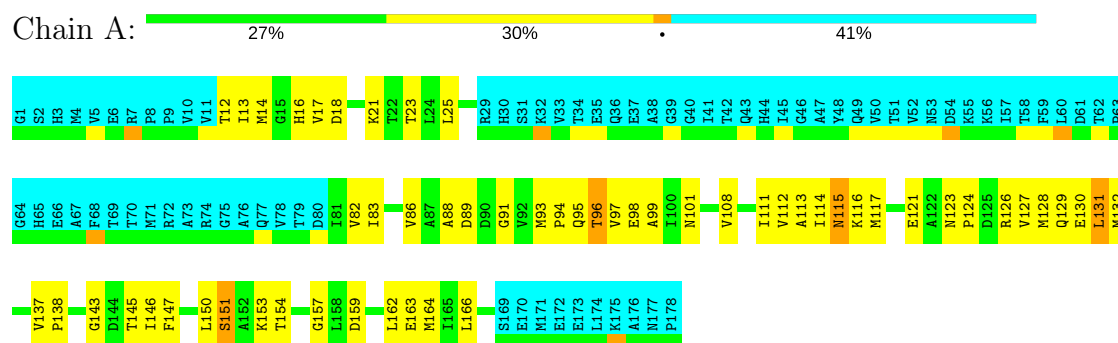• Molecule 1: Translation initiation factor IF-2

G1 S2 H3 M4 V5 E6 R7 P8 P9 V10 V11 T12 I13 M14 G15 H16 V17 D18 H19 G20 K21 T22 T23 L24 L25 R29 H30 S31 K32 V33 T34 E35 Q36 E37 A38 G39 G40 I41 T42 Q43 H44 I45 G46 A47 Y48 Q49 V50 T51 V52 N53 D54 K55 K56 I57 T58 F59 L60 D61 T62

P63 G64 H65 E66 A67 F68 T69 T70 M71 R72 A73 R74 G75 A76 Q77 V78 T79 D80 I81 V82 I83 L84 V85 V86 A87 A88 G91 V92 M93 P94 Q95 T96 I100 N101 H102 A103 K104 A105 A106 N107 I110 I111 V112 A113 I114 N115 K116 M117 D118 K119 N123 P124 D125 R126 V127 M128

Q129 E130 L131 M132 E133 Y134 P138 E139 E140 W141 T145 I146 F147 C148 K149 L150 S151 A152 K153 T154 K155 E156 G157 L158 L161 M164 I165 L166 S169 E170 M171 E172 E173 L174 K175 A176 N177 P178

4.2.18 Score per residue for model 18

• Molecule 1: Translation initiation factor IF-2

Chain A:	25%	30%	•	41%

G1 S2 H3 M4 V5 E6 R7 P8 P9 V10 V11 M14 G15 H16 V17 D18 H19 G20 K21 T22 T23 L24 L25 I28 R29 H30 S31 K32 V33 T34 E35 Q36 E37 A38 G39 G40 I41 T42 Q43 H44 I45 G46 A47 Y48 Q49 V50 T51 V52 N53 D54 K55 K56 I57 T58 F59 L60 D61 T62

P63 G64 H65 E66 A67 F68 T69 T70 M71 R72 A73 R74 G75 A76 Q77 V78 T79 D80 I83 V86 A87 A88 D89 D90 Q95 T96 V97 E98 A99 I100 N101 H102 A103 K104 N107 V108 I111 V112 A113 I114 N115 K116 M117 D118 N123 R126 V127 M128 Q129 E130 L131 M132 E133

L136 V137 P138 E139 E140 W141 G142 G143 D144 T145 I146 F147 L150 K153 T154 K155 E156 G157 L158 D159 H160 L161 L162 E163 L166 S169 E170 M171 E172 E173 L174 K175 A176 N177 P178

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *molecular dynamics.*

Of the 100 calculated structures, 18 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
CNS	structure solution	
CNS	refinement	

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)	2lkd_cs.str
Number of chemical shift lists	1
Total number of shifts	1695
Number of shifts mapped to atoms	1695
Number of unparsed shifts	0
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 ⓘ

6.1 Standard geometry ⓘ

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

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±0.04	0±1/814 (0.0±0.1%)	0.55±0.02	0±0/1108 (0.0±0.0%)
All	All	0.46	4/14652 (0.0%)	0.55	0/19944 (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	134	TYR	CE1-CZ	-8.54	1.27	1.38	17	2
1	A	134	TYR	CE2-CZ	7.77	1.48	1.38	17	2

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	134	TYR	Sidechain	2

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	801	827	825	53±8
2	A	28	12	12	4±2
All	All	14922	15102	15066	954

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:128:MET:HA	1:A:131:LEU:HD12	0.99	1.35	10	4
1:A:137:VAL:HB	1:A:143:GLY:HA3	0.98	1.33	7	15
1:A:150:LEU:HB2	1:A:157:GLY:HA3	0.93	1.39	1	14
1:A:128:MET:HA	1:A:131:LEU:HD23	0.90	1.43	11	3
1:A:111:ILE:HD13	1:A:146:ILE:HB	0.89	1.41	16	18
1:A:112:VAL:HG23	1:A:145:THR:HG21	0.88	1.42	6	15
1:A:150:LEU:HB3	1:A:157:GLY:HA3	0.87	1.42	7	12
1:A:139:GLU:HG2	1:A:146:ILE:HD13	0.84	1.48	17	5
1:A:150:LEU:CB	1:A:157:GLY:HA3	0.82	2.05	4	18
1:A:123:ASN:HD22	1:A:126:ARG:HB2	0.80	1.36	7	6
1:A:138:PRO:HB2	1:A:140:GLU:HG2	0.80	1.54	2	4
1:A:93:MET:HB3	1:A:94:PRO:HD2	0.80	1.51	17	17
1:A:114:ILE:HB	1:A:149:LYS:HA	0.78	1.56	17	8
1:A:132:MET:SD	1:A:138:PRO:HD2	0.77	2.20	10	3
1:A:84:LEU:HB3	1:A:112:VAL:HG13	0.75	1.58	12	2
1:A:116:LYS:HG2	2:A:179:GDP:C2	0.73	2.18	1	14
1:A:20:GLY:O	1:A:21:LYS:HG2	0.73	1.83	18	1
1:A:114:ILE:O	1:A:150:LEU:HG	0.73	1.84	5	14
1:A:84:LEU:HD12	1:A:86:VAL:HG13	0.73	1.60	8	3
1:A:140:GLU:HB2	1:A:141:TRP:CD1	0.73	2.18	17	1
1:A:131:LEU:HD12	1:A:136:LEU:HD21	0.73	1.61	8	1
1:A:21:LYS:HG3	1:A:23:THR:HB	0.72	1.59	18	1
1:A:113:ALA:HB1	1:A:150:LEU:HD11	0.71	1.61	7	1
1:A:116:LYS:HG2	2:A:179:GDP:N2	0.71	2.00	17	10
1:A:111:ILE:CD1	1:A:146:ILE:HB	0.71	2.14	3	18
1:A:113:ALA:HB1	1:A:150:LEU:HD21	0.71	1.62	5	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:MET:HA	1:A:131:LEU:CD2	0.71	2.15	11	3
1:A:140:GLU:HB2	1:A:141:TRP:HD1	0.70	1.46	17	1
1:A:124:PRO:O	1:A:128:MET:HG3	0.70	1.86	5	2
1:A:150:LEU:HB2	1:A:157:GLY:CA	0.70	2.15	1	9
1:A:13:ILE:HG13	1:A:25:LEU:HD21	0.70	1.62	8	2
1:A:153:LYS:HG3	2:A:179:GDP:C2	0.70	2.22	1	3
1:A:153:LYS:HB2	2:A:179:GDP:N1	0.69	2.02	8	8
1:A:88:ALA:HB2	1:A:114:ILE:CG2	0.69	2.18	8	18
1:A:131:LEU:HD23	1:A:147:PHE:HE2	0.69	1.46	2	2
1:A:138:PRO:HB3	1:A:147:PHE:CD1	0.69	2.23	13	2
1:A:88:ALA:HA	1:A:127:VAL:HG21	0.68	1.64	17	11
1:A:89:ASP:HB2	1:A:121:GLU:HB2	0.67	1.67	9	1
1:A:86:VAL:HG21	1:A:131:LEU:HD11	0.67	1.66	15	3
1:A:138:PRO:HA	1:A:147:PHE:CD1	0.66	2.25	6	14
1:A:14:MET:HB3	1:A:99:ALA:HB1	0.66	1.66	6	8
1:A:112:VAL:HG21	1:A:131:LEU:HD23	0.66	1.65	3	4
1:A:119:LYS:HE2	1:A:119:LYS:HA	0.66	1.66	12	1
1:A:21:LYS:HA	2:A:179:GDP:O1B	0.65	1.90	18	1
1:A:87:ALA:HA	1:A:115:ASN:OD1	0.65	1.91	15	9
1:A:21:LYS:CG	1:A:23:THR:HB	0.64	2.21	18	1
1:A:132:MET:HG2	1:A:141:TRP:HZ3	0.64	1.51	12	4
1:A:140:GLU:HG3	1:A:141:TRP:CD1	0.64	2.27	13	1
1:A:127:VAL:O	1:A:131:LEU:HG	0.64	1.93	6	4
1:A:82:VAL:HG21	1:A:102:HIS:HE1	0.64	1.52	11	1
1:A:13:ILE:HD11	1:A:25:LEU:HD23	0.64	1.69	15	1
1:A:21:LYS:CD	1:A:23:THR:HB	0.64	2.23	18	1
1:A:130:GLU:O	1:A:133:GLU:HG2	0.63	1.93	3	1
1:A:87:ALA:HB1	1:A:116:LYS:HD2	0.63	1.70	10	9
1:A:17:VAL:HA	2:A:179:GDP:O1B	0.63	1.94	10	1
1:A:21:LYS:HA	2:A:179:GDP:PB	0.62	2.34	18	1
1:A:132:MET:HA	1:A:136:LEU:H	0.62	1.54	12	8
1:A:137:VAL:HB	1:A:143:GLY:CA	0.62	2.20	7	2
1:A:104:LYS:HD3	1:A:136:LEU:HD21	0.62	1.72	4	3
1:A:131:LEU:HD23	1:A:147:PHE:CE2	0.62	2.30	2	3
1:A:86:VAL:O	1:A:114:ILE:HA	0.62	1.94	1	17
1:A:97:VAL:HG12	1:A:101:ASN:HD22	0.62	1.55	4	1
1:A:21:LYS:HD2	1:A:23:THR:HB	0.62	1.72	18	1
1:A:132:MET:SD	1:A:141:TRP:CZ3	0.61	2.93	6	2
1:A:123:ASN:ND2	1:A:126:ARG:HB2	0.61	2.09	7	2
1:A:20:GLY:HA3	1:A:24:LEU:HD23	0.61	1.71	7	3
1:A:95:GLN:HA	1:A:98:GLU:HG2	0.61	1.73	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:VAL:HG21	1:A:131:LEU:HD21	0.60	1.72	11	3
1:A:116:LYS:HD3	1:A:119:LYS:HE2	0.60	1.73	2	1
1:A:104:LYS:HA	1:A:104:LYS:HE2	0.60	1.73	10	1
1:A:12:THR:HB	1:A:82:VAL:HG22	0.60	1.73	3	4
1:A:128:MET:HA	1:A:131:LEU:HB2	0.60	1.73	2	1
1:A:81:ILE:HG21	1:A:111:ILE:HG12	0.59	1.75	2	3
1:A:21:LYS:HB2	2:A:179:GDP:O5'	0.59	1.98	18	1
1:A:132:MET:SD	1:A:141:TRP:HZ3	0.59	2.21	6	2
1:A:137:VAL:HG13	1:A:138:PRO:HD2	0.59	1.73	13	1
1:A:83:ILE:HA	1:A:111:ILE:O	0.58	1.97	14	17
1:A:132:MET:SD	1:A:137:VAL:HG13	0.58	2.38	10	2
1:A:114:ILE:HG21	1:A:124:PRO:HA	0.58	1.76	1	1
1:A:129:GLN:O	1:A:132:MET:HG3	0.58	1.98	15	5
1:A:115:ASN:HA	1:A:150:LEU:O	0.57	2.00	8	2
1:A:125:ASP:HA	1:A:128:MET:SD	0.57	2.40	11	5
1:A:123:ASN:HB3	1:A:126:ARG:HB3	0.57	1.75	10	1
1:A:128:MET:O	1:A:131:LEU:HB2	0.57	2.00	6	2
1:A:116:LYS:HA	1:A:118:ASP:OD1	0.57	2.00	16	8
1:A:88:ALA:HB2	1:A:114:ILE:HG21	0.56	1.77	9	8
1:A:156:GLU:HG3	1:A:157:GLY:N	0.56	2.16	5	5
1:A:88:ALA:HA	1:A:127:VAL:HG11	0.56	1.78	18	2
1:A:21:LYS:HB2	2:A:179:GDP:O2A	0.56	2.00	18	1
1:A:112:VAL:HG23	1:A:145:THR:CG2	0.56	2.30	8	16
1:A:128:MET:HG2	1:A:132:MET:CE	0.56	2.30	13	1
1:A:91:GLY:HA2	1:A:127:VAL:HB	0.56	1.77	9	10
1:A:20:GLY:O	1:A:24:LEU:HB2	0.55	2.00	18	3
1:A:123:ASN:HD22	1:A:126:ARG:CB	0.55	2.11	7	6
1:A:154:THR:HB	1:A:156:GLU:HG3	0.55	1.77	17	1
1:A:16:HIS:HB2	1:A:96:THR:OG1	0.55	2.01	6	18
1:A:129:GLN:O	1:A:132:MET:HG2	0.55	2.02	11	6
1:A:138:PRO:HA	1:A:145:THR:O	0.55	2.01	1	3
1:A:117:MET:HE3	1:A:124:PRO:HB3	0.55	1.79	17	4
1:A:131:LEU:HB3	1:A:136:LEU:HB2	0.55	1.78	5	3
1:A:83:ILE:HG12	1:A:111:ILE:HB	0.55	1.78	15	6
1:A:137:VAL:CB	1:A:143:GLY:HA3	0.54	2.21	7	13
1:A:117:MET:CE	1:A:124:PRO:HB3	0.54	2.32	17	7
1:A:131:LEU:HD13	1:A:147:PHE:CE2	0.54	2.38	17	1
1:A:128:MET:HG3	1:A:147:PHE:CD2	0.54	2.38	13	5
1:A:116:LYS:HD3	1:A:119:LYS:HD3	0.54	1.79	10	3
1:A:12:THR:HB	1:A:82:VAL:HG23	0.54	1.79	2	1
1:A:118:ASP:HB3	1:A:154:THR:OG1	0.54	2.02	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:MET:SD	1:A:149:LYS:HE2	0.53	2.42	2	2
1:A:138:PRO:HG2	1:A:141:TRP:CD2	0.53	2.38	2	4
1:A:113:ALA:HB1	1:A:150:LEU:CD2	0.53	2.34	18	9
1:A:146:ILE:HG21	1:A:164:MET:HB3	0.53	1.80	15	5
1:A:88:ALA:HB2	1:A:114:ILE:HG23	0.53	1.79	17	11
1:A:145:THR:HB	1:A:147:PHE:CE1	0.53	2.39	6	2
1:A:150:LEU:H	1:A:150:LEU:HD13	0.52	1.63	7	1
1:A:83:ILE:HD11	1:A:165:ILE:HD11	0.52	1.81	17	1
1:A:21:LYS:HB2	2:A:179:GDP:PA	0.52	2.45	18	1
1:A:117:MET:HB2	1:A:151:SER:HB3	0.52	1.82	17	3
1:A:18:ASP:HA	2:A:179:GDP:H5'	0.51	1.82	3	6
1:A:97:VAL:HG12	1:A:101:ASN:ND2	0.51	2.19	4	10
1:A:130:GLU:O	1:A:133:GLU:HB2	0.51	2.06	4	3
1:A:110:ILE:HB	1:A:145:THR:HG23	0.51	1.82	16	1
1:A:20:GLY:HA3	1:A:24:LEU:HD13	0.51	1.81	1	1
1:A:20:GLY:HA2	1:A:23:THR:OG1	0.51	2.06	7	5
1:A:14:MET:HB3	1:A:99:ALA:CB	0.51	2.35	14	1
1:A:128:MET:HG3	1:A:147:PHE:CE2	0.51	2.41	9	3
1:A:138:PRO:CB	1:A:140:GLU:HG2	0.51	2.35	14	4
1:A:103:ALA:CB	1:A:110:ILE:HD11	0.51	2.36	17	3
1:A:131:LEU:CD1	1:A:147:PHE:HE2	0.51	2.19	17	3
1:A:160:HIS:HA	1:A:163:GLU:HG2	0.50	1.83	6	2
1:A:132:MET:CE	1:A:138:PRO:HD3	0.50	2.36	13	1
1:A:132:MET:SD	1:A:138:PRO:HD3	0.50	2.46	13	1
1:A:100:ILE:O	1:A:104:LYS:HG2	0.50	2.06	10	6
1:A:127:VAL:HA	1:A:130:GLU:OE2	0.50	2.06	6	2
1:A:150:LEU:CB	1:A:157:GLY:CA	0.50	2.87	5	3
1:A:153:LYS:HG3	2:A:179:GDP:N1	0.50	2.21	6	3
1:A:115:ASN:O	1:A:116:LYS:HB2	0.50	2.06	1	14
1:A:139:GLU:CG	1:A:146:ILE:HD13	0.50	2.35	13	2
1:A:163:GLU:O	1:A:166:LEU:HG	0.50	2.06	1	1
1:A:21:LYS:HG3	1:A:23:THR:CB	0.50	2.35	18	1
1:A:19:HIS:NE2	1:A:90:ASP:HB3	0.50	2.22	18	3
1:A:159:ASP:O	1:A:163:GLU:HG3	0.49	2.07	2	4
1:A:118:ASP:CG	1:A:153:LYS:HB2	0.49	2.27	6	2
1:A:153:LYS:HB2	2:A:179:GDP:C2	0.49	2.42	8	1
1:A:128:MET:HA	1:A:131:LEU:CD1	0.49	2.24	17	3
1:A:159:ASP:O	1:A:162:LEU:HG	0.49	2.07	11	4
1:A:132:MET:HG2	1:A:136:LEU:O	0.49	2.07	4	1
1:A:114:ILE:HD11	1:A:147:PHE:HD2	0.49	1.66	8	1
1:A:115:ASN:ND2	2:A:179:GDP:C5	0.49	2.80	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ARG:O	1:A:130:GLU:HG2	0.49	2.08	18	3
1:A:127:VAL:O	1:A:131:LEU:HD22	0.49	2.07	14	3
1:A:14:MET:SD	1:A:99:ALA:HB1	0.49	2.48	7	2
1:A:17:VAL:HB	1:A:95:GLN:NE2	0.49	2.22	14	9
1:A:81:ILE:HD11	1:A:168:VAL:HG11	0.49	1.84	2	1
1:A:156:GLU:HG2	1:A:157:GLY:N	0.49	2.23	14	1
1:A:129:GLN:HG3	1:A:141:TRP:HH2	0.48	1.67	15	2
1:A:104:LYS:HE2	1:A:104:LYS:CA	0.48	2.39	10	1
1:A:21:LYS:HB3	2:A:179:GDP:O2B	0.48	2.08	4	1
1:A:131:LEU:HD13	1:A:147:PHE:HE2	0.48	1.67	17	1
1:A:125:ASP:HA	1:A:128:MET:HB3	0.48	1.85	17	2
1:A:24:LEU:O	1:A:28:ILE:HB	0.48	2.08	1	6
1:A:18:ASP:HA	2:A:179:GDP:C4'	0.48	2.38	2	1
1:A:164:MET:CE	1:A:164:MET:HA	0.48	2.39	6	4
1:A:86:VAL:HG23	1:A:114:ILE:HG13	0.48	1.85	18	1
1:A:127:VAL:HA	1:A:130:GLU:HG2	0.48	1.86	5	2
1:A:162:LEU:O	1:A:166:LEU:HG	0.48	2.09	5	1
1:A:131:LEU:HD12	1:A:136:LEU:HD13	0.48	1.84	4	1
1:A:132:MET:SD	1:A:137:VAL:HA	0.48	2.48	3	2
1:A:84:LEU:HD21	1:A:96:THR:HG22	0.47	1.86	10	1
1:A:19:HIS:HE1	1:A:91:GLY:O	0.47	1.92	16	3
1:A:132:MET:SD	1:A:141:TRP:CE3	0.47	3.08	10	3
1:A:13:ILE:HD12	1:A:25:LEU:HD21	0.47	1.87	11	1
1:A:151:SER:HB3	1:A:154:THR:OG1	0.47	2.09	12	4
1:A:21:LYS:HD3	2:A:179:GDP:C8	0.47	2.45	18	1
1:A:127:VAL:HA	1:A:130:GLU:HG3	0.47	1.87	1	2
1:A:132:MET:HG2	1:A:141:TRP:CZ3	0.47	2.40	12	1
1:A:81:ILE:CG2	1:A:111:ILE:HG12	0.47	2.40	10	4
1:A:159:ASP:O	1:A:163:GLU:HG2	0.47	2.09	12	2
1:A:139:GLU:HB2	1:A:146:ILE:HD13	0.46	1.88	10	2
1:A:16:HIS:CE1	1:A:17:VAL:HG12	0.46	2.45	14	7
1:A:100:ILE:HG12	1:A:136:LEU:HD11	0.46	1.87	11	1
1:A:138:PRO:HB3	1:A:147:PHE:CG	0.46	2.44	15	1
1:A:25:LEU:HD13	1:A:25:LEU:C	0.46	2.31	13	1
1:A:150:LEU:HD13	1:A:150:LEU:N	0.46	2.26	7	1
1:A:150:LEU:HB3	1:A:157:GLY:CA	0.46	2.36	12	1
1:A:145:THR:HB	1:A:147:PHE:HE1	0.46	1.70	7	2
1:A:17:VAL:HG23	2:A:179:GDP:O2B	0.46	2.10	18	2
1:A:86:VAL:HG12	1:A:96:THR:HG21	0.46	1.87	3	4
1:A:17:VAL:O	1:A:18:ASP:HB3	0.46	2.10	9	7
1:A:117:MET:SD	1:A:124:PRO:HB3	0.46	2.50	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:MET:HB3	1:A:94:PRO:CD	0.46	2.40	12	10
1:A:17:VAL:HA	2:A:179:GDP:O2B	0.46	2.10	2	1
1:A:111:ILE:HD12	1:A:146:ILE:HB	0.46	1.86	3	2
1:A:25:LEU:O	1:A:28:ILE:HG22	0.46	2.11	18	1
1:A:110:ILE:CG2	1:A:111:ILE:N	0.46	2.79	2	7
1:A:132:MET:HG2	1:A:137:VAL:HA	0.46	1.86	6	1
1:A:131:LEU:HD12	1:A:136:LEU:CD1	0.46	2.41	1	3
1:A:110:ILE:C	1:A:145:THR:HG23	0.45	2.32	7	4
1:A:110:ILE:HG22	1:A:111:ILE:N	0.45	2.27	5	3
1:A:139:GLU:HG2	1:A:145:THR:C	0.45	2.31	11	1
1:A:117:MET:HA	1:A:122:ALA:CB	0.45	2.41	7	1
1:A:139:GLU:HG3	1:A:145:THR:O	0.45	2.10	17	1
1:A:139:GLU:OE1	1:A:139:GLU:HA	0.45	2.10	10	1
1:A:16:HIS:HB2	1:A:96:THR:HG1	0.45	1.71	16	2
1:A:139:GLU:HG2	1:A:146:ILE:HA	0.45	1.87	16	1
1:A:27:ALA:HB1	1:A:155:LYS:HE3	0.45	1.87	11	1
1:A:84:LEU:HD12	1:A:131:LEU:HD21	0.44	1.89	16	1
1:A:118:ASP:CB	1:A:154:THR:HG23	0.44	2.42	12	3
1:A:128:MET:HB2	1:A:147:PHE:CD2	0.44	2.48	4	1
1:A:115:ASN:ND2	2:A:179:GDP:C6	0.44	2.86	1	5
1:A:17:VAL:HG23	2:A:179:GDP:O3B	0.44	2.13	14	1
1:A:112:VAL:HG11	1:A:131:LEU:CD2	0.44	2.42	9	1
1:A:157:GLY:HA2	1:A:160:HIS:HB3	0.44	1.89	14	1
1:A:21:LYS:HB2	2:A:179:GDP:O3B	0.44	2.12	11	1
1:A:93:MET:O	1:A:97:VAL:HG23	0.44	2.13	4	4
1:A:106:ALA:O	1:A:107:ASN:HB2	0.44	2.12	17	1
1:A:104:LYS:HD3	1:A:136:LEU:CD2	0.44	2.43	4	1
1:A:17:VAL:C	1:A:19:HIS:H	0.43	2.16	18	2
1:A:16:HIS:ND1	1:A:95:GLN:HG2	0.43	2.28	7	4
1:A:97:VAL:HA	1:A:100:ILE:HD12	0.43	1.88	2	2
1:A:158:LEU:O	1:A:162:LEU:HG	0.43	2.12	16	1
1:A:14:MET:SD	1:A:82:VAL:HG21	0.43	2.53	2	1
1:A:160:HIS:HA	1:A:163:GLU:CG	0.43	2.42	6	1
1:A:102:HIS:CG	1:A:103:ALA:N	0.43	2.86	17	1
1:A:92:VAL:HG11	1:A:134:TYR:HE2	0.43	1.73	1	1
1:A:134:TYR:N	1:A:134:TYR:CD1	0.43	2.86	14	1
1:A:131:LEU:HD12	1:A:136:LEU:HD12	0.43	1.91	14	1
1:A:100:ILE:HG23	1:A:136:LEU:HD11	0.43	1.90	1	1
1:A:116:LYS:HB3	1:A:119:LYS:HD3	0.43	1.91	4	1
1:A:25:LEU:HA	1:A:28:ILE:HG22	0.43	1.89	8	1
1:A:27:ALA:O	1:A:155:LYS:HE2	0.43	2.13	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:PRO:HB2	1:A:140:GLU:CG	0.43	2.43	1	1
1:A:114:ILE:O	1:A:150:LEU:HD23	0.42	2.14	8	2
1:A:108:VAL:HG22	1:A:109:PRO:HD2	0.42	1.91	12	1
1:A:138:PRO:HB3	1:A:140:GLU:HG2	0.42	1.89	4	2
1:A:22:THR:O	1:A:25:LEU:HG	0.42	2.14	3	1
1:A:129:GLN:O	1:A:133:GLU:HG2	0.42	2.14	18	2
1:A:110:ILE:HB	1:A:145:THR:OG1	0.42	2.14	17	1
1:A:115:ASN:ND2	1:A:116:LYS:HG3	0.42	2.29	7	1
1:A:164:MET:HA	1:A:164:MET:CE	0.42	2.45	14	3
1:A:100:ILE:HG21	1:A:134:TYR:HB3	0.42	1.91	4	1
1:A:138:PRO:HD3	1:A:147:PHE:CE1	0.42	2.50	1	1
1:A:138:PRO:HB3	1:A:147:PHE:HB2	0.42	1.91	2	1
1:A:153:LYS:HD2	2:A:179:GDP:N2	0.42	2.30	2	1
1:A:117:MET:N	1:A:151:SER:OG	0.42	2.52	11	2
1:A:164:MET:O	1:A:168:VAL:HG23	0.42	2.15	10	1
1:A:129:GLN:HG3	1:A:141:TRP:CH2	0.41	2.50	12	2
1:A:138:PRO:HG2	1:A:141:TRP:CG	0.41	2.50	2	1
1:A:103:ALA:HB1	1:A:110:ILE:HD11	0.41	1.91	17	1
1:A:155:LYS:HD3	1:A:158:LEU:HD12	0.41	1.90	18	4
1:A:131:LEU:CD2	1:A:147:PHE:CE2	0.41	3.03	18	1
1:A:21:LYS:HG2	2:A:179:GDP:PB	0.41	2.55	13	1
1:A:139:GLU:HG2	1:A:146:ILE:CD1	0.41	2.45	16	1
1:A:141:TRP:N	1:A:141:TRP:CD1	0.41	2.86	17	1
1:A:92:VAL:HG21	1:A:134:TYR:CE2	0.41	2.51	6	1
1:A:17:VAL:HG23	2:A:179:GDP:O1B	0.41	2.16	4	2
1:A:136:LEU:O	1:A:136:LEU:HG	0.41	2.15	10	2
1:A:117:MET:H	1:A:151:SER:HB2	0.41	1.75	12	1
1:A:117:MET:HE1	1:A:124:PRO:HD3	0.41	1.93	14	1
1:A:15:GLY:HA2	1:A:84:LEU:CD2	0.41	2.46	17	1
1:A:16:HIS:HA	1:A:95:GLN:HG2	0.41	1.92	18	1
1:A:86:VAL:HG12	1:A:96:THR:CG2	0.41	2.46	18	1
1:A:89:ASP:OD1	1:A:116:LYS:HD2	0.41	2.15	1	1
1:A:117:MET:N	1:A:151:SER:HB2	0.41	2.30	12	1
1:A:141:TRP:CD1	1:A:141:TRP:N	0.41	2.88	13	1
1:A:140:GLU:CD	1:A:140:GLU:H	0.41	2.20	5	1
1:A:125:ASP:HA	1:A:128:MET:HG2	0.41	1.92	10	1
1:A:152:ALA:HB3	2:A:179:GDP:O6	0.41	2.16	4	1
1:A:16:HIS:HB3	1:A:19:HIS:CE1	0.40	2.51	1	1
1:A:128:MET:HB2	1:A:147:PHE:CE2	0.40	2.51	4	2
1:A:130:GLU:HA	1:A:133:GLU:HG3	0.40	1.92	10	1
1:A:127:VAL:O	1:A:131:LEU:HD23	0.40	2.17	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:21:LYS:CD	2:A:179:GDP:C8	0.40	3.04	18	1
1:A:113:ALA:HA	1:A:148:CYS:O	0.40	2.16	3	1
1:A:84:LEU:HD13	1:A:84:LEU:C	0.40	2.36	1	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/178 (59%)	92±2 (87±2%)	12±2 (12±2%)	1±1 (1±1%)	20	66
All	All	1890/3204 (59%)	1649 (87%)	218 (12%)	23 (1%)	20	66

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	107	ASN	12
1	A	124	PRO	4
1	A	94	PRO	3
1	A	21	LYS	2
1	A	20	GLY	2

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	89/150 (59%)	80±2 (90±2%)	9±2 (10±2%)	13	57
All	All	1602/2700 (59%)	1440 (90%)	162 (10%)	13	57

All 31 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	96	THR	18
1	A	123	ASN	17
1	A	23	THR	14
1	A	166	LEU	10
1	A	89	ASP	9
1	A	108	VAL	8
1	A	25	LEU	7
1	A	24	LEU	7
1	A	154	THR	6
1	A	21	LYS	6
1	A	156	GLU	5
1	A	139	GLU	5
1	A	153	LYS	5
1	A	131	LEU	5
1	A	151	SER	5
1	A	150	LEU	4
1	A	164	MET	3
1	A	115	ASN	3
1	A	161	LEU	3
1	A	132	MET	3
1	A	84	LEU	3
1	A	110	ILE	3
1	A	136	LEU	2
1	A	86	VAL	2
1	A	102	HIS	2
1	A	118	ASP	2
1	A	159	ASP	1
1	A	126	ARG	1
1	A	149	LYS	1
1	A	98	GLU	1
1	A	95	GLN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	GDP	A	179	-	25,30,30	1.17±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	GDP	A	179	-	23,47,47	1.21±0.10	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	A	179	-	-	0±0,12,32,32	0±0,3,3,3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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There are no ring outliers.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

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 73% for the entire structure.

7.1 Chemical shift list 1

File name: 2lkd_cs.str

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	1695
Number of shifts mapped to atoms	1695
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	147	-0.54 ± 0.17	Should be applied
$^{13}C_\beta$	136	0.37 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	127	-0.10 ± 0.11	None needed (< 0.5 ppm)
^{15}N	129	-0.69 ± 0.14	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 90%, i.e. 1128 atoms were assigned a chemical shift out of a possible 1247. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	492/515 (96%)	198/205 (97%)	199/210 (95%)	95/100 (95%)
Sidechain	586/671 (87%)	348/385 (90%)	232/269 (86%)	6/17 (35%)

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	Total	**¹H**	**¹³C**	**¹⁵N**
Aromatic	50/61 (82%)	24/31 (77%)	21/21 (100%)	5/9 (56%)
Overall	1128/1247 (90%)	570/621 (92%)	452/500 (90%)	106/126 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1552 atoms were assigned a chemical shift out of a possible 2122. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**¹H**	**¹³C**	**¹⁵N**
Backbone	678/872 (78%)	275/347 (79%)	274/356 (77%)	129/169 (76%)
Sidechain	800/1131 (71%)	473/654 (72%)	319/438 (73%)	8/39 (21%)
Aromatic	74/119 (62%)	37/61 (61%)	32/41 (78%)	5/17 (29%)
Overall	1552/2122 (73%)	785/1062 (74%)	625/835 (75%)	142/225 (63%)

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	138	PRO	HG3	0.01	3.56 − 0.26	-5.8

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: