



Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2026 – 09:18 AM UTC

PDB ID : 2FV4 / pdb_00002fv4
Title : NMR solution structure of the yeast kinetochore Spc24/Spc25 globular domain
Authors : Schnell, J.R.; Chou, J.J.
Deposited on : 2006-01-29

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

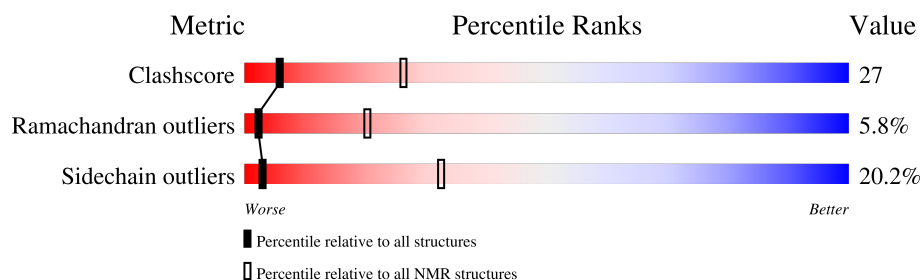
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	98	
2	B	77	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:134-A:152, A:158-A:173, A:183-A:221, B:156-B:184, B:188-B:194, B:199-B:213 (125)	0.78	7

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 and 6 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2347 atoms, of which 1176 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region.

Mol	Chain	Residues	Atoms						Trace
1	A	89	Total	C	H	N	O	S	0
			1363	432	677	123	128	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	GLY	-	cloning artifact	UNP P40014
A	125	SER	-	cloning artifact	UNP P40014
A	126	HIS	-	cloning artifact	UNP P40014
A	127	MET	-	cloning artifact	UNP P40014

- Molecule 2 is a protein called Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region.

Mol	Chain	Residues	Atoms					Trace
2	B	58	Total	C	H	N	O	0
			984	310	499	83	92	

There is a discrepancy between the modelled and reference sequences:

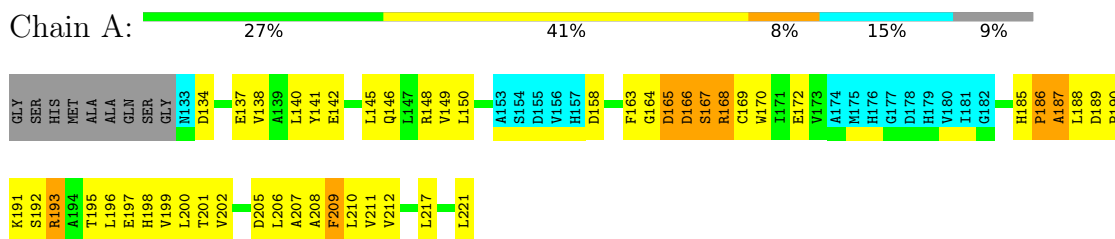
Chain	Residue	Modelled	Actual	Comment	Reference
B	137	MET	-	cloning artifact	UNP Q04477

4 Residue-property plots

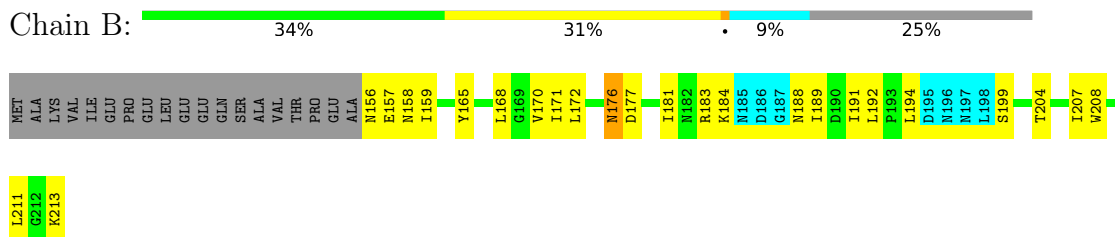
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region



- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

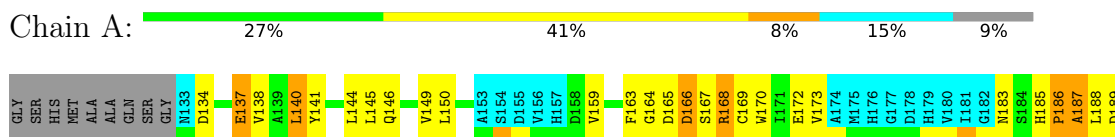


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

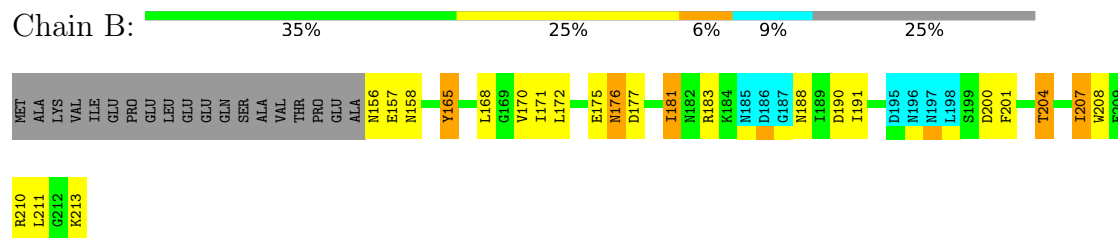
4.2.1 Score per residue for model 1

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region



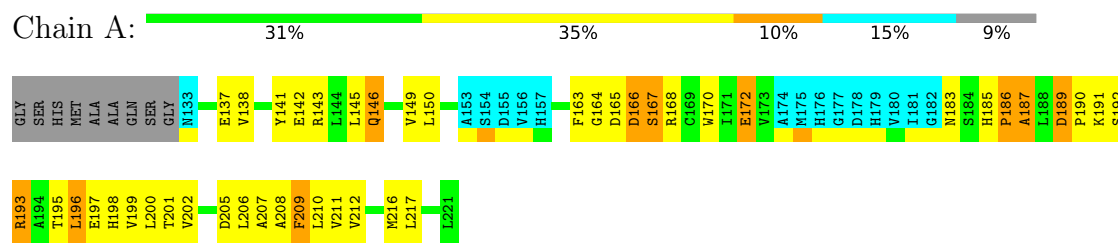


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

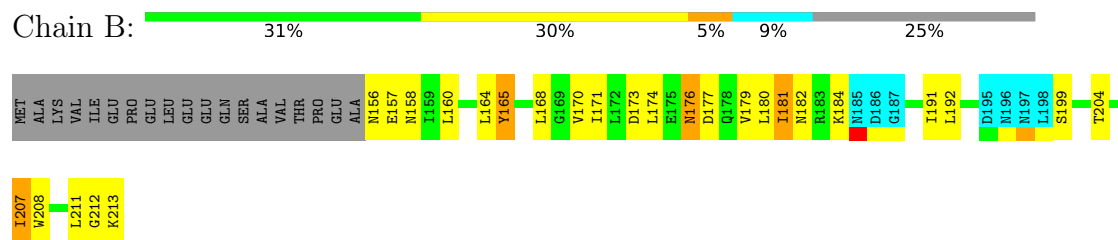


4.2.2 Score per residue for model 2

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

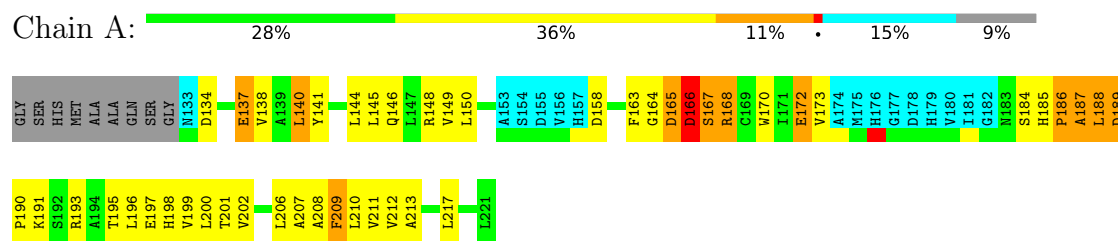


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

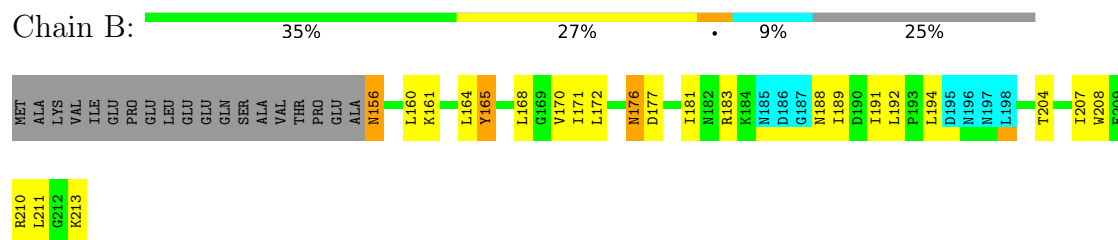


4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

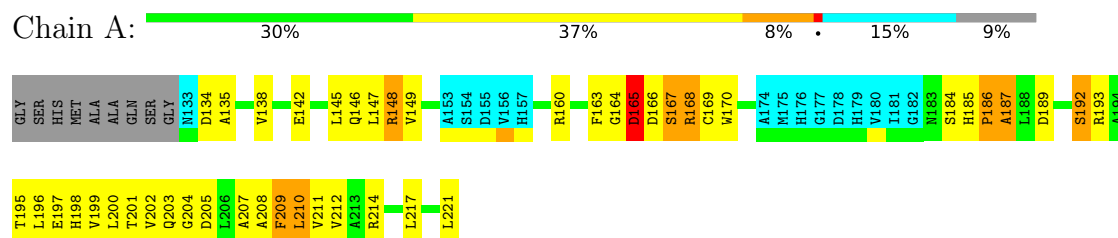


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

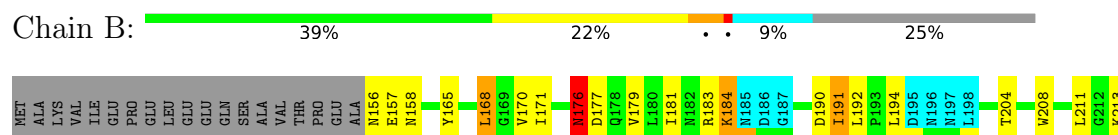


4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

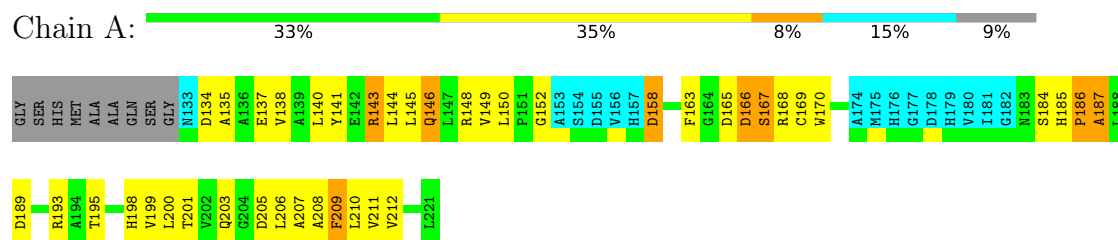


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

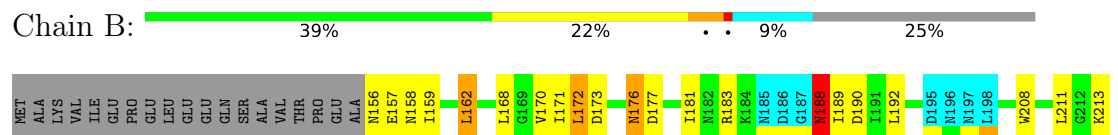


4.2.5 Score per residue for model 5

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

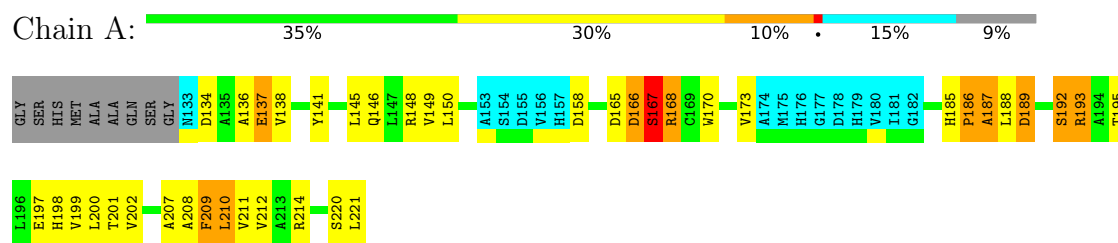


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

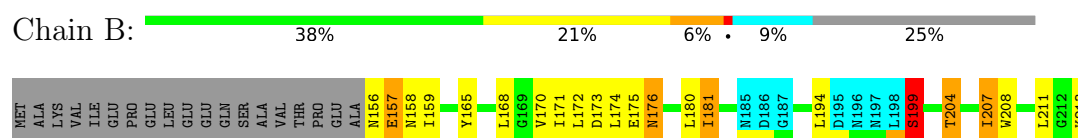


4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

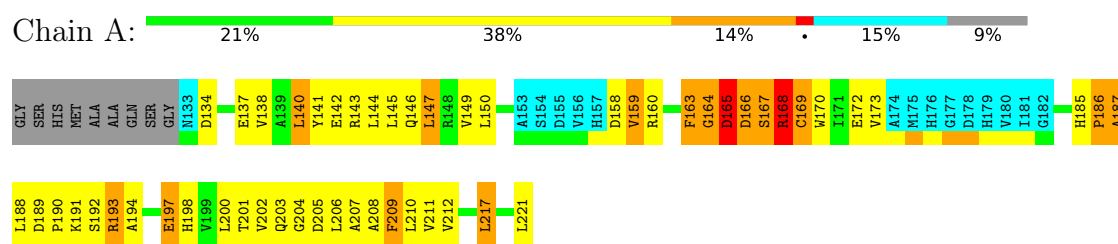


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

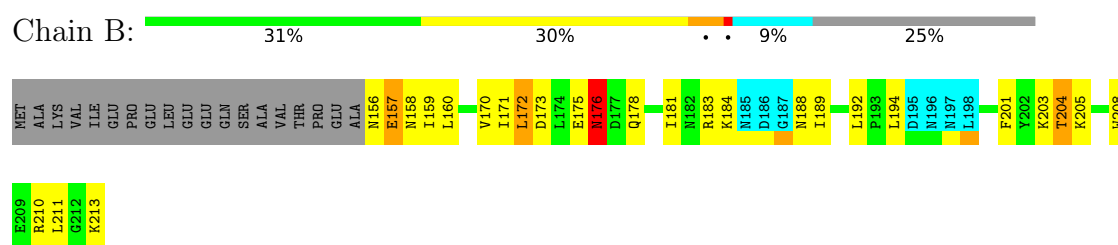


4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region



- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region



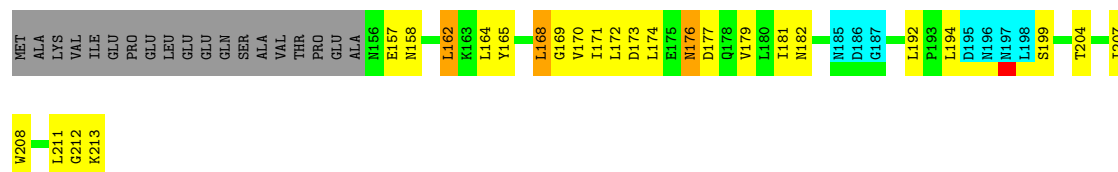
4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region



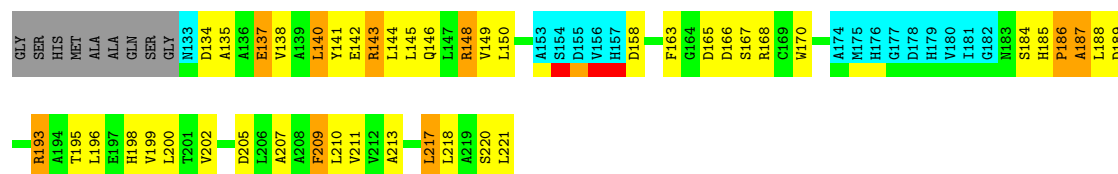


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region



4.2.9 Score per residue for model 9

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

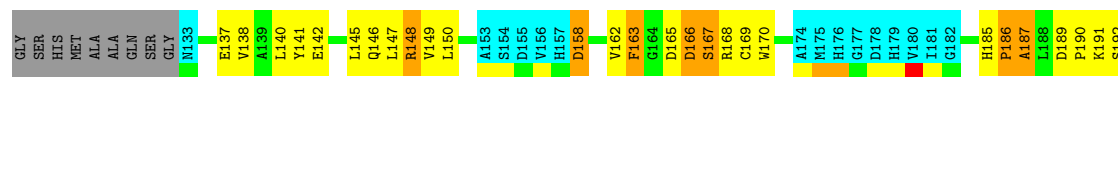


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region



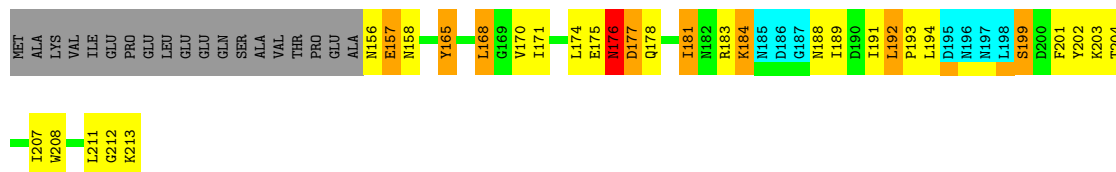
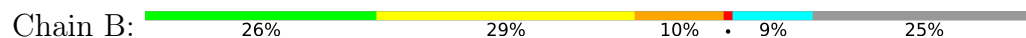
4.2.10 Score per residue for model 10

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region



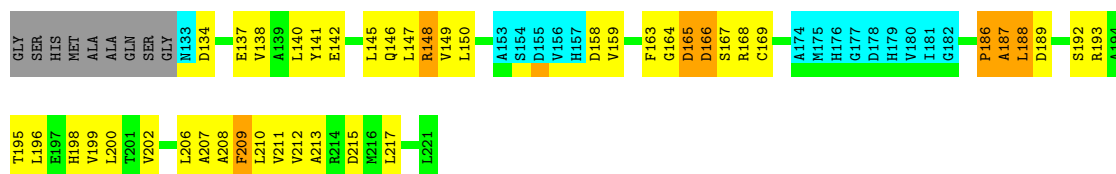


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

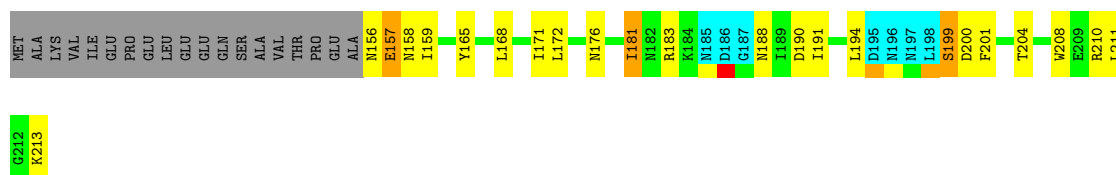


4.2.11 Score per residue for model 11

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

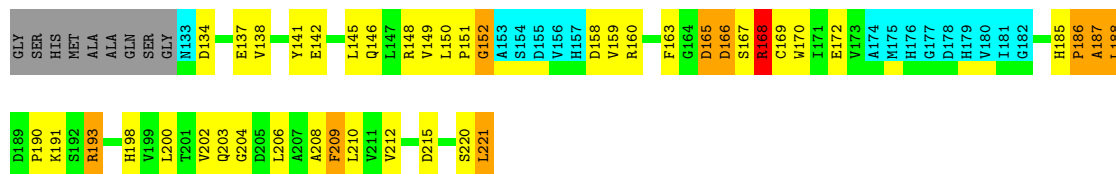


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

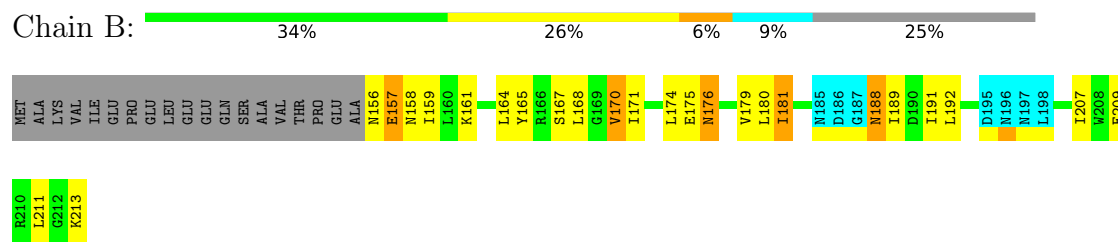


4.2.12 Score per residue for model 12

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

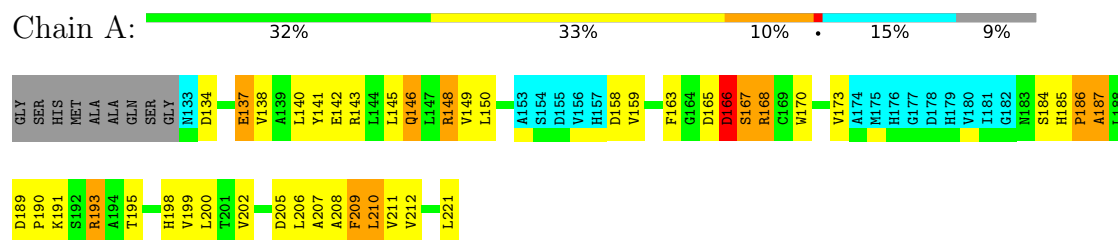


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

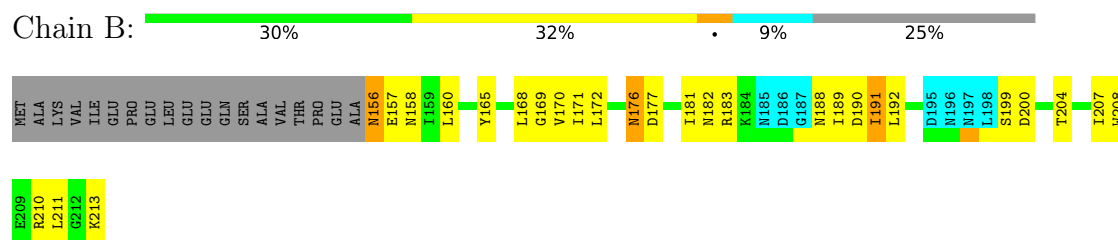


4.2.13 Score per residue for model 13

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

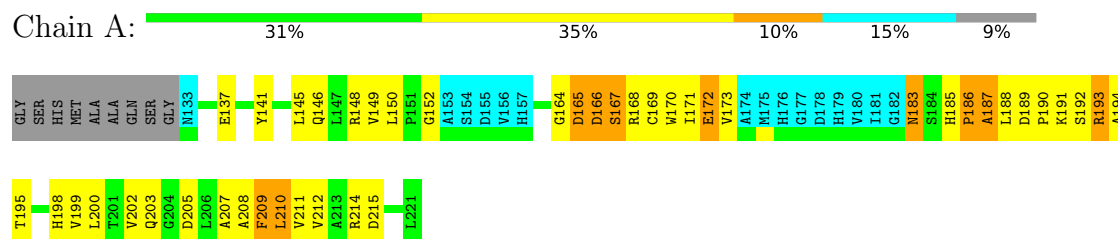


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

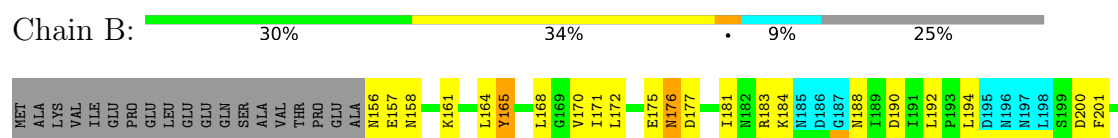


4.2.14 Score per residue for model 14

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region



- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region





4.2.15 Score per residue for model 15

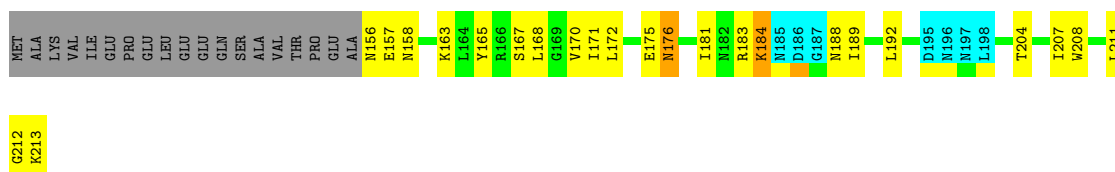
- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

Chain A:



- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

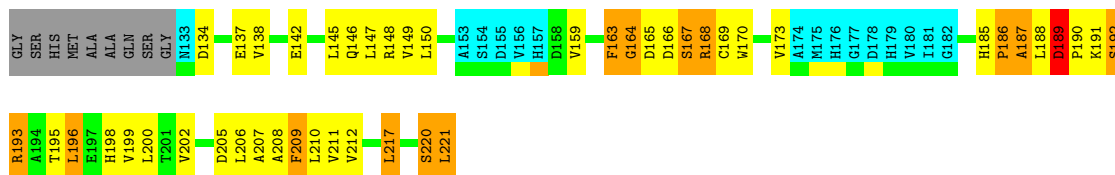
Chain B:



4.2.16 Score per residue for model 16

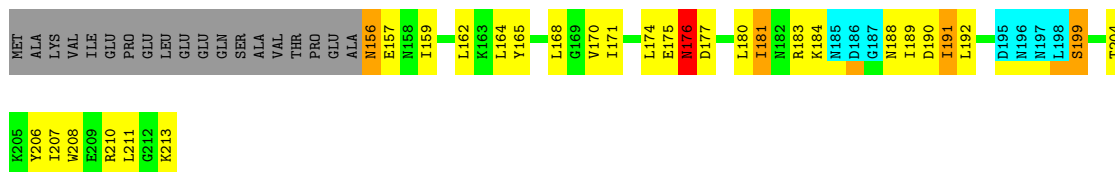
- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

Chain A:



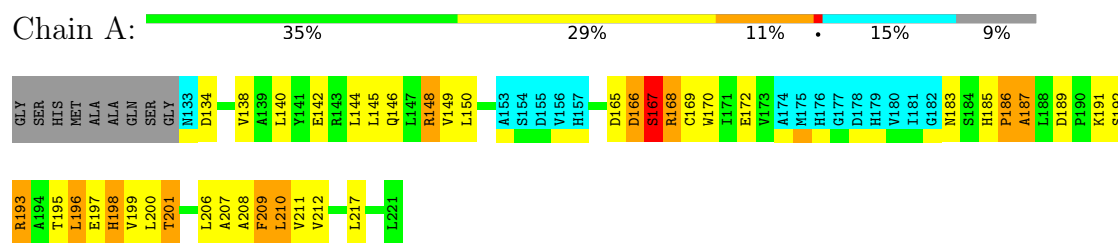
- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

Chain B:

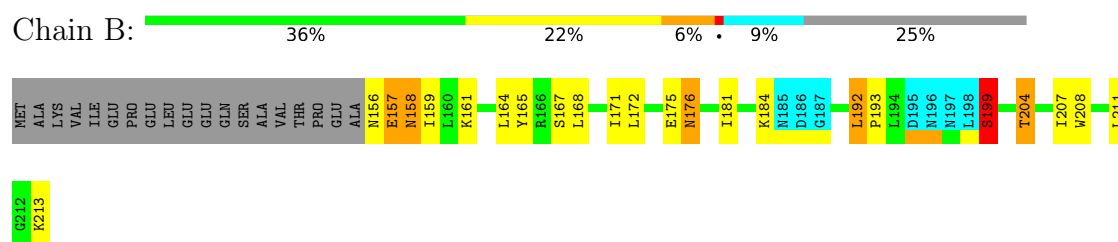


4.2.17 Score per residue for model 17

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

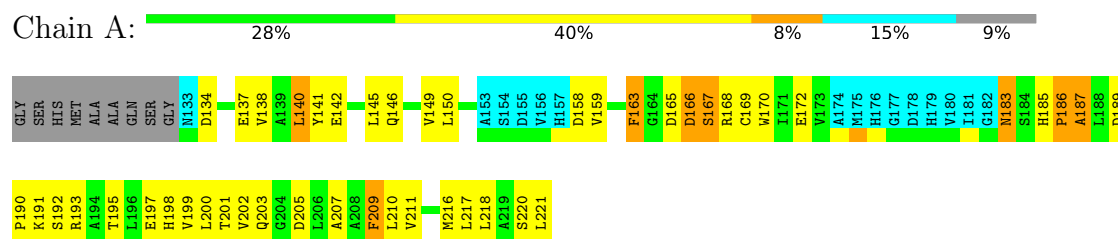


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

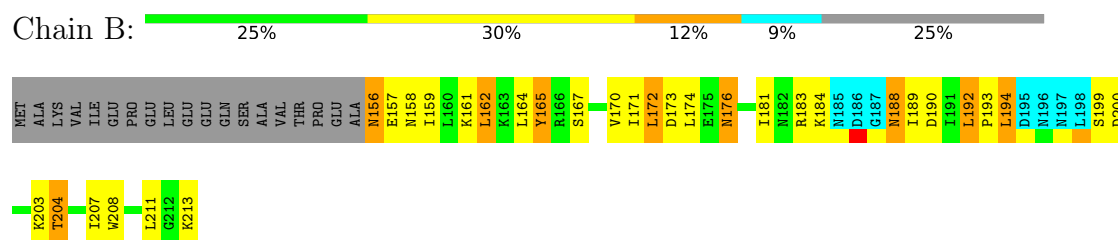


4.2.18 Score per residue for model 18

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

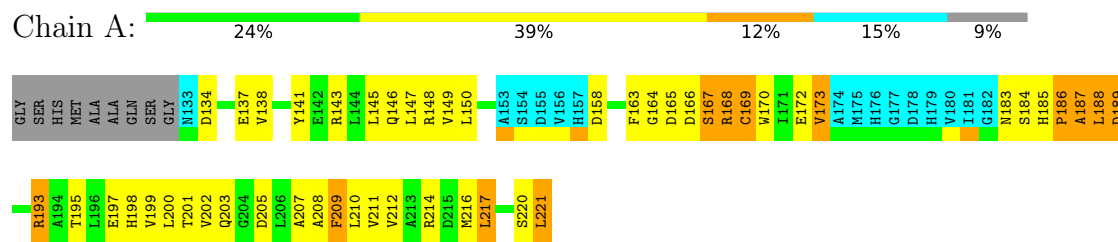


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

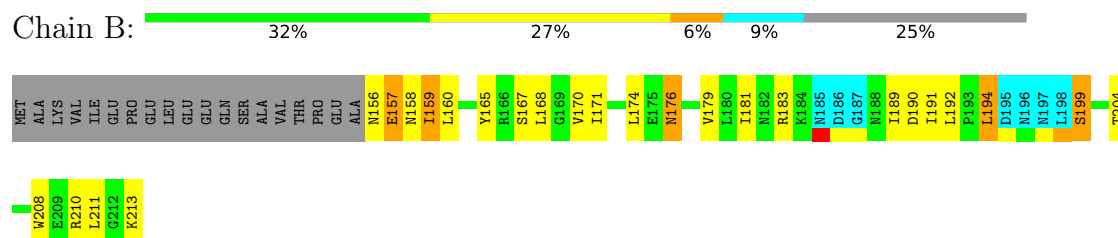


4.2.19 Score per residue for model 19

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region

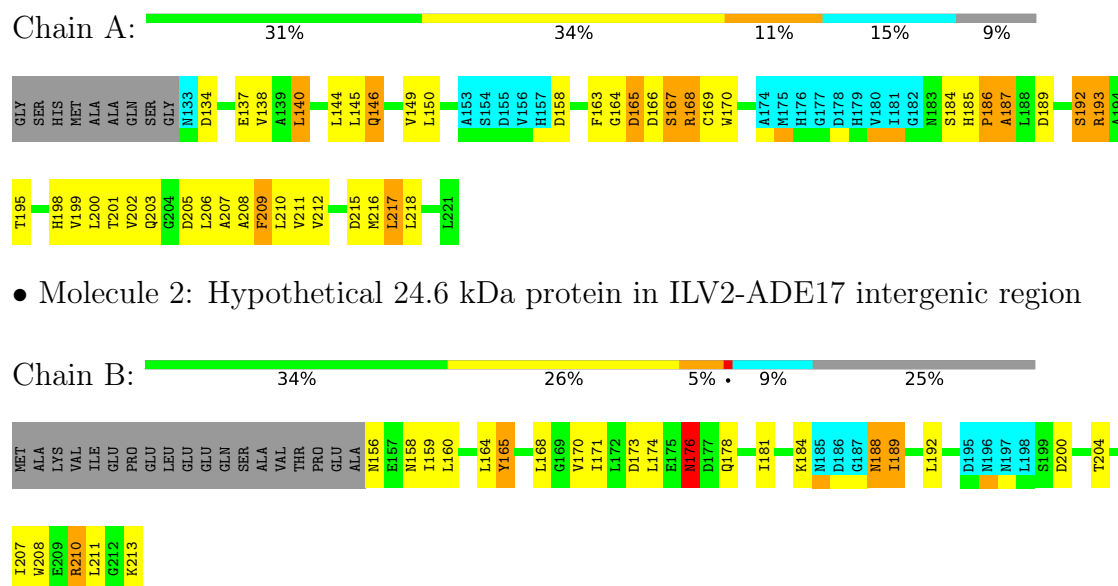


- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region

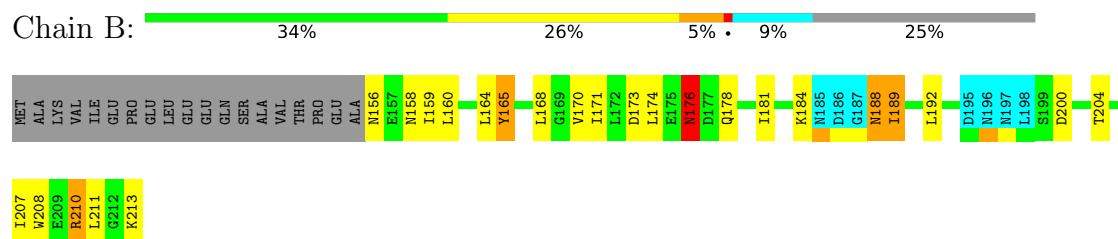


4.2.20 Score per residue for model 20

- Molecule 1: Hypothetical 25.2 kDa protein in AFG3-SEB2 intergenic region



- Molecule 2: Hypothetical 24.6 kDa protein in ILV2-ADE17 intergenic region



5 Refinement protocol and experimental data overview ⓘ

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

Of the 30 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
Xplor-NIH	refinement	2.11

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.50±0.01	0±0/588 (0.0± 0.0%)	1.20±0.01	0±0/799 (0.0± 0.1%)
2	B	1.37±0.01	0±0/439 (0.0± 0.0%)	1.21±0.01	0±0/589 (0.0± 0.0%)
All	All	1.44	0/20540 (0.0%)	1.20	7/27760 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	163	PHE	CA-CB-CG	-5.93	107.87	113.80	20	7

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	578	583	583	40±5
2	B	433	459	458	19±4
All	All	20220	20840	20820	1105

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:LEU:HD23	1:A:218:LEU:N	0.84	1.87	9	4
1:A:206:LEU:HD23	1:A:206:LEU:O	0.81	1.76	17	4
1:A:188:LEU:HD13	1:A:188:LEU:N	0.75	1.97	11	1
1:A:134:ASP:O	1:A:138:VAL:HG23	0.74	1.83	18	16
2:B:191:ILE:HD13	2:B:191:ILE:H	0.74	1.41	16	2
2:B:162:LEU:HD23	2:B:162:LEU:N	0.73	1.98	18	3
1:A:169:CYS:SG	1:A:217:LEU:HD11	0.73	2.23	7	2
1:A:207:ALA:O	1:A:211:VAL:HG23	0.73	1.83	8	19
1:A:145:LEU:HD12	2:B:165:TYR:CE1	0.72	2.20	6	3
1:A:220:SER:O	1:A:221:LEU:OXT	0.71	2.08	6	2
1:A:208:ALA:O	1:A:212:VAL:HG23	0.69	1.88	15	18
1:A:147:LEU:HD13	1:A:147:LEU:C	0.68	2.13	7	2
1:A:149:VAL:HG11	2:B:157:GLU:OE2	0.68	1.89	16	1
1:A:195:THR:O	1:A:199:VAL:HG23	0.67	1.88	9	17
1:A:210:LEU:HD23	1:A:210:LEU:O	0.67	1.89	1	6
1:A:166:ASP:O	1:A:168:ARG:N	0.67	2.26	13	9
1:A:145:LEU:HD12	2:B:165:TYR:CZ	0.67	2.25	13	3
1:A:210:LEU:C	1:A:210:LEU:HD23	0.66	2.16	9	3
1:A:145:LEU:HD12	2:B:165:TYR:CE2	0.66	2.25	19	4
1:A:209:PHE:CG	1:A:210:LEU:N	0.65	2.65	16	20
1:A:187:ALA:C	1:A:188:LEU:HD13	0.65	2.17	11	1
2:B:165:TYR:N	2:B:165:TYR:CD1	0.64	2.63	3	7
1:A:170:TRP:CH2	1:A:185:HIS:CG	0.64	2.86	1	17
1:A:166:ASP:OD2	1:A:217:LEU:HD12	0.64	1.92	11	1
1:A:145:LEU:HD21	2:B:208:TRP:CH2	0.63	2.28	8	1
1:A:186:PRO:O	1:A:187:ALA:HB2	0.63	1.94	11	18
1:A:209:PHE:C	1:A:209:PHE:CD1	0.63	2.77	9	20
1:A:145:LEU:HD21	2:B:208:TRP:CZ3	0.63	2.29	8	1
1:A:166:ASP:OD2	1:A:221:LEU:HD11	0.63	1.94	10	1
1:A:217:LEU:HD23	1:A:217:LEU:C	0.63	2.19	1	4
1:A:140:LEU:CD1	1:A:144:LEU:HD12	0.62	2.24	9	5
1:A:170:TRP:CH2	1:A:185:HIS:ND1	0.62	2.67	10	2
1:A:165:ASP:O	1:A:167:SER:N	0.62	2.32	1	4
1:A:214:ARG:HH12	2:B:168:LEU:HD11	0.62	1.54	4	1
1:A:145:LEU:HD21	1:A:214:ARG:HH21	0.62	1.54	4	1
1:A:193:ARG:NH2	1:A:194:ALA:HB2	0.62	2.09	7	2
1:A:170:TRP:CZ3	1:A:185:HIS:CD2	0.62	2.88	3	4
2:B:176:ASN:ND2	2:B:176:ASN:N	0.61	2.48	4	1
1:A:187:ALA:HB3	1:A:220:SER:OG	0.60	1.95	19	3
1:A:170:TRP:CH2	1:A:185:HIS:CE1	0.60	2.90	14	1
2:B:183:ARG:NH1	2:B:210:ARG:NH2	0.60	2.50	16	2
2:B:183:ARG:NH1	2:B:210:ARG:HH22	0.60	1.95	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:VAL:C	1:A:150:LEU:HD22	0.59	2.23	19	19
2:B:183:ARG:HH11	2:B:210:ARG:NH2	0.59	1.95	16	2
1:A:145:LEU:HD23	1:A:214:ARG:HH22	0.59	1.58	19	2
1:A:198:HIS:O	1:A:202:VAL:HG23	0.59	1.98	9	18
2:B:191:ILE:HD13	2:B:191:ILE:N	0.59	2.13	13	2
1:A:137:GLU:CG	2:B:174:LEU:HD11	0.58	2.27	10	2
1:A:165:ASP:OD2	1:A:221:LEU:HD11	0.58	1.97	6	1
1:A:170:TRP:CZ3	1:A:185:HIS:CG	0.58	2.90	10	1
1:A:147:LEU:HD23	1:A:148:ARG:N	0.58	2.13	10	1
2:B:168:LEU:CD1	2:B:208:TRP:CZ3	0.58	2.86	17	3
1:A:137:GLU:OE2	2:B:174:LEU:HD12	0.58	1.97	20	1
1:A:170:TRP:CZ2	1:A:185:HIS:CG	0.57	2.92	14	5
1:A:165:ASP:OD2	1:A:217:LEU:HD12	0.57	1.98	16	1
1:A:165:ASP:O	1:A:166:ASP:O	0.57	2.23	8	5
1:A:215:ASP:OD1	1:A:216:MET:N	0.57	2.38	20	1
1:A:188:LEU:HD23	1:A:220:SER:O	0.56	2.00	12	1
1:A:137:GLU:O	1:A:141:TYR:CD1	0.56	2.59	2	11
1:A:144:LEU:HD22	2:B:204:THR:HG21	0.56	1.78	17	4
1:A:163:PHE:CD1	1:A:163:PHE:N	0.56	2.72	9	8
2:B:156:ASN:O	2:B:158:ASN:N	0.56	2.39	12	13
1:A:163:PHE:CD2	1:A:217:LEU:HD21	0.56	2.36	19	1
2:B:183:ARG:NH2	2:B:210:ARG:NH2	0.56	2.53	13	1
2:B:183:ARG:NH2	2:B:210:ARG:HE	0.55	1.99	1	1
1:A:140:LEU:HD11	1:A:144:LEU:HD12	0.55	1.78	3	4
1:A:170:TRP:HE1	1:A:183:ASN:ND2	0.55	1.99	19	1
1:A:149:VAL:HG11	2:B:161:LYS:NZ	0.55	2.15	14	1
1:A:214:ARG:NH2	2:B:208:TRP:CE3	0.55	2.74	8	2
1:A:166:ASP:O	1:A:167:SER:C	0.55	2.49	3	3
2:B:156:ASN:CG	2:B:157:GLU:N	0.55	2.65	16	1
2:B:204:THR:O	2:B:208:TRP:CG	0.54	2.61	7	11
1:A:145:LEU:HD22	2:B:208:TRP:CH2	0.54	2.37	20	3
2:B:191:ILE:H	2:B:191:ILE:CD1	0.54	2.15	16	1
1:A:188:LEU:C	1:A:188:LEU:HD12	0.54	2.27	15	1
1:A:170:TRP:CH2	1:A:185:HIS:CD2	0.54	2.96	3	7
2:B:172:LEU:HD23	2:B:173:ASP:H	0.54	1.62	5	3
1:A:193:ARG:CG	1:A:193:ARG:HH11	0.54	2.15	8	12
1:A:148:ARG:HH11	1:A:148:ARG:CG	0.54	2.16	4	2
1:A:165:ASP:CG	1:A:217:LEU:HD21	0.54	2.28	20	1
2:B:176:ASN:N	2:B:176:ASN:OD1	0.54	2.41	16	4
1:A:193:ARG:NH2	1:A:197:GLU:OE2	0.54	2.41	6	1
1:A:193:ARG:CG	1:A:193:ARG:NH1	0.54	2.70	17	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:168:LEU:HD12	2:B:208:TRP:CH2	0.54	2.38	17	3
1:A:220:SER:C	1:A:221:LEU:OXT	0.54	2.50	6	1
2:B:157:GLU:CD	2:B:157:GLU:H	0.54	2.11	19	4
1:A:163:PHE:O	1:A:165:ASP:N	0.54	2.40	10	5
1:A:168:ARG:HH11	1:A:168:ARG:CG	0.54	2.16	13	2
2:B:188:ASN:O	2:B:189:ILE:O	0.53	2.25	20	1
1:A:142:GLU:OE1	1:A:148:ARG:NH2	0.53	2.41	4	2
1:A:166:ASP:C	1:A:168:ARG:H	0.53	2.12	17	5
1:A:170:TRP:CZ2	1:A:185:HIS:CD2	0.53	2.97	14	1
1:A:205:ASP:O	1:A:207:ALA:N	0.53	2.42	16	7
1:A:160:ARG:HE	1:A:170:TRP:CD1	0.53	2.22	4	1
2:B:158:ASN:OD1	2:B:159:ILE:N	0.53	2.41	17	2
2:B:211:LEU:C	2:B:213:LYS:N	0.53	2.65	7	20
1:A:190:PRO:O	1:A:192:SER:N	0.53	2.41	16	2
1:A:160:ARG:NH1	1:A:172:GLU:OE1	0.53	2.42	7	1
1:A:217:LEU:N	1:A:217:LEU:HD22	0.53	2.19	18	1
1:A:158:ASP:OD1	1:A:159:VAL:N	0.53	2.42	7	2
1:A:183:ASN:OD1	1:A:183:ASN:N	0.53	2.42	14	1
1:A:160:ARG:NE	1:A:172:GLU:OE2	0.53	2.42	15	1
1:A:190:PRO:C	1:A:192:SER:N	0.52	2.66	16	2
1:A:148:ARG:NH1	1:A:148:ARG:CG	0.52	2.72	11	3
2:B:176:ASN:C	2:B:176:ASN:ND2	0.52	2.68	10	1
1:A:193:ARG:NH1	1:A:193:ARG:CG	0.52	2.71	15	3
1:A:206:LEU:HD22	2:B:167:SER:HB3	0.52	1.82	17	1
1:A:137:GLU:HG2	2:B:174:LEU:HD11	0.52	1.80	10	1
1:A:142:GLU:CD	1:A:148:ARG:NH2	0.52	2.68	15	1
1:A:165:ASP:N	1:A:165:ASP:OD1	0.52	2.42	19	1
2:B:156:ASN:C	2:B:158:ASN:N	0.52	2.67	19	13
1:A:143:ARG:HH11	1:A:143:ARG:CG	0.52	2.17	9	2
1:A:205:ASP:C	1:A:207:ALA:N	0.52	2.67	20	11
1:A:134:ASP:OD1	1:A:135:ALA:N	0.52	2.42	9	4
1:A:137:GLU:O	1:A:141:TYR:CG	0.52	2.63	18	2
2:B:169:GLY:O	2:B:182:ASN:ND2	0.52	2.43	13	1
1:A:160:ARG:NH1	1:A:172:GLU:CD	0.52	2.67	7	1
1:A:168:ARG:CG	1:A:168:ARG:NH1	0.52	2.71	7	2
2:B:173:ASP:N	2:B:173:ASP:OD1	0.52	2.42	20	1
1:A:142:GLU:OE1	2:B:161:LYS:NZ	0.52	2.42	12	1
2:B:191:ILE:N	2:B:191:ILE:CD1	0.52	2.73	13	1
2:B:211:LEU:C	2:B:213:LYS:H	0.52	2.13	5	19
1:A:165:ASP:O	1:A:166:ASP:CB	0.52	2.58	19	3
1:A:149:VAL:HG23	2:B:161:LYS:NZ	0.52	2.20	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:198:HIS:ND1	1:A:198:HIS:C	0.52	2.67	17	1
1:A:186:PRO:O	1:A:187:ALA:CB	0.51	2.58	1	18
2:B:211:LEU:O	2:B:213:LYS:N	0.51	2.43	7	14
1:A:184:SER:OG	1:A:193:ARG:NE	0.51	2.42	4	2
1:A:143:ARG:CG	1:A:143:ARG:NH1	0.51	2.72	9	2
2:B:190:ASP:OD1	2:B:191:ILE:N	0.51	2.43	19	6
1:A:197:GLU:O	1:A:201:THR:HG23	0.51	2.05	6	9
1:A:144:LEU:HD21	2:B:200:ASP:HB3	0.51	1.83	20	1
1:A:140:LEU:CD1	1:A:144:LEU:HD11	0.51	2.35	15	1
1:A:184:SER:OG	1:A:193:ARG:NH2	0.51	2.42	15	1
1:A:196:LEU:HD13	1:A:196:LEU:C	0.51	2.30	8	1
1:A:158:ASP:N	1:A:158:ASP:OD1	0.51	2.43	10	1
2:B:200:ASP:OD1	2:B:201:PHE:N	0.51	2.44	1	1
1:A:149:VAL:HG23	2:B:161:LYS:HZ3	0.51	1.65	17	1
1:A:163:PHE:CE2	1:A:217:LEU:HD21	0.51	2.40	19	1
2:B:206:TYR:OH	2:B:210:ARG:NH1	0.51	2.43	16	1
1:A:149:VAL:CG1	2:B:161:LYS:NZ	0.51	2.73	14	1
1:A:137:GLU:OE1	1:A:137:GLU:N	0.51	2.44	18	1
1:A:145:LEU:O	1:A:214:ARG:NH1	0.51	2.42	1	1
1:A:137:GLU:CG	1:A:141:TYR:CE1	0.51	2.94	7	1
1:A:164:GLY:O	1:A:165:ASP:CB	0.51	2.58	14	1
1:A:146:GLN:NE2	1:A:164:GLY:O	0.50	2.45	20	4
1:A:148:ARG:CG	1:A:148:ARG:HH11	0.50	2.18	9	3
2:B:175:GLU:O	2:B:176:ASN:CB	0.50	2.59	10	2
1:A:166:ASP:CG	1:A:167:SER:H	0.50	2.13	1	1
1:A:209:PHE:CD1	1:A:210:LEU:N	0.50	2.79	6	16
2:B:183:ARG:HH12	2:B:210:ARG:HH21	0.50	1.50	3	1
2:B:191:ILE:CD1	2:B:191:ILE:N	0.50	2.74	16	1
1:A:165:ASP:O	1:A:169:CYS:SG	0.50	2.70	19	1
1:A:148:ARG:CG	1:A:148:ARG:NH1	0.50	2.72	8	2
1:A:147:LEU:HD23	1:A:147:LEU:C	0.50	2.32	10	1
1:A:160:ARG:HH11	1:A:172:GLU:CD	0.50	2.14	7	1
1:A:172:GLU:O	1:A:193:ARG:NH2	0.50	2.44	19	1
1:A:196:LEU:HD13	1:A:196:LEU:O	0.50	2.06	16	4
1:A:172:GLU:OE1	1:A:173:VAL:N	0.50	2.44	3	1
1:A:141:TYR:CE2	2:B:162:LEU:HD22	0.50	2.42	8	1
1:A:220:SER:O	1:A:221:LEU:O	0.50	2.30	12	1
1:A:145:LEU:HD23	2:B:208:TRP:CH2	0.50	2.41	1	2
1:A:166:ASP:O	1:A:167:SER:CB	0.49	2.59	7	7
2:B:160:LEU:O	2:B:160:LEU:HD23	0.49	2.07	13	2
1:A:142:GLU:CD	1:A:148:ARG:HH21	0.49	2.16	11	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:ARG:NH1	1:A:143:ARG:CG	0.49	2.74	13	3
1:A:166:ASP:CG	1:A:217:LEU:HD12	0.49	2.33	11	1
2:B:162:LEU:N	2:B:162:LEU:CD2	0.49	2.66	18	2
1:A:165:ASP:O	1:A:166:ASP:C	0.49	2.56	13	5
1:A:196:LEU:HD21	1:A:213:ALA:HB2	0.49	1.84	3	1
2:B:156:ASN:C	2:B:156:ASN:ND2	0.49	2.70	16	1
1:A:163:PHE:CD2	1:A:169:CYS:SG	0.48	3.03	1	1
1:A:166:ASP:OD1	1:A:166:ASP:N	0.48	2.42	5	2
1:A:210:LEU:C	1:A:210:LEU:CD2	0.48	2.86	19	3
2:B:201:PHE:CD2	2:B:202:TYR:N	0.48	2.82	10	1
1:A:192:SER:OG	1:A:216:MET:SD	0.48	2.70	18	2
1:A:164:GLY:O	1:A:165:ASP:O	0.48	2.32	15	2
2:B:183:ARG:NE	2:B:190:ASP:OD2	0.48	2.46	5	2
2:B:183:ARG:CZ	2:B:190:ASP:OD2	0.48	2.62	11	1
2:B:156:ASN:C	2:B:158:ASN:H	0.48	2.17	19	10
1:A:167:SER:O	1:A:168:ARG:C	0.48	2.56	12	4
1:A:217:LEU:C	1:A:217:LEU:CD2	0.48	2.85	20	2
1:A:142:GLU:CD	1:A:148:ARG:NE	0.48	2.71	13	1
1:A:167:SER:O	1:A:168:ARG:CB	0.48	2.59	14	1
1:A:137:GLU:CG	1:A:138:VAL:N	0.48	2.76	2	2
1:A:189:ASP:OD1	1:A:191:LYS:N	0.48	2.46	2	1
1:A:214:ARG:NH1	2:B:208:TRP:CB	0.48	2.77	8	1
1:A:188:LEU:N	1:A:188:LEU:CD1	0.47	2.70	11	1
1:A:198:HIS:O	1:A:202:VAL:CG2	0.47	2.62	16	12
2:B:172:LEU:HD23	2:B:173:ASP:N	0.47	2.24	5	1
1:A:193:ARG:CD	1:A:193:ARG:C	0.47	2.87	9	1
1:A:149:VAL:CG2	2:B:161:LYS:NZ	0.47	2.77	17	1
1:A:205:ASP:CG	2:B:184:LYS:HZ1	0.47	2.18	4	1
1:A:203:GLN:OE1	1:A:208:ALA:CB	0.47	2.62	5	2
1:A:142:GLU:CD	1:A:148:ARG:CZ	0.47	2.87	13	1
1:A:172:GLU:OE1	1:A:172:GLU:CA	0.47	2.62	14	1
1:A:195:THR:O	1:A:199:VAL:CG2	0.47	2.63	2	6
1:A:142:GLU:OE1	1:A:148:ARG:CZ	0.47	2.62	13	1
1:A:142:GLU:O	1:A:148:ARG:NH2	0.47	2.47	17	1
1:A:214:ARG:HH12	2:B:208:TRP:CB	0.47	2.22	8	1
2:B:183:ARG:O	2:B:184:LYS:C	0.47	2.58	15	1
1:A:142:GLU:N	1:A:142:GLU:CD	0.47	2.72	16	1
1:A:145:LEU:HD21	1:A:214:ARG:NH2	0.47	2.24	4	1
2:B:201:PHE:CZ	2:B:205:LYS:NZ	0.47	2.79	7	1
1:A:196:LEU:O	1:A:196:LEU:HD23	0.47	2.09	15	1
1:A:193:ARG:CB	1:A:193:ARG:CZ	0.47	2.91	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:173:ASP:O	2:B:173:ASP:CG	0.47	2.58	9	1
2:B:157:GLU:OE1	2:B:157:GLU:N	0.47	2.42	15	2
2:B:162:LEU:CD2	2:B:162:LEU:H	0.47	2.22	18	1
1:A:147:LEU:C	1:A:147:LEU:CD1	0.47	2.85	16	2
2:B:164:LEU:C	2:B:164:LEU:HD23	0.47	2.35	14	1
2:B:181:ILE:CD1	2:B:207:ILE:HG21	0.47	2.39	2	3
2:B:156:ASN:O	2:B:157:GLU:C	0.47	2.58	7	9
1:A:210:LEU:O	1:A:210:LEU:HD13	0.47	2.10	6	1
1:A:142:GLU:CD	2:B:161:LYS:NZ	0.47	2.73	12	1
1:A:190:PRO:C	1:A:192:SER:H	0.47	2.18	16	1
1:A:167:SER:O	1:A:168:ARG:O	0.46	2.33	12	11
2:B:188:ASN:CG	2:B:189:ILE:N	0.46	2.73	7	1
2:B:208:TRP:N	2:B:208:TRP:CD1	0.46	2.81	19	13
2:B:192:LEU:C	2:B:192:LEU:HD23	0.46	2.35	13	4
1:A:165:ASP:CG	1:A:166:ASP:N	0.46	2.72	12	1
1:A:205:ASP:C	1:A:207:ALA:H	0.46	2.18	19	8
1:A:189:ASP:CG	1:A:191:LYS:H	0.46	2.18	2	1
1:A:169:CYS:SG	1:A:186:PRO:O	0.46	2.70	16	2
1:A:158:ASP:OD1	1:A:158:ASP:N	0.46	2.48	5	1
1:A:203:GLN:C	1:A:205:ASP:N	0.46	2.71	15	3
1:A:203:GLN:C	1:A:205:ASP:H	0.46	2.19	18	4
1:A:145:LEU:HD23	1:A:214:ARG:NH2	0.46	2.26	19	1
1:A:207:ALA:O	1:A:211:VAL:CG2	0.46	2.64	1	10
2:B:164:LEU:O	2:B:165:TYR:C	0.46	2.57	16	5
1:A:137:GLU:CD	2:B:174:LEU:HD12	0.46	2.35	20	1
1:A:142:GLU:OE2	2:B:161:LYS:NZ	0.46	2.49	18	1
2:B:156:ASN:ND2	2:B:156:ASN:N	0.46	2.64	3	1
1:A:141:TYR:CE1	2:B:172:LEU:HD22	0.46	2.46	11	1
1:A:189:ASP:OD1	1:A:191:LYS:CB	0.46	2.64	2	1
1:A:214:ARG:NH2	2:B:168:LEU:HD21	0.46	2.26	4	1
2:B:200:ASP:N	2:B:200:ASP:OD1	0.46	2.49	9	1
2:B:169:GLY:CA	2:B:182:ASN:OD1	0.46	2.64	8	1
1:A:143:ARG:CG	1:A:143:ARG:HH11	0.46	2.24	13	2
1:A:170:TRP:CZ2	1:A:185:HIS:CB	0.46	2.99	15	2
1:A:196:LEU:HD11	1:A:213:ALA:HB2	0.46	1.88	9	2
1:A:166:ASP:CG	1:A:167:SER:N	0.45	2.74	1	1
1:A:170:TRP:NE1	1:A:183:ASN:OD1	0.45	2.48	8	1
1:A:134:ASP:OD1	2:B:158:ASN:ND2	0.45	2.47	15	1
1:A:166:ASP:C	1:A:168:ARG:N	0.45	2.74	8	6
1:A:137:GLU:HB3	2:B:174:LEU:HD11	0.45	1.87	6	2
1:A:188:LEU:CD2	1:A:189:ASP:H	0.45	2.24	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:207:ALA:O	1:A:208:ALA:C	0.45	2.59	7	2
1:A:211:VAL:HG21	2:B:212:GLY:CA	0.45	2.41	10	1
2:B:168:LEU:CD1	2:B:208:TRP:CH2	0.45	2.99	17	1
2:B:208:TRP:HA	2:B:211:LEU:HD12	0.45	1.88	8	5
1:A:164:GLY:O	1:A:165:ASP:C	0.45	2.60	7	1
1:A:145:LEU:HD13	2:B:165:TYR:CE1	0.45	2.47	10	2
1:A:142:GLU:OE1	1:A:148:ARG:NE	0.45	2.48	8	1
2:B:183:ARG:HH11	2:B:210:ARG:CZ	0.45	2.24	7	1
2:B:184:LYS:HZ3	2:B:213:LYS:C	0.45	2.19	15	1
1:A:217:LEU:HD22	1:A:217:LEU:H	0.45	1.70	18	1
1:A:206:LEU:O	1:A:206:LEU:CD2	0.45	2.62	2	2
2:B:176:ASN:N	2:B:176:ASN:HD22	0.45	2.07	4	1
1:A:214:ARG:HH12	2:B:208:TRP:CG	0.45	2.29	8	1
1:A:212:VAL:O	1:A:215:ASP:OD1	0.45	2.35	20	1
1:A:188:LEU:C	1:A:188:LEU:CD1	0.45	2.90	15	1
1:A:206:LEU:HD23	1:A:206:LEU:C	0.45	2.37	2	2
1:A:142:GLU:CD	1:A:148:ARG:HE	0.45	2.20	8	1
2:B:188:ASN:CG	2:B:189:ILE:H	0.45	2.20	15	2
1:A:210:LEU:HD13	2:B:168:LEU:HD23	0.45	1.89	10	1
1:A:145:LEU:CD1	2:B:165:TYR:CZ	0.45	2.99	11	1
1:A:188:LEU:O	1:A:189:ASP:CB	0.45	2.65	16	1
2:B:158:ASN:CG	2:B:159:ILE:N	0.45	2.75	19	2
1:A:145:LEU:O	1:A:146:GLN:C	0.44	2.59	13	20
2:B:156:ASN:OD1	2:B:156:ASN:N	0.44	2.49	13	1
1:A:188:LEU:O	1:A:189:ASP:CG	0.44	2.60	16	1
2:B:176:ASN:O	2:B:177:ASP:C	0.44	2.60	13	8
2:B:175:GLU:O	2:B:176:ASN:CG	0.44	2.60	6	4
1:A:137:GLU:HG3	2:B:174:LEU:HD11	0.44	1.88	19	3
1:A:188:LEU:HD22	1:A:188:LEU:H	0.44	1.72	11	1
1:A:190:PRO:O	1:A:191:LYS:C	0.44	2.60	2	10
1:A:172:GLU:CD	1:A:172:GLU:C	0.44	2.85	2	2
2:B:157:GLU:O	2:B:158:ASN:C	0.44	2.60	12	9
2:B:174:LEU:C	2:B:176:ASN:H	0.44	2.21	19	3
2:B:173:ASP:OD1	2:B:178:GLN:O	0.44	2.36	9	2
1:A:167:SER:C	1:A:168:ARG:CG	0.44	2.90	12	1
1:A:163:PHE:O	1:A:164:GLY:O	0.44	2.35	7	1
2:B:183:ARG:N	2:B:188:ASN:O	0.44	2.51	3	2
1:A:192:SER:O	1:A:193:ARG:C	0.44	2.60	16	4
1:A:141:TYR:O	2:B:165:TYR:OH	0.44	2.34	13	1
1:A:185:HIS:O	1:A:185:HIS:ND1	0.44	2.51	20	1
1:A:192:SER:CB	1:A:216:MET:SD	0.44	3.06	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:GLN:O	1:A:204:GLY:C	0.44	2.60	15	5
2:B:165:TYR:CD1	2:B:170:VAL:HG11	0.44	2.48	12	1
2:B:182:ASN:OD1	2:B:182:ASN:O	0.44	2.36	8	1
1:A:159:VAL:O	1:A:172:GLU:OE1	0.44	2.36	12	1
2:B:212:GLY:O	2:B:213:LYS:C	0.43	2.61	2	1
2:B:172:LEU:O	2:B:173:ASP:OD1	0.43	2.36	6	1
2:B:183:ARG:O	2:B:184:LYS:O	0.43	2.36	15	2
2:B:183:ARG:HH12	2:B:210:ARG:C	0.43	2.21	19	1
1:A:146:GLN:OE1	1:A:164:GLY:C	0.43	2.62	3	1
2:B:160:LEU:HD23	2:B:160:LEU:C	0.43	2.39	3	1
1:A:164:GLY:O	1:A:165:ASP:CG	0.43	2.62	11	1
2:B:175:GLU:C	2:B:176:ASN:CG	0.43	2.86	14	2
1:A:149:VAL:CG2	2:B:161:LYS:HZ3	0.43	2.26	17	1
1:A:134:ASP:OD2	2:B:158:ASN:OD1	0.43	2.36	6	1
2:B:173:ASP:O	2:B:173:ASP:OD2	0.43	2.37	9	1
2:B:192:LEU:HD23	2:B:193:PRO:HD2	0.43	1.90	18	3
2:B:169:GLY:O	2:B:182:ASN:OD1	0.43	2.36	8	1
2:B:171:ILE:HD11	2:B:182:ASN:ND2	0.43	2.29	9	1
1:A:137:GLU:CD	1:A:141:TYR:OH	0.43	2.61	14	3
1:A:205:ASP:OD1	1:A:207:ALA:N	0.43	2.48	4	1
2:B:210:ARG:O	2:B:213:LYS:OXT	0.43	2.36	11	1
1:A:187:ALA:O	1:A:220:SER:OG	0.43	2.35	6	1
2:B:192:LEU:C	2:B:192:LEU:CD2	0.43	2.92	13	2
1:A:183:ASN:N	1:A:193:ARG:HH21	0.43	2.12	2	1
1:A:196:LEU:C	1:A:196:LEU:CD1	0.43	2.92	8	1
1:A:191:LYS:O	1:A:192:SER:C	0.43	2.62	17	1
1:A:142:GLU:O	1:A:143:ARG:C	0.43	2.62	2	2
2:B:183:ARG:HH22	2:B:210:ARG:NH2	0.43	2.11	9	1
1:A:211:VAL:HG21	2:B:212:GLY:HA3	0.43	1.89	10	2
1:A:189:ASP:OD2	1:A:189:ASP:O	0.43	2.37	15	1
1:A:137:GLU:OE2	2:B:174:LEU:HD21	0.43	2.14	16	1
1:A:138:VAL:O	1:A:142:GLU:OE1	0.43	2.37	16	1
1:A:144:LEU:HD22	2:B:204:THR:CG2	0.43	2.43	17	1
1:A:145:LEU:CD2	1:A:214:ARG:HH21	0.43	2.24	4	1
1:A:193:ARG:O	1:A:197:GLU:OE1	0.43	2.37	7	1
2:B:175:GLU:O	2:B:176:ASN:OD1	0.43	2.37	7	1
2:B:188:ASN:OD1	2:B:189:ILE:N	0.43	2.50	16	2
1:A:215:ASP:O	1:A:215:ASP:OD1	0.43	2.37	11	1
2:B:164:LEU:C	2:B:164:LEU:CD2	0.43	2.92	14	1
1:A:166:ASP:OD1	1:A:167:SER:N	0.42	2.47	14	3
1:A:208:ALA:O	1:A:212:VAL:CG2	0.42	2.66	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:215:ASP:OD1	2:B:209:GLU:OE2	0.42	2.37	14	2
1:A:171:ILE:C	1:A:172:GLU:OE1	0.42	2.62	14	1
1:A:163:PHE:O	1:A:166:ASP:OD1	0.42	2.37	3	1
1:A:203:GLN:O	1:A:205:ASP:N	0.42	2.52	15	1
2:B:211:LEU:O	2:B:212:GLY:C	0.42	2.61	8	1
1:A:221:LEU:OXT	1:A:221:LEU:HG	0.42	2.13	19	1
2:B:159:ILE:CG1	2:B:160:LEU:N	0.42	2.82	7	1
2:B:200:ASP:OD1	2:B:201:PHE:CD2	0.42	2.73	14	1
2:B:170:VAL:HG22	2:B:181:ILE:HG23	0.42	1.89	16	1
1:A:172:GLU:OE1	1:A:183:ASN:CG	0.42	2.63	18	1
1:A:188:LEU:C	1:A:189:ASP:CG	0.42	2.88	19	1
2:B:210:ARG:O	2:B:211:LEU:C	0.42	2.63	20	1
1:A:209:PHE:O	1:A:210:LEU:C	0.42	2.62	6	1
1:A:166:ASP:C	1:A:167:SER:OG	0.42	2.62	7	2
1:A:164:GLY:O	1:A:165:ASP:OD1	0.42	2.37	11	1
2:B:207:ILE:CD1	2:B:208:TRP:NE1	0.42	2.83	13	1
1:A:172:GLU:OE1	1:A:172:GLU:C	0.42	2.62	3	1
2:B:176:ASN:C	2:B:177:ASP:CG	0.42	2.88	10	1
1:A:188:LEU:O	1:A:189:ASP:C	0.42	2.63	15	1
2:B:157:GLU:O	2:B:160:LEU:N	0.42	2.53	19	1
1:A:145:LEU:HD22	2:B:208:TRP:CZ2	0.42	2.50	3	1
1:A:172:GLU:OE1	1:A:172:GLU:N	0.42	2.52	14	1
1:A:189:ASP:O	1:A:192:SER:OG	0.42	2.37	6	1
1:A:193:ARG:CZ	1:A:193:ARG:CB	0.41	2.97	5	1
2:B:181:ILE:CG2	2:B:211:LEU:HD11	0.41	2.45	12	3
2:B:176:ASN:CG	2:B:176:ASN:O	0.41	2.62	18	1
1:A:169:CYS:SG	1:A:185:HIS:O	0.41	2.71	10	1
2:B:210:ARG:O	2:B:213:LYS:O	0.41	2.37	20	1
2:B:194:LEU:HD23	2:B:194:LEU:C	0.41	2.39	10	1
2:B:200:ASP:OD1	2:B:200:ASP:N	0.41	2.52	11	1
1:A:189:ASP:OD1	1:A:189:ASP:C	0.41	2.61	2	1
2:B:201:PHE:O	2:B:204:THR:OG1	0.41	2.37	11	1
2:B:189:ILE:O	2:B:189:ILE:HG23	0.41	2.15	5	2
1:A:134:ASP:OD1	1:A:134:ASP:N	0.41	2.52	8	1
1:A:172:GLU:O	1:A:173:VAL:HG23	0.41	2.15	14	1
1:A:164:GLY:C	1:A:165:ASP:O	0.41	2.64	15	1
2:B:162:LEU:HD23	2:B:162:LEU:H	0.41	1.69	18	1
2:B:189:ILE:O	2:B:190:ASP:OD1	0.41	2.39	18	1
1:A:220:SER:O	1:A:221:LEU:C	0.41	2.62	6	1
1:A:146:GLN:OE1	2:B:201:PHE:CE1	0.41	2.74	7	1
1:A:166:ASP:O	1:A:167:SER:OG	0.41	2.36	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:GLU:CG	1:A:183:ASN:H	0.41	2.29	17	1
1:A:192:SER:OG	1:A:216:MET:CG	0.41	2.69	18	1
1:A:173:VAL:O	1:A:173:VAL:HG13	0.41	2.15	19	1
1:A:172:GLU:C	1:A:172:GLU:OE2	0.41	2.64	2	1
1:A:141:TYR:CE1	2:B:172:LEU:HD13	0.41	2.51	5	1
1:A:163:PHE:O	1:A:164:GLY:C	0.41	2.63	7	2
2:B:168:LEU:HD13	2:B:168:LEU:O	0.41	2.15	8	1
1:A:165:ASP:OD2	1:A:169:CYS:SG	0.41	2.79	18	1
1:A:221:LEU:OXT	1:A:221:LEU:CG	0.41	2.69	19	1
2:B:182:ASN:O	2:B:211:LEU:HD23	0.41	2.16	2	1
1:A:163:PHE:CG	1:A:217:LEU:CD1	0.41	3.04	10	1
2:B:176:ASN:ND2	2:B:178:GLN:CB	0.41	2.84	10	1
1:A:151:PRO:O	1:A:152:GLY:O	0.41	2.39	12	1
1:A:215:ASP:OD1	1:A:215:ASP:C	0.41	2.63	20	1
1:A:210:LEU:HD23	1:A:210:LEU:C	0.41	2.41	7	1
1:A:170:TRP:CZ3	1:A:185:HIS:ND1	0.41	2.89	18	2
1:A:206:LEU:HD22	2:B:167:SER:CB	0.41	2.46	17	1
1:A:165:ASP:CG	1:A:166:ASP:H	0.40	2.23	12	1
1:A:170:TRP:CH2	1:A:185:HIS:CB	0.40	3.04	5	1
1:A:166:ASP:HB3	1:A:221:LEU:HD11	0.40	1.93	16	1
1:A:165:ASP:C	1:A:165:ASP:OD1	0.40	2.63	3	1
1:A:165:ASP:OD2	1:A:217:LEU:HD21	0.40	2.16	20	1
2:B:158:ASN:O	2:B:159:ILE:C	0.40	2.63	5	1
1:A:149:VAL:O	1:A:150:LEU:HD22	0.40	2.17	11	1
1:A:218:LEU:N	1:A:218:LEU:CD1	0.40	2.85	18	1
2:B:204:THR:O	2:B:208:TRP:CD2	0.40	2.75	18	1
1:A:140:LEU:HG	2:B:174:LEU:HD21	0.40	1.93	18	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	73/98 (74%)	62±2 (85±2%)	6±2 (8±2%)	5±1 (7±2%)	2	17
2	B	49/77 (64%)	42±2 (86±3%)	4±1 (9±3%)	2±1 (4±1%)	3	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2440/3500 (70%)	2087 (86%)	212 (9%)	141 (6%)	2	20

All 20 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	186	PRO	20
2	B	176	ASN	20
1	A	187	ALA	19
1	A	168	ARG	18
1	A	166	ASP	9
2	B	157	GLU	9
1	A	167	SER	9
1	A	165	ASP	7
1	A	206	LEU	5
2	B	188	ASN	5
2	B	184	LYS	4
2	B	199	SER	4
1	A	152	GLY	3
1	A	164	GLY	2
1	A	188	LEU	2
1	A	189	ASP	1
1	A	191	LYS	1
1	A	192	SER	1
1	A	173	VAL	1
2	B	189	ILE	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	62/78 (79%)	49±2 (80±4%)	13±2 (20±4%)	3	32
2	B	49/71 (69%)	39±2 (80±5%)	10±2 (20±5%)	3	32
All	All	2220/2980 (74%)	1771 (80%)	449 (20%)	3	32

All 73 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	209	PHE	20
2	B	171	ILE	20
2	B	181	ILE	20
1	A	189	ASP	18
1	A	200	LEU	18
2	B	170	VAL	16
1	A	193	ARG	16
2	B	168	LEU	15
2	B	207	ILE	14
1	A	148	ARG	14
2	B	192	LEU	13
2	B	204	THR	12
1	A	140	LEU	11
1	A	217	LEU	11
1	A	167	SER	11
2	B	172	LEU	10
2	B	191	ILE	9
1	A	169	CYS	9
1	A	188	LEU	8
1	A	166	ASP	8
1	A	221	LEU	8
2	B	165	TYR	7
1	A	192	SER	7
1	A	210	LEU	7
2	B	159	ILE	7
1	A	159	VAL	6
1	A	201	THR	6
2	B	199	SER	6
1	A	147	LEU	6
1	A	137	GLU	5
1	A	146	GLN	5
1	A	196	LEU	5
2	B	179	VAL	5
2	B	176	ASN	5
1	A	184	SER	5
1	A	173	VAL	5
1	A	172	GLU	4
2	B	180	LEU	4
2	B	156	ASN	4
1	A	158	ASP	4
2	B	162	LEU	4
1	A	168	ARG	4
1	A	206	LEU	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	167	SER	4
1	A	183	ASN	3
1	A	220	SER	3
2	B	164	LEU	3
1	A	165	ASP	3
2	B	194	LEU	3
1	A	162	VAL	3
1	A	216	MET	2
2	B	160	LEU	2
2	B	173	ASP	2
1	A	143	ARG	2
1	A	198	HIS	2
2	B	188	ASN	2
1	A	138	VAL	2
2	B	177	ASP	2
2	B	175	GLU	1
2	B	161	LYS	1
1	A	149	VAL	1
1	A	144	LEU	1
1	A	197	GLU	1
2	B	178	GLN	1
1	A	145	LEU	1
2	B	183	ARG	1
2	B	184	LYS	1
1	A	142	GLU	1
2	B	203	LYS	1
1	A	214	ARG	1
2	B	163	LYS	1
2	B	158	ASN	1
2	B	210	ARG	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 [i](#)

There are no oligosaccharides 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

No chemical shift data were provided