



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 10:57 PM BST

PDB ID : 2K7A
Title : Ensemble Structures of the binary complex between the SH3 and SH2 domain of interleukin-2 tyrosine kinase.
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Deposited on : 2008-08-08

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

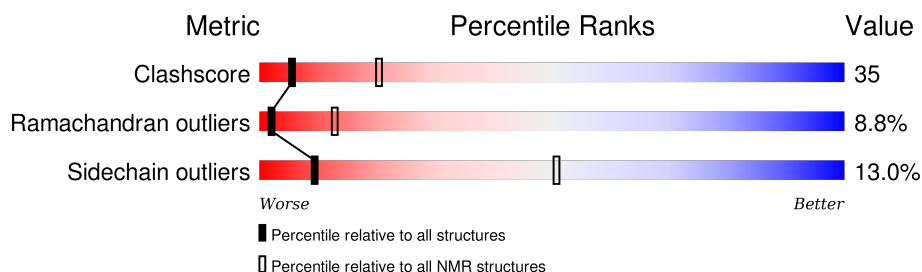
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	63	
2	B	110	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 6 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:171-A:184, A:188-A:231, B:232-B:297, B:302-B:339 (162)	0.48	6

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2749 atoms, of which 1345 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SH3 domain of Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms						Trace
1	A	63	Total	C	H	N	O	S	0
			993	328	473	82	109	1	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	GLY	-	EXPRESSION TAG	UNP Q03526
A	170	SER	-	EXPRESSION TAG	UNP Q03526

- Molecule 2 is a protein called SH2 domain of Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms						Trace
2	B	108	Total	C	H	N	O	S	0
			1756	565	872	150	166	3	

There are 3 discrepancies between the modelled and reference sequences:

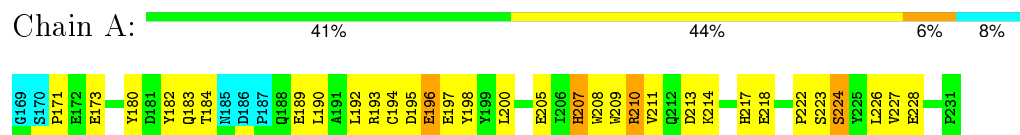
Chain	Residue	Modelled	Actual	Comment	Reference
B	230	GLY	-	EXPRESSION TAG	UNP Q03526
B	231	SER	-	EXPRESSION TAG	UNP Q03526
B	339	GLY	-	EXPRESSION TAG	UNP Q03526

4 Residue-property plots

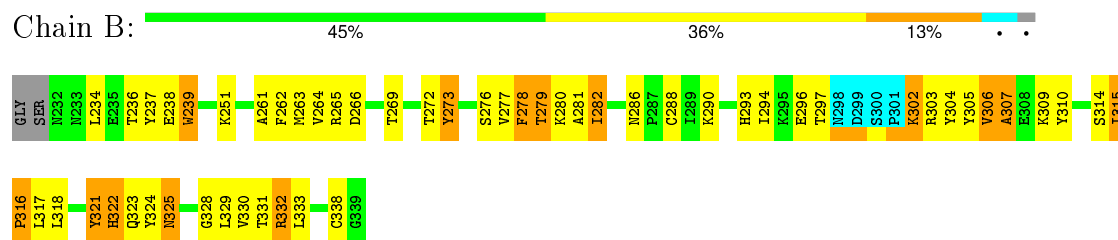
4.1 Average score per residue in the NMR ensemble

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: SH3 domain of Tyrosine-protein kinase ITK/TSK



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

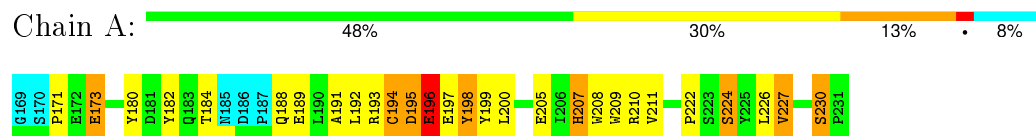


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

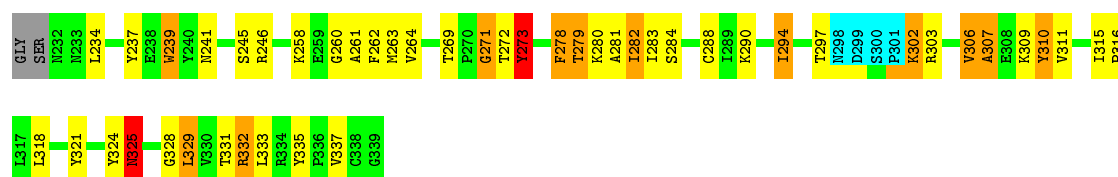
4.2.1 Score per residue for model 1

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK





4.2.2 Score per residue for model 2

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK



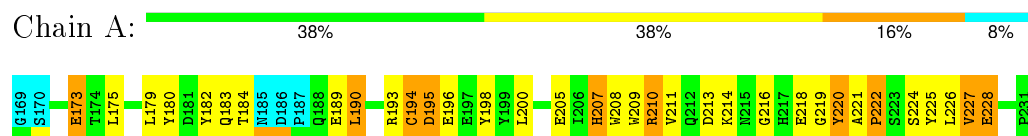
4.2.3 Score per residue for model 3

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

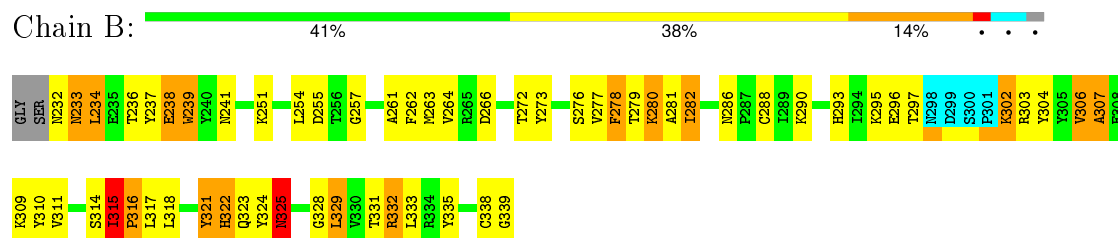


- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK



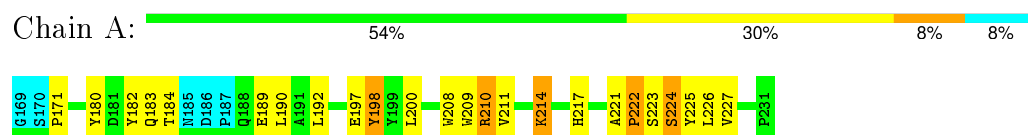


- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

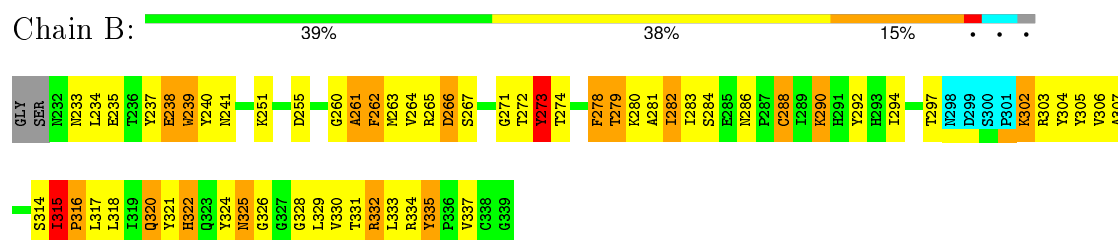


4.2.5 Score per residue for model 5

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

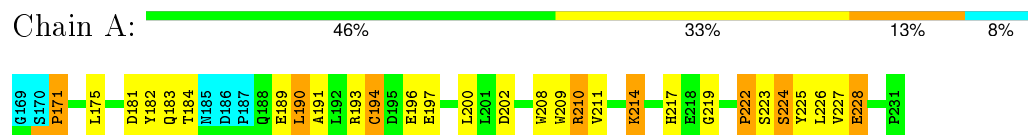


- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK



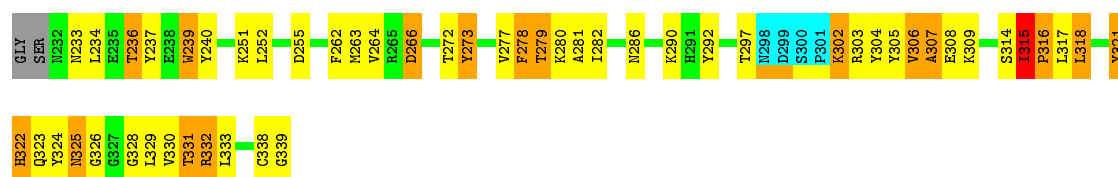
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK



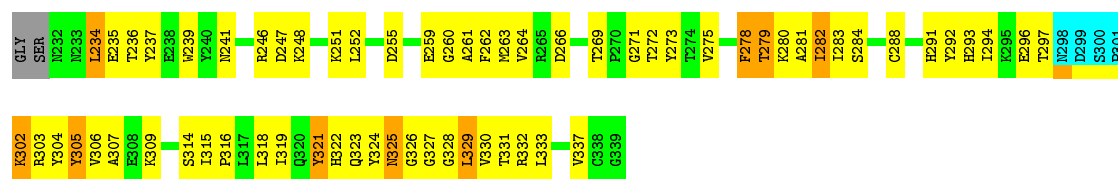


4.2.7 Score per residue for model 7

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

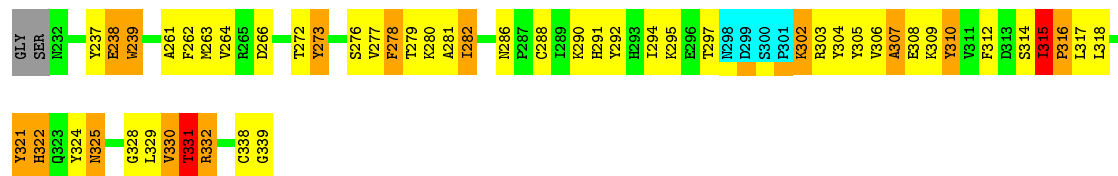


4.2.8 Score per residue for model 8

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

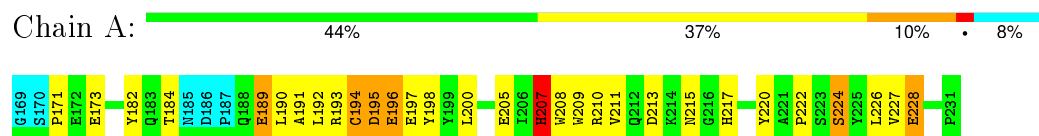


- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

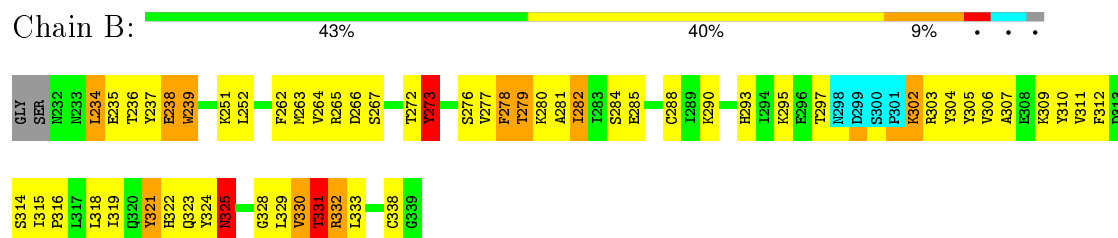


4.2.9 Score per residue for model 9

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

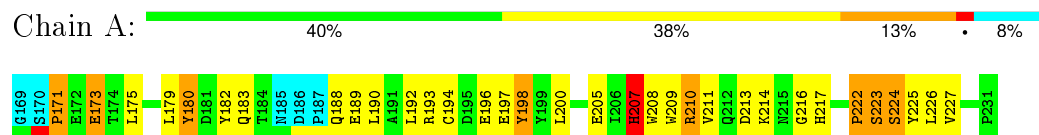


- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

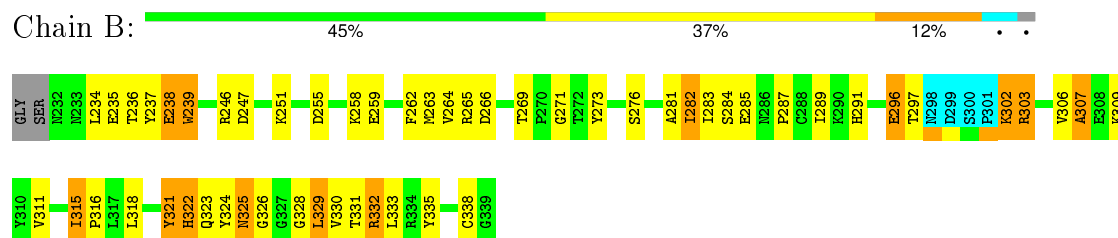


4.2.10 Score per residue for model 10

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

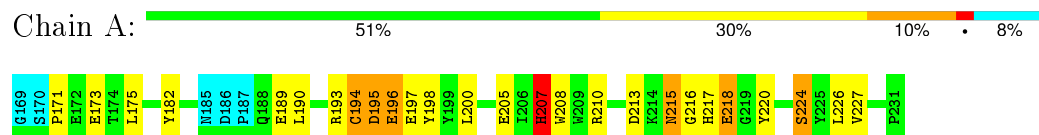


- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK



4.2.11 Score per residue for model 11

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK



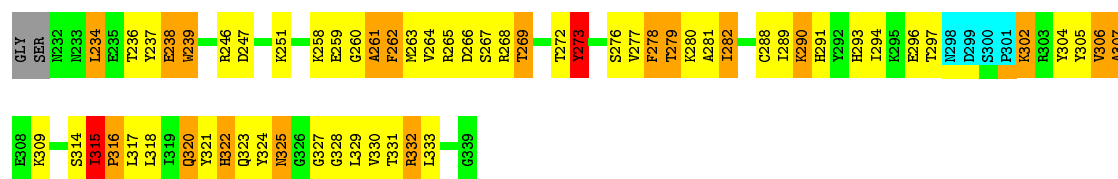


4.2.12 Score per residue for model 12

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

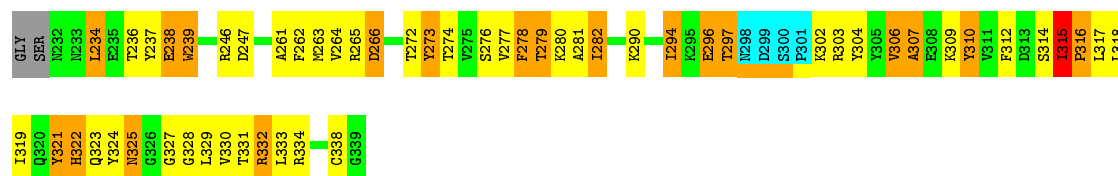


4.2.13 Score per residue for model 13

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

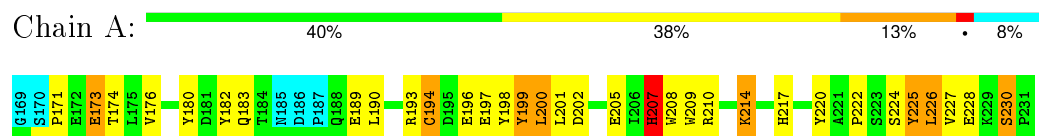


- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

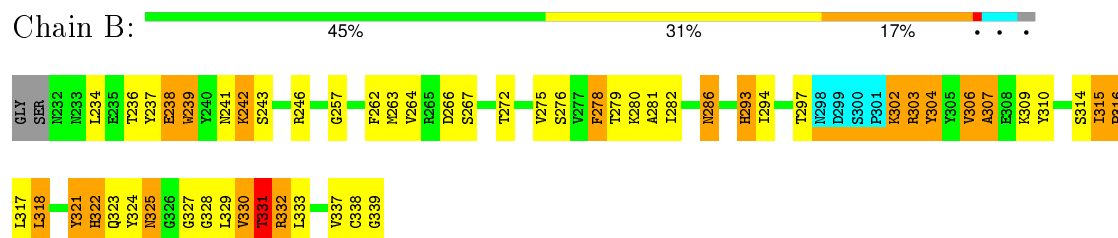


4.2.14 Score per residue for model 14

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

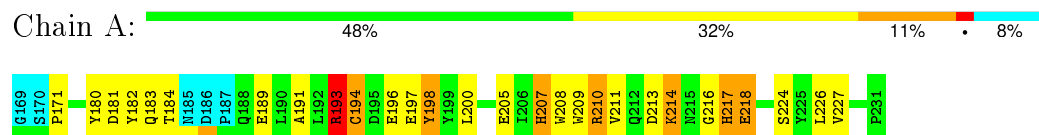


- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

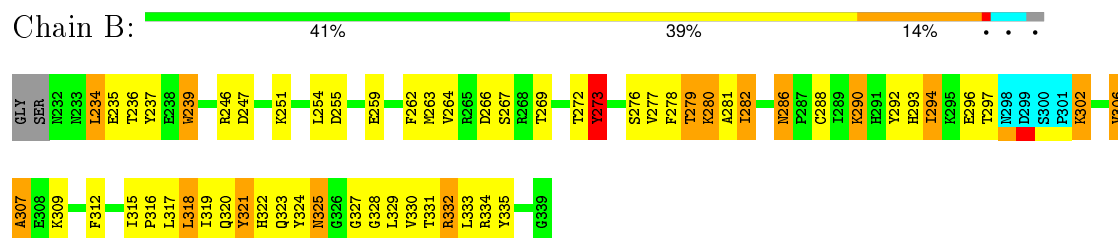


4.2.15 Score per residue for model 15

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

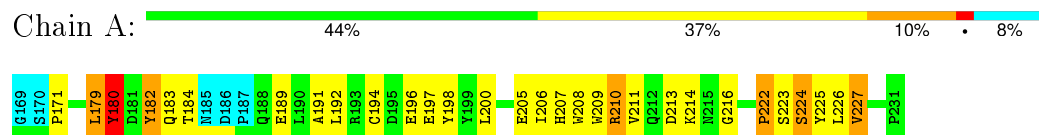


- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK



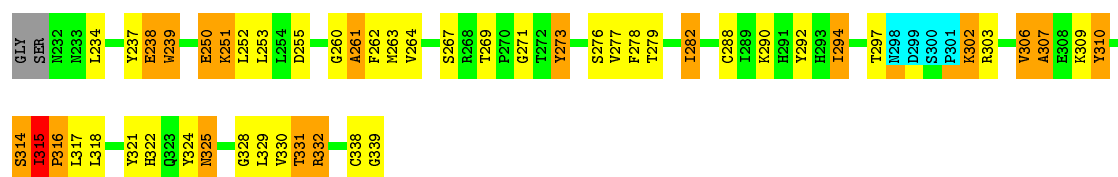
4.2.16 Score per residue for model 16

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK



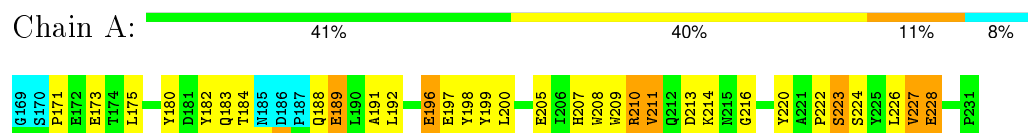
- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK



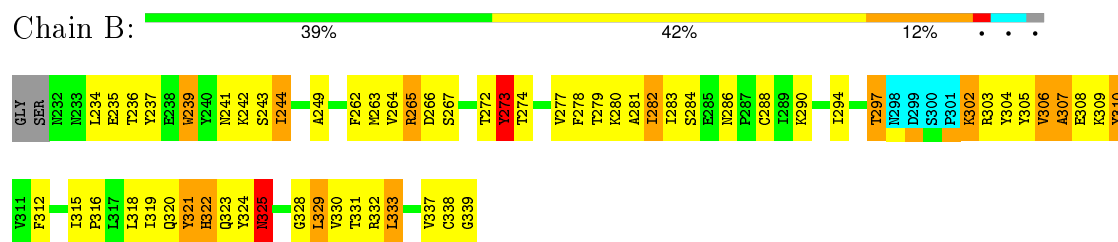


4.2.17 Score per residue for model 17

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

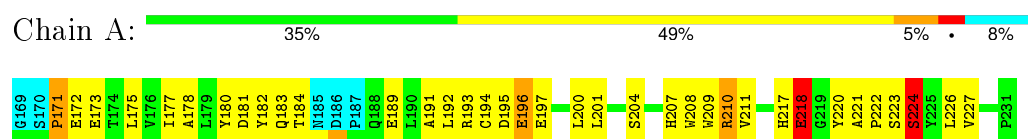


- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

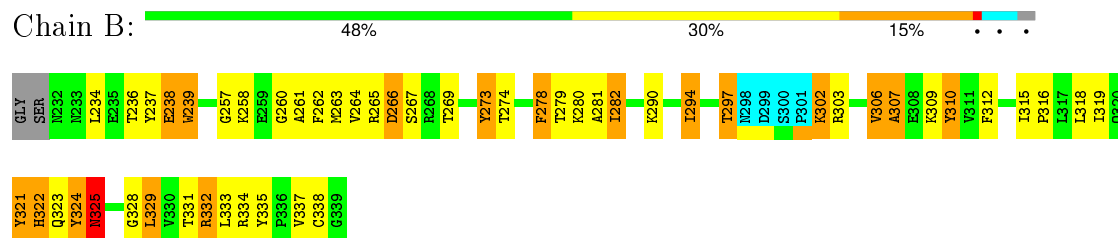


4.2.18 Score per residue for model 18

- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK



4.2.19 Score per residue for model 19

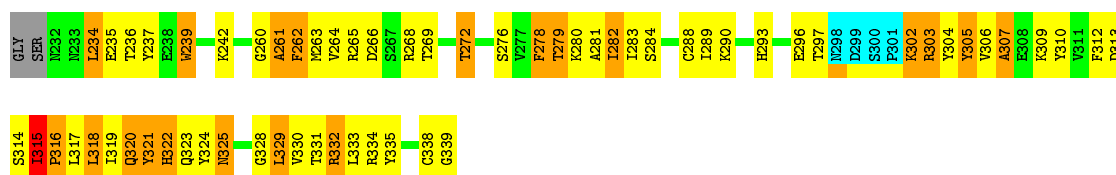
- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

Chain A: 



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

Chain B: 



4.2.20 Score per residue for model 20

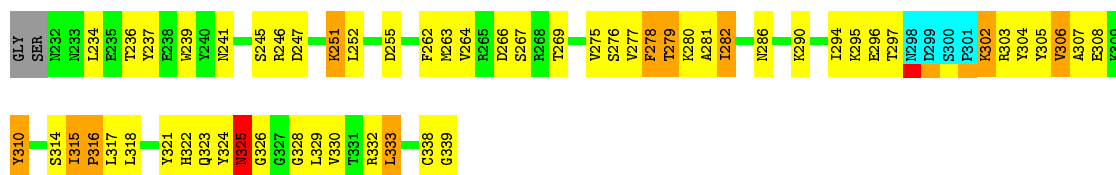
- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

Chain A: 



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

Chain B: 



5 Refinement protocol and experimental data overview

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

Of the 60 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
xplor-nih	refinement	2.19

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)	BMRB entry 16809
Number of chemical shift lists	2
Total number of shifts	3776
Number of shifts mapped to atoms	3776
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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	487	446	446	36±6
2	B	855	850	848	62±6
All	All	26840	25920	25880	1871

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:277:VAL:HG21	2:B:292:TYR:CE2	0.91	2.00	15	1
2:B:277:VAL:HG21	2:B:292:TYR:CD2	0.90	2.00	15	1
1:A:175:LEU:O	1:A:176:VAL:HG13	0.86	1.71	20	2
2:B:292:TYR:CD2	2:B:329:LEU:HD22	0.84	2.06	15	3
1:A:224:SER:OG	2:B:330:VAL:HG21	0.81	1.75	15	8
1:A:224:SER:OG	2:B:330:VAL:HG11	0.80	1.76	11	5
1:A:222:PRO:O	1:A:226:LEU:HD13	0.79	1.77	17	3
1:A:209:TRP:O	1:A:210:ARG:O	0.76	2.04	12	12
1:A:208:TRP:HE1	2:B:328:GLY:C	0.76	1.84	2	19
2:B:318:LEU:HD23	2:B:318:LEU:O	0.76	1.80	9	5
2:B:324:TYR:CD2	2:B:325:ASN:ND2	0.75	2.55	18	3
1:A:194:CYS:O	1:A:195:ASP:CB	0.74	2.35	9	6
2:B:306:VAL:HG13	2:B:306:VAL:O	0.73	1.83	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:321:TYR:CE2	2:B:322:HIS:CD2	0.73	2.77	15	2
1:A:226:LEU:O	1:A:227:VAL:HG13	0.73	1.83	17	16
2:B:318:LEU:O	2:B:318:LEU:HD23	0.72	1.84	8	12
2:B:314:SER:O	2:B:316:PRO:N	0.72	2.23	12	11
1:A:222:PRO:O	1:A:226:LEU:HD12	0.72	1.83	20	12
2:B:330:VAL:HG22	2:B:330:VAL:O	0.72	1.82	14	3
2:B:306:VAL:O	2:B:306:VAL:HG13	0.72	1.85	17	1
1:A:208:TRP:CE2	2:B:329:LEU:O	0.71	2.43	7	5
1:A:179:LEU:HD23	1:A:225:TYR:O	0.71	1.84	4	2
2:B:306:VAL:O	2:B:306:VAL:HG23	0.71	1.86	2	7
1:A:201:LEU:N	1:A:201:LEU:HD12	0.71	2.01	13	1
1:A:180:TYR:CZ	1:A:225:TYR:CG	0.71	2.79	16	1
2:B:330:VAL:O	2:B:330:VAL:HG22	0.70	1.84	11	1
1:A:209:TRP:O	1:A:211:VAL:HG13	0.70	1.85	7	3
1:A:194:CYS:O	1:A:195:ASP:CG	0.70	2.29	9	4
2:B:306:VAL:HG23	2:B:306:VAL:O	0.70	1.87	1	4
1:A:208:TRP:CZ2	2:B:329:LEU:O	0.69	2.45	5	10
2:B:263:MET:HG3	2:B:264:VAL:H	0.68	1.46	1	14
1:A:180:TYR:CD2	1:A:225:TYR:CE1	0.68	2.81	16	1
2:B:325:ASN:N	2:B:325:ASN:ND2	0.68	2.41	18	4
2:B:263:MET:CG	2:B:264:VAL:H	0.68	2.01	17	9
2:B:273:TYR:H	2:B:294:ILE:HD11	0.67	1.49	18	3
1:A:210:ARG:O	1:A:211:VAL:HG13	0.67	1.90	5	8
2:B:291:HIS:O	2:B:292:TYR:CD1	0.66	2.49	8	2
1:A:180:TYR:CE2	1:A:225:TYR:CD1	0.66	2.84	16	1
1:A:190:LEU:HD22	1:A:217:HIS:O	0.66	1.91	10	1
2:B:306:VAL:O	2:B:307:ALA:HB3	0.66	1.91	9	3
2:B:324:TYR:CG	2:B:325:ASN:ND2	0.66	2.64	9	3
2:B:241:ASN:ND2	2:B:263:MET:SD	0.65	2.70	14	4
1:A:180:TYR:CE2	1:A:225:TYR:CE1	0.65	2.84	16	1
1:A:208:TRP:HE1	2:B:328:GLY:CA	0.65	2.04	15	12
2:B:325:ASN:ND2	2:B:325:ASN:N	0.65	2.44	2	1
2:B:315:ILE:HD12	2:B:315:ILE:H	0.65	1.52	14	2
1:A:182:TYR:CE1	1:A:183:GLN:O	0.64	2.51	7	6
1:A:196:GLU:OE1	1:A:196:GLU:N	0.64	2.30	3	3
1:A:198:TYR:N	1:A:198:TYR:CD1	0.64	2.65	15	5
1:A:180:TYR:CZ	1:A:225:TYR:CD1	0.64	2.86	16	1
2:B:306:VAL:HG22	2:B:318:LEU:HD11	0.64	1.70	3	10
2:B:315:ILE:N	2:B:315:ILE:HD13	0.64	2.07	10	1
1:A:192:LEU:HD22	1:A:198:TYR:OH	0.64	1.93	1	1
1:A:206:ILE:N	1:A:206:ILE:HD12	0.64	2.08	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:273:TYR:N	2:B:273:TYR:CD1	0.64	2.65	17	6
2:B:273:TYR:CD1	2:B:273:TYR:N	0.63	2.65	9	9
1:A:184:THR:OG1	1:A:191:ALA:N	0.63	2.31	17	9
2:B:315:ILE:O	2:B:317:LEU:N	0.63	2.32	19	11
2:B:318:LEU:HD21	2:B:322:HIS:CE1	0.63	2.28	3	2
2:B:263:MET:CG	2:B:264:VAL:N	0.63	2.62	17	20
1:A:215:ASN:ND2	1:A:217:HIS:NE2	0.63	2.46	11	1
2:B:315:ILE:N	2:B:316:PRO:CD	0.63	2.61	9	9
2:B:304:TYR:CD1	2:B:304:TYR:N	0.63	2.63	3	4
2:B:306:VAL:HG12	2:B:318:LEU:HD11	0.62	1.71	16	2
1:A:180:TYR:CD1	1:A:180:TYR:N	0.62	2.66	16	6
1:A:193:ARG:O	1:A:196:GLU:HB3	0.62	1.95	3	5
2:B:279:THR:HG23	2:B:279:THR:O	0.62	1.93	8	1
1:A:214:LYS:H	1:A:214:LYS:HZ3	0.62	1.36	10	2
2:B:278:PHE:CD1	2:B:279:THR:N	0.62	2.67	8	19
2:B:237:TYR:CG	2:B:239:TRP:CZ2	0.62	2.87	17	20
2:B:324:TYR:N	2:B:324:TYR:CD1	0.62	2.67	9	2
2:B:322:HIS:CE1	2:B:328:GLY:H	0.62	2.12	10	3
2:B:328:GLY:O	2:B:329:LEU:HD22	0.62	1.94	17	2
1:A:198:TYR:CD1	1:A:198:TYR:N	0.62	2.68	10	2
2:B:310:TYR:N	2:B:310:TYR:CD1	0.62	2.68	2	8
1:A:175:LEU:HD12	1:A:175:LEU:N	0.62	2.10	17	3
1:A:223:SER:H	2:B:330:VAL:HG12	0.62	1.53	2	1
2:B:324:TYR:CE2	2:B:325:ASN:ND2	0.61	2.68	9	3
2:B:282:ILE:HD12	2:B:288:CYS:SG	0.61	2.36	5	10
2:B:310:TYR:CD1	2:B:310:TYR:N	0.61	2.69	1	3
1:A:179:LEU:HD21	1:A:227:VAL:CG2	0.61	2.24	4	1
1:A:228:GLU:N	1:A:228:GLU:CD	0.61	2.54	9	2
2:B:244:ILE:HG21	2:B:265:ARG:NE	0.61	2.11	17	1
2:B:333:LEU:H	2:B:333:LEU:HD12	0.61	1.55	17	1
2:B:266:ASP:OD1	2:B:266:ASP:N	0.61	2.34	6	2
2:B:306:VAL:O	2:B:307:ALA:HB2	0.61	1.95	11	12
1:A:228:GLU:CD	1:A:228:GLU:N	0.61	2.53	20	3
2:B:322:HIS:CE1	2:B:329:LEU:HD23	0.61	2.31	11	5
1:A:184:THR:OG1	1:A:191:ALA:HB2	0.60	1.96	13	2
2:B:322:HIS:CE1	2:B:328:GLY:N	0.60	2.69	10	2
2:B:292:TYR:OH	2:B:330:VAL:HG12	0.60	1.97	15	1
2:B:333:LEU:HD12	2:B:333:LEU:H	0.60	1.57	11	3
1:A:197:GLU:O	1:A:198:TYR:CD1	0.60	2.54	3	5
1:A:182:TYR:CD1	1:A:183:GLN:N	0.60	2.70	3	3
2:B:240:TYR:CE1	2:B:266:ASP:OD1	0.60	2.55	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:190:LEU:HD21	1:A:217:HIS:O	0.60	1.97	14	7
2:B:315:ILE:HB	2:B:316:PRO:CD	0.59	2.27	12	11
1:A:199:TYR:CE2	1:A:214:LYS:NZ	0.59	2.67	2	1
1:A:175:LEU:C	1:A:176:VAL:HG22	0.59	2.17	20	2
1:A:192:LEU:HD11	1:A:222:PRO:HD2	0.59	1.75	7	6
2:B:273:TYR:N	2:B:294:ILE:HD11	0.59	2.12	13	5
2:B:324:TYR:O	2:B:326:GLY:N	0.59	2.36	3	5
1:A:174:THR:HG23	1:A:175:LEU:N	0.59	2.12	20	1
2:B:321:TYR:CE2	2:B:322:HIS:NE2	0.58	2.71	15	1
2:B:325:ASN:HD22	2:B:325:ASN:N	0.58	1.95	18	4
1:A:196:GLU:OE1	1:A:198:TYR:CE1	0.58	2.57	17	3
1:A:182:TYR:CD2	1:A:183:GLN:N	0.58	2.71	14	6
2:B:237:TYR:CD2	2:B:239:TRP:CZ2	0.58	2.91	20	14
2:B:288:CYS:SG	2:B:290:LYS:NZ	0.58	2.76	5	1
1:A:199:TYR:O	1:A:211:VAL:HG12	0.58	1.99	17	2
1:A:208:TRP:NE1	2:B:328:GLY:C	0.58	2.57	14	5
2:B:282:ILE:HD12	2:B:288:CYS:CB	0.58	2.29	8	10
2:B:307:ALA:HB2	2:B:328:GLY:O	0.58	1.99	7	1
2:B:297:THR:OG1	2:B:297:THR:O	0.57	2.19	13	2
1:A:193:ARG:O	1:A:195:ASP:N	0.57	2.37	9	3
2:B:279:THR:O	2:B:281:ALA:N	0.57	2.38	7	15
1:A:205:GLU:OE1	1:A:207:HIS:NE2	0.57	2.38	8	14
2:B:297:THR:O	2:B:302:LYS:O	0.57	2.22	1	9
1:A:182:TYR:CZ	1:A:183:GLN:O	0.57	2.58	10	8
2:B:321:TYR:CZ	2:B:326:GLY:O	0.57	2.57	20	2
1:A:214:LYS:H	1:A:214:LYS:NZ	0.57	1.98	10	1
1:A:178:ALA:HB3	1:A:196:GLU:OE2	0.57	2.00	3	1
1:A:182:TYR:CG	1:A:183:GLN:N	0.57	2.73	20	10
1:A:224:SER:CB	2:B:330:VAL:HG21	0.57	2.29	7	5
1:A:194:CYS:C	1:A:196:GLU:H	0.56	2.03	18	7
1:A:189:GLU:OE1	1:A:208:TRP:CZ3	0.56	2.58	14	5
1:A:193:ARG:O	1:A:194:CYS:C	0.56	2.42	3	9
2:B:314:SER:O	2:B:315:ILE:C	0.56	2.43	8	11
2:B:310:TYR:CE1	2:B:321:TYR:OH	0.56	2.55	16	3
1:A:196:GLU:OE1	1:A:197:GLU:N	0.56	2.39	7	3
2:B:315:ILE:O	2:B:318:LEU:N	0.56	2.25	13	8
1:A:210:ARG:NE	1:A:220:TYR:CZ	0.56	2.74	11	1
2:B:321:TYR:O	2:B:325:ASN:ND2	0.56	2.39	20	5
2:B:321:TYR:HH	2:B:322:HIS:CE1	0.56	2.18	2	4
1:A:205:GLU:OE1	1:A:207:HIS:CD2	0.56	2.59	9	2
1:A:175:LEU:N	1:A:175:LEU:HD12	0.56	2.16	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:233:ASN:C	2:B:235:GLU:H	0.56	2.04	5	1
2:B:258:LYS:NZ	2:B:335:TYR:CZ	0.56	2.73	1	1
2:B:315:ILE:HD13	2:B:315:ILE:N	0.56	2.16	3	1
2:B:324:TYR:CD1	2:B:324:TYR:N	0.56	2.74	2	2
1:A:195:ASP:O	1:A:196:GLU:O	0.55	2.24	3	4
1:A:182:TYR:CE2	1:A:183:GLN:O	0.55	2.59	15	7
1:A:196:GLU:OE1	1:A:198:TYR:CZ	0.55	2.59	16	4
2:B:324:TYR:CG	2:B:325:ASN:N	0.55	2.75	1	3
2:B:324:TYR:O	2:B:325:ASN:C	0.55	2.45	3	20
1:A:214:LYS:CE	1:A:214:LYS:H	0.55	2.15	10	2
1:A:189:GLU:N	1:A:189:GLU:OE1	0.55	2.39	15	2
1:A:175:LEU:O	1:A:176:VAL:CG1	0.55	2.51	20	2
2:B:297:THR:O	2:B:297:THR:HG23	0.55	2.00	11	1
2:B:329:LEU:HD11	2:B:333:LEU:CD1	0.55	2.32	5	3
1:A:197:GLU:O	1:A:214:LYS:CE	0.55	2.54	6	4
1:A:180:TYR:HD1	1:A:180:TYR:N	0.55	1.99	16	1
2:B:266:ASP:N	2:B:266:ASP:OD1	0.55	2.39	18	2
2:B:297:THR:HG22	2:B:303:ARG:O	0.55	2.02	18	1
2:B:277:VAL:N	2:B:290:LYS:O	0.55	2.39	16	10
1:A:194:CYS:O	1:A:195:ASP:HB2	0.55	2.00	9	1
2:B:330:VAL:CG2	2:B:330:VAL:O	0.55	2.55	14	3
2:B:250:GLU:O	2:B:253:LEU:N	0.54	2.38	16	1
2:B:304:TYR:N	2:B:304:TYR:CD1	0.54	2.67	14	7
2:B:306:VAL:O	2:B:307:ALA:CB	0.54	2.55	9	12
2:B:304:TYR:CG	2:B:315:ILE:HD13	0.54	2.37	5	1
2:B:306:VAL:O	2:B:306:VAL:CG1	0.54	2.55	16	1
2:B:278:PHE:CD1	2:B:278:PHE:C	0.54	2.80	18	9
1:A:209:TRP:CH2	1:A:223:SER:OG	0.54	2.59	13	4
2:B:321:TYR:CD1	2:B:321:TYR:O	0.54	2.60	3	4
2:B:323:GLN:O	2:B:333:LEU:O	0.54	2.25	18	15
2:B:316:PRO:O	2:B:320:GLN:NE2	0.54	2.41	12	3
2:B:297:THR:N	2:B:303:ARG:O	0.54	2.41	7	3
2:B:262:PHE:CZ	2:B:319:ILE:HD12	0.54	2.38	19	1
1:A:189:GLU:OE1	1:A:189:GLU:N	0.54	2.40	8	2
2:B:282:ILE:HD11	2:B:290:LYS:NZ	0.54	2.16	19	2
1:A:222:PRO:O	1:A:226:LEU:CD1	0.54	2.56	18	12
2:B:328:GLY:O	2:B:329:LEU:HD23	0.54	2.02	5	2
1:A:197:GLU:O	1:A:214:LYS:NZ	0.54	2.41	6	6
1:A:214:LYS:CD	1:A:214:LYS:H	0.54	2.16	19	3
2:B:312:PHE:CZ	2:B:321:TYR:CD1	0.54	2.95	18	1
2:B:259:GLU:OE2	2:B:280:LYS:N	0.54	2.41	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:296:GLU:N	2:B:296:GLU:OE1	0.54	2.40	15	1
1:A:202:ASP:C	1:A:204:SER:H	0.54	2.06	3	1
1:A:176:VAL:CG2	1:A:198:TYR:O	0.54	2.56	14	2
1:A:193:ARG:N	1:A:196:GLU:OE1	0.54	2.41	12	1
1:A:193:ARG:H	1:A:196:GLU:CD	0.53	2.05	12	1
1:A:196:GLU:OE1	1:A:214:LYS:NZ	0.53	2.38	15	1
1:A:215:ASN:O	1:A:215:ASN:ND2	0.53	2.40	11	1
1:A:201:LEU:N	1:A:201:LEU:CD1	0.53	2.71	13	1
2:B:338:CYS:SG	2:B:339:GLY:N	0.53	2.81	20	9
2:B:319:ILE:O	2:B:319:ILE:HG22	0.53	2.02	18	2
1:A:189:GLU:OE2	1:A:208:TRP:CZ3	0.53	2.62	9	1
2:B:314:SER:O	2:B:316:PRO:CD	0.53	2.57	12	11
1:A:197:GLU:C	1:A:198:TYR:CD1	0.53	2.81	8	4
2:B:238:GLU:CD	2:B:238:GLU:N	0.53	2.62	5	6
1:A:189:GLU:OE2	1:A:208:TRP:CE3	0.53	2.61	9	1
2:B:259:GLU:N	2:B:259:GLU:OE1	0.53	2.42	10	1
2:B:277:VAL:HG23	2:B:290:LYS:O	0.53	2.02	15	1
2:B:333:LEU:N	2:B:333:LEU:HD12	0.53	2.19	14	4
2:B:284:SER:OG	2:B:285:GLU:N	0.53	2.40	9	1
2:B:265:ARG:O	2:B:274:THR:N	0.53	2.42	18	3
2:B:324:TYR:CD2	2:B:325:ASN:N	0.53	2.76	1	2
2:B:266:ASP:OD1	2:B:267:SER:N	0.53	2.41	20	4
2:B:333:LEU:HD12	2:B:333:LEU:N	0.53	2.17	9	7
1:A:207:HIS:CD2	1:A:208:TRP:H	0.53	2.22	2	4
2:B:263:MET:SD	2:B:337:VAL:O	0.53	2.67	1	4
2:B:321:TYR:OH	2:B:322:HIS:CE1	0.53	2.62	13	4
1:A:194:CYS:O	1:A:196:GLU:N	0.53	2.41	18	7
2:B:258:LYS:NZ	2:B:335:TYR:CE1	0.53	2.72	18	2
2:B:263:MET:HG3	2:B:264:VAL:N	0.53	2.19	14	3
2:B:249:ALA:HB2	2:B:265:ARG:HE	0.53	1.62	17	1
2:B:263:MET:O	2:B:276:SER:N	0.53	2.42	15	14
2:B:312:PHE:CZ	2:B:321:TYR:CD2	0.53	2.96	8	5
1:A:196:GLU:CD	1:A:196:GLU:N	0.53	2.62	1	1
2:B:233:ASN:O	2:B:240:TYR:CE2	0.52	2.62	5	1
1:A:193:ARG:NH2	1:A:213:ASP:OD2	0.52	2.42	15	1
1:A:189:GLU:OE2	1:A:208:TRP:CZ2	0.52	2.62	12	2
2:B:331:THR:O	2:B:332:ARG:C	0.52	2.47	19	10
2:B:330:VAL:O	2:B:330:VAL:CG2	0.52	2.56	11	1
1:A:189:GLU:OE2	2:B:332:ARG:NH2	0.52	2.41	18	1
2:B:304:TYR:CD2	2:B:315:ILE:HD13	0.52	2.40	6	5
2:B:262:PHE:CD1	2:B:262:PHE:C	0.52	2.83	6	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:272:THR:O	2:B:293:HIS:NE2	0.52	2.42	12	3
2:B:321:TYR:O	2:B:325:ASN:OD1	0.52	2.28	20	3
1:A:208:TRP:CD1	2:B:328:GLY:O	0.52	2.62	11	2
2:B:259:GLU:OE1	2:B:259:GLU:N	0.52	2.42	7	1
1:A:189:GLU:OE1	1:A:208:TRP:CH2	0.52	2.62	19	1
1:A:196:GLU:OE2	1:A:214:LYS:NZ	0.52	2.42	16	1
2:B:317:LEU:O	2:B:320:GLN:N	0.52	2.33	19	3
1:A:211:VAL:HG22	1:A:219:GLY:O	0.52	2.04	4	1
2:B:320:GLN:N	2:B:320:GLN:OE1	0.52	2.42	12	1
2:B:331:THR:O	2:B:332:ARG:O	0.52	2.28	9	7
2:B:306:VAL:CG2	2:B:306:VAL:O	0.52	2.58	1	3
1:A:196:GLU:N	1:A:196:GLU:CD	0.52	2.63	3	1
1:A:197:GLU:C	1:A:198:TYR:CG	0.52	2.83	3	4
2:B:278:PHE:C	2:B:278:PHE:CD1	0.52	2.83	8	10
2:B:295:LYS:O	2:B:303:ARG:O	0.52	2.28	9	5
2:B:275:VAL:CG2	2:B:294:ILE:HD11	0.52	2.35	14	3
2:B:321:TYR:O	2:B:321:TYR:CD1	0.51	2.63	12	5
1:A:224:SER:O	1:A:226:LEU:N	0.51	2.40	14	3
1:A:218:GLU:N	1:A:218:GLU:OE1	0.51	2.44	4	1
2:B:333:LEU:CD1	2:B:333:LEU:H	0.51	2.19	9	2
2:B:322:HIS:CD2	2:B:329:LEU:HD23	0.51	2.39	9	1
2:B:315:ILE:N	2:B:316:PRO:HD2	0.51	2.20	9	9
1:A:190:LEU:HD21	1:A:219:GLY:N	0.51	2.21	4	1
2:B:272:THR:CG2	2:B:294:ILE:O	0.51	2.58	12	4
1:A:193:ARG:O	1:A:196:GLU:CD	0.51	2.48	12	2
2:B:321:TYR:CE2	2:B:322:HIS:CE1	0.51	2.98	10	5
2:B:306:VAL:CG1	2:B:306:VAL:O	0.51	2.59	15	2
2:B:321:TYR:CD2	2:B:322:HIS:CD2	0.51	2.99	3	1
1:A:201:LEU:HD12	1:A:201:LEU:N	0.51	2.21	14	1
1:A:208:TRP:NE1	2:B:328:GLY:O	0.51	2.44	9	2
1:A:177:ILE:HG23	1:A:196:GLU:O	0.51	2.06	18	1
2:B:258:LYS:NZ	2:B:335:TYR:OH	0.51	2.43	10	1
2:B:314:SER:C	2:B:316:PRO:HD2	0.51	2.26	12	11
2:B:262:PHE:O	2:B:262:PHE:CG	0.51	2.64	5	3
1:A:223:SER:H	2:B:330:VAL:CG1	0.51	2.18	3	2
2:B:332:ARG:O	2:B:333:LEU:C	0.50	2.48	11	4
1:A:224:SER:C	1:A:226:LEU:H	0.50	2.08	14	4
1:A:222:PRO:C	1:A:226:LEU:HD13	0.50	2.25	19	1
2:B:318:LEU:CD2	2:B:322:HIS:CD2	0.50	2.93	12	1
2:B:262:PHE:CG	2:B:333:LEU:HG	0.50	2.41	5	4
2:B:315:ILE:H	2:B:315:ILE:CD1	0.50	2.19	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:315:ILE:HD12	2:B:315:ILE:N	0.50	2.21	14	1
1:A:214:LYS:H	1:A:214:LYS:CD	0.50	2.18	5	2
2:B:240:TYR:CZ	2:B:266:ASP:OD2	0.50	2.65	6	1
1:A:191:ALA:O	1:A:192:LEU:HD23	0.50	2.05	9	1
2:B:306:VAL:O	2:B:306:VAL:CG2	0.50	2.59	19	4
1:A:181:ASP:OD1	1:A:194:CYS:SG	0.50	2.68	7	2
1:A:188:GLN:OE1	2:B:309:LYS:NZ	0.50	2.40	1	2
2:B:233:ASN:C	2:B:235:GLU:N	0.50	2.64	5	1
2:B:319:ILE:O	2:B:323:GLN:HG2	0.50	2.07	18	2
2:B:232:ASN:O	2:B:234:LEU:N	0.50	2.44	4	1
2:B:307:ALA:C	2:B:309:LYS:H	0.50	2.10	19	14
1:A:213:ASP:O	1:A:216:GLY:N	0.50	2.41	10	9
1:A:205:GLU:O	1:A:209:TRP:NE1	0.50	2.44	12	4
1:A:206:ILE:H	1:A:206:ILE:HD12	0.50	1.66	8	1
1:A:193:ARG:O	1:A:194:CYS:O	0.50	2.30	3	5
1:A:193:ARG:O	1:A:196:GLU:N	0.50	2.44	2	2
2:B:296:GLU:OE1	2:B:303:ARG:NH1	0.50	2.45	10	1
2:B:309:LYS:NZ	2:B:327:GLY:O	0.50	2.45	7	1
1:A:182:TYR:OH	2:B:332:ARG:NH1	0.50	2.45	12	1
2:B:297:THR:H	2:B:303:ARG:CB	0.50	2.20	3	1
1:A:200:LEU:C	1:A:201:LEU:HD12	0.50	2.26	13	1
2:B:239:TRP:O	2:B:264:VAL:O	0.50	2.29	3	16
2:B:305:TYR:C	2:B:305:TYR:CD1	0.50	2.85	9	2
2:B:286:ASN:OD1	2:B:286:ASN:N	0.50	2.45	20	2
2:B:328:GLY:C	2:B:329:LEU:HD22	0.50	2.27	14	1
1:A:173:GLU:CD	1:A:173:GLU:N	0.50	2.65	3	4
2:B:262:PHE:C	2:B:262:PHE:CD1	0.50	2.85	5	8
2:B:260:GLY:O	2:B:261:ALA:C	0.50	2.49	5	7
2:B:324:TYR:C	2:B:325:ASN:ND2	0.50	2.66	1	2
1:A:198:TYR:O	1:A:199:TYR:O	0.50	2.29	14	2
1:A:180:TYR:N	1:A:180:TYR:CD1	0.49	2.79	19	6
2:B:314:SER:O	2:B:317:LEU:N	0.49	2.44	20	6
1:A:193:ARG:O	1:A:196:GLU:CB	0.49	2.60	15	8
2:B:233:ASN:O	2:B:235:GLU:N	0.49	2.45	5	1
2:B:291:HIS:O	2:B:292:TYR:CG	0.49	2.65	8	2
2:B:305:TYR:O	2:B:305:TYR:CG	0.49	2.64	19	3
2:B:234:LEU:C	2:B:236:THR:N	0.49	2.66	19	16
1:A:182:TYR:C	1:A:182:TYR:CD1	0.49	2.86	10	5
1:A:178:ALA:HB3	1:A:193:ARG:O	0.49	2.07	18	1
1:A:225:TYR:OH	2:B:331:THR:CG2	0.49	2.61	5	1
2:B:260:GLY:O	2:B:262:PHE:N	0.49	2.45	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:322:HIS:NE2	2:B:329:LEU:HD23	0.49	2.23	14	3
1:A:209:TRP:CD2	1:A:223:SER:OG	0.49	2.64	19	1
2:B:305:TYR:CD1	2:B:305:TYR:C	0.49	2.86	3	4
1:A:179:LEU:HB3	1:A:180:TYR:CE1	0.49	2.42	10	1
1:A:192:LEU:O	1:A:193:ARG:NE	0.49	2.45	1	1
1:A:213:ASP:N	1:A:213:ASP:OD1	0.49	2.43	20	1
2:B:234:LEU:O	2:B:236:THR:N	0.49	2.46	19	9
1:A:183:GLN:NE2	1:A:184:THR:O	0.49	2.45	5	1
2:B:321:TYR:CZ	2:B:322:HIS:CD2	0.49	3.01	15	1
2:B:315:ILE:HB	2:B:316:PRO:HD3	0.49	1.84	12	3
2:B:279:THR:CG2	2:B:279:THR:O	0.49	2.61	8	1
1:A:209:TRP:O	1:A:210:ARG:C	0.49	2.51	12	10
2:B:303:ARG:CZ	2:B:304:TYR:OH	0.49	2.60	2	1
2:B:303:ARG:NE	2:B:304:TYR:OH	0.49	2.46	2	1
2:B:292:TYR:CE2	2:B:329:LEU:HD22	0.49	2.42	6	3
2:B:263:MET:HG2	2:B:264:VAL:N	0.49	2.23	12	8
1:A:210:ARG:NH2	1:A:220:TYR:OH	0.49	2.43	14	5
1:A:226:LEU:O	1:A:227:VAL:HG23	0.49	2.08	11	2
2:B:286:ASN:O	2:B:286:ASN:ND2	0.49	2.45	5	1
1:A:209:TRP:CE2	1:A:223:SER:OG	0.49	2.56	19	1
1:A:184:THR:OG1	1:A:191:ALA:CA	0.48	2.61	16	5
2:B:333:LEU:CD1	2:B:333:LEU:N	0.48	2.76	4	7
1:A:210:ARG:NE	1:A:220:TYR:CE2	0.48	2.81	9	3
2:B:330:VAL:HG13	2:B:331:THR:HG22	0.48	1.83	7	1
2:B:323:GLN:C	2:B:324:TYR:CD1	0.48	2.87	15	1
2:B:238:GLU:N	2:B:238:GLU:CD	0.48	2.67	9	5
1:A:192:LEU:C	1:A:193:ARG:HE	0.48	2.11	1	1
1:A:228:GLU:CD	1:A:228:GLU:H	0.48	2.09	9	4
2:B:234:LEU:C	2:B:236:THR:H	0.48	2.11	6	4
1:A:209:TRP:N	1:A:221:ALA:O	0.48	2.44	5	3
2:B:303:ARG:NH2	2:B:304:TYR:OH	0.48	2.46	17	1
2:B:322:HIS:CD2	2:B:329:LEU:HD12	0.48	2.44	8	2
2:B:319:ILE:HG22	2:B:319:ILE:O	0.48	2.08	11	2
1:A:213:ASP:OD1	1:A:214:LYS:N	0.48	2.46	3	1
2:B:315:ILE:HD13	2:B:315:ILE:H	0.48	1.68	8	1
1:A:181:ASP:OD2	1:A:194:CYS:SG	0.48	2.71	8	1
2:B:283:ILE:CG2	2:B:284:SER:N	0.48	2.76	10	7
1:A:224:SER:C	1:A:226:LEU:N	0.48	2.67	18	5
1:A:216:GLY:O	1:A:217:HIS:O	0.48	2.31	15	1
1:A:190:LEU:HD11	1:A:217:HIS:HB3	0.48	1.85	13	4
2:B:315:ILE:CB	2:B:316:PRO:CD	0.48	2.92	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:307:ALA:C	2:B:309:LYS:N	0.48	2.67	19	15
2:B:321:TYR:HH	2:B:327:GLY:HA3	0.48	1.68	13	2
2:B:283:ILE:HG23	2:B:284:SER:N	0.48	2.23	10	3
1:A:214:LYS:N	1:A:214:LYS:HZ3	0.48	2.05	10	1
1:A:209:TRP:CZ3	1:A:223:SER:OG	0.48	2.60	13	1
1:A:192:LEU:HD11	1:A:222:PRO:CD	0.47	2.38	7	3
2:B:324:TYR:CD1	2:B:325:ASN:ND2	0.47	2.82	9	2
1:A:224:SER:OG	2:B:330:VAL:CG2	0.47	2.61	3	3
2:B:281:ALA:O	2:B:282:ILE:O	0.47	2.32	18	8
1:A:193:ARG:C	1:A:196:GLU:OE2	0.47	2.52	3	3
1:A:173:GLU:N	1:A:173:GLU:CD	0.47	2.67	4	4
1:A:184:THR:HG23	1:A:189:GLU:O	0.47	2.08	7	1
1:A:192:LEU:HD22	1:A:198:TYR:CZ	0.47	2.44	5	1
1:A:225:TYR:CD2	2:B:330:VAL:CG2	0.47	2.97	5	1
2:B:297:THR:OG1	2:B:303:ARG:CA	0.47	2.62	1	1
1:A:190:LEU:HD12	1:A:191:ALA:O	0.47	2.09	6	1
1:A:207:HIS:O	1:A:208:TRP:CD2	0.47	2.67	12	1
2:B:277:VAL:O	2:B:290:LYS:N	0.47	2.43	4	4
2:B:242:LYS:HD2	2:B:243:SER:H	0.47	1.69	14	1
2:B:266:ASP:OD1	2:B:266:ASP:O	0.47	2.33	19	3
2:B:297:THR:OG1	2:B:303:ARG:N	0.47	2.48	1	2
1:A:226:LEU:C	1:A:227:VAL:HG22	0.47	2.30	4	1
2:B:296:GLU:OE2	2:B:296:GLU:N	0.47	2.47	20	1
1:A:210:ARG:NE	1:A:220:TYR:CE1	0.47	2.83	14	1
2:B:322:HIS:CG	2:B:329:LEU:HD12	0.47	2.44	16	2
2:B:329:LEU:O	2:B:331:THR:N	0.47	2.47	11	1
2:B:246:ARG:HH11	2:B:265:ARG:HH21	0.47	1.53	11	1
2:B:238:GLU:O	2:B:241:ASN:ND2	0.47	2.48	5	1
2:B:315:ILE:CD1	2:B:315:ILE:N	0.47	2.72	10	2
2:B:296:GLU:N	2:B:296:GLU:CD	0.47	2.68	15	1
2:B:250:GLU:O	2:B:252:LEU:N	0.47	2.47	16	1
2:B:302:LYS:HA	2:B:311:VAL:HG11	0.47	1.86	1	1
2:B:305:TYR:OH	2:B:308:GLU:OE2	0.47	2.32	6	5
2:B:279:THR:O	2:B:279:THR:HG23	0.47	2.10	11	2
2:B:315:ILE:H	2:B:315:ILE:HD13	0.47	1.70	16	1
2:B:241:ASN:O	2:B:244:ILE:HG22	0.47	2.09	17	1
2:B:329:LEU:CD1	2:B:333:LEU:CD1	0.47	2.93	12	1
2:B:318:LEU:HD21	2:B:322:HIS:NE2	0.47	2.24	12	1
2:B:272:THR:HG23	2:B:296:GLU:CD	0.47	2.29	15	1
1:A:205:GLU:OE1	1:A:207:HIS:CE1	0.47	2.67	8	3
2:B:329:LEU:C	2:B:331:THR:H	0.47	2.13	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:ASP:OD2	1:A:210:ARG:CZ	0.47	2.63	6	1
2:B:304:TYR:CG	2:B:315:ILE:CD1	0.47	2.97	5	1
2:B:317:LEU:C	2:B:319:ILE:N	0.47	2.65	19	3
1:A:190:LEU:HD23	1:A:211:VAL:HG23	0.47	1.85	10	1
2:B:322:HIS:NE2	2:B:328:GLY:N	0.47	2.63	17	1
1:A:223:SER:OG	2:B:290:LYS:NZ	0.47	2.41	17	1
2:B:315:ILE:C	2:B:317:LEU:N	0.46	2.69	19	6
1:A:207:HIS:O	1:A:223:SER:OG	0.46	2.33	19	2
1:A:225:TYR:CD1	2:B:330:VAL:CG2	0.46	2.98	10	2
1:A:190:LEU:CD2	1:A:217:HIS:O	0.46	2.62	10	2
2:B:266:ASP:O	2:B:266:ASP:OD1	0.46	2.33	12	3
1:A:222:PRO:HB3	2:B:330:VAL:HG23	0.46	1.87	14	2
1:A:210:ARG:O	1:A:211:VAL:CG1	0.46	2.63	5	5
1:A:206:ILE:O	2:B:292:TYR:CE1	0.46	2.68	16	1
1:A:189:GLU:CA	1:A:189:GLU:OE1	0.46	2.64	17	1
2:B:303:ARG:HD2	2:B:303:ARG:N	0.46	2.25	3	1
1:A:182:TYR:O	1:A:192:LEU:O	0.46	2.34	5	4
1:A:208:TRP:CE3	1:A:220:TYR:O	0.46	2.68	7	2
1:A:182:TYR:OH	1:A:189:GLU:OE1	0.46	2.34	2	5
1:A:175:LEU:N	1:A:175:LEU:CD1	0.46	2.79	17	2
1:A:202:ASP:C	1:A:204:SER:N	0.46	2.68	3	1
1:A:225:TYR:O	1:A:226:LEU:HD12	0.46	2.11	14	1
2:B:321:TYR:CE2	2:B:322:HIS:ND1	0.46	2.84	11	4
2:B:332:ARG:O	2:B:333:LEU:O	0.46	2.34	17	3
2:B:302:LYS:CD	2:B:302:LYS:N	0.46	2.79	3	1
2:B:239:TRP:CD1	2:B:239:TRP:N	0.46	2.82	13	1
1:A:222:PRO:C	1:A:226:LEU:HD12	0.46	2.31	1	2
1:A:230:SER:O	1:A:230:SER:OG	0.46	2.33	8	1
1:A:200:LEU:CD2	1:A:202:ASP:H	0.46	2.24	14	1
2:B:303:ARG:HG3	2:B:304:TYR:CD1	0.46	2.45	13	1
2:B:312:PHE:HD2	2:B:318:LEU:N	0.46	2.09	19	1
2:B:285:GLU:O	2:B:288:CYS:SG	0.46	2.69	3	1
2:B:239:TRP:N	2:B:239:TRP:CD1	0.46	2.82	18	3
2:B:272:THR:CG2	2:B:293:HIS:CE1	0.46	2.99	19	2
2:B:269:THR:O	2:B:272:THR:O	0.46	2.33	19	1
2:B:318:LEU:HD21	2:B:322:HIS:CD2	0.46	2.45	12	1
2:B:246:ARG:CG	2:B:247:ASP:N	0.46	2.79	13	7
2:B:321:TYR:CG	2:B:322:HIS:N	0.46	2.84	19	1
1:A:202:ASP:O	1:A:204:SER:N	0.46	2.49	3	1
1:A:197:GLU:O	1:A:198:TYR:CG	0.46	2.69	14	2
2:B:310:TYR:CE1	2:B:321:TYR:CE1	0.45	3.04	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:331:THR:O	2:B:334:ARG:NE	0.45	2.48	5	1
1:A:190:LEU:HD23	1:A:211:VAL:CG2	0.45	2.41	10	1
2:B:318:LEU:O	2:B:322:HIS:HB2	0.45	2.11	19	1
1:A:226:LEU:O	1:A:227:VAL:CG1	0.45	2.62	9	7
1:A:206:ILE:CD1	1:A:206:ILE:N	0.45	2.78	8	1
2:B:239:TRP:O	2:B:264:VAL:N	0.45	2.47	13	2
1:A:196:GLU:OE1	1:A:197:GLU:O	0.45	2.34	17	2
2:B:241:ASN:ND2	2:B:263:MET:CE	0.45	2.79	20	2
1:A:182:TYR:HB3	1:A:192:LEU:HD12	0.45	1.87	1	2
1:A:230:SER:OG	1:A:230:SER:O	0.45	2.34	12	1
2:B:325:ASN:N	2:B:325:ASN:HD22	0.45	2.09	20	1
2:B:250:GLU:O	2:B:251:LYS:C	0.45	2.54	16	1
1:A:193:ARG:N	1:A:196:GLU:CD	0.45	2.70	12	1
1:A:193:ARG:N	1:A:196:GLU:OE2	0.45	2.50	1	1
1:A:207:HIS:N	1:A:207:HIS:ND1	0.45	2.63	15	1
2:B:255:ASP:OD1	2:B:255:ASP:O	0.45	2.34	6	5
1:A:218:GLU:H	1:A:218:GLU:CD	0.45	2.14	11	3
1:A:180:TYR:C	1:A:194:CYS:SG	0.45	2.95	18	1
1:A:189:GLU:OE2	1:A:208:TRP:CH2	0.45	2.69	7	2
1:A:200:LEU:HD23	1:A:201:LEU:N	0.45	2.26	18	1
1:A:222:PRO:O	1:A:226:LEU:CG	0.45	2.64	12	3
1:A:182:TYR:CD1	1:A:182:TYR:C	0.45	2.89	7	4
2:B:267:SER:OG	2:B:272:THR:O	0.45	2.35	17	1
1:A:174:THR:OG1	1:A:175:LEU:N	0.45	2.50	12	1
2:B:329:LEU:CD1	2:B:333:LEU:HD13	0.45	2.41	15	1
1:A:196:GLU:CD	1:A:198:TYR:OH	0.45	2.55	14	2
1:A:183:GLN:CD	1:A:184:THR:N	0.45	2.70	5	1
2:B:315:ILE:N	2:B:315:ILE:HD12	0.45	2.23	20	1
2:B:273:TYR:O	2:B:293:HIS:CD2	0.45	2.70	11	2
2:B:264:VAL:CG1	2:B:265:ARG:N	0.45	2.79	9	7
2:B:335:TYR:CD1	2:B:335:TYR:N	0.45	2.85	5	1
2:B:329:LEU:N	2:B:329:LEU:CD2	0.45	2.80	9	1
2:B:310:TYR:CE2	2:B:321:TYR:OH	0.45	2.62	9	1
1:A:219:GLY:O	1:A:221:ALA:N	0.45	2.50	4	1
1:A:174:THR:O	1:A:174:THR:HG23	0.45	2.10	13	2
2:B:272:THR:O	2:B:273:TYR:O	0.44	2.35	11	5
1:A:190:LEU:HD21	1:A:217:HIS:C	0.44	2.33	8	1
1:A:216:GLY:O	1:A:218:GLU:OE2	0.44	2.34	11	1
2:B:245:SER:OG	2:B:246:ARG:N	0.44	2.51	1	1
2:B:240:TYR:CZ	2:B:266:ASP:CG	0.44	2.91	6	1
2:B:317:LEU:O	2:B:319:ILE:N	0.44	2.50	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:207:HIS:O	1:A:208:TRP:CG	0.44	2.70	12	1
1:A:200:LEU:HD22	1:A:203:SER:N	0.44	2.27	3	1
1:A:181:ASP:CG	1:A:194:CYS:SG	0.44	2.96	8	1
1:A:197:GLU:CG	1:A:214:LYS:HZ1	0.44	2.26	19	2
2:B:233:ASN:OD1	2:B:233:ASN:O	0.44	2.36	4	1
2:B:321:TYR:C	2:B:321:TYR:CD1	0.44	2.86	11	5
2:B:286:ASN:N	2:B:286:ASN:OD1	0.44	2.50	11	1
1:A:189:GLU:CD	1:A:208:TRP:CH2	0.44	2.91	19	1
1:A:180:TYR:CD2	1:A:225:TYR:CD1	0.44	3.05	16	1
2:B:302:LYS:HB3	2:B:311:VAL:HG11	0.44	1.89	4	1
1:A:184:THR:OG1	1:A:190:LEU:C	0.44	2.56	4	1
2:B:307:ALA:O	2:B:309:LYS:N	0.44	2.51	19	1
2:B:286:ASN:ND2	2:B:286:ASN:C	0.44	2.71	15	1
2:B:233:ASN:O	2:B:233:ASN:OD1	0.44	2.36	3	1
2:B:251:LYS:CG	2:B:252:LEU:N	0.44	2.81	7	5
2:B:297:THR:OG1	2:B:302:LYS:C	0.44	2.56	1	2
1:A:194:CYS:C	1:A:196:GLU:N	0.44	2.70	18	4
1:A:197:GLU:HG3	1:A:214:LYS:HZ1	0.44	1.73	19	1
1:A:202:ASP:O	1:A:202:ASP:CG	0.44	2.55	3	1
1:A:206:ILE:O	1:A:223:SER:CB	0.44	2.66	3	1
1:A:202:ASP:CG	1:A:210:ARG:CZ	0.44	2.86	6	1
1:A:207:HIS:C	1:A:208:TRP:CG	0.44	2.91	12	1
2:B:292:TYR:OH	2:B:330:VAL:CG1	0.44	2.66	15	1
1:A:173:GLU:CD	1:A:173:GLU:H	0.44	2.16	8	2
1:A:228:GLU:O	1:A:228:GLU:OE2	0.44	2.36	9	2
2:B:242:LYS:C	2:B:244:ILE:H	0.44	2.15	17	1
2:B:272:THR:OG1	2:B:296:GLU:OE2	0.44	2.35	12	1
1:A:173:GLU:H	1:A:173:GLU:CD	0.44	2.16	1	2
2:B:327:GLY:C	2:B:329:LEU:H	0.44	2.17	14	1
1:A:190:LEU:HD13	1:A:191:ALA:N	0.44	2.28	8	1
2:B:333:LEU:N	2:B:333:LEU:CD1	0.44	2.81	12	3
2:B:322:HIS:C	2:B:324:TYR:N	0.44	2.71	14	2
1:A:208:TRP:HB3	1:A:220:TYR:HB3	0.44	1.90	3	1
1:A:176:VAL:O	1:A:197:GLU:CD	0.44	2.55	14	2
2:B:267:SER:OG	2:B:274:THR:OG1	0.43	2.36	3	1
2:B:303:ARG:NH1	2:B:304:TYR:OH	0.43	2.51	13	1
1:A:190:LEU:HD23	1:A:219:GLY:CA	0.43	2.44	6	2
2:B:319:ILE:O	2:B:319:ILE:CG2	0.43	2.66	18	1
2:B:266:ASP:OD1	2:B:273:TYR:CE1	0.43	2.72	10	1
2:B:331:THR:HG23	2:B:331:THR:O	0.43	2.13	7	1
1:A:224:SER:OG	1:A:225:TYR:N	0.43	2.51	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:315:ILE:N	2:B:315:ILE:CD1	0.43	2.80	14	1
2:B:262:PHE:CG	2:B:262:PHE:O	0.43	2.71	6	2
1:A:205:GLU:OE2	1:A:207:HIS:NE2	0.43	2.52	9	1
1:A:228:GLU:OE2	1:A:228:GLU:O	0.43	2.37	4	2
1:A:196:GLU:C	1:A:196:GLU:OE1	0.43	2.57	17	1
1:A:208:TRP:CD1	2:B:328:GLY:C	0.43	2.91	14	1
2:B:318:LEU:CD2	2:B:322:HIS:HD1	0.43	2.26	13	1
2:B:281:ALA:O	2:B:286:ASN:OD1	0.43	2.36	2	2
2:B:319:ILE:O	2:B:323:GLN:CG	0.43	2.66	19	2
2:B:315:ILE:CD1	2:B:315:ILE:H	0.43	2.25	20	1
2:B:257:GLY:C	2:B:280:LYS:HZ3	0.43	2.16	14	1
2:B:318:LEU:O	2:B:318:LEU:CD2	0.43	2.63	8	4
1:A:215:ASN:CG	1:A:217:HIS:NE2	0.43	2.71	11	1
2:B:303:ARG:H	2:B:311:VAL:HG12	0.43	1.72	10	1
2:B:289:ILE:CG2	2:B:291:HIS:NE2	0.43	2.81	10	2
1:A:194:CYS:SG	1:A:194:CYS:O	0.43	2.76	4	1
2:B:267:SER:OG	2:B:293:HIS:NE2	0.43	2.46	14	1
2:B:257:GLY:O	2:B:280:LYS:NZ	0.43	2.44	18	1
1:A:221:ALA:HB1	1:A:226:LEU:HD11	0.43	1.91	18	2
2:B:271:GLY:O	2:B:296:GLU:OE2	0.43	2.37	11	3
1:A:223:SER:OG	1:A:224:SER:N	0.43	2.51	16	1
2:B:281:ALA:C	2:B:288:CYS:HG	0.43	2.17	17	1
2:B:306:VAL:HG12	2:B:318:LEU:CD1	0.43	2.43	12	1
1:A:205:GLU:OE1	1:A:208:TRP:O	0.43	2.36	20	1
2:B:297:THR:OG1	2:B:302:LYS:O	0.43	2.28	15	1
1:A:196:GLU:OE1	1:A:198:TYR:CE2	0.43	2.72	16	1
1:A:227:VAL:CG1	2:B:282:ILE:HG23	0.43	2.44	16	1
1:A:198:TYR:CE1	1:A:213:ASP:CG	0.43	2.92	9	1
1:A:207:HIS:ND1	1:A:207:HIS:N	0.43	2.65	8	1
1:A:195:ASP:O	1:A:195:ASP:CG	0.43	2.56	4	1
1:A:184:THR:OG1	1:A:191:ALA:CB	0.43	2.67	13	1
1:A:180:TYR:CE1	1:A:225:TYR:HB3	0.42	2.49	16	1
2:B:255:ASP:O	2:B:255:ASP:OD1	0.42	2.37	16	4
1:A:181:ASP:OD1	1:A:181:ASP:O	0.42	2.36	18	3
2:B:318:LEU:C	2:B:318:LEU:HD23	0.42	2.34	9	1
2:B:312:PHE:CD2	2:B:318:LEU:N	0.42	2.87	19	1
2:B:294:ILE:O	2:B:296:GLU:OE2	0.42	2.36	20	1
1:A:189:GLU:OE1	1:A:208:TRP:CE3	0.42	2.72	11	2
1:A:218:GLU:OE1	1:A:218:GLU:O	0.42	2.37	2	1
2:B:320:GLN:OE1	2:B:320:GLN:CA	0.42	2.67	12	1
1:A:193:ARG:O	1:A:196:GLU:CG	0.42	2.66	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:196:GLU:OE1	1:A:198:TYR:OH	0.42	2.36	20	1
1:A:181:ASP:OD1	1:A:194:CYS:N	0.42	2.52	8	1
1:A:181:ASP:O	1:A:181:ASP:OD1	0.42	2.36	6	1
1:A:223:SER:O	1:A:226:LEU:O	0.42	2.37	18	1
1:A:225:TYR:CD1	2:B:330:VAL:HG21	0.42	2.49	10	1
1:A:221:ALA:CB	1:A:226:LEU:HD11	0.42	2.45	8	1
1:A:190:LEU:CD2	1:A:219:GLY:N	0.42	2.83	6	1
1:A:196:GLU:CA	1:A:196:GLU:OE1	0.42	2.67	11	1
2:B:319:ILE:O	2:B:323:GLN:CD	0.42	2.58	19	1
2:B:273:TYR:H	2:B:294:ILE:CD1	0.42	2.23	13	1
1:A:217:HIS:CD2	1:A:217:HIS:N	0.42	2.87	11	1
2:B:318:LEU:CD2	2:B:318:LEU:O	0.42	2.65	18	2
2:B:267:SER:OG	2:B:269:THR:OG1	0.42	2.34	12	1
2:B:323:GLN:O	2:B:324:TYR:CD1	0.42	2.72	3	1
2:B:285:GLU:O	2:B:287:PRO:O	0.42	2.38	10	1
2:B:321:TYR:CE1	2:B:325:ASN:OD1	0.42	2.73	1	1
2:B:297:THR:H	2:B:303:ARG:HB3	0.42	1.75	3	1
1:A:226:LEU:O	1:A:227:VAL:CG2	0.42	2.68	11	2
2:B:332:ARG:HH21	2:B:334:ARG:HH22	0.42	1.57	5	1
2:B:265:ARG:N	2:B:274:THR:O	0.42	2.44	17	2
1:A:208:TRP:NE1	2:B:328:GLY:CA	0.42	2.82	17	1
1:A:196:GLU:H	1:A:196:GLU:CD	0.42	2.18	1	1
1:A:220:TYR:CD1	1:A:220:TYR:N	0.42	2.88	3	1
2:B:272:THR:OG1	2:B:296:GLU:CD	0.42	2.58	13	2
2:B:311:VAL:HG12	2:B:312:PHE:N	0.42	2.30	9	1
1:A:222:PRO:HD2	1:A:226:LEU:HD11	0.42	1.92	19	1
1:A:182:TYR:HH	1:A:189:GLU:CD	0.42	2.18	6	1
1:A:171:PRO:O	1:A:172:GLU:C	0.42	2.58	18	1
1:A:211:VAL:CG2	1:A:219:GLY:H	0.42	2.27	4	1
2:B:258:LYS:NZ	2:B:259:GLU:O	0.42	2.53	12	1
2:B:318:LEU:CD2	2:B:322:HIS:ND1	0.42	2.83	3	1
1:A:182:TYR:CZ	1:A:184:THR:OG1	0.41	2.73	9	2
2:B:322:HIS:NE2	2:B:327:GLY:CA	0.41	2.83	15	1
1:A:196:GLU:OE1	1:A:196:GLU:C	0.41	2.59	16	1
1:A:207:HIS:O	2:B:329:LEU:O	0.41	2.38	12	1
2:B:322:HIS:NE2	2:B:327:GLY:HA2	0.41	2.30	15	1
1:A:198:TYR:CD1	1:A:213:ASP:OD1	0.41	2.73	11	1
2:B:303:ARG:CD	2:B:304:TYR:CZ	0.41	3.03	9	1
2:B:318:LEU:HD23	2:B:322:HIS:ND1	0.41	2.31	20	1
2:B:321:TYR:OH	2:B:322:HIS:NE2	0.41	2.49	13	1
1:A:223:SER:O	1:A:226:LEU:N	0.41	2.46	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:TYR:CE1	1:A:225:TYR:CD1	0.41	3.09	16	1
2:B:267:SER:C	2:B:269:THR:N	0.41	2.74	16	1
2:B:263:MET:CE	2:B:337:VAL:O	0.41	2.69	18	1
1:A:202:ASP:CG	1:A:210:ARG:NE	0.41	2.74	6	1
1:A:228:GLU:H	1:A:228:GLU:CD	0.41	2.19	20	1
1:A:176:VAL:HG12	1:A:228:GLU:HA	0.41	1.93	14	1
1:A:176:VAL:HG22	1:A:198:TYR:O	0.41	2.16	13	1
2:B:304:TYR:CD2	2:B:315:ILE:CD1	0.41	3.04	19	2
2:B:315:ILE:O	2:B:316:PRO:C	0.41	2.58	5	1
2:B:267:SER:C	2:B:269:THR:H	0.41	2.19	16	1
2:B:251:LYS:O	2:B:254:LEU:N	0.41	2.53	15	2
2:B:294:ILE:O	2:B:296:GLU:OE1	0.41	2.38	15	1
1:A:202:ASP:OD1	1:A:202:ASP:O	0.41	2.39	3	1
2:B:272:THR:OG1	2:B:296:GLU:OE1	0.41	2.39	3	1
2:B:281:ALA:N	2:B:286:ASN:OD1	0.41	2.54	14	1
2:B:303:ARG:CG	2:B:304:TYR:CE1	0.41	3.03	13	1
2:B:240:TYR:OH	2:B:266:ASP:OD2	0.41	2.35	6	1
2:B:271:GLY:O	2:B:272:THR:OG1	0.41	2.39	5	2
2:B:288:CYS:SG	2:B:289:ILE:N	0.41	2.94	2	2
1:A:218:GLU:N	1:A:218:GLU:CD	0.41	2.73	7	1
2:B:248:LYS:O	2:B:252:LEU:CB	0.41	2.69	7	1
2:B:333:LEU:H	2:B:333:LEU:CD1	0.41	2.28	14	1
1:A:190:LEU:HD13	1:A:217:HIS:CB	0.41	2.46	6	1
1:A:217:HIS:O	1:A:218:GLU:CB	0.41	2.69	18	2
1:A:182:TYR:O	1:A:192:LEU:C	0.41	2.58	9	1
2:B:257:GLY:C	2:B:280:LYS:NZ	0.41	2.74	4	1
2:B:273:TYR:O	2:B:294:ILE:CG1	0.41	2.69	17	1
1:A:209:TRP:C	1:A:210:ARG:O	0.41	2.59	12	1
2:B:322:HIS:CE1	2:B:327:GLY:CA	0.41	3.04	12	1
1:A:222:PRO:O	1:A:226:LEU:HG	0.41	2.16	12	1
1:A:229:LYS:O	1:A:230:SER:OG	0.41	2.37	12	1
2:B:325:ASN:CG	2:B:326:GLY:H	0.41	2.18	20	1
1:A:217:HIS:N	1:A:217:HIS:CD2	0.41	2.89	14	1
2:B:269:THR:O	2:B:271:GLY:N	0.41	2.54	16	1
2:B:303:ARG:CD	2:B:304:TYR:CE1	0.41	3.04	7	1
2:B:305:TYR:O	2:B:305:TYR:CD1	0.41	2.74	19	1
1:A:202:ASP:OD1	1:A:204:SER:OG	0.41	2.37	13	1
2:B:262:PHE:CD1	2:B:262:PHE:O	0.40	2.74	6	1
2:B:271:GLY:O	2:B:296:GLU:OE1	0.40	2.38	10	1
2:B:317:LEU:C	2:B:319:ILE:H	0.40	2.19	19	1
2:B:268:ARG:O	2:B:269:THR:C	0.40	2.59	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:237:TYR:CD2	2:B:239:TRP:CH2	0.40	3.09	1	1
2:B:242:LYS:H	2:B:242:LYS:HD2	0.40	1.75	14	1
2:B:262:PHE:CE1	2:B:319:ILE:HG23	0.40	2.50	13	1
1:A:215:ASN:CB	1:A:217:HIS:NE2	0.40	2.83	9	1
1:A:189:GLU:CD	1:A:220:TYR:O	0.40	2.60	4	1
1:A:225:TYR:CE2	2:B:330:VAL:HG22	0.40	2.51	5	1
2:B:276:SER:OG	2:B:291:HIS:CE1	0.40	2.75	2	1
2:B:331:THR:O	2:B:331:THR:OG1	0.40	2.32	1	1
2:B:237:TYR:HB3	2:B:239:TRP:CE2	0.40	2.52	11	1
1:A:214:LYS:HD3	1:A:214:LYS:N	0.40	2.32	2	1
2:B:321:TYR:CZ	2:B:322:HIS:NE2	0.40	2.89	15	1
1:A:180:TYR:CD1	1:A:225:TYR:CD1	0.40	3.10	5	1
1:A:179:LEU:CD1	1:A:225:TYR:O	0.40	2.69	16	1
2:B:303:ARG:NE	2:B:313:ASP:OD1	0.40	2.55	19	1
2:B:310:TYR:CZ	2:B:321:TYR:OH	0.40	2.71	3	1
2:B:323:GLN:C	2:B:333:LEU:O	0.40	2.60	14	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	57/63 (90%)	44±3 (77±5%)	9±2 (15±4%)	4±1 (8±2%)	2	16
2	B	102/110 (93%)	76±3 (75±3%)	16±3 (16±3%)	10±2 (9±2%)	2	11
All	All	3180/3460 (92%)	2408 (76%)	493 (16%)	279 (9%)	2	13

All 45 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	282	ILE	20
2	B	325	ASN	20
2	B	302	LYS	18
2	B	307	ALA	17
1	A	171	PRO	16

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Mol	Chain	Res	Type	Models (Total)
2	B	332	ARG	16
1	A	210	ARG	15
2	B	280	LYS	15
2	B	306	VAL	13
1	A	194	CYS	11
2	B	315	ILE	11
2	B	316	PRO	11
2	B	273	TYR	10
1	A	222	PRO	8
2	B	261	ALA	8
2	B	235	GLU	7
1	A	207	HIS	7
1	A	195	ASP	6
2	B	331	THR	5
2	B	330	VAL	4
1	A	196	GLU	4
2	B	334	ARG	4
2	B	333	LEU	3
1	A	230	SER	3
2	B	233	ASN	2
1	A	176	VAL	2
1	A	209	TRP	2
1	A	193	ARG	2
1	A	218	GLU	2
1	A	199	TYR	2
1	A	225	TYR	1
1	A	224	SER	1
1	A	203	SER	1
1	A	180	TYR	1
1	A	227	VAL	1
2	B	251	LYS	1
2	B	234	LEU	1
2	B	314	SER	1
2	B	271	GLY	1
1	A	220	TYR	1
1	A	189	GLU	1
2	B	303	ARG	1
2	B	250	GLU	1
2	B	243	SER	1
1	A	217	HIS	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	53/57 (93%)	46±1 (87±3%)	7±1 (13±3%)	9 51
2	B	93/98 (95%)	81±3 (87±3%)	12±3 (13±3%)	9 51
All	All	2920/3100 (94%)	2540 (87%)	380 (13%)	9 51

All 69 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	200	LEU	19
2	B	239	TRP	17
2	B	321	TYR	15
2	B	278	PHE	15
1	A	224	SER	14
1	A	173	GLU	14
2	B	322	HIS	13
1	A	207	HIS	12
2	B	310	TYR	12
2	B	279	THR	11
2	B	273	TYR	11
2	B	234	LEU	11
2	B	238	GLU	10
1	A	214	LYS	10
2	B	269	THR	10
2	B	315	ILE	10
2	B	329	LEU	9
1	A	227	VAL	8
1	A	196	GLU	8
2	B	325	ASN	7
1	A	198	TYR	6
2	B	294	ILE	6
1	A	190	LEU	6
2	B	331	THR	6
2	B	286	ASN	6
2	B	318	LEU	5
1	A	228	GLU	5
1	A	223	SER	5

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Mol	Chain	Res	Type	Models (Total)
2	B	251	LYS	5
2	B	303	ARG	5
1	A	180	TYR	5
1	A	230	SER	4
2	B	293	HIS	4
2	B	297	THR	4
2	B	338	CYS	4
2	B	266	ASP	4
1	A	218	GLU	4
2	B	290	LYS	4
1	A	211	VAL	4
2	B	335	TYR	4
2	B	296	GLU	3
2	B	320	GLN	3
2	B	314	SER	3
2	B	305	TYR	3
1	A	193	ARG	3
2	B	262	PHE	3
2	B	272	THR	3
2	B	267	SER	2
2	B	304	TYR	2
1	A	176	VAL	2
2	B	242	LYS	2
1	A	189	GLU	2
2	B	246	ARG	1
1	A	182	TYR	1
1	A	215	ASN	1
2	B	324	TYR	1
1	A	203	SER	1
2	B	236	THR	1
1	A	188	GLN	1
2	B	244	ILE	1
2	B	337	VAL	1
2	B	265	ARG	1
2	B	330	VAL	1
1	A	204	SER	1
2	B	245	SER	1
2	B	268	ARG	1
2	B	288	CYS	1
1	A	179	LEU	1
1	A	226	LEU	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 81% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16809

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	1939
Number of shifts mapped to atoms	1939
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	171	2.54 ± 0.12	Should be applied
$^{13}\text{C}_\beta$	161	2.49 ± 0.16	Should be applied
$^{13}\text{C}'$	158	4.56 ± 0.15	Should be applied
^{15}N	159	0.61 ± 0.44	None needed (imprecise)

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 81%, i.e. 1673 atoms were assigned a chemical shift out of a possible 2063. 23 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	782/796 (98%)	314/317 (99%)	315/324 (97%)	153/155 (99%)
Sidechain	776/1040 (75%)	433/612 (71%)	328/382 (86%)	15/46 (33%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	115/227 (51%)	76/117 (65%)	36/101 (36%)	3/9 (33%)
Overall	1673/2063 (81%)	823/1046 (79%)	679/807 (84%)	171/210 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1745 atoms were assigned a chemical shift out of a possible 2150. 23 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	816/837 (97%)	328/333 (98%)	329/342 (96%)	159/162 (98%)
Sidechain	814/1086 (75%)	457/640 (71%)	340/398 (85%)	17/48 (35%)
Aromatic	115/227 (51%)	76/117 (65%)	36/101 (36%)	3/9 (33%)
Overall	1745/2150 (81%)	861/1090 (79%)	705/841 (84%)	179/219 (82%)

7.1.4 Statistically unusual chemical shifts ⓘ

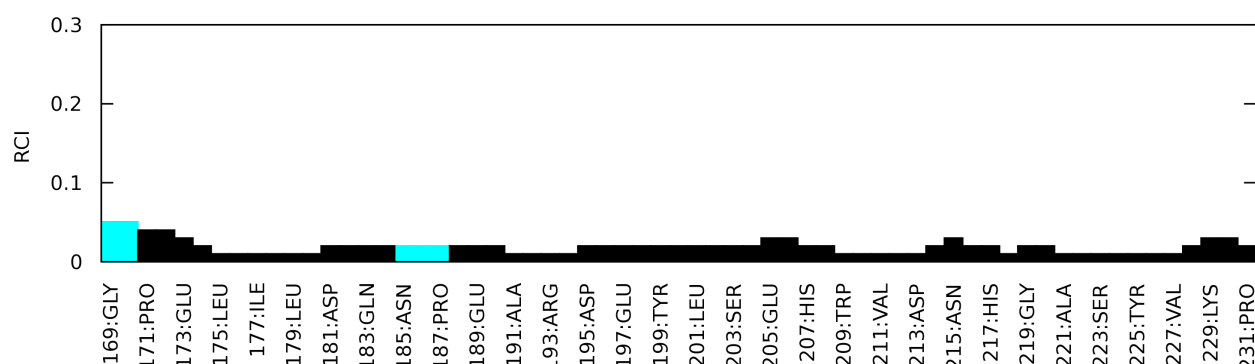
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	303	ARG	NE	119.27	92.63 – 76.73	21.8
2	B	265	ARG	NE	118.55	92.63 – 76.73	21.3
1	A	223	SER	HB3	1.61	5.25 – 2.45	-8.0
1	A	223	SER	HB2	1.80	5.18 – 2.58	-8.0
2	B	333	LEU	HB3	-1.20	3.34 – -0.26	-7.6
2	B	239	TRP	CD1	114.31	136.18 – 116.78	-6.3
2	B	237	TYR	HB3	0.47	4.75 – 0.95	-6.3
1	A	203	SER	HB3	2.16	5.25 – 2.45	-6.0
1	A	222	PRO	HG2	0.32	3.48 – 0.38	-5.2
2	B	285	GLU	C	166.79	186.83 – 167.03	-5.1
2	B	331	THR	C	165.68	183.43 – 165.73	-5.0
2	B	287	PRO	CG	21.76	32.66 – 21.76	-5.0

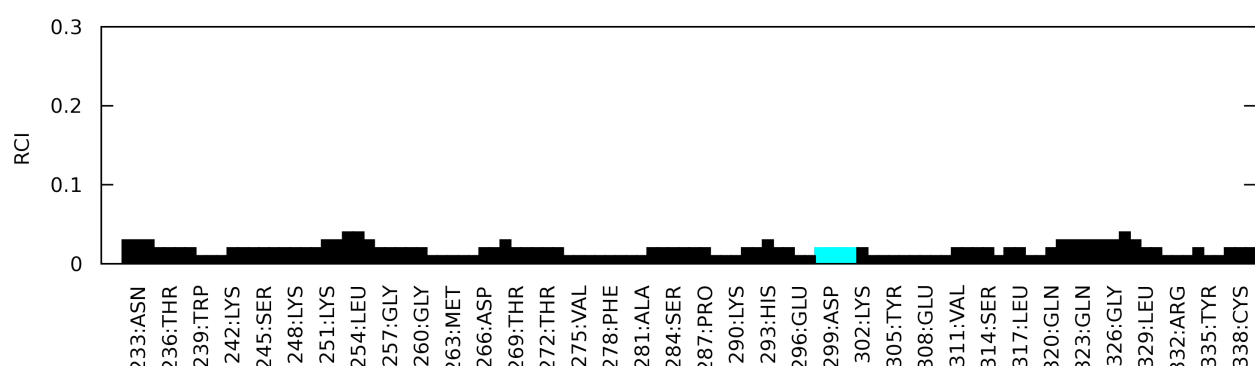
7.1.5 Random Coil Index (RCI) plots ⓘ

The images below report *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:



Random coil index (RCI) for chain B:



7.2 Chemical shift list 2

File name: BMRB entry 16809

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping [i](#)

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	1837
Number of shifts mapped to atoms	1837
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	11

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	171	2.79 ± 0.16	Should be applied
$^{13}\text{C}_\beta$	161	2.43 ± 0.11	Should be applied
$^{13}\text{C}'$	58	2.98 ± 0.16	Should be applied
^{15}N	159	0.52 ± 0.38	None needed (imprecise)

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 1576 atoms were assigned a chemical shift out of a possible 2063. 23 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	685/796 (86%)	314/317 (99%)	218/324 (67%)	153/155 (99%)
Sidechain	776/1040 (75%)	433/612 (71%)	328/382 (86%)	15/46 (33%)
Aromatic	115/227 (51%)	76/117 (65%)	36/101 (36%)	3/9 (33%)
Overall	1576/2063 (76%)	823/1046 (79%)	582/807 (72%)	171/210 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1645 atoms were assigned a chemical shift out of a possible 2150. 23 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	716/837 (86%)	328/333 (98%)	229/342 (67%)	159/162 (98%)
Sidechain	814/1086 (75%)	457/640 (71%)	340/398 (85%)	17/48 (35%)
Aromatic	115/227 (51%)	76/117 (65%)	36/101 (36%)	3/9 (33%)
Overall	1645/2150 (77%)	861/1090 (79%)	605/841 (72%)	179/219 (82%)

7.2.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	303	ARG	NE	119.29	92.63 – 76.73	21.8
2	B	265	ARG	NE	118.52	92.63 – 76.73	21.3
1	A	223	SER	HB2	1.76	5.18 – 2.58	-8.2
1	A	223	SER	HB3	1.58	5.25 – 2.45	-8.1
2	B	333	LEU	HB3	-1.20	3.34 – -0.26	-7.6
2	B	239	TRP	CD1	114.38	136.18 – 116.78	-6.2
2	B	237	TYR	HB3	0.53	4.75 – 0.95	-6.1

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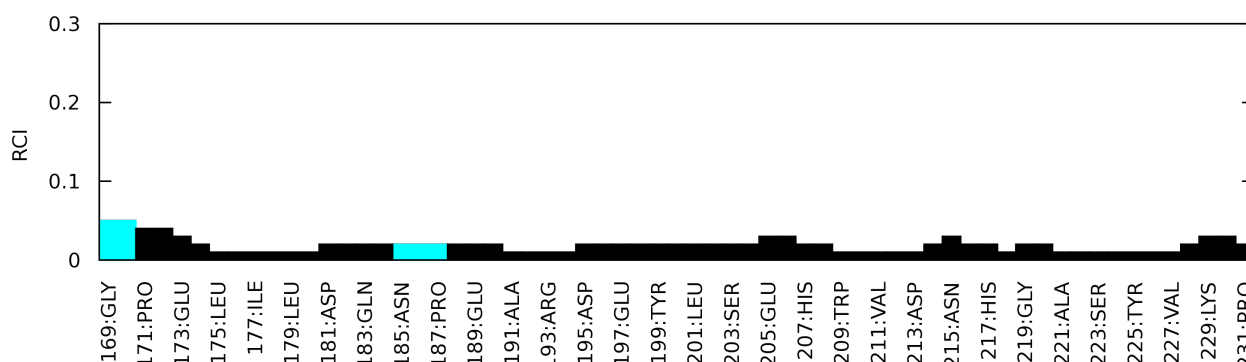
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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	203	SER	HB3	2.15	5.25 – 2.45	-6.1
1	A	222	PRO	HG2	0.21	3.48 – 0.38	-5.5
1	A	222	PRO	HG3	0.18	3.56 – 0.26	-5.2
2	B	287	PRO	CG	21.76	32.66 – 21.76	-5.0

7.2.5 Random Coil Index (RCI) plots [i](#)

The images below report *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:



Random coil index (RCI) for chain B:

