



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 06:03 AM UTC

PDB ID : 2BRU / pdb_00002bru
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 ⓘ symbol.

The types of validation reports are described at

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

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

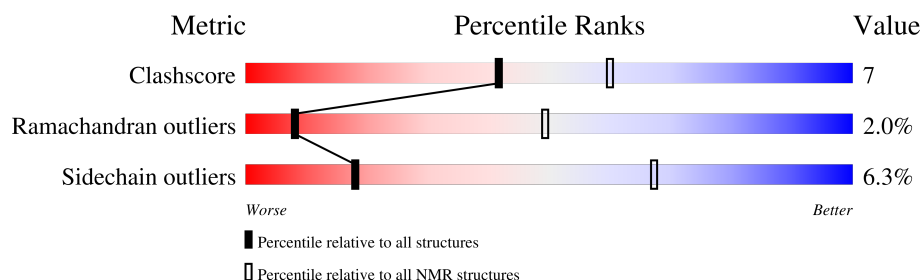
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	401	
1	B	401	
2	C	186	

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)	1.24	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 1 single-model cluster was found.

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

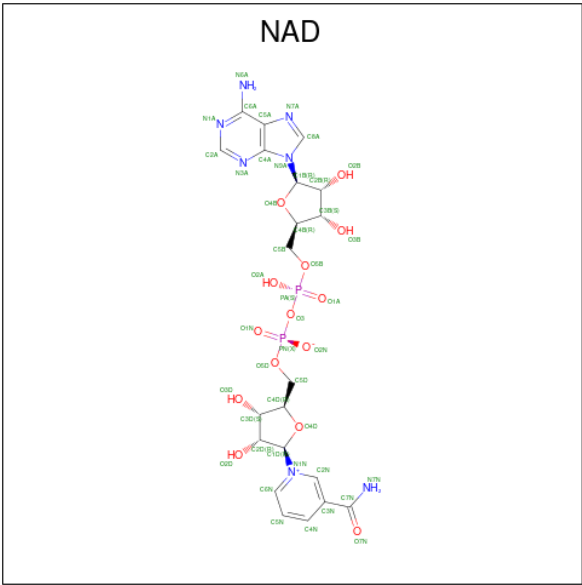
- Molecule 1 is a protein called NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA.

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 (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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 (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



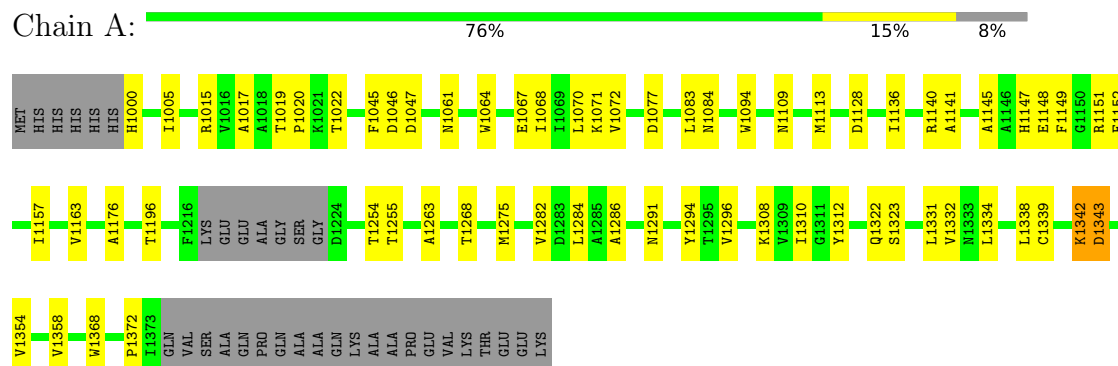
Mol	Chain	Residues	Atoms					
4	C	1	Total	C	H	N	O	P
			55	21	7	7	17	3

4 Residue-property plots

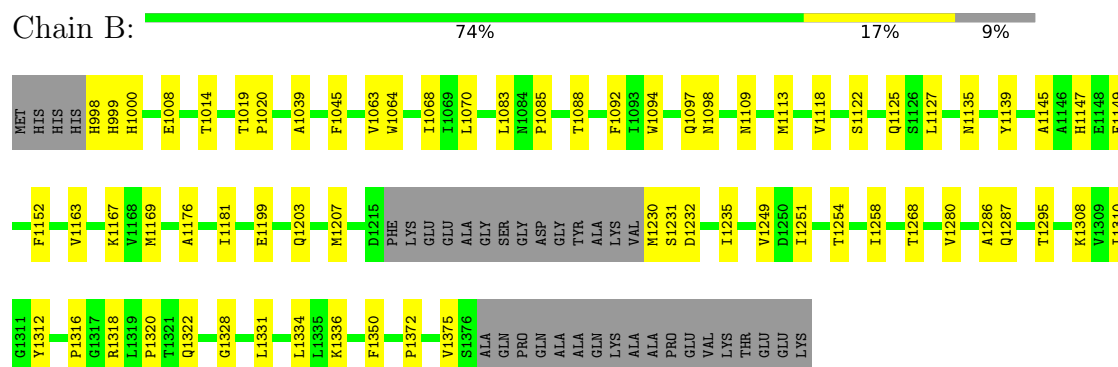
4.1 Average score per residue in the NMR ensemble

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

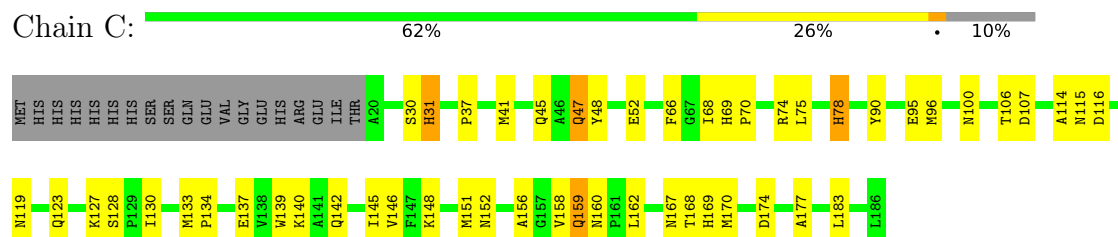
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA



• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA



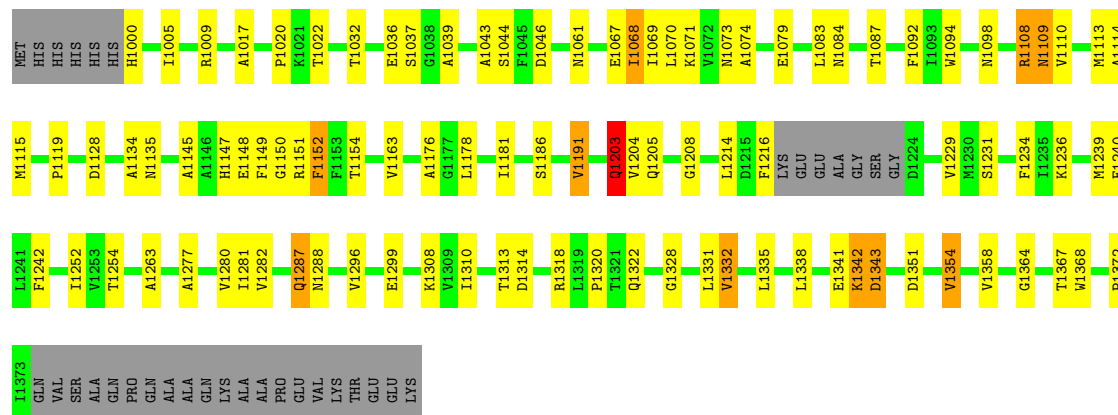
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

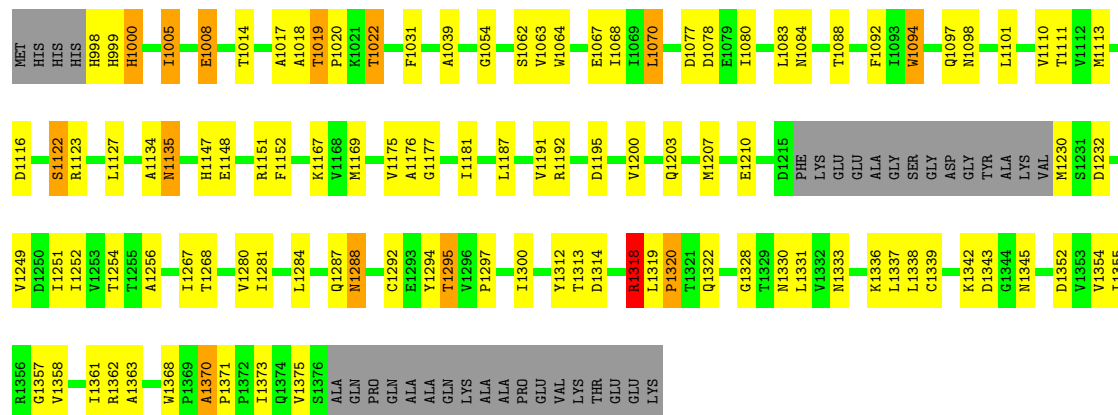
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A: 



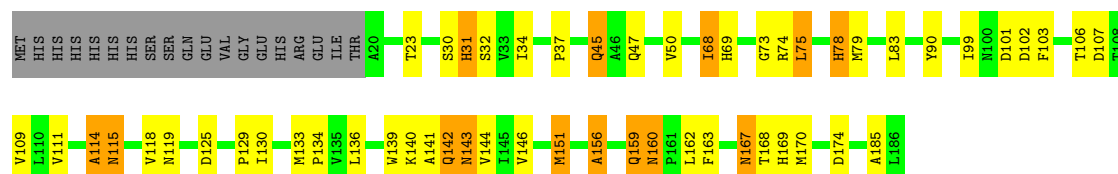
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

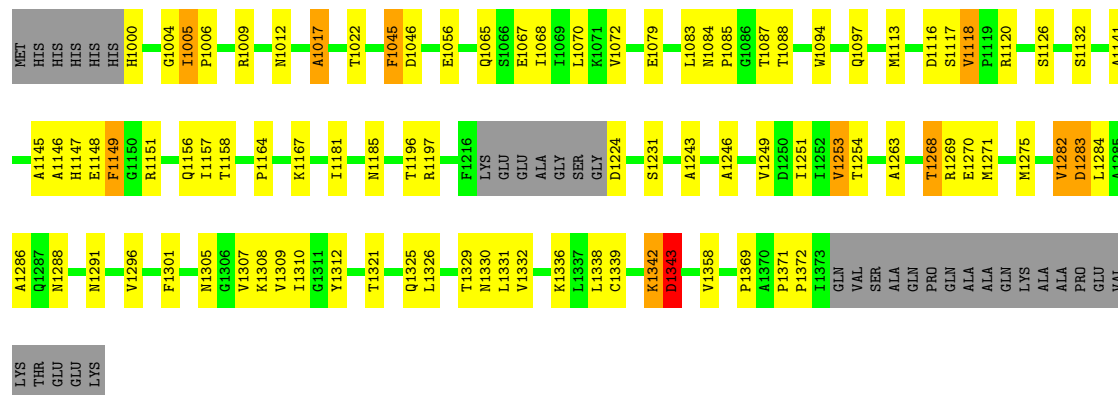
Chain C: 



4.2.2 Score per residue for model 2

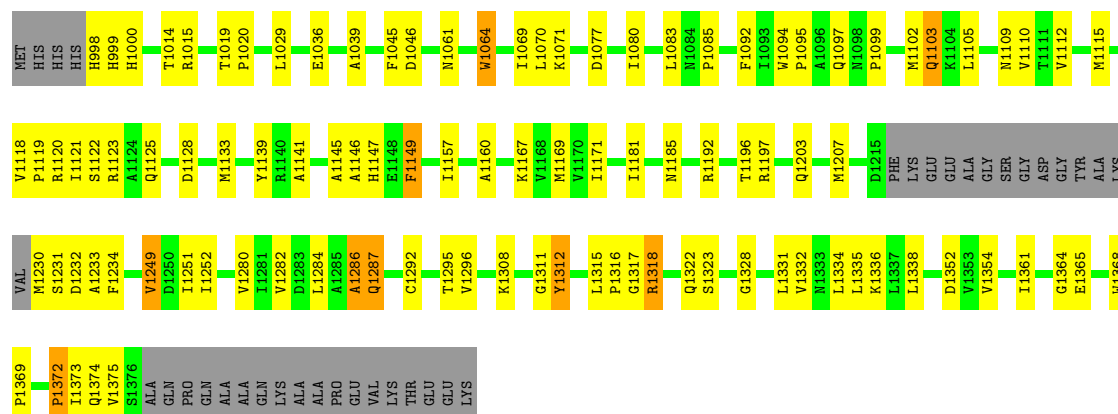
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A:  69% 20% 8%



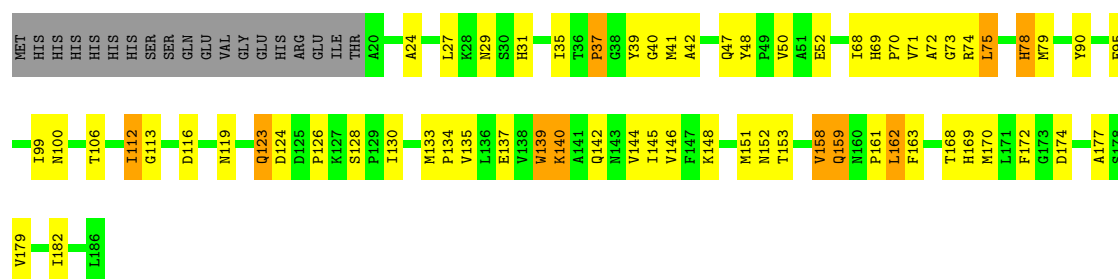
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B:  65% 23% 9%

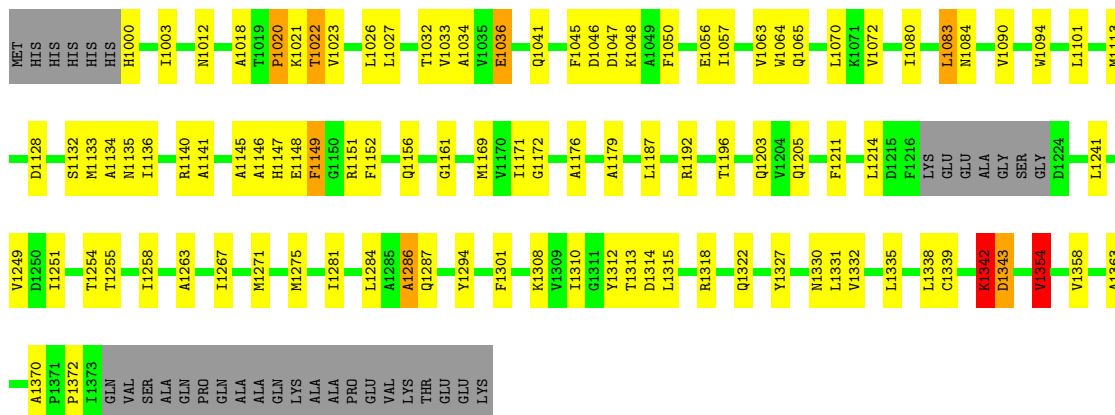


• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C:  55% 30% 5% 10%

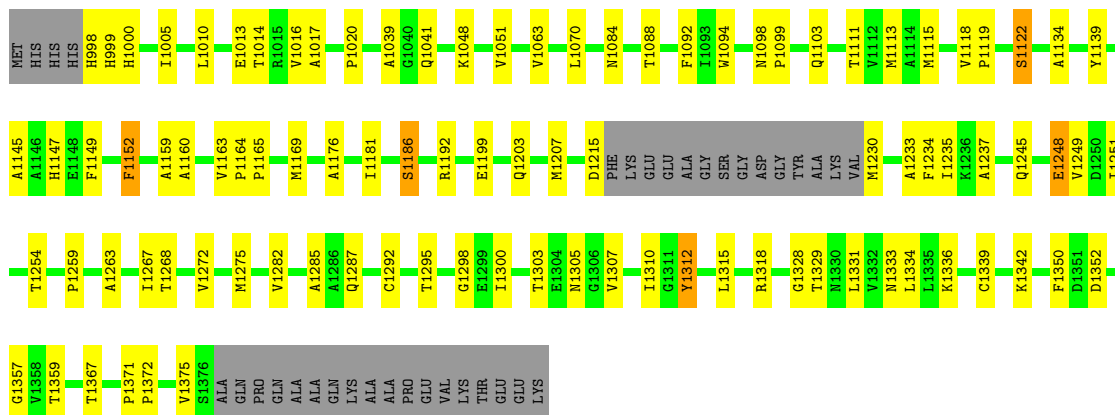


Chain A: 



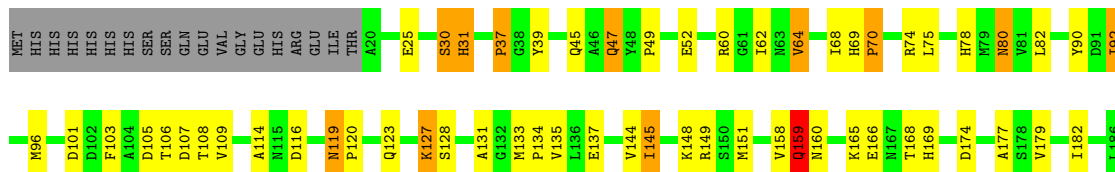
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

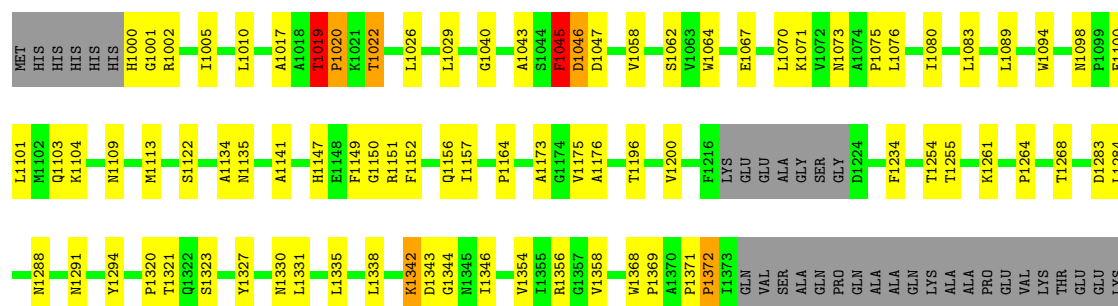
Chain C: 



4.2.5 Score per residue for model 5

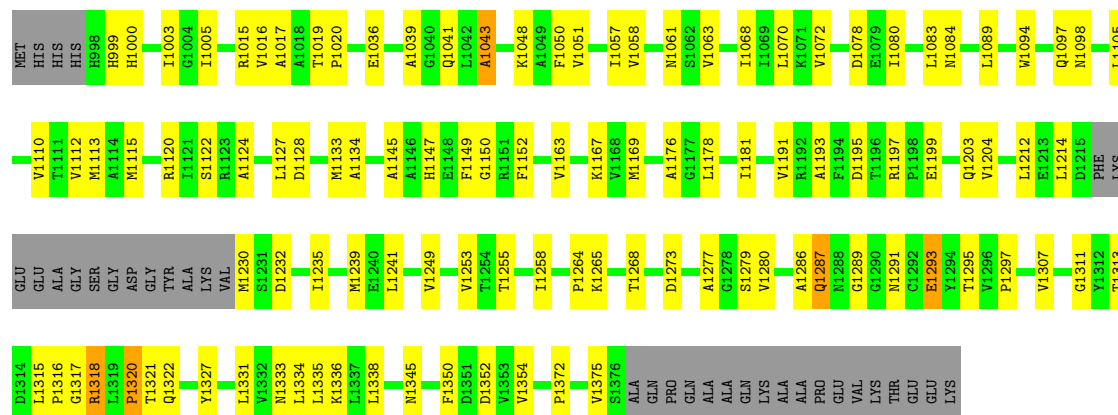
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A: 



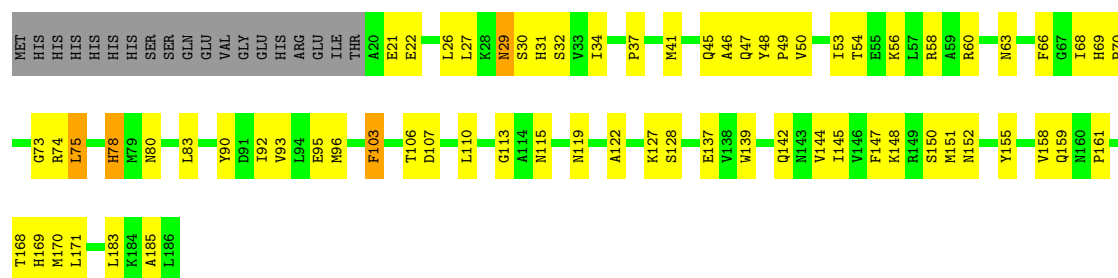
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 64% 26% 9%



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

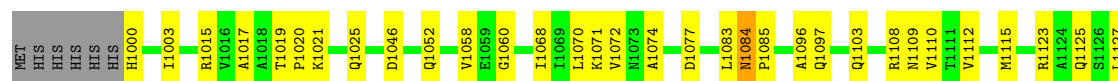
Chain C: 53% 34% 10%

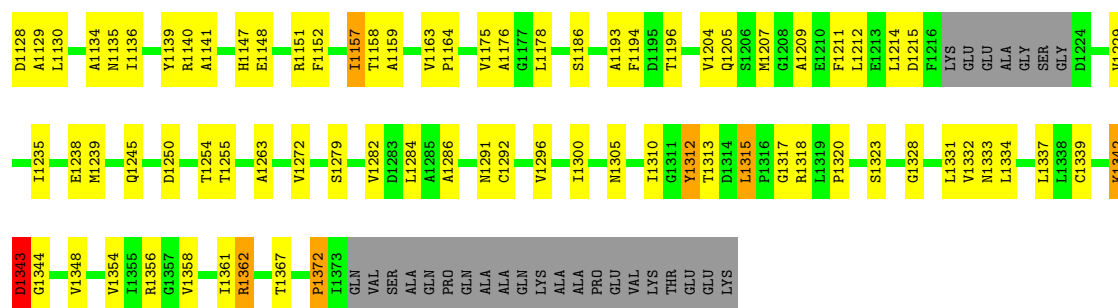


4.2.6 Score per residue for model 6

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

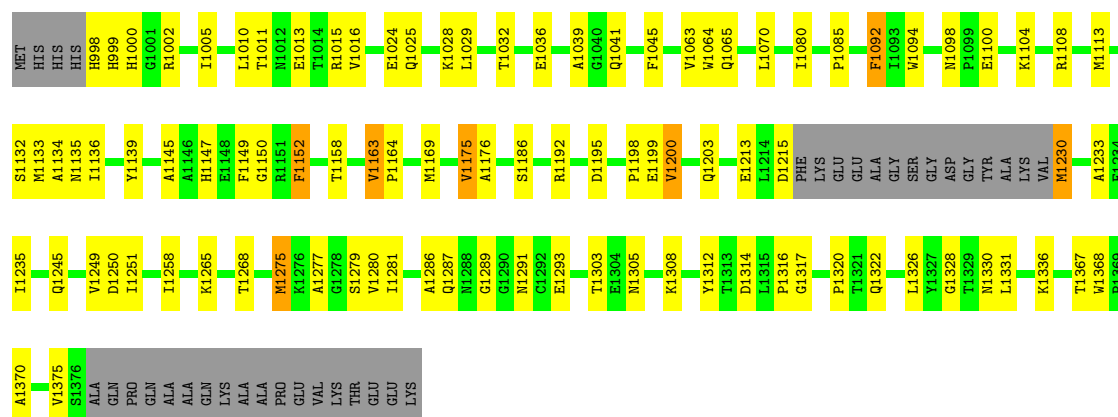
Chain A: 64% 25% 8%





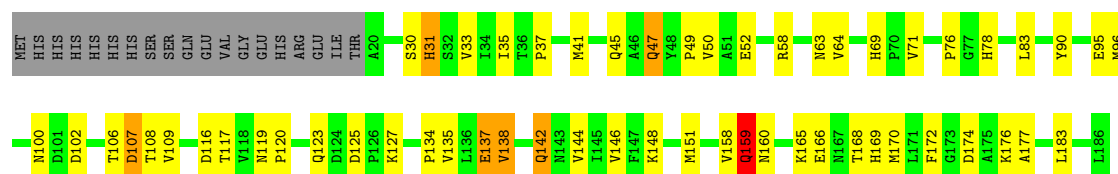
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 67% 22% 9%



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

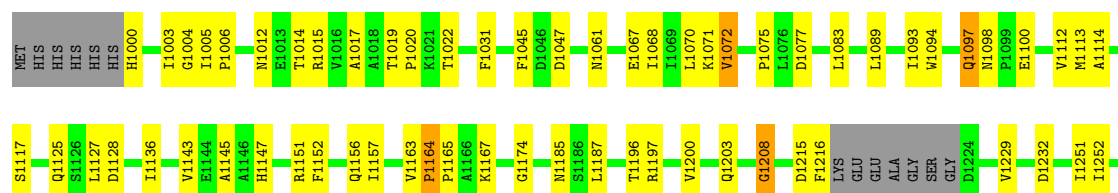
Chain C: 59% 27% 10%



4.2.7 Score per residue for model 7

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain A: 67% 23% 8%





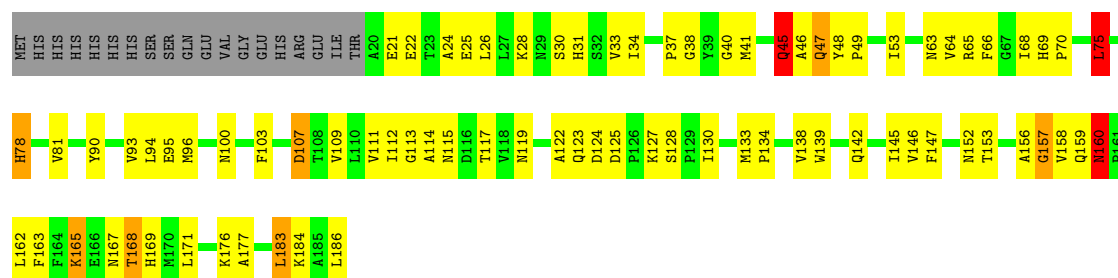
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 63% 24% 9%



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

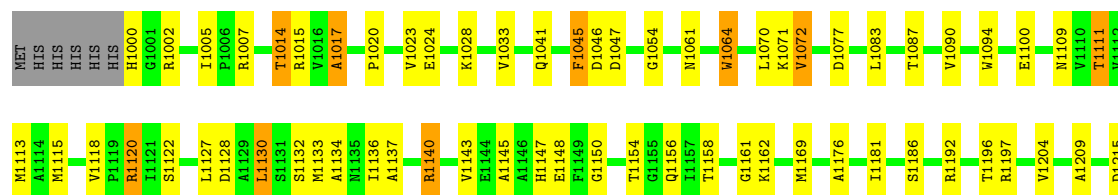
Chain C: 47% 38% 10%

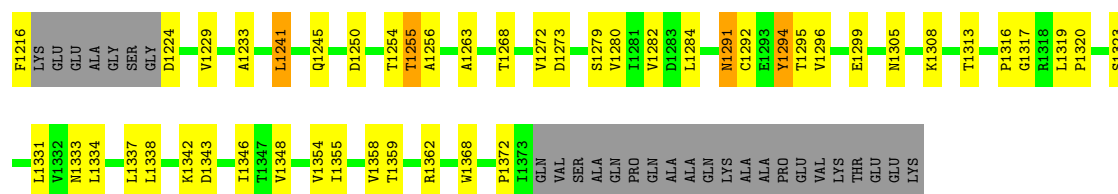


4.2.8 Score per residue for model 8

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

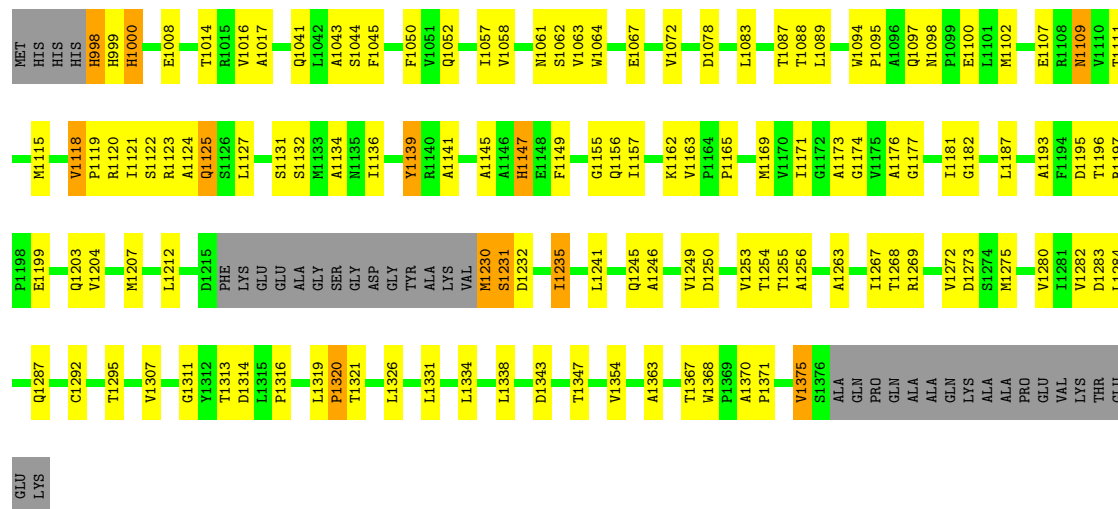
Chain A: 64% 25% 8%





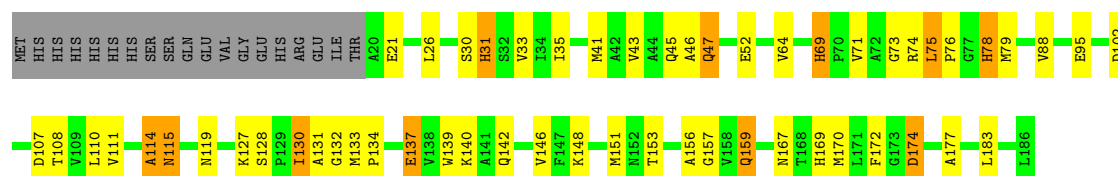
• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 60% 28% 9%



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

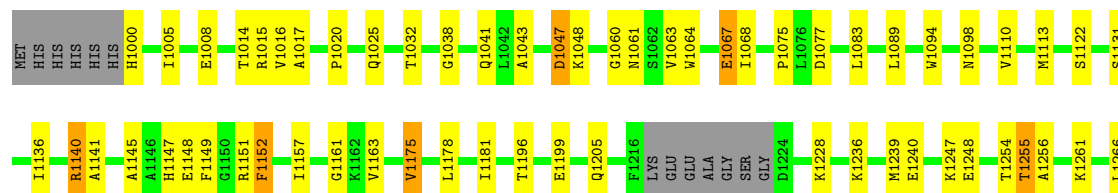
Chain C: 60% 24% 6% 10%

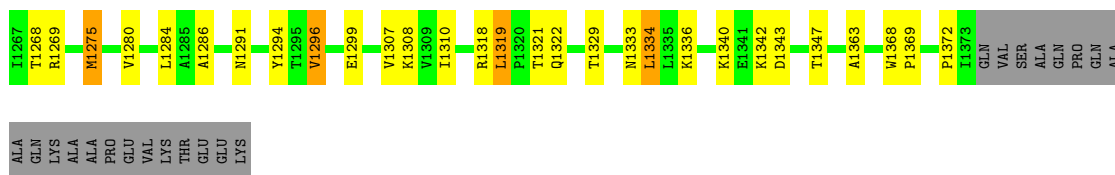


4.2.9 Score per residue for model 9

• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

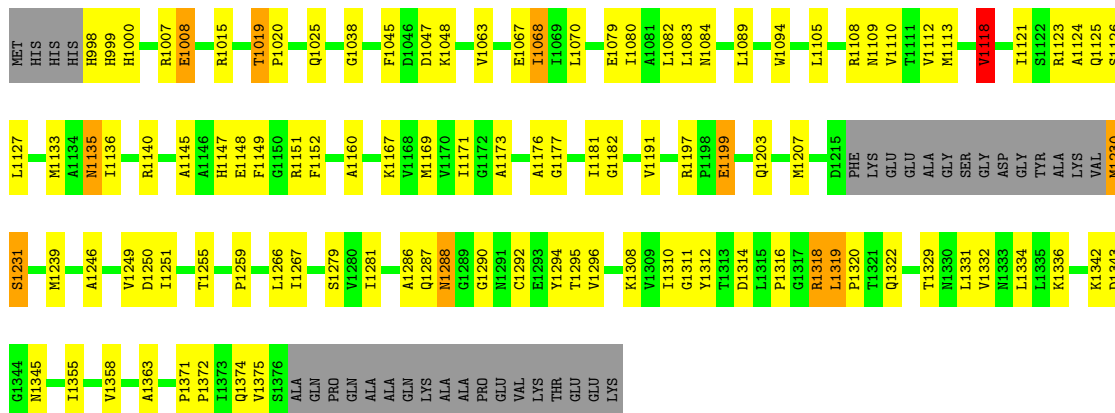
Chain A: 69% 20% 8%



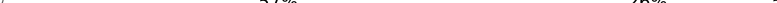


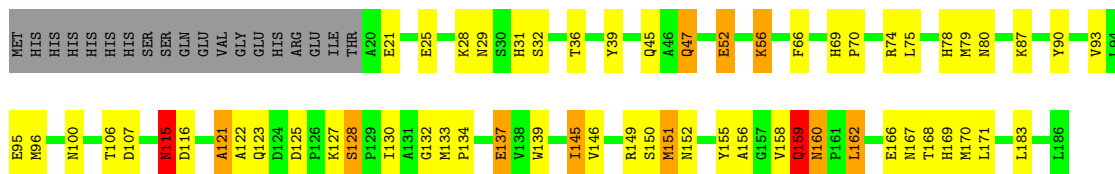
● Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 64% 24% 9%



- Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

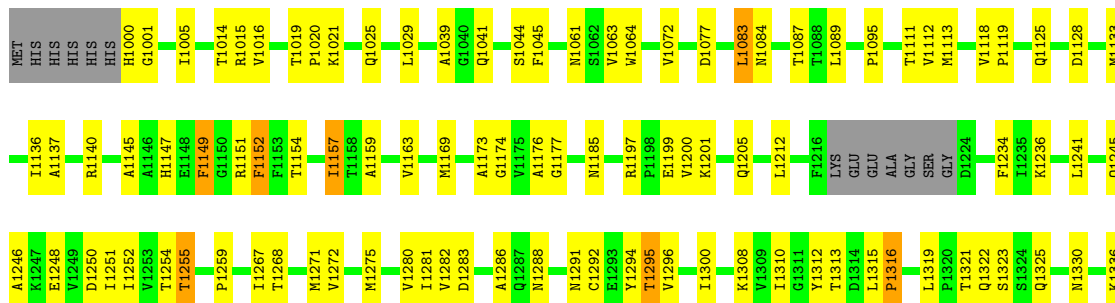
Chain C:  57% 26% 5% 10%

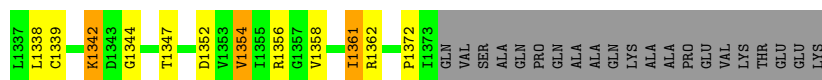


4.2.10 Score per residue for model 10

- Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

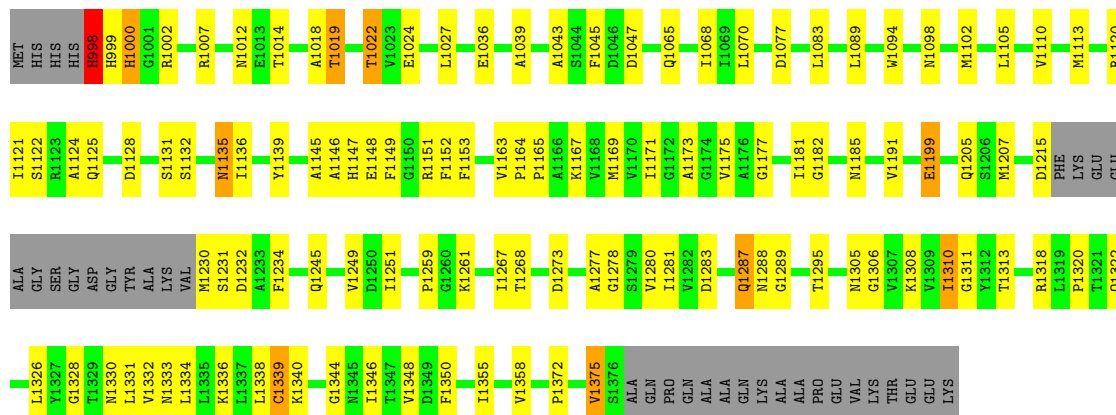
Chain A: 64% 25% 8%





• Molecule 1: NAD(P) TRANSHYDROGENASE SUBUNIT ALPHA

Chain B: 63% 26% 9%



• Molecule 2: NAD(P) TRANSHYDROGENASE SUBUNIT BETA

Chain C: 55% 27% 8% 10%



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.

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	0.99±0.01	4±1/2779 (0.1± 0.0%)	1.66±0.02	37±6/3776 (1.0± 0.2%)
1	B	1.03±0.01	6±2/2773 (0.2± 0.1%)	1.67±0.03	34±9/3768 (0.9± 0.2%)
2	C	1.06±0.02	5±1/1297 (0.4± 0.1%)	1.75±0.04	24±5/1764 (1.4± 0.3%)
All	All	1.02	151/68490 (0.2%)	1.68	950/93080 (1.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	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	31	HIS	CD2-NE2	-8.99	1.27	1.37	9	10
1	A	1000	HIS	CD2-NE2	-8.83	1.28	1.37	8	9
1	B	1375	VAL	C-N	-8.76	1.21	1.33	9	10
1	B	1147	HIS	CD2-NE2	-8.72	1.28	1.37	5	10
2	C	78	HIS	CD2-NE2	-8.54	1.28	1.37	9	9
1	B	999	HIS	CD2-NE2	-8.27	1.28	1.37	10	8
1	B	1000	HIS	CD2-NE2	-8.23	1.28	1.37	9	10
1	A	1372	PRO	C-N	-8.22	1.21	1.33	10	10
1	B	998	HIS	CD2-NE2	-8.18	1.28	1.37	1	6
2	C	69	HIS	CD2-NE2	-8.01	1.29	1.37	9	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	1147	HIS	CD2-NE2	-7.94	1.29	1.37	3	10
2	C	169	HIS	CD2-NE2	-7.68	1.29	1.37	1	10
1	B	999	HIS	CG-ND1	-7.42	1.30	1.38	6	5
2	C	139	TRP	NE1-CE2	-6.77	1.30	1.37	3	1
1	B	1000	HIS	CG-ND1	-6.53	1.31	1.38	1	5
1	A	1000	HIS	CG-ND1	-6.22	1.31	1.38	2	5
1	B	998	HIS	CG-ND1	-6.17	1.31	1.38	3	3
2	C	169	HIS	CG-ND1	-6.12	1.31	1.38	8	3
1	B	1371	PRO	CA-C	6.09	1.55	1.51	1	1
2	C	78	HIS	CG-ND1	-5.99	1.31	1.38	7	4
2	C	31	HIS	CG-ND1	-5.78	1.31	1.38	4	5
1	A	1147	HIS	CG-ND1	-5.72	1.31	1.38	9	5
2	C	69	HIS	CG-ND1	-5.26	1.32	1.38	9	2
1	B	1088	THR	CA-CB	5.13	1.59	1.52	3	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(°)	Ideal(°)	Models	
								Worst	Total
1	B	1012	ASN	OD1-CG-ND2	-10.71	111.89	122.60	10	2
1	A	1152	PHE	CA-CB-CG	9.79	123.59	113.80	10	6
1	A	1342	LYS	O-C-N	-9.77	110.92	123.32	9	10
1	A	1147	HIS	CB-CG-CD2	-9.67	118.63	131.20	1	8
2	C	30	SER	N-CA-C	9.64	124.14	112.38	3	7
2	C	167	ASN	CA-CB-CG	9.58	122.18	112.60	1	5
1	B	1215	ASP	CA-CB-CG	9.06	121.66	112.60	10	2
1	B	1098	ASN	CA-C-N	8.87	128.19	118.97	8	2
1	B	1098	ASN	C-N-CA	8.87	128.19	118.97	8	2
1	A	1296	VAL	N-CA-C	-8.68	99.66	107.56	1	6
1	A	1147	HIS	CB-CG-ND1	8.63	135.65	122.70	1	3
2	C	115	ASN	CA-CB-CG	8.51	121.11	112.60	9	3
1	A	1046	ASP	N-CA-C	8.49	120.85	110.41	8	3
1	B	1125	GLN	OE1-CD-NE2	-8.35	114.25	122.60	3	2
2	C	159	GLN	OE1-CD-NE2	-8.34	114.26	122.60	9	2
1	B	1136	ILE	N-CA-C	-8.29	102.46	110.42	9	1
2	C	139	TRP	CG-CD2-CE3	8.23	142.13	133.90	10	4
1	A	1025	GLN	OE1-CD-NE2	-8.21	114.39	122.60	9	1
1	B	1135	ASN	OD1-CG-ND2	-8.19	114.41	122.60	1	4
2	C	137	GLU	N-CA-C	8.18	128.21	110.80	8	3
1	A	1061	ASN	OD1-CG-ND2	-8.14	114.46	122.60	10	4
2	C	100	ASN	OD1-CG-ND2	-8.13	114.47	122.60	7	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	1249	VAL	N-CA-C	8.13	118.91	110.05	2	1
1	A	1047	ASP	CA-CB-CG	8.09	120.69	112.60	5	4
2	C	107	ASP	CA-CB-CG	8.03	120.63	112.60	8	2
1	B	999	HIS	CB-CG-CD2	-8.02	120.78	131.20	2	6
2	C	119	ASN	OD1-CG-ND2	-8.01	114.59	122.60	6	2
1	B	998	HIS	CB-CG-CD2	-8.01	120.79	131.20	1	7
1	B	1374	GLN	OE1-CD-NE2	-7.99	114.61	122.60	3	3
1	B	1149	PHE	CA-CB-CG	7.95	121.75	113.80	9	7
1	A	1343	ASP	CA-CB-CG	7.93	120.53	112.60	6	4
1	A	1368	TRP	CG-CD2-CE3	7.93	141.83	133.90	8	3
1	B	1097	GLN	OE1-CD-NE2	-7.87	114.73	122.60	2	6
1	A	1128	ASP	CA-CB-CG	7.78	120.38	112.60	4	6
1	A	1125	GLN	N-CA-C	7.70	122.35	112.34	6	2
1	A	1118	VAL	CA-C-N	7.65	127.70	119.90	10	2
1	A	1118	VAL	C-N-CA	7.65	127.70	119.90	10	2
1	A	1149	PHE	CA-CB-CG	7.63	121.43	113.80	9	7
1	B	1370	ALA	CA-C-N	7.61	125.21	119.66	6	3
1	B	1370	ALA	C-N-CA	7.61	125.21	119.66	6	3
1	B	1230	MET	O-C-N	-7.55	110.92	123.00	7	8
2	C	103	PHE	CA-CB-CG	7.55	121.35	113.80	4	2
2	C	31	HIS	CB-CG-CD2	-7.54	121.39	131.20	1	7
2	C	69	HIS	CB-CG-CD2	-7.49	121.46	131.20	6	6
1	A	1017	ALA	N-CA-C	7.47	119.07	111.07	2	3
1	A	1371	PRO	N-CA-C	7.47	117.64	110.47	3	2
1	A	1322	GLN	OE1-CD-NE2	-7.44	115.16	122.60	4	2
1	B	1147	HIS	CB-CG-CD2	-7.42	121.55	131.20	8	8
1	A	1109	ASN	OD1-CG-ND2	-7.40	115.20	122.60	5	4
1	A	1205	GLN	OE1-CD-NE2	-7.40	115.20	122.60	6	5
1	A	1291	ASN	CA-CB-CG	7.40	120.00	112.60	6	4
2	C	142	GLN	N-CA-C	7.33	120.14	111.71	6	2
1	B	1041	GLN	OE1-CD-NE2	-7.32	115.28	122.60	5	2
1	A	1005	ILE	O-C-N	-7.32	116.76	121.37	2	1
2	C	114	ALA	N-CA-C	7.29	126.34	110.80	8	2
1	A	1156	GLN	OE1-CD-NE2	-7.26	115.33	122.60	7	4
2	C	152	ASN	OD1-CG-ND2	-7.25	115.35	122.60	5	3
1	A	1094	TRP	CG-CD2-CE3	7.23	141.13	133.90	5	4
2	C	149	ARG	N-CA-C	-7.22	100.51	111.56	4	2
2	C	124	ASP	N-CA-C	7.21	120.20	111.40	2	1
2	C	185	ALA	N-CA-C	7.21	118.82	110.97	1	1
2	C	160	ASN	OD1-CG-ND2	-7.20	115.40	122.60	9	4
1	B	1092	PHE	CA-CB-CG	7.19	120.99	113.80	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1103	GLN	OE1-CD-NE2	-7.19	115.41	122.60	5	2
1	B	1330	ASN	OD1-CG-ND2	-7.18	115.42	122.60	7	3
1	A	1000	HIS	CA-CB-CG	7.18	120.98	113.80	3	1
2	C	160	ASN	CA-CB-CG	7.17	119.77	112.60	7	2
1	B	1232	ASP	CA-CB-CG	7.12	119.72	112.60	8	4
2	C	143	ASN	OD1-CG-ND2	-7.11	115.49	122.60	1	1
1	B	1094	TRP	CA-C-N	7.02	126.54	119.24	7	6
1	B	1094	TRP	C-N-CA	7.02	126.54	119.24	7	6
1	B	1103	GLN	OE1-CD-NE2	-7.00	115.60	122.60	2	2
1	B	1288	ASN	OD1-CG-ND2	-6.99	115.61	122.60	1	2
1	A	1261	LYS	CA-C-N	6.98	127.39	119.93	9	3
1	A	1261	LYS	C-N-CA	6.98	127.39	119.93	9	3
1	B	1045	PHE	CA-CB-CG	6.96	120.76	113.80	2	1
2	C	123	GLN	OE1-CD-NE2	-6.95	115.65	122.60	7	3
1	B	1312	TYR	N-CA-C	6.95	119.74	108.41	3	3
1	B	1109	ASN	OD1-CG-ND2	-6.95	115.65	122.60	3	1
2	C	128	SER	CA-C-N	6.94	126.19	118.97	4	6
2	C	128	SER	C-N-CA	6.94	126.19	118.97	4	6
1	A	1330	ASN	CA-CB-CG	6.93	119.53	112.60	10	2
2	C	158	VAL	N-CA-C	6.93	119.41	109.51	6	3
1	A	1064	TRP	CE2-CD2-CG	-6.89	98.93	107.20	10	4
1	A	1163	VAL	CA-C-N	6.88	124.61	119.66	3	1
1	A	1163	VAL	C-N-CA	6.88	124.61	119.66	3	1
1	B	1000	HIS	CB-CG-CD2	-6.87	122.27	131.20	4	3
1	A	1305	ASN	OD1-CG-ND2	-6.86	115.74	122.60	7	1
1	A	1000	HIS	CB-CG-CD2	-6.86	122.29	131.20	1	4
1	A	1073	ASN	CA-CB-CG	6.86	119.46	112.60	5	1
1	A	1098	ASN	N-CA-C	6.86	124.96	109.81	9	2
2	C	100	ASN	CA-CB-CG	6.86	119.46	112.60	7	2
2	C	124	ASP	CA-CB-CG	6.85	119.45	112.60	7	1
1	A	1199	GLU	N-CA-C	6.83	121.22	112.34	10	1
1	B	1246	ALA	N-CA-C	6.83	119.59	111.33	9	4
2	C	78	HIS	CB-CG-CD2	-6.79	122.37	131.20	10	3
1	B	1286	ALA	N-CA-C	6.77	119.52	111.33	6	4
1	B	1098	ASN	O-C-N	-6.76	115.10	121.05	10	1
1	B	1318	ARG	N-CA-C	6.76	125.20	110.80	2	5
1	B	1310	ILE	N-CA-CB	-6.72	105.54	112.06	10	2
2	C	169	HIS	CB-CG-CD2	-6.71	122.48	131.20	5	4
2	C	63	ASN	OD1-CG-ND2	-6.70	115.90	122.60	3	2
1	A	1002	ARG	N-CA-C	-6.70	97.44	108.76	5	2
1	B	1371	PRO	O-C-N	-6.69	118.23	121.31	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	1152	PHE	CA-CB-CG	6.68	120.48	113.80	4	5
1	A	1046	ASP	CA-CB-CG	6.68	119.28	112.60	6	2
2	C	167	ASN	OD1-CG-ND2	-6.67	115.92	122.60	9	2
1	A	1342	LYS	N-CA-C	6.67	118.72	110.91	2	3
1	B	1147	HIS	CB-CG-ND1	6.66	132.69	122.70	8	2
1	B	1296	VAL	N-CA-C	-6.65	100.15	107.73	3	3
1	B	1122	SER	N-CA-C	6.64	119.12	111.02	5	4
1	A	1084	ASN	N-CA-C	-6.63	101.43	109.72	6	2
1	A	1314	ASP	CA-CB-CG	6.61	119.21	112.60	4	3
1	A	1296	VAL	CA-C-O	-6.61	115.42	119.12	10	1
1	B	1072	VAL	N-CA-C	-6.60	104.73	110.74	5	1
1	B	1368	TRP	CE2-CD2-CG	-6.60	99.28	107.20	2	1
1	B	1195	ASP	CA-CB-CG	6.59	119.19	112.60	5	2
2	C	78	HIS	CA-CB-CG	6.57	120.37	113.80	5	4
1	B	1275	MET	N-CA-C	6.54	118.75	110.24	6	2
1	B	1125	GLN	CG-CD-NE2	6.54	126.20	116.40	3	1
1	B	1008	GLU	N-CA-C	6.53	118.73	110.24	9	3
1	A	1305	ASN	CA-CB-CG	6.52	119.12	112.60	6	2
1	B	1070	LEU	N-CA-C	-6.51	98.12	108.73	1	1
1	B	1291	ASN	CA-CB-CG	6.49	119.09	112.60	6	2
2	C	119	ASN	CA-C-N	6.49	127.95	119.84	6	6
2	C	119	ASN	C-N-CA	6.49	127.95	119.84	6	6
1	B	1047	ASP	CA-CB-CG	6.49	119.09	112.60	10	2
1	B	1078	ASP	CA-CB-CG	6.48	119.08	112.60	1	3
2	C	183	LEU	N-CA-C	6.48	120.29	112.38	7	2
1	A	1084	ASN	CA-CB-CG	6.48	119.08	112.60	4	2
1	A	1351	ASP	CA-CB-CG	6.46	119.06	112.60	1	1
1	B	1017	ALA	N-CA-C	6.45	118.31	111.28	8	1
1	A	1215	ASP	CA-CB-CG	6.42	119.02	112.60	7	2
1	A	1268	THR	N-CA-C	6.42	119.08	110.35	2	1
1	B	1098	ASN	OD1-CG-ND2	-6.41	116.19	122.60	5	3
1	A	1057	ILE	CB-CA-C	6.41	118.59	111.80	4	1
1	A	1094	TRP	CE2-CD2-CG	-6.40	99.52	107.20	5	6
1	A	1318	ARG	N-CA-C	6.38	120.63	112.34	1	1
1	B	999	HIS	CB-CG-ND1	6.38	132.27	122.70	4	3
1	A	1064	TRP	CG-CD2-CE3	6.37	140.27	133.90	10	3
1	B	1258	ILE	N-CA-C	-6.37	103.15	108.63	6	2
1	B	1181	ILE	N-CA-C	-6.35	104.14	110.30	3	1
1	A	1164	PRO	CA-C-N	6.34	126.31	119.78	5	2
1	A	1164	PRO	C-N-CA	6.34	126.31	119.78	5	2
1	B	1277	ALA	N-CA-C	6.33	118.50	110.33	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1301	PHE	CA-CB-CG	6.31	120.11	113.80	4	1
1	B	1052	GLN	OE1-CD-NE2	-6.31	116.29	122.60	8	1
1	B	1118	VAL	CA-C-N	6.29	126.32	119.90	9	1
1	B	1118	VAL	C-N-CA	6.29	126.32	119.90	9	1
1	A	1229	VAL	N-CA-C	6.29	116.77	110.23	7	3
2	C	69	HIS	CA-C-N	6.28	125.50	118.97	10	5
2	C	69	HIS	C-N-CA	6.28	125.50	118.97	10	5
1	A	1231	SER	N-CA-C	6.26	120.48	109.96	2	1
1	B	1094	TRP	CG-CD2-CE3	6.26	140.16	133.90	10	5
2	C	159	GLN	CG-CD-NE2	6.26	125.79	116.40	6	2
2	C	160	ASN	CA-C-N	6.25	126.72	119.47	1	3
2	C	160	ASN	C-N-CA	6.25	126.72	119.47	1	3
1	A	1263	ALA	CA-C-N	6.25	126.62	119.93	2	5
1	A	1263	ALA	C-N-CA	6.25	126.62	119.93	2	5
2	C	106	THR	CA-CB-OG1	-6.25	100.22	109.60	4	1
1	A	1341	GLU	N-CA-C	6.25	118.17	111.36	1	1
1	B	1295	THR	CA-CB-OG1	-6.25	100.23	109.60	3	1
1	B	1288	ASN	CA-CB-CG	6.24	118.84	112.60	10	1
1	A	1012	ASN	OD1-CG-ND2	-6.23	116.37	122.60	7	2
1	B	1314	ASP	CA-CB-CG	6.23	118.83	112.60	1	3
1	B	1197	ARG	CA-C-N	6.23	125.64	118.85	5	4
1	B	1197	ARG	C-N-CA	6.23	125.64	118.85	5	4
1	A	1064	TRP	CB-CG-CD1	-6.22	117.57	126.90	5	1
1	A	1041	GLN	OE1-CD-NE2	-6.21	116.39	122.60	4	2
1	A	1074	ALA	N-CA-C	6.20	116.73	109.60	1	1
2	C	80	ASN	CA-CB-CG	6.20	118.80	112.60	3	2
1	B	1245	GLN	OE1-CD-NE2	-6.20	116.40	122.60	10	4
1	B	1135	ASN	CB-CG-ND2	6.19	125.69	116.40	10	2
1	A	1224	ASP	CA-CB-CG	6.19	118.79	112.60	8	1
1	A	1135	ASN	CA-CB-CG	6.18	118.78	112.60	1	1
1	A	1025	GLN	CG-CD-NE2	6.18	125.67	116.40	9	1
1	A	1319	LEU	CA-C-N	6.18	125.40	118.97	9	2
1	A	1319	LEU	C-N-CA	6.18	125.40	118.97	9	2
1	A	1224	ASP	CA-C-N	6.17	126.96	119.99	3	2
1	A	1224	ASP	C-N-CA	6.17	126.96	119.99	3	2
1	A	1098	ASN	CA-C-N	6.16	125.89	119.05	7	1
1	A	1098	ASN	C-N-CA	6.16	125.89	119.05	7	1
2	C	78	HIS	N-CA-C	6.13	119.59	111.75	10	2
1	A	1019	THR	CA-C-N	6.12	127.50	119.84	5	1
1	A	1019	THR	C-N-CA	6.12	127.50	119.84	5	1
1	A	1045	PHE	N-CA-C	-6.12	97.76	110.80	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1077	ASP	CA-CB-CG	6.12	118.72	112.60	7	1
1	B	1061	ASN	OD1-CG-ND2	-6.11	116.49	122.60	8	2
2	C	45	GLN	N-CA-C	6.11	123.81	110.80	7	2
1	B	1109	ASN	CB-CG-ND2	6.10	125.56	116.40	3	2
1	A	1325	GLN	OE1-CD-NE2	-6.10	116.50	122.60	2	1
2	C	139	TRP	CE2-CD2-CG	-6.08	99.90	107.20	7	5
2	C	142	GLN	OE1-CD-NE2	-6.07	116.53	122.60	2	2
1	A	1185	ASN	OD1-CG-ND2	-6.07	116.53	122.60	10	2
2	C	165	LYS	N-CA-C	6.07	117.88	110.41	4	1
1	B	1061	ASN	CA-CB-CG	6.05	118.65	112.60	7	1
1	B	1019	THR	O-C-N	-6.03	117.85	121.71	2	1
1	B	1345	ASN	OD1-CG-ND2	-6.03	116.57	122.60	9	3
1	A	1322	GLN	CG-CD-NE2	6.03	125.44	116.40	4	2
2	C	139	TRP	CB-CG-CD1	-6.01	117.88	126.90	2	5
1	A	1064	TRP	CG-CD1-NE1	-6.00	102.39	110.20	10	2
2	C	101	ASP	O-C-N	6.00	128.27	122.03	4	1
1	A	1122	SER	N-CA-C	6.00	118.30	111.11	5	2
1	B	1230	MET	CA-C-N	5.99	132.49	121.70	7	3
1	B	1230	MET	C-N-CA	5.99	132.49	121.70	7	3
2	C	27	LEU	N-CA-C	5.99	118.58	111.33	2	1
1	B	1205	GLN	OE1-CD-NE2	-5.98	116.62	122.60	10	1
2	C	22	GLU	N-CA-C	-5.98	104.68	111.14	10	1
1	A	1158	THR	O-C-N	-5.96	116.28	122.84	3	1
2	C	152	ASN	CA-CB-CG	5.95	118.55	112.60	10	1
1	B	1373	ILE	CB-CA-C	5.95	119.79	111.34	7	1
2	C	96	MET	N-CA-C	5.94	119.55	111.17	7	1
1	B	1254	THR	CA-C-O	5.94	127.10	120.92	1	2
1	A	1077	ASP	N-CA-C	5.94	118.52	111.33	8	3
1	A	1286	ALA	N-CA-C	5.93	123.42	110.80	4	2
1	A	1288	ASN	OD1-CG-ND2	-5.92	116.68	122.60	1	3
1	B	1254	THR	CB-CA-C	5.92	121.37	111.30	7	2
2	C	36	THR	CA-C-N	5.92	125.88	119.78	9	1
2	C	36	THR	C-N-CA	5.92	125.88	119.78	9	1
1	A	1203	GLN	OE1-CD-NE2	-5.92	116.69	122.60	4	3
1	B	1094	TRP	CE2-CD2-CG	-5.92	100.10	107.20	9	4
1	A	1249	VAL	N-CA-C	5.91	117.66	109.80	3	2
1	B	1005	ILE	CA-C-N	5.91	125.81	119.85	1	2
1	B	1005	ILE	C-N-CA	5.91	125.81	119.85	1	2
1	B	1019	THR	CA-C-N	5.89	125.37	119.24	1	3
1	B	1019	THR	C-N-CA	5.89	125.37	119.24	1	3
1	A	1368	TRP	CE2-CD2-CG	-5.89	100.14	107.20	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	159	GLN	CB-CG-CD	5.88	122.60	112.60	6	1
1	B	1288	ASN	CB-CG-ND2	5.88	125.22	116.40	9	1
2	C	88	VAL	N-CA-C	-5.88	101.48	107.89	3	1
2	C	88	VAL	CA-C-N	5.87	127.18	119.84	10	3
2	C	88	VAL	C-N-CA	5.87	127.18	119.84	10	3
1	A	1196	THR	N-CA-C	-5.87	104.96	111.36	8	1
1	B	1175	VAL	N-CA-C	5.87	116.52	110.36	10	1
2	C	69	HIS	CB-CG-ND1	5.86	131.50	122.70	3	2
1	A	1084	ASN	OD1-CG-ND2	-5.86	116.74	122.60	10	2
1	B	1045	PHE	N-CA-C	-5.86	97.41	107.61	8	1
2	C	169	HIS	CB-CG-ND1	5.85	131.48	122.70	5	2
1	B	1371	PRO	N-CA-CB	-5.85	99.91	103.19	8	1
1	A	1352	ASP	CA-CB-CG	5.85	118.45	112.60	10	1
2	C	80	ASN	OD1-CG-ND2	-5.84	116.76	122.60	9	2
1	A	1294	TYR	N-CA-C	5.83	119.92	112.34	8	1
1	A	1214	LEU	CA-C-O	5.82	127.33	120.69	4	1
1	B	1315	LEU	CA-C-O	-5.82	113.27	118.63	5	1
1	B	1256	ALA	N-CA-C	5.81	123.17	110.80	7	1
2	C	47	GLN	CA-C-O	-5.80	114.72	120.70	7	1
1	A	1067	GLU	N-CA-C	5.80	120.09	113.19	2	1
1	B	1330	ASN	CA-CB-CG	5.80	118.40	112.60	6	1
2	C	47	GLN	N-CA-C	5.80	117.68	111.36	6	1
1	A	1132	SER	N-CA-C	5.80	117.68	111.36	3	2
2	C	29	ASN	OD1-CG-ND2	-5.78	116.83	122.60	2	3
1	A	1185	ASN	CB-CG-ND2	5.77	125.05	116.40	10	1
1	B	1283	ASP	CA-CB-CG	5.76	118.36	112.60	10	1
2	C	145	ILE	N-CA-CB	-5.75	105.69	111.90	2	1
2	C	140	LYS	N-CA-C	5.75	123.06	110.80	2	1
1	B	1284	LEU	N-CA-C	-5.75	104.62	111.69	1	1
1	A	1000	HIS	CB-CG-ND1	5.74	131.32	122.70	1	2
1	B	1125	GLN	N-CA-C	5.73	118.30	111.71	9	2
2	C	41	MET	N-CA-C	5.73	118.27	111.33	3	1
2	C	31	HIS	CB-CG-ND1	5.73	131.30	122.70	7	2
1	B	1253	VAL	N-CA-CB	-5.72	105.94	111.89	3	1
1	B	1371	PRO	CA-C-N	5.72	126.99	119.84	4	3
1	B	1371	PRO	C-N-CA	5.72	126.99	119.84	4	3
1	A	1333	ASN	OD1-CG-ND2	-5.71	116.89	122.60	6	2
2	C	130	ILE	N-CA-CB	5.70	118.05	111.90	8	1
2	C	115	ASN	OD1-CG-ND2	-5.69	116.91	122.60	3	4
1	A	1342	LYS	CA-C-N	5.69	131.94	121.70	2	1
1	A	1342	LYS	C-N-CA	5.69	131.94	121.70	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1094	TRP	CA-C-N	5.68	125.80	119.32	5	4
1	A	1094	TRP	C-N-CA	5.68	125.80	119.32	5	4
1	A	1228	LYS	CB-CA-C	-5.68	101.35	110.79	9	1
1	B	1094	TRP	CB-CG-CD1	-5.68	118.38	126.90	4	2
1	A	1258	ILE	CA-C-N	5.67	126.00	119.93	4	1
1	A	1258	ILE	C-N-CA	5.67	126.00	119.93	4	1
1	A	1064	TRP	CD1-CG-CD2	5.67	115.37	106.30	10	2
1	A	1291	ASN	OD1-CG-ND2	-5.67	116.93	122.60	6	3
1	A	1315	LEU	N-CA-C	5.66	121.24	113.77	6	1
1	A	1159	ALA	N-CA-C	-5.66	106.42	113.38	6	2
1	B	1205	GLN	CG-CD-NE2	5.65	124.88	116.40	10	1
2	C	159	GLN	N-CA-C	5.64	122.81	110.80	6	3
1	B	1147	HIS	CA-CB-CG	5.64	119.44	113.80	9	1
1	A	1295	THR	CA-C-N	-5.64	118.77	122.60	10	1
1	A	1295	THR	C-N-CA	-5.64	118.77	122.60	10	1
1	B	1343	ASP	CA-CB-CG	5.62	118.22	112.60	1	4
1	A	1295	THR	CA-CB-OG1	-5.62	101.17	109.60	3	1
2	C	24	ALA	O-C-N	5.61	127.85	122.07	2	1
1	B	1371	PRO	CA-C-O	-5.61	116.86	120.90	8	1
1	B	1031	PHE	CA-CB-CG	-5.61	108.19	113.80	1	1
1	B	1084	ASN	OD1-CG-ND2	-5.60	117.00	122.60	9	2
1	B	1315	LEU	CA-C-N	5.59	125.95	119.47	5	1
1	B	1315	LEU	C-N-CA	5.59	125.95	119.47	5	1
1	A	1283	ASP	CA-CB-CG	5.58	118.18	112.60	2	1
1	B	1122	SER	O-C-N	-5.58	116.11	122.08	5	1
2	C	106	THR	CA-CB-CG2	5.57	119.96	110.50	6	2
2	C	47	GLN	OE1-CD-NE2	-5.57	117.03	122.60	9	2
1	B	1296	VAL	CA-C-O	-5.56	116.01	119.12	2	1
1	B	1111	THR	CA-CB-OG1	-5.56	101.26	109.60	8	1
1	B	1107	GLU	N-CA-C	5.56	117.02	111.07	8	1
1	A	1120	ARG	N-CA-C	5.55	121.03	113.37	2	1
1	A	1319	LEU	N-CA-C	-5.54	99.33	108.75	10	1
1	A	1330	ASN	OD1-CG-ND2	-5.54	117.06	122.60	2	1
1	A	1216	PHE	CA-CB-CG	5.54	119.34	113.80	7	1
1	B	1361	ILE	O-C-N	-5.53	117.99	122.97	1	1
1	A	1197	ARG	CA-C-N	5.53	125.20	119.56	3	4
1	A	1197	ARG	C-N-CA	5.53	125.20	119.56	3	4
1	A	1109	ASN	CA-CB-CG	5.53	118.13	112.60	8	1
2	C	174	ASP	CA-CB-CG	5.53	118.13	112.60	8	1
1	B	998	HIS	CB-CG-ND1	5.51	130.97	122.70	1	3
1	B	1025	GLN	OE1-CD-NE2	-5.51	117.09	122.60	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	168	THR	N-CA-CB	-5.51	102.33	110.49	7	1
1	B	1235	ILE	CA-CB-CG1	5.50	119.75	110.40	8	1
1	A	1087	THR	N-CA-C	5.49	118.32	110.24	8	2
1	A	1256	ALA	N-CA-C	5.49	118.58	108.58	9	1
1	A	1211	PHE	N-CA-C	-5.49	99.79	108.73	4	1
1	B	1164	PRO	CA-C-O	-5.48	116.40	120.73	6	1
1	A	1061	ASN	N-CA-C	5.48	117.96	111.33	7	1
1	A	1038	GLY	N-CA-C	-5.48	107.38	113.79	9	1
1	A	1061	ASN	CB-CG-ND2	5.48	124.62	116.40	10	1
1	A	1145	ALA	CA-C-O	-5.48	115.26	120.90	9	1
1	B	1330	ASN	CB-CG-ND2	5.47	124.60	116.40	1	1
1	A	1115	MET	N-CA-C	5.46	117.99	111.71	1	1
1	B	1352	ASP	CA-CB-CG	5.46	118.06	112.60	5	2
1	B	1293	GLU	N-CA-C	5.45	119.19	112.54	5	1
1	B	1084	ASN	CB-CG-ND2	5.45	124.57	116.40	9	1
2	C	119	ASN	CA-CB-CG	5.45	118.05	112.60	4	4
2	C	125	ASP	CA-C-N	5.45	125.53	119.87	7	3
2	C	125	ASP	C-N-CA	5.45	125.53	119.87	7	3
1	B	1353	VAL	N-CA-C	5.43	116.81	110.62	7	1
1	A	1094	TRP	CB-CG-CD1	-5.43	118.76	126.90	2	3
1	A	1012	ASN	CA-CB-CG	-5.42	107.18	112.60	2	1
1	A	1343	ASP	N-CA-CB	5.42	119.72	110.50	4	1
1	B	1263	ALA	N-CA-C	5.42	117.40	109.71	8	1
2	C	156	ALA	N-CA-C	-5.42	104.92	112.45	3	1
2	C	139	TRP	CG-CD1-NE1	-5.41	103.16	110.20	2	2
1	A	1255	THR	N-CA-C	5.41	120.00	113.41	9	2
2	C	131	ALA	N-CA-C	5.40	118.11	110.50	4	1
1	A	1368	TRP	O-C-N	-5.39	115.39	121.43	1	1
1	A	1354	VAL	N-CA-CB	5.39	119.57	110.56	3	1
1	B	1087	THR	CB-CA-C	5.38	118.50	109.89	8	1
1	A	1114	ALA	CA-C-O	5.38	126.34	120.58	1	1
1	A	1241	LEU	N-CA-C	-5.38	105.33	111.14	4	1
2	C	106	THR	CA-C-O	5.37	126.81	120.96	2	1
1	A	1277	ALA	N-CA-C	5.37	117.01	110.41	1	1
1	A	1181	ILE	CA-C-N	5.36	125.89	119.94	2	2
1	A	1181	ILE	C-N-CA	5.36	125.89	119.94	2	2
1	B	1305	ASN	CA-CB-CG	5.36	117.96	112.60	10	3
1	A	1008	GLU	N-CA-C	5.36	118.41	110.48	9	1
1	B	1164	PRO	CA-C-N	5.35	125.29	119.78	3	1
1	B	1164	PRO	C-N-CA	5.35	125.29	119.78	3	1
1	B	1061	ASN	N-CA-C	5.35	118.91	112.38	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	1195	ASP	N-CA-C	-5.34	100.95	109.07	3	1
1	B	1019	THR	CA-C-O	-5.34	115.14	120.96	9	2
2	C	163	PHE	CA-CB-CG	5.34	119.14	113.80	7	2
1	A	1097	GLN	N-CA-C	-5.33	106.28	112.89	7	2
1	B	1052	GLN	CG-CD-NE2	5.33	124.40	116.40	8	1
2	C	177	ALA	N-CA-C	5.33	117.78	111.33	7	1
1	B	1064	TRP	CB-CG-CD1	-5.33	118.90	126.90	8	1
1	A	1117	SER	N-CA-C	5.33	119.49	113.15	2	1
2	C	116	ASP	CA-CB-CG	5.33	117.92	112.60	10	1
1	B	1185	ASN	OD1-CG-ND2	-5.32	117.28	122.60	10	2
2	C	45	GLN	CA-CB-CG	5.32	124.73	114.10	3	2
1	B	1064	TRP	N-CA-C	5.31	117.07	111.28	6	1
1	A	1174	GLY	O-C-N	-5.31	118.08	122.92	3	1
1	A	1361	ILE	O-C-N	-5.31	117.66	123.18	10	1
1	A	1236	LYS	N-CA-C	-5.30	105.58	111.36	10	1
1	B	1269	ARG	N-CA-C	5.30	117.47	111.11	8	1
1	A	1154	THR	N-CA-CB	-5.29	100.92	109.60	3	1
1	A	1281	ILE	N-CA-C	-5.29	99.33	106.85	3	1
1	A	1052	GLN	OE1-CD-NE2	-5.29	117.31	122.60	6	1
1	B	1305	ASN	OD1-CG-ND2	-5.29	117.31	122.60	7	1
2	C	34	ILE	N-CA-CB	5.29	117.40	111.21	7	1
1	A	1273	ASP	N-CA-C	5.28	117.78	111.71	3	1
2	C	139	TRP	CD1-CG-CD2	5.27	114.73	106.30	8	1
1	A	1201	LYS	N-CA-C	5.27	117.43	111.11	10	1
1	B	1306	GLY	O-C-N	-5.27	116.72	122.41	10	1
1	A	1356	ARG	CA-C-O	-5.26	115.27	120.90	10	1
1	B	1094	TRP	CG-CD1-NE1	-5.25	103.37	110.20	7	3
1	B	1303	THR	CB-CA-C	5.25	118.40	109.53	6	1
1	A	1312	TYR	N-CA-C	5.25	116.81	108.67	6	1
1	B	1071	LYS	N-CA-CB	-5.25	102.56	111.69	7	1
1	A	1143	VAL	N-CA-CB	-5.25	105.11	110.62	7	1
1	A	1370	ALA	CA-C-N	5.24	125.78	120.38	4	1
1	A	1370	ALA	C-N-CA	5.24	125.78	120.38	4	1
1	B	1241	LEU	N-CA-C	-5.24	105.48	111.14	3	1
1	A	1338	LEU	N-CA-C	5.24	116.79	111.14	3	1
1	A	1056	GLU	N-CA-C	-5.23	101.93	110.20	2	1
1	A	1332	VAL	N-CA-C	-5.23	105.40	110.42	1	2
1	A	1005	ILE	N-CA-C	-5.23	102.01	107.60	10	2
2	C	135	VAL	CB-CA-C	5.22	117.63	111.32	4	1
1	A	1287	GLN	N-CA-C	5.22	116.97	111.28	4	1
1	B	1316	PRO	CA-C-N	5.21	125.87	120.03	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	1316	PRO	C-N-CA	5.21	125.87	120.03	8	1
1	A	1354	VAL	N-CA-C	-5.20	105.78	110.82	4	2
1	B	1368	TRP	CB-CG-CD1	-5.19	119.11	126.90	8	1
2	C	81	VAL	N-CA-C	-5.19	105.44	110.42	7	1
2	C	54	THR	CA-C-N	5.18	127.18	120.44	5	1
2	C	54	THR	C-N-CA	5.18	127.18	120.44	5	1
1	A	1141	ALA	N-CA-C	-5.18	105.55	111.14	3	1
1	B	1128	ASP	CA-CB-CG	5.18	117.78	112.60	7	1
1	B	1368	TRP	N-CA-C	-5.18	103.25	109.72	6	1
1	B	1128	ASP	CA-C-O	5.17	126.49	120.49	7	1
1	A	1204	VAL	N-CA-CB	-5.17	104.50	110.55	1	1
1	B	1261	LYS	O-C-N	-5.17	117.80	121.83	10	1
2	C	29	ASN	CA-CB-CG	5.17	117.77	112.60	5	1
2	C	145	ILE	CB-CA-C	5.17	118.89	111.81	9	1
1	B	1373	ILE	N-CA-CB	-5.16	105.40	111.60	1	1
1	A	1356	ARG	CA-C-N	5.16	125.67	119.94	5	1
1	A	1356	ARG	C-N-CA	5.16	125.67	119.94	5	1
1	A	1313	THR	CA-C-O	5.16	125.89	120.42	6	1
2	C	56	LYS	N-CA-C	5.16	116.59	111.07	5	1
1	A	1087	THR	CA-CB-OG1	-5.16	101.86	109.60	10	1
1	B	1186	SER	CA-CB-OG	5.15	121.41	111.10	4	1
1	A	1133	MET	N-CA-C	5.15	117.64	111.71	10	1
1	B	1109	ASN	N-CA-C	5.13	118.81	112.24	9	1
1	B	1124	ALA	N-CA-C	5.13	116.88	111.28	10	1
1	B	1139	TYR	N-CA-C	-5.13	105.59	111.14	10	1
1	A	1068	ILE	CA-CB-CG1	5.13	119.12	110.40	1	1
1	A	1299	GLU	N-CA-C	5.13	117.21	109.41	8	2
1	A	1245	GLN	OE1-CD-NE2	-5.13	117.47	122.60	6	2
1	A	1044	SER	N-CA-C	5.12	121.51	113.72	1	1
1	B	1157	ILE	N-CA-C	-5.12	99.32	107.15	2	1
1	A	1287	GLN	OE1-CD-NE2	-5.11	117.49	122.60	1	1
1	B	1250	ASP	N-CA-C	-5.11	105.27	112.12	3	1
1	A	1120	ARG	CA-CB-CG	5.11	124.32	114.10	3	1
2	C	66	PHE	CA-CB-CG	5.11	118.91	113.80	3	1
2	C	145	ILE	CA-CB-CG2	5.11	119.18	110.50	4	1
1	A	1084	ASN	CA-C-N	5.11	125.38	119.92	1	1
1	A	1084	ASN	C-N-CA	5.11	125.38	119.92	1	1
1	B	1128	ASP	N-CA-C	5.11	117.06	109.25	7	1
1	A	1111	THR	CA-CB-OG1	-5.10	101.94	109.60	8	1
1	A	1005	ILE	CA-C-N	5.10	126.22	120.66	2	1
1	A	1005	ILE	C-N-CA	5.10	126.22	120.66	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1277	ALA	N-CA-CB	-5.10	102.70	110.45	3	1
2	C	100	ASN	CB-CG-ND2	5.10	124.05	116.40	2	1
1	B	1314	ASP	N-CA-C	5.10	120.41	113.37	9	1
2	C	68	ILE	N-CA-CB	5.09	117.37	112.28	1	1
1	B	1327	TYR	N-CA-C	-5.09	105.42	110.97	7	1
1	B	1319	LEU	CA-C-N	5.08	126.20	119.84	1	1
1	B	1319	LEU	C-N-CA	5.08	126.20	119.84	1	1
1	B	1254	THR	CA-CB-CG2	5.08	119.13	110.50	7	1
2	C	115	ASN	CB-CG-ND2	5.08	124.02	116.40	5	1
1	A	1326	LEU	CA-C-O	-5.07	115.04	120.42	7	1
2	C	43	VAL	N-CA-C	5.07	117.39	111.05	8	1
2	C	108	THR	N-CA-C	5.07	116.53	108.67	10	1
1	A	1095	PRO	N-CA-C	5.07	120.49	113.65	10	1
1	B	1368	TRP	CG-CD1-NE1	-5.07	103.61	110.20	3	2
1	A	1234	PHE	CA-C-O	-5.07	115.48	120.70	10	1
1	B	1325	GLN	OE1-CD-NE2	-5.06	117.54	122.60	7	1
1	B	1273	ASP	N-CA-C	5.06	120.36	113.37	8	1
2	C	153	THR	CA-CB-CG2	5.06	119.11	110.50	2	1
1	B	1094	TRP	CB-CA-C	5.06	115.47	110.71	1	1
1	B	1077	ASP	N-CA-C	5.06	118.71	112.54	1	1
1	B	1064	TRP	CE2-CD2-CG	-5.06	101.13	107.20	1	1
1	A	1143	VAL	CA-C-O	-5.06	115.88	121.29	8	1
1	A	1154	THR	N-CA-C	5.05	116.43	109.15	3	1
1	A	1098	ASN	O-C-N	-5.05	116.60	121.05	1	1
1	B	1084	ASN	CA-CB-CG	5.05	117.65	112.60	9	1
1	A	1229	VAL	CB-CA-C	-5.05	105.42	111.88	8	1
1	B	1044	SER	CA-C-O	5.05	127.41	121.40	8	1
1	B	1372	PRO	N-CA-C	5.05	119.12	111.19	10	1
1	A	1094	TRP	CG-CD1-NE1	-5.04	103.64	110.20	3	1
2	C	125	ASP	CA-CB-CG	5.04	117.64	112.60	1	1
1	B	1094	TRP	CD1-CG-CD2	5.04	114.36	106.30	9	1
2	C	165	LYS	N-CA-CB	-5.04	103.40	110.25	7	1
1	A	1269	ARG	N-CA-C	5.03	117.16	111.02	2	1
1	B	1287	GLN	CG-CD-NE2	5.03	123.95	116.40	2	1
1	B	1234	PHE	CA-CB-CG	5.03	118.83	113.80	10	1
1	A	1164	PRO	N-CA-C	5.02	116.83	110.70	6	1
1	A	1247	LYS	N-CA-C	5.02	118.50	112.38	9	1
1	B	1039	ALA	CA-C-N	5.02	125.66	119.99	1	1
1	B	1039	ALA	C-N-CA	5.02	125.66	119.99	1	1
1	B	1084	ASN	CA-C-N	5.02	126.11	119.84	4	1
1	B	1084	ASN	C-N-CA	5.02	126.11	119.84	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	46	ALA	N-CA-C	5.02	119.03	113.01	7	1
2	C	108	THR	CA-CB-OG1	-5.02	102.08	109.60	4	1
1	B	1174	GLY	CA-C-O	-5.01	116.27	122.03	8	1
1	A	1330	ASN	O-C-N	5.01	127.23	122.07	5	1
1	B	1212	LEU	N-CA-C	5.01	116.64	108.63	5	1
1	B	1163	VAL	CA-C-N	5.01	123.27	119.66	6	1
1	B	1163	VAL	C-N-CA	5.01	123.27	119.66	6	1
1	A	1368	TRP	CB-CG-CD1	-5.00	119.39	126.90	1	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	B	1139	TYR	Sidechain	4
1	A	1294	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
2	C	48	TYR	Sidechain	2
1	A	1318	ARG	Sidechain	2
1	A	1362	ARG	Sidechain	2
1	A	1108	ARG	Sidechain	1
2	C	39	TYR	Sidechain	1
1	A	1327	TYR	Sidechain	1
2	C	60	ARG	Sidechain	1
1	B	1327	TYR	Sidechain	1
2	C	155	TYR	Sidechain	1
1	A	1123	ARG	Sidechain	1
1	A	1139	TYR	Sidechain	1
2	C	58	ARG	Sidechain	1
1	A	1007	ARG	Sidechain	1
1	A	1192	ARG	Sidechain	1
1	A	1255	THR	Peptide	1
1	A	1269	ARG	Sidechain	1
1	B	998	HIS	Peptide	1

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	2735	579	2770	36±5
1	B	2729	582	2778	42±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	929

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
2:C:151:MET:SD	2:C:170:MET:HE1	0.76	2.21	8	1
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
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:163:PHE:HA	2:C:170:MET:HE2	0.67	1.64	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:1203:GLN:HG2	2:C:74:ARG:HG3	0.66	1.67	1	3
1:A:1133:MET:HA	1:A:1136:ILE:HD12	0.66	1.66	8	2
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:1009:ARG:NH1	1:A:1079:GLU:HG2	0.65	2.06	1	1
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
2:C:162:LEU:HA	2:C:168:THR:HB	0.65	1.68	1	1
1:A:1145:ALA:HB1	1:A:1251:ILE:HD12	0.65	1.67	4	5
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:A:1115:MET:HE3	1:A:1129:ALA:HB2	0.64	1.69	6	1
2:C:72:ALA:HB3	2:C:79:MET:SD	0.64	2.33	2	1
2:C:66:PHE:HB2	2:C:93:VAL:HA	0.64	1.68	7	4
1:B:1182:GLY:HA2	1:B:1207:MET:HE1	0.64	1.67	7	4
1:B:1083:LEU:HD21	1:B:1089:LEU:HD13	0.64	1.69	8	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:1169:MET:HE3	1:B:1171:ILE:HD11	0.63	1.70	10	4
1:A:1018:ALA:HB1	1:A:1022:THR:HB	0.62	1.70	4	1
1:B:1157:ILE:HG23	1:B:1162:LYS:HG2	0.62	1.71	8	1
1:A:1113:MET:SD	1:A:1338:LEU:HD21	0.62	2.33	7	3
1:A:1339:CYS:SG	1:A:1342:LYS:HA	0.62	2.34	2	1
2:C:37:PRO:HD2	2:C:68:ILE:HG12	0.62	1.69	10	4
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:1080:ILE:HA	1:B:1083:LEU:HD12	0.61	1.71	5	2
1:B:1267:ILE:HG21	1:B:1281:ILE:HD13	0.61	1.71	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:1151:ARG:NH2	1:A:1164:PRO:HB2	0.61	2.10	2	1
2:C:24:ALA:HB1	2:C:186:LEU:HA	0.61	1.71	7	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:1120:ARG:HB2	1:B:1375:VAL:HG13	0.59	1.74	3	1
1:B:1181:ILE:HG12	1:B:1191:VAL:HG11	0.59	1.74	5	2
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:B:1328:GLY:HA2	1:B:1331:LEU:HD12	0.58	1.73	4	5
1:A:1246:ALA:HB1	1:A:1275:MET:HG2	0.58	1.75	2	2
1:B:1125:GLN:HA	1:B:1128:ASP:HB3	0.58	1.74	10	1
1:B:1167:LYS:HB2	1:B:1249:VAL:HA	0.58	1.74	5	5
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: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
2:C:20:ALA:HA	2:C:171:LEU:HD21	0.58	1.76	3	1
1:B:1207:MET:SD	2:C:75:LEU:HG	0.58	2.37	7	1
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:A:1169:MET:HE3	1:A:1171:ILE:HD11	0.57	1.76	4	1
1:B:1005:ILE:HG23	1:B:1017:ALA:HB3	0.57	1.75	1	3
1:B:1016:VAL:HG21	1:B:1039:ALA:HB1	0.57	1.75	3	4
1:B:1113:MET:SD	1:B:1334:LEU:HD21	0.57	2.39	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:1312:TYR:HB2	1:B:1315:LEU:HG	0.57	1.74	2	3
1:A:1300:ILE:HG12	1:A:1310:ILE:HG12	0.57	1.75	6	2
1:A:1113:MET:HE1	1:A:1338:LEU:HD11	0.57	1.75	8	4
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
2:C:34:ILE:HB	2:C:109:VAL:HG13	0.56	1.75	1	1
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
1:B:1083:LEU:HD11	1:B:1089:LEU:HD22	0.56	1.78	9	2
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:B:1332:VAL:HG12	1:B:1336:LYS:HE3	0.55	1.76	2	2
1:A:1157:ILE:HG13	2:C:70:PRO:HB3	0.55	1.78	5	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
2:C:73:GLY:C	2:C:74:ARG:HD2	0.55	2.26	1	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
1:B:1230:MET:N	1:B:1231:SER:HG	0.55	1.99	7	3
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:1043:ALA:HA	1:B:1320:PRO:HB2	0.54	1.79	10	2
1:B:1118:VAL:HG12	1:B:1124:ALA:HB1	0.54	1.77	8	3
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
2:C:151:MET:HB2	2:C:170:MET:HE1	0.54	1.78	1	1
1:A:1115:MET:SD	1:A:1334:LEU:HD22	0.54	2.43	8	3
1:A:1090:VAL:HG13	1:A:1113:MET:HB2	0.54	1.78	4	1
1:B:1349:ASP:HB3	1:B:1355:ILE:HG21	0.54	1.79	7	1
1:A:1136:ILE:HG23	1:A:1319:LEU:HD23	0.54	1.80	9	1
1:A:1136:ILE:HD11	1:A:1326:LEU:HB2	0.54	1.80	7	1
1:B:1085:PRO:HB3	1:B:1109:ASN:HB2	0.53	1.80	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:96:MET:SD	2:C:134:PRO:HB2	0.53	2.43	6	1
1:A:1070:LEU:HD21	1:A:1335:LEU:HD11	0.53	1.81	4	1
1:B:1300:ILE:HG12	1:B:1310:ILE:HG12	0.53	1.79	7	1
1:A:1169:MET:HA	1:A:1192:ARG:O	0.53	2.03	4	1
1:B:1022:THR:HG21	1:B:1328:GLY:HA3	0.53	1.80	1	1
1:B:1085:PRO:HA	1:B:1108:ARG:O	0.53	2.04	7	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:A:1132:SER:HB3	1:A:1326:LEU:HB3	0.53	1.80	2	1
1:B:1181:ILE:HG22	1:B:1207:MET:HG2	0.53	1.79	4	1
1:B:1355:ILE:HA	1:B:1358:VAL:HG12	0.53	1.81	9	4
1:B:1339:CYS:SG	1:B:1344:GLY:N	0.53	2.82	10	1
1:A:1252:ILE:HB	1:A:1281:ILE:HG12	0.53	1.80	1	1
2:C:35:ILE:O	2:C:37:PRO:HD3	0.53	2.03	6	1
1:A:1109:ASN:HA	1:A:1364:GLY:HA2	0.53	1.79	1	1
1:B:1095:PRO:HB3	1:B:1102:MET:HE2	0.53	1.78	2	3
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
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
1:B:1029:LEU:HD21	1:B:1336:LYS:HG2	0.52	1.80	6	2
1:B:1141:ALA:HB2	1:B:1284:LEU:HD21	0.52	1.82	7	2
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:1192:ARG:HG2	1:B:1210:GLU:HB2	0.52	1.80	3	2
1:A:1255:THR:HG22	1:A:1284:LEU:HD13	0.52	1.81	8	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:1031:PHE:HZ	1:A:1339:CYS:HG	0.52	1.45	7	1
1:A:1267:ILE:HA	1:A:1271:MET:SD	0.51	2.45	10	1
1:A:1178:LEU:HD13	1:A:1203:GLN:HG2	0.51	1.81	1	1
2:C:148:LYS:HE3	2:C:151:MET:SD	0.51	2.46	4	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
1:A:1110:VAL:HG23	1:A:1112:VAL:HG23	0.51	1.82	6	1
1:A:1024:GLU:O	1:A:1028:LYS:HG2	0.51	2.06	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:1026:LEU:HD21	1:A:1332:VAL:HG22	0.50	1.83	4	1
1:B:1015:ARG:HG3	1:B:1317:GLY:HA2	0.50	1.82	2	4
1:A:1320:PRO:HD2	1:B:1150:GLY:HA2	0.50	1.84	5	3
1:B:1007:ARG:HB2	1:B:1039:ALA:HA	0.50	1.84	10	1
1:B:1118:VAL:HG21	1:B:1128:ASP:HA	0.50	1.83	2	1
2:C:165:LYS:HB2	2:C:168:THR:HB	0.50	1.80	10	2
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:1181:ILE:HA	1:A:1191:VAL:HG11	0.50	1.84	1	1
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:1292:CYS:HB3	1:A:1295:THR:OG1	0.50	2.06	10	3
1:B:1292:CYS:HB3	1:B:1295:THR:OG1	0.50	2.07	8	4
3:B:1:NAD:H3D	3:B:1:NAD:O1N	0.50	2.07	3	1
1:B:1338:LEU:HD13	1:B:1346:ILE:HG23	0.50	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:1019:THR:HG21	1:A:1325:GLN:HA	0.49	1.84	10	1
1:A:1140:ARG:HD3	1:A:1319:LEU:HD13	0.49	1.82	3	1
1:A:1194:PHE:HB2	1:A:1212:LEU:HD12	0.49	1.84	6	1
1:B:1249:VAL:HG23	1:B:1275:MET:HE3	0.49	1.84	4	2
1:B:1275:MET:SD	1:B:1281:ILE:HD11	0.49	2.48	6	1
1:B:1239:MET:HE1	1:B:1266:LEU:HA	0.49	1.83	9	1
1:B:998:HIS:HB2	1:B:1000:HIS:HB2	0.49	1.82	10	1
1:B:1025:GLN:HE22	1:B:1329:THR:HG23	0.49	1.68	3	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:1250:ASP:O	1:B:1279:SER:HB3	0.49	2.08	6	2
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
2:C:35:ILE:HG22	2:C:37:PRO:HD3	0.49	1.84	2	1
1:A:1252:ILE:HD12	1:A:1281:ILE:HG12	0.49	1.84	10	2

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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
1:B:1115:MET:HE2	1:B:1331:LEU:HD23	0.49	1.83	8	3
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:A:1277:ALA:HB1	1:B:1045:PHE:HA	0.49	1.83	7	2
1:B:1155:GLY:HA3	1:B:1165:PRO:HG3	0.49	1.84	8	1
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
1:A:1070:LEU:HB3	1:A:1331:LEU:HD13	0.48	1.84	7	2
1:A:1096:ALA:HB3	1:A:1097:GLN:NE2	0.48	2.23	6	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
1:A:1080:ILE:HD11	1:A:1101:LEU:HG	0.48	1.84	5	1
2:C:115:ASN:ND2	2:C:116:ASP:H	0.48	2.06	10	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:1298:GLY:HA2	1:B:1312:TYR:HA	0.48	1.84	4	1
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:A:1152:PHE:CD1	1:B:1322:GLN:HG2	0.48	2.43	9	4
1:B:1094:TRP:HB2	1:B:1098:ASN:ND2	0.48	2.24	1	2
2:C:109:VAL:HG11	2:C:138:VAL:HG23	0.48	1.86	6	1
2:C:79:MET:HA	2:C:82:LEU:HD12	0.48	1.85	10	1
2:C:148:LYS:HE3	4:C:1001:NAP:O2B	0.48	2.09	10	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:B:1002:ARG:HG3	1:B:1032:THR:HB	0.48	1.85	6	1
2:C:37:PRO:HG2	2:C:68:ILE:HG13	0.48	1.83	1	1
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:145:ILE:HG13	2:C:171:LEU:HB2	0.48	1.86	7	2
1:A:1016:VAL:HG21	1:A:1039:ALA:HB1	0.48	1.84	10	1
1:B:1251:ILE:HA	1:B:1280:VAL:O	0.47	2.09	1	1
1:A:1022:THR:HB	1:A:1332:VAL:HG21	0.47	1.85	2	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:1214:LEU:HG	1:A:1216:PHE:HB2	0.47	1.84	1	1
1:A:1167:LYS:HB2	1:A:1249:VAL:HA	0.47	1.85	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:1003:ILE:HG12	1:B:1068:ILE:HB	0.47	1.85	5	2
1:A:1025:GLN:OE1	1:A:1336:LYS:HE2	0.47	2.10	10	1
2:C:118:VAL:HG12	2:C:136:LEU:HB2	0.47	1.86	1	1
1:B:1105:LEU:HD13	1:B:1112:VAL:HG21	0.47	1.85	7	4
1:B:1264:PRO:O	1:B:1291:ASN:HA	0.47	2.09	5	1
1:A:1250:ASP:O	1:A:1279:SER:HB3	0.47	2.08	8	2
1:A:1312:TYR:HB2	1:A:1315:LEU:HG	0.47	1.84	6	1
1:A:1029:LEU:HA	1:A:1342:LYS:HE3	0.47	1.84	10	1
2:C:34:ILE:HG12	2:C:106:THR:HG21	0.47	1.87	1	1
1:B:1284:LEU:HD23	1:B:1315:LEU:HD13	0.47	1.85	2	1
2:C:144:VAL:HB	2:C:168:THR:HA	0.47	1.86	2	2
1:A:1061:ASN:HA	1:A:1064:TRP:CD1	0.47	2.40	8	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:1113:MET:HE1	1:B:1338:LEU:HD21	0.47	1.86	1	1
2:C:160:ASN:HD22	2:C:162:LEU:HD12	0.47	1.70	1	1
2:C:30:SER:CA	2:C:107:ASP:HB3	0.47	2.40	4	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
1:B:1064:TRP:CZ3	1:B:1083:LEU:HG	0.47	2.45	2	1
1:A:1172:GLY:O	1:A:1255:THR:HB	0.47	2.09	4	1
1:A:1019:THR:HG21	1:A:1321:THR:HG23	0.47	1.87	5	1
1:A:1029:LEU:HA	1:A:1342:LYS:HE2	0.47	1.86	5	1
1:B:1111:THR:HG23	1:B:1362:ARG:HA	0.47	1.86	7	2
1:A:1148:GLU:HB3	1:A:1308:LYS:HG3	0.47	1.86	2	1
2:C:179:VAL:HA	2:C:182:ILE:HG12	0.47	1.86	2	2
2:C:48:TYR:HB2	2:C:49:PRO:HD3	0.47	1.87	3	2
1:B:1357:GLY:CA	1:B:1370:ALA:HB2	0.47	2.39	1	1
1:B:1272:VAL:HG11	1:B:1303:THR:HG21	0.47	1.86	4	1
1:A:1152:PHE:HE1	1:B:1136:ILE:HD13	0.47	1.68	10	1
1:A:1071:LYS:HE3	1:A:1073:ASN:O	0.47	2.10	1	1
2:C:109:VAL:HB	2:C:144:VAL:HA	0.47	1.86	4	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
1:A:1069:ILE:HG12	1:A:1087:THR:HG21	0.46	1.87	1	1
1:B:1169:MET:O	1:B:1252:ILE:HA	0.46	2.09	2	1
1:A:1080:ILE:HA	1:A:1083:LEU:HD23	0.46	1.86	4	2
1:B:1199:GLU:O	1:B:1203:GLN:HG2	0.46	2.09	3	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

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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:B:1169:MET:HA	1:B:1192:ARG:O	0.46	2.10	2	2
1:B:1350:PHE:HE1	1:B:1359:THR:HB	0.46	1.70	3	1
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:A:1120:ARG:HD3	1:A:1130:LEU:HD13	0.46	1.88	8	1
1:B:1146:ALA:HB2	1:B:1153:PHE:HE1	0.46	1.70	3	2
1:B:1252:ILE:HB	1:B:1281:ILE:HG12	0.46	1.87	1	1
1:B:1016:VAL:HG12	1:B:1043:ALA:HB2	0.46	1.87	5	1
1:B:1267:ILE:HG22	1:B:1272:VAL:HG22	0.46	1.87	8	1
1:A:1150:GLY:HA2	1:B:1320:PRO:HG2	0.46	1.87	5	3
1:A:1301:PHE:HB3	1:A:1309:VAL:HB	0.46	1.87	2	1
1:B:1051:VAL:HG23	1:B:1057:ILE:HG12	0.46	1.88	5	1
2:C:44:ALA:HB2	4:C:1001:NAP:N6A	0.46	2.25	10	1
1:A:1070:LEU:HD22	1:A:1331:LEU:HD22	0.46	1.87	8	3
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:1132:SER:HB2	1:A:1330:ASN:OD1	0.46	2.11	4	1
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
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
2:C:109:VAL:HG21	2:C:138:VAL:HG23	0.46	1.86	7	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:1122:SER:HB3	2:C:133:MET:HE2	0.45	1.87	1	1
1:B:1133:MET:HB3	1:B:1316:PRO:HB3	0.45	1.88	5	4
1:A:1161:GLY:HA3	1:B:1329:THR:HG21	0.45	1.88	4	2
1:B:1010:LEU:HB3	1:B:1013:GLU:HB2	0.45	1.89	6	2
1:B:1035:VAL:HB	1:B:1057:ILE:HD13	0.45	1.88	7	1
1:A:1329:THR:HB	1:B:1160:ALA:HB1	0.45	1.86	9	1
1:B:1007:ARG:NH1	1:B:1038:GLY:HA3	0.45	2.26	9	1
1:B:1113:MET:HE3	1:B:1359:THR:OG1	0.45	2.12	4	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:B:1112:VAL:HB	1:B:1361:ILE:HB	0.45	1.86	2	1
1:B:1070:LEU:HD22	1:B:1331:LEU:HB3	0.45	1.88	4	1
2:C:113:GLY:HA2	2:C:147:PHE:O	0.45	2.11	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1204:VAL:HG13	1:A:1209:ALA:HB3	0.45	1.87	6	2
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: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:1083:LEU:HD12	1:A:1110:VAL:HG11	0.45	1.88	9	1
1:A:1335:LEU:HA	1:A:1338:LEU:HB2	0.45	1.86	1	1
1:A:1025:GLN:HB3	1:A:1332:VAL:HG11	0.45	1.87	6	2
1:B:1132:SER:HB3	1:B:1326:LEU:HB3	0.45	1.89	6	2
1:A:1337:LEU:HD13	1:A:1355:ILE:HD11	0.45	1.88	8	1
1:A:1058:VAL:HB	1:A:1062:SER:HB2	0.45	1.88	5	1
1:A:1112:VAL:HB	1:A:1361:ILE:HB	0.45	1.88	6	2
1:A:1158:THR:O	2:C:70:PRO:HB3	0.45	2.12	3	1
1:A:1034:ALA:HA	1:A:1056:GLU:HB3	0.45	1.88	4	1
2:C:146:VAL:HB	2:C:170:MET:HA	0.45	1.86	8	2
1:B:1167:LYS:HA	1:B:1190:ILE:O	0.45	2.12	7	1
1:B:1132:SER:O	1:B:1136:ILE:HG12	0.45	2.11	8	1
1:B:1199:GLU:HB2	2:C:155:TYR:CE1	0.45	2.41	9	1
1:A:1173:ALA:HA	1:A:1177:GLY:HA3	0.45	1.86	10	1
2:C:174:ASP:HA	4:C:1001:NAP:N1A	0.45	2.27	1	1
1:A:1275:MET:SD	1:A:1281:ILE:HD11	0.45	2.52	4	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: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:B:1089:LEU:O	1:B:1112:VAL:HA	0.45	2.12	5	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:A:1071:LYS:HB2	1:A:1091:SER:OG	0.45	2.12	3	1
1:A:1135:ASN:ND2	1:A:1179:ALA:HB2	0.45	2.27	4	1
1:A:1010:LEU:HD12	1:A:1076:LEU:HD11	0.45	1.89	5	1
1:B:1328:GLY:O	1:B:1332:VAL:HG23	0.45	2.12	10	2
1:A:1047:ASP:HA	1:A:1050:PHE:HD2	0.45	1.71	4	1
1:B:1016:VAL:CG2	1:B:1039:ALA:HB1	0.45	2.42	5	1
1:B:1050:PHE:HB2	1:B:1057:ILE:HD11	0.45	1.86	5	2
1:B:1279:SER:O	1:B:1307:VAL:HA	0.45	2.12	5	1
1:A:1015:ARG:HG3	1:A:1317:GLY:HA2	0.45	1.88	6	2
1:A:1113:MET:SD	1:A:1348:VAL:HG13	0.45	2.51	8	1
1:B:1207:MET:SD	2:C:75:LEU:HD22	0.44	2.52	1	1

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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:A:1312:TYR:CB	1:A:1315:LEU:HG	0.44	2.42	6	2
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:B:1339:CYS:SG	1:B:1342:LYS:HA	0.44	2.52	4	2
1:B:1178:LEU:HD22	2:C:75:LEU:HG	0.44	1.89	5	1
1:B:1338:LEU:O	1:B:1347:THR:HB	0.44	2.11	8	1
1:A:1328:GLY:O	1:A:1332:VAL:HG23	0.44	2.13	1	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:B:1125:GLN:HG3	1:B:1131:SER:HB3	0.44	1.88	10	1
1:B:1080:ILE:HD11	1:B:1101:LEU:HD12	0.44	1.89	1	1
1:A:1275:MET:HB2	1:A:1307:VAL:HG21	0.44	1.88	2	1
1:A:1140:ARG:NH1	1:A:1318:ARG:O	0.44	2.50	6	2
2:C:128:SER:OG	2:C:158:VAL:HG21	0.44	2.11	5	1
2:C:33:VAL:O	2:C:64:VAL:HA	0.44	2.12	7	3
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: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: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: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
1:B:1021:LYS:O	1:B:1025:GLN:HG3	0.44	2.12	3	1
1:B:1079:GLU:HA	1:B:1082:LEU:HD12	0.44	1.88	9	2
2:C:122:ALA:HA	2:C:128:SER:CB	0.44	2.43	5	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:A:1312:TYR:O	1:A:1315:LEU:HG	0.43	2.13	3	1
1:B:1002:ARG:NH2	1:B:1065:GLN:O	0.43	2.50	10	2
1:B:1156:GLN:H	1:B:1163:VAL:HB	0.43	1.74	8	1
1:A:1016:VAL:HG23	1:A:1039:ALA:HB1	0.43	1.90	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: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:1169:MET:O	1:A:1252:ILE:HA	0.43	2.14	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:1332:VAL:O	1:B:1336:LYS:HG3	0.43	2.12	2	1
1:B:1120:ARG:HH12	1:B:1128:ASP:CG	0.43	2.21	10	2
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:A:1131:SER:HA	1:A:1175:VAL:HG21	0.43	1.89	9	1
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
1:B:1102:MET:HA	1:B:1105:LEU:HD12	0.43	1.90	10	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:1323:SER:O	1:A:1327:TYR:HB3	0.43	2.14	5	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
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:1356:ARG:HG3	1:B:1371:PRO:HD3	0.43	1.90	7	1
1:B:1121:ILE:HD12	1:B:1123:ARG:HB3	0.43	1.91	9	1
1:A:1045:PHE:HA	1:B:1277:ALA:HB1	0.43	1.91	10	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
2:C:31:HIS:O	2:C:62:ILE:HG23	0.43	2.13	4	1
1:A:1146:ALA:HA	1:A:1149:PHE:HB2	0.43	1.91	4	2
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:1111:THR:HG23	1:A:1362:ARG:HG3	0.43	1.91	10	1
2:C:42:ALA:HB2	2:C:79:MET:HB3	0.43	1.89	2	1
1:B:1305:ASN:OD1	1:B:1307:VAL:HG23	0.43	2.14	7	1
2:C:39:TYR:CD1	2:C:74:ARG:HD3	0.43	2.49	9	1
1:B:1092:PHE:CD1	1:B:1116:ASP:HB3	0.42	2.48	1	1
1:B:1069:ILE:HG22	1:B:1071:LYS:HB2	0.42	1.89	2	1
1:A:1330:ASN:ND2	1:B:1160:ALA:HB2	0.42	2.29	4	1
1:A:1342:LYS:HA	1:A:1344:GLY:H	0.42	1.73	5	1
1:A:1070:LEU:HD23	1:A:1090:VAL:HB	0.42	1.91	8	1
1:B:1136:ILE:HG21	1:B:1316:PRO:HA	0.42	1.89	6	1
2:C:148:LYS:NZ	4:C:1001:NAP:O3B	0.42	2.52	8	1
2:C:116:ASP:HB3	2:C:130:ILE:HD13	0.42	1.91	9	1
2:C:118:VAL:HG23	2:C:162:LEU:HD13	0.42	1.90	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1339:CYS:HB3	1:A:1342:LYS:HG2	0.42	1.91	4	1
1:A:1162:LYS:HZ2	2:C:95:GLU:CD	0.42	2.22	8	1
1:A:1060:GLY:O	1:A:1063:VAL:HG12	0.42	2.14	9	1
2:C:24:ALA:HB2	2:C:182:ILE:HG22	0.42	1.90	10	1
1:A:1287:GLN:HA	1:A:1313:THR:HG23	0.42	1.92	1	1
1:B:1023:VAL:HG22	1:B:1033:VAL:HG11	0.42	1.91	3	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: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:B:1119:PRO:HG2	1:B:1357:GLY:HA3	0.42	1.90	4	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: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:1040:GLY:HA2	1:A:1043:ALA:HB3	0.42	1.91	5	1
1:A:1083:LEU:HD11	1:A:1089:LEU:HD13	0.42	1.92	10	1
1:A:1243:ALA:HB2	1:A:1271:MET:HE2	0.42	1.91	2	1
2:C:41:MET:HE3	2:C:112:ILE:HG13	0.42	1.91	7	2
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: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:1149:PHE:CE1	1:A:1151:ARG:HD2	0.42	2.50	4	1
1:B:1100:GLU:CD	1:B:1100:GLU:H	0.42	2.23	8	1
1:B:1120:ARG:HB3	3:B:1:NAD:H1D	0.42	1.92	10	1
2:C:44:ALA:HB2	4:C:1001:NAP:H62A	0.42	1.74	10	1
2:C:111:VAL:HG13	2:C:114:ALA:HB3	0.42	1.91	10	1
2:C:72:ALA:HA	4:C:1001:NAP:H52N	0.42	1.91	2	1
2:C:38:GLY:HA3	2:C:114:ALA:HB2	0.42	1.91	7	1
1:A:1041:GLN:HE22	1:A:1047:ASP:HB2	0.42	1.75	9	1
1:B:1119:PRO:HB2	1:B:1121:ILE:HG12	0.42	1.91	2	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: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:B:1068:ILE:HD11	1:B:1346:ILE:HD11	0.42	1.91	10	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1193:ALA:O	1:A:1211:PHE:HA	0.41	2.15	6	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: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:B:1164:PRO:HA	1:B:1165:PRO:HD3	0.41	1.74	4	2
1:B:1263:ALA:CB	1:B:1285:ALA:HB1	0.41	2.45	4	1
1:A:1135:ASN:HA	1:A:1176:ALA:HA	0.41	1.92	5	1
2:C:129:PRO:HD2	2:C:156:ALA:HB2	0.41	1.92	1	1
1:A:1068:ILE:HG12	1:A:1088:THR:HB	0.41	1.92	2	1
1:B:1119:PRO:CG	1:B:1357:GLY:HA3	0.41	2.45	4	1
2:C:65:ARG:NH2	2:C:94:LEU:HD22	0.41	2.30	7	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
1:A:1069:ILE:HG12	1:A:1087:THR:CG2	0.41	2.45	1	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:1254:THR:HG22	1:A:1291:ASN:HB2	0.41	1.92	10	1
2:C:26:LEU:HA	2:C:29:ASN:HB3	0.41	1.90	5	1
1:A:1216:PHE:HE1	1:A:1233:ALA:HB1	0.41	1.74	8	1
1:A:1239:MET:SD	1:A:1242:PHE:HD2	0.41	2.39	1	1
1:B:1109:ASN:HA	1:B:1364:GLY:CA	0.41	2.46	2	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:B:1127:LEU:HD22	1:B:1354:VAL:HG11	0.41	1.92	7	1
1:A:1215:ASP:H	1:A:1241:LEU:HD21	0.41	1.75	8	1
1:A:1333:ASN:HA	1:A:1336:LYS:HD2	0.41	1.92	9	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: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:1346:ILE:HG22	1:B:1348:VAL:HG23	0.41	1.91	10	1
1:A:1043:ALA:HA	1:A:1320:PRO:HB2	0.41	1.92	1	1
1:A:1020:PRO:HD2	1:A:1045:PHE:CD2	0.41	2.50	4	1
1:A:1164:PRO:HA	1:A:1165:PRO:HD2	0.41	1.79	7	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:B:1148:GLU:HG3	1:B:1300:ILE:HD13	0.41	1.92	1	1
1:B:1295:THR:O	1:B:1297:PRO:HD3	0.41	2.16	1	1
2:C:47:GLN:O	2:C:50:VAL:HG12	0.41	2.15	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1003:ILE:HD13	1:A:1335:LEU:HD13	0.41	1.93	4	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:B:1149:PHE:CZ	1:B:1250:ASP:HB3	0.41	2.51	8	1
2:C:26:LEU:HB3	2:C:108:THR:OG1	0.41	2.15	8	1
1:A:1125:GLN:HA	1:A:1128:ASP:HB3	0.41	1.92	10	1
1:A:1009:ARG:HH11	1:A:1079:GLU:HG2	0.41	1.75	2	1
1:B:1092:PHE:HZ	1:B:1133:MET:HG3	0.41	1.75	6	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: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:B:1177:GLY:O	1:B:1181:ILE:HG13	0.40	2.17	1	1
1:B:1350:PHE:HB2	1:B:1362:ARG:NH1	0.40	2.31	3	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:70:PRO:HG3	2:C:96:MET:SD	0.40	2.56	4	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: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
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: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
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
2:C:180:ASP:O	2:C:183:LEU:HG	0.40	2.16	10	1
1:A:1140:ARG:CZ	1:A:1318:ARG:HB3	0.40	2.46	3	1
2:C:45:GLN:HG3	2:C:176:LYS:HG3	0.40	1.92	7	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
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
1:B:1192:ARG:HH12	1:B:1248:GLU:CD	0.40	2.25	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:116:ASP:HA	2:C:119:ASN:CB	0.40	2.46	4	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

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%)	14	63
1	B	361/401 (90%)	322±3 (89±1%)	34±3 (9±1%)	6±2 (2±1%)	10	55
2	C	165/186 (89%)	132±3 (80±2%)	25±3 (15±2%)	8±1 (5±1%)	3	24
All	All	8890/9880 (90%)	7769 (87%)	941 (11%)	180 (2%)	8	49

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	31	HIS	5
2	C	137	GLU	5
1	B	1318	ARG	4
2	C	78	HIS	4
1	B	1372	PRO	4
1	B	1259	PRO	4
2	C	115	ASN	4
1	B	1231	SER	4
1	B	1175	VAL	3
1	B	1256	ALA	3
2	C	114	ALA	3

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Mol	Chain	Res	Type	Models (Total)
1	B	1233	ALA	3
2	C	158	VAL	3
1	A	1001	GLY	3
1	A	1363	ALA	3
2	C	45	GLN	3
1	A	1372	PRO	3
1	A	1154	THR	2
1	A	1208	GLY	2
1	B	1122	SER	2
1	B	1232	ASP	2
2	C	71	VAL	2
2	C	99	ILE	2
2	C	140	LYS	2
1	B	1346	ILE	2
2	C	138	VAL	2
1	B	1235	ILE	2
2	C	37	PRO	2
2	C	70	PRO	2
2	C	127	LYS	2
2	C	96	MET	2
2	C	63	ASN	2
1	A	1256	ALA	2
1	B	1363	ALA	2
2	C	132	GLY	2
1	A	1037	SER	1
1	A	1092	PHE	1
1	B	1054	GLY	1
1	B	1295	THR	1
2	C	130	ILE	1
2	C	141	ALA	1
2	C	156	ALA	1
1	B	1160	ALA	1
1	B	1286	ALA	1
1	B	1369	PRO	1
1	A	1010	LEU	1
1	A	1015	ARG	1
2	C	68	ILE	1
2	C	100	ASN	1
2	C	154	GLY	1
1	B	1099	PRO	1
1	B	1159	ALA	1
2	C	105	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	1020	PRO	1
1	B	1043	ALA	1
2	C	185	ALA	1
1	A	1060	GLY	1
1	A	1074	ALA	1
1	A	1085	PRO	1
1	B	1011	THR	1
1	B	1198	PRO	1
1	B	1314	ASP	1
2	C	76	PRO	1
2	C	107	ASP	1
2	C	117	THR	1
1	A	1297	PRO	1
1	B	1012	ASN	1
1	B	1030	GLY	1
1	B	1085	PRO	1
1	B	1290	GLY	1
1	B	1297	PRO	1
2	C	157	GLY	1
2	C	160	ASN	1
1	A	1054	GLY	1
1	A	1072	VAL	1
1	A	1120	ARG	1
1	A	1359	THR	1
2	C	69	HIS	1
2	C	87	LYS	1
2	C	121	ALA	1
2	C	162	LEU	1
2	C	183	LEU	1
1	B	1289	GLY	1
2	C	86	ALA	1
2	C	89	PRO	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	288/317 (91%)	271±2 (94±1%)	17±2 (6±1%)	19 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	290/317 (91%)	274±2 (95±1%)	16±2 (5±1%)	21 71
2	C	135/153 (88%)	123±2 (91±2%)	12±2 (9±2%)	11 57
All	All	7130/7870 (91%)	6680 (94%)	450 (6%)	18 67

All 205 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
1	A	1020	PRO	9
1	A	1083	LEU	9
1	B	1287	GLN	9
2	C	159	GLN	9
1	A	1282	VAL	7
1	B	1014	THR	7
1	A	1254	THR	6
1	B	1020	PRO	6
2	C	52	GLU	6
2	C	127	LYS	6
1	B	1199	GLU	6
1	A	1067	GLU	5
1	B	1019	THR	5
1	B	1063	VAL	5
2	C	45	GLN	5
1	A	1196	THR	5
1	B	1350	PHE	5
2	C	21	GLU	5
1	A	1022	THR	4
1	A	1032	THR	4
1	B	1068	ILE	4
1	B	1135	ASN	4
1	B	1268	THR	4
2	C	140	LYS	4
1	A	1072	VAL	4
1	A	1343	ASP	4
1	B	1077	ASP	4
1	B	1196	THR	4
1	A	1045	PHE	4
1	A	1100	GLU	4
1	B	1367	THR	4
1	A	1255	THR	4

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Mol	Chain	Res	Type	Models (Total)
1	B	1045	PHE	4
1	A	1014	THR	4
1	A	1046	ASP	3
1	B	1022	THR	3
2	C	50	VAL	3
2	C	115	ASN	3
2	C	151	MET	3
1	A	1158	THR	3
1	A	1268	THR	3
1	B	1103	GLN	3
1	B	1373	ILE	3
2	C	90	TYR	3
1	A	1122	SER	3
1	A	1130	LEU	3
2	C	22	GLU	3
2	C	152	ASN	3
1	A	1313	THR	3
1	B	1048	LYS	3
1	B	1118	VAL	3
2	C	166	GLU	3
1	A	1019	THR	3
1	A	1071	LYS	3
1	A	1108	ARG	2
1	A	1119	PRO	2
1	A	1354	VAL	2
1	B	1008	GLU	2
1	B	1084	ASN	2
1	B	1288	ASN	2
1	B	1294	TYR	2
1	B	1313	THR	2
1	B	1352	ASP	2
2	C	79	MET	2
2	C	142	GLN	2
1	A	1312	TYR	2
1	A	1321	THR	2
1	A	1369	PRO	2
1	A	1371	PRO	2
2	C	75	LEU	2
2	C	112	ILE	2
2	C	126	PRO	2
2	C	161	PRO	2
1	A	1047	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	1063	VAL	2
1	A	1077	ASP	2
1	A	1084	ASN	2
1	A	1294	TYR	2
1	A	1316	PRO	2
1	B	1088	THR	2
1	B	1213	GLU	2
1	B	1214	LEU	2
2	C	60	ARG	2
2	C	117	THR	2
2	C	176	LYS	2
1	A	1021	LYS	2
1	A	1048	LYS	2
1	A	1342	LYS	2
1	B	1041	GLN	2
2	C	92	ILE	2
1	B	1230	MET	2
1	B	1258	ILE	2
1	B	1273	ASP	2
1	B	1321	THR	2
2	C	103	PHE	2
2	C	150	SER	2
1	A	1157	ILE	2
1	B	1085	PRO	2
1	B	1113	MET	2
2	C	102	ASP	2
2	C	123	GLN	2
1	B	1342	LYS	2
2	C	26	LEU	2
1	A	1241	LEU	2
1	A	1248	GLU	2
1	A	1068	ILE	1
1	A	1110	VAL	1
1	A	1191	VAL	1
1	A	1203	GLN	1
1	A	1367	THR	1
1	B	1062	SER	1
1	B	1312	TYR	1
2	C	23	THR	1
2	C	83	LEU	1
2	C	101	ASP	1
1	A	1085	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	1116	ASP	1
1	A	1126	SER	1
1	A	1253	VAL	1
1	A	1270	GLU	1
1	A	1329	THR	1
1	B	1064	TRP	1
1	B	1099	PRO	1
1	B	1120	ARG	1
1	B	1231	SER	1
1	B	1365	GLU	1
1	B	1372	PRO	1
2	C	37	PRO	1
2	C	162	LEU	1
1	A	1123	ARG	1
1	A	1202	GLU	1
1	A	1303	THR	1
1	B	1032	THR	1
1	B	1059	GLU	1
1	B	1111	THR	1
1	B	1125	GLN	1
1	B	1232	ASP	1
2	C	68	ILE	1
2	C	78	HIS	1
2	C	85	GLU	1
2	C	155	TYR	1
1	A	1027	LEU	1
1	A	1036	GLU	1
1	A	1065	GLN	1
1	A	1101	LEU	1
1	A	1310	ILE	1
1	A	1338	LEU	1
1	B	1051	VAL	1
1	B	1234	PHE	1
1	B	1248	GLU	1
1	B	1282	VAL	1
2	C	25	GLU	1
2	C	49	PRO	1
2	C	64	VAL	1
2	C	80	ASN	1
2	C	145	ILE	1
1	B	1058	VAL	1
1	B	1061	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	B	1297	PRO	1
1	A	1058	VAL	1
1	B	1036	GLU	1
1	B	1100	GLU	1
1	B	1158	THR	1
1	B	1175	VAL	1
1	B	1200	VAL	1
1	B	1308	LYS	1
2	C	108	THR	1
2	C	120	PRO	1
2	C	135	VAL	1
2	C	165	LYS	1
1	A	1093	ILE	1
1	A	1232	ASP	1
1	B	1122	SER	1
2	C	147	PHE	1
2	C	184	LYS	1
1	A	1127	LEU	1
1	A	1154	THR	1
1	A	1156	GLN	1
1	A	1273	ASP	1
1	A	1346	ILE	1
1	B	998	HIS	1
1	B	1000	HIS	1
1	B	1067	GLU	1
1	B	1109	ASN	1
1	B	1119	PRO	1
1	B	1235	ILE	1
1	A	1015	ARG	1
1	A	1175	VAL	1
1	A	1199	GLU	1
1	A	1275	MET	1
1	A	1334	LEU	1
1	B	1126	SER	1
1	B	1319	LEU	1
2	C	56	LYS	1
2	C	107	ASP	1
1	A	1041	GLN	1
1	A	1259	PRO	1
1	A	1288	ASN	1
1	B	1339	CYS	1
1	B	1340	LYS	1

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Mol	Chain	Res	Type	Models (Total)
2	C	96	MET	1
2	C	119	ASN	1
2	C	139	TRP	1
2	C	169	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	46,48,48	1.46±0.09	6±1 (12±2%)
4	NAP	C	1001	-	50,52,52	1.52±0.08	6±1 (12±2%)

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	Counts	Bond angles	
						RMSZ	#Z>2
3	NAD	B	1	-	64,73,73	2.09±0.15	13±1 (20±1%)
4	NAP	C	1001	-	71,80,80	1.88±0.15	14±2 (19±2%)

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±0,35,67,67	0±0,5,5,5
3	NAD	B	1	-	-	0±0,30,62,62	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	7.29	1.43	1.35	1	10
4	C	1001	NAP	C2N-N1N	7.04	1.42	1.35	1	10
4	C	1001	NAP	PA-O3	4.76	1.64	1.59	1	6
3	B	1	NAD	O4D-C1D	4.63	1.47	1.40	4	8
3	B	1	NAD	C5A-N7A	4.50	1.30	1.39	4	10
4	C	1001	NAP	C5A-N7A	4.24	1.31	1.39	2	10
4	C	1001	NAP	O4D-C1D	3.85	1.45	1.40	9	10
4	C	1001	NAP	PN-O3	3.67	1.63	1.59	3	2
4	C	1001	NAP	C3N-C7N	3.44	1.55	1.50	3	4
3	B	1	NAD	PA-O3	3.24	1.63	1.59	5	3
3	B	1	NAD	C6N-N1N	3.19	1.42	1.35	6	9
4	C	1001	NAP	C6N-N1N	3.10	1.42	1.35	5	9
4	C	1001	NAP	C4A-N9A	2.94	1.31	1.37	8	6
3	B	1	NAD	C8A-N9A	2.84	1.32	1.37	3	4
3	B	1	NAD	C3N-C7N	2.68	1.54	1.50	9	3
3	B	1	NAD	C4A-N9A	2.54	1.32	1.37	10	9
4	C	1001	NAP	P2B-O2X	2.50	1.45	1.54	8	4
4	C	1001	NAP	C8A-N7A	2.49	1.36	1.31	10	2
3	B	1	NAD	C8A-N7A	2.14	1.35	1.31	1	1
3	B	1	NAD	C5N-C4N	2.12	1.42	1.38	8	1
4	C	1001	NAP	P2B-O2B	2.09	1.63	1.59	8	1
3	B	1	NAD	C2N-C3N	2.01	1.42	1.39	5	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(°)	Ideal(°)	Models	
								Worst	Total
4	C	1001	NAP	C4D-O4D-C1D	10.37	100.43	109.92	10	9
3	B	1	NAD	C4D-O4D-C1D	8.60	102.05	109.92	8	9
3	B	1	NAD	C5A-C4A-N3A	7.78	116.01	126.72	2	10
3	B	1	NAD	N3A-C4A-N9A	7.65	140.18	127.17	4	10
4	C	1001	NAP	O4B-C1B-N9A	6.64	120.84	108.09	4	8
4	C	1001	NAP	N3A-C4A-N9A	6.59	138.38	127.17	9	10
4	C	1001	NAP	C5A-C4A-N3A	6.46	117.82	126.72	1	10
3	B	1	NAD	C6A-C5A-C4A	5.99	125.36	117.18	2	10
3	B	1	NAD	O4B-C1B-N9A	5.56	118.77	108.09	7	10
4	C	1001	NAP	C6A-C5A-N7A	5.36	121.75	132.09	1	10
3	B	1	NAD	N3A-C2A-N1A	5.22	120.68	128.58	9	10
3	B	1	NAD	C6A-C5A-N7A	5.01	122.44	132.09	2	10
4	C	1001	NAP	N3A-C2A-N1A	4.94	121.10	128.58	5	10
3	B	1	NAD	C4B-O4B-C1B	4.59	99.34	109.47	3	8
4	C	1001	NAP	C6A-C5A-C4A	4.29	123.03	117.18	4	9
3	B	1	NAD	C2A-N3A-C4A	4.07	121.78	111.83	6	10
4	C	1001	NAP	C6N-N1N-C2N	3.75	118.68	121.88	1	8
3	B	1	NAD	C4A-C5A-N7A	3.57	114.66	110.58	4	4
4	C	1001	NAP	C2A-N3A-C4A	3.49	120.34	111.83	1	10
4	C	1001	NAP	C4B-O4B-C1B	3.45	101.85	109.47	3	9
3	B	1	NAD	C4A-N9A-C8A	3.32	109.22	105.74	1	9
4	C	1001	NAP	O2B-P2B-O1X	3.25	97.75	109.33	4	7
3	B	1	NAD	C5N-C4N-C3N	3.24	123.55	120.36	5	3
3	B	1	NAD	O4B-C1B-C2B	3.22	99.74	106.62	6	3
4	C	1001	NAP	C4A-C5A-N7A	3.10	114.12	110.58	2	7
3	B	1	NAD	C6N-N1N-C2N	2.98	119.35	121.88	4	7
4	C	1001	NAP	C4A-N9A-C8A	2.92	108.81	105.74	6	7
3	B	1	NAD	C5A-C4A-N9A	2.75	102.81	105.81	4	1
4	C	1001	NAP	C2A-N1A-C6A	2.71	123.17	118.73	7	5
4	C	1001	NAP	N6A-C6A-N1A	2.64	124.25	118.38	1	4
3	B	1	NAD	O5D-C5D-C4D	2.63	117.96	108.99	8	1
4	C	1001	NAP	C5N-C4N-C3N	2.60	122.92	120.36	4	1
4	C	1001	NAP	O4B-C4B-C5B	2.57	117.58	109.33	10	1
4	C	1001	NAP	C2D-C3D-C4D	2.55	97.69	102.61	2	1
3	B	1	NAD	N9A-C8A-N7A	2.50	110.39	113.94	1	4
3	B	1	NAD	N6A-C6A-N1A	2.50	123.95	118.38	2	2
3	B	1	NAD	C2A-N1A-C6A	2.47	122.79	118.73	9	4
4	C	1001	NAP	C2N-C3N-C4N	2.47	121.13	118.26	9	1
4	C	1001	NAP	O7N-C7N-C3N	2.36	122.49	119.60	4	2
3	B	1	NAD	O4B-C4B-C5B	2.32	116.78	109.33	7	6

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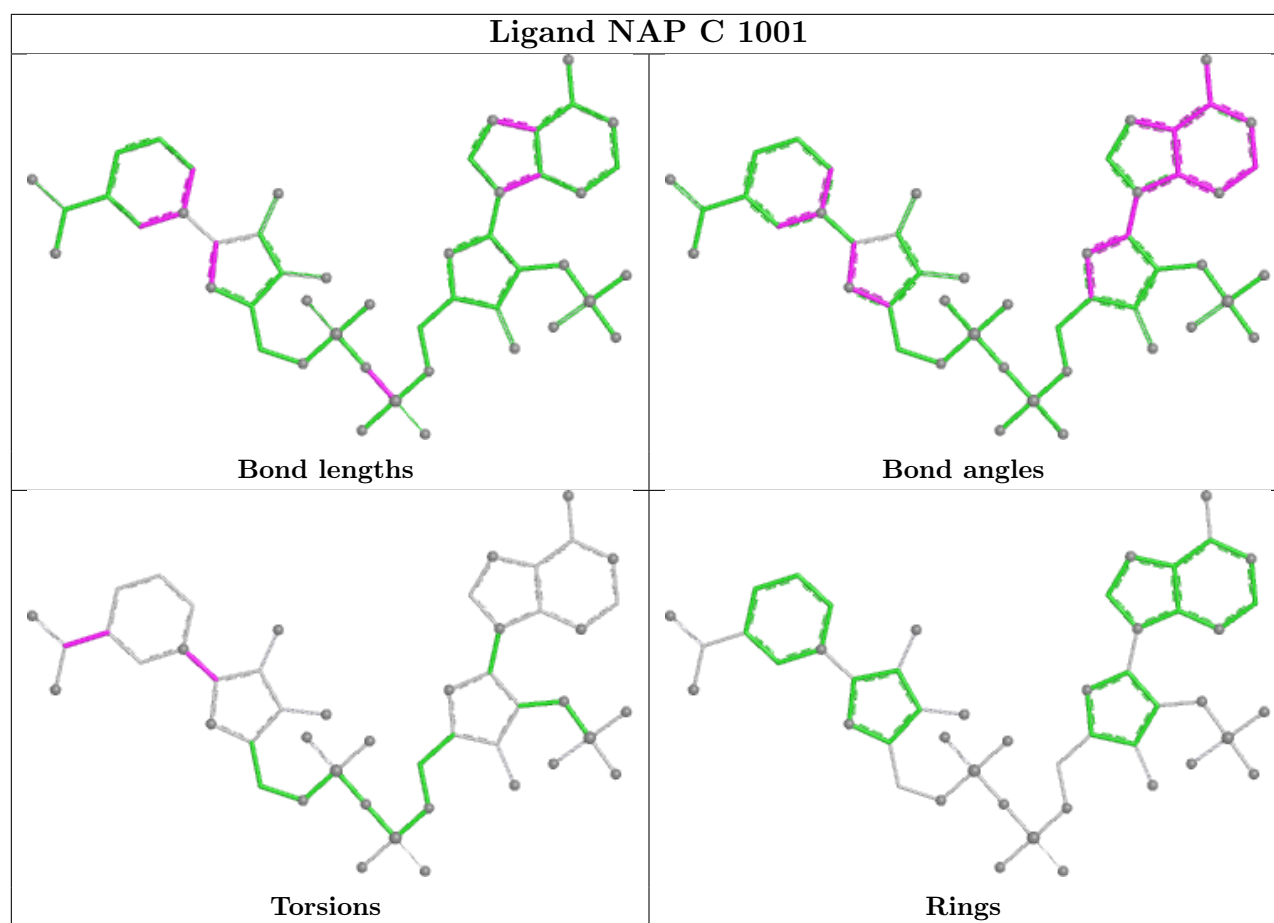
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	C	1001	NAP	N9A-C8A-N7A	2.28	110.69	113.94	6	3
4	C	1001	NAP	C3N-C7N-N7N	2.26	114.95	117.74	4	2
4	C	1001	NAP	C3B-C2B-C1B	2.06	106.75	102.81	9	1
4	C	1001	NAP	O2X-P2B-O1X	2.06	118.85	110.83	4	1

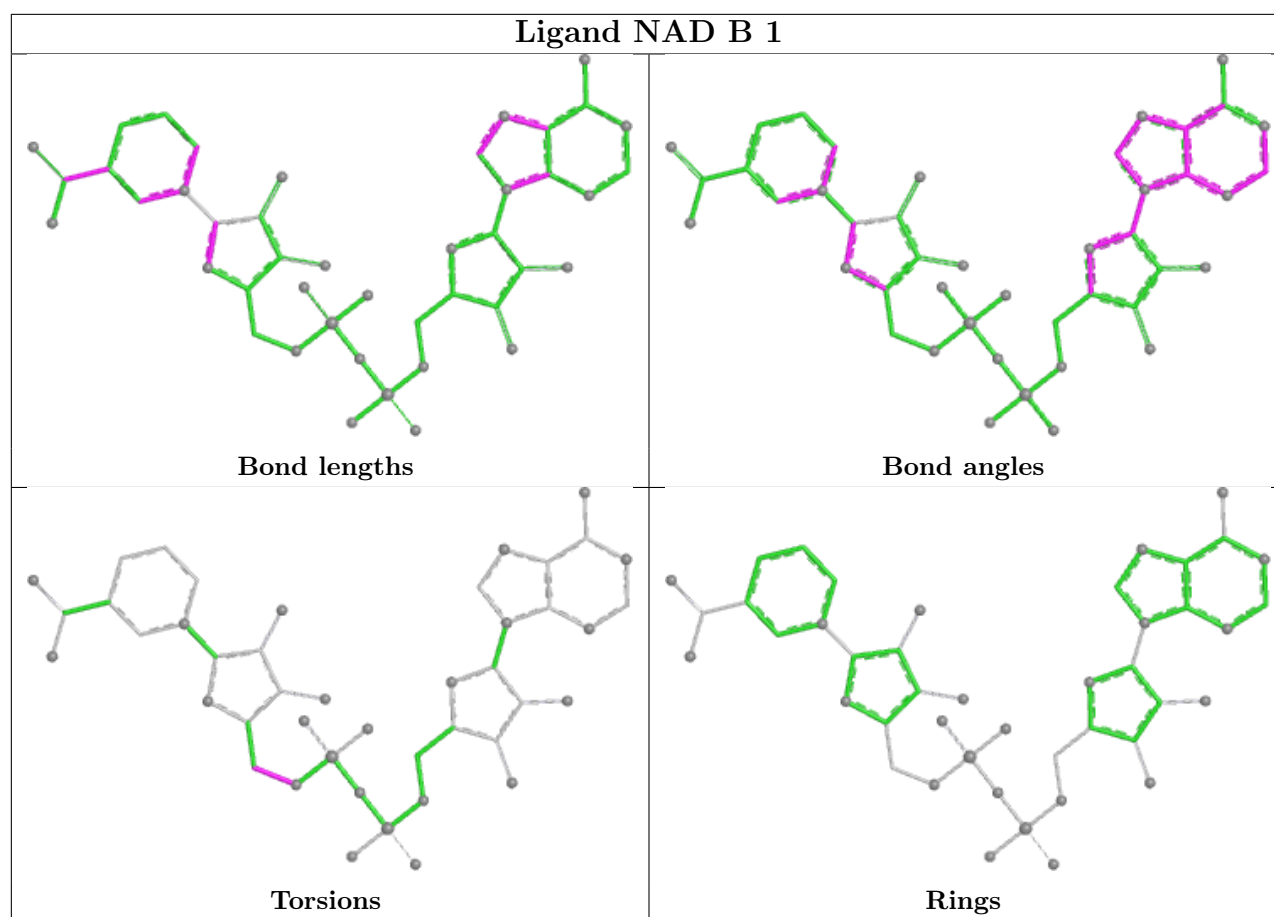
There are no chirality outliers.

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 than 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.





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