Full wwPDB NMR Structure Validation Report (i)

Jun 14, 2020 – 12:20 pm BST

PDB ID	:	2BRU
Title	:	Complex of the domain I and domain III of Escherichia coli transhydrogenase
Authors	:	Johansson, T.; Pedersen, A.; Leckner, J.; Karlsson, B.G.
Deposited on	:	2005-05-11

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

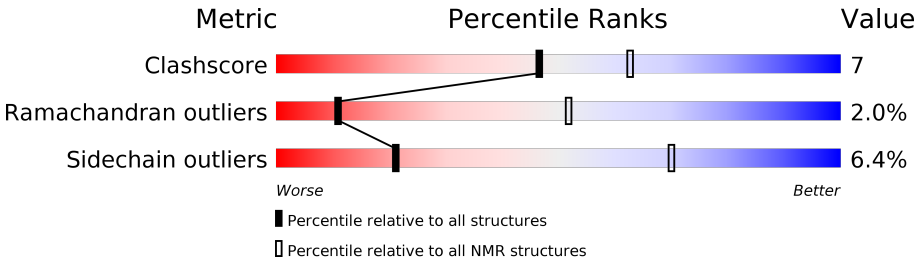
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment 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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	401	73% 18% 8%
1	B	401	72% 19% 9%
2	C	186	58% 31% • 10%

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:1000-A:1216, A:1224-A:1373, B:998-B:1215, B:1230-B:1376, C:20-C:186 (899)	0.72	3

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

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

The models can be grouped into 2 clusters and 4 single-model clusters were found.

Cluster number	Models
1	4, 6, 7, 8
2	2, 3
Single-model clusters	1; 5; 9; 10

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8268 atoms, of which 1440 are hydrogens and 0 are deuteriums.

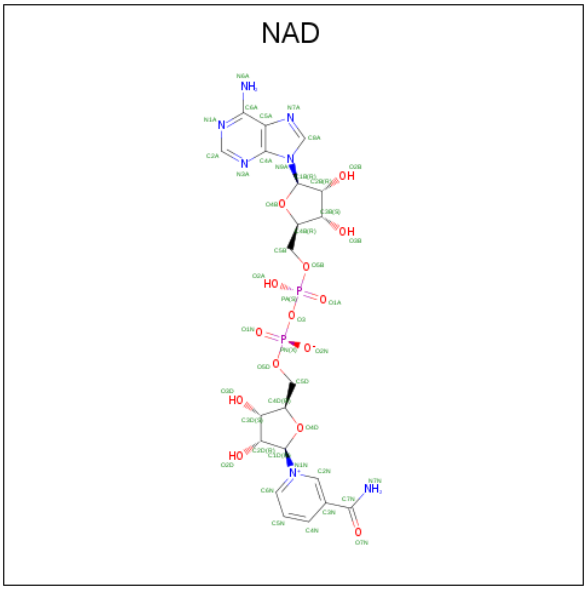
- Molecule 1 is a protein called NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms						Trace
1	A	367	Total	C	H	N	O	S	1
			3314	1734	579	464	525	12	
1	B	365	Total	C	H	N	O	S	1
			3311	1729	582	467	521	12	

- Molecule 2 is a protein called NAD(P) TRANSHYDROGENASE SUBUNIT BETA.

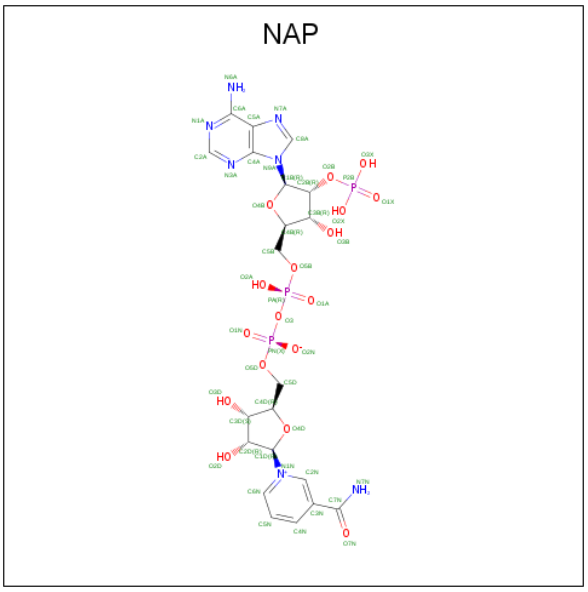
Mol	Chain	Residues	Atoms						Trace
2	C	167	Total	C	H	N	O	S	0
			1536	809	264	215	242	6	

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						
3	B	1	Total	C	H	N	O	P	
			52	21	8	7	14	2	

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
4	C	1	55	21	7	7	17	3

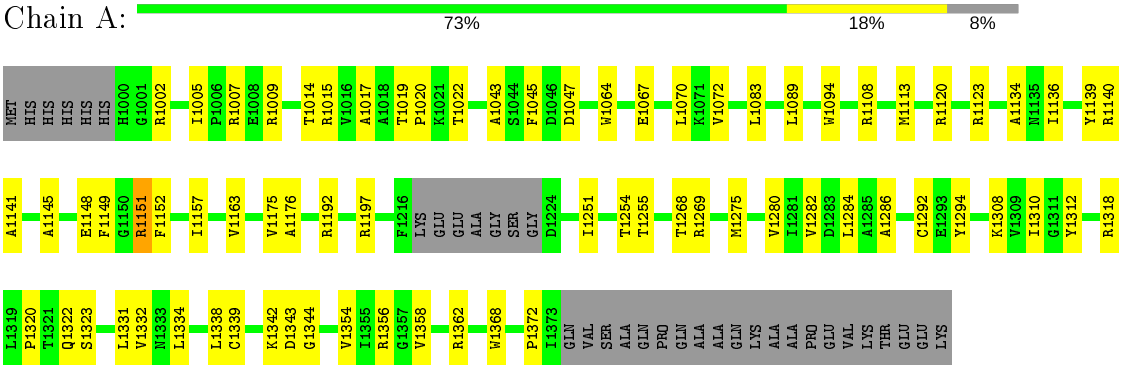
4 Residue-property plots

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.

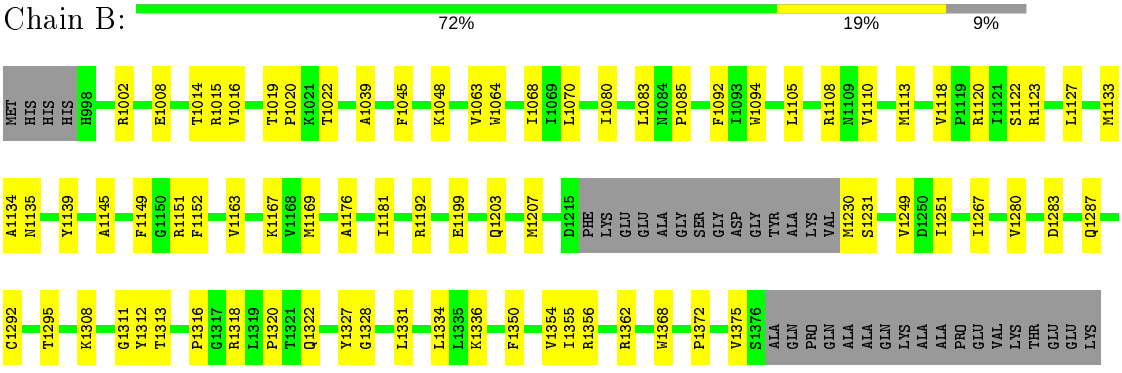
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:



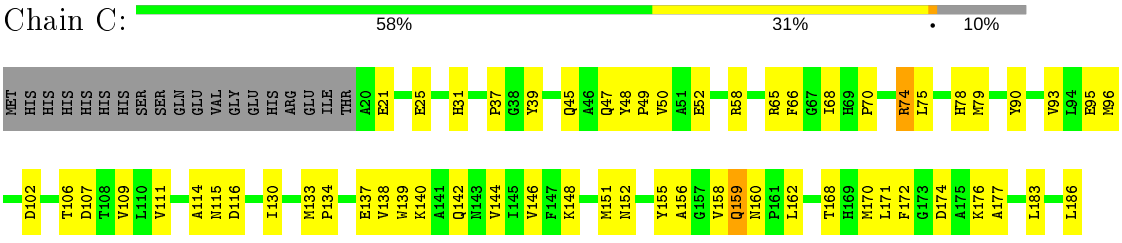
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C:



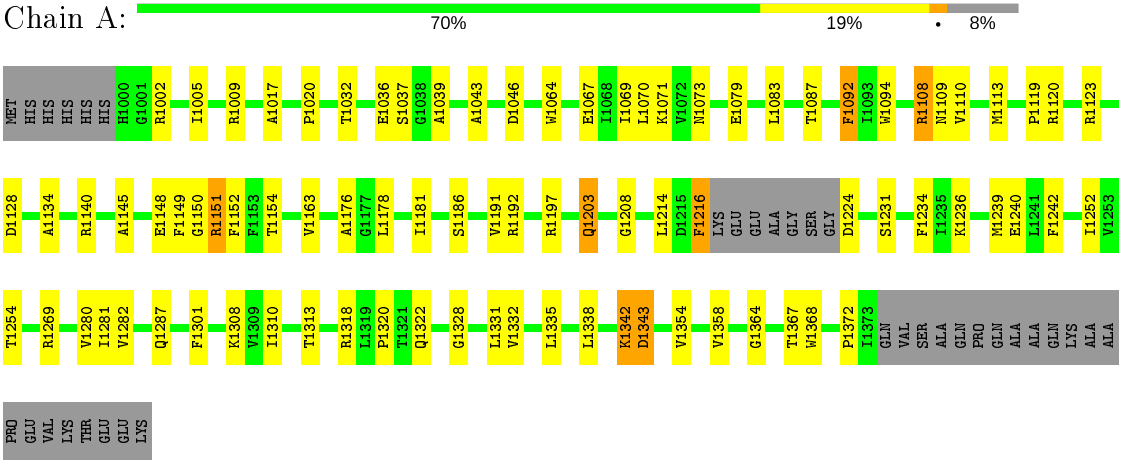
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

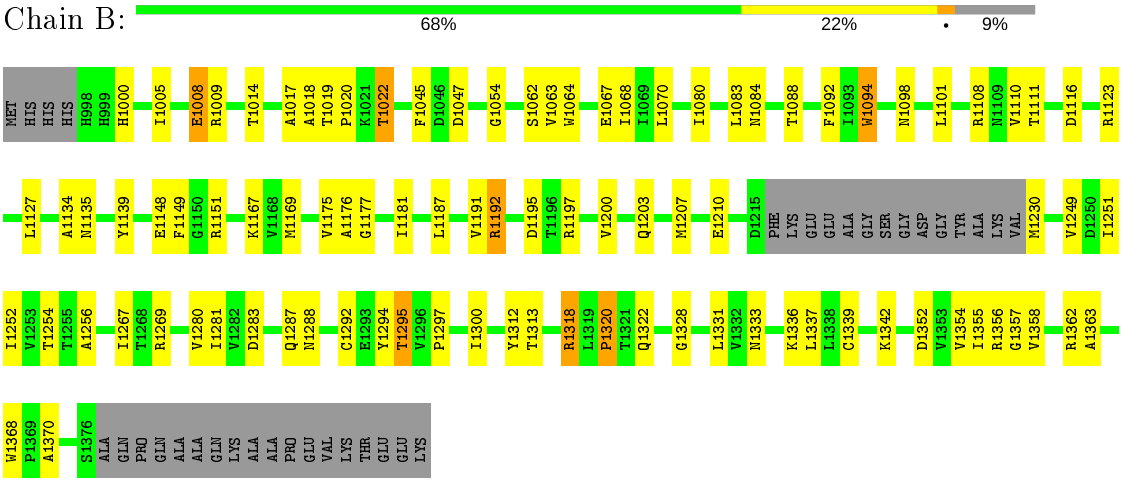
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:



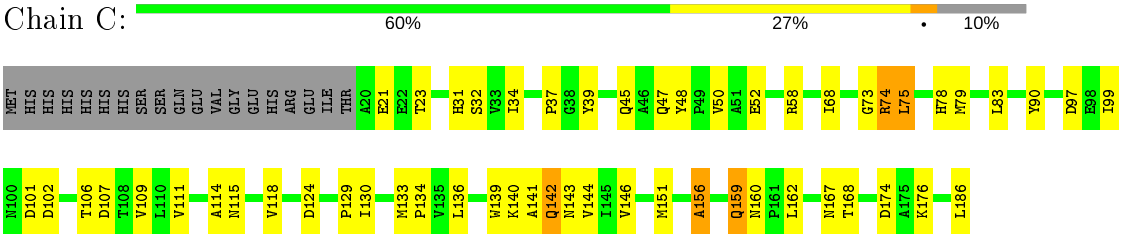
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

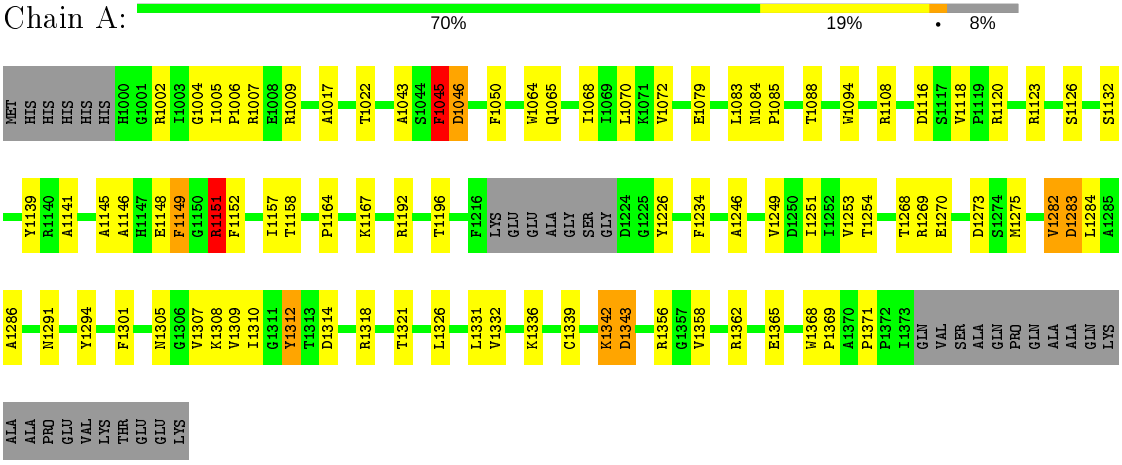
Chain C:



4.2.2 Score per residue for model 2

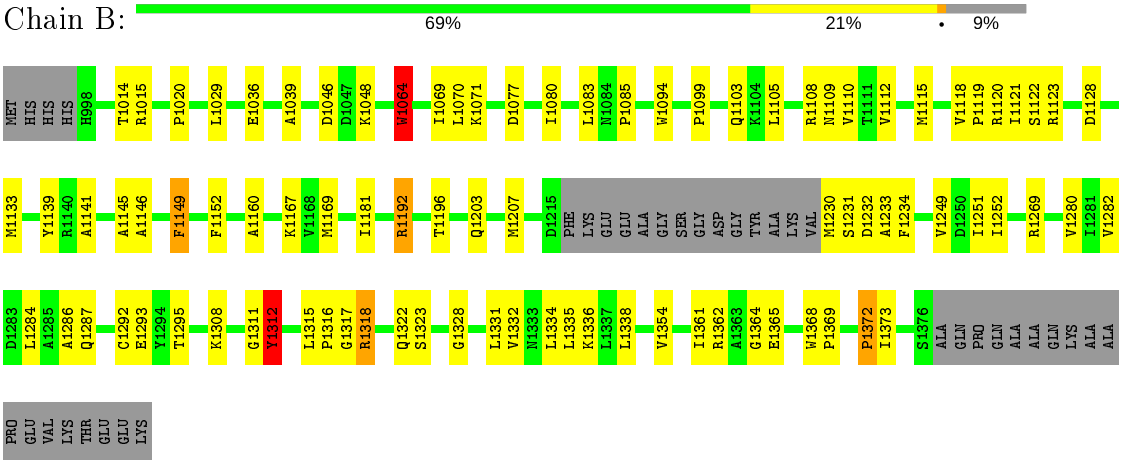
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:



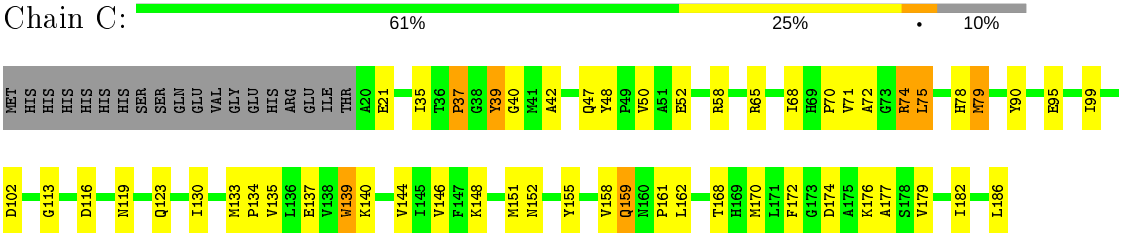
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

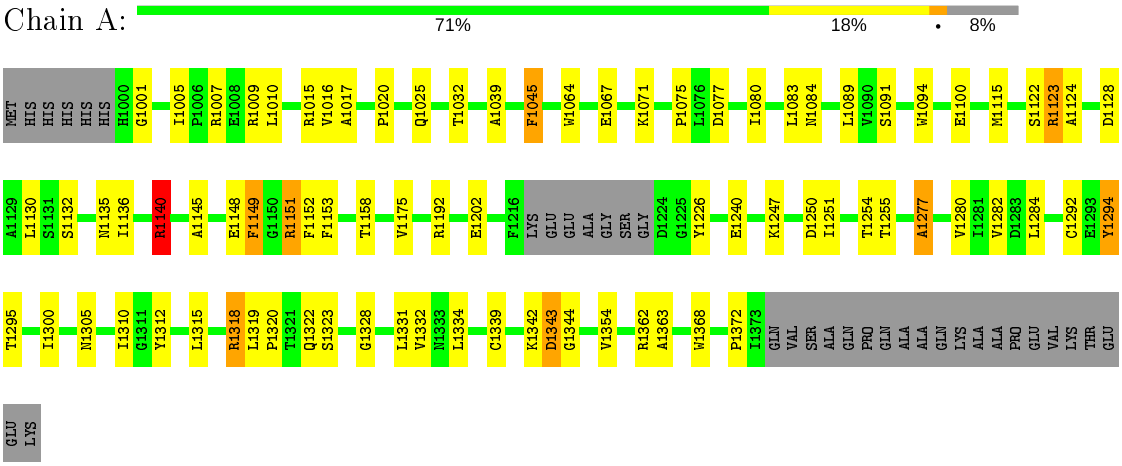
Chain C:



4.2.3 Score per residue for model 3 (medoid)

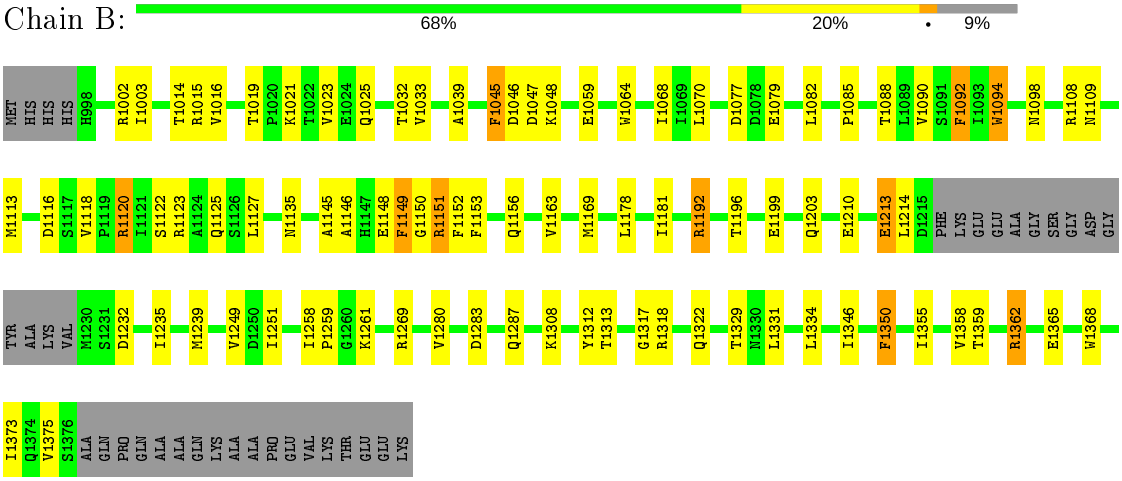
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:



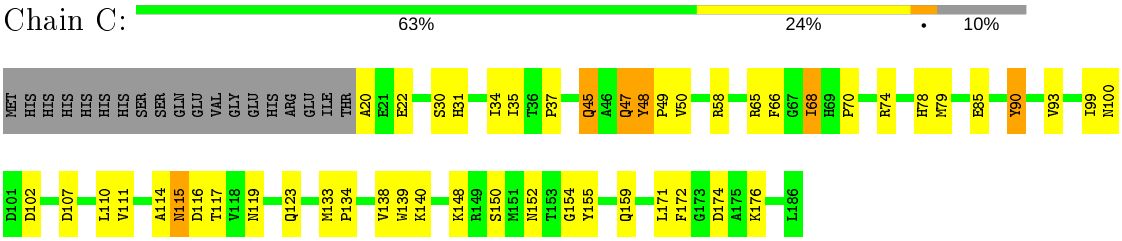
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

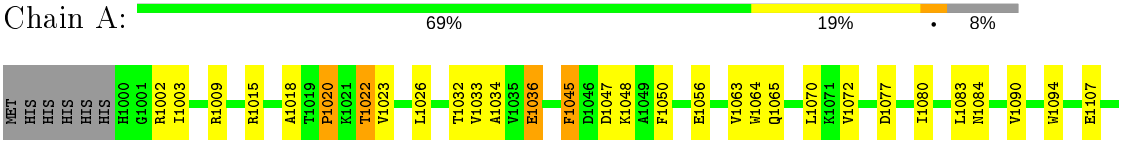
Chain C:

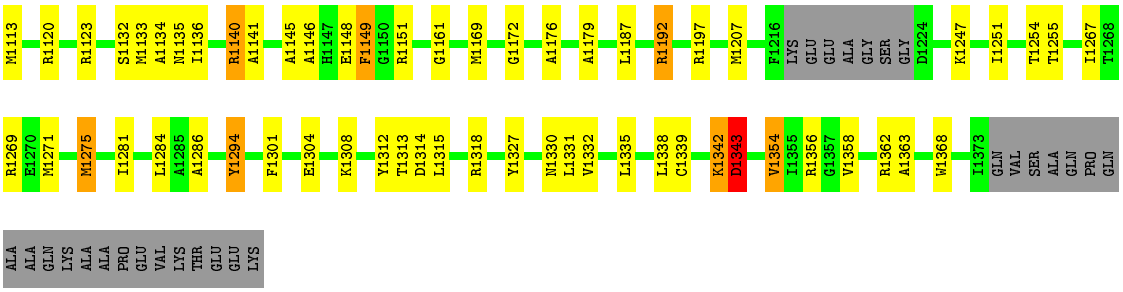


4.2.4 Score per residue for model 4

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

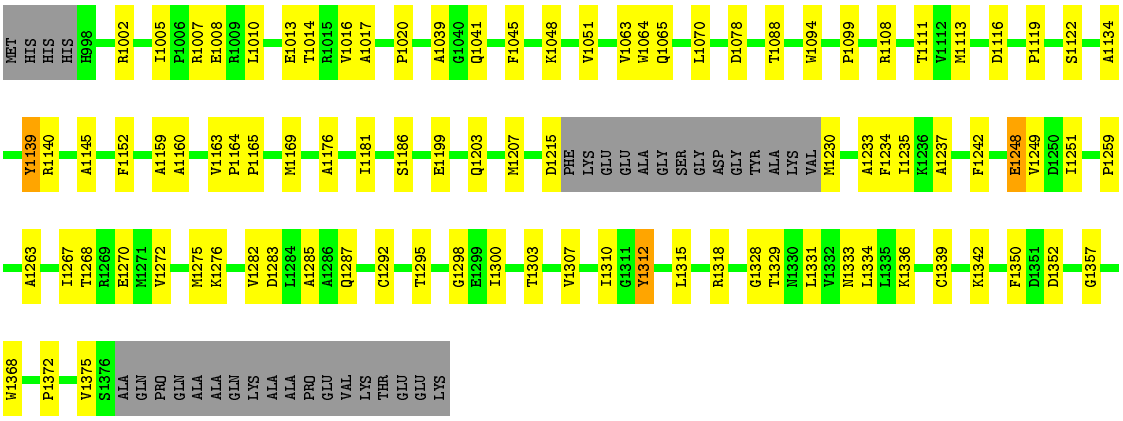
Chain A:





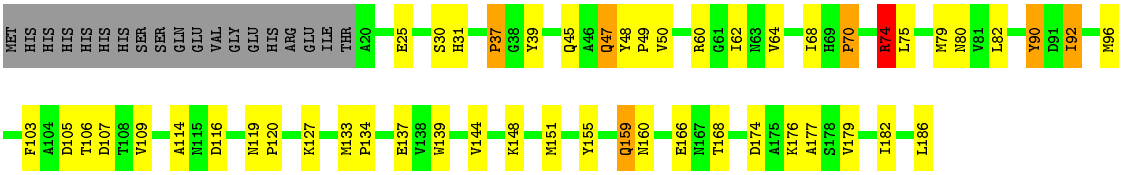
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

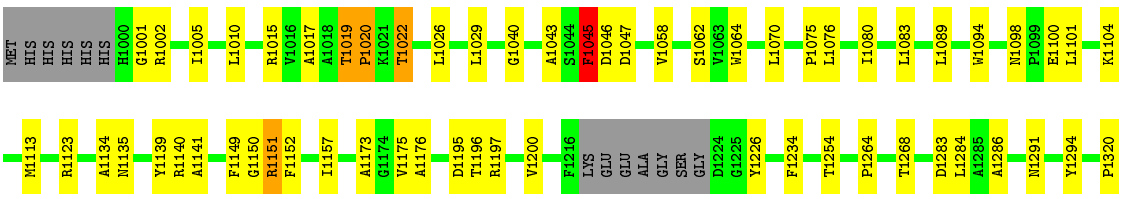
Chain C:

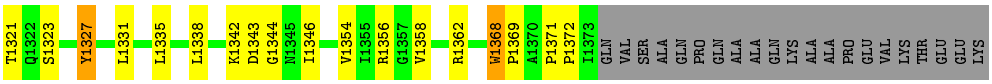


4.2.5 Score per residue for model 5

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

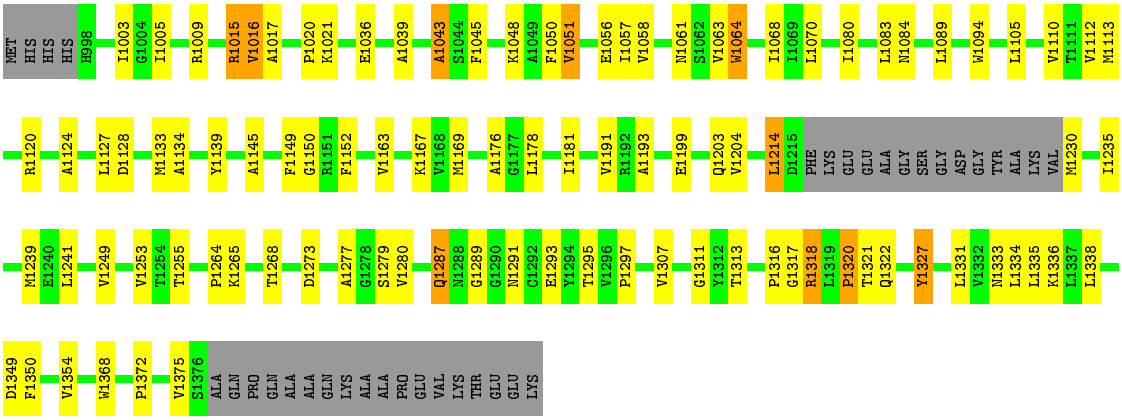
Chain A:





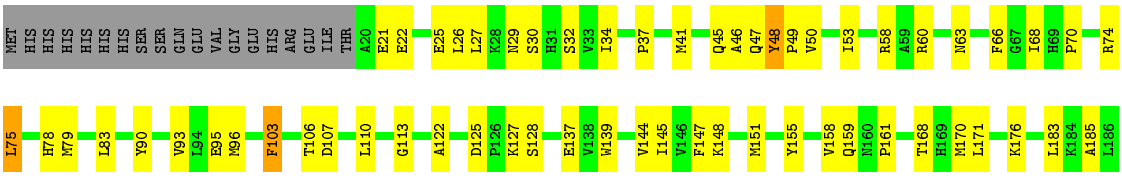
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

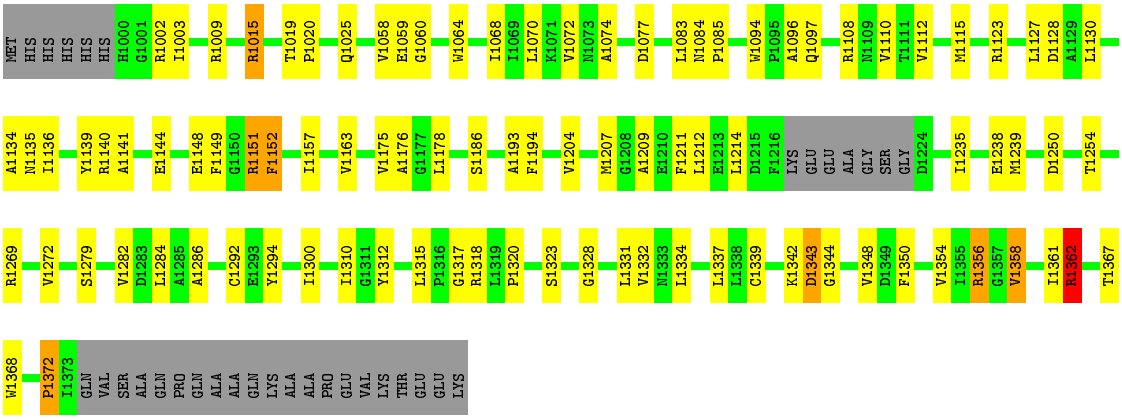
Chain C:



4.2.6 Score per residue for model 6

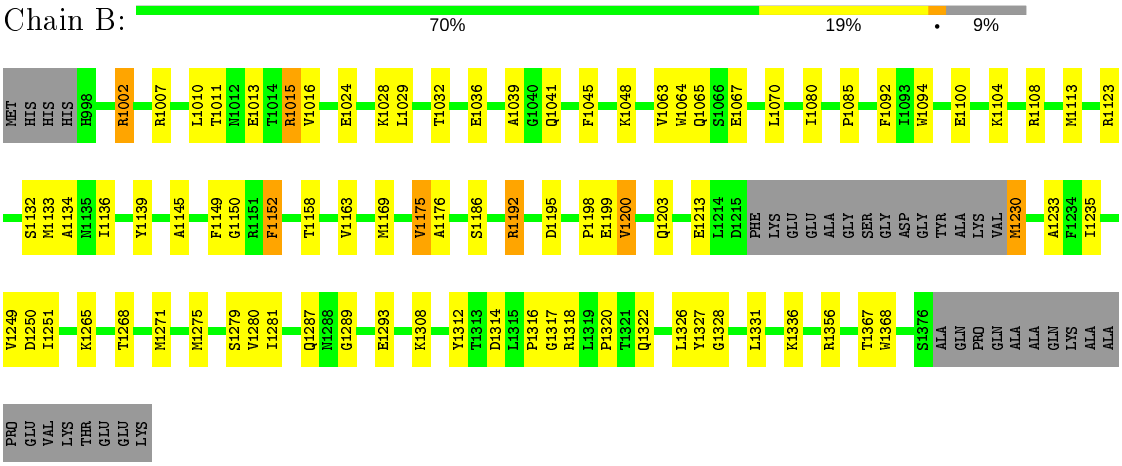
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:



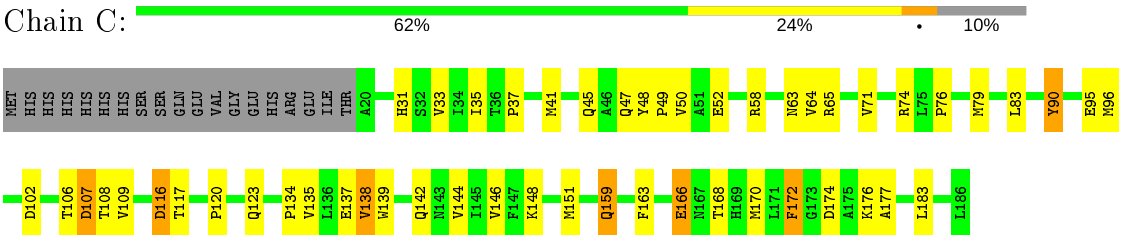
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

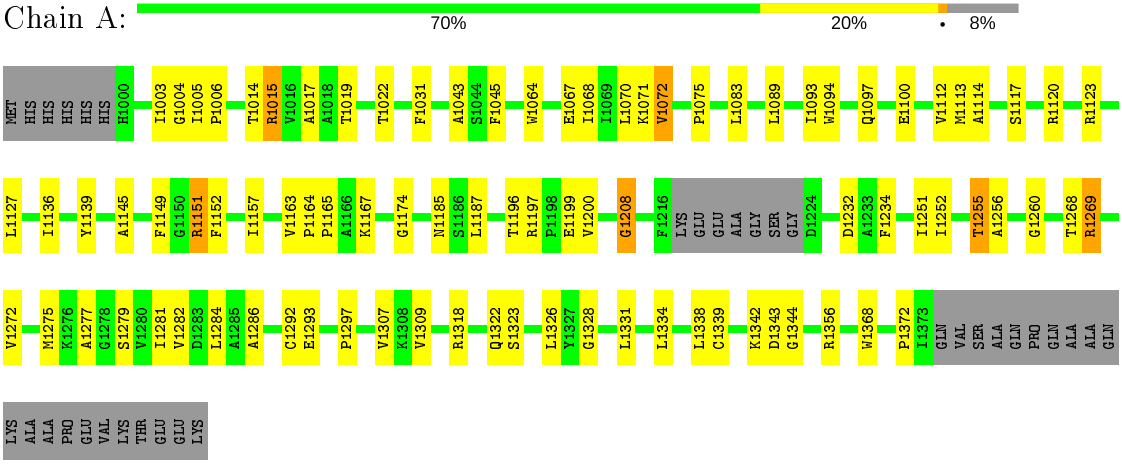
Chain C:



4.2.7 Score per residue for model 7

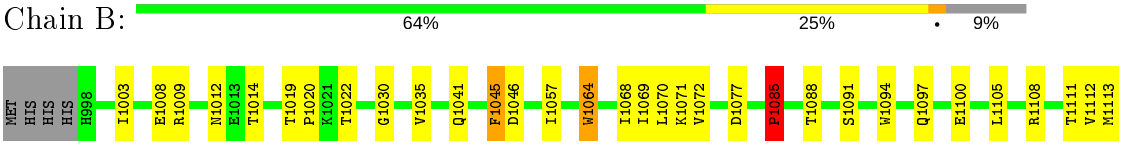
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

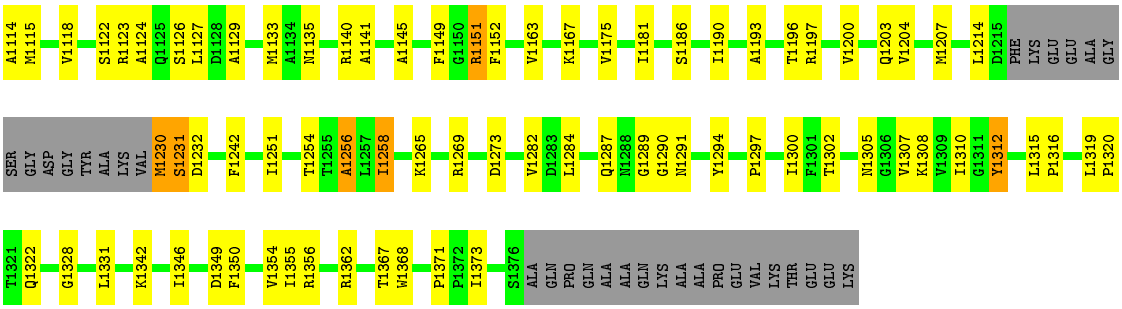
Chain A:



• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:





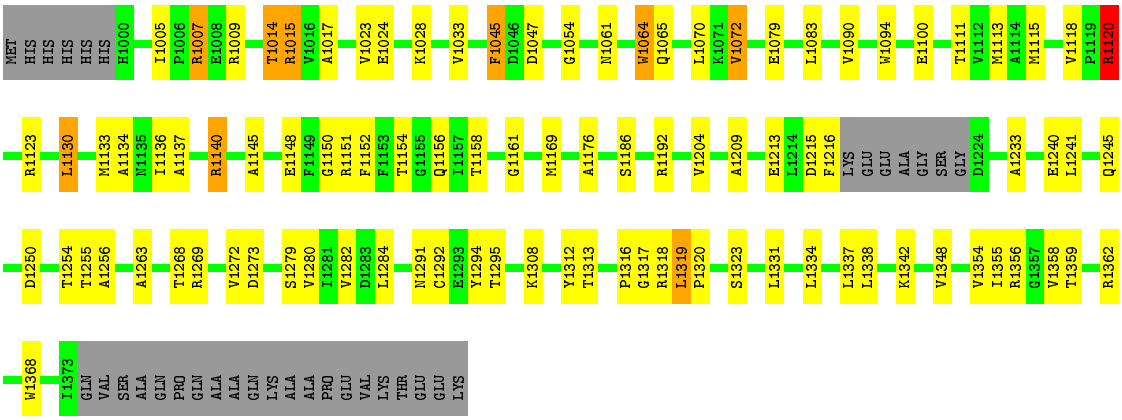
• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C:

4.2.8 Score per residue for model 8

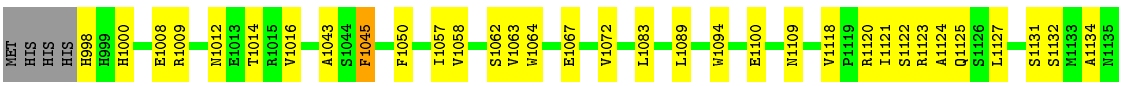
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

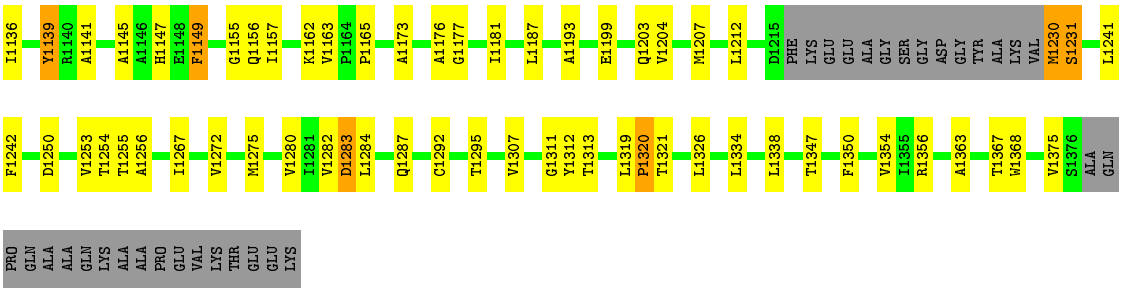
Chain A:



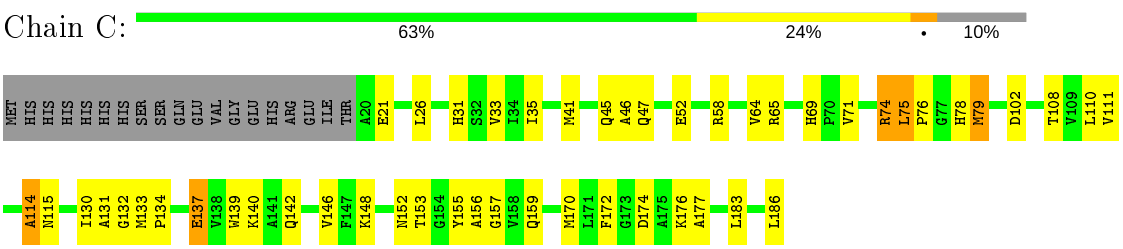
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:



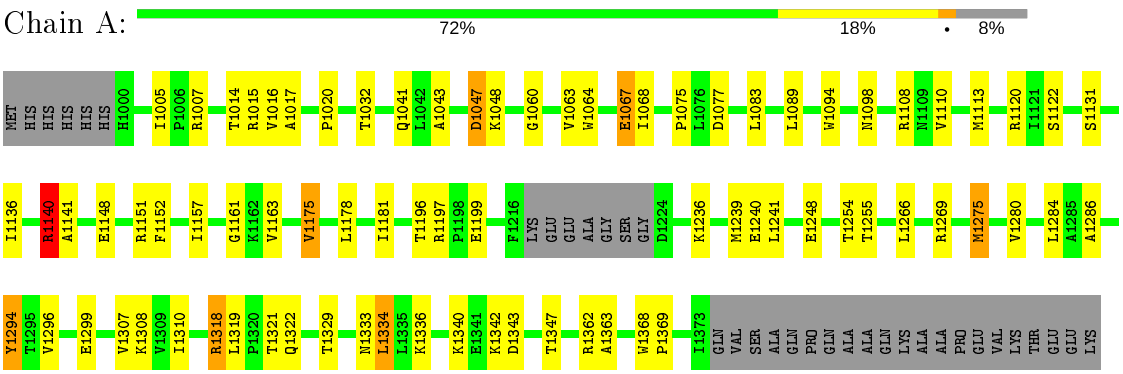


• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

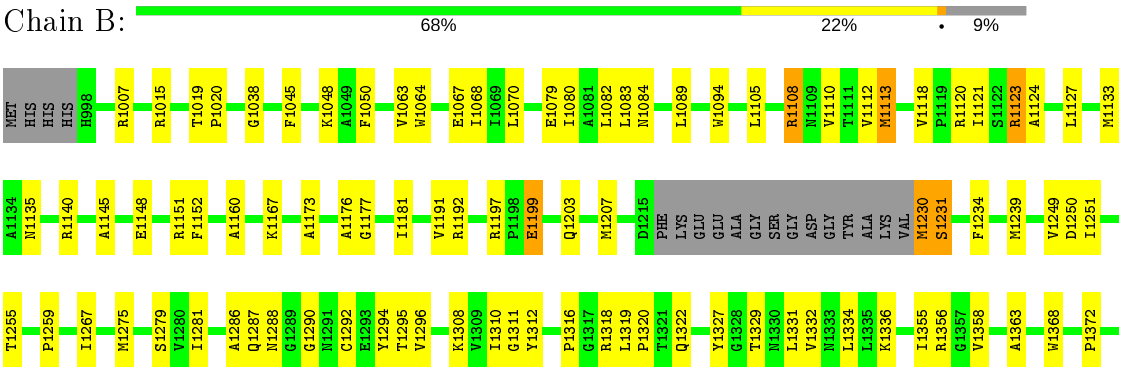


4.2.9 Score per residue for model 9

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

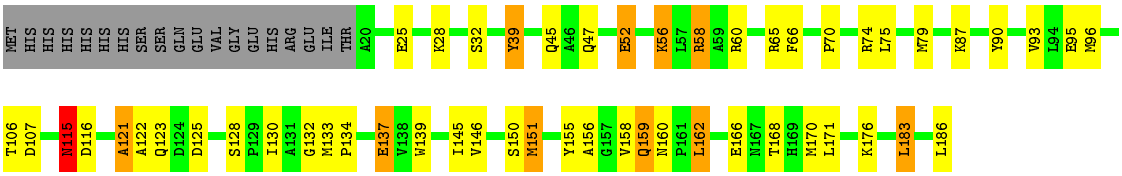


• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

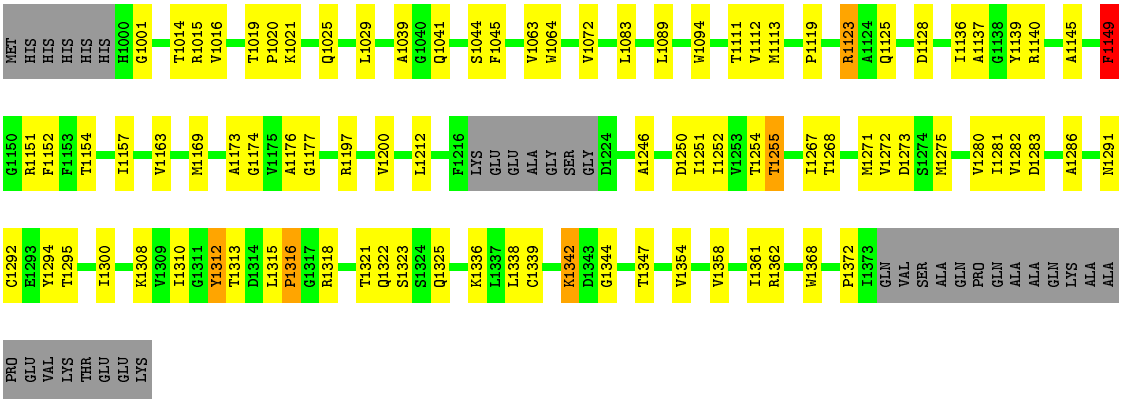
Chain C:



4.2.10 Score per residue for model 10

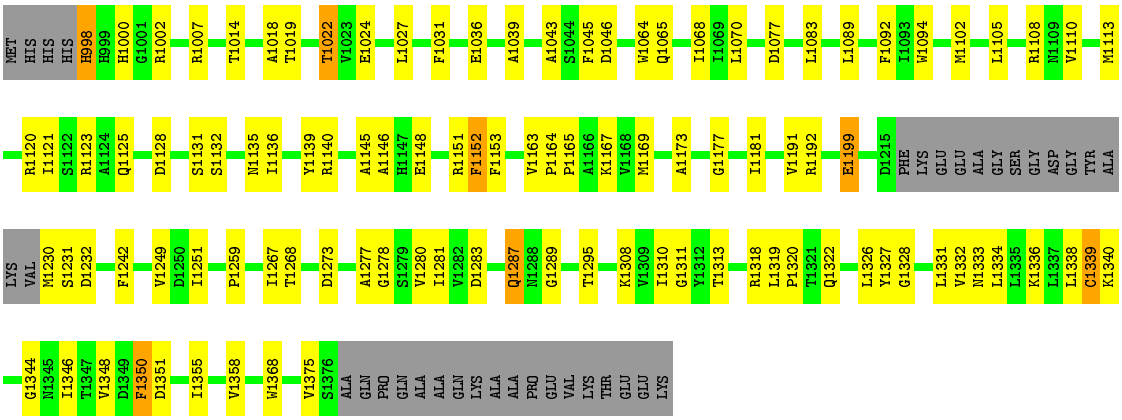
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:



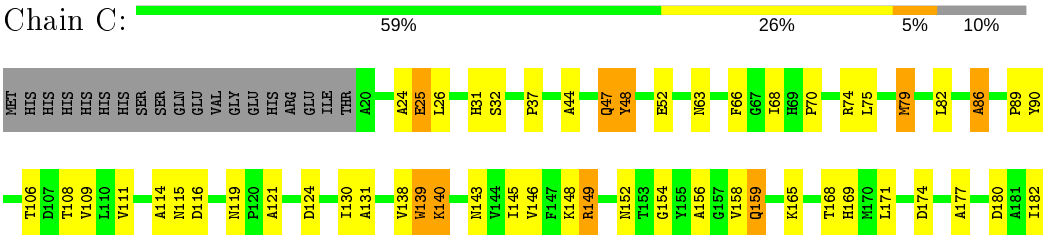
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C:


59%
26%
5%
10%
MET HIS HIS HIS HIS HIS HIS SER SER GLN GLU VAL GLY GLU HIS ARG GLU ILE THR A20 A24 E25 L26 H31 S32 P37 A44 Q47 Y48 E52 N63 F66 G67 I68 H69 F70 R74 L75 M79 L82 A86 P89 Y90 V93 M96
T106 D107 T108 V109 L110 V111 A114 N115 D116 N119 P120 A121 D124 I130 A131 V138 W139 K140 N143 V144 I145 V146 F147 K148 R149 N152 T153 G154 Y155 A156 G157 V158 Q159 K165 T168 H169 M170 L171 D174 A177 D180 A181 I182 L183 L186

5 Refinement protocol and experimental data overview

The models were refined using the following method: *RIGID BODY MINIMIZATION, MOLECULAR DYNAMICS SIMULATION*.

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	
X-PLOR	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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.82±0.01	1±1/2779 (0.0± 0.0%)	1.38±0.02	27±6/3776 (0.7± 0.2%)
1	B	0.83±0.01	0±1/2773 (0.0± 0.0%)	1.36±0.02	24±3/3768 (0.6± 0.1%)
2	C	0.83±0.01	0±0/1297 (0.0± 0.0%)	1.41±0.03	10±2/1764 (0.6± 0.1%)
All	All	0.83	17/68490 (0.0%)	1.38	605/93080 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.2±1.9
1	B	0.0±0.0	1.2±0.9
2	C	0.0±0.0	0.9±0.7
All	All	0	43

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	139	TRP	NE1-CE2	-5.80	1.30	1.37	3	1
1	A	1064	TRP	CD1-NE1	-5.78	1.28	1.38	10	1
1	B	1375	VAL	C-N	-5.64	1.21	1.34	9	3
2	C	139	TRP	CD1-NE1	-5.48	1.28	1.38	7	1
2	C	52	GLU	CD-OE1	-5.40	1.19	1.25	1	1
1	A	1094	TRP	CD1-NE1	-5.34	1.28	1.38	5	1
1	A	1372	PRO	C-N	-5.31	1.21	1.34	10	4
1	A	1240	GLU	CD-OE2	-5.30	1.19	1.25	8	1
1	B	1008	GLU	CD-OE2	-5.16	1.20	1.25	4	1
2	C	25	GLU	CD-OE1	-5.09	1.20	1.25	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	1199	GLU	CD-OE2	-5.04	1.20	1.25	7	1
1	A	1368	TRP	CG-CD2	-5.03	1.35	1.43	2	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	1064	TRP	CD1-CG-CD2	11.34	115.37	106.30	10	10
1	B	1356	ARG	NE-CZ-NH1	10.98	125.79	120.30	9	4
1	B	1356	ARG	NE-CZ-NH2	-10.97	114.81	120.30	1	2
2	C	139	TRP	CD1-CG-CD2	10.54	114.73	106.30	8	10
1	A	1064	TRP	CE2-CD2-CG	-10.46	98.93	107.30	10	10
1	B	1108	ARG	NE-CZ-NH1	10.12	125.36	120.30	4	3
1	A	1192	ARG	NE-CZ-NH2	-10.10	115.25	120.30	2	3
1	B	1094	TRP	CD1-CG-CD2	10.07	114.36	106.30	9	10
1	A	1123	ARG	NE-CZ-NH2	-10.06	115.27	120.30	5	5
1	B	1368	TRP	CE2-CD2-CG	-10.02	99.28	107.30	2	8
1	A	1318	ARG	NE-CZ-NH1	10.00	125.30	120.30	7	4
1	B	1312	TYR	CB-CG-CD2	-9.86	115.08	121.00	8	5
1	B	1108	ARG	NE-CZ-NH2	-9.85	115.38	120.30	2	3
1	A	1362	ARG	NE-CZ-NH2	-9.75	115.42	120.30	2	4
1	A	1094	TRP	CE2-CD2-CG	-9.72	99.52	107.30	5	10
1	A	1094	TRP	CD1-CG-CD2	9.57	113.96	106.30	4	10
1	A	1368	TRP	CD1-CG-CD2	9.46	113.86	106.30	3	10
1	A	1151	ARG	NE-CZ-NH2	-9.26	115.67	120.30	5	4
2	C	139	TRP	CE2-CD2-CG	-9.24	99.90	107.30	7	10
2	C	139	TRP	CG-CD2-CE3	9.14	142.13	133.90	10	4
1	B	1197	ARG	NE-CZ-NH2	-9.14	115.73	120.30	9	3
1	B	1094	TRP	CE2-CD2-CG	-9.00	100.10	107.30	9	10
1	A	1368	TRP	CE2-CD2-CG	-8.95	100.14	107.30	8	10
1	B	1064	TRP	CD1-CG-CD2	8.92	113.44	106.30	7	10
1	A	1197	ARG	NE-CZ-NH1	8.90	124.75	120.30	4	3
1	A	1368	TRP	CG-CD2-CE3	8.81	141.83	133.90	8	4
2	C	65	ARG	NE-CZ-NH1	8.81	124.70	120.30	7	4
1	A	1151	ARG	NE-CZ-NH1	8.76	124.68	120.30	7	5
1	A	1356	ARG	NE-CZ-NH2	-8.66	115.97	120.30	6	4
1	B	1269	ARG	NE-CZ-NH2	-8.66	115.97	120.30	3	4
2	C	74	ARG	NE-CZ-NH1	8.59	124.59	120.30	7	5
1	A	1318	ARG	NE-CZ-NH2	-8.58	116.01	120.30	1	5
1	B	1368	TRP	CD1-CG-CD2	8.40	113.02	106.30	2	10
1	B	1123	ARG	NE-CZ-NH1	8.37	124.48	120.30	6	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	1009	ARG	NE-CZ-NH2	-8.36	116.12	120.30	1	2
1	B	1140	ARG	NE-CZ-NH1	8.35	124.47	120.30	4	3
1	B	1192	ARG	NE-CZ-NH2	-8.33	116.14	120.30	1	5
1	A	1002	ARG	NE-CZ-NH1	8.28	124.44	120.30	1	3
1	A	1294	TYR	CB-CG-CD2	-8.21	116.08	121.00	3	4
2	C	60	ARG	NE-CZ-NH2	-8.19	116.21	120.30	7	3
1	A	1140	ARG	NE-CZ-NH1	8.15	124.38	120.30	1	3
2	C	90	TYR	CB-CG-CD2	-8.14	116.12	121.00	6	4
1	A	1094	TRP	CG-CD2-CE3	8.04	141.13	133.90	5	4
1	B	1002	ARG	NE-CZ-NH1	8.01	124.30	120.30	3	1
1	B	1269	ARG	NE-CZ-NH1	7.95	124.27	120.30	1	2
2	C	74	ARG	NE-CZ-NH2	-7.95	116.33	120.30	6	4
1	A	1015	ARG	NE-CZ-NH1	7.94	124.27	120.30	5	5
1	A	1153	PHE	CB-CG-CD2	-7.86	115.30	120.80	3	1
1	B	1242	PHE	CB-CG-CD2	-7.85	115.30	120.80	4	4
1	B	1242	PHE	CB-CG-CD1	7.82	126.27	120.80	4	1
2	C	155	TYR	CB-CG-CD2	-7.79	116.33	121.00	4	1
1	B	1123	ARG	NE-CZ-NH2	-7.74	116.43	120.30	6	4
1	A	1002	ARG	NE-CZ-NH2	-7.72	116.44	120.30	1	2
1	B	1064	TRP	CE2-CD2-CG	-7.71	101.13	107.30	1	10
1	A	1064	TRP	CG-CD1-NE1	-7.71	102.39	110.10	10	5
1	A	1197	ARG	NE-CZ-NH2	-7.70	116.45	120.30	4	3
1	A	1312	TYR	CB-CG-CD2	-7.67	116.40	121.00	10	3
1	A	1123	ARG	NE-CZ-NH1	7.65	124.12	120.30	10	5
1	A	1009	ARG	NE-CZ-NH2	-7.63	116.48	120.30	3	4
1	A	1192	ARG	NE-CZ-NH1	7.61	124.11	120.30	2	2
1	A	1108	ARG	NE-CZ-NH2	-7.58	116.51	120.30	2	2
1	A	1009	ARG	NE-CZ-NH1	7.50	124.05	120.30	4	1
1	B	1283	ASP	CB-CG-OD1	7.49	125.04	118.30	4	5
1	A	1120	ARG	NE-CZ-NH1	7.49	124.05	120.30	4	4
2	C	48	TYR	CB-CG-CD2	-7.43	116.54	121.00	6	6
1	A	1342	LYS	O-C-N	-7.37	110.92	122.70	9	9
1	B	1230	MET	O-C-N	-7.36	110.92	122.70	7	7
1	A	1120	ARG	NE-CZ-NH2	-7.32	116.64	120.30	1	3
1	A	1007	ARG	NE-CZ-NH1	7.27	123.94	120.30	3	3
1	A	1269	ARG	NE-CZ-NH2	-7.26	116.67	120.30	1	2
1	A	1064	TRP	CB-CG-CD1	-7.26	117.57	127.00	5	3
2	C	39	TYR	CB-CG-CD2	-7.25	116.65	121.00	1	3
1	B	1092	PHE	CB-CG-CD2	-7.20	115.76	120.80	3	2
2	C	149	ARG	NE-CZ-NH1	7.15	123.88	120.30	10	1
1	A	1064	TRP	CG-CD2-CE3	7.08	140.27	133.90	10	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	1009	ARG	NE-CZ-NH1	7.06	123.83	120.30	7	3
2	C	139	TRP	CB-CG-CD1	-7.02	117.88	127.00	2	6
1	A	1140	ARG	NE-CZ-NH2	-7.01	116.79	120.30	9	4
1	A	1015	ARG	NE-CZ-NH2	-6.96	116.82	120.30	5	1
1	B	1094	TRP	CG-CD2-CE3	6.96	140.16	133.90	10	6
2	C	139	TRP	CG-CD1-NE1	-6.94	103.16	110.10	2	6
1	B	1151	ARG	NE-CZ-NH1	6.92	123.76	120.30	7	2
1	A	1149	PHE	CB-CG-CD2	-6.91	115.96	120.80	6	3
1	A	1269	ARG	NE-CZ-NH1	6.78	123.69	120.30	8	5
1	A	1356	ARG	NE-CZ-NH1	6.75	123.67	120.30	4	3
1	B	1094	TRP	CG-CD1-NE1	-6.73	103.37	110.10	7	5
1	A	1362	ARG	NE-CZ-NH1	6.71	123.65	120.30	3	3
1	B	1230	MET	CA-C-N	6.70	131.93	117.20	7	6
1	B	1094	TRP	CB-CG-CD1	-6.63	118.38	127.00	4	8
1	B	1139	TYR	CB-CG-CD2	-6.62	117.03	121.00	10	4
1	B	1151	ARG	NE-CZ-NH2	-6.60	117.00	120.30	7	1
1	B	1349	ASP	CB-CG-OD1	6.56	124.20	118.30	5	1
1	A	1077	ASP	CB-CG-OD1	6.53	124.17	118.30	4	1
1	B	1318	ARG	NE-CZ-NH2	-6.52	117.04	120.30	2	3
1	B	1368	TRP	CG-CD1-NE1	-6.49	103.61	110.10	3	3
1	B	1050	PHE	CB-CG-CD2	-6.48	116.26	120.80	9	1
1	A	1273	ASP	CB-CG-OD1	6.47	124.13	118.30	2	1
1	A	1094	TRP	CG-CD1-NE1	-6.46	103.64	110.10	3	5
1	B	1002	ARG	NE-CZ-NH2	-6.46	117.07	120.30	6	2
2	C	91	ASP	CB-CG-OD1	6.45	124.11	118.30	7	1
2	C	58	ARG	NE-CZ-NH1	6.42	123.51	120.30	9	1
1	B	1031	PHE	CB-CG-CD2	-6.40	116.32	120.80	10	1
1	B	1064	TRP	CG-CD1-NE1	-6.39	103.71	110.10	8	4
1	A	1046	ASP	CB-CG-OD1	6.38	124.05	118.30	2	1
2	C	137	GLU	N-CA-C	6.38	128.21	111.00	8	1
1	B	1140	ARG	NE-CZ-NH2	-6.38	117.11	120.30	10	1
1	B	1368	TRP	NE1-CE2-CD2	6.37	113.67	107.30	2	1
1	A	1007	ARG	NE-CZ-NH2	-6.37	117.11	120.30	2	3
1	A	1094	TRP	CB-CG-CD1	-6.34	118.76	127.00	2	3
2	C	124	ASP	CB-CG-OD1	6.32	123.99	118.30	1	1
1	A	1368	TRP	CG-CD1-NE1	-6.29	103.81	110.10	4	6
1	B	1064	TRP	CB-CG-CD1	-6.23	118.90	127.00	8	3
2	C	147	PHE	CB-CG-CD2	-6.22	116.44	120.80	7	1
2	C	97	ASP	CB-CG-OD1	6.22	123.90	118.30	1	1
1	B	1008	GLU	OE1-CD-OE2	-6.22	115.84	123.30	1	2
1	A	1050	PHE	CB-CG-CD2	-6.22	116.45	120.80	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	1120	ARG	NE-CZ-NH2	-6.22	117.19	120.30	3	1
1	B	1192	ARG	NE-CZ-NH1	6.21	123.41	120.30	2	2
1	A	1139	TYR	CB-CG-CD2	-6.20	117.28	121.00	10	3
2	C	65	ARG	NE-CZ-NH2	-6.18	117.21	120.30	2	3
1	A	1314	ASP	CB-CG-OD1	6.16	123.85	118.30	2	2
1	B	1234	PHE	CB-CG-CD1	-6.13	116.51	120.80	9	1
1	B	1368	TRP	CB-CG-CD1	-6.07	119.11	127.00	8	2
2	C	186	LEU	CA-CB-CG	6.06	129.23	115.30	9	3
1	B	1007	ARG	NE-CZ-NH2	-6.03	117.28	120.30	6	1
1	A	1139	TYR	CB-CG-CD1	-6.03	117.38	121.00	5	1
1	A	1342	LYS	CA-C-N	6.00	130.41	117.20	4	8
1	B	1312	TYR	CB-CG-CD1	5.98	124.59	121.00	8	2
1	B	1045	PHE	CB-CG-CD2	-5.97	116.62	120.80	3	1
1	B	1015	ARG	NE-CZ-NH2	-5.96	117.32	120.30	6	1
1	B	1318	ARG	NE-CZ-NH1	5.95	123.27	120.30	2	1
1	A	1294	TYR	CB-CG-CD1	-5.94	117.44	121.00	4	2
1	A	1128	ASP	CB-CG-OD1	5.94	123.64	118.30	1	3
1	A	1327	TYR	CB-CG-CD2	-5.92	117.45	121.00	5	1
1	B	1273	ASP	CB-CG-OD1	5.92	123.63	118.30	7	1
1	A	1240	GLU	OE1-CD-OE2	-5.88	116.24	123.30	3	1
1	A	1226	TYR	CB-CG-CD2	-5.87	117.48	121.00	5	1
2	C	103	PHE	CB-CG-CD2	-5.86	116.70	120.80	4	1
1	A	1368	TRP	CB-CG-CD1	-5.85	119.39	127.00	1	2
1	A	1226	TYR	CB-CG-CD1	-5.83	117.50	121.00	3	1
2	C	58	ARG	NE-CZ-NH2	5.81	123.20	120.30	8	3
1	A	1108	ARG	NE-CZ-NH1	5.79	123.19	120.30	9	1
1	A	1286	ALA	CB-CA-C	-5.76	101.46	110.10	5	1
2	C	163	PHE	CB-CG-CD2	-5.74	116.79	120.80	6	2
1	B	1350	PHE	CB-CG-CD2	-5.71	116.81	120.80	10	2
2	C	172	PHE	CB-CG-CD2	-5.69	116.82	120.80	6	1
2	C	114	ALA	N-CA-C	5.68	126.34	111.00	8	1
1	A	1275	MET	CA-CB-CG	5.67	122.95	113.30	4	1
2	C	149	ARG	NE-CZ-NH2	-5.67	117.47	120.30	10	1
1	B	1051	VAL	CG1-CB-CG2	-5.66	101.84	110.90	5	1
1	B	1319	LEU	CA-CB-CG	5.65	128.29	115.30	10	2
2	C	107	ASP	CB-CG-OD1	5.64	123.38	118.30	7	1
1	B	1362	ARG	NE-CZ-NH1	5.63	123.11	120.30	2	2
2	C	137	GLU	OE1-CD-OE2	-5.60	116.58	123.30	9	1
1	B	1152	PHE	CB-CG-CD2	-5.60	116.88	120.80	10	3
1	B	1149	PHE	CB-CG-CD2	-5.59	116.89	120.80	3	3
2	C	166	GLU	OE1-CD-OE2	-5.59	116.60	123.30	6	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	1213	GLU	OE1-CD-OE2	-5.56	116.62	123.30	3	1
1	B	1197	ARG	NE-CZ-NH1	5.51	123.05	120.30	1	1
1	B	1327	TYR	CB-CG-CD1	-5.50	117.70	121.00	6	3
2	C	174	ASP	CB-CG-OD1	5.48	123.23	118.30	3	1
1	A	1283	ASP	CB-CG-OD1	5.47	123.23	118.30	2	1
1	B	1327	TYR	CB-CG-CD2	-5.45	117.73	121.00	10	1
1	A	1047	ASP	CB-CG-OD1	5.45	123.20	118.30	5	1
1	B	1293	GLU	OE1-CD-OE2	-5.43	116.78	123.30	2	1
1	B	1120	ARG	NE-CZ-NH1	5.43	123.01	120.30	5	1
1	A	1241	LEU	CA-CB-CG	5.41	127.75	115.30	9	1
2	C	106	THR	CA-CB-CG2	5.40	119.96	112.40	6	2
1	A	1368	TRP	NE1-CE2-CZ2	-5.35	124.51	130.40	8	1
1	B	1064	TRP	CG-CD2-CE3	5.35	138.72	133.90	8	1
1	B	1056	GLU	OE1-CD-OE2	-5.34	116.89	123.30	5	1
1	A	1234	PHE	CB-CG-CD2	-5.33	117.07	120.80	7	2
1	B	1296	VAL	N-CA-C	-5.32	96.65	111.00	9	1
1	A	1277	ALA	N-CA-CB	-5.29	102.70	110.10	3	1
1	A	1358	VAL	CG1-CB-CG2	-5.28	102.44	110.90	6	1
1	A	1043	ALA	CB-CA-C	-5.28	102.18	110.10	2	2
1	A	1152	PHE	CB-CG-CD1	5.28	124.50	120.80	6	1
1	B	1116	ASP	CB-CG-OD1	5.26	123.04	118.30	4	1
1	A	1059	GLU	OE1-CD-OE2	-5.26	116.98	123.30	6	1
1	B	1318	ARG	N-CA-C	5.26	125.20	111.00	2	2
1	A	1045	PHE	CB-CG-CD2	-5.24	117.14	120.80	3	2
1	B	1015	ARG	NE-CZ-NH1	5.23	122.92	120.30	5	1
1	B	1016	VAL	CA-CB-CG1	5.22	118.74	110.90	5	1
2	C	111	VAL	CG1-CB-CG2	-5.22	102.55	110.90	3	1
1	B	1047	ASP	CB-CG-OD2	5.22	122.99	118.30	3	1
1	B	1232	ASP	CB-CG-OD2	5.21	122.99	118.30	7	1
2	C	139	TRP	NE1-CE2-CD2	5.20	112.50	107.30	5	1
1	B	1368	TRP	CG-CD2-CE3	5.18	138.56	133.90	5	1
1	A	1098	ASN	N-CA-C	5.17	124.96	111.00	9	1
1	A	1304	GLU	OE1-CD-OE2	-5.16	117.11	123.30	4	1
1	A	1195	ASP	CB-CG-OD1	5.16	122.94	118.30	5	1
2	C	45	GLN	CA-CB-CG	5.15	124.73	113.40	3	1
1	B	1234	PHE	CB-CG-CD2	5.14	124.40	120.80	9	1
1	A	1343	ASP	CB-CG-OD1	5.10	122.89	118.30	4	1
1	B	1294	TYR	CB-CG-CD1	-5.10	117.94	121.00	7	1
1	A	1107	GLU	OE1-CD-OE2	-5.10	117.18	123.30	4	1
1	B	1007	ARG	NE-CZ-NH1	5.10	122.85	120.30	4	1
1	B	1254	THR	CA-C-N	-5.09	106.00	117.20	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	50	VAL	CG1-CB-CG2	5.09	119.05	110.90	4	1
1	B	1175	VAL	CA-CB-CG2	5.09	118.53	110.90	6	1
2	C	60	ARG	NE-CZ-NH1	5.09	122.84	120.30	7	1
1	B	1100	GLU	OE1-CD-OE2	-5.08	117.20	123.30	7	1
1	A	1343	ASP	N-CA-CB	5.07	119.72	110.60	4	1
1	A	1319	LEU	CA-CB-CG	5.05	126.91	115.30	8	1
1	A	1079	GLU	OE1-CD-OE2	-5.05	117.25	123.30	8	1
1	A	1094	TRP	NE1-CE2-CD2	5.04	112.34	107.30	9	1
1	B	1239	MET	CA-CB-CG	5.04	121.87	113.30	9	1
2	C	52	GLU	OE1-CD-OE2	-5.04	117.25	123.30	1	1
1	B	1108	ARG	NH1-CZ-NH2	-5.03	113.86	119.40	4	1
1	B	1045	PHE	N-CA-C	-5.03	97.41	111.00	8	1
1	B	1046	ASP	CB-CG-OD1	5.03	122.82	118.30	10	1
1	A	1002	ARG	N-CA-C	-5.02	97.44	111.00	5	1
2	C	183	LEU	CA-CB-CG	5.02	126.84	115.30	9	1
1	A	1213	GLU	OE1-CD-OE2	-5.01	117.29	123.30	8	1
1	B	1128	ASP	CB-CG-OD1	5.01	122.81	118.30	5	1
1	B	1351	ASP	CB-CG-OD2	5.00	122.80	118.30	10	1
1	A	1144	GLU	OE1-CD-OE2	-5.00	117.30	123.30	6	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	1294	TYR	Sidechain	4
1	B	1139	TYR	Sidechain	4
1	B	1318	ARG	Sidechain	3
2	C	90	TYR	Sidechain	3
1	A	1045	PHE	Peptide	3
1	B	1312	TYR	Sidechain	3
1	A	1140	ARG	Sidechain	3
1	A	1362	ARG	Sidechain	2
1	A	1318	ARG	Sidechain	2
2	C	48	TYR	Sidechain	2
1	B	1327	TYR	Sidechain	1
1	A	1123	ARG	Sidechain	1
1	A	1139	TYR	Sidechain	1
2	C	58	ARG	Sidechain	1
1	A	1255	THR	Peptide	1
1	A	1327	TYR	Sidechain	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
2	C	60	ARG	Sidechain	1
2	C	155	TYR	Sidechain	1
1	A	1269	ARG	Sidechain	1
1	B	998	HIS	Peptide	1
1	A	1108	ARG	Sidechain	1
1	A	1007	ARG	Sidechain	1
2	C	39	TYR	Sidechain	1
1	A	1192	ARG	Sidechain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2735	579	2770	35±5
1	B	2729	582	2778	40±5
2	C	1272	264	1273	22±5
3	B	44	8	26	0±0
4	C	48	7	25	1±1
All	All	68280	14400	68720	892

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1186:SER:HB3	1:B:1187:LEU:HA	0.88	1.44	8	2
2:C:120:PRO:HG2	2:C:160:ASN:HB2	0.81	1.52	4	1
2:C:162:LEU:HA	2:C:168:THR:HG22	0.77	1.56	9	2
1:B:1016:VAL:HB	1:B:1043:ALA:HB2	0.77	1.57	8	1
1:A:1187:LEU:HA	1:B:1186:SER:HB3	0.77	1.56	7	2
1:B:1152:PHE:HB2	1:B:1163:VAL:HG11	0.76	1.57	4	6
1:A:1134:ALA:HB1	1:A:1176:ALA:HB2	0.75	1.56	8	5
2:C:40:GLY:HA3	2:C:113:GLY:HA3	0.74	1.57	2	2
1:A:1152:PHE:HB2	1:A:1163:VAL:HG11	0.74	1.59	10	4
1:A:1151:ARG:HA	1:B:1322:GLN:HB2	0.73	1.61	10	8
2:C:130:ILE:HG12	2:C:156:ALA:HB2	0.73	1.59	8	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1015:ARG:HD2	1:A:1072:VAL:HG11	0.72	1.60	8	3
1:B:1070:LEU:HD13	1:B:1331:LEU:HD13	0.71	1.62	3	3
2:C:148:LYS:HD3	2:C:170:MET:SD	0.71	2.25	2	2
2:C:41:MET:SD	2:C:83:LEU:HD11	0.70	2.27	5	2
1:B:1287:GLN:HB3	1:B:1313:THR:HG23	0.68	1.65	10	3
2:C:146:VAL:HG21	2:C:162:LEU:HB3	0.68	1.63	7	2
1:A:1136:ILE:HD13	1:A:1323:SER:HA	0.68	1.66	7	5
1:B:1134:ALA:HB1	1:B:1176:ALA:HB2	0.68	1.66	4	5
1:A:1135:ASN:HB2	1:A:1175:VAL:HG12	0.67	1.64	3	3
1:A:1023:VAL:HG22	1:A:1033:VAL:HG11	0.67	1.64	8	2
2:C:121:ALA:HA	2:C:125:ASP:HB3	0.67	1.67	9	1
1:B:1215:ASP:HB3	1:B:1237:ALA:HB1	0.67	1.67	4	1
1:A:1133:MET:HA	1:A:1136:ILE:HD12	0.66	1.66	8	2
1:B:1203:GLN:HG2	2:C:74:ARG:HG3	0.66	1.67	1	3
1:A:1005:ILE:HG23	1:A:1017:ALA:HB3	0.66	1.67	3	7
1:A:1141:ALA:HB2	1:A:1284:LEU:HD21	0.66	1.68	9	5
1:B:1145:ALA:HB1	1:B:1251:ILE:HD12	0.65	1.68	4	7
1:A:1070:LEU:HD13	1:A:1331:LEU:HD13	0.65	1.67	5	3
1:B:1195:ASP:HB3	1:B:1200:VAL:HG21	0.65	1.67	6	2
1:A:1009:ARG:NH1	1:A:1079:GLU:HG2	0.65	2.06	1	1
1:A:1145:ALA:HB1	1:A:1251:ILE:HD12	0.65	1.67	4	5
2:C:162:LEU:HA	2:C:168:THR:HB	0.65	1.68	1	1
2:C:107:ASP:HA	2:C:142:GLN:HB2	0.65	1.69	6	2
1:A:1305:ASN:HA	1:B:1046:ASP:HB2	0.65	1.69	3	2
2:C:133:MET:SD	2:C:134:PRO:HD2	0.65	2.32	4	7
1:A:1061:ASN:HA	1:A:1064:TRP:HD1	0.64	1.51	8	1
1:B:1083:LEU:HD21	1:B:1089:LEU:HD13	0.64	1.69	8	1
2:C:66:PHE:HB2	2:C:93:VAL:HA	0.64	1.68	7	4
2:C:72:ALA:HB3	2:C:79:MET:SD	0.64	2.33	2	1
1:A:1003:ILE:HG12	1:A:1068:ILE:HB	0.64	1.69	6	1
1:B:1212:LEU:HB3	1:B:1241:LEU:HD21	0.64	1.67	8	1
1:A:1157:ILE:HG21	2:C:70:PRO:HB2	0.64	1.68	2	1
1:A:1148:GLU:HB3	1:A:1308:LYS:HD2	0.63	1.68	4	3
1:B:1123:ARG:HG3	1:B:1354:VAL:HG21	0.63	1.70	2	3
1:B:1199:GLU:HB2	2:C:155:TYR:HE1	0.63	1.53	9	1
1:A:1254:THR:HB	1:A:1283:ASP:HA	0.63	1.68	10	3
1:A:1148:GLU:HB2	1:A:1310:ILE:HD11	0.63	1.69	2	5
2:C:30:SER:HA	2:C:107:ASP:HB3	0.63	1.69	4	3
1:B:1157:ILE:HG23	1:B:1162:LYS:HG2	0.62	1.71	8	1
1:A:1018:ALA:HB1	1:A:1022:THR:HB	0.62	1.70	4	1
1:A:1113:MET:SD	1:A:1338:LEU:HD21	0.62	2.33	7	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:37:PRO:HD2	2:C:68:ILE:HG12	0.62	1.69	10	4
1:A:1339:CYS:SG	1:A:1342:LYS:HA	0.62	2.34	2	1
2:C:174:ASP:HB3	2:C:177:ALA:HB3	0.62	1.72	4	5
2:C:47:GLN:HG2	2:C:82:LEU:HB3	0.62	1.71	4	2
2:C:143:ASN:HA	2:C:167:ASN:HB2	0.62	1.71	1	1
1:B:1267:ILE:HG21	1:B:1281:ILE:HD13	0.61	1.71	9	2
1:B:1080:ILE:HA	1:B:1083:LEU:HD12	0.61	1.71	5	2
1:B:1070:LEU:HD22	1:B:1331:LEU:HD22	0.61	1.72	7	5
2:C:41:MET:HA	2:C:46:ALA:HB3	0.61	1.72	8	2
1:B:1181:ILE:HG22	1:B:1207:MET:SD	0.61	2.36	8	5
2:C:24:ALA:HB1	2:C:186:LEU:HA	0.61	1.71	7	1
1:A:1151:ARG:NH2	1:A:1164:PRO:HB2	0.61	2.10	2	1
1:B:1169:MET:HB2	1:B:1249:VAL:HG11	0.61	1.71	4	6
2:C:151:MET:SD	2:C:170:MET:SD	0.61	2.98	6	1
1:A:1322:GLN:HB2	1:B:1151:ARG:HA	0.61	1.73	7	5
2:C:145:ILE:HG12	2:C:171:LEU:HB2	0.61	1.73	9	1
2:C:99:ILE:HG13	2:C:102:ASP:HB2	0.61	1.71	1	1
2:C:25:GLU:HA	2:C:28:LYS:HE2	0.60	1.73	9	2
1:B:1295:THR:HG23	1:B:1311:GLY:HA3	0.60	1.73	10	5
1:A:1014:THR:HB	1:A:1320:PRO:HB3	0.60	1.72	8	1
1:A:1296:VAL:HB	1:A:1299:GLU:HB2	0.60	1.74	9	1
1:A:1328:GLY:HA2	1:A:1331:LEU:HD12	0.59	1.74	3	3
1:B:1181:ILE:HG12	1:B:1191:VAL:HG11	0.59	1.74	5	2
1:B:1120:ARG:HB2	1:B:1375:VAL:HG13	0.59	1.74	3	1
1:B:1070:LEU:HB3	1:B:1331:LEU:HD13	0.59	1.72	2	4
1:B:1199:GLU:HB2	2:C:74:ARG:NH2	0.59	2.13	10	1
1:A:1124:ALA:HB2	1:A:1354:VAL:HG11	0.59	1.75	3	1
1:A:1246:ALA:HB1	1:A:1275:MET:HG2	0.58	1.75	2	2
1:B:1328:GLY:HA2	1:B:1331:LEU:HD12	0.58	1.73	4	5
1:B:1125:GLN:HA	1:B:1128:ASP:HB3	0.58	1.74	10	1
1:B:1230:MET:N	1:B:1231:SER:HG	0.58	1.96	8	3
2:C:111:VAL:HB	2:C:146:VAL:HA	0.58	1.75	8	4
1:A:1118:VAL:HG22	1:A:1358:VAL:HG22	0.58	1.74	2	2
1:B:1167:LYS:HB2	1:B:1249:VAL:HA	0.58	1.74	5	5
1:B:1148:GLU:HB3	1:B:1308:LYS:HD2	0.58	1.74	3	2
1:B:1193:ALA:HB3	1:B:1204:VAL:HG11	0.58	1.74	8	1
1:B:1173:ALA:HA	1:B:1177:GLY:HA3	0.58	1.75	9	3
2:C:39:TYR:HB2	2:C:114:ALA:HB2	0.58	1.76	4	1
2:C:70:PRO:HD3	2:C:96:MET:HB2	0.58	1.74	4	1
1:B:1207:MET:SD	2:C:75:LEU:HG	0.58	2.37	7	1
2:C:20:ALA:HA	2:C:171:LEU:HD21	0.58	1.76	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:1127:LEU:HG	1:B:1334:LEU:HA	0.58	1.76	8	2
2:C:90:TYR:HA	2:C:93:VAL:HB	0.58	1.74	7	2
1:B:1214:LEU:HG	1:B:1241:LEU:HD22	0.57	1.73	5	1
1:B:1335:LEU:HD23	1:B:1338:LEU:HD12	0.57	1.75	2	2
1:B:1113:MET:SD	1:B:1334:LEU:HD21	0.57	2.39	10	2
1:B:1016:VAL:HG21	1:B:1039:ALA:HB1	0.57	1.75	3	4
1:B:1005:ILE:HG23	1:B:1017:ALA:HB3	0.57	1.75	1	3
1:A:1254:THR:HG21	1:A:1291:ASN:HB2	0.57	1.76	2	2
1:B:1118:VAL:HG22	1:B:1358:VAL:HG23	0.57	1.76	3	1
1:A:1300:ILE:HG12	1:A:1310:ILE:HG12	0.57	1.75	6	2
1:B:1312:TYR:HB2	1:B:1315:LEU:HG	0.57	1.74	2	3
1:B:1120:ARG:HB2	1:B:1375:VAL:HG11	0.57	1.77	10	1
1:A:1280:VAL:HG22	1:A:1308:LYS:HB2	0.56	1.75	10	2
1:B:1083:LEU:HD11	1:B:1089:LEU:HD22	0.56	1.78	9	2
1:A:1157:ILE:HD13	2:C:95:GLU:HB3	0.56	1.77	2	3
2:C:116:ASP:HA	2:C:119:ASN:HB2	0.56	1.75	3	3
2:C:34:ILE:HB	2:C:109:VAL:HG13	0.56	1.75	1	1
2:C:68:ILE:HB	2:C:95:GLU:HA	0.56	1.77	5	1
1:B:1083:LEU:HD22	1:B:1110:VAL:HG11	0.56	1.76	5	1
1:B:1145:ALA:HA	1:B:1280:VAL:HG11	0.56	1.76	10	5
1:A:1157:ILE:HG12	2:C:70:PRO:HG2	0.56	1.78	10	1
1:A:1267:ILE:HG23	1:A:1271:MET:SD	0.56	2.41	4	1
1:A:1157:ILE:HG13	2:C:70:PRO:HB3	0.55	1.78	5	2
1:B:1332:VAL:HG12	1:B:1336:LYS:HE3	0.55	1.76	2	2
1:B:1041:GLN:NE2	1:B:1046:ASP:HA	0.55	2.16	7	1
1:B:1141:ALA:HA	1:B:1282:VAL:HG11	0.55	1.78	2	3
2:C:122:ALA:HB1	2:C:133:MET:HB3	0.55	1.77	7	2
1:A:1075:PRO:HG2	1:A:1089:LEU:HD21	0.55	1.78	5	4
1:B:1120:ARG:HB2	1:B:1375:VAL:HG21	0.55	1.78	8	1
2:C:109:VAL:HG11	2:C:138:VAL:HG21	0.55	1.78	10	1
2:C:32:SER:HB2	2:C:106:THR:HA	0.55	1.78	1	2
2:C:148:LYS:HE3	2:C:151:MET:HA	0.55	1.79	5	1
1:A:1004:GLY:O	1:A:1006:PRO:HD3	0.54	2.01	7	2
1:B:1118:VAL:HG12	1:B:1124:ALA:HB1	0.54	1.77	8	3
1:B:1043:ALA:HA	1:B:1320:PRO:HB2	0.54	1.79	10	2
1:A:1354:VAL:O	1:A:1358:VAL:HG23	0.54	2.02	10	6
1:B:1267:ILE:HB	1:B:1292:CYS:HA	0.54	1.79	4	2
1:A:1137:ALA:HB2	1:A:1316:PRO:HG3	0.54	1.80	8	2
1:A:1115:MET:SD	1:A:1334:LEU:HD22	0.54	2.43	8	3
1:A:1136:ILE:HG23	1:A:1319:LEU:HD23	0.54	1.80	9	1
1:B:1349:ASP:HB3	1:B:1355:ILE:HG21	0.54	1.79	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1090:VAL:HG13	1:A:1113:MET:HB2	0.54	1.78	4	1
1:A:1136:ILE:HD11	1:A:1326:LEU:HB2	0.54	1.80	7	1
2:C:96:MET:SD	2:C:134:PRO:HB2	0.53	2.43	6	1
1:B:1085:PRO:HB3	1:B:1109:ASN:HB2	0.53	1.80	3	2
1:B:1300:ILE:HG12	1:B:1310:ILE:HG12	0.53	1.79	7	1
1:A:1070:LEU:HD21	1:A:1335:LEU:HD11	0.53	1.81	4	1
1:A:1169:MET:HA	1:A:1192:ARG:O	0.53	2.03	4	1
1:A:1113:MET:SD	1:A:1334:LEU:HD21	0.53	2.43	9	1
1:B:1286:ALA:HA	1:B:1290:GLY:HA2	0.53	1.80	9	1
1:B:1085:PRO:HA	1:B:1108:ARG:O	0.53	2.04	7	1
1:B:1022:THR:HG21	1:B:1328:GLY:HA3	0.53	1.80	1	1
1:B:1181:ILE:HG22	1:B:1207:MET:HG2	0.53	1.79	4	1
1:A:1132:SER:HB3	1:A:1326:LEU:HB3	0.53	1.80	2	1
1:B:1339:CYS:SG	1:B:1344:GLY:N	0.53	2.82	10	1
1:B:1355:ILE:HA	1:B:1358:VAL:HG12	0.53	1.81	9	4
2:C:35:ILE:O	2:C:37:PRO:HD3	0.53	2.03	6	1
1:A:1252:ILE:HB	1:A:1281:ILE:HG12	0.53	1.80	1	1
1:A:1339:CYS:SG	1:A:1344:GLY:HA2	0.53	2.44	6	3
2:C:157:GLY:O	2:C:160:ASN:HB2	0.53	2.04	7	1
1:A:1109:ASN:HA	1:A:1364:GLY:HA2	0.53	1.79	1	1
2:C:121:ALA:HA	2:C:124:ASP:HB3	0.53	1.80	10	1
1:A:1145:ALA:HA	1:A:1280:VAL:HG11	0.52	1.81	1	4
2:C:148:LYS:O	2:C:172:PHE:HA	0.52	2.04	6	4
1:A:1113:MET:HB3	1:A:1358:VAL:HG12	0.52	1.82	10	2
1:B:1029:LEU:HD21	1:B:1336:LYS:HG2	0.52	1.80	6	2
1:A:1031:PHE:HZ	1:A:1339:CYS:HG	0.52	1.44	7	1
1:B:1141:ALA:HB2	1:B:1284:LEU:HD21	0.52	1.82	7	2
1:A:1255:THR:HG22	1:A:1284:LEU:HD13	0.52	1.81	8	2
1:B:1192:ARG:HG2	1:B:1210:GLU:HB2	0.52	1.80	3	2
2:C:53:ILE:HD13	2:C:183:LEU:HA	0.52	1.81	7	2
1:A:1031:PHE:HZ	1:A:1339:CYS:SG	0.52	2.28	7	1
2:C:52:GLU:HB3	2:C:183:LEU:HB2	0.52	1.81	8	2
1:B:1181:ILE:HG23	1:B:1191:VAL:HG11	0.52	1.81	1	2
2:C:145:ILE:HG23	2:C:171:LEU:HB2	0.52	1.82	5	1
1:A:1267:ILE:HA	1:A:1271:MET:SD	0.51	2.45	10	1
2:C:148:LYS:HE3	2:C:151:MET:SD	0.51	2.46	4	1
1:A:1178:LEU:HD13	1:A:1203:GLN:HG2	0.51	1.81	1	1
1:B:1124:ALA:HB2	1:B:1354:VAL:HG22	0.51	1.82	5	1
1:B:1123:ARG:HD2	1:B:1337:LEU:HD21	0.51	1.81	1	1
1:B:1254:THR:HG23	1:B:1283:ASP:HA	0.51	1.82	8	1
1:A:1067:GLU:HB3	1:A:1068:ILE:HD12	0.51	1.82	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1024:GLU:O	1:A:1028:LYS:HG2	0.51	2.06	8	1
1:A:1110:VAL:HG23	1:A:1112:VAL:HG23	0.51	1.82	6	1
1:A:1161:GLY:HA3	1:B:1326:LEU:HA	0.51	1.83	8	1
1:B:1125:GLN:NE2	1:B:1131:SER:HB3	0.51	2.19	8	1
2:C:41:MET:SD	2:C:79:MET:HB2	0.51	2.46	8	1
1:A:1236:LYS:O	1:A:1240:GLU:HG3	0.51	2.06	9	2
1:B:1003:ILE:HG12	1:B:1068:ILE:HD12	0.51	1.81	7	1
1:A:1149:PHE:CZ	1:A:1250:ASP:HB3	0.50	2.41	10	2
1:B:1258:ILE:HB	1:B:1261:LYS:HB2	0.50	1.84	3	1
2:C:73:GLY:C	2:C:74:ARG:HD2	0.50	2.26	1	1
1:A:1026:LEU:HD21	1:A:1332:VAL:HG22	0.50	1.83	4	1
1:B:1007:ARG:HB2	1:B:1039:ALA:HA	0.50	1.84	10	1
1:A:1320:PRO:HD2	1:B:1150:GLY:HA2	0.50	1.84	5	3
1:B:1015:ARG:HG3	1:B:1317:GLY:HA2	0.50	1.82	2	4
2:C:165:LYS:HB2	2:C:168:THR:HB	0.50	1.80	10	2
1:B:1118:VAL:HG21	1:B:1128:ASP:HA	0.50	1.83	2	1
1:B:1083:LEU:HB3	1:B:1110:VAL:HG11	0.50	1.84	9	4
2:C:156:ALA:HB1	2:C:158:VAL:HG22	0.50	1.84	9	1
1:B:1122:SER:HB2	2:C:133:MET:HA	0.50	1.82	4	3
1:B:1148:GLU:HB2	1:B:1310:ILE:HD11	0.50	1.83	10	2
1:A:1292:CYS:HB3	1:A:1295:THR:OG1	0.50	2.06	10	3
1:B:1088:THR:HA	1:B:1111:THR:HB	0.50	1.83	1	2
2:C:123:GLN:HB2	2:C:135:VAL:HG22	0.50	1.82	2	1
1:A:1181:ILE:HA	1:A:1191:VAL:HG11	0.50	1.84	1	1
1:B:1292:CYS:HB3	1:B:1295:THR:OG1	0.50	2.07	8	4
1:B:1338:LEU:HD13	1:B:1346:ILE:HG23	0.50	1.84	10	1
3:B:1:NAD:O1N	3:B:1:NAD:H3D	0.50	2.07	3	1
1:A:1019:THR:HG21	1:A:1325:GLN:HA	0.49	1.84	10	1
1:A:1140:ARG:HG3	1:A:1315:LEU:HD22	0.49	1.82	4	2
1:B:1127:LEU:HD23	1:B:1334:LEU:HD12	0.49	1.83	5	2
1:A:1194:PHE:HB2	1:A:1212:LEU:HD12	0.49	1.84	6	1
1:A:1140:ARG:HD3	1:A:1319:LEU:HD13	0.49	1.82	3	1
1:B:998:HIS:HB2	1:B:1000:HIS:HB2	0.49	1.82	10	1
1:B:1275:MET:SD	1:B:1281:ILE:HD11	0.49	2.48	6	1
1:B:1203:GLN:OE1	2:C:74:ARG:HA	0.49	2.07	8	3
1:A:1089:LEU:HD23	1:A:1112:VAL:HG22	0.49	1.83	7	1
1:B:1025:GLN:HE22	1:B:1329:THR:HG23	0.49	1.68	3	1
1:B:1121:ILE:HG22	2:C:131:ALA:HB1	0.49	1.82	8	1
1:A:1174:GLY:HA2	1:A:1197:ARG:NH2	0.49	2.23	10	1
1:B:1250:ASP:O	1:B:1279:SER:HB3	0.49	2.08	6	2
1:A:1252:ILE:HD12	1:A:1281:ILE:HG12	0.49	1.84	10	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1157:ILE:HB	2:C:95:GLU:HG2	0.49	1.85	9	1
2:C:35:ILE:HG22	2:C:37:PRO:HD3	0.49	1.84	2	1
1:B:1333:ASN:HA	1:B:1336:LYS:HD2	0.49	1.85	1	4
1:A:1015:ARG:HB3	1:A:1072:VAL:HG11	0.49	1.84	7	1
1:B:1058:VAL:HB	1:B:1062:SER:HB2	0.49	1.84	8	1
1:B:1155:GLY:HA3	1:B:1165:PRO:HG3	0.49	1.84	8	1
1:A:1277:ALA:HB1	1:B:1045:PHE:HA	0.49	1.83	7	2
1:A:1096:ALA:HB3	1:A:1097:GLN:NE2	0.48	2.23	6	1
1:A:1070:LEU:HB3	1:A:1331:LEU:HD13	0.48	1.84	7	2
1:A:1036:GLU:HB3	1:A:1039:ALA:HB2	0.48	1.85	1	1
2:C:107:ASP:HA	2:C:142:GLN:HB3	0.48	1.83	1	1
2:C:153:THR:HG23	2:C:157:GLY:HA3	0.48	1.85	7	2
2:C:160:ASN:HB3	2:C:162:LEU:HD12	0.48	1.84	9	1
2:C:115:ASN:ND2	2:C:116:ASP:H	0.48	2.06	10	1
1:A:1080:ILE:HD11	1:A:1101:LEU:HG	0.48	1.84	5	1
2:C:75:LEU:HB2	2:C:78:HIS:HB2	0.48	1.85	8	1
1:B:1235:ILE:O	1:B:1239:MET:HG2	0.48	2.09	5	2
1:B:1268:THR:HA	1:B:1293:GLU:HG3	0.48	1.85	5	2
1:B:1015:ARG:NH1	1:B:1133:MET:SD	0.48	2.87	9	1
1:B:1067:GLU:HB2	1:B:1068:ILE:HD12	0.48	1.86	9	1
1:B:1298:GLY:HA2	1:B:1312:TYR:HA	0.48	1.84	4	1
1:A:1152:PHE:CD1	1:B:1322:GLN:HG2	0.48	2.43	9	4
2:C:148:LYS:HE3	4:C:1001:NAP:O2B	0.48	2.09	10	1
2:C:79:MET:HA	2:C:82:LEU:HD12	0.48	1.85	10	1
2:C:109:VAL:HG11	2:C:138:VAL:HG23	0.48	1.86	6	1
1:B:1094:TRP:HB2	1:B:1098:ASN:ND2	0.48	2.24	1	2
1:B:1002:ARG:HG3	1:B:1032:THR:HB	0.48	1.85	6	1
1:B:1123:ARG:HA	2:C:134:PRO:HD3	0.48	1.84	3	2
1:B:1300:ILE:HG23	1:B:1310:ILE:HG12	0.48	1.85	4	1
1:A:1016:VAL:HG21	1:A:1039:ALA:HB1	0.48	1.84	10	1
2:C:145:ILE:HG13	2:C:171:LEU:HB2	0.48	1.86	7	2
2:C:144:VAL:HB	2:C:168:THR:HG23	0.48	1.85	5	2
1:A:1127:LEU:HD21	1:A:1337:LEU:HD22	0.48	1.85	6	1
2:C:37:PRO:HG2	2:C:68:ILE:HG13	0.48	1.83	1	1
1:A:1140:ARG:HD3	1:A:1319:LEU:HB2	0.47	1.85	8	1
2:C:71:VAL:HG22	2:C:76:PRO:HB3	0.47	1.85	8	1
2:C:115:ASN:ND2	2:C:154:GLY:HA3	0.47	2.24	10	1
1:A:1022:THR:HB	1:A:1332:VAL:HG21	0.47	1.85	2	1
1:B:1251:ILE:HA	1:B:1280:VAL:O	0.47	2.09	1	1
1:A:1025:GLN:OE1	1:A:1336:LYS:HE2	0.47	2.10	10	1
1:B:1003:ILE:HG12	1:B:1068:ILE:HB	0.47	1.85	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1167:LYS:HB2	1:A:1249:VAL:HA	0.47	1.85	2	1
1:A:1214:LEU:HG	1:A:1216:PHE:HB2	0.47	1.84	1	1
1:A:1250:ASP:O	1:A:1279:SER:HB3	0.47	2.08	8	2
1:A:1029:LEU:HA	1:A:1342:LYS:HE3	0.47	1.84	10	1
1:B:1264:PRO:O	1:B:1291:ASN:HA	0.47	2.09	5	1
1:B:1105:LEU:HD13	1:B:1112:VAL:HG21	0.47	1.85	7	4
1:A:1312:TYR:HB2	1:A:1315:LEU:HG	0.47	1.84	6	1
2:C:118:VAL:HG12	2:C:136:LEU:HB2	0.47	1.86	1	1
1:A:1061:ASN:HA	1:A:1064:TRP:CD1	0.47	2.40	8	1
2:C:144:VAL:HB	2:C:168:THR:HA	0.47	1.86	2	2
1:B:1284:LEU:HD23	1:B:1315:LEU:HD13	0.47	1.85	2	1
2:C:34:ILE:HG12	2:C:106:THR:HG21	0.47	1.87	1	1
1:A:1178:LEU:HB3	1:A:1207:MET:SD	0.47	2.49	6	1
1:A:1185:ASN:ND2	1:A:1208:GLY:HA3	0.47	2.25	7	1
1:B:1253:VAL:HG12	1:B:1255:THR:HG23	0.47	1.86	8	2
1:B:1104:LYS:O	1:B:1108:ARG:HG2	0.47	2.08	6	1
2:C:49:PRO:O	2:C:183:LEU:HD11	0.47	2.09	6	1
2:C:30:SER:CA	2:C:107:ASP:HB3	0.47	2.40	4	1
2:C:160:ASN:HD22	2:C:162:LEU:HD12	0.47	1.70	1	1
1:A:1029:LEU:HA	1:A:1342:LYS:HE2	0.47	1.86	5	1
1:A:1019:THR:HG21	1:A:1321:THR:HG23	0.47	1.87	5	1
1:A:1172:GLY:O	1:A:1255:THR:HB	0.47	2.09	4	1
1:B:1064:TRP:CZ3	1:B:1083:LEU:HG	0.47	2.45	2	1
2:C:48:TYR:HB2	2:C:49:PRO:HD3	0.47	1.87	3	2
1:B:1111:THR:HG23	1:B:1362:ARG:HA	0.47	1.86	7	2
1:B:1248:GLU:O	1:B:1276:LYS:NZ	0.47	2.47	4	1
2:C:179:VAL:HA	2:C:182:ILE:HG12	0.47	1.86	2	2
1:A:1148:GLU:HB3	1:A:1308:LYS:HG3	0.47	1.86	2	1
1:A:1152:PHE:HE1	1:B:1136:ILE:HD13	0.47	1.68	10	1
1:B:1272:VAL:HG11	1:B:1303:THR:HG21	0.47	1.86	4	1
1:B:1357:GLY:CA	1:B:1370:ALA:HB2	0.47	2.39	1	1
2:C:35:ILE:HG12	2:C:110:LEU:HB2	0.47	1.85	8	1
1:A:1178:LEU:HD23	1:A:1181:ILE:HD12	0.47	1.86	9	1
2:C:109:VAL:HB	2:C:144:VAL:HA	0.47	1.86	4	1
1:A:1071:LYS:HE3	1:A:1073:ASN:O	0.47	2.10	1	1
1:A:1322:GLN:HG2	1:B:1152:PHE:CD1	0.46	2.46	7	1
1:B:1302:THR:HG23	1:B:1308:LYS:HG2	0.46	1.86	7	1
1:A:1080:ILE:HA	1:A:1083:LEU:HD23	0.46	1.86	4	2
1:B:1169:MET:O	1:B:1252:ILE:HA	0.46	2.09	2	1
1:B:1199:GLU:O	1:B:1203:GLN:HG2	0.46	2.09	3	1
1:A:1069:ILE:HG12	1:A:1087:THR:HG21	0.46	1.87	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:1275:MET:HB2	1:B:1307:VAL:HG21	0.46	1.87	4	2
1:B:1265:LYS:NZ	1:B:1289:GLY:O	0.46	2.49	6	3
1:A:1157:ILE:HD13	2:C:95:GLU:HB2	0.46	1.86	9	1
1:A:1120:ARG:HD3	1:A:1130:LEU:HD13	0.46	1.88	8	1
1:B:1169:MET:HA	1:B:1192:ARG:O	0.46	2.10	2	2
1:A:1339:CYS:HB3	1:A:1344:GLY:HA2	0.46	1.87	7	1
1:B:1200:VAL:HB	1:B:1203:GLN:NE2	0.46	2.25	7	1
1:B:1350:PHE:HE1	1:B:1359:THR:HB	0.46	1.70	3	1
1:B:1146:ALA:HB2	1:B:1153:PHE:HE1	0.46	1.70	3	2
1:B:1267:ILE:HG22	1:B:1272:VAL:HG22	0.46	1.87	8	1
1:B:1016:VAL:HG12	1:B:1043:ALA:HB2	0.46	1.87	5	1
1:B:1252:ILE:HB	1:B:1281:ILE:HG12	0.46	1.87	1	1
1:A:1150:GLY:HA2	1:B:1320:PRO:HG2	0.46	1.87	5	3
2:C:44:ALA:HB2	4:C:1001:NAP:N6A	0.46	2.25	10	1
1:B:1051:VAL:HG23	1:B:1057:ILE:HG12	0.46	1.88	5	1
1:A:1301:PHE:HB3	1:A:1309:VAL:HB	0.46	1.87	2	1
1:A:1070:LEU:HD22	1:A:1331:LEU:HD22	0.46	1.87	8	3
1:A:1268:THR:O	1:A:1272:VAL:HG23	0.46	2.10	7	3
1:B:1008:GLU:HG3	1:B:1072:VAL:HB	0.46	1.87	7	2
1:A:1080:ILE:HG21	1:A:1104:LYS:HB3	0.46	1.87	5	1
1:B:1193:ALA:HB3	1:B:1204:VAL:HG21	0.46	1.88	5	2
2:C:34:ILE:HG13	2:C:103:PHE:HA	0.46	1.88	5	1
2:C:109:VAL:HG21	2:C:138:VAL:HG23	0.46	1.86	7	1
1:A:1132:SER:HB2	1:A:1330:ASN:OD1	0.46	2.11	4	1
1:B:1109:ASN:HA	1:B:1364:GLY:HA3	0.46	1.88	2	1
1:B:1178:LEU:HA	1:B:1181:ILE:HD12	0.46	1.86	3	1
1:A:1338:LEU:HD23	1:A:1346:ILE:HG23	0.46	1.88	5	1
1:A:1368:TRP:CD1	1:A:1369:PRO:HA	0.46	2.46	5	1
1:B:1133:MET:HB3	1:B:1316:PRO:HB3	0.45	1.88	5	4
1:B:1010:LEU:HB3	1:B:1013:GLU:HB2	0.45	1.89	6	2
1:B:1007:ARG:NH1	1:B:1038:GLY:HA3	0.45	2.26	9	1
1:A:1329:THR:HB	1:B:1160:ALA:HB1	0.45	1.86	9	1
1:A:1161:GLY:HA3	1:B:1329:THR:HG21	0.45	1.88	4	2
1:B:1035:VAL:HB	1:B:1057:ILE:HD13	0.45	1.88	7	1
1:B:1113:MET:SD	1:B:1338:LEU:HD11	0.45	2.51	5	1
1:B:1080:ILE:HG22	1:B:1108:ARG:HG3	0.45	1.86	9	1
1:A:1263:ALA:HB1	1:A:1291:ASN:ND2	0.45	2.26	8	1
1:B:1139:TYR:HD2	1:B:1319:LEU:HD21	0.45	1.71	8	1
1:A:1204:VAL:HG13	1:A:1209:ALA:HB3	0.45	1.87	6	2
2:C:113:GLY:HA2	2:C:147:PHE:O	0.45	2.11	5	1
1:A:1083:LEU:HD12	1:A:1110:VAL:HG11	0.45	1.88	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1167:LYS:N	1:A:1167:LYS:HD2	0.45	2.27	7	1
1:B:1115:MET:HB3	1:B:1129:ALA:CB	0.45	2.41	7	1
1:B:1070:LEU:HD22	1:B:1331:LEU:HB3	0.45	1.88	4	1
1:B:1112:VAL:HB	1:B:1361:ILE:HB	0.45	1.86	2	1
1:A:1337:LEU:HD13	1:A:1355:ILE:HD11	0.45	1.88	8	1
1:B:1132:SER:HB3	1:B:1326:LEU:HB3	0.45	1.89	6	2
1:A:1025:GLN:HB3	1:A:1332:VAL:HG11	0.45	1.87	6	2
1:A:1335:LEU:HA	1:A:1338:LEU:HB2	0.45	1.86	1	1
1:A:1112:VAL:HB	1:A:1361:ILE:HB	0.45	1.88	6	2
1:A:1058:VAL:HB	1:A:1062:SER:HB2	0.45	1.88	5	1
1:B:1132:SER:O	1:B:1136:ILE:HG12	0.45	2.11	8	1
2:C:146:VAL:HB	2:C:170:MET:HA	0.45	1.86	8	2
1:A:1173:ALA:HA	1:A:1177:GLY:HA3	0.45	1.86	10	1
1:B:1199:GLU:HB2	2:C:155:TYR:CE1	0.45	2.41	9	1
1:B:1167:LYS:HA	1:B:1190:ILE:O	0.45	2.12	7	1
1:A:1034:ALA:HA	1:A:1056:GLU:HB3	0.45	1.88	4	1
1:A:1158:THR:O	2:C:70:PRO:HB3	0.45	2.12	3	1
1:A:1186:SER:O	1:B:1186:SER:HB3	0.45	2.12	6	1
2:C:116:ASP:HB2	4:C:1001:NAP:H51N	0.45	1.88	6	1
2:C:151:MET:HG2	2:C:170:MET:SD	0.45	2.51	9	1
1:A:1275:MET:SD	1:A:1281:ILE:HD11	0.45	2.52	4	1
2:C:174:ASP:HA	4:C:1001:NAP:N1A	0.45	2.27	1	1
1:A:1111:THR:HG21	1:A:1348:VAL:HG21	0.45	1.88	8	1
1:A:1176:ALA:HB3	1:A:1255:THR:HG21	0.45	1.88	10	1
2:C:149:ARG:NH2	4:C:1001:NAP:N6A	0.45	2.65	10	1
1:B:1089:LEU:O	1:B:1112:VAL:HA	0.45	2.12	5	1
1:B:1115:MET:SD	1:B:1334:LEU:HD13	0.45	2.51	2	1
2:C:130:ILE:HB	2:C:133:MET:HB2	0.45	1.88	2	1
1:A:1010:LEU:HD12	1:A:1076:LEU:HD11	0.45	1.89	5	1
1:A:1135:ASN:ND2	1:A:1179:ALA:HB2	0.45	2.27	4	1
1:A:1071:LYS:HB2	1:A:1091:SER:OG	0.45	2.12	3	1
1:A:1113:MET:SD	1:A:1348:VAL:HG13	0.45	2.51	8	1
1:B:1050:PHE:HB2	1:B:1057:ILE:HD11	0.45	1.86	5	2
1:A:1015:ARG:HG3	1:A:1317:GLY:HA2	0.45	1.88	6	2
1:B:1328:GLY:O	1:B:1332:VAL:HG23	0.45	2.12	10	2
1:B:1016:VAL:CG2	1:B:1039:ALA:HB1	0.45	2.42	5	1
1:B:1279:SER:O	1:B:1307:VAL:HA	0.45	2.12	5	1
1:A:1047:ASP:HA	1:A:1050:PHE:HD2	0.45	1.71	4	1
1:B:1255:THR:HA	1:B:1284:LEU:HD22	0.44	1.89	8	1
2:C:115:ASN:HD21	2:C:154:GLY:HA3	0.44	1.72	10	1
1:A:1312:TYR:CB	1:A:1315:LEU:HG	0.44	2.42	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:144:VAL:HB	2:C:168:THR:HG22	0.44	1.87	1	1
1:B:1207:MET:SD	2:C:75:LEU:HD22	0.44	2.52	1	1
1:B:1338:LEU:O	1:B:1347:THR:HB	0.44	2.11	8	1
1:B:1178:LEU:HD22	2:C:75:LEU:HG	0.44	1.89	5	1
1:B:1339:CYS:SG	1:B:1342:LYS:HA	0.44	2.52	4	2
1:B:1125:GLN:HG3	1:B:1131:SER:HB3	0.44	1.88	10	1
1:B:1018:ALA:HB1	1:B:1022:THR:HB	0.44	1.89	1	2
2:C:68:ILE:HD11	2:C:93:VAL:HG13	0.44	1.88	7	1
1:A:1328:GLY:O	1:A:1332:VAL:HG23	0.44	2.13	1	1
2:C:33:VAL:O	2:C:64:VAL:HA	0.44	2.12	7	3
1:A:1021:LYS:HB2	1:A:1325:GLN:NE2	0.44	2.27	10	1
2:C:66:PHE:HB2	2:C:93:VAL:HG22	0.44	1.89	10	1
2:C:128:SER:OG	2:C:158:VAL:HG21	0.44	2.11	5	1
1:A:1140:ARG:NH1	1:A:1318:ARG:O	0.44	2.50	6	2
1:B:1068:ILE:HA	1:B:1088:THR:HB	0.44	1.88	7	1
1:B:1091:SER:O	1:B:1114:ALA:HA	0.44	2.12	7	1
1:A:1275:MET:HB2	1:A:1307:VAL:HG21	0.44	1.88	2	1
1:B:1080:ILE:HD11	1:B:1101:LEU:HD12	0.44	1.89	1	1
2:C:34:ILE:HG12	2:C:106:THR:OG1	0.44	2.12	5	1
1:A:1255:THR:HA	1:A:1284:LEU:HB2	0.44	1.89	7	1
2:C:137:GLU:HB3	2:C:139:TRP:NE1	0.44	2.28	2	1
1:B:1090:VAL:HG13	1:B:1113:MET:HB2	0.44	1.90	3	1
2:C:122:ALA:HA	2:C:128:SER:CB	0.44	2.43	5	1
1:B:1079:GLU:HA	1:B:1082:LEU:HD12	0.44	1.88	9	2
1:B:1021:LYS:O	1:B:1025:GLN:HG3	0.44	2.12	3	1
1:B:1113:MET:HA	1:B:1358:VAL:O	0.44	2.12	9	1
1:B:1036:GLU:HB3	1:B:1039:ALA:HB2	0.44	1.89	10	2
2:C:30:SER:HB3	2:C:32:SER:O	0.43	2.12	5	1
1:B:1156:GLN:H	1:B:1163:VAL:HB	0.43	1.74	8	1
1:B:1002:ARG:NH2	1:B:1065:GLN:O	0.43	2.50	10	2
1:A:1312:TYR:O	1:A:1315:LEU:HG	0.43	2.13	3	1
1:A:1045:PHE:HD1	1:B:1277:ALA:HB3	0.43	1.73	5	1
2:C:27:LEU:HD21	2:C:110:LEU:HD21	0.43	1.90	5	1
1:B:1080:ILE:HG21	1:B:1104:LYS:HB3	0.43	1.89	6	1
1:A:1269:ARG:HG3	1:A:1293:GLU:HB3	0.43	1.90	7	1
1:A:1016:VAL:HG23	1:A:1039:ALA:HB1	0.43	1.90	3	1
1:A:1169:MET:O	1:A:1252:ILE:HA	0.43	2.14	10	1
1:A:1214:LEU:HD11	1:A:1238:GLU:HA	0.43	1.89	6	1
1:A:1275:MET:HB3	1:A:1307:VAL:HG21	0.43	1.89	9	2
1:A:1044:SER:HB3	1:B:1278:GLY:HA2	0.43	1.91	10	1
1:A:1169:MET:HG3	1:A:1212:LEU:HD11	0.43	1.90	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:1102:MET:HA	1:B:1105:LEU:HD12	0.43	1.90	10	1
1:A:1131:SER:HA	1:A:1175:VAL:HG21	0.43	1.89	9	1
1:A:1003:ILE:HA	1:A:1068:ILE:O	0.43	2.12	7	1
1:A:1097:GLN:NE2	1:A:1260:GLY:HA2	0.43	2.29	7	1
1:B:1332:VAL:O	1:B:1336:LYS:HG3	0.43	2.12	2	1
1:A:1342:LYS:N	1:A:1343:ASP:HB3	0.43	2.29	1	1
1:B:1111:THR:HA	1:B:1363:ALA:H	0.43	1.74	1	1
1:B:1127:LEU:HD11	1:B:1337:LEU:HD13	0.43	1.89	1	1
1:A:1140:ARG:NH2	1:B:1147:HIS:O	0.43	2.51	8	1
2:C:133:MET:HG2	4:C:1001:NAP:O3D	0.43	2.14	8	1
2:C:148:LYS:NZ	2:C:152:ASN:OD1	0.43	2.51	2	2
1:A:1323:SER:O	1:A:1327:TYR:HB3	0.43	2.14	5	1
1:A:1167:LYS:HB3	1:A:1249:VAL:HG12	0.43	1.89	2	1
2:C:34:ILE:HD11	2:C:102:ASP:HB3	0.43	1.90	3	1
1:A:1045:PHE:HA	1:B:1277:ALA:HB1	0.43	1.91	10	1
1:B:1280:VAL:HG22	1:B:1308:LYS:HB2	0.43	1.90	2	2
1:A:1331:LEU:O	1:A:1335:LEU:HG	0.43	2.14	5	1
1:B:1121:ILE:HD12	1:B:1123:ARG:HB3	0.43	1.91	9	1
1:B:1356:ARG:HG3	1:B:1371:PRO:HD3	0.43	1.90	7	1
2:C:31:HIS:O	2:C:62:ILE:HG23	0.43	2.13	4	1
1:B:1230:MET:SD	1:B:1234:PHE:CD2	0.43	3.12	2	1
1:A:1132:SER:O	1:A:1135:ASN:HB3	0.43	2.14	3	1
1:A:1111:THR:HG23	1:A:1362:ARG:HG3	0.43	1.91	10	1
1:B:1024:GLU:O	1:B:1028:LYS:HG3	0.43	2.13	6	1
1:B:1008:GLU:OE2	1:B:1071:LYS:HG2	0.43	2.14	7	1
1:B:1256:ALA:HB3	1:B:1291:ASN:OD1	0.43	2.14	7	1
1:A:1146:ALA:HA	1:A:1149:PHE:HB2	0.43	1.91	4	2
2:C:39:TYR:CD1	2:C:74:ARG:HD3	0.43	2.49	9	1
1:B:1305:ASN:OD1	1:B:1307:VAL:HG23	0.43	2.14	7	1
2:C:42:ALA:HB2	2:C:79:MET:HB3	0.43	1.89	2	1
1:A:1070:LEU:HD23	1:A:1090:VAL:HB	0.42	1.91	8	1
1:A:1342:LYS:HA	1:A:1344:GLY:H	0.42	1.73	5	1
1:A:1330:ASN:ND2	1:B:1160:ALA:HB2	0.42	2.29	4	1
1:B:1069:ILE:HG22	1:B:1071:LYS:HB2	0.42	1.89	2	1
1:B:1092:PHE:CD1	1:B:1116:ASP:HB3	0.42	2.48	1	1
2:C:148:LYS:NZ	4:C:1001:NAP:O3B	0.42	2.52	8	1
1:B:1136:ILE:HG21	1:B:1316:PRO:HA	0.42	1.89	6	1
2:C:116:ASP:HB3	2:C:130:ILE:HD13	0.42	1.91	9	1
2:C:24:ALA:HB2	2:C:182:ILE:HG22	0.42	1.90	10	1
1:A:1060:GLY:O	1:A:1063:VAL:HG12	0.42	2.14	9	1
1:A:1339:CYS:HB3	1:A:1342:LYS:HG2	0.42	1.91	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:118:VAL:HG23	2:C:162:LEU:HD13	0.42	1.90	1	1
1:A:1173:ALA:HB3	1:A:1200:VAL:HG21	0.42	1.91	10	2
2:C:115:ASN:HB3	4:C:1001:NAP:O1N	0.42	2.13	9	1
1:B:1023:VAL:HG22	1:B:1033:VAL:HG11	0.42	1.91	3	1
1:A:1287:GLN:HA	1:A:1313:THR:HG23	0.42	1.92	1	1
1:A:1196:THR:HG23	1:A:1234:PHE:CE2	0.42	2.49	5	1
1:A:1163:VAL:HG22	1:B:1326:LEU:HD21	0.42	1.91	6	1
1:A:1174:GLY:HA2	1:A:1200:VAL:HG11	0.42	1.92	7	1
1:B:1119:PRO:HG2	1:B:1357:GLY:HA3	0.42	1.90	4	1
1:B:1000:HIS:HA	1:B:1067:GLU:HB2	0.42	1.92	1	1
2:C:118:VAL:O	2:C:162:LEU:HD11	0.42	2.14	1	1
1:A:1083:LEU:HD11	1:A:1089:LEU:HD13	0.42	1.92	10	1
1:A:1040:GLY:HA2	1:A:1043:ALA:HB3	0.42	1.91	5	1
1:A:1253:VAL:HA	1:A:1282:VAL:HG23	0.42	1.91	2	1
2:C:146:VAL:HG21	2:C:162:LEU:HG	0.42	1.90	2	1
1:A:1045:PHE:CZ	1:A:1321:THR:HG23	0.42	2.50	10	1
2:C:48:TYR:CZ	2:C:86:ALA:HA	0.42	2.50	10	1
1:A:1127:LEU:HD23	1:A:1334:LEU:HD12	0.42	1.91	7	1
1:B:1254:THR:HG23	1:B:1291:ASN:HB2	0.42	1.92	7	1
1:B:1120:ARG:HB3	3:B:1:NAD:H1D	0.42	1.92	10	1
2:C:111:VAL:HG13	2:C:114:ALA:HB3	0.42	1.91	10	1
2:C:44:ALA:HB2	4:C:1001:NAP:H62A	0.42	1.74	10	1
1:A:1149:PHE:CE1	1:A:1151:ARG:HD2	0.42	2.50	4	1
1:A:1041:GLN:HE22	1:A:1047:ASP:HB2	0.42	1.75	9	1
2:C:38:GLY:HA3	2:C:114:ALA:HB2	0.42	1.91	7	1
2:C:72:ALA:HA	4:C:1001:NAP:H52N	0.42	1.91	2	1
1:B:1068:ILE:HD11	1:B:1346:ILE:HD11	0.42	1.91	10	1
1:A:1022:THR:O	1:A:1026:LEU:HG	0.42	2.15	5	1
1:A:1272:VAL:HG21	1:A:1292:CYS:SG	0.42	2.55	6	1
1:A:1140:ARG:HH11	1:A:1319:LEU:HD13	0.42	1.75	9	1
1:A:1036:GLU:HG2	1:A:1063:VAL:HG11	0.42	1.91	4	1
2:C:64:VAL:HG13	2:C:92:ILE:HD12	0.42	1.92	4	1
1:B:1119:PRO:HB2	1:B:1121:ILE:HG12	0.42	1.91	2	1
1:A:1193:ALA:O	1:A:1211:PHE:HA	0.41	2.15	6	1
1:A:1239:MET:SD	1:A:1266:LEU:O	0.41	2.78	9	1
1:B:1140:ARG:HH11	1:B:1319:LEU:HD13	0.41	1.75	9	1
1:A:1071:LYS:HE2	1:A:1075:PRO:HA	0.41	1.91	7	1
1:B:1126:SER:OG	1:B:1127:LEU:HD12	0.41	2.14	7	1
1:A:1065:GLN:NE2	1:A:1084:ASN:HD21	0.41	2.13	2	1
1:B:1146:ALA:HA	1:B:1149:PHE:HB2	0.41	1.92	2	1
1:B:1164:PRO:HA	1:B:1165:PRO:HD3	0.41	1.74	4	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1135:ASN:HA	1:A:1176:ALA:HA	0.41	1.92	5	1
1:B:1263:ALA:CB	1:B:1285:ALA:HB1	0.41	2.45	4	1
1:B:1125:GLN:HE21	1:B:1131:SER:HB3	0.41	1.75	8	1
1:A:1338:LEU:HG	1:A:1347:THR:O	0.41	2.15	10	1
2:C:65:ARG:NH2	2:C:94:LEU:HD22	0.41	2.30	7	1
1:B:1119:PRO:CG	1:B:1357:GLY:HA3	0.41	2.45	4	1
1:A:1068:ILE:HG12	1:A:1088:THR:HB	0.41	1.92	2	1
2:C:129:PRO:HD2	2:C:156:ALA:HB2	0.41	1.92	1	1
1:A:1254:THR:HG22	1:A:1291:ASN:HB2	0.41	1.92	10	1
1:A:1292:CYS:SG	1:A:1309:VAL:HG11	0.41	2.55	7	1
1:B:1115:MET:HB3	1:B:1129:ALA:HB2	0.41	1.91	7	1
1:B:1118:VAL:CG1	1:B:1124:ALA:HB1	0.41	2.45	7	1
1:A:1069:ILE:HG12	1:A:1087:THR:CG2	0.41	2.45	1	1
1:A:1216:PHE:HE1	1:A:1233:ALA:HB1	0.41	1.74	8	1
2:C:26:LEU:HA	2:C:29:ASN:HB3	0.41	1.90	5	1
1:A:1215:ASP:H	1:A:1241:LEU:HD21	0.41	1.75	8	1
1:A:1264:PRO:HG2	1:A:1291:ASN:ND2	0.41	2.31	5	1
1:A:1356:ARG:NH1	1:A:1367:THR:O	0.41	2.53	6	1
1:A:1333:ASN:HA	1:A:1336:LYS:HD2	0.41	1.92	9	1
1:B:1127:LEU:HD22	1:B:1354:VAL:HG11	0.41	1.92	7	1
1:B:1109:ASN:HA	1:B:1364:GLY:CA	0.41	2.46	2	1
1:A:1239:MET:SD	1:A:1242:PHE:HD2	0.41	2.39	1	1
1:B:1346:ILE:HG22	1:B:1348:VAL:HG23	0.41	1.91	10	1
1:A:1098:ASN:HB3	1:A:1101:LEU:HB3	0.41	1.93	5	1
2:C:58:ARG:NH1	2:C:63:ASN:HA	0.41	2.30	5	1
1:B:1015:ARG:HG2	1:B:1323:SER:HB3	0.41	1.93	2	1
2:C:148:LYS:HE3	2:C:150:SER:O	0.41	2.16	3	1
1:A:1169:MET:SD	1:A:1245:GLN:HB3	0.41	2.55	8	1
1:B:1121:ILE:HB	2:C:131:ALA:O	0.41	2.16	10	1
1:A:1164:PRO:HA	1:A:1165:PRO:HD2	0.41	1.79	7	1
1:A:1020:PRO:HD2	1:A:1045:PHE:CD2	0.41	2.50	4	1
1:A:1043:ALA:HA	1:A:1320:PRO:HB2	0.41	1.92	1	1
2:C:26:LEU:HB3	2:C:108:THR:OG1	0.41	2.15	8	1
1:B:1149:PHE:CZ	1:B:1250:ASP:HB3	0.41	2.51	8	1
1:A:1125:GLN:HA	1:A:1128:ASP:HB3	0.41	1.92	10	1
1:A:1264:PRO:HG2	1:A:1291:ASN:HD21	0.41	1.76	5	1
1:B:1258:ILE:HG23	3:B:1:NAD:H8A	0.41	1.93	7	1
2:C:48:TYR:CD1	2:C:49:PRO:HD3	0.41	2.50	7	1
1:A:1003:ILE:HD13	1:A:1335:LEU:HD13	0.41	1.93	4	1
2:C:47:GLN:O	2:C:50:VAL:HG12	0.41	2.15	3	1
1:B:1148:GLU:HG3	1:B:1300:ILE:HD13	0.41	1.92	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:1295:THR:O	1:B:1297:PRO:HD3	0.41	2.16	1	1
1:B:1092:PHE:HZ	1:B:1133:MET:HG3	0.41	1.75	6	1
1:B:1015:ARG:HD3	1:B:1133:MET:SD	0.41	2.55	9	1
1:B:1176:ALA:HB3	1:B:1255:THR:HG21	0.41	1.91	9	1
2:C:128:SER:HB3	2:C:158:VAL:HG21	0.41	1.93	9	1
1:A:1114:ALA:HB3	1:A:1117:SER:HB2	0.41	1.92	7	1
2:C:37:PRO:HG3	2:C:41:MET:SD	0.41	2.57	7	1
1:A:1009:ARG:HH11	1:A:1079:GLU:HG2	0.41	1.75	2	1
1:B:1350:PHE:HB2	1:B:1362:ARG:NH1	0.40	2.31	3	1
1:B:1177:GLY:O	1:B:1181:ILE:HG13	0.40	2.17	1	1
1:B:1024:GLU:HA	1:B:1027:LEU:HD12	0.40	1.93	10	1
2:C:108:THR:HA	2:C:143:ASN:O	0.40	2.16	10	1
1:B:1003:ILE:HA	1:B:1068:ILE:O	0.40	2.16	5	1
1:A:1348:VAL:HB	1:A:1362:ARG:NH2	0.40	2.30	6	1
1:A:1016:VAL:HG12	1:A:1043:ALA:HB2	0.40	1.93	9	1
1:A:1340:LYS:HD2	1:A:1347:THR:HG21	0.40	1.92	9	1
1:A:1151:ARG:NH2	1:A:1279:SER:OG	0.40	2.54	7	1
1:B:1064:TRP:HA	1:B:1069:ILE:HD11	0.40	1.92	7	1
2:C:70:PRO:HG3	2:C:96:MET:SD	0.40	2.56	4	1
1:A:1332:VAL:O	1:A:1336:LYS:HG3	0.40	2.17	2	1
1:A:1148:GLU:HG3	1:A:1300:ILE:HD13	0.40	1.92	3	1
1:B:1092:PHE:HD1	1:B:1116:ASP:HB3	0.40	1.75	3	1
1:B:1152:PHE:HE2	1:B:1156:GLN:NE2	0.40	2.13	3	1
2:C:35:ILE:HG12	2:C:110:LEU:HD12	0.40	1.93	3	1
2:C:180:ASP:O	2:C:183:LEU:HG	0.40	2.16	10	1
2:C:50:VAL:HA	2:C:53:ILE:HG22	0.40	1.93	5	1
1:A:1235:ILE:O	1:A:1239:MET:HG2	0.40	2.16	6	1
2:C:32:SER:HB2	2:C:106:THR:OG1	0.40	2.17	9	1
1:A:1152:PHE:HB2	1:A:1163:VAL:CG1	0.40	2.47	9	1
2:C:52:GLU:O	2:C:56:LYS:HE2	0.40	2.16	9	1
2:C:45:GLN:HG3	2:C:176:LYS:HG3	0.40	1.92	7	1
1:A:1140:ARG:CZ	1:A:1318:ARG:HB3	0.40	2.46	3	1
1:B:1036:GLU:HB2	1:B:1063:VAL:HG11	0.40	1.94	5	1
1:B:1200:VAL:HA	1:B:1203:GLN:HG2	0.40	1.92	6	1
2:C:116:ASP:HA	2:C:119:ASN:CB	0.40	2.46	4	1
1:A:1113:MET:HA	1:A:1358:VAL:O	0.40	2.17	1	1
1:A:1231:SER:O	1:A:1234:PHE:HB3	0.40	2.16	1	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	363/401 (91%)	323±5 (89±1%)	36±5 (10±1%)	4±1 (1±0%)	18 66
1	B	361/401 (90%)	322±3 (89±1%)	34±3 (9±1%)	6±2 (2±1%)	13 57
2	C	165/186 (89%)	132±3 (80±2%)	25±3 (15±2%)	8±1 (5±1%)	4 26
All	All	8890/9880 (90%)	7769 (87%)	941 (11%)	180 (2%)	11 52

All 90 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	C	75	LEU	8
1	A	1343	ASP	7
1	B	1320	PRO	6
2	C	159	GLN	6
1	A	1286	ALA	6
2	C	137	GLU	5
2	C	31	HIS	5
2	C	78	HIS	4
1	B	1259	PRO	4
1	B	1372	PRO	4
1	B	1231	SER	4
2	C	115	ASN	4
1	B	1318	ARG	4
1	B	1256	ALA	3
1	B	1233	ALA	3
1	A	1001	GLY	3
1	B	1175	VAL	3
2	C	158	VAL	3
2	C	114	ALA	3
1	A	1372	PRO	3
2	C	45	GLN	3
1	A	1363	ALA	3
1	B	1232	ASP	2
2	C	37	PRO	2
2	C	132	GLY	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	C	99	ILE	2
1	B	1346	ILE	2
1	B	1122	SER	2
1	B	1363	ALA	2
2	C	71	VAL	2
2	C	127	LYS	2
1	A	1208	GLY	2
2	C	96	MET	2
1	A	1256	ALA	2
2	C	70	PRO	2
2	C	140	LYS	2
1	A	1154	THR	2
1	B	1235	ILE	2
2	C	63	ASN	2
2	C	138	VAL	2
1	B	1369	PRO	1
1	B	1198	PRO	1
1	A	1359	THR	1
2	C	86	ALA	1
1	A	1074	ALA	1
2	C	141	ALA	1
1	A	1297	PRO	1
2	C	121	ALA	1
1	A	1072	VAL	1
2	C	160	ASN	1
1	B	1297	PRO	1
2	C	107	ASP	1
2	C	105	ASP	1
1	B	1030	GLY	1
2	C	183	LEU	1
2	C	89	PRO	1
2	C	130	ILE	1
1	B	1159	ALA	1
1	B	1043	ALA	1
2	C	162	LEU	1
1	B	1295	THR	1
2	C	69	HIS	1
1	A	1092	PHE	1
2	C	157	GLY	1
1	B	1290	GLY	1
2	C	100	ASN	1
1	B	1160	ALA	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	C	185	ALA	1
1	A	1037	SER	1
1	A	1054	GLY	1
1	A	1085	PRO	1
1	A	1060	GLY	1
1	B	1054	GLY	1
1	B	1289	GLY	1
2	C	87	LYS	1
1	B	1085	PRO	1
1	B	1012	ASN	1
1	B	1011	THR	1
1	A	1010	LEU	1
2	C	117	THR	1
1	A	1120	ARG	1
2	C	76	PRO	1
2	C	68	ILE	1
1	B	1099	PRO	1
1	B	1314	ASP	1
1	A	1020	PRO	1
1	A	1015	ARG	1
2	C	154	GLY	1
2	C	156	ALA	1
1	B	1286	ALA	1

6.3.2 Protein sidechains (i)

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	288/317 (91%)	272±3 (95±1%)	16±3 (5±1%)	25	74
1	B	290/317 (91%)	274±2 (94±1%)	17±2 (6±1%)	24	73
2	C	135/153 (88%)	122±2 (90±1%)	13±2 (10±1%)	12	58
All	All	7130/7870 (91%)	6677 (94%)	453 (6%)	21	70

All 198 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	C	47	GLN	10
2	C	79	MET	10
2	C	159	GLN	9
1	B	1287	GLN	9
2	C	176	LYS	9
1	B	1045	PHE	8
1	B	1014	THR	7
1	A	1282	VAL	7
1	A	1020	PRO	7
1	B	1048	LYS	6
1	A	1083	LEU	6
1	A	1254	THR	6
1	B	1020	PRO	6
1	A	1045	PHE	6
1	A	1149	PHE	6
1	B	1199	GLU	6
2	C	21	GLU	5
1	B	1149	PHE	5
1	B	1350	PHE	5
1	A	1343	ASP	5
1	B	1135	ASN	5
1	B	1063	VAL	5
2	C	45	GLN	5
1	B	1019	THR	5
1	A	1032	THR	4
1	A	1100	GLU	4
1	A	1067	GLU	4
1	A	1014	THR	4
2	C	140	LYS	4
1	B	1077	ASP	4
2	C	25	GLU	4
1	A	1072	VAL	3
2	C	90	TYR	3
2	C	166	GLU	3
1	B	1084	ASN	3
1	B	1196	THR	3
1	A	1313	THR	3
1	A	1046	ASP	3
1	B	1373	ILE	3
1	A	1019	THR	3
2	C	74	ARG	3
1	B	1113	MET	3
1	A	1077	ASP	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	C	152	ASN	3
2	C	50	VAL	3
1	A	1196	THR	3
1	B	1367	THR	3
2	C	115	ASN	3
2	C	52	GLU	3
2	C	151	MET	3
1	A	1084	ASN	3
2	C	155	TYR	3
2	C	123	GLN	3
2	C	102	ASP	3
1	A	1130	LEU	3
1	B	1214	LEU	3
1	A	1152	PHE	3
1	B	1022	THR	3
2	C	22	GLU	3
1	A	1022	THR	3
1	B	1288	ASN	2
1	A	1273	ASP	2
1	A	1321	THR	2
1	A	1047	ASP	2
1	A	1294	TYR	2
1	A	1369	PRO	2
2	C	26	LEU	2
2	C	142	GLN	2
2	C	58	ARG	2
1	B	1120	ARG	2
1	A	1247	LYS	2
1	B	1064	TRP	2
1	B	1085	PRO	2
1	B	1067	GLU	2
2	C	161	PRO	2
1	B	1041	GLN	2
1	B	1213	GLU	2
1	B	1230	MET	2
1	A	1065	GLN	2
1	A	1301	PHE	2
2	C	103	PHE	2
1	A	1122	SER	2
1	B	1365	GLU	2
1	A	1312	TYR	2
1	B	1273	ASP	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	1268	THR	2
1	A	1119	PRO	2
1	B	1100	GLU	2
2	C	186	LEU	2
1	A	1158	THR	2
2	C	117	THR	2
1	B	1352	ASP	2
1	A	1371	PRO	2
1	A	1108	ARG	2
1	B	1294	TYR	2
1	B	1313	THR	2
1	A	1268	THR	2
1	B	1321	THR	2
1	A	1048	LYS	2
2	C	75	LEU	2
1	A	1123	ARG	2
1	A	1255	THR	2
1	B	1097	GLN	1
1	B	1339	CYS	1
2	C	120	PRO	1
2	C	78	HIS	1
1	B	1051	VAL	1
1	B	1232	ASP	1
2	C	101	ASP	1
1	A	1093	ILE	1
1	A	1041	GLN	1
1	A	1224	ASP	1
2	C	119	ASN	1
2	C	37	PRO	1
1	B	1021	LYS	1
1	A	1316	PRO	1
1	B	1078	ASP	1
1	B	998	HIS	1
1	B	1342	LYS	1
2	C	116	ASP	1
1	B	1047	ASP	1
1	A	1126	SER	1
2	C	125	ASP	1
1	A	1203	GLN	1
2	C	147	PHE	1
1	A	1199	GLU	1
1	A	1207	MET	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	1372	PRO	1
1	B	1058	VAL	1
1	A	1092	PHE	1
2	C	107	ASP	1
1	B	1109	ASN	1
1	B	1032	THR	1
1	B	1008	GLU	1
1	A	1156	GLN	1
1	A	1063	VAL	1
1	A	1202	GLU	1
1	B	1088	THR	1
2	C	139	TRP	1
1	A	1354	VAL	1
1	B	1012	ASN	1
1	A	1110	VAL	1
2	C	96	MET	1
1	B	1231	SER	1
2	C	108	THR	1
1	B	1308	LYS	1
1	A	1270	GLU	1
2	C	56	LYS	1
1	B	1312	TYR	1
1	A	1154	THR	1
2	C	135	VAL	1
1	B	1297	PRO	1
1	B	1036	GLU	1
1	B	1152	PHE	1
1	B	1000	HIS	1
1	A	1151	ARG	1
1	B	1258	ILE	1
2	C	169	HIS	1
1	B	1059	GLU	1
2	C	23	THR	1
1	B	1158	THR	1
1	A	1248	GLU	1
1	A	1350	PHE	1
1	B	1061	ASN	1
2	C	85	GLU	1
2	C	150	SER	1
1	B	1282	VAL	1
1	A	1085	PRO	1
2	C	83	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	1232	ASP	1
2	C	92	ILE	1
1	A	1365	GLU	1
1	A	1338	LEU	1
1	A	1226	TYR	1
1	A	1058	VAL	1
2	C	49	PRO	1
1	B	1065	GLN	1
1	A	1175	VAL	1
1	B	1340	LYS	1
1	A	1116	ASP	1
1	B	1200	VAL	1
1	B	1234	PHE	1
1	A	1275	MET	1
1	A	1036	GLU	1
1	B	1068	ILE	1
1	B	1270	GLU	1
1	A	1367	THR	1
1	B	1103	GLN	1
1	B	1275	MET	1
1	B	1248	GLU	1
1	B	1099	PRO	1
1	A	1216	PHE	1
1	B	1125	GLN	1
1	A	1015	ARG	1
1	A	1334	LEU	1
2	C	80	ASN	1
1	B	1271	MET	1
1	B	1062	SER	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	NAD	B	1	-	42,48,48	1.29±0.08	0±0 (0±1%)
4	NAP	C	1001	-	45,52,52	1.37±0.08	1±0 (1±1%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	NAD	B	1	-	50,73,73	1.33±0.11	0±0 (0±0%)
4	NAP	C	1001	-	56,80,80	1.34±0.05	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	C	1001	-	-	0±0,31,67,67	0±0,5,5,5
3	NAD	B	1	-	-	0±0,26,62,62	0±0,5,5,5

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	1	NAD	C2N-N1N	6.59	1.43	1.35	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	C	1001	NAP	C2N-N1N	6.37	1.42	1.35	1	7

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	1	NAD	N3A-C2A-N1A	5.12	120.68	128.68	9	1
3	B	1	NAD	C4A-C5A-N7A	5.05	114.66	109.40	4	1

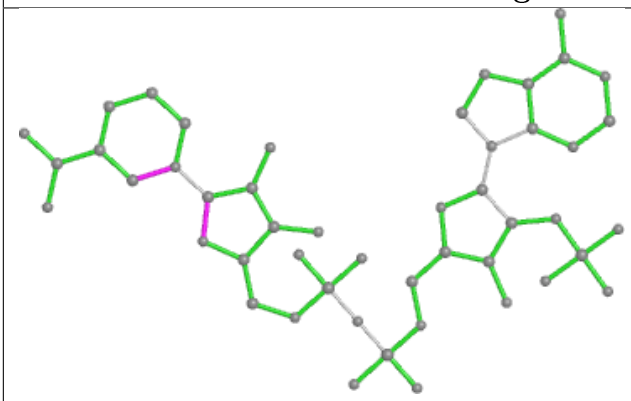
There are no chirality outliers.

There are no torsion outliers.

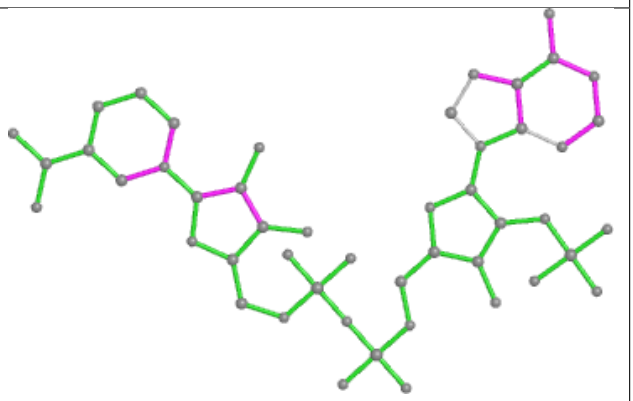
There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

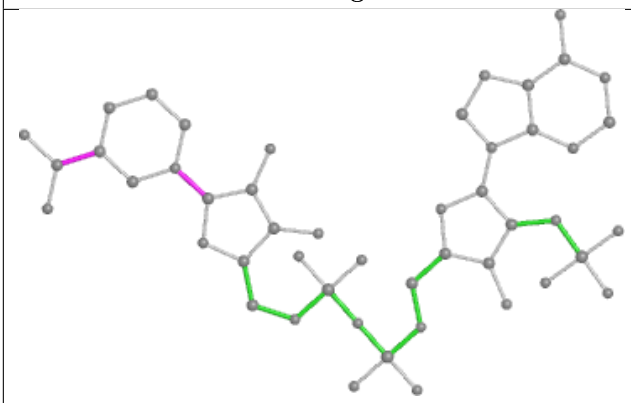
Ligand NAP C 1001



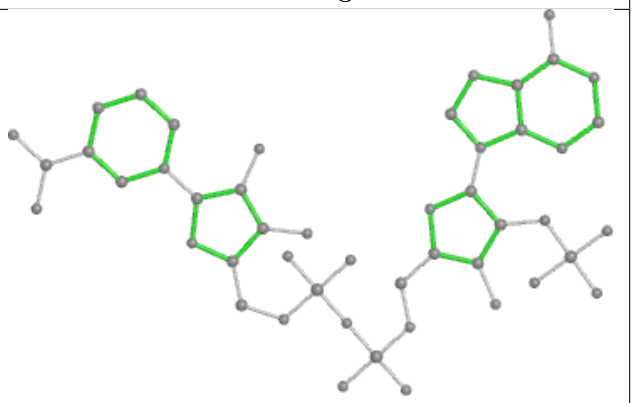
Bond lengths



Bond angles

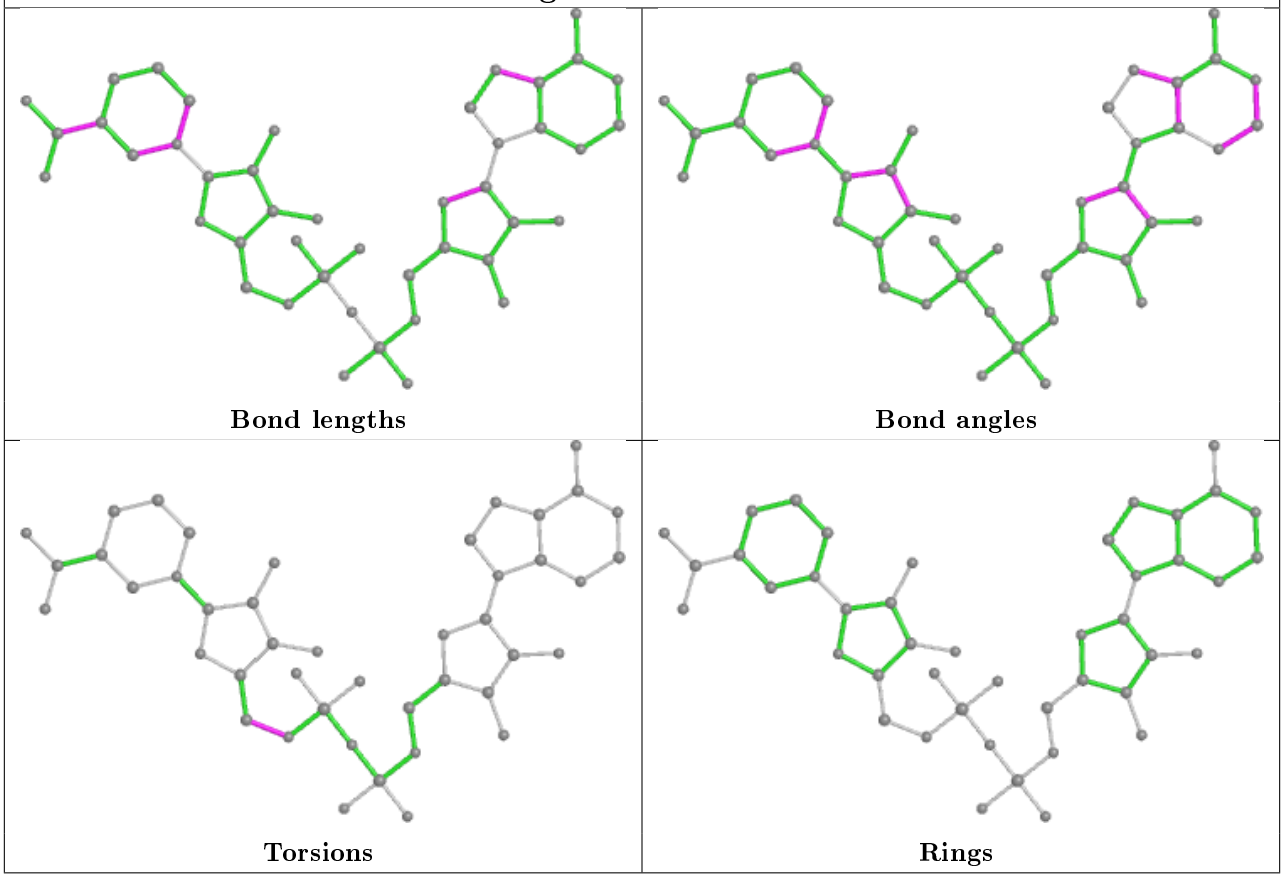


Torsions



Rings

Ligand NAD B 1



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