



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 07:02 AM BST

PDB ID : 3EZB
Title : COMPLEX OF THE AMINO TERMINAL DOMAIN OF ENZYME I AND
THE HISTIDINE-CONTAINING PHOSPHOCARRIER PROTEIN HPR
FROM ESCHERICHIA COLI
Authors : Clore, G.M.; Garrett, D.S.; Gronenborn, A.M.
Deposited on : 1998-11-03

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

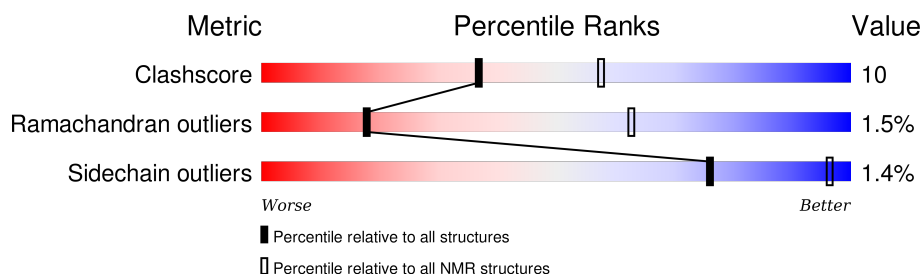
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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	259	
2	B	85	

2 Ensemble composition and analysis ⓘ

This entry contains 40 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. No representative model was identified.

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:1-A:236, B:301-B:385 (321)	Not calculated	Not calculated

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5319 atoms, of which 2691 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I).

Mol	Chain	Residues	Atoms						Trace
1	A	259	Total	C	H	N	O	S	0
			4026	1243	2038	337	403	5	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	ARG	LEU	CONFLICT	UNP P08839

- Molecule 2 is a protein called PROTEIN (PHOSPHOCARRIER PROTEIN HPR).

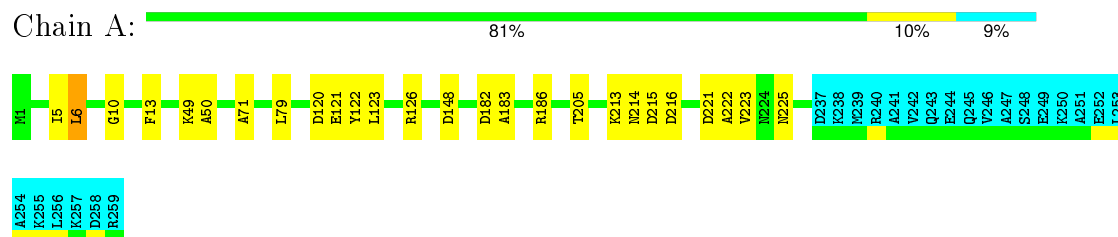
Mol	Chain	Residues	Atoms						Trace
2	B	85	Total	C	H	N	O	S	0
			1293	401	653	107	130	2	

4 Residue-property plots [i](#)

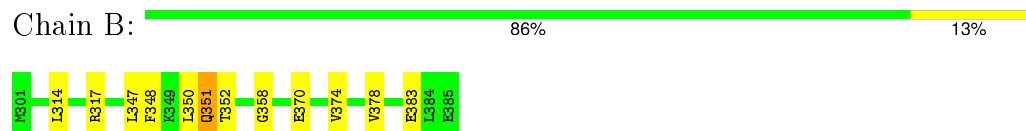
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)



- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

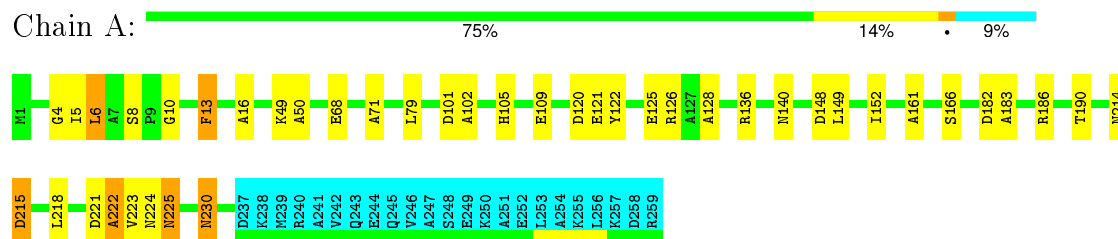


4.2 Scores per residue for each member of the ensemble

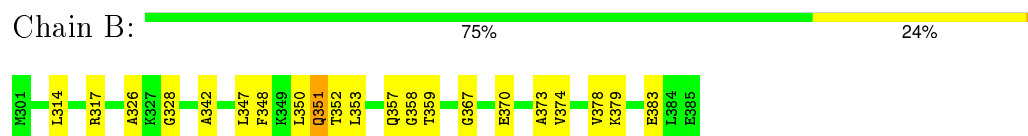
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

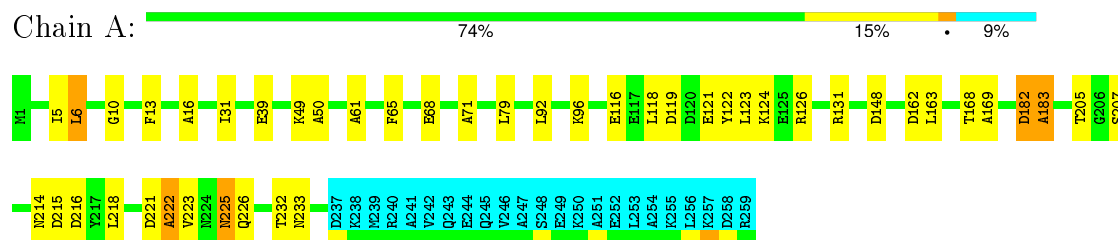


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

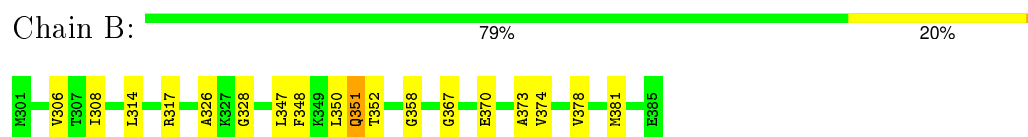


4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

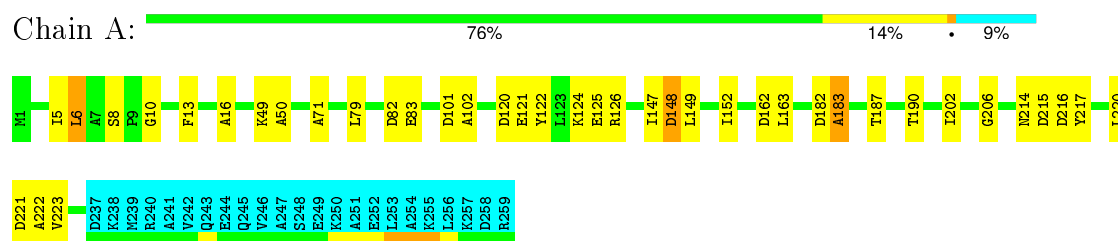


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

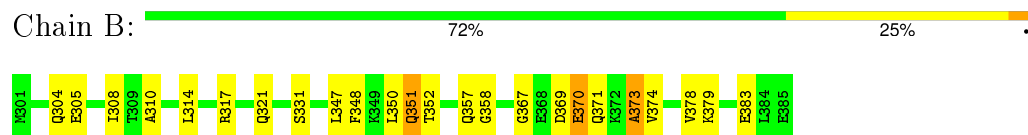


4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

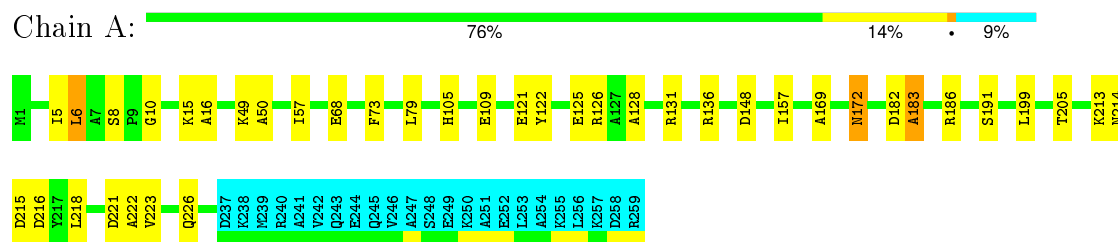


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

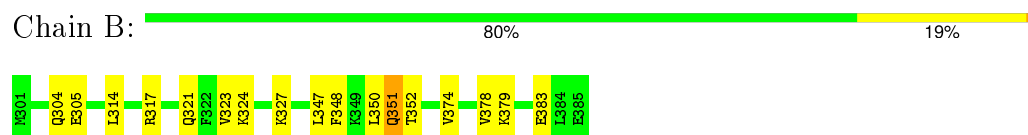


4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

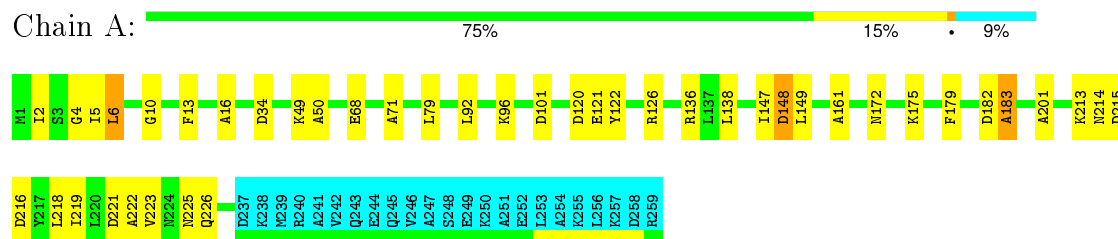


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

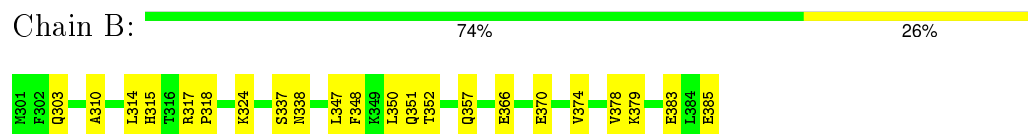


4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

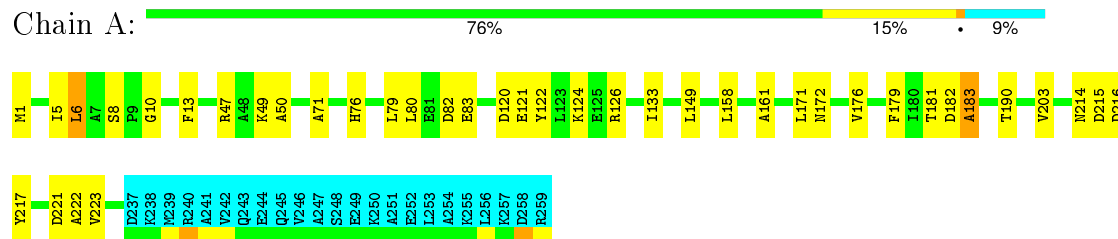


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)




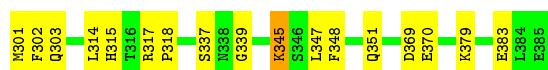
4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)



- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

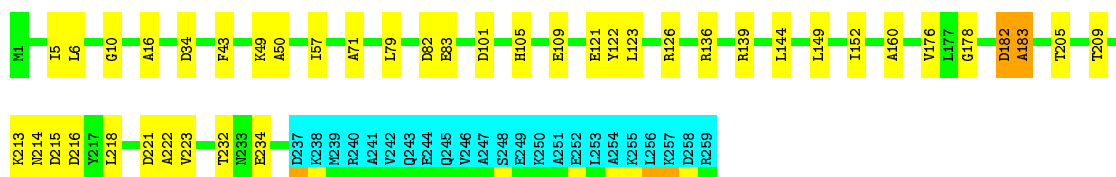
Chain B: 



4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

Chain A: 



- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

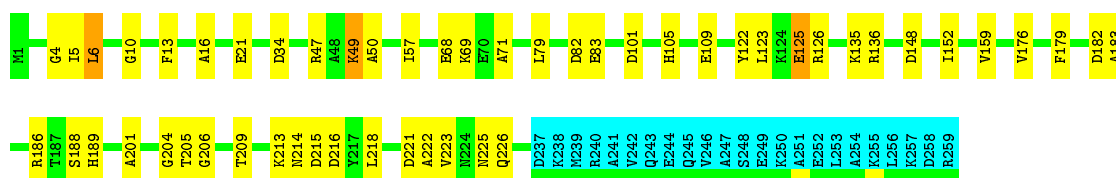
Chain B: 




4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

Chain A: 



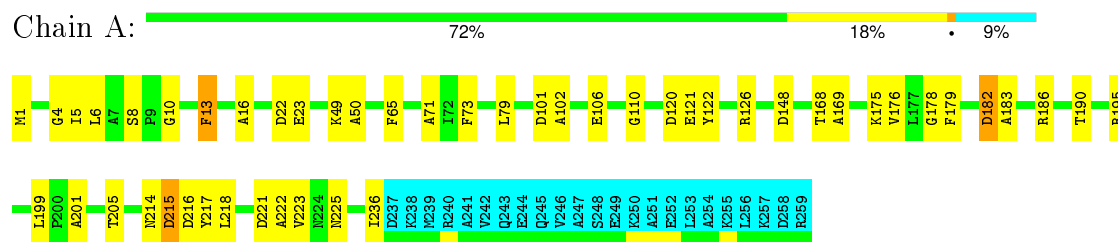
- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

Chain B: 

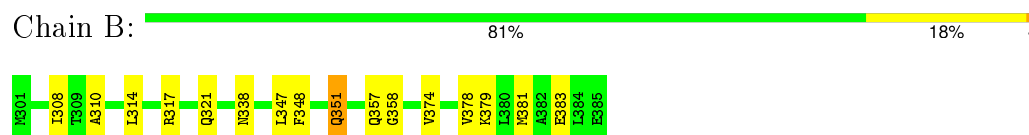


4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

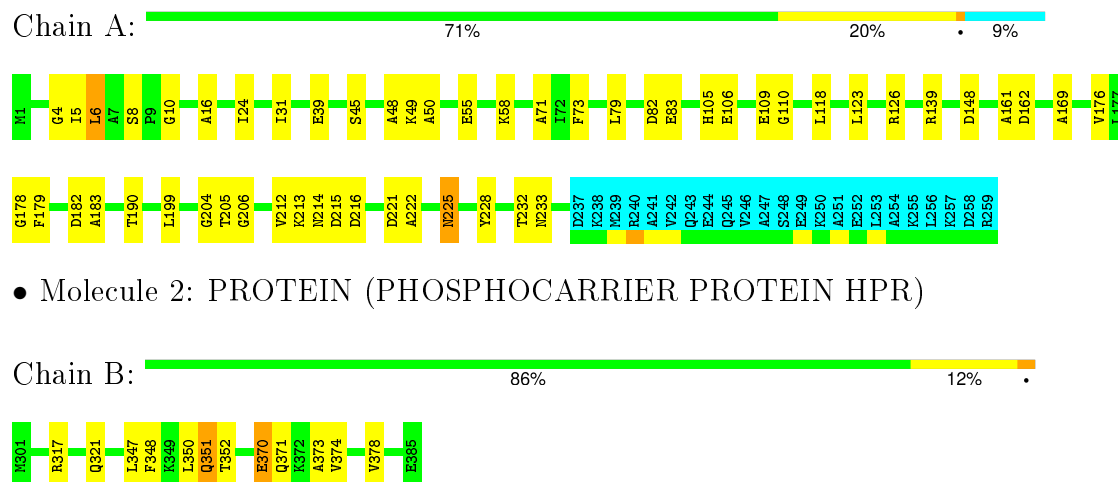


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)



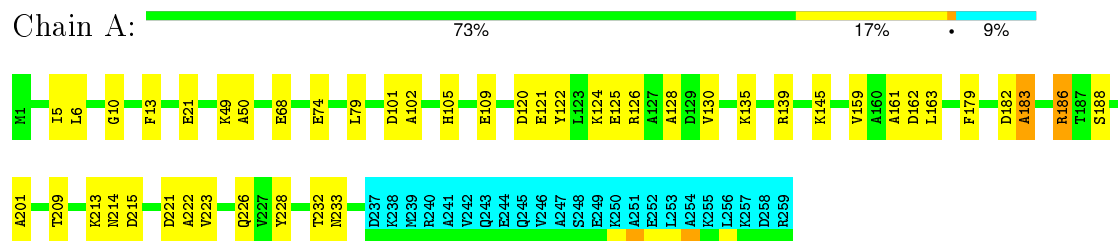
4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

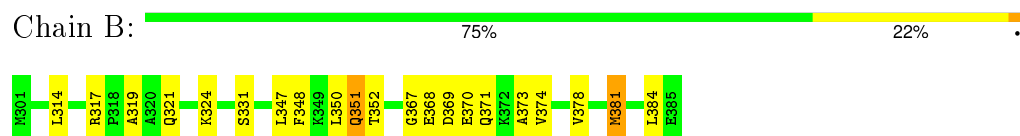


4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

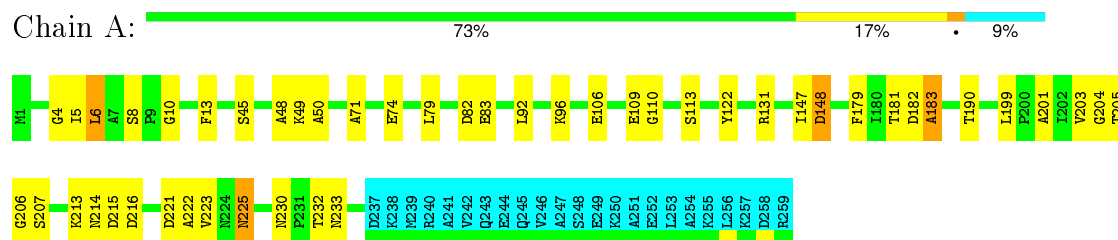


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

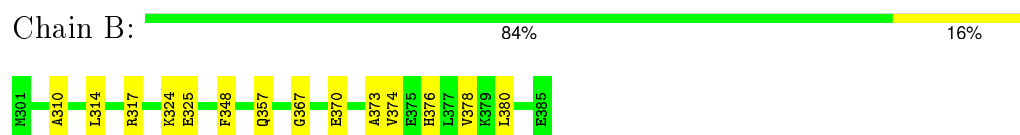


4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

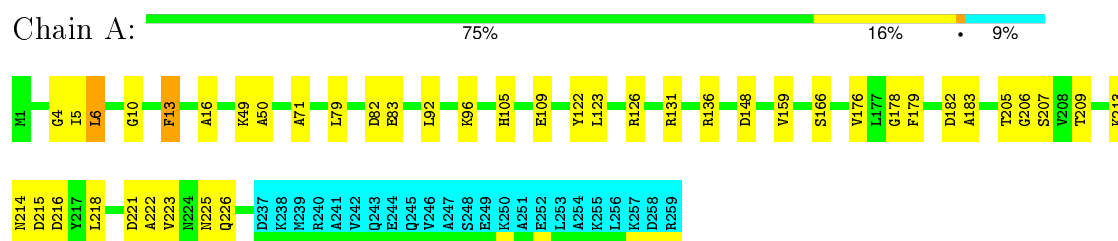


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

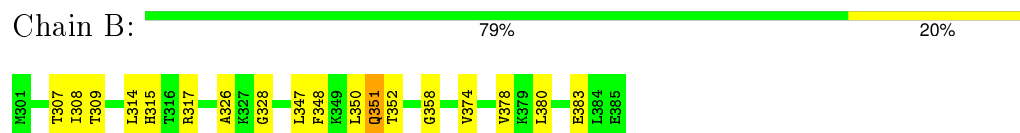


4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

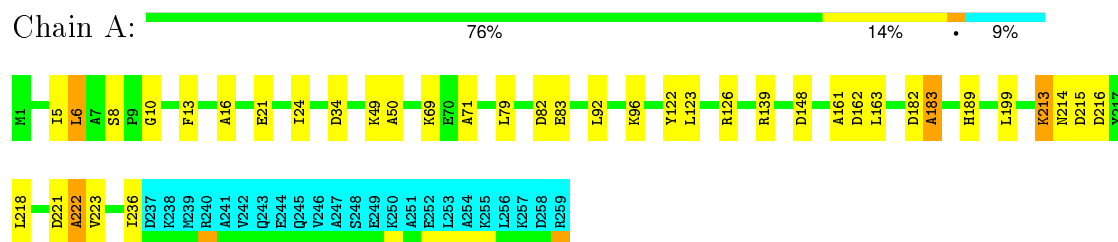


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

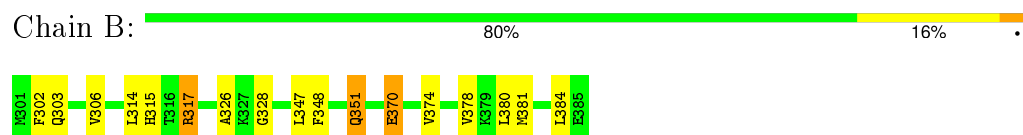


4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

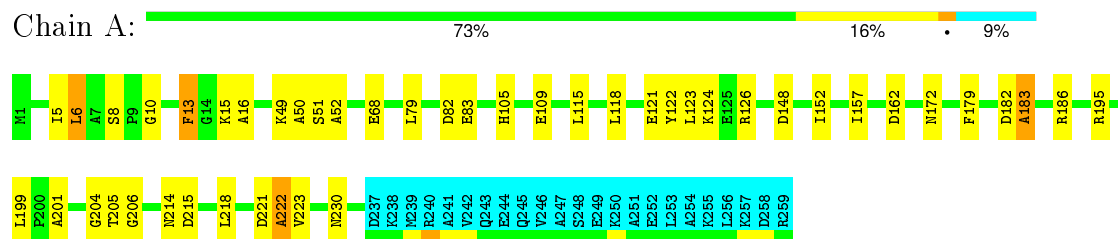


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

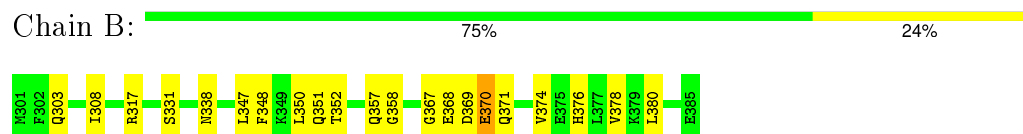


4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

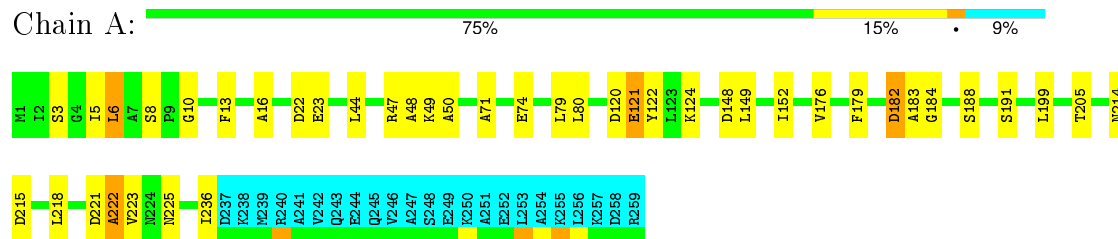


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)



4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)



- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

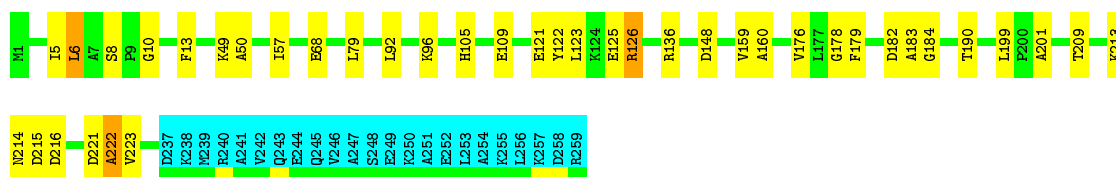
Chain B: 74% 25%



4.2.17 Score per residue for model 17

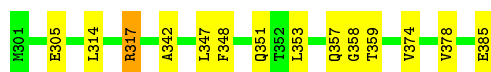
- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

Chain A: 76% 14% 9%



- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

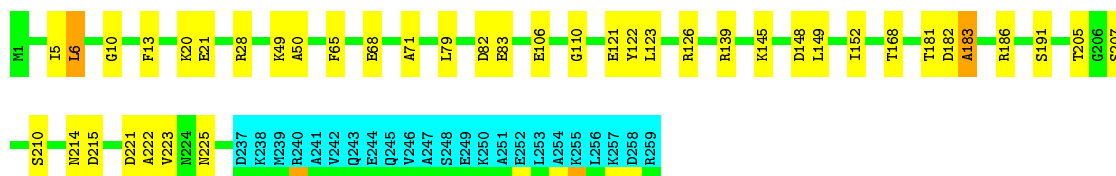
Chain B: 84% 15%



4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

Chain A: 75% 15% 9%



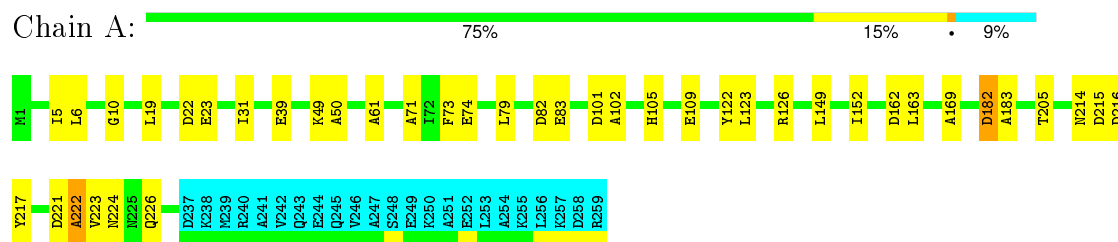
- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

Chain B: 75% 22%

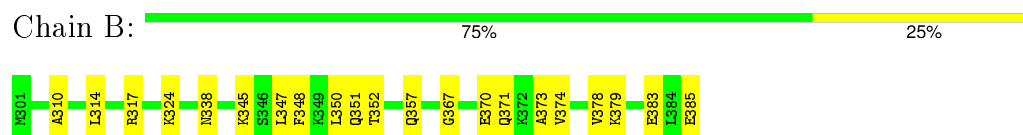


4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

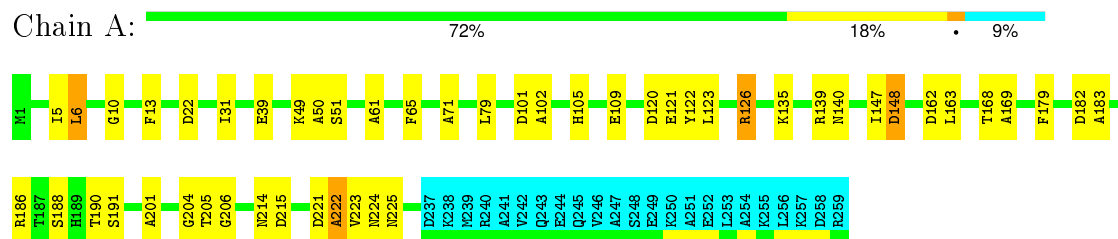


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

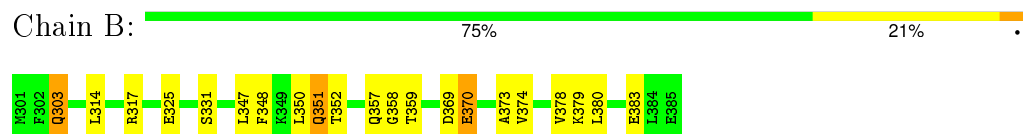


4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

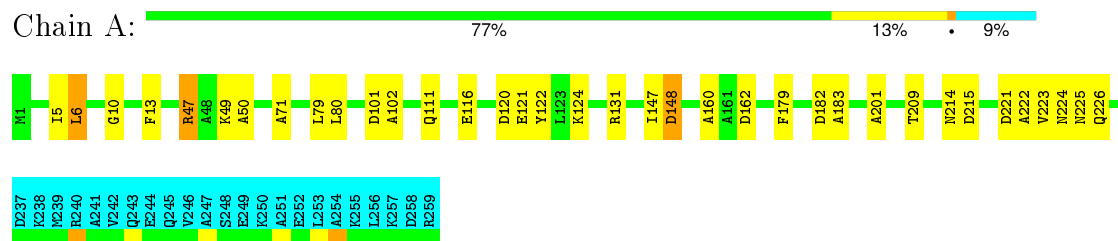


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

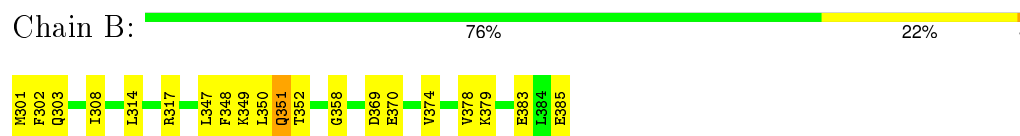


4.2.21 Score per residue for model 21

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

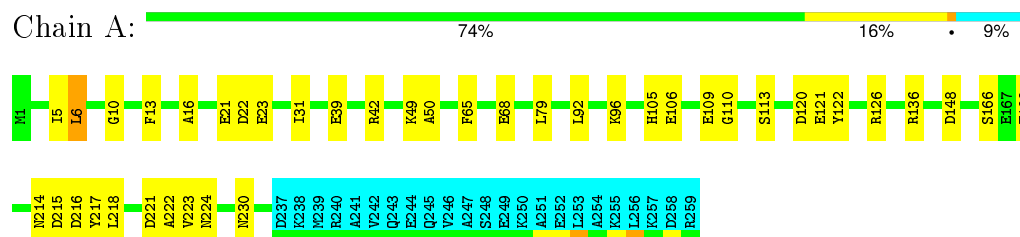


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

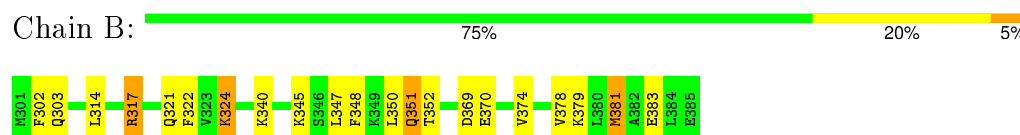


4.2.22 Score per residue for model 22

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

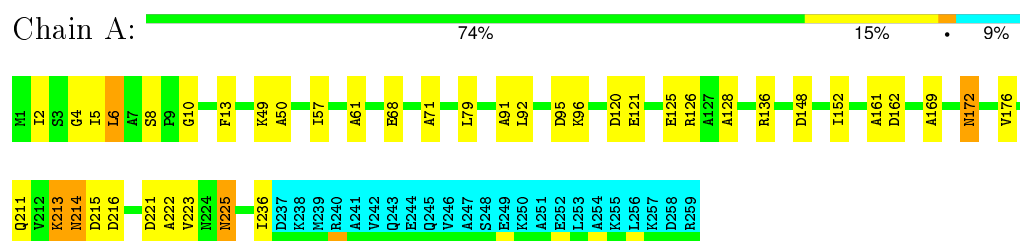


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

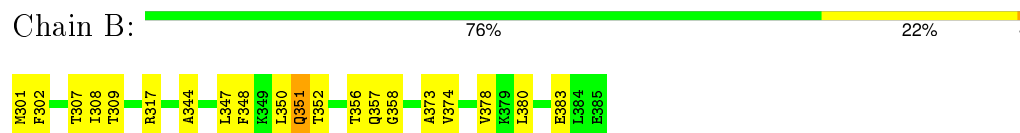


4.2.23 Score per residue for model 23

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

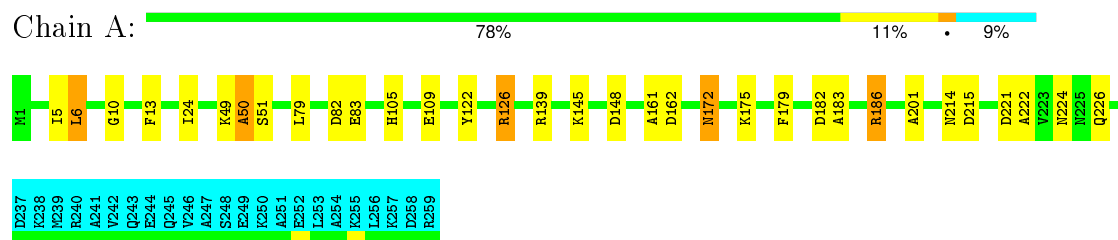


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

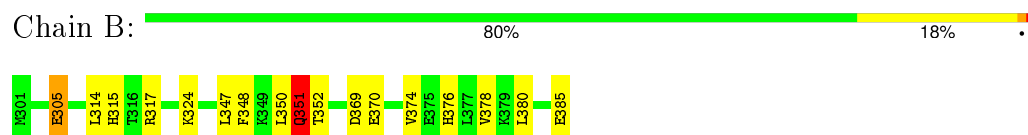


4.2.24 Score per residue for model 24

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

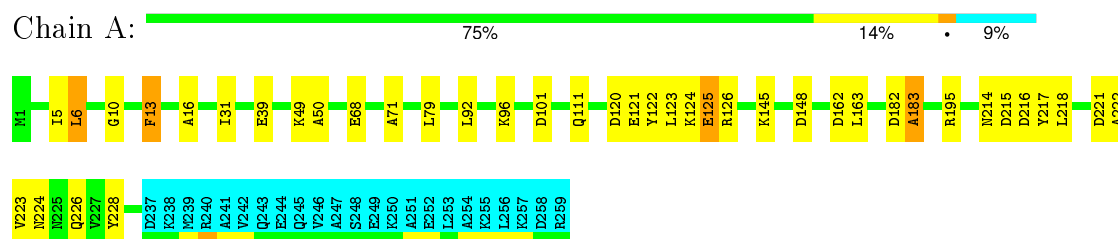


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

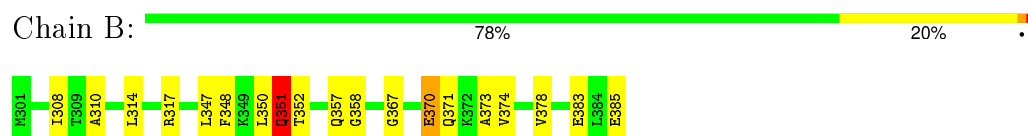


4.2.25 Score per residue for model 25

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

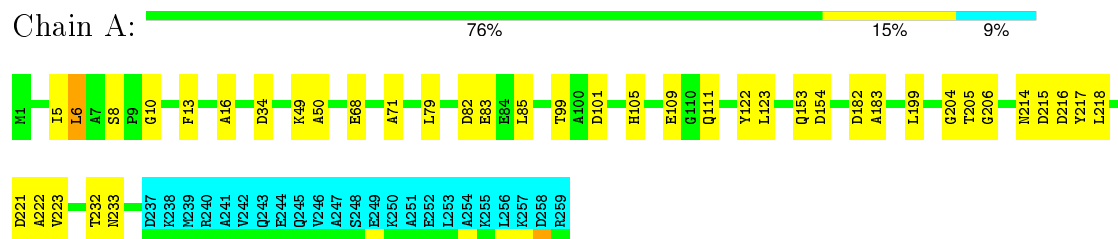


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

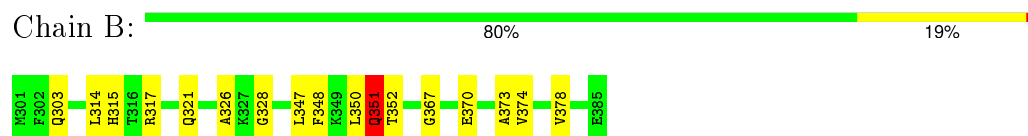


4.2.26 Score per residue for model 26

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

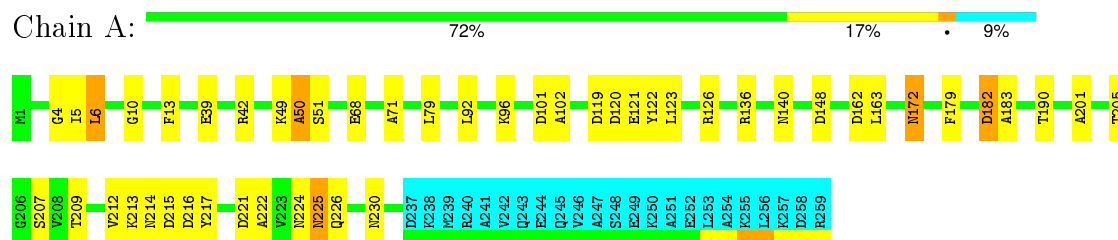


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

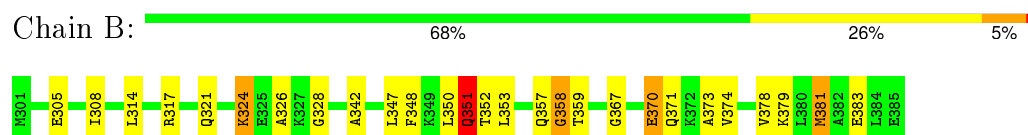


4.2.27 Score per residue for model 27

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

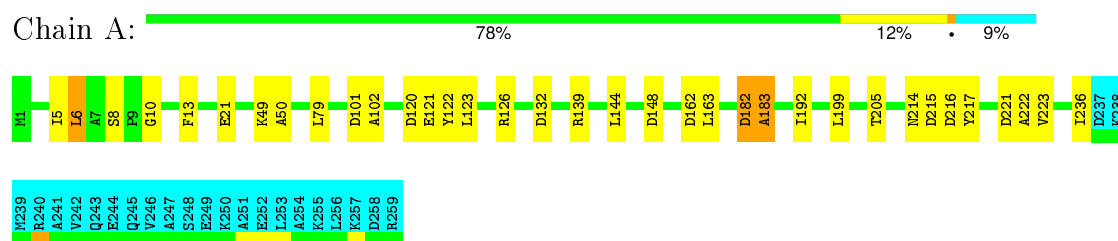


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

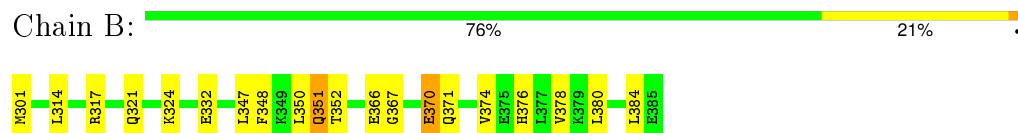


4.2.28 Score per residue for model 28

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

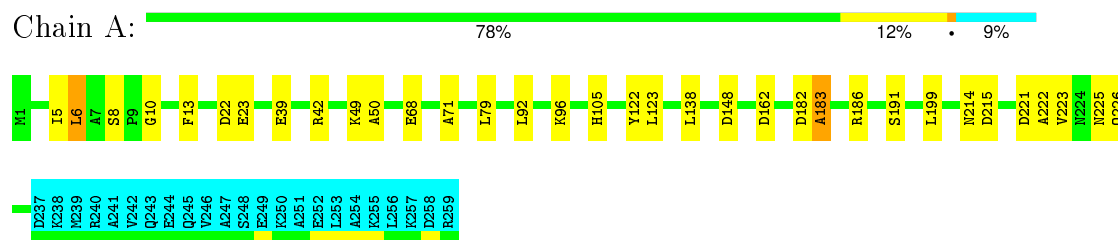


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

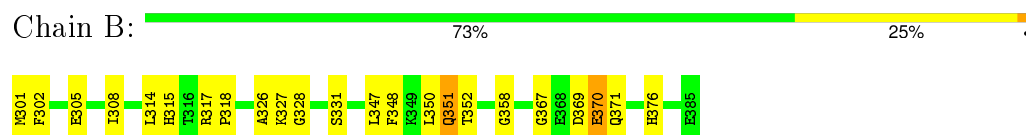


4.2.29 Score per residue for model 29

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

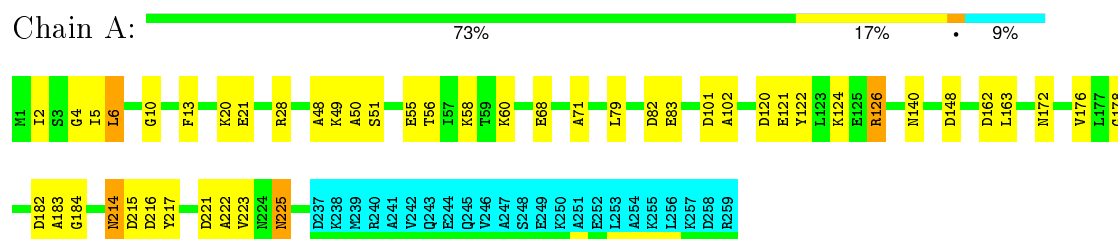


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

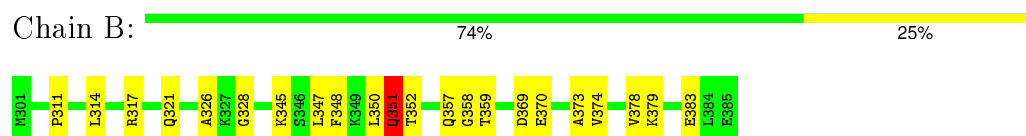


4.2.30 Score per residue for model 30

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

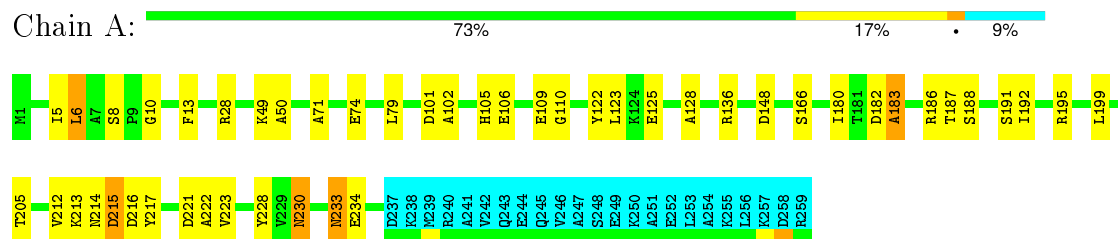


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)



4.2.31 Score per residue for model 31

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)



- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

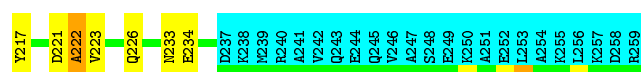
Chain B: 



4.2.32 Score per residue for model 32

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

Chain A: 



- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

Chain B: 



4.2.33 Score per residue for model 33

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

Chain A: 



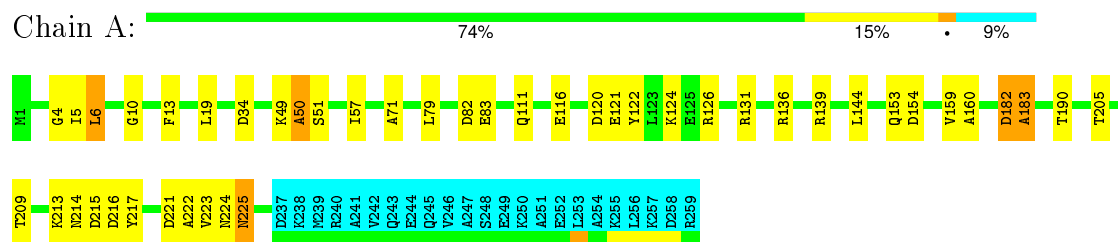
- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

Chain B: 

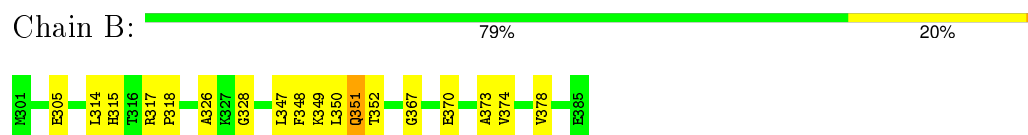


4.2.34 Score per residue for model 34

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

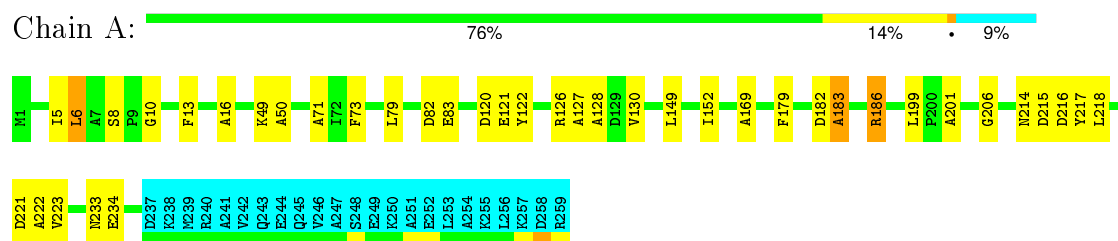


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

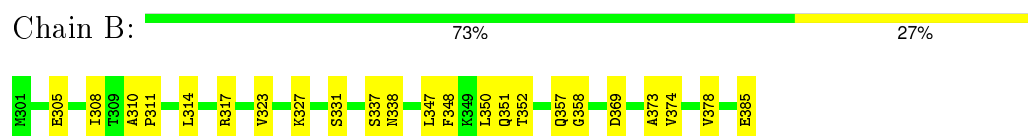


4.2.35 Score per residue for model 35

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

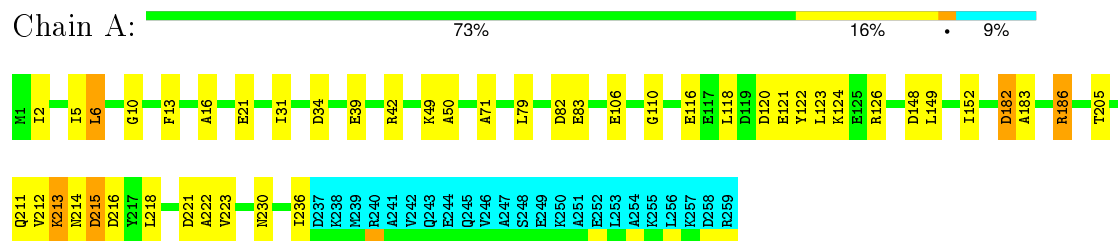


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

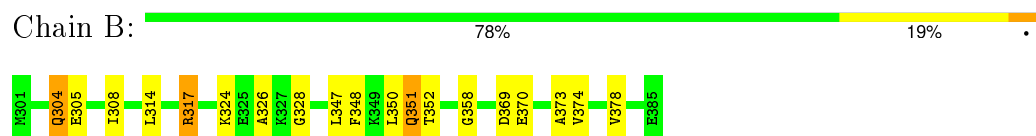


4.2.36 Score per residue for model 36

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

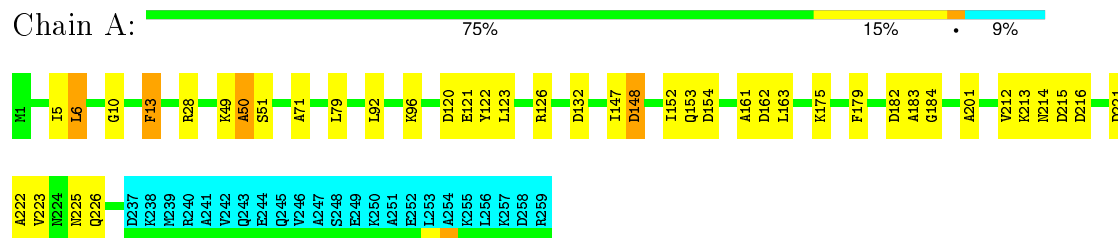


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

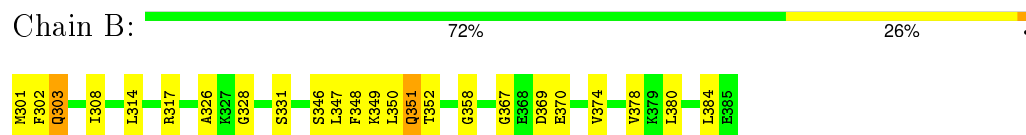


4.2.37 Score per residue for model 37

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

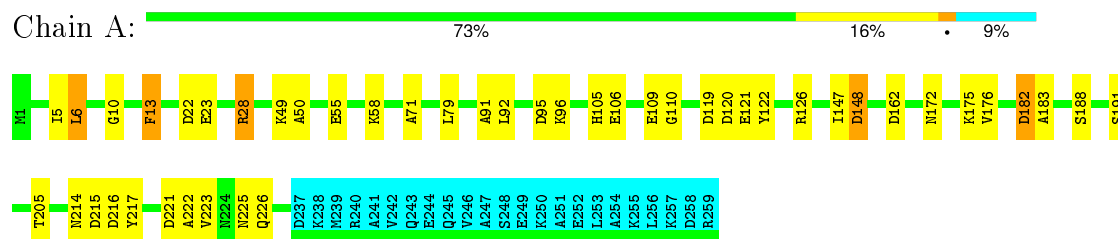


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

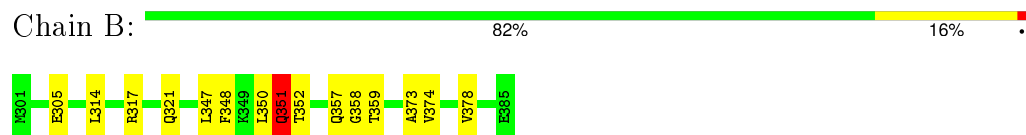


4.2.38 Score per residue for model 38

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

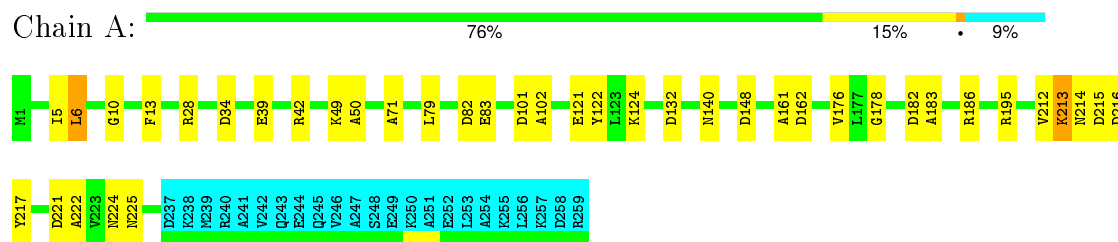


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

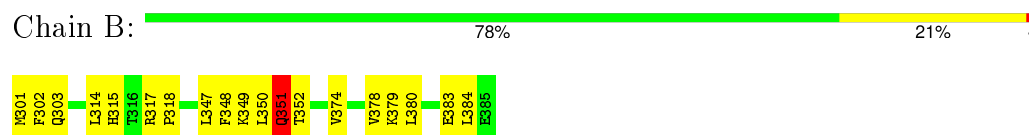


4.2.39 Score per residue for model 39

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)

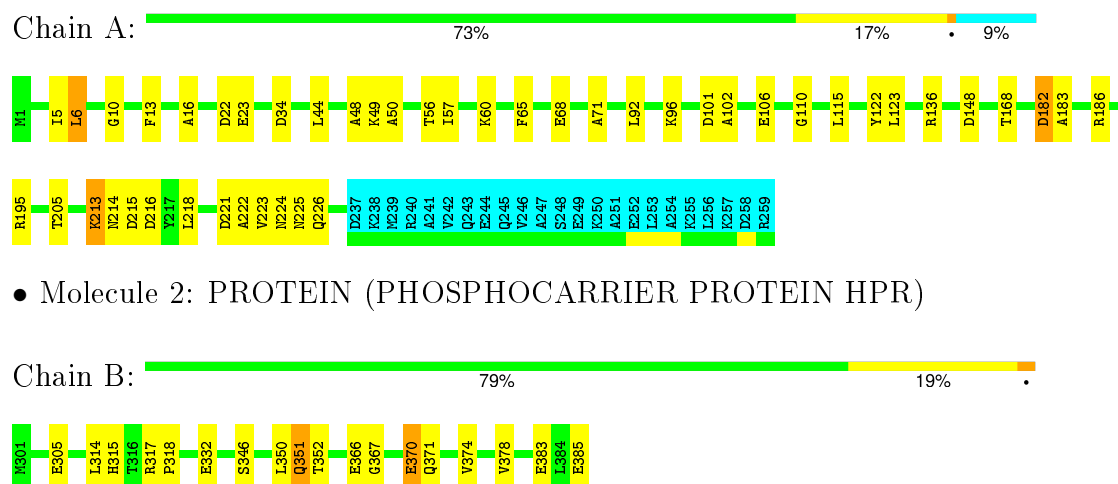


- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)



4.2.40 Score per residue for model 40

- Molecule 1: PROTEIN (PHOSPHOTRANSFER SYSTEM, ENZYME I)



- Molecule 2: PROTEIN (PHOSPHOCARRIER PROTEIN HPR)

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 40 calculated structures, 40 were deposited, based on the following criterion: *REGULARIZED MEAN STRUCTURE*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	

No chemical shift data was provided. 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	1805	1847	1847	37±6
2	B	640	653	650	20±4
All	All	97799	99997	99876	1972

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:LEU:HD22	2:B:347:LEU:HD23	0.93	1.40	24	38
1:A:10:GLY:O	1:A:222:ALA:HB3	0.81	1.76	28	40
1:A:123:LEU:HD22	2:B:351:GLN:O	0.80	1.76	7	14
1:A:79:LEU:HD11	2:B:348:PHE:CE2	0.78	2.14	22	39
1:A:79:LEU:HD11	2:B:348:PHE:CZ	0.73	2.18	3	24
1:A:16:ALA:HB3	1:A:216:ASP:OD1	0.73	1.83	2	1
1:A:126:ARG:HE	2:B:351:GLN:HE22	0.67	1.30	34	3
1:A:126:ARG:NE	2:B:351:GLN:HE22	0.65	1.89	10	4
1:A:122:TYR:CE1	1:A:126:ARG:NH1	0.65	2.64	22	6
1:A:172:ASN:ND2	1:A:175:LYS:NZ	0.65	2.45	5	1
1:A:172:ASN:ND2	1:A:172:ASN:H	0.65	1.89	23	1
1:A:71:ALA:CB	2:B:317:ARG:NH1	0.64	2.60	34	9
1:A:126:ARG:NE	2:B:351:GLN:HE21	0.63	1.91	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ARG:NE	2:B:351:GLN:NE2	0.63	2.47	23	9
2:B:350:LEU:O	2:B:352:THR:N	0.63	2.32	24	35
2:B:346:SER:CB	2:B:349:LYS:HZ3	0.63	2.07	31	3
1:A:233:ASN:ND2	1:A:234:GLU:H	0.63	1.91	31	1
2:B:317:ARG:NH2	2:B:321:GLN:NE2	0.62	2.47	18	3
2:B:351:GLN:HE21	2:B:351:GLN:N	0.62	1.92	39	3
1:A:79:LEU:HD21	2:B:348:PHE:CE1	0.62	2.28	27	21
1:A:122:TYR:CZ	1:A:126:ARG:NH1	0.62	2.68	18	3
2:B:351:GLN:NE2	2:B:351:GLN:N	0.62	2.48	39	3
1:A:4:GLY:H	1:A:225:ASN:HD21	0.61	1.37	1	10
1:A:233:ASN:ND2	1:A:234:GLU:N	0.60	2.49	31	1
2:B:317:ARG:NE	2:B:321:GLN:NE2	0.60	2.49	38	4
1:A:126:ARG:NH2	2:B:314:LEU:O	0.60	2.34	13	2
1:A:126:ARG:HE	2:B:351:GLN:NE2	0.60	1.95	22	3
1:A:214:ASN:N	1:A:214:ASN:HD22	0.60	1.94	30	2
1:A:152:ILE:N	1:A:152:ILE:HD12	0.59	2.11	23	3
1:A:4:GLY:H	1:A:225:ASN:ND2	0.59	1.95	1	5
1:A:232:THR:HG22	1:A:233:ASN:N	0.59	2.12	10	5
2:B:301:MET:SD	2:B:302:PHE:N	0.59	2.76	18	1
1:A:159:VAL:HG12	1:A:209:THR:HG22	0.59	1.74	34	4
1:A:13:PHE:CD1	1:A:13:PHE:N	0.59	2.71	9	18
2:B:370:GLU:OE1	2:B:370:GLU:N	0.58	2.35	29	5
2:B:370:GLU:N	2:B:370:GLU:OE1	0.58	2.36	11	4
1:A:13:PHE:N	1:A:13:PHE:CD1	0.58	2.70	26	17
2:B:331:SER:OG	2:B:369:ASP:N	0.57	2.36	16	9
2:B:317:ARG:HH21	2:B:321:GLN:NE2	0.57	1.97	18	6
2:B:347:LEU:O	2:B:351:GLN:NE2	0.57	2.38	9	6
1:A:4:GLY:N	1:A:225:ASN:HD21	0.57	1.98	5	1
2:B:374:VAL:O	2:B:378:VAL:HG23	0.57	1.99	38	38
2:B:317:ARG:NH2	2:B:321:GLN:HE22	0.57	1.98	18	2
1:A:182:ASP:OD1	1:A:209:THR:HG23	0.57	1.99	13	2
1:A:172:ASN:N	1:A:172:ASN:ND2	0.57	2.50	23	1
1:A:126:ARG:NE	2:B:351:GLN:OE1	0.57	2.38	1	4
1:A:172:ASN:ND2	1:A:175:LYS:H	0.57	1.98	24	1
1:A:131:ARG:HE	1:A:135:LYS:NZ	0.56	1.98	33	1
1:A:111:GLN:HE21	2:B:348:PHE:CB	0.56	2.13	26	3
1:A:186:ARG:HE	1:A:195:ARG:HH21	0.56	1.42	15	1
1:A:126:ARG:HH21	2:B:351:GLN:NE2	0.56	1.98	7	2
2:B:323:VAL:CG1	2:B:327:LYS:HZ2	0.56	2.14	4	1
1:A:47:ARG:NH2	1:A:80:LEU:O	0.56	2.39	21	4
1:A:71:ALA:HB2	2:B:317:ARG:NH1	0.56	2.16	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ARG:CZ	2:B:351:GLN:HE21	0.56	2.14	23	1
1:A:152:ILE:CD1	1:A:152:ILE:N	0.56	2.69	23	1
1:A:216:ASP:OD1	1:A:217:TYR:N	0.55	2.39	19	16
2:B:370:GLU:OE1	2:B:371:GLN:N	0.55	2.40	28	7
1:A:126:ARG:CZ	2:B:351:GLN:NE2	0.55	2.70	17	3
2:B:351:GLN:N	2:B:351:GLN:OE1	0.55	2.39	25	5
1:A:221:ASP:OD2	1:A:226:GLN:N	0.55	2.39	4	9
2:B:351:GLN:HE21	2:B:351:GLN:CA	0.55	2.14	39	2
1:A:126:ARG:NH1	2:B:351:GLN:OE1	0.55	2.39	28	2
1:A:22:ASP:OD1	1:A:23:GLU:N	0.55	2.40	29	7
1:A:233:ASN:OD1	1:A:234:GLU:N	0.55	2.40	32	2
2:B:379:LYS:O	2:B:383:GLU:N	0.55	2.40	7	18
2:B:351:GLN:OE1	2:B:351:GLN:N	0.55	2.39	38	2
1:A:182:ASP:N	1:A:182:ASP:OD1	0.55	2.40	38	7
1:A:121:GLU:CD	1:A:121:GLU:H	0.55	2.05	37	1
2:B:321:GLN:HE22	2:B:324:LYS:NZ	0.55	1.98	4	1
2:B:323:VAL:CG1	2:B:327:LYS:NZ	0.55	2.70	4	2
1:A:186:ARG:HE	1:A:195:ARG:HH12	0.55	1.45	39	1
1:A:105:HIS:NE2	1:A:109:GLU:OE1	0.55	2.40	38	13
1:A:162:ASP:OD1	1:A:163:LEU:N	0.55	2.40	14	11
1:A:126:ARG:CG	2:B:351:GLN:HE22	0.55	2.14	1	1
1:A:79:LEU:HD11	2:B:348:PHE:CD2	0.54	2.37	10	13
1:A:39:GLU:OE2	1:A:42:ARG:NH1	0.54	2.40	29	4
1:A:22:ASP:OD1	1:A:22:ASP:N	0.54	2.40	33	1
1:A:182:ASP:OD1	1:A:182:ASP:N	0.54	2.41	40	6
1:A:120:ASP:OD1	1:A:121:GLU:N	0.54	2.40	21	21
1:A:221:ASP:O	1:A:223:VAL:N	0.54	2.41	32	32
1:A:121:GLU:O	1:A:124:LYS:N	0.54	2.41	30	12
1:A:179:PHE:O	1:A:201:ALA:HB1	0.54	2.02	17	14
2:B:308:ILE:O	2:B:358:GLY:N	0.54	2.39	13	14
1:A:116:GLU:OE2	1:A:131:ARG:NH2	0.54	2.41	21	2
1:A:61:ALA:HB2	1:A:169:ALA:HB1	0.54	1.80	2	4
2:B:302:PHE:CD1	2:B:303:GLN:N	0.54	2.75	8	8
1:A:221:ASP:OD2	1:A:225:ASN:N	0.54	2.41	37	6
1:A:55:GLU:OE1	1:A:58:LYS:NZ	0.54	2.41	38	3
1:A:152:ILE:N	1:A:152:ILE:CD1	0.54	2.71	8	2
2:B:317:ARG:CZ	2:B:321:GLN:NE2	0.54	2.70	38	2
1:A:49:LYS:CG	1:A:50:ALA:N	0.54	2.71	8	1
1:A:126:ARG:CD	2:B:351:GLN:HE22	0.54	2.16	1	3
2:B:321:GLN:NE2	2:B:384:LEU:HD21	0.54	2.17	7	1
2:B:326:ALA:O	2:B:328:GLY:N	0.54	2.41	29	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:GLU:OE1	1:A:125:GLU:N	0.54	2.41	25	1
1:A:221:ASP:CG	1:A:226:GLN:H	0.54	2.07	37	9
1:A:122:TYR:OH	2:B:315:HIS:N	0.54	2.41	26	3
1:A:10:GLY:O	1:A:221:ASP:O	0.53	2.26	13	38
1:A:105:HIS:CD2	1:A:109:GLU:OE1	0.53	2.61	22	14
1:A:125:GLU:O	1:A:128:ALA:HB3	0.53	2.02	23	5
2:B:317:ARG:NH2	2:B:321:GLN:OE1	0.53	2.41	26	2
1:A:19:LEU:HD21	1:A:149:LEU:HD21	0.53	1.79	19	1
1:A:221:ASP:OD1	1:A:222:ALA:N	0.53	2.41	37	8
1:A:57:ILE:CD1	1:A:136:ARG:HH22	0.53	2.17	17	6
1:A:21:GLU:OE1	1:A:139:ARG:NH2	0.53	2.41	18	1
1:A:214:ASN:OD1	1:A:215:ASP:N	0.53	2.42	39	2
1:A:122:TYR:O	1:A:126:ARG:NH1	0.53	2.42	3	2
1:A:195:ARG:HH11	1:A:195:ARG:CG	0.53	2.17	25	1
1:A:4:GLY:N	1:A:225:ASN:ND2	0.53	2.57	5	1
1:A:123:LEU:HD23	1:A:126:ARG:HH22	0.53	1.63	2	4
1:A:224:ASN:ND2	1:A:226:GLN:OE1	0.53	2.42	27	2
2:B:340:LYS:NZ	2:B:352:THR:O	0.53	2.40	22	1
2:B:305:GLU:N	2:B:305:GLU:OE1	0.53	2.42	38	6
1:A:233:ASN:HD22	1:A:234:GLU:H	0.53	1.45	31	1
1:A:126:ARG:CZ	2:B:351:GLN:HE22	0.53	2.17	10	2
1:A:21:GLU:OE1	1:A:21:GLU:N	0.53	2.42	30	2
1:A:214:ASN:ND2	1:A:214:ASN:O	0.53	2.42	23	1
2:B:321:GLN:OE1	2:B:324:LYS:NZ	0.53	2.41	27	2
1:A:214:ASN:O	1:A:215:ASP:CB	0.53	2.56	19	40
1:A:101:ASP:OD1	1:A:102:ALA:N	0.53	2.42	9	13
2:B:385:GLU:N	2:B:385:GLU:OE1	0.53	2.41	25	2
2:B:351:GLN:N	2:B:351:GLN:NE2	0.53	2.57	9	1
2:B:337:SER:O	2:B:338:ASN:ND2	0.52	2.42	5	1
1:A:125:GLU:N	1:A:125:GLU:OE1	0.52	2.42	8	1
1:A:233:ASN:N	1:A:233:ASN:HD22	0.52	2.00	31	1
2:B:304:GLN:OE1	2:B:305:GLU:N	0.52	2.42	32	1
1:A:221:ASP:OD1	1:A:221:ASP:N	0.52	2.42	5	6
1:A:21:GLU:N	1:A:21:GLU:OE1	0.52	2.42	22	3
2:B:310:ALA:N	2:B:357:GLN:OE1	0.52	2.43	32	1
2:B:357:GLN:O	2:B:359:THR:N	0.52	2.43	17	7
1:A:182:ASP:OD2	1:A:206:GLY:N	0.52	2.43	13	1
1:A:214:ASN:O	1:A:214:ASN:ND2	0.52	2.42	30	1
1:A:221:ASP:OD2	1:A:224:ASN:N	0.52	2.42	20	4
1:A:126:ARG:NH1	2:B:314:LEU:O	0.52	2.43	34	1
2:B:351:GLN:CA	2:B:351:GLN:HE21	0.52	2.16	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:GLU:CD	2:B:324:LYS:NZ	0.52	2.63	11	3
1:A:224:ASN:OD1	1:A:226:GLN:NE2	0.52	2.41	40	2
1:A:68:GLU:OE1	2:B:317:ARG:NH1	0.52	2.42	18	17
1:A:71:ALA:HB3	2:B:317:ARG:CD	0.52	2.35	14	23
2:B:381:MET:SD	2:B:381:MET:O	0.52	2.68	11	3
2:B:331:SER:OG	2:B:368:GLU:N	0.52	2.42	15	3
1:A:126:ARG:NH2	2:B:319:ALA:CB	0.52	2.73	11	1
1:A:122:TYR:OH	2:B:314:LEU:O	0.52	2.27	22	32
1:A:122:TYR:OH	1:A:126:ARG:NH1	0.51	2.43	9	4
1:A:182:ASP:O	1:A:183:ALA:O	0.51	2.29	4	20
1:A:186:ARG:NH2	1:A:195:ARG:NH1	0.51	2.58	40	1
1:A:71:ALA:CB	2:B:317:ARG:HH11	0.51	2.18	13	6
1:A:121:GLU:N	1:A:121:GLU:OE1	0.51	2.41	18	3
1:A:149:LEU:O	1:A:152:ILE:HD12	0.51	2.05	7	8
1:A:31:ILE:HD13	1:A:39:GLU:HG3	0.51	1.82	36	5
1:A:212:VAL:HG12	1:A:213:LYS:N	0.51	2.20	37	6
1:A:214:ASN:ND2	1:A:214:ASN:N	0.51	2.58	30	2
1:A:65:PHE:CE1	1:A:168:THR:O	0.51	2.64	18	5
2:B:304:GLN:NE2	2:B:305:GLU:O	0.51	2.44	16	3
1:A:172:ASN:O	1:A:176:VAL:HG23	0.51	2.06	6	3
1:A:92:LEU:O	1:A:96:LYS:N	0.51	2.40	2	15
2:B:304:GLN:CD	2:B:305:GLU:N	0.51	2.64	32	4
1:A:160:ALA:C	1:A:209:THR:HG21	0.50	2.25	34	4
2:B:317:ARG:NH1	2:B:321:GLN:CG	0.50	2.74	10	1
2:B:385:GLU:OE1	2:B:385:GLU:N	0.50	2.44	5	3
1:A:221:ASP:N	1:A:221:ASP:OD1	0.50	2.44	38	3
1:A:221:ASP:OD2	1:A:224:ASN:ND2	0.50	2.44	34	2
2:B:381:MET:O	2:B:381:MET:CE	0.50	2.59	27	1
1:A:221:ASP:C	1:A:223:VAL:N	0.50	2.64	17	36
1:A:101:ASP:N	1:A:101:ASP:OD1	0.50	2.43	7	3
1:A:176:VAL:HG11	1:A:179:PHE:CE1	0.50	2.42	6	6
2:B:380:LEU:O	2:B:383:GLU:N	0.50	2.42	13	2
1:A:69:LYS:NZ	1:A:189:HIS:NE2	0.50	2.51	8	2
2:B:370:GLU:CD	2:B:371:GLN:N	0.50	2.65	29	2
1:A:123:LEU:CD2	1:A:126:ARG:HH21	0.50	2.19	32	5
1:A:123:LEU:CD2	1:A:126:ARG:HH22	0.50	2.20	18	4
1:A:74:GLU:OE2	2:B:324:LYS:NZ	0.50	2.43	19	2
2:B:323:VAL:CG1	2:B:327:LYS:HZ3	0.50	2.20	35	1
1:A:195:ARG:NH1	1:A:195:ARG:CG	0.50	2.71	25	1
2:B:321:GLN:CD	2:B:324:LYS:NZ	0.50	2.65	22	1
1:A:213:LYS:N	1:A:216:ASP:OD2	0.50	2.41	12	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ILE:HD11	1:A:136:ARG:HH22	0.50	1.67	4	1
1:A:182:ASP:O	1:A:182:ASP:OD1	0.50	2.30	15	6
1:A:136:ARG:HH12	1:A:166:SER:CB	0.49	2.20	13	4
2:B:367:GLY:O	2:B:370:GLU:OE1	0.49	2.29	29	2
2:B:315:HIS:CD2	2:B:318:PRO:CD	0.49	2.95	5	7
1:A:162:ASP:N	1:A:162:ASP:OD1	0.49	2.42	29	5
1:A:121:GLU:H	1:A:121:GLU:CD	0.49	2.09	17	1
2:B:306:VAL:HG22	2:B:307:THR:N	0.49	2.22	33	1
1:A:111:GLN:NE2	2:B:348:PHE:CB	0.49	2.75	25	1
1:A:79:LEU:HD13	2:B:347:LEU:HB3	0.49	1.84	22	20
1:A:47:ARG:CG	1:A:47:ARG:NH1	0.49	2.74	8	1
2:B:303:GLN:CD	2:B:303:GLN:N	0.49	2.66	20	3
1:A:182:ASP:OD2	1:A:206:GLY:O	0.49	2.31	26	10
1:A:47:ARG:NH1	1:A:47:ARG:CG	0.49	2.73	21	1
1:A:6:LEU:HD11	1:A:8:SER:O	0.49	2.07	6	3
1:A:172:ASN:ND2	1:A:175:LYS:HZ1	0.49	2.05	5	1
1:A:106:GLU:O	1:A:110:GLY:N	0.49	2.43	9	9
1:A:8:SER:CB	1:A:199:LEU:O	0.49	2.60	14	12
1:A:24:ILE:HD11	1:A:139:ARG:NH1	0.49	2.22	24	2
1:A:172:ASN:OD1	1:A:172:ASN:N	0.49	2.45	30	1
2:B:374:VAL:O	2:B:378:VAL:CG2	0.49	2.61	36	13
2:B:376:HIS:O	2:B:380:LEU:N	0.49	2.45	28	3
1:A:221:ASP:C	1:A:223:VAL:H	0.49	2.11	23	18
1:A:4:GLY:O	1:A:225:ASN:ND2	0.49	2.46	5	1
1:A:16:ALA:HB2	1:A:218:LEU:HD12	0.49	1.84	5	16
2:B:305:GLU:H	2:B:305:GLU:CD	0.49	2.11	24	2
2:B:370:GLU:OE2	2:B:371:GLN:NE2	0.49	2.41	10	1
2:B:305:GLU:N	2:B:305:GLU:CD	0.49	2.67	3	3
2:B:322:PHE:CE1	2:B:381:MET:SD	0.49	3.06	22	1
1:A:82:ASP:OD1	1:A:83:GLU:N	0.48	2.46	6	19
1:A:161:ALA:O	1:A:182:ASP:OD1	0.48	2.31	37	9
2:B:381:MET:CE	2:B:381:MET:O	0.48	2.61	33	2
2:B:301:MET:N	2:B:366:GLU:OE1	0.48	2.46	7	2
2:B:346:SER:OG	2:B:349:LYS:NZ	0.48	2.42	37	1
1:A:101:ASP:OD1	1:A:138:LEU:HD22	0.48	2.08	5	1
1:A:230:ASN:O	1:A:230:ASN:ND2	0.48	2.45	15	2
1:A:47:ARG:HH11	1:A:47:ARG:CG	0.48	2.21	21	1
1:A:19:LEU:HD12	1:A:160:ALA:HB2	0.48	1.85	34	1
1:A:5:ILE:O	1:A:5:ILE:HG22	0.48	2.09	7	6
1:A:5:ILE:O	1:A:6:LEU:O	0.48	2.31	39	34
1:A:122:TYR:OH	1:A:126:ARG:CZ	0.48	2.62	36	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:ARG:HH11	1:A:139:ARG:HG2	0.48	1.69	14	1
1:A:192:ILE:N	1:A:192:ILE:HD12	0.48	2.23	28	1
2:B:345:LYS:NZ	2:B:345:LYS:CB	0.48	2.77	6	1
2:B:380:LEU:O	2:B:384:LEU:CD2	0.48	2.62	39	6
1:A:182:ASP:OD2	1:A:207:SER:N	0.48	2.46	13	2
1:A:131:ARG:CG	1:A:131:ARG:NH1	0.48	2.76	2	1
1:A:126:ARG:NH1	2:B:351:GLN:CD	0.48	2.67	24	1
1:A:105:HIS:HB2	1:A:138:LEU:HD21	0.48	1.86	29	1
2:B:385:GLU:CD	2:B:385:GLU:H	0.48	2.11	17	2
2:B:381:MET:SD	2:B:381:MET:C	0.48	2.92	33	2
1:A:69:LYS:NZ	1:A:189:HIS:CE1	0.48	2.81	14	1
2:B:310:ALA:O	2:B:357:GLN:CG	0.48	2.61	3	6
1:A:214:ASN:O	1:A:215:ASP:OD1	0.48	2.31	1	2
2:B:326:ALA:C	2:B:328:GLY:N	0.48	2.68	29	11
2:B:305:GLU:CD	2:B:305:GLU:N	0.47	2.67	24	1
1:A:182:ASP:OD1	1:A:182:ASP:O	0.47	2.32	22	3
1:A:20:LYS:NZ	1:A:20:LYS:CB	0.47	2.76	30	2
2:B:350:LEU:C	2:B:352:THR:N	0.47	2.68	29	23
2:B:351:GLN:NE2	2:B:351:GLN:CA	0.47	2.77	39	1
1:A:149:LEU:O	1:A:152:ILE:CD1	0.47	2.62	36	6
1:A:101:ASP:OD1	1:A:141:ILE:HG21	0.47	2.08	33	1
1:A:65:PHE:CE2	1:A:168:THR:O	0.47	2.66	9	1
2:B:305:GLU:OE1	2:B:305:GLU:N	0.47	2.46	27	1
1:A:49:LYS:O	1:A:50:ALA:C	0.47	2.53	8	40
2:B:310:ALA:O	2:B:357:GLN:OE1	0.47	2.33	32	1
2:B:303:GLN:N	2:B:303:GLN:CD	0.47	2.68	37	2
1:A:39:GLU:OE2	1:A:42:ARG:NH2	0.47	2.46	22	1
1:A:34:ASP:N	1:A:34:ASP:OD1	0.47	2.46	39	1
1:A:24:ILE:HD11	1:A:139:ARG:HH11	0.47	1.70	24	1
2:B:346:SER:CB	2:B:349:LYS:NZ	0.47	2.77	31	3
1:A:126:ARG:CD	2:B:351:GLN:NE2	0.47	2.77	36	2
1:A:140:ASN:N	1:A:140:ASN:HD22	0.47	2.06	39	3
2:B:385:GLU:CD	2:B:385:GLU:N	0.47	2.68	21	2
1:A:186:ARG:CG	1:A:186:ARG:NH1	0.47	2.76	33	3
1:A:22:ASP:OD2	1:A:144:LEU:HD11	0.47	2.08	33	1
1:A:49:LYS:HB3	1:A:49:LYS:HZ3	0.47	1.68	31	1
1:A:49:LYS:CG	1:A:50:ALA:H	0.47	2.21	8	1
1:A:68:GLU:CD	2:B:317:ARG:NH1	0.47	2.67	8	4
1:A:28:ARG:NH1	1:A:28:ARG:CG	0.47	2.76	38	4
1:A:101:ASP:OD1	1:A:101:ASP:N	0.47	2.47	26	4
1:A:232:THR:CG2	1:A:233:ASN:N	0.47	2.78	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:ILE:CG2	1:A:205:THR:HG21	0.47	2.40	31	1
2:B:309:THR:C	2:B:357:GLN:HE22	0.47	2.12	32	1
1:A:123:LEU:HD23	1:A:126:ARG:HH21	0.47	1.70	28	2
1:A:176:VAL:CG1	1:A:178:GLY:O	0.47	2.63	30	7
2:B:338:ASN:ND2	2:B:338:ASN:O	0.47	2.48	9	2
1:A:5:ILE:HG22	1:A:5:ILE:O	0.47	2.10	9	9
1:A:74:GLU:OE1	2:B:324:LYS:NZ	0.47	2.45	33	4
1:A:126:ARG:NH2	2:B:351:GLN:CD	0.47	2.68	7	1
2:B:367:GLY:O	2:B:370:GLU:OE2	0.46	2.34	25	8
1:A:73:PHE:CZ	1:A:169:ALA:HB2	0.46	2.45	4	5
1:A:139:ARG:NH1	1:A:144:LEU:CD2	0.46	2.78	34	2
1:A:230:ASN:C	1:A:230:ASN:HD22	0.46	2.13	31	2
2:B:351:GLN:H	2:B:351:GLN:NE2	0.46	2.07	9	1
1:A:119:ASP:N	1:A:119:ASP:OD1	0.46	2.47	27	1
1:A:56:THR:CG2	1:A:60:LYS:NZ	0.46	2.79	30	1
1:A:149:LEU:O	1:A:172:ASN:ND2	0.46	2.49	5	1
2:B:332:GLU:N	2:B:332:GLU:OE1	0.46	2.41	28	1
1:A:172:ASN:C	1:A:172:ASN:HD22	0.46	2.14	24	2
1:A:126:ARG:NH2	2:B:315:HIS:C	0.46	2.69	24	1
1:A:186:ARG:CD	1:A:186:ARG:N	0.46	2.79	24	1
1:A:186:ARG:O	1:A:191:SER:OG	0.46	2.33	20	5
1:A:115:LEU:O	1:A:118:LEU:N	0.46	2.45	15	1
2:B:351:GLN:NE2	2:B:351:GLN:H	0.46	2.08	14	2
1:A:161:ALA:O	1:A:162:ASP:OD1	0.46	2.34	10	1
1:A:139:ARG:CG	1:A:139:ARG:NH1	0.46	2.77	14	1
1:A:181:THR:C	1:A:205:THR:HG1	0.46	2.14	33	1
1:A:8:SER:OG	1:A:201:ALA:N	0.46	2.48	23	1
1:A:182:ASP:OD1	1:A:205:THR:OG1	0.46	2.34	40	14
1:A:21:GLU:OE2	1:A:135:LYS:NZ	0.46	2.48	8	1
2:B:347:LEU:HD11	2:B:351:GLN:HE22	0.46	1.69	8	4
2:B:304:GLN:HE22	2:B:305:GLU:C	0.46	2.14	36	1
2:B:307:THR:O	2:B:309:THR:HG23	0.46	2.11	13	3
1:A:2:ILE:CD1	1:A:211:GLN:HE22	0.45	2.24	36	1
1:A:186:ARG:C	1:A:188:SER:H	0.45	2.15	31	3
2:B:344:ALA:HA	2:B:350:LEU:HD11	0.45	1.87	23	1
1:A:175:LYS:N	1:A:175:LYS:CD	0.45	2.80	9	1
1:A:186:ARG:NE	1:A:195:ARG:NH1	0.45	2.63	39	1
1:A:8:SER:OG	1:A:199:LEU:O	0.45	2.34	12	4
1:A:214:ASN:O	1:A:215:ASP:CG	0.45	2.55	31	3
1:A:214:ASN:O	1:A:215:ASP:OD2	0.45	2.35	36	2
2:B:347:LEU:O	2:B:351:GLN:OE1	0.45	2.34	13	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:TYR:OH	2:B:315:HIS:CA	0.45	2.64	29	4
1:A:139:ARG:HH11	1:A:139:ARG:CG	0.45	2.24	14	1
2:B:381:MET:C	2:B:381:MET:SD	0.45	2.95	11	1
2:B:347:LEU:CD1	2:B:351:GLN:HE22	0.45	2.24	8	4
1:A:131:ARG:CG	1:A:131:ARG:HH11	0.45	2.25	2	1
2:B:356:THR:O	2:B:357:GLN:C	0.45	2.55	23	1
2:B:370:GLU:CD	2:B:371:GLN:H	0.45	2.15	29	1
1:A:179:PHE:N	1:A:179:PHE:CD1	0.45	2.84	20	1
1:A:49:LYS:O	1:A:51:SER:N	0.45	2.50	24	5
2:B:383:GLU:O	2:B:385:GLU:OE2	0.45	2.35	19	3
2:B:311:PRO:CD	2:B:385:GLU:O	0.45	2.65	35	1
1:A:214:ASN:N	1:A:214:ASN:OD1	0.45	2.50	4	2
1:A:121:GLU:N	1:A:121:GLU:CD	0.45	2.69	37	1
2:B:345:LYS:O	2:B:345:LYS:CG	0.45	2.64	22	1
1:A:121:GLU:O	1:A:125:GLU:OE1	0.45	2.34	17	1
1:A:214:ASN:O	1:A:214:ASN:OD1	0.45	2.34	7	2
1:A:147:ILE:O	1:A:148:ASP:O	0.45	2.35	3	7
1:A:79:LEU:HD22	2:B:347:LEU:CD2	0.45	2.38	15	3
2:B:325:GLU:OE1	2:B:380:LEU:HD22	0.45	2.12	12	3
1:A:207:SER:O	1:A:207:SER:OG	0.45	2.33	12	2
1:A:126:ARG:HH11	1:A:126:ARG:CG	0.45	2.24	30	1
1:A:2:ILE:O	1:A:225:ASN:O	0.45	2.35	30	2
1:A:126:ARG:HH21	2:B:315:HIS:C	0.45	2.14	14	2
1:A:131:ARG:NH1	1:A:131:ARG:CG	0.45	2.78	13	3
2:B:317:ARG:HH21	2:B:321:GLN:HE22	0.45	1.54	11	2
2:B:306:VAL:CG2	2:B:307:THR:N	0.45	2.80	33	1
1:A:186:ARG:CB	1:A:186:ARG:NH1	0.45	2.80	40	1
1:A:58:LYS:NZ	1:A:70:GLU:OE2	0.44	2.49	33	1
1:A:16:ALA:N	1:A:216:ASP:O	0.44	2.50	10	2
2:B:304:GLN:NE2	2:B:305:GLU:N	0.44	2.66	36	1
1:A:68:GLU:OE2	2:B:317:ARG:NH1	0.44	2.50	2	1
2:B:379:LYS:O	2:B:383:GLU:OE2	0.44	2.36	33	1
2:B:366:GLU:OE1	2:B:370:GLU:OE1	0.44	2.36	32	1
1:A:162:ASP:OD1	1:A:162:ASP:N	0.44	2.50	38	1
1:A:79:LEU:CD1	2:B:348:PHE:CZ	0.44	2.99	3	1
1:A:182:ASP:OD2	1:A:205:THR:OG1	0.44	2.36	13	1
2:B:338:ASN:O	2:B:338:ASN:OD1	0.44	2.34	15	1
1:A:34:ASP:O	1:A:34:ASP:OD1	0.44	2.36	7	7
2:B:321:GLN:HE21	2:B:384:LEU:HD21	0.44	1.72	7	1
2:B:322:PHE:CD1	2:B:381:MET:SD	0.44	3.11	22	1
2:B:366:GLU:OE2	2:B:370:GLU:OE2	0.44	2.36	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:367:GLY:H	2:B:370:GLU:CD	0.44	2.16	26	7
1:A:234:GLU:OE1	1:A:234:GLU:N	0.44	2.44	7	1
1:A:116:GLU:CD	1:A:131:ARG:NH2	0.44	2.70	34	1
1:A:109:GLU:OE2	1:A:113:SER:OG	0.44	2.35	12	1
1:A:126:ARG:NH1	1:A:126:ARG:CG	0.44	2.81	30	1
1:A:158:LEU:HD22	1:A:171:LEU:HD11	0.44	1.89	6	1
1:A:188:SER:O	1:A:191:SER:OG	0.44	2.36	20	1
1:A:182:ASP:C	1:A:182:ASP:OD1	0.44	2.56	6	5
2:B:382:ALA:HB3	2:B:383:GLU:OE2	0.44	2.12	33	1
2:B:342:ALA:HB3	2:B:353:LEU:HD11	0.43	1.89	1	3
1:A:122:TYR:OH	2:B:314:LEU:C	0.43	2.56	29	4
1:A:149:LEU:O	1:A:152:ILE:HD13	0.43	2.13	1	1
1:A:172:ASN:N	1:A:172:ASN:HD22	0.43	2.09	23	1
1:A:56:THR:HG22	1:A:60:LYS:HZ3	0.43	1.73	40	1
1:A:172:ASN:N	1:A:172:ASN:OD1	0.43	2.47	4	1
1:A:119:ASP:O	1:A:119:ASP:OD1	0.43	2.37	2	2
2:B:304:GLN:OE1	2:B:305:GLU:O	0.43	2.35	36	1
2:B:350:LEU:C	2:B:352:THR:H	0.43	2.16	24	3
1:A:139:ARG:HH11	1:A:144:LEU:CD2	0.43	2.26	34	1
1:A:221:ASP:OD1	1:A:226:GLN:O	0.43	2.36	29	5
1:A:16:ALA:HB2	1:A:218:LEU:CD1	0.43	2.43	7	2
1:A:39:GLU:CD	1:A:42:ARG:NH2	0.43	2.72	22	1
2:B:337:SER:C	2:B:338:ASN:ND2	0.43	2.72	5	1
1:A:125:GLU:OE1	1:A:187:THR:O	0.43	2.37	3	1
1:A:31:ILE:HG21	1:A:39:GLU:HG3	0.43	1.88	19	2
1:A:45:SER:O	1:A:48:ALA:HB3	0.43	2.13	10	2
1:A:3:SER:CB	1:A:225:ASN:OD1	0.43	2.67	16	1
1:A:215:ASP:OD1	1:A:215:ASP:C	0.43	2.57	1	2
1:A:2:ILE:CD1	1:A:211:GLN:OE1	0.43	2.67	23	1
1:A:115:LEU:CD1	2:B:351:GLN:OE1	0.43	2.67	40	1
1:A:139:ARG:HH12	1:A:144:LEU:HD23	0.43	1.73	28	1
2:B:304:GLN:NE2	2:B:305:GLU:OE2	0.43	2.51	3	1
1:A:116:GLU:C	1:A:118:LEU:N	0.43	2.72	2	2
1:A:131:ARG:HE	1:A:135:LYS:CE	0.43	2.26	33	1
1:A:186:ARG:HH11	1:A:186:ARG:CG	0.43	2.27	33	1
2:B:306:VAL:HG13	2:B:306:VAL:O	0.43	2.13	7	1
2:B:332:GLU:OE1	2:B:366:GLU:O	0.43	2.36	28	2
1:A:48:ALA:O	1:A:51:SER:OG	0.43	2.35	30	1
1:A:44:LEU:O	1:A:48:ALA:N	0.43	2.51	40	2
1:A:47:ARG:CG	1:A:47:ARG:HH11	0.43	2.27	8	1
1:A:186:ARG:N	1:A:186:ARG:CD	0.43	2.82	35	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:230:ASN:ND2	1:A:230:ASN:O	0.43	2.52	22	1
1:A:126:ARG:HH21	2:B:347:LEU:HD11	0.43	1.74	35	1
1:A:136:ARG:NH1	1:A:136:ARG:CG	0.43	2.81	27	1
1:A:21:GLU:CG	1:A:139:ARG:HH21	0.43	2.27	28	1
1:A:186:ARG:NE	1:A:195:ARG:HH21	0.43	2.09	15	1
2:B:321:GLN:OE1	2:B:384:LEU:CD2	0.43	2.66	11	1
2:B:301:MET:CG	2:B:302:PHE:N	0.43	2.82	37	7
2:B:317:ARG:HH12	2:B:321:GLN:NE2	0.43	2.12	10	1
1:A:204:GLY:O	1:A:205:THR:C	0.43	2.57	12	7
1:A:127:ALA:O	1:A:130:VAL:N	0.43	2.52	35	1
1:A:99:THR:OG1	1:A:101:ASP:OD1	0.43	2.35	26	1
1:A:224:ASN:CG	1:A:226:GLN:HE21	0.42	2.17	21	1
1:A:131:ARG:HH11	1:A:131:ARG:CG	0.42	2.28	13	1
1:A:161:ALA:O	1:A:162:ASP:CG	0.42	2.58	24	1
1:A:186:ARG:O	1:A:188:SER:N	0.42	2.52	31	1
1:A:181:THR:O	1:A:205:THR:OG1	0.42	2.38	18	1
1:A:15:LYS:O	1:A:157:ILE:N	0.42	2.39	4	2
2:B:321:GLN:NE2	2:B:324:LYS:NZ	0.42	2.66	22	1
1:A:28:ARG:HH11	1:A:28:ARG:CG	0.42	2.28	38	1
1:A:215:ASP:O	1:A:215:ASP:OD1	0.42	2.38	36	1
1:A:34:ASP:OD1	1:A:34:ASP:O	0.42	2.36	14	2
2:B:369:ASP:O	2:B:370:GLU:C	0.42	2.58	33	9
1:A:188:SER:OG	1:A:191:SER:OG	0.42	2.36	38	2
1:A:121:GLU:O	1:A:122:TYR:C	0.42	2.58	30	9
1:A:118:LEU:HD13	1:A:123:LEU:HD13	0.42	1.91	33	2
1:A:186:ARG:NH1	1:A:186:ARG:CG	0.42	2.80	1	1
1:A:153:GLN:O	1:A:154:ASP:OD1	0.42	2.37	37	3
1:A:24:ILE:CG1	1:A:139:ARG:HH12	0.42	2.27	14	1
1:A:120:ASP:OD1	1:A:121:GLU:OE2	0.42	2.37	37	1
1:A:224:ASN:N	1:A:224:ASN:HD22	0.42	2.13	25	1
1:A:13:PHE:CD2	1:A:219:ILE:HG23	0.42	2.50	5	1
2:B:324:LYS:NZ	2:B:324:LYS:CB	0.42	2.82	24	1
2:B:332:GLU:OE1	2:B:332:GLU:N	0.42	2.45	32	2
2:B:351:GLN:CA	2:B:351:GLN:NE2	0.42	2.83	26	1
2:B:346:SER:O	2:B:346:SER:OG	0.42	2.36	37	1
1:A:132:ASP:O	1:A:132:ASP:OD1	0.42	2.38	28	2
1:A:182:ASP:OD1	1:A:182:ASP:C	0.42	2.57	14	3
2:B:351:GLN:O	2:B:351:GLN:CD	0.42	2.58	23	1
2:B:346:SER:OG	2:B:346:SER:O	0.42	2.36	40	1
1:A:186:ARG:CG	1:A:186:ARG:HH11	0.42	2.27	31	1
1:A:230:ASN:ND2	1:A:230:ASN:C	0.42	2.73	31	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:ASN:HD22	1:A:140:ASN:N	0.42	2.12	20	1
1:A:28:ARG:CG	1:A:28:ARG:NH1	0.42	2.81	39	2
2:B:349:LYS:O	2:B:352:THR:OG1	0.42	2.33	33	1
1:A:49:LYS:CB	1:A:49:LYS:HZ3	0.42	2.28	31	1
1:A:224:ASN:ND2	1:A:226:GLN:NE2	0.42	2.68	21	1
1:A:101:ASP:OD1	1:A:101:ASP:C	0.42	2.59	25	1
1:A:214:ASN:OD1	1:A:215:ASP:OD2	0.42	2.37	3	1
1:A:159:VAL:CG1	1:A:209:THR:HG22	0.42	2.45	11	2
1:A:126:ARG:NH2	2:B:347:LEU:HD11	0.42	2.29	23	1
1:A:122:TYR:OH	1:A:126:ARG:NH2	0.42	2.53	27	1
1:A:130:VAL:CG2	2:B:351:GLN:NE2	0.42	2.83	11	1
1:A:116:GLU:O	1:A:118:LEU:N	0.41	2.53	2	1
2:B:370:GLU:CG	2:B:371:GLN:N	0.41	2.83	19	1
1:A:186:ARG:C	1:A:188:SER:N	0.41	2.73	31	2
1:A:152:ILE:O	1:A:175:LYS:NZ	0.41	2.40	37	1
1:A:226:GLN:NE2	1:A:228:TYR:OH	0.41	2.52	11	2
1:A:101:ASP:C	1:A:101:ASP:OD1	0.41	2.59	5	1
2:B:370:GLU:OE1	2:B:370:GLU:C	0.41	2.58	14	2
1:A:49:LYS:CB	1:A:49:LYS:NZ	0.41	2.82	31	1
2:B:347:LEU:O	2:B:351:GLN:CD	0.41	2.59	21	1
1:A:224:ASN:O	1:A:224:ASN:OD1	0.41	2.37	21	1
1:A:135:LYS:NZ	1:A:139:ARG:NH2	0.41	2.67	11	1
2:B:321:GLN:CD	2:B:324:LYS:HZ1	0.41	2.16	22	1
2:B:317:ARG:HH21	2:B:321:GLN:CD	0.41	2.19	38	2
1:A:192:ILE:HD13	1:A:195:ARG:HH22	0.41	1.74	31	1
1:A:79:LEU:O	1:A:85:LEU:HD12	0.41	2.15	26	1
1:A:186:ARG:NE	1:A:195:ARG:HH22	0.41	2.13	9	1
1:A:126:ARG:CZ	2:B:351:GLN:OE1	0.41	2.68	28	1
1:A:172:ASN:HD22	1:A:175:LYS:HZ1	0.41	1.58	5	1
2:B:349:LYS:O	2:B:350:LEU:C	0.41	2.59	34	3
1:A:202:ILE:CD1	1:A:220:LEU:HD11	0.41	2.46	3	1
1:A:172:ASN:ND2	1:A:176:VAL:HG23	0.41	2.31	23	1
2:B:326:ALA:C	2:B:328:GLY:H	0.41	2.19	29	1
1:A:132:ASP:OD1	1:A:132:ASP:O	0.41	2.39	37	1
1:A:43:PHE:C	1:A:43:PHE:CD1	0.41	2.94	7	1
2:B:310:ALA:O	2:B:357:GLN:CD	0.41	2.59	35	2
1:A:136:ARG:CG	1:A:136:ARG:NH1	0.41	2.84	5	1
1:A:214:ASN:OD1	1:A:214:ASN:N	0.41	2.54	14	2
1:A:21:GLU:OE1	1:A:147:ILE:HD11	0.41	2.15	33	1
1:A:214:ASN:OD1	1:A:214:ASN:O	0.41	2.39	40	1
1:A:149:LEU:O	1:A:172:ASN:OD1	0.41	2.39	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:HIS:CG	1:A:133:ILE:HD11	0.41	2.50	6	1
1:A:182:ASP:CG	1:A:205:THR:OG1	0.41	2.59	38	1
2:B:306:VAL:CG1	2:B:381:MET:SD	0.41	3.09	2	2
1:A:232:THR:HG22	1:A:233:ASN:H	0.41	1.72	10	1
2:B:370:GLU:C	2:B:370:GLU:OE1	0.41	2.59	18	1
1:A:56:THR:CG2	1:A:60:LYS:HZ3	0.41	2.29	30	1
1:A:181:THR:O	1:A:203:VAL:C	0.41	2.60	12	2
1:A:91:ALA:O	1:A:95:ASP:N	0.41	2.43	38	2
2:B:385:GLU:N	2:B:385:GLU:CD	0.41	2.74	24	1
1:A:230:ASN:OD1	1:A:230:ASN:O	0.41	2.39	27	1
1:A:179:PHE:O	1:A:201:ALA:CB	0.41	2.69	12	1
2:B:350:LEU:O	2:B:351:GLN:C	0.40	2.60	27	3
1:A:49:LYS:HZ1	1:A:140:ASN:CA	0.40	2.29	30	1
2:B:337:SER:C	2:B:339:GLY:N	0.40	2.73	6	1
1:A:172:ASN:HD22	1:A:175:LYS:NZ	0.40	2.10	5	1
1:A:233:ASN:N	1:A:233:ASN:ND2	0.40	2.68	31	1
1:A:22:ASP:N	1:A:22:ASP:OD1	0.40	2.55	20	1
1:A:28:ARG:HH11	1:A:28:ARG:HG2	0.40	1.77	38	1
2:B:351:GLN:CA	2:B:351:GLN:OE1	0.40	2.69	17	1
1:A:121:GLU:O	1:A:121:GLU:CD	0.40	2.60	7	1
1:A:51:SER:OG	1:A:52:ALA:N	0.40	2.53	15	1
2:B:357:GLN:C	2:B:359:THR:N	0.40	2.75	17	1
1:A:127:ALA:O	1:A:128:ALA:C	0.40	2.59	33	2
1:A:233:ASN:HD22	1:A:234:GLU:N	0.40	2.11	31	1
1:A:136:ARG:O	1:A:140:ASN:CG	0.40	2.60	27	1
1:A:135:LYS:NZ	1:A:139:ARG:HE	0.40	2.15	20	1
1:A:207:SER:OG	1:A:210:SER:OG	0.40	2.37	18	1
1:A:182:ASP:O	1:A:182:ASP:CG	0.40	2.60	15	1
1:A:172:ASN:OD1	1:A:172:ASN:O	0.40	2.40	15	1
2:B:373:ALA:O	2:B:374:VAL:C	0.40	2.60	3	1
2:B:337:SER:O	2:B:338:ASN:OD1	0.40	2.39	35	1
2:B:310:ALA:O	2:B:312:ASN:N	0.40	2.54	32	1
1:A:120:ASP:C	1:A:120:ASP:OD1	0.40	2.60	20	1
1:A:110:GLY:O	1:A:113:SER:OG	0.40	2.39	22	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	235/259 (91%)	218±2 (93±1%)	14±2 (6±1%)	3±1 (1±0%)	19	64
2	B	83/85 (98%)	75±2 (91±2%)	6±1 (8±2%)	2±1 (2±1%)	14	56
All	All	12720/13760 (92%)	11730 (92%)	795 (6%)	195 (2%)	18	63

All 13 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	6	LEU	40
1	A	183	ALA	39
2	B	351	GLN	35
1	A	148	ASP	33
2	B	373	ALA	17
1	A	222	ALA	10
2	B	358	GLY	8
1	A	184	GLY	5
1	A	50	ALA	4
2	B	311	PRO	1
2	B	357	GLN	1
1	A	187	THR	1
2	B	327	LYS	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	195/214 (91%)	193±1 (99±1%)	2±1 (1±1%)	81	97
2	B	70/70 (100%)	69±1 (98±2%)	1±1 (2±2%)	64	94
All	All	10599/11360 (93%)	10452 (99%)	147 (1%)	76	96

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

Mol	Chain	Res	Type	Models (Total)
2	B	370	GLU	13
1	A	225	ASN	13
2	B	351	GLN	11
1	A	182	ASP	11
1	A	190	THR	10
1	A	213	LYS	8
1	A	13	PHE	8
2	B	317	ARG	6
1	A	186	ARG	5
2	B	381	MET	5
1	A	145	LYS	5
2	B	324	LYS	5
1	A	215	ASP	5
1	A	172	ASN	4
1	A	126	ARG	4
2	B	345	LYS	4
2	B	303	GLN	4
1	A	230	ASN	3
1	A	1	MET	2
1	A	125	GLU	2
2	B	376	HIS	2
1	A	214	ASN	2
2	B	304	GLN	2
2	B	338	ASN	2
1	A	121	GLU	1
1	A	47	ARG	1
2	B	305	GLU	1
2	B	379	LYS	1
2	B	357	GLN	1
1	A	233	ASN	1
1	A	232	THR	1
1	A	49	LYS	1
2	B	383	GLU	1
1	A	175	LYS	1
1	A	28	ARG	1

6.3.3 RNA ⓘ

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

No chemical shift data were provided