



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 05:19 am GMT

PDB ID : 2MZI  
Title : NMR Solution Structure of the PRO Form of Human Matrilysin (proMMP-7)  
in Complex with Anionic Membrane  
Authors : Prior, S.H.; Van Doren, S.R.  
Deposited on : 2015-02-12

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

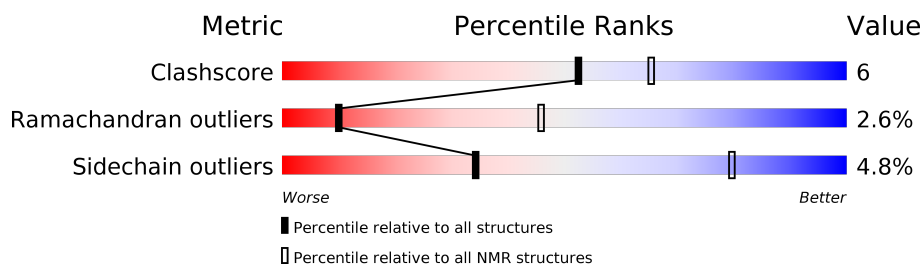
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 21%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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	250	78%15% . . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
5	A	C3S	431	20	-
5	A	C3S	432	20	-
5	A	C3S	433	20	-
5	A	C3S	434	20	-
5	A	C3S	435	20	-
5	A	C3S	436	20	-

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:2-A:75, A:82-A:244 (237)	0.69	5

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

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

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

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

### 3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10109 atoms, of which 2165 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrilysin.

Mol	Chain	Residues	Atoms						Trace
1	A	248	Total	C	H	N	O	S	0
			3847	1240	1895	339	364	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	GLU	ENGINEERED MUTATION	UNP P09237

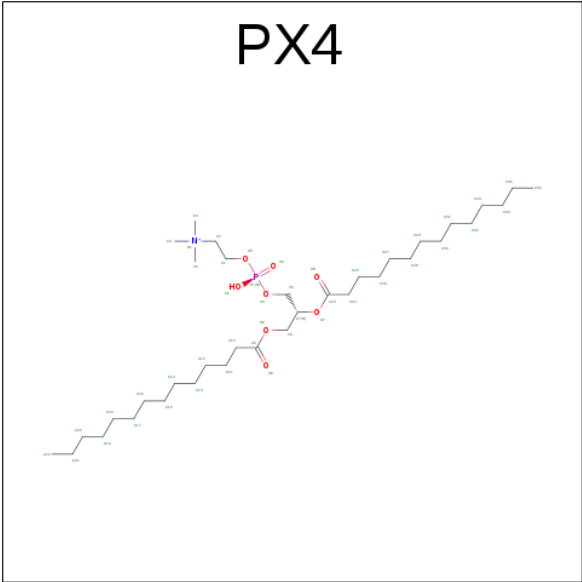
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
3	A	2	Total	Zn
			2	2

- Molecule 4 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C<sub>36</sub>H<sub>73</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

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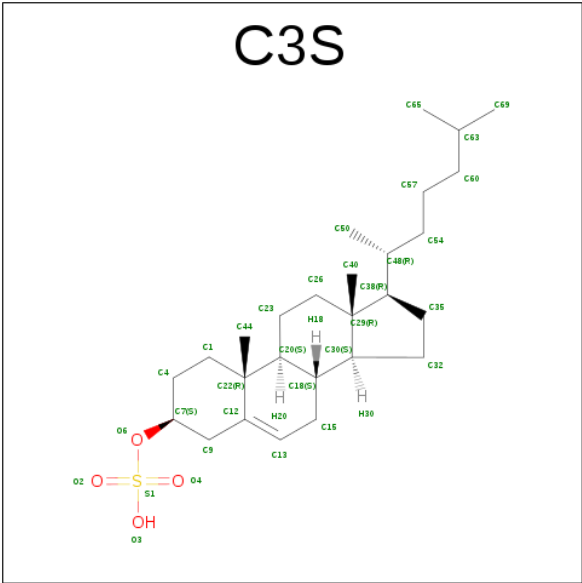
[illegible]

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Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

- Molecule 5 is CHOLEST-5-EN-3-YL HYDROGEN SULFATE (three-letter code: C3S) (formula: C<sub>27</sub>H<sub>46</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms				
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1

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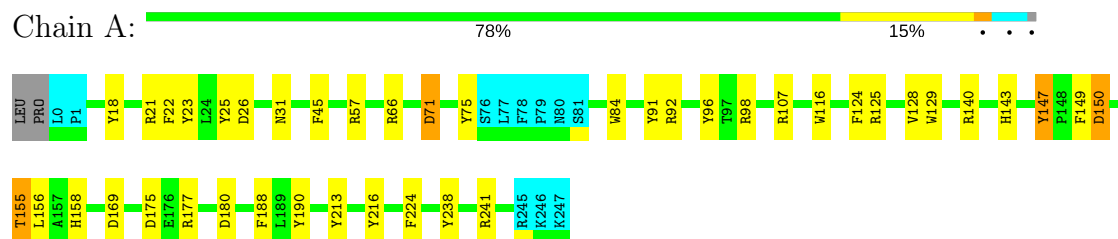
Mol	Chain	Residues	Atoms				
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Matrilysin

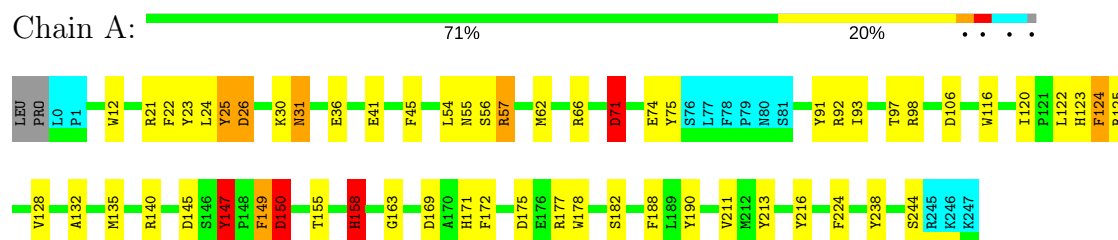


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

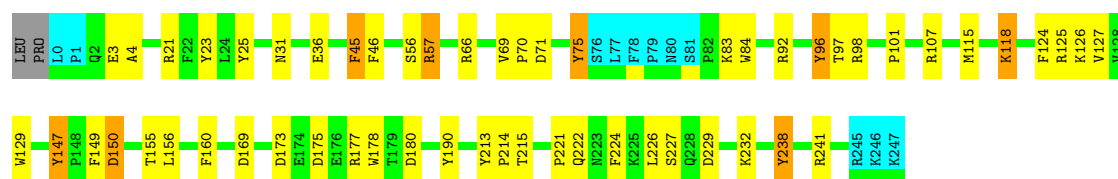
- Molecule 1: Matrilysin



#### 4.2.2 Score per residue for model 2

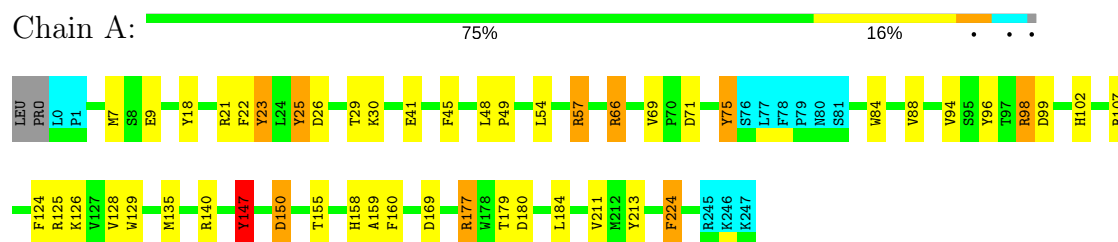
- Molecule 1: Matrilysin





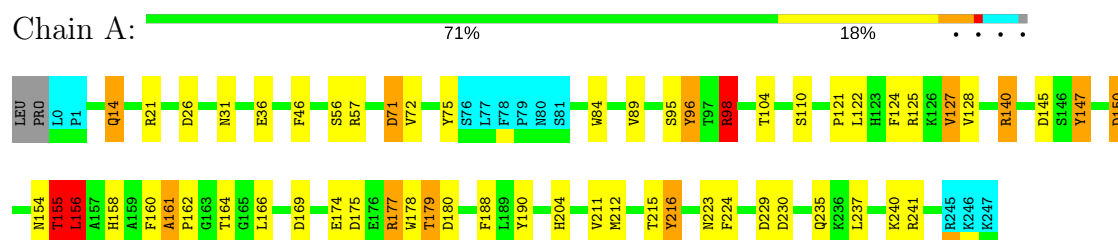
### 4.2.3 Score per residue for model 3

- Molecule 1: Matrilysin



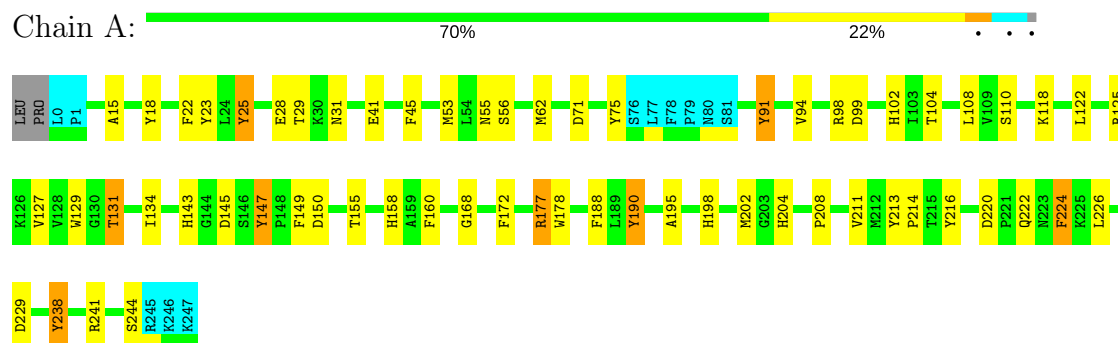
### 4.2.4 Score per residue for model 4

- Molecule 1: Matrilysin



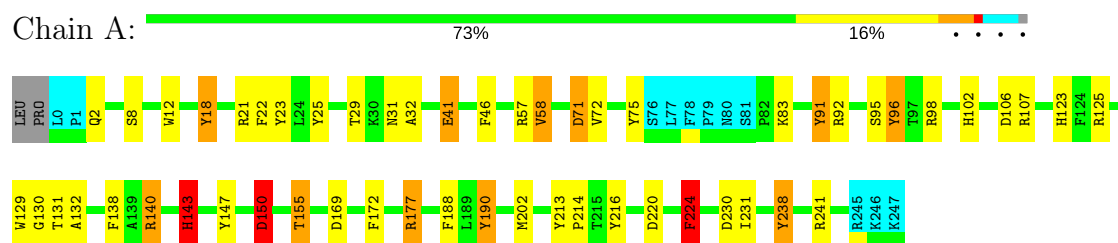
### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Matrilysin



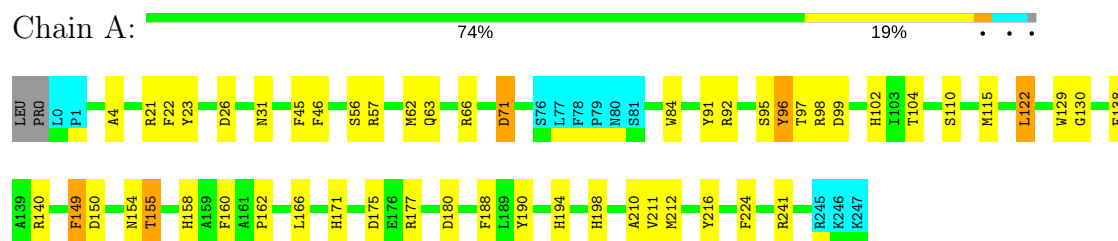
### 4.2.6 Score per residue for model 6

- Molecule 1: Matrilysin



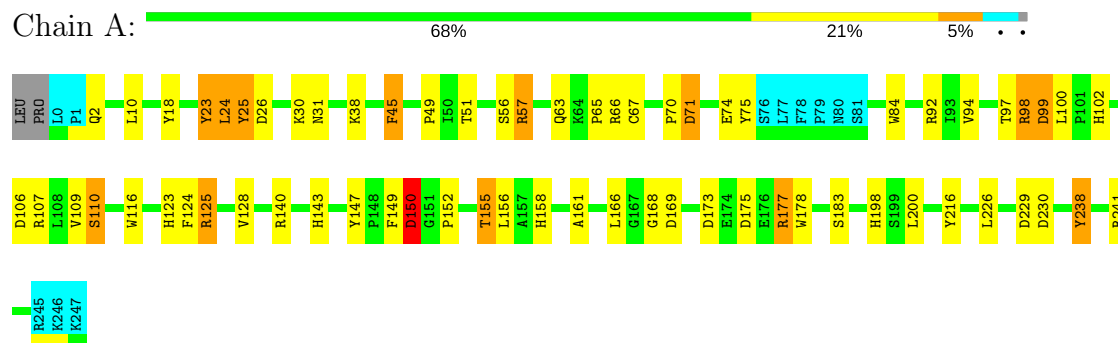
### 4.2.7 Score per residue for model 7

- Molecule 1: Matrilysin



### 4.2.8 Score per residue for model 8

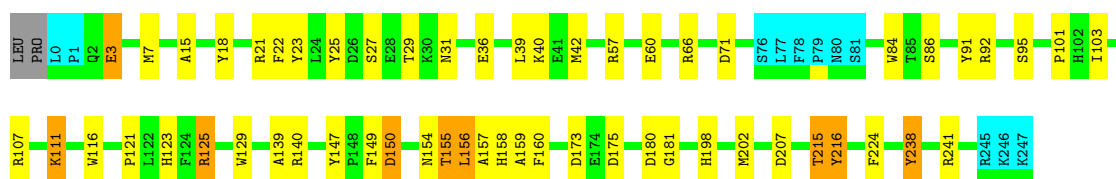
- Molecule 1: Matrilysin



### 4.2.9 Score per residue for model 9

- Molecule 1: Matrilysin

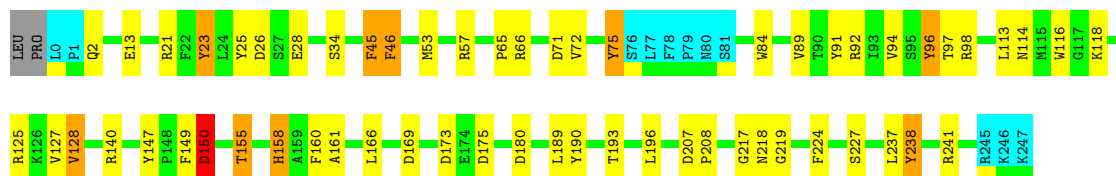




#### 4.2.10 Score per residue for model 10

- Molecule 1: Matrilysin

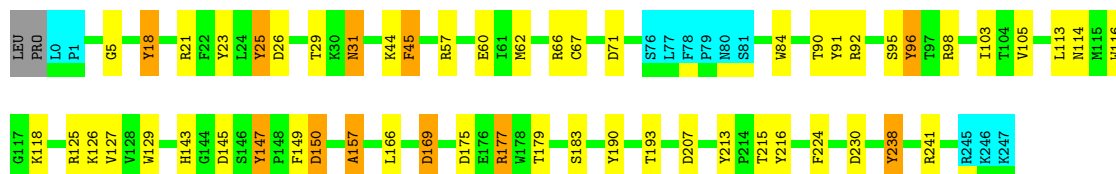
Chain A: 71% 20%



#### 4.2.11 Score per residue for model 11

- Molecule 1: Matrilysin

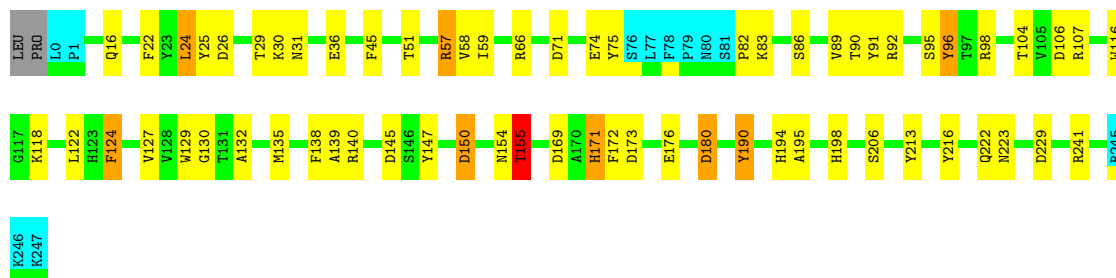
Chain A: 73% 18%



#### 4.2.12 Score per residue for model 12

- Molecule 1: Matrilysin

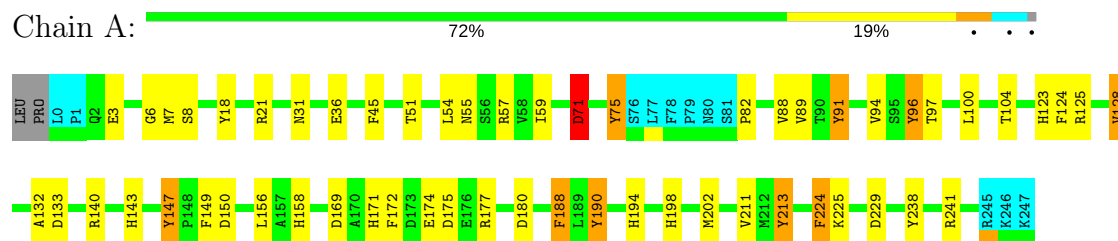
Chain A: 69% 22%





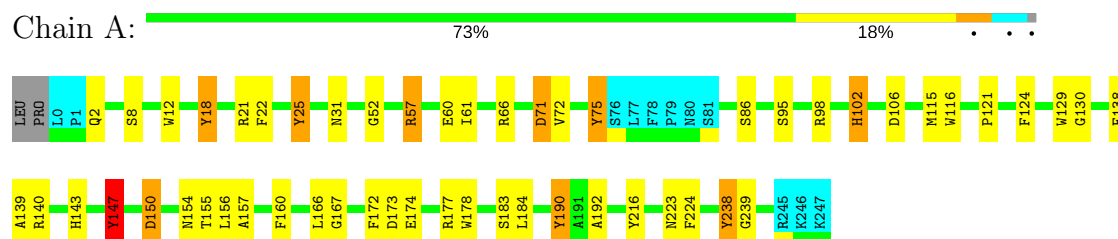
### 4.2.13 Score per residue for model 13

- Molecule 1: Matrilysin



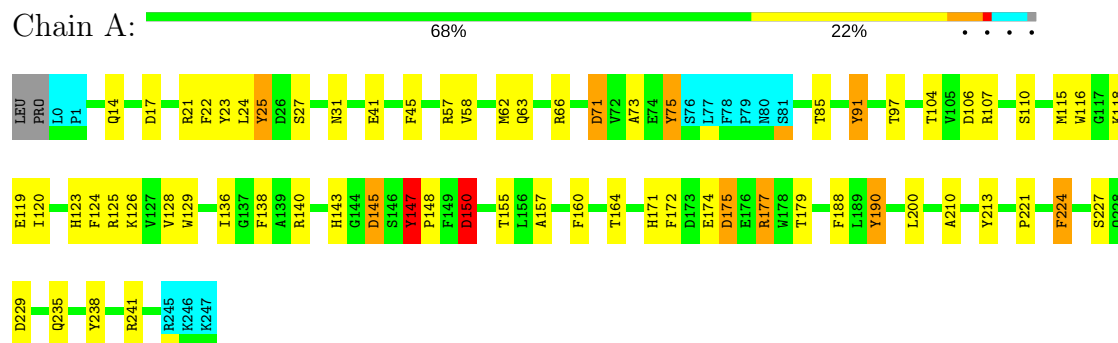
### 4.2.14 Score per residue for model 14

- Molecule 1: Matrilysin



### 4.2.15 Score per residue for model 15

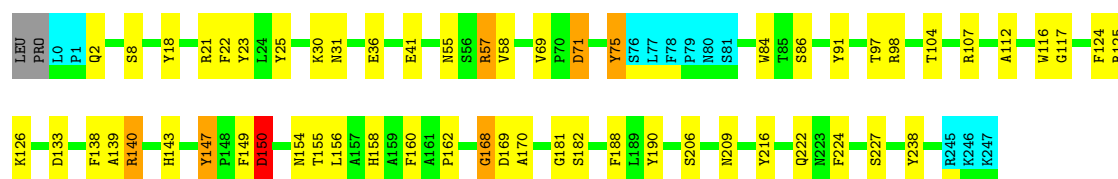
- Molecule 1: Matrilysin



### 4.2.16 Score per residue for model 16

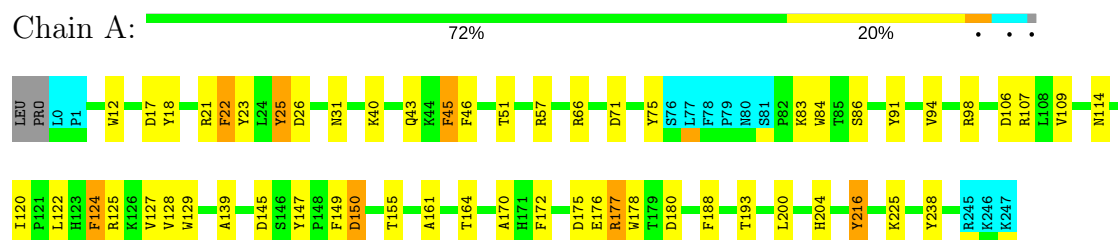
- Molecule 1: Matrilysin





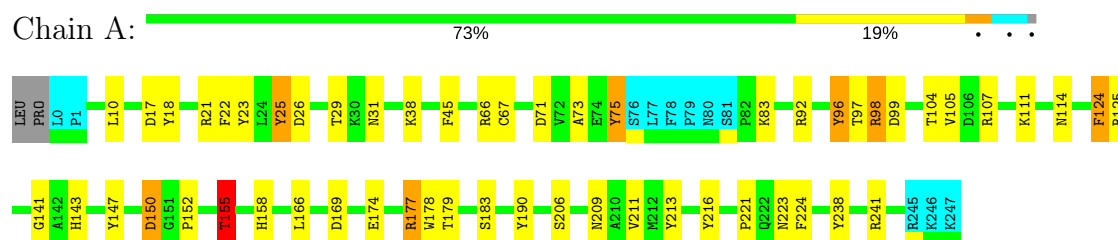
#### 4.2.17 Score per residue for model 17

- Molecule 1: Matrilysin



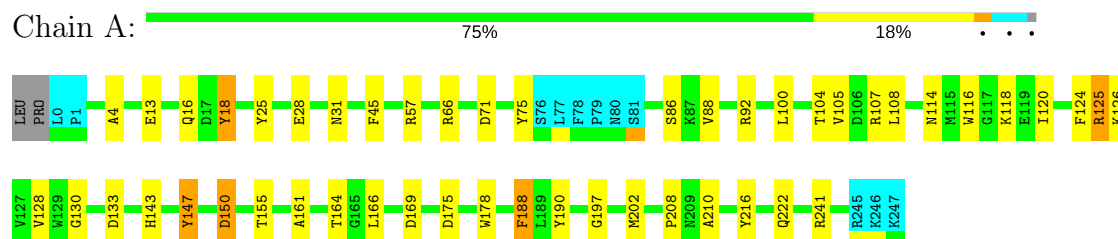
#### 4.2.18 Score per residue for model 18

- Molecule 1: Matrilysin



#### 4.2.19 Score per residue for model 19

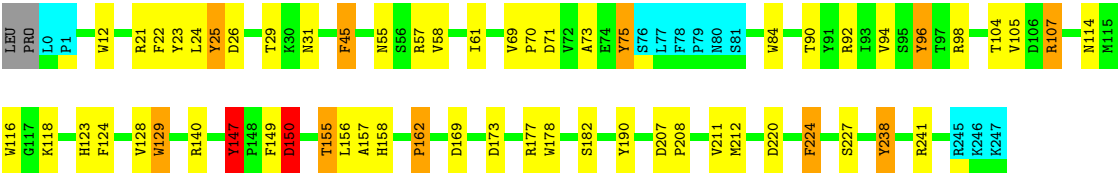
- Molecule 1: Matrilysin



#### 4.2.20 Score per residue for model 20

- Molecule 1: Matrilysin

Chain A: 



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 10000 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
HADDOCK	structure solution	2.1
GROMOS	refinement	4.5.7

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2mzi_cs.str
Number of chemical shift lists	1
Total number of shifts	797
Number of shifts mapped to atoms	797
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	21%

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: ZN, CA, C3S, PX4

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	0.52±0.00	0±0/1912 (0.0±0.0%)	2.02±0.04	56±8/2587 (2.2±0.3%)
All	All	0.52	0/38240 (0.0%)	2.02	1128/51740 (2.2%)

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	7.2±2.1
All	All	0	144

There are no bond-length outliers.

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	A	177	ARG	NE-CZ-NH2	-19.51	110.54	120.30	5	12
1	A	140	ARG	NE-CZ-NH2	-18.98	110.81	120.30	14	12
1	A	140	ARG	NE-CZ-NH1	18.27	129.44	120.30	1	8
1	A	125	ARG	NE-CZ-NH2	-17.59	111.51	120.30	2	11
1	A	57	ARG	NE-CZ-NH2	-17.59	111.51	120.30	1	8
1	A	92	ARG	NE-CZ-NH2	-17.51	111.55	120.30	19	9
1	A	92	ARG	NE-CZ-NH1	16.90	128.75	120.30	20	7
1	A	125	ARG	NE-CZ-NH1	16.21	128.41	120.30	2	9
1	A	66	ARG	NE-CZ-NH1	14.71	127.65	120.30	2	12
1	A	21	ARG	NE-CZ-NH1	-14.63	112.99	120.30	9	11
1	A	66	ARG	NE-CZ-NH2	-14.42	113.09	120.30	3	7
1	A	75	TYR	CB-CG-CD2	-14.09	112.54	121.00	19	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	71	ASP	CB-CG-OD1	13.81	130.73	118.30	4	12
1	A	46	PHE	CB-CG-CD2	-13.80	111.14	120.80	10	5
1	A	91	TYR	CB-CG-CD2	-13.35	112.99	121.00	13	7
1	A	160	PHE	CB-CG-CD2	13.29	130.10	120.80	9	6
1	A	190	TYR	CB-CG-CD2	-13.14	113.11	121.00	19	11
1	A	107	ARG	NE-CZ-NH1	13.12	126.86	120.30	3	9
1	A	98	ARG	NE-CZ-NH1	13.06	126.83	120.30	18	12
1	A	173	ASP	CB-CG-OD2	-12.80	106.78	118.30	14	3
1	A	75	TYR	CB-CG-CD1	12.79	128.68	121.00	2	6
1	A	190	TYR	CB-CG-CD1	12.52	128.51	121.00	11	7
1	A	23	TYR	CB-CG-CD2	-12.45	113.53	121.00	16	4
1	A	25	TYR	CB-CG-CD2	-12.18	113.69	121.00	18	4
1	A	172	PHE	CB-CG-CD2	-11.99	112.41	120.80	14	5
1	A	224	PHE	CB-CG-CD1	-11.89	112.48	120.80	16	5
1	A	160	PHE	CB-CG-CD1	-11.72	112.59	120.80	9	4
1	A	124	PHE	CB-CG-CD1	-11.44	112.79	120.80	1	4
1	A	45	PHE	CB-CG-CD1	11.36	128.75	120.80	12	8
1	A	241	ARG	NE-CZ-NH1	-11.33	114.63	120.30	19	8
1	A	238	TYR	CB-CG-CD1	-11.28	114.23	121.00	1	7
1	A	96	TYR	CB-CG-CD2	-11.13	114.32	121.00	11	7
1	A	224	PHE	CB-CG-CD2	11.09	128.56	120.80	16	3
1	A	25	TYR	CB-CG-CD1	-10.98	114.41	121.00	11	6
1	A	71	ASP	CB-CG-OD2	10.94	128.14	118.30	14	12
1	A	21	ARG	NE-CZ-NH2	10.67	125.63	120.30	9	11
1	A	138	PHE	CB-CG-CD2	-10.66	113.34	120.80	16	3
1	A	45	PHE	CB-CG-CD2	-10.23	113.64	120.80	12	5
1	A	211	VAL	CA-CB-CG1	10.23	126.24	110.90	3	5
1	A	57	ARG	NE-CZ-NH1	10.20	125.40	120.30	1	5
1	A	155	THR	CA-CB-CG2	10.12	126.57	112.40	12	5
1	A	169	ASP	CB-CG-OD2	10.04	127.33	118.30	2	6
1	A	145	ASP	CB-CG-OD1	9.95	127.25	118.30	17	6
1	A	140	ARG	CD-NE-CZ	9.95	137.53	123.60	4	5
1	A	140	ARG	NH1-CZ-NH2	9.83	130.21	119.40	14	1
1	A	124	PHE	CB-CG-CD2	-9.77	113.96	120.80	20	6
1	A	23	TYR	CB-CG-CD1	-9.77	115.14	121.00	9	2
1	A	98	ARG	NE-CZ-NH2	9.75	125.17	120.30	1	6
1	A	147	TYR	CB-CG-CD2	-9.37	115.38	121.00	3	7
1	A	220	ASP	CB-CG-OD1	9.36	126.72	118.30	5	2
1	A	25	TYR	CG-CD1-CE1	-9.35	113.82	121.30	11	2
1	A	71	ASP	OD1-CG-OD2	-9.34	105.55	123.30	7	18
1	A	169	ASP	CB-CG-OD1	9.18	126.56	118.30	1	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	177	ARG	CD-NE-CZ	9.16	136.43	123.60	11	2
1	A	51	THR	CA-CB-CG2	9.07	125.10	112.40	8	3
1	A	91	TYR	CB-CG-CD1	-9.05	115.57	121.00	6	6
1	A	216	TYR	CB-CG-CD1	8.97	126.38	121.00	18	8
1	A	241	ARG	NE-CZ-NH2	-8.96	115.82	120.30	11	11
1	A	96	TYR	CG-CD1-CE1	-8.88	114.19	121.30	10	1
1	A	18	TYR	CB-CG-CD1	-8.78	115.73	121.00	18	3
1	A	230	ASP	CB-CG-OD1	8.76	126.19	118.30	11	2
1	A	175	ASP	CB-CG-OD2	8.72	126.15	118.30	9	6
1	A	22	PHE	CB-CG-CD2	-8.67	114.73	120.80	20	6
1	A	145	ASP	OD1-CG-OD2	-8.60	106.96	123.30	17	3
1	A	172	PHE	CB-CG-CD1	8.49	126.74	120.80	14	4
1	A	216	TYR	CB-CG-CD2	-8.46	115.92	121.00	1	6
1	A	56	SER	N-CA-CB	-8.35	97.98	110.50	2	3
1	A	116	TRP	CD1-NE1-CE2	8.23	116.41	109.00	16	4
1	A	145	ASP	CB-CG-OD2	8.20	125.68	118.30	17	1
1	A	188	PHE	CB-CG-CD2	-8.16	115.09	120.80	13	5
1	A	175	ASP	CB-CG-OD1	-8.13	110.98	118.30	2	5
1	A	207	ASP	CB-CG-OD1	8.13	125.61	118.30	20	2
1	A	75	TYR	CG-CD1-CE1	8.11	127.79	121.30	16	3
1	A	180	ASP	CB-CG-OD2	-8.10	111.01	118.30	13	5
1	A	138	PHE	CB-CG-CD1	-8.07	115.15	120.80	15	2
1	A	173	ASP	CB-CG-OD1	7.95	125.45	118.30	14	5
1	A	149	PHE	CB-CG-CD2	-7.94	115.24	120.80	13	4
1	A	29	THR	CA-CB-CG2	7.88	123.44	112.40	3	6
1	A	238	TYR	CB-CG-CD2	-7.88	116.27	121.00	6	3
1	A	147	TYR	CG-CD2-CE2	-7.86	115.01	121.30	3	2
1	A	26	ASP	CB-CG-OD1	7.82	125.34	118.30	17	4
1	A	106	ASP	CB-CG-OD2	7.79	125.31	118.30	6	6
1	A	96	TYR	CD1-CE1-CZ	7.78	126.80	119.80	10	2
1	A	66	ARG	CD-NE-CZ	7.76	134.47	123.60	2	1
1	A	84	TRP	CE2-CD2-CG	7.76	113.50	107.30	8	3
1	A	116	TRP	NE1-CE2-CD2	-7.65	99.65	107.30	20	5
1	A	159	ALA	N-CA-CB	7.64	120.80	110.10	3	2
1	A	69	VAL	CA-CB-CG1	7.63	122.34	110.90	3	3
1	A	84	TRP	CD1-NE1-CE2	7.62	115.86	109.00	4	1
1	A	23	TYR	CD1-CE1-CZ	-7.61	112.95	119.80	3	4
1	A	213	TYR	CB-CG-CD1	-7.60	116.44	121.00	13	3
1	A	238	TYR	CG-CD1-CE1	7.60	127.38	121.30	10	3
1	A	84	TRP	NE1-CE2-CD2	-7.54	99.76	107.30	4	3
1	A	53	MET	CB-CA-C	7.54	125.47	110.40	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	75	TYR	CG-CD2-CE2	-7.50	115.30	121.30	17	1
1	A	102	HIS	CA-CB-CG	7.50	126.34	113.60	7	1
1	A	21	ARG	CD-NE-CZ	7.49	134.09	123.60	16	1
1	A	216	TYR	CG-CD2-CE2	-7.47	115.32	121.30	19	4
1	A	106	ASP	CB-CG-OD1	7.45	125.00	118.30	17	2
1	A	139	ALA	CB-CA-C	7.44	121.26	110.10	9	3
1	A	84	TRP	CD1-CG-CD2	-7.43	100.35	106.30	8	2
1	A	178	TRP	CD1-NE1-CE2	7.41	115.67	109.00	5	4
1	A	129	TRP	CZ3-CH2-CZ2	-7.41	112.71	121.60	11	2
1	A	226	LEU	CB-CG-CD2	7.40	123.58	111.00	5	2
1	A	180	ASP	CB-CA-C	7.33	125.06	110.40	2	2
1	A	26	ASP	CB-CG-OD2	7.33	124.89	118.30	12	3
1	A	180	ASP	CB-CG-OD1	7.32	124.89	118.30	13	3
1	A	56	SER	CB-CA-C	7.29	123.96	110.10	7	1
1	A	193	THR	CA-CB-CG2	7.29	122.61	112.40	10	1
1	A	86	SER	N-CA-CB	-7.29	99.56	110.50	9	4
1	A	97	THR	CA-CB-CG2	7.28	122.59	112.40	8	2
1	A	23	TYR	CG-CD2-CE2	-7.28	115.48	121.30	1	2
1	A	178	TRP	NE1-CE2-CD2	-7.26	100.03	107.30	5	4
1	A	98	ARG	CD-NE-CZ	7.26	133.77	123.60	14	1
1	A	36	GLU	OE1-CD-OE2	-7.24	114.62	123.30	12	3
1	A	62	MET	CA-CB-CG	7.23	125.60	113.30	7	4
1	A	25	TYR	N-CA-CB	7.20	123.57	110.60	17	1
1	A	107	ARG	NE-CZ-NH2	-7.11	116.75	120.30	9	3
1	A	18	TYR	CB-CG-CD2	-7.10	116.74	121.00	16	5
1	A	213	TYR	CB-CG-CD2	-7.09	116.75	121.00	11	5
1	A	8	SER	N-CA-CB	-7.08	99.88	110.50	14	3
1	A	227	SER	N-CA-CB	-7.07	99.90	110.50	2	4
1	A	177	ARG	NH1-CZ-NH2	7.06	127.17	119.40	7	2
1	A	188	PHE	CB-CG-CD1	7.05	125.74	120.80	5	4
1	A	18	TYR	CG-CD1-CE1	-7.02	115.68	121.30	14	2
1	A	104	THR	CA-CB-CG2	7.01	122.21	112.40	20	2
1	A	96	TYR	CB-CG-CD1	6.99	125.19	121.00	11	3
1	A	220	ASP	CB-CG-OD2	-6.98	112.02	118.30	5	1
1	A	95	SER	CB-CA-C	6.97	123.35	110.10	7	5
1	A	17	ASP	CB-CG-OD2	6.97	124.57	118.30	18	1
1	A	155	THR	OG1-CB-CG2	-6.96	93.99	110.00	5	3
1	A	12	TRP	CD1-NE1-CE2	6.95	115.26	109.00	6	2
1	A	65	PRO	N-CA-CB	6.93	111.62	103.30	10	2
1	A	229	ASP	CB-CG-OD1	6.93	124.53	118.30	12	5
1	A	182	SER	N-CA-CB	-6.90	100.14	110.50	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	127	VAL	CA-CB-CG2	6.90	121.25	110.90	17	5
1	A	84	TRP	NE1-CE2-CZ2	6.88	137.96	130.40	4	1
1	A	70	PRO	N-CA-CB	6.86	111.53	103.30	20	2
1	A	164	THR	CA-CB-CG2	6.86	122.00	112.40	19	1
1	A	56	SER	C-N-CA	6.84	138.81	121.70	4	2
1	A	12	TRP	CE3-CZ3-CH2	6.83	128.72	121.20	1	1
1	A	221	PRO	N-CA-CB	6.81	111.47	103.30	2	1
1	A	190	TYR	CG-CD1-CE1	-6.79	115.87	121.30	16	3
1	A	25	TYR	CD1-CE1-CZ	-6.78	113.70	119.80	6	3
1	A	147	TYR	CB-CG-CD1	-6.77	116.94	121.00	2	5
1	A	125	ARG	NH1-CZ-NH2	-6.77	111.95	119.40	18	4
1	A	18	TYR	CG-CD2-CE2	-6.75	115.90	121.30	13	1
1	A	213	TYR	CG-CD2-CE2	-6.75	115.90	121.30	11	1
1	A	238	TYR	CG-CD2-CE2	-6.73	115.92	121.30	9	6
1	A	73	ALA	N-CA-CB	-6.72	100.69	110.10	15	1
1	A	41	GLU	OE1-CD-OE2	-6.72	115.23	123.30	1	4
1	A	65	PRO	N-CD-CG	6.72	113.28	103.20	8	2
1	A	105	VAL	CB-CA-C	6.72	124.17	111.40	19	1
1	A	90	THR	CA-CB-OG1	6.70	123.07	109.00	12	1
1	A	88	VAL	CA-CB-CG2	6.68	120.93	110.90	19	1
1	A	238	TYR	CZ-CE2-CD2	6.64	125.78	119.80	9	6
1	A	24	LEU	CB-CA-C	6.64	122.81	110.20	12	3
1	A	150	ASP	CB-CG-OD1	-6.63	112.33	118.30	20	6
1	A	156	LEU	CB-CG-CD2	6.63	122.27	111.00	4	1
1	A	174	GLU	OE1-CD-OE2	-6.61	115.36	123.30	14	2
1	A	214	PRO	N-CA-CB	6.61	111.23	103.30	6	2
1	A	230	ASP	CB-CG-OD2	-6.60	112.36	118.30	6	3
1	A	178	TRP	CE2-CD2-CG	6.58	112.57	107.30	8	3
1	A	97	THR	CA-CB-OG1	6.58	122.82	109.00	15	2
1	A	57	ARG	CD-NE-CZ	6.58	132.81	123.60	13	5
1	A	12	TRP	CA-CB-CG	6.57	126.19	113.70	1	1
1	A	149	PHE	CB-CG-CD1	-6.57	116.20	120.80	7	2
1	A	4	ALA	N-CA-CB	-6.57	100.90	110.10	19	3
1	A	150	ASP	N-CA-CB	6.56	122.41	110.60	20	1
1	A	132	ALA	CB-CA-C	6.56	119.94	110.10	12	2
1	A	123	HIS	CA-CB-CG	6.53	124.71	113.60	13	3
1	A	229	ASP	CB-CG-OD2	6.53	124.18	118.30	8	4
1	A	72	VAL	CB-CA-C	6.53	123.81	111.40	6	2
1	A	101	PRO	N-CA-CB	6.51	111.11	103.30	9	1
1	A	98	ARG	CA-CB-CG	-6.51	99.08	113.40	11	1
1	A	241	ARG	CD-NE-CZ	6.48	132.68	123.60	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	210	ALA	N-CA-CB	-6.48	101.03	110.10	19	1
1	A	145	ASP	N-CA-CB	6.45	122.21	110.60	15	1
1	A	169	ASP	OD1-CG-OD2	-6.45	111.05	123.30	20	8
1	A	12	TRP	CZ3-CH2-CZ2	-6.43	113.88	121.60	1	1
1	A	129	TRP	CB-CG-CD2	6.43	134.95	126.60	6	2
1	A	121	PRO	N-CA-CB	6.42	111.00	103.30	4	1
1	A	213	TYR	CD1-CE1-CZ	-6.42	114.02	119.80	13	1
1	A	6	GLY	C-N-CA	6.41	137.74	121.70	13	1
1	A	7	MET	CG-SD-CE	6.39	110.42	100.20	9	1
1	A	132	ALA	N-CA-CB	-6.38	101.17	110.10	1	3
1	A	91	TYR	CG-CD2-CE2	-6.37	116.20	121.30	6	3
1	A	192	ALA	CB-CA-C	-6.37	100.55	110.10	14	1
1	A	195	ALA	N-CA-CB	-6.33	101.24	110.10	12	2
1	A	147	TYR	N-CA-CB	6.31	121.95	110.60	4	2
1	A	54	LEU	CB-CG-CD1	-6.30	100.29	111.00	1	1
1	A	46	PHE	CZ-CE2-CD2	-6.30	112.54	120.10	10	1
1	A	99	ASP	CB-CG-OD2	6.28	123.95	118.30	5	1
1	A	176	GLU	OE1-CD-OE2	-6.28	115.77	123.30	12	1
1	A	207	ASP	N-CA-CB	-6.27	99.32	110.60	9	2
1	A	168	GLY	CA-C-O	-6.26	109.33	120.60	16	1
1	A	46	PHE	CB-CG-CD1	6.25	125.17	120.80	10	1
1	A	105	VAL	CA-CB-CG1	6.24	120.26	110.90	18	2
1	A	177	ARG	NE-CZ-NH1	6.22	123.41	120.30	1	6
1	A	213	TYR	CG-CD1-CE1	-6.21	116.33	121.30	3	1
1	A	116	TRP	CG-CD1-NE1	-6.17	103.93	110.10	16	1
1	A	92	ARG	CD-NE-CZ	6.16	132.23	123.60	9	3
1	A	8	SER	CB-CA-C	6.16	121.81	110.10	6	1
1	A	116	TRP	CE2-CD2-CG	6.15	112.22	107.30	20	2
1	A	13	GLU	OE1-CD-OE2	-6.14	115.93	123.30	10	2
1	A	104	THR	CA-CB-OG1	6.13	121.86	109.00	15	5
1	A	212	MET	CA-CB-CG	6.12	123.71	113.30	4	1
1	A	128	VAL	CA-CB-CG2	6.12	120.09	110.90	10	4
1	A	91	TYR	CG-CD1-CE1	-6.12	116.40	121.30	10	3
1	A	60	GLU	OE1-CD-OE2	-6.12	115.96	123.30	9	1
1	A	46	PHE	CG-CD1-CE1	-6.12	114.07	120.80	10	1
1	A	150	ASP	CB-CG-OD2	-6.08	112.83	118.30	8	3
1	A	89	VAL	CA-CB-CG1	6.08	120.02	110.90	4	1
1	A	116	TRP	NE1-CE2-CZ2	6.07	137.08	130.40	9	2
1	A	23	TYR	CZ-CE2-CD2	-6.06	114.34	119.80	15	2
1	A	157	ALA	C-N-CA	6.06	136.85	121.70	9	1
1	A	198	HIS	O-C-N	-6.06	113.00	122.70	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	TRP	CB-CG-CD2	6.05	134.47	126.60	9	2
1	A	155	THR	N-CA-CB	6.05	121.79	110.30	10	1
1	A	98	ARG	NH1-CZ-NH2	-6.05	112.75	119.40	18	2
1	A	125	ARG	CD-NE-CZ	6.04	132.05	123.60	8	6
1	A	135	MET	CG-SD-CE	6.03	109.85	100.20	3	2
1	A	238	TYR	CD1-CG-CD2	6.01	124.51	117.90	1	1
1	A	115	MET	CG-SD-CE	6.01	109.81	100.20	2	2
1	A	70	PRO	N-CD-CG	6.01	112.21	103.20	8	2
1	A	92	ARG	NH1-CZ-NH2	6.00	126.00	119.40	18	1
1	A	172	PHE	CZ-CE2-CD2	5.99	127.29	120.10	1	1
1	A	12	TRP	CE2-CD2-CE3	-5.99	111.51	118.70	6	1
1	A	200	LEU	CB-CA-C	-5.99	98.82	110.20	17	2
1	A	160	PHE	CG-CD2-CE2	-5.99	114.21	120.80	3	1
1	A	190	TYR	CZ-CE2-CD2	-5.99	114.41	119.80	5	1
1	A	149	PHE	C-N-CA	5.99	136.67	121.70	7	3
1	A	12	TRP	NE1-CE2-CD2	-5.97	101.33	107.30	6	1
1	A	148	PRO	N-CD-CG	5.97	112.16	103.20	15	1
1	A	188	PHE	O-C-N	-5.97	113.15	122.70	4	1
1	A	89	VAL	CA-CB-CG2	5.95	119.82	110.90	13	1
1	A	229	ASP	C-N-CA	5.94	136.56	121.70	15	1
1	A	36	GLU	N-CA-CB	-5.93	99.93	110.60	2	1
1	A	156	LEU	CB-CG-CD1	5.91	121.05	111.00	9	2
1	A	22	PHE	CB-CG-CD1	-5.90	116.67	120.80	16	4
1	A	110	SER	N-CA-CB	-5.89	101.67	110.50	7	3
1	A	109	VAL	CA-CB-CG2	5.88	119.72	110.90	17	2
1	A	86	SER	CB-CA-C	5.87	121.24	110.10	19	2
1	A	94	VAL	CA-CB-CG2	5.86	119.70	110.90	8	4
1	A	152	PRO	N-CD-CG	5.85	111.98	103.20	18	1
1	A	149	PHE	CA-CB-CG	5.84	127.92	113.90	7	1
1	A	103	ILE	CA-CB-CG1	5.83	122.09	111.00	9	1
1	A	28	GLU	O-C-N	-5.83	113.37	122.70	10	1
1	A	94	VAL	CA-CB-CG1	5.82	119.63	110.90	3	1
1	A	143	HIS	CA-CB-CG	5.81	123.48	113.60	11	4
1	A	58	VAL	CG1-CB-CG2	-5.81	101.61	110.90	15	1
1	A	116	TRP	CH2-CZ2-CE2	5.80	123.20	117.40	14	3
1	A	149	PHE	CG-CD2-CE2	5.80	127.18	120.80	9	2
1	A	158	HIS	CB-CA-C	5.80	122.00	110.40	1	1
1	A	31	ASN	N-CA-CB	5.80	121.04	110.60	11	1
1	A	188	PHE	CZ-CE2-CD2	5.79	127.05	120.10	15	1
1	A	178	TRP	CG-CD1-NE1	-5.79	104.31	110.10	18	1
1	A	107	ARG	CD-NE-CZ	5.78	131.70	123.60	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	178	TRP	CH2-CZ2-CE2	5.78	123.18	117.40	4	1
1	A	99	ASP	CB-CG-OD1	5.78	123.50	118.30	8	2
1	A	22	PHE	CZ-CE2-CD2	-5.78	113.17	120.10	15	1
1	A	26	ASP	CB-CA-C	5.76	121.92	110.40	3	2
1	A	58	VAL	CB-CA-C	5.76	122.34	111.40	6	1
1	A	12	TRP	NE1-CE2-CZ2	5.75	136.73	130.40	17	1
1	A	244	SER	CB-CA-C	5.75	121.02	110.10	1	2
1	A	12	TRP	CG-CD2-CE3	5.75	139.07	133.90	14	1
1	A	116	TRP	CE3-CZ3-CH2	-5.75	114.88	121.20	16	1
1	A	51	THR	CA-CB-OG1	5.75	121.07	109.00	17	1
1	A	194	HIS	CA-CB-CG	5.74	123.36	113.60	13	2
1	A	178	TRP	CD1-CG-CD2	-5.74	101.71	106.30	8	1
1	A	133	ASP	CB-CG-OD1	5.74	123.46	118.30	19	2
1	A	84	TRP	CB-CG-CD1	-5.73	119.55	127.00	11	3
1	A	96	TYR	CB-CA-C	5.73	121.86	110.40	13	2
1	A	164	THR	C-N-CA	5.73	134.33	122.30	19	2
1	A	215	THR	CA-CB-CG2	5.73	120.42	112.40	11	1
1	A	30	LYS	C-N-CA	5.72	136.01	121.70	8	2
1	A	136	ILE	CA-CB-CG1	5.72	121.87	111.00	15	1
1	A	190	TYR	CG-CD2-CE2	-5.71	116.73	121.30	19	1
1	A	213	TYR	CA-CB-CG	5.71	124.24	113.40	5	1
1	A	178	TRP	NE1-CE2-CZ2	5.68	136.65	130.40	18	4
1	A	127	VAL	CG1-CB-CG2	5.68	119.99	110.90	10	1
1	A	90	THR	CA-CB-CG2	5.68	120.35	112.40	11	1
1	A	237	LEU	CB-CG-CD2	-5.68	101.35	111.00	4	1
1	A	129	TRP	CE3-CZ3-CH2	5.68	127.45	121.20	11	1
1	A	111	LYS	C-N-CA	5.68	135.89	121.70	18	1
1	A	113	LEU	CB-CG-CD2	5.67	120.63	111.00	11	1
1	A	75	TYR	CZ-CE2-CD2	5.66	124.90	119.80	16	1
1	A	227	SER	CB-CA-C	5.65	120.83	110.10	20	1
1	A	45	PHE	CA-CB-CG	5.64	127.45	113.90	2	2
1	A	129	TRP	NE1-CE2-CD2	-5.64	101.66	107.30	11	2
1	A	88	VAL	C-N-CA	5.63	135.78	121.70	3	1
1	A	26	ASP	OD1-CG-OD2	-5.62	112.61	123.30	1	1
1	A	129	TRP	CG-CD1-NE1	5.61	115.71	110.10	3	1
1	A	225	LYS	CB-CA-C	5.61	121.62	110.40	17	1
1	A	18	TYR	CD1-CG-CD2	5.60	124.06	117.90	13	1
1	A	171	HIS	CB-CA-C	5.60	121.60	110.40	15	2
1	A	45	PHE	CG-CD2-CE2	-5.59	114.65	120.80	3	1
1	A	46	PHE	CD1-CE1-CZ	-5.59	113.39	120.10	4	1
1	A	212	MET	CG-SD-CE	5.59	109.14	100.20	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	60	GLU	O-C-N	-5.58	113.78	122.70	9	2
1	A	59	ILE	CA-CB-CG2	5.57	122.04	110.90	13	1
1	A	212	MET	CB-CA-C	5.57	121.54	110.40	20	1
1	A	104	THR	O-C-N	-5.57	113.79	122.70	7	1
1	A	45	PHE	CA-C-N	5.57	129.45	117.20	5	1
1	A	73	ALA	CB-CA-C	-5.57	101.75	110.10	20	2
1	A	121	PRO	N-CD-CG	5.56	111.55	103.20	14	1
1	A	94	VAL	C-N-CA	5.55	135.59	121.70	10	1
1	A	17	ASP	CB-CG-OD1	5.55	123.30	118.30	17	1
1	A	91	TYR	CZ-CE2-CD2	5.54	124.79	119.80	13	1
1	A	208	PRO	N-CD-CG	5.54	111.51	103.20	20	2
1	A	41	GLU	O-C-N	-5.54	113.84	122.70	15	1
1	A	154	ASN	C-N-CA	5.53	135.53	121.70	7	2
1	A	193	THR	OG1-CB-CG2	-5.53	97.28	110.00	11	1
1	A	128	VAL	C-N-CA	5.53	135.52	121.70	8	2
1	A	27	SER	N-CA-CB	-5.53	102.21	110.50	15	2
1	A	131	THR	CA-CB-OG1	5.50	120.55	109.00	5	1
1	A	12	TRP	CB-CG-CD1	-5.50	119.85	127.00	20	1
1	A	25	TYR	CB-CA-C	5.50	121.39	110.40	5	1
1	A	152	PRO	N-CA-CB	5.49	109.89	103.30	8	1
1	A	158	HIS	CA-CB-CG	5.48	122.92	113.60	5	2
1	A	164	THR	OG1-CB-CG2	-5.47	97.41	110.00	17	1
1	A	83	LYS	O-C-N	-5.47	113.94	122.70	18	1
1	A	84	TRP	CG-CD1-NE1	5.47	115.57	110.10	17	1
1	A	241	ARG	N-CA-CB	-5.47	100.76	110.60	8	1
1	A	89	VAL	CB-CA-C	5.46	121.78	111.40	12	2
1	A	124	PHE	CD1-CE1-CZ	5.46	126.65	120.10	12	2
1	A	29	THR	OG1-CB-CG2	-5.45	97.47	110.00	9	2
1	A	59	ILE	CA-CB-CG1	5.44	121.34	111.00	12	1
1	A	139	ALA	N-CA-CB	5.44	117.72	110.10	17	1
1	A	133	ASP	C-N-CA	5.44	135.29	121.70	19	1
1	A	57	ARG	C-N-CA	5.43	135.28	121.70	9	2
1	A	116	TRP	CZ3-CH2-CZ2	-5.43	115.08	121.60	14	1
1	A	84	TRP	CD2-CE3-CZ3	5.42	125.85	118.80	10	1
1	A	58	VAL	CA-CB-CG1	5.42	119.03	110.90	16	1
1	A	3	GLU	OE1-CD-OE2	-5.42	116.79	123.30	9	1
1	A	241	ARG	NH1-CZ-NH2	-5.42	113.44	119.40	6	1
1	A	40	LYS	C-N-CA	5.42	135.24	121.70	17	1
1	A	46	PHE	CG-CD2-CE2	5.41	126.75	120.80	7	1
1	A	45	PHE	CG-CD1-CE1	-5.41	114.85	120.80	1	1
1	A	204	HIS	N-CA-C	5.41	125.60	111.00	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	170	ALA	CB-CA-C	5.41	118.21	110.10	17	2
1	A	29	THR	CA-CB-OG1	-5.40	97.66	109.00	6	1
1	A	5	GLY	C-N-CA	5.40	133.63	122.30	11	1
1	A	58	VAL	CA-CB-CG2	5.39	118.99	110.90	12	1
1	A	232	LYS	CA-C-N	5.39	126.98	116.20	2	1
1	A	161	ALA	N-CA-CB	-5.37	102.59	110.10	10	2
1	A	237	LEU	CB-CG-CD1	-5.36	101.89	111.00	10	1
1	A	100	LEU	CB-CG-CD2	5.36	120.10	111.00	19	1
1	A	238	TYR	C-N-CA	5.35	133.54	122.30	9	1
1	A	161	ALA	CB-CA-C	-5.35	102.08	110.10	4	3
1	A	176	GLU	N-CA-CB	-5.35	100.97	110.60	17	1
1	A	84	TRP	CG-CD2-CE3	5.35	138.71	133.90	11	1
1	A	2	GLN	CB-CA-C	5.34	121.08	110.40	6	1
1	A	238	TYR	CD1-CE1-CZ	-5.34	114.99	119.80	10	1
1	A	41	GLU	CA-CB-CG	5.34	125.15	113.40	16	1
1	A	124	PHE	CG-CD1-CE1	-5.33	114.93	120.80	1	2
1	A	85	THR	CA-CB-OG1	5.33	120.20	109.00	15	1
1	A	23	TYR	N-CA-CB	-5.33	101.01	110.60	2	1
1	A	74	GLU	CB-CA-C	5.32	121.03	110.40	1	2
1	A	42	MET	N-CA-C	5.32	125.36	111.00	9	1
1	A	129	TRP	CD1-NE1-CE2	-5.31	104.22	109.00	3	2
1	A	206	SER	C-N-CA	5.31	134.98	121.70	16	1
1	A	193	THR	O-C-N	-5.31	114.20	122.70	17	1
1	A	129	TRP	C-N-CA	5.30	133.44	122.30	12	2
1	A	135	MET	CA-CB-CG	5.30	122.31	113.30	1	1
1	A	223	ASN	C-N-CA	5.30	134.96	121.70	4	3
1	A	157	ALA	CB-CA-C	5.30	118.05	110.10	11	1
1	A	111	LYS	N-CA-CB	-5.28	101.11	110.60	9	1
1	A	84	TRP	CH2-CZ2-CE2	5.27	122.67	117.40	7	1
1	A	67	CYS	CB-CA-C	-5.26	99.87	110.40	8	1
1	A	99	ASP	CA-CB-CG	5.25	124.95	113.40	18	1
1	A	121	PRO	C-N-CA	5.25	134.82	121.70	9	1
1	A	43	GLN	N-CA-CB	5.25	120.05	110.60	17	1
1	A	67	CYS	CA-CB-SG	-5.25	104.56	114.00	11	1
1	A	57	ARG	N-CA-CB	-5.24	101.16	110.60	19	1
1	A	44	LYS	CA-CB-CG	5.24	124.93	113.40	11	1
1	A	239	GLY	O-C-N	-5.24	114.32	122.70	14	1
1	A	23	TYR	CG-CD1-CE1	5.23	125.49	121.30	3	1
1	A	143	HIS	N-CA-CB	-5.23	101.18	110.60	6	2
1	A	91	TYR	CD1-CE1-CZ	5.23	124.51	119.80	15	1
1	A	82	PRO	N-CD-CG	5.23	111.05	103.20	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	32	ALA	N-CA-CB	5.23	117.42	110.10	6	1
1	A	209	ASN	C-N-CA	5.22	134.76	121.70	18	1
1	A	116	TRP	CB-CG-CD2	5.22	133.39	126.60	1	2
1	A	10	LEU	CB-CG-CD1	5.22	119.87	111.00	8	1
1	A	145	ASP	CB-CA-C	-5.22	99.96	110.40	11	1
1	A	61	ILE	CB-CA-C	5.22	122.03	111.60	14	1
1	A	62	MET	N-CA-CB	-5.22	101.21	110.60	5	1
1	A	45	PHE	CB-CA-C	5.22	120.83	110.40	10	1
1	A	207	ASP	CB-CG-OD2	-5.21	113.61	118.30	20	1
1	A	106	ASP	OD1-CG-OD2	-5.21	113.40	123.30	14	1
1	A	125	ARG	N-CA-CB	-5.21	101.22	110.60	10	1
1	A	98	ARG	CB-CA-C	5.21	120.82	110.40	8	1
1	A	218	ASN	C-N-CA	5.21	133.23	122.30	10	1
1	A	3	GLU	C-N-CA	5.20	134.71	121.70	2	1
1	A	3	GLU	O-C-N	-5.20	114.38	122.70	9	1
1	A	57	ARG	O-C-N	-5.19	114.40	122.70	9	1
1	A	12	TRP	CH2-CZ2-CE2	5.19	122.59	117.40	17	1
1	A	200	LEU	CB-CG-CD2	5.19	119.82	111.00	15	1
1	A	129	TRP	CE2-CD2-CG	5.18	111.45	107.30	20	1
1	A	215	THR	N-CA-CB	-5.18	100.45	110.30	2	1
1	A	100	LEU	CB-CG-CD1	5.18	119.81	111.00	13	1
1	A	188	PHE	CG-CD1-CE1	5.16	126.48	120.80	16	1
1	A	18	TYR	N-CA-CB	-5.16	101.31	110.60	6	1
1	A	211	VAL	CG1-CB-CG2	-5.16	102.64	110.90	13	2
1	A	190	TYR	O-C-N	-5.16	114.44	122.70	14	1
1	A	23	TYR	CD1-CG-CD2	5.16	123.57	117.90	1	1
1	A	52	GLY	CA-C-O	-5.16	111.31	120.60	14	1
1	A	24	LEU	C-N-CA	5.16	134.59	121.70	15	1
1	A	65	PRO	CA-N-CD	-5.16	104.28	111.50	8	1
1	A	147	TYR	CD1-CG-CD2	5.15	123.57	117.90	3	1
1	A	129	TRP	CD1-CG-CD2	-5.15	102.18	106.30	15	1
1	A	215	THR	CA-CB-OG1	5.14	119.80	109.00	4	1
1	A	18	TYR	CD1-CE1-CZ	5.14	124.43	119.80	17	2
1	A	120	ILE	CA-CB-CG1	5.13	120.74	111.00	1	1
1	A	226	LEU	CB-CG-CD1	-5.13	102.28	111.00	8	1
1	A	106	ASP	CA-CB-CG	5.12	124.68	113.40	17	1
1	A	211	VAL	O-C-N	-5.12	114.51	122.70	1	1
1	A	231	ILE	O-C-N	-5.12	114.52	122.70	6	1
1	A	208	PRO	N-CA-CB	5.11	109.44	103.30	10	3
1	A	91	TYR	CB-CA-C	5.11	120.62	110.40	11	1
1	A	54	LEU	CB-CG-CD2	-5.11	102.32	111.00	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	TYR	C-N-CA	5.10	134.45	121.70	8	1
1	A	102	HIS	N-CA-C	5.09	124.75	111.00	5	1
1	A	84	TRP	CE2-CD2-CE3	-5.09	112.59	118.70	2	1
1	A	128	VAL	CA-CB-CG1	5.09	118.54	110.90	13	1
1	A	202	MET	CG-SD-CE	-5.09	92.05	100.20	19	1
1	A	224	PHE	CB-CA-C	5.09	120.58	110.40	6	1
1	A	14	GLN	CG-CD-OE1	-5.09	111.42	121.60	15	1
1	A	108	LEU	O-C-N	-5.09	114.56	122.70	5	1
1	A	95	SER	O-C-N	-5.08	114.57	122.70	4	1
1	A	206	SER	O-C-N	-5.08	114.58	122.70	18	1
1	A	28	GLU	CA-CB-CG	5.07	124.56	113.40	5	1
1	A	206	SER	N-CA-CB	-5.07	102.90	110.50	12	1
1	A	210	ALA	CB-CA-C	-5.06	102.51	110.10	7	1
1	A	131	THR	CA-CB-CG2	-5.06	105.32	112.40	6	1
1	A	96	TYR	CG-CD2-CE2	-5.06	117.25	121.30	13	1
1	A	29	THR	C-N-CA	5.06	134.34	121.70	6	1
1	A	149	PHE	CZ-CE2-CD2	-5.05	114.04	120.10	9	1
1	A	48	LEU	CB-CG-CD1	5.05	119.58	111.00	3	1
1	A	116	TRP	CA-CB-CG	5.04	123.28	113.70	15	1
1	A	163	GLY	O-C-N	5.04	130.76	122.70	1	1
1	A	93	ILE	CA-CB-CG2	5.04	120.97	110.90	1	1
1	A	53	MET	O-C-N	5.04	130.75	122.70	5	1
1	A	2	GLN	N-CA-CB	-5.04	101.54	110.60	10	1
1	A	122	LEU	O-C-N	5.03	130.75	122.70	7	1
1	A	174	GLU	CA-CB-CG	5.03	124.47	113.40	14	1
1	A	194	HIS	N-CA-CB	-5.03	101.55	110.60	12	1
1	A	112	ALA	N-CA-CB	-5.02	103.07	110.10	16	1
1	A	69	VAL	CA-CB-CG2	5.02	118.43	110.90	2	1
1	A	15	ALA	N-CA-CB	-5.02	103.07	110.10	5	1
1	A	210	ALA	C-N-CA	5.02	134.25	121.70	15	1
1	A	220	ASP	CB-CA-C	-5.01	100.38	110.40	20	1
1	A	102	HIS	O-C-N	5.01	130.72	122.70	14	1
1	A	183	SER	N-CA-CB	5.00	118.01	110.50	11	1
1	A	63	GLN	CA-CB-CG	5.00	124.41	113.40	8	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	238	TYR	Sidechain	11

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	18	TYR	Sidechain	8
1	A	96	TYR	Sidechain	7
1	A	190	TYR	Sidechain	7
1	A	149	PHE	Sidechain,Peptide	6
1	A	147	TYR	Sidechain	6
1	A	213	TYR	Sidechain	5
1	A	91	TYR	Sidechain	5
1	A	25	TYR	Sidechain	5
1	A	45	PHE	Sidechain	4
1	A	216	TYR	Sidechain	4
1	A	157	ALA	Peptide	4
1	A	23	TYR	Sidechain	4
1	A	22	PHE	Sidechain	4
1	A	188	PHE	Sidechain	4
1	A	75	TYR	Sidechain	3
1	A	140	ARG	Peptide,Sidechain	3
1	A	71	ASP	Sidechain	3
1	A	143	HIS	Mainchain,Sidechain	3
1	A	198	HIS	Sidechain	2
1	A	168	GLY	Peptide	2
1	A	124	PHE	Sidechain	2
1	A	66	ARG	Sidechain	2
1	A	138	PHE	Sidechain	2
1	A	123	HIS	Sidechain	2
1	A	158	HIS	Sidechain	2
1	A	57	ARG	Sidechain	1
1	A	46	PHE	Peptide	1
1	A	28	GLU	Mainchain	1
1	A	49	PRO	Mainchain	1
1	A	197	GLY	Peptide	1
1	A	133	ASP	Peptide	1
1	A	169	ASP	Sidechain	1
1	A	129	TRP	Peptide	1
1	A	219	GLY	Peptide	1
1	A	30	LYS	Peptide	1
1	A	167	GLY	Mainchain	1
1	A	240	LYS	Mainchain	1
1	A	235	GLN	Sidechain	1
1	A	150	ASP	Peptide	1
1	A	204	HIS	Sidechain	1
1	A	125	ARG	Sidechain	1
1	A	181	GLY	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	179	THR	Peptide	1
1	A	36	GLU	Mainchain	1
1	A	41	GLU	Peptide	1
1	A	160	PHE	Sidechain	1
1	A	107	ARG	Sidechain	1
1	A	130	GLY	Peptide	1
1	A	183	SER	Mainchain	1
1	A	215	THR	Mainchain	1
1	A	14	GLN	Mainchain	1
1	A	177	ARG	Sidechain	1
1	A	224	PHE	Sidechain	1
1	A	102	HIS	Sidechain	1
1	A	61	ILE	Mainchain	1
1	A	241	ARG	Sidechain	1
1	A	98	ARG	Sidechain	1
1	A	95	SER	Mainchain	1
1	A	139	ALA	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	1861	1796	1796	4±2
4	A	5796	0	9072	122±10
5	A	192	270	272	3±2
All	All	157060	41320	222802	2459

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:384:PX4:H50	4:A:427:PX4:H60	0.91	1.43	1	1
4:A:328:PX4:H39	4:A:351:PX4:H23	0.90	1.41	12	1
4:A:386:PX4:H42	4:A:417:PX4:H38	0.85	1.47	3	1
4:A:308:PX4:H17	4:A:326:PX4:H55	0.84	1.49	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:367:PX4:H16	4:A:399:PX4:H47	0.84	1.48	17	1
4:A:353:PX4:H53	4:A:361:PX4:H21	0.84	1.47	13	1
4:A:309:PX4:H17	4:A:328:PX4:H24	0.84	1.47	20	1
4:A:372:PX4:H31	4:A:410:PX4:H66	0.84	1.50	6	1
4:A:316:PX4:H17	4:A:352:PX4:H19	0.84	1.48	17	1
4:A:381:PX4:H14	4:A:394:PX4:H47	0.82	1.49	6	1
4:A:327:PX4:H23	4:A:348:PX4:H47	0.82	1.49	18	1
4:A:326:PX4:H35	4:A:355:PX4:H31	0.82	1.50	5	1
4:A:359:PX4:H64	4:A:375:PX4:H43	0.82	1.52	15	1
4:A:329:PX4:H19	4:A:335:PX4:H26	0.82	1.52	11	1
4:A:327:PX4:H35	4:A:359:PX4:H60	0.82	1.52	10	1
4:A:313:PX4:H25	4:A:362:PX4:H26	0.81	1.52	15	1
4:A:345:PX4:H46	4:A:358:PX4:H16	0.81	1.53	13	1
4:A:319:PX4:H67	4:A:319:PX4:H34	0.81	1.49	16	1
4:A:386:PX4:H16	4:A:402:PX4:H14	0.81	1.50	16	1
4:A:412:PX4:H50	4:A:424:PX4:H48	0.81	1.51	14	1
4:A:417:PX4:H21	4:A:421:PX4:H61	0.80	1.52	20	1
4:A:392:PX4:H47	4:A:425:PX4:H16	0.80	1.53	19	1
4:A:306:PX4:H52	4:A:342:PX4:H25	0.80	1.52	9	1
4:A:382:PX4:H46	4:A:423:PX4:H32	0.79	1.53	20	1
4:A:367:PX4:H38	4:A:389:PX4:H29	0.78	1.56	14	1
4:A:373:PX4:H50	4:A:410:PX4:H19	0.78	1.54	15	1
4:A:369:PX4:H52	4:A:419:PX4:H19	0.78	1.56	6	1
4:A:308:PX4:H42	4:A:332:PX4:H38	0.78	1.55	17	1
4:A:390:PX4:H31	4:A:416:PX4:H33	0.77	1.56	11	1
4:A:328:PX4:H58	4:A:347:PX4:H53	0.77	1.55	14	1
4:A:352:PX4:H40	4:A:375:PX4:H44	0.77	1.56	18	1
4:A:384:PX4:H59	4:A:427:PX4:H63	0.77	1.57	13	1
4:A:398:PX4:H30	4:A:399:PX4:H34	0.77	1.54	6	1
4:A:374:PX4:H69	4:A:429:PX4:H63	0.76	1.54	20	1
4:A:319:PX4:H62	4:A:343:PX4:H23	0.76	1.56	1	1
4:A:365:PX4:H63	4:A:376:PX4:H23	0.75	1.57	14	1
4:A:322:PX4:H66	4:A:430:PX4:H69	0.75	1.57	17	1
4:A:324:PX4:H53	4:A:333:PX4:H28	0.75	1.59	13	1
4:A:366:PX4:H47	4:A:403:PX4:H16	0.75	1.59	12	2
4:A:360:PX4:H66	4:A:379:PX4:H39	0.75	1.57	12	1
4:A:323:PX4:H61	4:A:325:PX4:H62	0.75	1.57	20	1
4:A:383:PX4:H61	4:A:394:PX4:H50	0.75	1.55	2	1
4:A:397:PX4:H56	4:A:430:PX4:H27	0.75	1.56	16	1
4:A:365:PX4:H30	4:A:383:PX4:H35	0.75	1.57	19	1
4:A:429:PX4:H69	4:A:430:PX4:H31	0.74	1.59	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:306:PX4:H62	4:A:342:PX4:H39	0.74	1.59	11	1
4:A:329:PX4:H42	4:A:335:PX4:H59	0.74	1.57	7	1
4:A:332:PX4:H47	4:A:348:PX4:H47	0.74	1.58	13	1
4:A:370:PX4:H17	4:A:430:PX4:H50	0.74	1.58	8	3
4:A:391:PX4:H28	4:A:408:PX4:H56	0.74	1.59	5	1
4:A:373:PX4:H59	4:A:406:PX4:H26	0.73	1.59	11	1
4:A:371:PX4:H18	4:A:401:PX4:H33	0.73	1.59	17	1
4:A:369:PX4:H30	4:A:429:PX4:H66	0.73	1.60	17	1
4:A:327:PX4:H21	4:A:348:PX4:H22	0.73	1.58	4	1
4:A:313:PX4:H17	4:A:329:PX4:H48	0.73	1.58	4	1
4:A:409:PX4:H17	4:A:412:PX4:H19	0.73	1.60	4	1
4:A:333:PX4:H48	4:A:364:PX4:H53	0.73	1.61	20	1
4:A:341:PX4:H30	4:A:356:PX4:H29	0.73	1.60	17	1
4:A:330:PX4:H20	4:A:337:PX4:H16	0.73	1.59	14	2
4:A:385:PX4:H59	4:A:387:PX4:H54	0.73	1.58	18	1
4:A:306:PX4:H48	4:A:342:PX4:H22	0.73	1.59	9	2
4:A:325:PX4:H57	4:A:353:PX4:H54	0.73	1.59	7	1
4:A:370:PX4:H48	4:A:381:PX4:H47	0.73	1.61	12	1
4:A:372:PX4:H65	4:A:420:PX4:H69	0.73	1.61	4	1
4:A:382:PX4:H66	4:A:397:PX4:H40	0.73	1.59	10	1
4:A:389:PX4:H16	4:A:399:PX4:H46	0.73	1.60	5	1
4:A:365:PX4:H30	4:A:369:PX4:H41	0.72	1.59	1	1
4:A:393:PX4:H16	4:A:419:PX4:H20	0.72	1.61	16	1
4:A:323:PX4:H37	4:A:347:PX4:H20	0.72	1.58	8	1
4:A:361:PX4:H57	4:A:403:PX4:H34	0.72	1.62	12	1
4:A:417:PX4:H22	4:A:418:PX4:H26	0.72	1.59	16	1
4:A:317:PX4:H20	4:A:326:PX4:H16	0.72	1.61	16	1
4:A:347:PX4:H46	4:A:360:PX4:H19	0.72	1.61	12	1
4:A:316:PX4:H53	4:A:343:PX4:H26	0.72	1.62	7	1
4:A:344:PX4:H47	4:A:354:PX4:H9	0.72	1.61	19	1
4:A:383:PX4:H30	4:A:405:PX4:H72	0.71	1.61	1	1
4:A:311:PX4:H20	4:A:324:PX4:H69	0.71	1.63	7	1
4:A:317:PX4:H24	4:A:326:PX4:H21	0.71	1.61	8	1
4:A:375:PX4:H28	4:A:407:PX4:H29	0.71	1.63	14	1
4:A:307:PX4:H49	4:A:337:PX4:H53	0.71	1.60	17	1
4:A:366:PX4:H57	4:A:403:PX4:H50	0.71	1.61	1	1
4:A:353:PX4:H23	4:A:361:PX4:H32	0.71	1.61	7	1
4:A:338:PX4:H46	4:A:347:PX4:H57	0.71	1.63	6	1
4:A:345:PX4:H62	4:A:359:PX4:H17	0.71	1.60	3	1
4:A:316:PX4:H41	4:A:399:PX4:H68	0.71	1.61	6	1
4:A:316:PX4:H50	4:A:343:PX4:H24	0.70	1.62	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:307:PX4:H22	4:A:337:PX4:H52	0.70	1.63	15	1
4:A:367:PX4:H42	4:A:389:PX4:H33	0.70	1.61	14	1
4:A:334:PX4:H70	4:A:373:PX4:H33	0.70	1.63	8	1
4:A:397:PX4:H19	4:A:423:PX4:H61	0.70	1.63	4	1
4:A:308:PX4:H17	4:A:426:PX4:H45	0.70	1.62	9	1
4:A:413:PX4:H35	4:A:428:PX4:H34	0.70	1.63	6	1
4:A:324:PX4:H18	4:A:324:PX4:H1	0.70	1.63	5	1
4:A:333:PX4:H20	5:A:432:C3S:H443	0.70	1.61	4	1
4:A:395:PX4:H60	4:A:405:PX4:H31	0.70	1.62	2	1
4:A:332:PX4:H37	4:A:350:PX4:H22	0.70	1.64	2	1
4:A:365:PX4:H21	4:A:383:PX4:H31	0.70	1.64	12	1
4:A:324:PX4:H38	4:A:368:PX4:H41	0.70	1.64	11	1
4:A:360:PX4:H37	4:A:393:PX4:H72	0.70	1.61	11	1
4:A:312:PX4:H49	4:A:324:PX4:H26	0.70	1.62	11	1
4:A:369:PX4:H44	4:A:429:PX4:H65	0.69	1.64	14	1
4:A:369:PX4:H20	4:A:430:PX4:H16	0.69	1.64	8	1
4:A:373:PX4:H16	4:A:389:PX4:H49	0.69	1.64	19	1
4:A:397:PX4:H67	4:A:411:PX4:H42	0.69	1.64	1	1
4:A:369:PX4:H51	4:A:419:PX4:H57	0.69	1.62	8	1
4:A:397:PX4:H66	4:A:423:PX4:H68	0.69	1.64	12	1
4:A:347:PX4:H61	4:A:360:PX4:H47	0.69	1.63	20	1
4:A:371:PX4:H20	4:A:401:PX4:H41	0.69	1.65	5	1
4:A:428:PX4:H72	4:A:429:PX4:H56	0.69	1.64	5	1
4:A:391:PX4:H16	4:A:427:PX4:H14	0.69	1.63	2	1
4:A:343:PX4:H17	4:A:356:PX4:H46	0.69	1.65	17	1
4:A:308:PX4:H59	4:A:326:PX4:H26	0.69	1.62	18	1
4:A:343:PX4:H48	4:A:356:PX4:H51	0.69	1.64	4	1
4:A:388:PX4:H17	4:A:391:PX4:H50	0.68	1.63	18	1
4:A:369:PX4:H58	4:A:429:PX4:H21	0.68	1.64	19	1
4:A:370:PX4:H62	4:A:381:PX4:H60	0.68	1.65	3	1
4:A:388:PX4:H27	4:A:388:PX4:H48	0.68	1.65	7	1
4:A:386:PX4:H58	4:A:402:PX4:H25	0.68	1.64	9	1
4:A:371:PX4:H19	4:A:386:PX4:H53	0.68	1.64	19	1
4:A:394:PX4:H51	4:A:430:PX4:H59	0.68	1.66	20	1
4:A:318:PX4:H53	4:A:357:PX4:H23	0.68	1.65	6	1
4:A:388:PX4:H67	4:A:390:PX4:H58	0.68	1.65	11	1
4:A:365:PX4:H52	4:A:396:PX4:H49	0.68	1.66	6	1
4:A:316:PX4:H21	4:A:321:PX4:H16	0.68	1.65	3	1
4:A:408:PX4:H67	4:A:427:PX4:H62	0.68	1.66	2	1
4:A:339:PX4:H42	4:A:346:PX4:H66	0.68	1.66	20	1
4:A:365:PX4:H55	4:A:383:PX4:H23	0.68	1.66	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:358:PX4:H23	4:A:358:PX4:H54	0.68	1.66	11	1
4:A:322:PX4:H38	4:A:344:PX4:H41	0.68	1.65	9	1
4:A:315:PX4:H57	4:A:350:PX4:H19	0.68	1.66	20	1
4:A:352:PX4:H7	4:A:352:PX4:O6	0.68	1.89	20	1
4:A:366:PX4:H22	4:A:403:PX4:H32	0.68	1.64	18	1
4:A:393:PX4:H21	4:A:429:PX4:H38	0.68	1.67	4	1
4:A:376:PX4:H17	4:A:388:PX4:H19	0.67	1.65	4	1
4:A:316:PX4:H32	4:A:318:PX4:H40	0.67	1.67	14	1
4:A:307:PX4:H29	4:A:327:PX4:H56	0.67	1.64	2	1
4:A:318:PX4:H22	4:A:321:PX4:H51	0.67	1.65	7	1
4:A:322:PX4:H50	4:A:337:PX4:H17	0.67	1.65	13	1
4:A:365:PX4:H55	4:A:376:PX4:H55	0.67	1.64	18	1
4:A:306:PX4:H36	4:A:342:PX4:H41	0.67	1.66	13	1
4:A:327:PX4:H23	4:A:338:PX4:H58	0.67	1.65	12	1
4:A:312:PX4:H20	4:A:346:PX4:H19	0.67	1.64	10	1
4:A:400:PX4:H33	4:A:401:PX4:H67	0.67	1.67	20	1
4:A:320:PX4:H35	4:A:332:PX4:H38	0.67	1.64	7	1
4:A:320:PX4:H63	4:A:334:PX4:H59	0.67	1.66	2	1
4:A:322:PX4:H69	4:A:369:PX4:H31	0.67	1.67	15	1
4:A:309:PX4:H22	4:A:328:PX4:H24	0.67	1.65	10	1
4:A:347:PX4:H53	4:A:351:PX4:H43	0.67	1.66	3	1
4:A:365:PX4:H47	4:A:383:PX4:H16	0.67	1.65	13	1
4:A:369:PX4:H18	4:A:429:PX4:H54	0.67	1.67	17	1
4:A:374:PX4:H64	4:A:381:PX4:H69	0.66	1.66	13	1
4:A:397:PX4:H16	4:A:411:PX4:H23	0.66	1.66	19	1
4:A:347:PX4:H22	4:A:351:PX4:H30	0.66	1.66	20	1
4:A:387:PX4:H31	4:A:416:PX4:H57	0.66	1.67	4	1
4:A:400:PX4:H20	4:A:401:PX4:H14	0.66	1.67	9	1
4:A:310:PX4:H50	4:A:333:PX4:H48	0.66	1.67	15	1
4:A:328:PX4:H51	4:A:347:PX4:H16	0.66	1.67	14	1
4:A:365:PX4:O3	4:A:369:PX4:H7	0.66	1.90	8	1
4:A:383:PX4:H21	4:A:396:PX4:H50	0.66	1.65	18	1
4:A:325:PX4:H45	4:A:325:PX4:H67	0.66	1.67	3	1
4:A:345:PX4:H49	4:A:358:PX4:H16	0.66	1.67	7	1
4:A:376:PX4:H14	4:A:390:PX4:H9	0.66	1.67	11	1
4:A:357:PX4:H26	4:A:363:PX4:H24	0.66	1.68	3	1
4:A:317:PX4:H36	4:A:326:PX4:H32	0.66	1.68	14	1
4:A:305:PX4:H38	4:A:310:PX4:H33	0.66	1.68	19	1
4:A:365:PX4:H27	4:A:369:PX4:H62	0.66	1.66	4	1
4:A:372:PX4:H17	4:A:420:PX4:H55	0.66	1.66	4	1
4:A:375:PX4:H21	4:A:392:PX4:H31	0.66	1.68	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:319:PX4:H21	4:A:352:PX4:H17	0.66	1.69	6	1
4:A:336:PX4:H17	4:A:354:PX4:H15	0.66	1.65	7	1
4:A:305:PX4:H67	4:A:426:PX4:H67	0.65	1.66	11	1
4:A:386:PX4:H28	4:A:401:PX4:H44	0.65	1.69	2	1
4:A:397:PX4:H48	4:A:423:PX4:H60	0.65	1.67	16	1
4:A:414:PX4:O6	4:A:426:PX4:H6	0.65	1.91	9	1
4:A:317:PX4:H40	4:A:326:PX4:H37	0.65	1.66	7	1
4:A:316:PX4:H64	4:A:389:PX4:H72	0.65	1.66	16	1
4:A:309:PX4:H19	4:A:328:PX4:H31	0.65	1.69	12	1
4:A:323:PX4:H18	4:A:328:PX4:H2	0.65	1.68	11	1
4:A:330:PX4:H69	4:A:415:PX4:H67	0.65	1.68	9	1
4:A:315:PX4:H53	4:A:332:PX4:H21	0.65	1.69	1	1
4:A:371:PX4:H14	4:A:373:PX4:H20	0.65	1.68	5	1
4:A:305:PX4:H36	4:A:310:PX4:H34	0.65	1.69	4	1
4:A:305:PX4:H50	4:A:312:PX4:H47	0.65	1.69	13	1
4:A:404:PX4:H33	4:A:418:PX4:H72	0.65	1.67	11	1
4:A:326:PX4:H60	4:A:353:PX4:H63	0.65	1.68	13	1
4:A:371:PX4:H68	4:A:399:PX4:H30	0.65	1.69	6	1
4:A:386:PX4:H47	4:A:417:PX4:H58	0.65	1.68	17	1
4:A:384:PX4:H50	4:A:389:PX4:H23	0.65	1.66	15	1
4:A:369:PX4:H25	4:A:430:PX4:H24	0.65	1.67	10	1
4:A:329:PX4:H51	4:A:355:PX4:H46	0.65	1.69	13	1
4:A:369:PX4:H18	4:A:429:PX4:H49	0.65	1.69	6	1
4:A:308:PX4:H32	4:A:332:PX4:H31	0.65	1.69	8	1
4:A:428:PX4:H52	4:A:430:PX4:H25	0.64	1.69	11	1
4:A:335:PX4:H53	4:A:363:PX4:H54	0.64	1.67	20	1
4:A:318:PX4:H28	4:A:357:PX4:H28	0.64	1.69	15	1
4:A:387:PX4:H71	4:A:403:PX4:H35	0.64	1.67	12	1
4:A:428:PX4:H24	4:A:429:PX4:H22	0.64	1.70	9	1
4:A:394:PX4:H38	4:A:400:PX4:H69	0.64	1.69	5	1
4:A:308:PX4:H20	4:A:326:PX4:H54	0.64	1.67	2	1
4:A:373:PX4:H18	4:A:406:PX4:H49	0.64	1.69	8	1
4:A:341:PX4:H64	4:A:352:PX4:H56	0.64	1.68	17	1
4:A:403:PX4:H47	4:A:421:PX4:H17	0.64	1.69	16	1
4:A:320:PX4:H64	4:A:340:PX4:H22	0.64	1.67	3	1
4:A:317:PX4:H30	4:A:325:PX4:H25	0.64	1.69	7	1
4:A:305:PX4:H45	4:A:311:PX4:H68	0.64	1.66	4	1
4:A:338:PX4:H16	4:A:344:PX4:H47	0.64	1.68	20	2
4:A:415:PX4:H32	4:A:421:PX4:H29	0.64	1.69	20	1
4:A:335:PX4:H46	4:A:354:PX4:H46	0.64	1.68	3	1
4:A:376:PX4:H50	4:A:376:PX4:H20	0.64	1.68	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:319:PX4:O2	4:A:336:PX4:H9	0.64	1.93	8	1
4:A:335:PX4:H64	4:A:347:PX4:H68	0.64	1.70	11	1
4:A:383:PX4:H38	4:A:419:PX4:H60	0.64	1.68	12	1
4:A:392:PX4:H14	4:A:392:PX4:H6	0.64	1.70	4	1
4:A:317:PX4:H50	4:A:325:PX4:H30	0.64	1.70	8	1
4:A:377:PX4:H59	4:A:377:PX4:H29	0.64	1.68	19	1
4:A:334:PX4:H64	5:A:432:C3S:H443	0.64	1.68	2	1
5:A:436:C3S:H402	5:A:436:C3S:H501	0.64	1.70	17	2
4:A:365:PX4:H50	4:A:407:PX4:H47	0.63	1.68	13	1
4:A:366:PX4:H16	4:A:378:PX4:H20	0.63	1.69	18	2
4:A:371:PX4:H59	4:A:389:PX4:C5	0.63	2.22	15	1
4:A:369:PX4:H42	4:A:430:PX4:H45	0.63	1.67	11	1
4:A:308:PX4:H69	4:A:355:PX4:H45	0.63	1.69	20	1
4:A:370:PX4:H16	4:A:394:PX4:H15	0.63	1.68	3	2
4:A:383:PX4:H25	4:A:383:PX4:H52	0.63	1.69	14	1
4:A:382:PX4:H54	4:A:404:PX4:H45	0.63	1.70	12	1
4:A:339:PX4:H61	4:A:357:PX4:H59	0.63	1.68	9	1
4:A:328:PX4:H17	4:A:347:PX4:H20	0.63	1.69	7	1
4:A:324:PX4:H42	4:A:346:PX4:H33	0.63	1.70	16	1
4:A:371:PX4:H19	4:A:402:PX4:H22	0.63	1.69	7	1
4:A:380:PX4:H16	4:A:385:PX4:H10	0.63	1.69	19	1
4:A:375:PX4:H70	4:A:405:PX4:H37	0.63	1.71	3	1
1:A:222:GLN:O	4:A:317:PX4:H1	0.63	1.94	12	3
4:A:326:PX4:H39	4:A:326:PX4:H66	0.63	1.71	1	1
4:A:373:PX4:H28	4:A:406:PX4:H52	0.63	1.71	14	1
4:A:321:PX4:H59	4:A:357:PX4:H40	0.63	1.71	17	1
4:A:376:PX4:H61	4:A:390:PX4:H30	0.63	1.70	8	1
4:A:312:PX4:H53	4:A:346:PX4:H61	0.63	1.69	16	1
4:A:308:PX4:H24	4:A:320:PX4:H50	0.63	1.71	16	1
4:A:371:PX4:H59	4:A:389:PX4:H13	0.63	1.68	15	1
4:A:336:PX4:H23	4:A:354:PX4:H27	0.63	1.70	9	1
4:A:338:PX4:H40	4:A:344:PX4:H28	0.63	1.70	2	1
4:A:388:PX4:H2	4:A:391:PX4:H15	0.63	1.71	8	1
4:A:375:PX4:O6	4:A:392:PX4:H6	0.63	1.93	5	1
1:A:107:ARG:HG3	4:A:315:PX4:H46	0.62	1.71	20	2
4:A:376:PX4:H25	4:A:396:PX4:H26	0.62	1.70	17	1
4:A:365:PX4:H62	4:A:407:PX4:H58	0.62	1.71	9	1
4:A:318:PX4:H17	4:A:357:PX4:H27	0.62	1.71	1	1
4:A:389:PX4:H16	4:A:399:PX4:H53	0.62	1.70	1	1
4:A:318:PX4:H26	4:A:342:PX4:H18	0.62	1.69	9	2
4:A:311:PX4:H52	4:A:313:PX4:H52	0.62	1.68	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:307:PX4:H57	4:A:348:PX4:H66	0.62	1.70	2	1
4:A:306:PX4:H53	4:A:342:PX4:H27	0.62	1.69	11	1
4:A:318:PX4:H59	4:A:336:PX4:H34	0.62	1.71	19	1
4:A:305:PX4:H24	4:A:311:PX4:H16	0.62	1.70	15	1
4:A:410:PX4:H18	4:A:410:PX4:H2	0.62	1.70	15	1
4:A:306:PX4:H16	4:A:358:PX4:H46	0.62	1.71	9	1
4:A:341:PX4:H10	4:A:356:PX4:O6	0.62	1.94	8	1
4:A:386:PX4:H31	4:A:417:PX4:H67	0.62	1.71	19	1
4:A:380:PX4:H16	4:A:385:PX4:H23	0.62	1.71	20	1
4:A:309:PX4:H32	4:A:347:PX4:H40	0.62	1.69	3	1
4:A:330:PX4:H62	4:A:337:PX4:H34	0.62	1.71	11	1
4:A:365:PX4:H46	4:A:376:PX4:H49	0.62	1.72	2	1
4:A:307:PX4:H69	4:A:430:PX4:H66	0.62	1.71	2	1
4:A:365:PX4:H22	4:A:370:PX4:H26	0.62	1.70	10	1
4:A:361:PX4:H58	4:A:378:PX4:H42	0.62	1.70	7	1
4:A:397:PX4:H16	4:A:411:PX4:H21	0.62	1.71	10	1
4:A:316:PX4:H52	4:A:352:PX4:H46	0.62	1.71	8	1
4:A:335:PX4:H46	4:A:354:PX4:H49	0.62	1.69	16	1
4:A:306:PX4:H59	4:A:359:PX4:H56	0.62	1.72	12	1
4:A:337:PX4:H20	4:A:355:PX4:H31	0.62	1.72	13	1
4:A:383:PX4:H59	4:A:394:PX4:H30	0.62	1.71	17	1
4:A:306:PX4:H57	4:A:359:PX4:H46	0.62	1.71	9	1
4:A:396:PX4:H27	4:A:407:PX4:H21	0.62	1.72	1	1
4:A:335:PX4:H17	4:A:347:PX4:H53	0.62	1.72	5	1
4:A:429:PX4:H54	4:A:430:PX4:H23	0.61	1.72	14	1
1:A:125:ARG:HH21	4:A:359:PX4:H14	0.61	1.55	19	1
4:A:386:PX4:H44	4:A:417:PX4:H66	0.61	1.71	15	1
4:A:310:PX4:H72	4:A:364:PX4:H69	0.61	1.72	9	1
4:A:376:PX4:H54	4:A:376:PX4:H24	0.61	1.72	3	1
4:A:308:PX4:H55	4:A:403:PX4:H39	0.61	1.70	6	1
4:A:389:PX4:O1	4:A:401:PX4:H13	0.61	1.93	20	1
4:A:325:PX4:H10	4:A:325:PX4:H14	0.61	1.71	5	1
4:A:320:PX4:H44	4:A:402:PX4:H66	0.61	1.72	18	1
4:A:410:PX4:H29	4:A:424:PX4:H27	0.61	1.70	1	1
4:A:368:PX4:H50	4:A:414:PX4:H29	0.61	1.72	13	1
4:A:369:PX4:H55	4:A:429:PX4:H21	0.61	1.72	11	1
4:A:371:PX4:H68	4:A:375:PX4:H65	0.61	1.72	11	1
4:A:366:PX4:H32	4:A:402:PX4:H30	0.61	1.72	7	1
4:A:400:PX4:H3	4:A:401:PX4:O1	0.61	1.96	14	1
4:A:413:PX4:H60	4:A:422:PX4:H64	0.61	1.73	4	1
4:A:312:PX4:H16	4:A:346:PX4:H47	0.61	1.71	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:317:PX4:H54	4:A:330:PX4:H33	0.61	1.73	7	1
4:A:308:PX4:H30	4:A:320:PX4:H58	0.61	1.71	5	1
4:A:331:PX4:H54	4:A:344:PX4:H34	0.61	1.72	20	1
4:A:394:PX4:H31	4:A:400:PX4:H20	0.61	1.73	6	1
4:A:343:PX4:H57	4:A:350:PX4:H17	0.61	1.70	10	3
4:A:396:PX4:H31	4:A:407:PX4:H27	0.61	1.73	16	1
4:A:368:PX4:H8	4:A:406:PX4:O6	0.61	1.96	1	1
4:A:394:PX4:H43	4:A:405:PX4:H33	0.61	1.71	3	1
4:A:351:PX4:H42	4:A:419:PX4:H69	0.61	1.72	13	1
4:A:338:PX4:H20	4:A:344:PX4:H53	0.61	1.72	17	1
4:A:376:PX4:H20	4:A:396:PX4:H49	0.61	1.71	17	1
4:A:360:PX4:H62	4:A:429:PX4:H36	0.61	1.72	16	1
4:A:319:PX4:H54	4:A:341:PX4:H55	0.61	1.72	3	1
4:A:358:PX4:H66	4:A:407:PX4:H42	0.61	1.72	13	1
4:A:324:PX4:H30	4:A:346:PX4:H60	0.61	1.71	6	1
4:A:340:PX4:H9	4:A:340:PX4:H16	0.61	1.71	6	1
4:A:382:PX4:H46	4:A:423:PX4:H56	0.61	1.71	4	1
4:A:327:PX4:H16	4:A:351:PX4:H4	0.60	1.73	14	1
4:A:372:PX4:O2	4:A:380:PX4:H20	0.60	1.96	12	1
4:A:401:PX4:H63	4:A:405:PX4:H36	0.60	1.72	4	1
4:A:395:PX4:H33	4:A:402:PX4:H60	0.60	1.73	3	1
4:A:370:PX4:H17	4:A:430:PX4:H46	0.60	1.71	18	1
4:A:319:PX4:H17	4:A:352:PX4:H50	0.60	1.73	19	1
4:A:321:PX4:H54	4:A:342:PX4:H35	0.60	1.74	15	1
4:A:414:PX4:H50	4:A:426:PX4:H21	0.60	1.71	12	1
4:A:315:PX4:H57	4:A:350:PX4:H21	0.60	1.73	1	1
4:A:388:PX4:H61	4:A:403:PX4:H65	0.60	1.73	5	1
4:A:384:PX4:H62	5:A:434:C3S:H601	0.60	1.71	14	1
4:A:376:PX4:H65	4:A:390:PX4:H51	0.60	1.72	19	1
4:A:404:PX4:H29	4:A:417:PX4:H24	0.60	1.73	15	1
4:A:322:PX4:H65	4:A:365:PX4:H40	0.60	1.72	10	1
4:A:340:PX4:H28	5:A:432:C3S:H262	0.60	1.73	9	1
4:A:401:PX4:H71	4:A:405:PX4:H29	0.60	1.73	7	1
4:A:403:PX4:H17	4:A:421:PX4:H51	0.60	1.73	7	1
4:A:426:PX4:H15	4:A:426:PX4:H13	0.60	1.72	5	1
4:A:399:PX4:H38	5:A:435:C3S:H693	0.60	1.73	6	1
4:A:321:PX4:H69	4:A:427:PX4:H33	0.60	1.72	11	1
4:A:309:PX4:H58	4:A:345:PX4:H41	0.60	1.74	9	1
4:A:404:PX4:H23	4:A:418:PX4:H27	0.60	1.73	9	1
4:A:387:PX4:H20	4:A:415:PX4:H22	0.60	1.73	1	1
4:A:308:PX4:H36	4:A:332:PX4:H27	0.60	1.73	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:413:PX4:H31	4:A:429:PX4:H32	0.60	1.72	4	1
4:A:306:PX4:H22	4:A:358:PX4:H47	0.60	1.73	5	2
4:A:403:PX4:H46	4:A:421:PX4:H17	0.60	1.74	7	1
4:A:365:PX4:C24	4:A:383:PX4:H23	0.60	2.27	17	1
4:A:322:PX4:H32	4:A:331:PX4:H25	0.60	1.73	4	1
4:A:306:PX4:H56	4:A:342:PX4:H29	0.60	1.73	9	1
4:A:411:PX4:H28	4:A:423:PX4:H58	0.60	1.71	20	1
4:A:305:PX4:H57	4:A:312:PX4:H59	0.60	1.74	5	2
4:A:370:PX4:H17	4:A:430:PX4:C26	0.60	2.27	8	1
4:A:369:PX4:H46	4:A:419:PX4:H17	0.60	1.72	3	1
4:A:346:PX4:H38	5:A:431:C3S:H691	0.59	1.74	17	1
4:A:320:PX4:H24	4:A:326:PX4:H60	0.59	1.74	4	1
4:A:333:PX4:H22	4:A:340:PX4:H52	0.59	1.72	13	1
4:A:375:PX4:H68	4:A:392:PX4:H29	0.59	1.74	8	1
4:A:384:PX4:H23	4:A:405:PX4:H20	0.59	1.72	11	1
4:A:348:PX4:H34	4:A:359:PX4:H54	0.59	1.74	10	1
4:A:395:PX4:H30	4:A:401:PX4:H40	0.59	1.75	9	1
4:A:316:PX4:H21	4:A:352:PX4:H25	0.59	1.74	7	1
4:A:322:PX4:H72	4:A:337:PX4:H59	0.59	1.73	13	1
4:A:316:PX4:H16	4:A:321:PX4:H11	0.59	1.71	17	1
4:A:387:PX4:H26	4:A:416:PX4:H19	0.59	1.75	15	1
4:A:406:PX4:H70	4:A:426:PX4:H54	0.59	1.73	9	1
4:A:422:PX4:H53	4:A:425:PX4:H53	0.59	1.73	14	1
4:A:369:PX4:H62	4:A:430:PX4:H42	0.59	1.74	2	1
4:A:313:PX4:H29	4:A:362:PX4:H56	0.59	1.73	16	1
4:A:386:PX4:H52	4:A:402:PX4:H22	0.59	1.74	18	1
4:A:411:PX4:H64	4:A:412:PX4:H71	0.59	1.73	18	1
4:A:370:PX4:H50	4:A:381:PX4:H17	0.59	1.72	10	1
4:A:308:PX4:H47	4:A:361:PX4:H63	0.59	1.73	20	1
4:A:404:PX4:H21	4:A:418:PX4:H17	0.59	1.74	17	1
4:A:412:PX4:H17	4:A:424:PX4:H54	0.59	1.74	8	1
4:A:404:PX4:H40	4:A:417:PX4:H39	0.59	1.74	7	1
4:A:362:PX4:H67	4:A:415:PX4:H67	0.59	1.74	14	1
4:A:415:PX4:H32	4:A:418:PX4:H66	0.59	1.74	14	1
4:A:327:PX4:H71	4:A:429:PX4:H37	0.59	1.74	8	1
4:A:391:PX4:H31	4:A:407:PX4:H31	0.59	1.75	4	1
4:A:368:PX4:H61	4:A:426:PX4:H58	0.59	1.75	9	1
4:A:342:PX4:H39	4:A:407:PX4:H37	0.59	1.74	2	1
4:A:371:PX4:H18	4:A:401:PX4:C17	0.59	2.28	17	1
4:A:371:PX4:H65	4:A:384:PX4:H19	0.59	1.73	19	1
4:A:310:PX4:H53	4:A:364:PX4:H55	0.59	1.75	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:306:PX4:H20	4:A:358:PX4:H47	0.59	1.73	4	1
4:A:405:PX4:H56	4:A:407:PX4:H23	0.59	1.73	1	1
4:A:336:PX4:H50	4:A:338:PX4:H28	0.59	1.74	3	1
4:A:369:PX4:H30	4:A:381:PX4:H67	0.59	1.74	2	1
4:A:387:PX4:H47	4:A:421:PX4:H16	0.59	1.72	8	1
4:A:404:PX4:O1	4:A:418:PX4:H3	0.59	1.98	16	1
4:A:397:PX4:H3	4:A:411:PX4:O6	0.59	1.98	4	1
4:A:324:PX4:H58	4:A:334:PX4:H55	0.59	1.74	10	1
4:A:305:PX4:H28	4:A:311:PX4:H30	0.59	1.72	5	1
4:A:338:PX4:H69	4:A:359:PX4:H32	0.59	1.74	3	1
4:A:351:PX4:H19	4:A:359:PX4:H32	0.59	1.75	16	1
4:A:312:PX4:H20	4:A:339:PX4:H22	0.59	1.75	1	1
4:A:366:PX4:H22	4:A:403:PX4:H20	0.59	1.74	7	1
4:A:369:PX4:H59	4:A:393:PX4:H29	0.59	1.74	7	1
4:A:321:PX4:H48	4:A:342:PX4:H35	0.58	1.73	16	1
4:A:382:PX4:H53	4:A:423:PX4:H39	0.58	1.75	1	1
4:A:339:PX4:H18	4:A:339:PX4:H2	0.58	1.74	7	1
4:A:307:PX4:H54	4:A:332:PX4:H30	0.58	1.73	13	1
4:A:400:PX4:H24	4:A:401:PX4:H17	0.58	1.74	8	2
4:A:386:PX4:H67	4:A:426:PX4:H64	0.58	1.73	18	1
4:A:325:PX4:H23	4:A:362:PX4:H55	0.58	1.74	9	1
4:A:315:PX4:H43	4:A:381:PX4:H70	0.58	1.76	8	1
4:A:341:PX4:H45	4:A:367:PX4:H35	0.58	1.73	11	1
4:A:339:PX4:H28	4:A:346:PX4:H67	0.58	1.76	4	1
4:A:359:PX4:H6	4:A:359:PX4:H18	0.58	1.74	7	1
4:A:370:PX4:H30	4:A:430:PX4:H60	0.58	1.75	11	1
4:A:334:PX4:H39	4:A:426:PX4:H25	0.58	1.75	3	1
4:A:366:PX4:H37	4:A:378:PX4:H61	0.58	1.75	7	1
4:A:409:PX4:H5	4:A:412:PX4:O6	0.58	1.98	5	1
4:A:329:PX4:H34	4:A:360:PX4:H33	0.58	1.75	14	1
4:A:387:PX4:H17	4:A:421:PX4:H20	0.58	1.74	2	2
4:A:380:PX4:H33	4:A:385:PX4:H35	0.58	1.75	8	1
4:A:354:PX4:H66	4:A:416:PX4:H70	0.58	1.73	5	1
4:A:396:PX4:O6	4:A:407:PX4:H9	0.58	1.97	12	1
4:A:313:PX4:H17	4:A:355:PX4:H50	0.58	1.75	20	1
4:A:314:PX4:H15	4:A:314:PX4:H13	0.58	1.76	7	1
4:A:372:PX4:H17	4:A:380:PX4:H27	0.58	1.75	7	1
4:A:328:PX4:H49	4:A:347:PX4:H16	0.58	1.73	5	1
4:A:399:PX4:H22	4:A:424:PX4:H24	0.58	1.75	5	1
4:A:422:PX4:H36	4:A:425:PX4:H61	0.58	1.74	5	1
4:A:308:PX4:H42	4:A:350:PX4:H26	0.58	1.76	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:385:PX4:H68	4:A:415:PX4:H35	0.58	1.76	14	1
4:A:327:PX4:H22	4:A:338:PX4:H58	0.58	1.75	2	1
4:A:409:PX4:H33	5:A:434:C3S:H403	0.58	1.75	17	1
4:A:338:PX4:O1	4:A:344:PX4:H3	0.58	1.98	9	1
4:A:325:PX4:H17	4:A:353:PX4:H20	0.58	1.74	1	1
4:A:307:PX4:H33	4:A:337:PX4:H71	0.58	1.74	20	1
4:A:392:PX4:H48	4:A:427:PX4:H47	0.58	1.75	7	1
4:A:324:PX4:O1	4:A:334:PX4:H6	0.58	1.99	16	1
4:A:387:PX4:H26	4:A:416:PX4:H17	0.58	1.75	18	1
4:A:327:PX4:H4	4:A:348:PX4:H18	0.58	1.75	19	1
4:A:406:PX4:H32	4:A:410:PX4:H61	0.58	1.76	1	1
4:A:409:PX4:H66	4:A:412:PX4:H65	0.58	1.75	8	1
4:A:367:PX4:H60	4:A:412:PX4:H52	0.58	1.76	16	1
4:A:305:PX4:H32	4:A:310:PX4:H34	0.58	1.76	18	1
4:A:316:PX4:H30	4:A:318:PX4:H47	0.58	1.74	20	1
4:A:375:PX4:H64	4:A:405:PX4:H66	0.58	1.76	3	1
4:A:337:PX4:H68	4:A:397:PX4:H43	0.58	1.76	13	1
4:A:324:PX4:H55	4:A:334:PX4:H51	0.58	1.76	4	1
4:A:314:PX4:H57	4:A:354:PX4:H38	0.57	1.74	13	1
4:A:365:PX4:H24	4:A:396:PX4:H49	0.57	1.76	9	1
4:A:347:PX4:H21	4:A:360:PX4:H22	0.57	1.76	5	1
4:A:375:PX4:H32	4:A:427:PX4:H27	0.57	1.76	6	1
4:A:328:PX4:H43	4:A:338:PX4:H62	0.57	1.75	12	1
4:A:323:PX4:H46	4:A:325:PX4:C6	0.57	2.29	5	1
4:A:377:PX4:H48	4:A:420:PX4:H46	0.57	1.74	5	1
4:A:319:PX4:H47	4:A:341:PX4:H65	0.57	1.75	18	1
4:A:327:PX4:H27	4:A:348:PX4:H51	0.57	1.76	18	1
4:A:423:PX4:H68	4:A:430:PX4:H36	0.57	1.76	18	1
4:A:316:PX4:H57	4:A:319:PX4:H45	0.57	1.73	3	1
4:A:323:PX4:H14	4:A:353:PX4:O7	0.57	1.99	7	1
4:A:310:PX4:H21	4:A:311:PX4:H17	0.57	1.76	19	1
4:A:373:PX4:H28	4:A:401:PX4:H37	0.57	1.77	5	1
4:A:364:PX4:H45	4:A:372:PX4:H44	0.57	1.75	6	1
4:A:371:PX4:H47	4:A:373:PX4:H23	0.57	1.77	14	1
1:A:125:ARG:CZ	4:A:306:PX4:H53	0.57	2.30	8	1
4:A:377:PX4:H55	4:A:377:PX4:H25	0.57	1.76	19	1
4:A:373:PX4:H47	4:A:406:PX4:H17	0.57	1.75	11	1
4:A:365:PX4:H15	4:A:383:PX4:H19	0.57	1.77	4	1
4:A:353:PX4:H29	4:A:355:PX4:H67	0.57	1.76	20	1
4:A:373:PX4:H17	4:A:406:PX4:H49	0.57	1.76	13	1
4:A:327:PX4:H30	4:A:348:PX4:H51	0.57	1.74	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:420:PX4:H27	4:A:422:PX4:H49	0.57	1.75	10	1
4:A:365:PX4:H53	4:A:383:PX4:H34	0.57	1.76	7	1
4:A:310:PX4:H44	4:A:364:PX4:H65	0.57	1.75	13	1
4:A:343:PX4:H28	4:A:352:PX4:H52	0.57	1.75	2	1
4:A:338:PX4:H28	4:A:344:PX4:H25	0.57	1.75	16	1
4:A:316:PX4:H49	4:A:321:PX4:H24	0.57	1.75	12	1
4:A:322:PX4:H69	4:A:327:PX4:H44	0.57	1.76	13	1
4:A:316:PX4:O1	4:A:352:PX4:H14	0.57	2.00	8	1
4:A:375:PX4:H15	4:A:405:PX4:O3	0.57	2.00	8	1
4:A:375:PX4:H22	4:A:405:PX4:H47	0.57	1.77	15	1
4:A:375:PX4:H59	4:A:399:PX4:H67	0.57	1.75	12	1
4:A:353:PX4:H19	4:A:361:PX4:H54	0.57	1.77	4	1
4:A:312:PX4:H47	4:A:324:PX4:H16	0.57	1.77	20	3
4:A:316:PX4:H64	4:A:350:PX4:H66	0.57	1.76	6	1
4:A:409:PX4:H51	4:A:428:PX4:H28	0.57	1.76	8	1
1:A:2:GLN:HE22	1:A:57:ARG:CZ	0.57	2.12	8	1
4:A:316:PX4:H21	4:A:321:PX4:H22	0.57	1.75	16	1
4:A:306:PX4:H56	4:A:321:PX4:H17	0.57	1.75	15	1
4:A:320:PX4:H52	4:A:334:PX4:H28	0.57	1.75	10	1
4:A:370:PX4:H66	4:A:381:PX4:H64	0.57	1.75	3	1
4:A:394:PX4:H33	4:A:400:PX4:H65	0.57	1.77	5	1
4:A:414:PX4:H25	5:A:432:C3S:H693	0.57	1.77	6	1
4:A:324:PX4:H71	4:A:408:PX4:H71	0.57	1.76	9	1
4:A:414:PX4:H55	4:A:426:PX4:H63	0.57	1.76	7	1
1:A:88:VAL:HG11	4:A:306:PX4:H46	0.56	1.75	13	1
4:A:331:PX4:H23	4:A:337:PX4:H25	0.56	1.77	16	1
4:A:379:PX4:H20	4:A:422:PX4:H46	0.56	1.77	15	1
4:A:422:PX4:H13	4:A:425:PX4:O8	0.56	2.00	10	1
4:A:395:PX4:H32	4:A:402:PX4:H56	0.56	1.76	1	1
4:A:396:PX4:H53	4:A:407:PX4:H58	0.56	1.76	20	1
4:A:389:PX4:H59	4:A:401:PX4:H36	0.56	1.77	7	1
4:A:380:PX4:H38	4:A:420:PX4:H66	0.56	1.76	7	1
4:A:397:PX4:H53	4:A:423:PX4:H60	0.56	1.77	13	1
4:A:318:PX4:H21	4:A:357:PX4:H38	0.56	1.76	2	1
4:A:331:PX4:H62	4:A:354:PX4:H28	0.56	1.77	18	1
4:A:412:PX4:H61	4:A:424:PX4:H58	0.56	1.77	11	1
4:A:343:PX4:H69	4:A:350:PX4:H29	0.56	1.77	1	1
4:A:369:PX4:O4	4:A:419:PX4:H5	0.56	2.01	13	1
4:A:370:PX4:H60	4:A:370:PX4:H33	0.56	1.77	13	1
4:A:336:PX4:H17	4:A:354:PX4:H50	0.56	1.76	17	1
4:A:409:PX4:H48	4:A:412:PX4:H19	0.56	1.77	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:411:PX4:H49	4:A:412:PX4:H51	0.56	1.77	12	1
4:A:313:PX4:H14	4:A:313:PX4:H12	0.56	1.76	11	1
4:A:387:PX4:H38	4:A:421:PX4:H44	0.56	1.77	9	1
4:A:409:PX4:H17	4:A:412:PX4:H22	0.56	1.77	8	1
4:A:327:PX4:H19	4:A:348:PX4:H29	0.56	1.77	16	1
4:A:387:PX4:H59	4:A:421:PX4:H55	0.56	1.76	16	1
4:A:392:PX4:H17	4:A:425:PX4:H20	0.56	1.76	10	1
4:A:315:PX4:H49	4:A:332:PX4:H21	0.56	1.76	1	1
4:A:368:PX4:H22	5:A:436:C3S:H571	0.56	1.78	1	1
4:A:371:PX4:H68	4:A:373:PX4:H59	0.56	1.77	20	1
4:A:331:PX4:O2	4:A:337:PX4:H3	0.56	2.00	7	1
4:A:338:PX4:H24	4:A:344:PX4:H21	0.56	1.77	13	1
4:A:384:PX4:H18	4:A:384:PX4:O3	0.56	2.01	6	1
4:A:345:PX4:H63	4:A:359:PX4:H50	0.56	1.77	4	1
4:A:400:PX4:H27	4:A:401:PX4:H17	0.56	1.77	10	1
4:A:372:PX4:H36	4:A:406:PX4:H33	0.56	1.77	13	1
4:A:352:PX4:H34	4:A:407:PX4:H35	0.56	1.76	8	1
4:A:381:PX4:H29	4:A:418:PX4:H37	0.56	1.75	9	1
4:A:340:PX4:H25	4:A:356:PX4:H64	0.56	1.77	3	1
4:A:306:PX4:H17	4:A:342:PX4:H19	0.56	1.77	6	1
4:A:318:PX4:H20	4:A:342:PX4:H52	0.56	1.78	16	1
4:A:415:PX4:H22	4:A:415:PX4:H51	0.56	1.76	16	1
4:A:351:PX4:H28	4:A:359:PX4:H19	0.56	1.77	19	1
4:A:396:PX4:H3	4:A:407:PX4:O1	0.56	2.01	19	1
4:A:315:PX4:H42	4:A:374:PX4:H64	0.56	1.77	15	1
4:A:380:PX4:H17	4:A:420:PX4:O2	0.56	2.00	15	1
4:A:409:PX4:H11	5:A:434:C3S:H92	0.56	1.78	7	1
4:A:406:PX4:H49	4:A:414:PX4:H26	0.56	1.77	14	1
4:A:409:PX4:H32	4:A:412:PX4:H33	0.56	1.78	4	1
1:A:23:TYR:CE1	1:A:72:VAL:HG21	0.56	2.36	10	1
4:A:392:PX4:H50	4:A:425:PX4:H53	0.56	1.78	17	1
4:A:376:PX4:H19	4:A:396:PX4:H25	0.56	1.76	18	1
4:A:318:PX4:H31	4:A:342:PX4:H65	0.56	1.76	19	1
4:A:338:PX4:H32	4:A:344:PX4:H23	0.56	1.76	12	1
4:A:343:PX4:H41	4:A:425:PX4:H70	0.56	1.78	5	1
4:A:305:PX4:H28	4:A:310:PX4:H56	0.56	1.78	14	1
4:A:316:PX4:H25	4:A:321:PX4:H32	0.56	1.76	14	1
4:A:315:PX4:H26	4:A:332:PX4:H24	0.56	1.78	16	1
4:A:354:PX4:H37	4:A:409:PX4:H42	0.56	1.77	18	1
4:A:366:PX4:H12	4:A:403:PX4:O2	0.56	2.01	12	1
4:A:397:PX4:H21	4:A:411:PX4:O5	0.56	2.00	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:322:PX4:H11	4:A:344:PX4:O1	0.56	2.01	7	1
4:A:333:PX4:H14	5:A:432:C3S:H30	0.55	1.76	17	1
4:A:330:PX4:H33	4:A:337:PX4:H47	0.55	1.77	5	1
4:A:377:PX4:H25	4:A:377:PX4:H58	0.55	1.77	13	1
4:A:318:PX4:H70	4:A:389:PX4:H40	0.55	1.78	14	1
4:A:388:PX4:H13	4:A:388:PX4:H15	0.55	1.77	14	1
4:A:400:PX4:H47	4:A:405:PX4:H16	0.55	1.78	5	2
4:A:311:PX4:O8	4:A:329:PX4:H10	0.55	2.01	16	1
4:A:386:PX4:H23	4:A:402:PX4:H48	0.55	1.76	18	1
4:A:406:PX4:O1	4:A:410:PX4:H15	0.55	2.01	19	1
4:A:403:PX4:O2	4:A:421:PX4:H10	0.55	2.00	15	1
4:A:417:PX4:H20	4:A:418:PX4:H22	0.55	1.77	20	1
4:A:348:PX4:H38	4:A:359:PX4:H58	0.55	1.79	7	1
4:A:394:PX4:H56	4:A:395:PX4:H59	0.55	1.78	14	1
4:A:312:PX4:H27	4:A:345:PX4:H30	0.55	1.76	17	1
4:A:322:PX4:H33	4:A:344:PX4:H34	0.55	1.76	18	1
4:A:403:PX4:H46	4:A:421:PX4:H49	0.55	1.78	15	1
4:A:306:PX4:H36	4:A:345:PX4:H64	0.55	1.77	12	1
4:A:400:PX4:O2	4:A:405:PX4:H14	0.55	2.02	20	1
4:A:361:PX4:H62	5:A:431:C3S:H42	0.55	1.79	18	1
4:A:383:PX4:H52	4:A:396:PX4:H50	0.55	1.77	19	1
4:A:413:PX4:H27	4:A:428:PX4:H41	0.55	1.77	15	1
4:A:403:PX4:H21	4:A:421:PX4:H51	0.55	1.78	10	1
4:A:382:PX4:H51	4:A:423:PX4:H20	0.55	1.78	9	1
4:A:371:PX4:H60	4:A:406:PX4:H61	0.55	1.77	20	1
4:A:378:PX4:H21	4:A:403:PX4:H20	0.55	1.78	3	1
4:A:343:PX4:H40	4:A:410:PX4:H45	0.55	1.77	3	1
4:A:365:PX4:H65	4:A:396:PX4:H61	0.55	1.77	7	1
4:A:393:PX4:H18	4:A:419:PX4:H16	0.55	1.78	5	1
4:A:366:PX4:H68	4:A:404:PX4:H41	0.55	1.76	13	1
4:A:383:PX4:H21	4:A:430:PX4:H57	0.55	1.79	13	1
4:A:327:PX4:O1	4:A:348:PX4:H16	0.55	2.01	14	1
4:A:306:PX4:H48	4:A:342:PX4:H21	0.55	1.78	19	1
4:A:403:PX4:H36	4:A:417:PX4:H34	0.55	1.78	9	1
4:A:317:PX4:H29	4:A:326:PX4:H50	0.55	1.77	3	1
4:A:343:PX4:H54	4:A:350:PX4:H49	0.55	1.78	3	1
4:A:382:PX4:H51	4:A:423:PX4:H52	0.55	1.77	2	1
4:A:305:PX4:H62	4:A:363:PX4:H55	0.55	1.77	16	1
4:A:344:PX4:H66	4:A:419:PX4:H41	0.55	1.77	4	1
4:A:315:PX4:H53	4:A:332:PX4:C11	0.55	2.30	1	1
4:A:389:PX4:H32	4:A:399:PX4:H59	0.55	1.79	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:366:PX4:H64	4:A:403:PX4:H40	0.55	1.78	5	1
4:A:319:PX4:H64	4:A:384:PX4:H68	0.55	1.79	8	1
4:A:319:PX4:H14	4:A:319:PX4:H10	0.55	1.79	4	1
4:A:385:PX4:H17	5:A:433:C3S:H443	0.55	1.78	10	1
4:A:351:PX4:H50	4:A:359:PX4:H32	0.55	1.77	9	1
4:A:330:PX4:H51	4:A:337:PX4:H29	0.55	1.77	20	1
4:A:388:PX4:H51	4:A:388:PX4:H31	0.55	1.78	7	1
4:A:307:PX4:H19	4:A:327:PX4:H44	0.55	1.78	5	1
4:A:313:PX4:H45	4:A:355:PX4:H49	0.55	1.79	15	1
4:A:415:PX4:H61	4:A:418:PX4:H69	0.55	1.78	12	1
4:A:338:PX4:H56	4:A:344:PX4:H61	0.55	1.77	11	1
4:A:382:PX4:H54	4:A:423:PX4:H49	0.55	1.76	5	1
4:A:319:PX4:H63	4:A:352:PX4:H55	0.55	1.79	6	1
4:A:353:PX4:H47	4:A:361:PX4:H24	0.55	1.79	6	1
4:A:365:PX4:H47	4:A:383:PX4:H23	0.55	1.78	17	1
1:A:115:MET:HB2	4:A:315:PX4:H4	0.55	1.78	15	1
4:A:420:PX4:H36	4:A:422:PX4:H26	0.55	1.78	15	1
4:A:332:PX4:H46	4:A:348:PX4:H5	0.55	1.77	4	1
4:A:363:PX4:H20	4:A:363:PX4:H10	0.55	1.79	1	1
4:A:378:PX4:H34	4:A:408:PX4:H70	0.55	1.79	1	1
4:A:317:PX4:H47	4:A:330:PX4:H28	0.55	1.79	7	1
4:A:330:PX4:H17	4:A:355:PX4:H24	0.55	1.78	6	1
4:A:383:PX4:H53	4:A:407:PX4:H54	0.55	1.79	14	1
4:A:375:PX4:H55	4:A:384:PX4:H18	0.55	1.79	17	1
4:A:333:PX4:H25	4:A:364:PX4:H36	0.55	1.79	15	1
4:A:369:PX4:H48	4:A:419:PX4:H51	0.55	1.79	20	1
4:A:398:PX4:H67	4:A:404:PX4:H58	0.55	1.77	3	1
4:A:336:PX4:H71	4:A:409:PX4:H31	0.55	1.79	5	1
4:A:320:PX4:H51	4:A:334:PX4:H17	0.54	1.78	16	1
4:A:389:PX4:H64	4:A:399:PX4:H39	0.54	1.78	15	1
4:A:365:PX4:H48	4:A:419:PX4:H52	0.54	1.79	20	1
4:A:376:PX4:H12	4:A:390:PX4:O6	0.54	2.02	3	1
4:A:312:PX4:H24	4:A:324:PX4:H16	0.54	1.78	6	1
4:A:383:PX4:H55	4:A:394:PX4:H48	0.54	1.78	2	1
4:A:315:PX4:H40	4:A:350:PX4:H30	0.54	1.77	16	1
4:A:391:PX4:H36	4:A:408:PX4:H60	0.54	1.79	19	1
4:A:415:PX4:H24	5:A:433:C3S:H442	0.54	1.78	15	1
4:A:397:PX4:H24	4:A:411:PX4:H49	0.54	1.78	20	1
4:A:351:PX4:H50	4:A:359:PX4:H42	0.54	1.78	5	1
4:A:404:PX4:H67	4:A:404:PX4:H35	0.54	1.78	18	1
4:A:364:PX4:H65	4:A:364:PX4:H39	0.54	1.77	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:392:PX4:H57	4:A:425:PX4:H26	0.54	1.79	19	1
4:A:319:PX4:H50	4:A:356:PX4:H14	0.54	1.79	15	1
4:A:365:PX4:H58	4:A:370:PX4:H40	0.54	1.79	11	1
4:A:307:PX4:H16	4:A:337:PX4:H54	0.54	1.79	1	1
4:A:310:PX4:H70	4:A:424:PX4:H42	0.54	1.79	5	1
4:A:367:PX4:H21	4:A:367:PX4:H48	0.54	1.78	17	1
4:A:325:PX4:H24	4:A:355:PX4:H22	0.54	1.78	8	1
4:A:380:PX4:H56	4:A:380:PX4:H29	0.54	1.80	18	1
4:A:409:PX4:H49	4:A:428:PX4:H21	0.54	1.79	18	1
4:A:308:PX4:H69	4:A:371:PX4:H43	0.54	1.80	11	1
4:A:336:PX4:H55	4:A:344:PX4:H43	0.54	1.78	11	1
4:A:305:PX4:H39	4:A:333:PX4:H61	0.54	1.79	6	1
4:A:316:PX4:H65	4:A:343:PX4:H52	0.54	1.79	17	1
4:A:310:PX4:H11	4:A:333:PX4:H50	0.54	1.78	16	1
4:A:388:PX4:H60	4:A:391:PX4:H17	0.54	1.79	12	1
4:A:376:PX4:H20	4:A:383:PX4:H24	0.54	1.79	11	1
4:A:346:PX4:H40	4:A:361:PX4:H65	0.54	1.78	10	1
4:A:308:PX4:H16	4:A:320:PX4:H16	0.54	1.78	14	2
4:A:335:PX4:H62	4:A:347:PX4:H67	0.54	1.79	2	1
4:A:418:PX4:H31	4:A:423:PX4:H30	0.54	1.79	10	1
4:A:397:PX4:H16	4:A:429:PX4:H12	0.54	1.79	14	1
4:A:312:PX4:H3	4:A:346:PX4:O3	0.54	2.02	2	1
4:A:317:PX4:H40	4:A:361:PX4:H34	0.54	1.79	15	1
4:A:371:PX4:H24	4:A:402:PX4:H63	0.54	1.79	12	1
4:A:386:PX4:H55	4:A:417:PX4:H17	0.54	1.80	12	1
4:A:415:PX4:H45	4:A:416:PX4:H8	0.54	1.79	20	1
4:A:331:PX4:H43	4:A:398:PX4:H39	0.54	1.79	7	1
4:A:310:PX4:O6	4:A:313:PX4:H5	0.54	2.02	2	1
4:A:340:PX4:H35	4:A:389:PX4:H67	0.54	1.79	17	1
4:A:392:PX4:H69	4:A:425:PX4:H71	0.54	1.80	15	1
4:A:347:PX4:H52	4:A:351:PX4:H50	0.54	1.78	12	1
4:A:323:PX4:H63	4:A:328:PX4:H58	0.54	1.80	11	1
4:A:395:PX4:O2	4:A:402:PX4:H12	0.54	2.03	9	1
4:A:368:PX4:H69	4:A:426:PX4:H66	0.54	1.80	9	1
4:A:328:PX4:H44	4:A:353:PX4:H66	0.54	1.78	3	1
4:A:372:PX4:H34	4:A:406:PX4:H34	0.54	1.78	6	1
4:A:332:PX4:H18	4:A:348:PX4:H57	0.54	1.78	16	1
1:A:103:ILE:HD13	4:A:350:PX4:H46	0.54	1.78	11	1
4:A:378:PX4:H65	4:A:414:PX4:H46	0.54	1.78	1	1
4:A:400:PX4:H30	4:A:401:PX4:H57	0.54	1.79	3	1
4:A:312:PX4:O1	4:A:324:PX4:H2	0.54	2.02	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:O7	4:A:397:PX4:H47	0.54	2.02	7	1
4:A:385:PX4:H50	4:A:415:PX4:H16	0.54	1.78	5	1
4:A:428:PX4:H49	4:A:430:PX4:H30	0.54	1.80	5	1
4:A:310:PX4:H49	4:A:364:PX4:H61	0.54	1.80	8	1
4:A:426:PX4:H72	5:A:432:C3S:H352	0.54	1.80	16	1
4:A:305:PX4:H58	4:A:324:PX4:H64	0.54	1.80	20	1
4:A:375:PX4:H60	4:A:405:PX4:H63	0.54	1.80	3	1
4:A:365:PX4:H33	4:A:419:PX4:H63	0.54	1.80	7	1
4:A:376:PX4:H19	4:A:396:PX4:H17	0.53	1.79	15	1
4:A:385:PX4:H41	5:A:433:C3S:H602	0.53	1.78	15	1
4:A:316:PX4:H11	4:A:318:PX4:O8	0.53	2.03	3	1
4:A:308:PX4:H38	4:A:350:PX4:H50	0.53	1.80	16	1
4:A:322:PX4:H19	4:A:331:PX4:H26	0.53	1.80	12	1
4:A:310:PX4:H52	4:A:333:PX4:H59	0.53	1.79	9	1
4:A:317:PX4:H25	4:A:326:PX4:H16	0.53	1.80	7	1
1:A:131:THR:O	4:A:321:PX4:H11	0.53	2.03	5	1
4:A:375:PX4:H28	4:A:427:PX4:H21	0.53	1.79	13	1
4:A:341:PX4:H19	4:A:356:PX4:H25	0.53	1.79	14	1
4:A:333:PX4:H50	4:A:364:PX4:H46	0.53	1.78	12	1
4:A:428:PX4:H22	4:A:429:PX4:H17	0.53	1.81	10	1
4:A:323:PX4:H34	4:A:345:PX4:H37	0.53	1.80	9	1
4:A:308:PX4:H23	4:A:320:PX4:H25	0.53	1.81	3	1
4:A:323:PX4:H48	4:A:361:PX4:H28	0.53	1.81	5	1
4:A:316:PX4:H52	4:A:343:PX4:H47	0.53	1.80	13	1
4:A:379:PX4:H11	5:A:434:C3S:O2	0.53	2.03	14	1
4:A:330:PX4:H60	4:A:331:PX4:H23	0.53	1.80	17	1
4:A:397:PX4:H10	4:A:411:PX4:O6	0.53	2.03	16	1
4:A:362:PX4:H41	4:A:364:PX4:H61	0.53	1.80	18	1
4:A:374:PX4:H50	4:A:430:PX4:H51	0.53	1.79	18	1
4:A:384:PX4:O6	4:A:401:PX4:H13	0.53	2.02	12	1
4:A:381:PX4:H21	4:A:394:PX4:H51	0.53	1.81	10	1
4:A:323:PX4:H20	4:A:353:PX4:H53	0.53	1.81	20	1
4:A:378:PX4:H61	4:A:386:PX4:H61	0.53	1.79	3	1
4:A:385:PX4:H18	4:A:385:PX4:H1	0.53	1.81	7	1
4:A:359:PX4:H71	4:A:376:PX4:H26	0.53	1.79	5	1
4:A:376:PX4:H27	4:A:396:PX4:H26	0.53	1.79	13	1
4:A:370:PX4:H28	4:A:383:PX4:H26	0.53	1.79	19	1
4:A:330:PX4:O8	4:A:331:PX4:H3	0.53	2.04	4	1
4:A:314:PX4:H40	4:A:352:PX4:H38	0.53	1.80	4	1
4:A:370:PX4:H55	4:A:394:PX4:H52	0.53	1.81	9	1
4:A:428:PX4:H13	4:A:428:PX4:O6	0.53	2.04	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:314:PX4:H56	4:A:336:PX4:H35	0.53	1.79	20	1
4:A:371:PX4:H62	4:A:389:PX4:H26	0.53	1.79	2	1
4:A:386:PX4:H52	4:A:426:PX4:H50	0.53	1.80	2	1
4:A:325:PX4:H36	4:A:355:PX4:H32	0.53	1.79	15	1
4:A:327:PX4:H64	4:A:344:PX4:H53	0.53	1.80	3	1
4:A:320:PX4:H52	4:A:334:PX4:H59	0.53	1.80	6	1
4:A:358:PX4:H24	4:A:358:PX4:H57	0.53	1.81	2	1
4:A:334:PX4:H57	4:A:334:PX4:H24	0.53	1.79	16	1
4:A:333:PX4:H16	5:A:432:C3S:H231	0.53	1.80	19	1
4:A:367:PX4:H57	5:A:434:C3S:H12	0.53	1.80	5	1
4:A:395:PX4:H32	4:A:402:PX4:H69	0.53	1.81	12	1
4:A:393:PX4:H32	4:A:416:PX4:H34	0.53	1.80	11	1
4:A:318:PX4:H19	4:A:342:PX4:H42	0.53	1.80	1	1
4:A:358:PX4:H49	4:A:359:PX4:H47	0.53	1.80	1	1
4:A:395:PX4:H16	4:A:402:PX4:H47	0.53	1.80	3	1
4:A:403:PX4:H51	4:A:421:PX4:H17	0.53	1.81	5	1
4:A:415:PX4:H57	4:A:418:PX4:H51	0.53	1.81	13	1
4:A:357:PX4:H17	4:A:363:PX4:H22	0.53	1.80	6	1
4:A:410:PX4:H16	5:A:435:C3S:H441	0.53	1.81	11	1
4:A:325:PX4:O6	4:A:330:PX4:H7	0.53	2.05	13	2
4:A:350:PX4:H57	4:A:402:PX4:H43	0.53	1.79	14	1
4:A:327:PX4:H45	4:A:383:PX4:H64	0.53	1.79	8	1
4:A:362:PX4:H39	4:A:367:PX4:H41	0.53	1.81	19	1
4:A:373:PX4:H55	4:A:399:PX4:H19	0.53	1.79	12	1
4:A:396:PX4:H20	4:A:407:PX4:H49	0.53	1.81	11	2
4:A:401:PX4:H63	4:A:405:PX4:H29	0.53	1.81	4	1
4:A:313:PX4:H50	4:A:329:PX4:H26	0.53	1.80	7	1
4:A:411:PX4:H17	4:A:412:PX4:H48	0.53	1.81	5	1
4:A:320:PX4:H55	4:A:334:PX4:H50	0.52	1.79	13	1
4:A:365:PX4:H17	4:A:369:PX4:H9	0.52	1.79	13	1
4:A:375:PX4:H17	4:A:405:PX4:H13	0.52	1.80	18	1
4:A:370:PX4:H4	4:A:430:PX4:H15	0.52	1.82	19	1
4:A:346:PX4:H20	4:A:358:PX4:H25	0.52	1.78	12	1
4:A:366:PX4:H27	4:A:386:PX4:H58	0.52	1.80	12	1
4:A:391:PX4:H20	4:A:427:PX4:H16	0.52	1.80	10	1
4:A:323:PX4:H67	4:A:329:PX4:H65	0.52	1.80	20	1
4:A:369:PX4:H47	4:A:419:PX4:H17	0.52	1.80	13	1
4:A:393:PX4:H67	4:A:421:PX4:H45	0.52	1.81	13	1
4:A:404:PX4:H39	4:A:417:PX4:H29	0.52	1.81	8	1
4:A:392:PX4:H38	4:A:407:PX4:H30	0.52	1.81	19	1
4:A:305:PX4:H48	4:A:311:PX4:H31	0.52	1.79	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:380:PX4:H19	4:A:420:PX4:H22	0.52	1.81	10	1
4:A:343:PX4:H60	4:A:350:PX4:H48	0.52	1.80	17	1
4:A:333:PX4:H60	4:A:333:PX4:H30	0.52	1.79	12	1
4:A:404:PX4:H55	4:A:415:PX4:H49	0.52	1.80	12	1
4:A:381:PX4:H25	4:A:395:PX4:H23	0.52	1.81	4	1
4:A:321:PX4:H41	4:A:399:PX4:H57	0.52	1.82	9	1
4:A:397:PX4:H24	4:A:428:PX4:H46	0.52	1.81	3	1
4:A:376:PX4:H32	4:A:396:PX4:H30	0.52	1.82	13	1
4:A:325:PX4:H50	4:A:361:PX4:H23	0.52	1.82	6	1
4:A:400:PX4:H50	4:A:405:PX4:H16	0.52	1.81	6	1
4:A:337:PX4:H71	4:A:381:PX4:H62	0.52	1.80	17	1
4:A:391:PX4:H10	4:A:427:PX4:H1	0.52	1.80	19	1
4:A:330:PX4:H19	4:A:337:PX4:H16	0.52	1.79	11	1
4:A:399:PX4:O6	4:A:424:PX4:H3	0.52	2.04	4	1
4:A:321:PX4:H17	4:A:342:PX4:H27	0.52	1.80	1	1
4:A:320:PX4:H33	4:A:361:PX4:H65	0.52	1.80	20	1
4:A:323:PX4:H62	4:A:328:PX4:H48	0.52	1.80	2	1
4:A:428:PX4:H14	4:A:429:PX4:H51	0.52	1.80	17	1
4:A:314:PX4:H61	4:A:336:PX4:H35	0.52	1.80	16	1
4:A:413:PX4:H24	4:A:419:PX4:H26	0.52	1.82	18	1
4:A:383:PX4:H37	4:A:388:PX4:H42	0.52	1.79	19	1
4:A:351:PX4:H23	4:A:359:PX4:H38	0.52	1.81	4	1
4:A:385:PX4:H22	5:A:433:C3S:H403	0.52	1.80	1	1
4:A:326:PX4:H70	4:A:353:PX4:H50	0.52	1.81	6	1
4:A:397:PX4:H57	4:A:423:PX4:H61	0.52	1.81	14	1
4:A:384:PX4:H69	4:A:392:PX4:H65	0.52	1.82	9	1
4:A:325:PX4:H65	4:A:353:PX4:H60	0.52	1.82	7	1
4:A:308:PX4:H31	4:A:315:PX4:H42	0.52	1.80	6	1
4:A:323:PX4:H16	4:A:353:PX4:H49	0.52	1.81	18	1
4:A:319:PX4:H54	4:A:343:PX4:H27	0.52	1.81	12	1
4:A:315:PX4:H56	4:A:332:PX4:H17	0.52	1.81	20	2
4:A:310:PX4:H23	4:A:311:PX4:H51	0.52	1.79	4	1
4:A:374:PX4:H71	4:A:419:PX4:H70	0.52	1.81	4	1
4:A:395:PX4:H47	4:A:401:PX4:H49	0.52	1.80	10	1
4:A:365:PX4:H19	4:A:369:PX4:H22	0.52	1.81	1	1
4:A:375:PX4:H56	4:A:400:PX4:H69	0.52	1.81	1	1
4:A:391:PX4:H21	4:A:427:PX4:H21	0.52	1.82	5	1
4:A:343:PX4:H22	4:A:356:PX4:H54	0.52	1.82	14	1
4:A:365:PX4:H37	4:A:369:PX4:H36	0.52	1.81	2	1
4:A:391:PX4:H30	4:A:407:PX4:H24	0.52	1.82	2	1
4:A:322:PX4:H59	4:A:330:PX4:H31	0.52	1.82	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:386:PX4:H52	4:A:417:PX4:H32	0.52	1.82	16	1
4:A:366:PX4:H64	4:A:390:PX4:H34	0.52	1.81	19	1
4:A:373:PX4:H19	4:A:386:PX4:H56	0.52	1.81	15	1
4:A:416:PX4:H49	4:A:421:PX4:H27	0.52	1.80	3	1
4:A:314:PX4:H24	4:A:336:PX4:H20	0.52	1.82	18	1
4:A:374:PX4:H57	4:A:381:PX4:H58	0.52	1.80	9	1
4:A:329:PX4:H69	4:A:387:PX4:H37	0.52	1.82	9	1
4:A:373:PX4:H41	4:A:378:PX4:H62	0.52	1.81	3	1
4:A:375:PX4:H31	4:A:407:PX4:H41	0.52	1.81	6	1
4:A:369:PX4:H56	4:A:419:PX4:H54	0.52	1.80	12	1
4:A:394:PX4:H56	4:A:430:PX4:H58	0.52	1.82	4	1
4:A:355:PX4:H38	4:A:397:PX4:H44	0.52	1.82	10	1
4:A:339:PX4:H46	4:A:363:PX4:H17	0.52	1.82	9	1
4:A:368:PX4:H4	5:A:436:C3S:C13	0.52	2.35	9	1
4:A:351:PX4:H69	4:A:360:PX4:H47	0.51	1.80	18	1
4:A:368:PX4:H18	5:A:436:C3S:H691	0.51	1.81	18	1
4:A:351:PX4:C14	4:A:359:PX4:H19	0.51	2.34	19	1
4:A:405:PX4:H60	4:A:407:PX4:H68	0.51	1.82	15	1
4:A:369:PX4:H21	4:A:374:PX4:H60	0.51	1.82	4	1
4:A:395:PX4:H21	4:A:401:PX4:H57	0.51	1.82	9	1
4:A:347:PX4:H60	4:A:354:PX4:H34	0.51	1.81	1	1
4:A:330:PX4:H24	4:A:337:PX4:H22	0.51	1.83	14	1
4:A:412:PX4:H61	4:A:424:PX4:H57	0.51	1.82	16	1
4:A:388:PX4:H22	4:A:396:PX4:H44	0.51	1.81	18	1
4:A:385:PX4:H46	4:A:415:PX4:H14	0.51	1.81	15	2
4:A:393:PX4:H14	4:A:419:PX4:O5	0.51	2.06	11	1
4:A:331:PX4:H28	4:A:337:PX4:H28	0.51	1.81	3	2
4:A:332:PX4:H23	4:A:348:PX4:H67	0.51	1.82	4	1
4:A:310:PX4:H51	4:A:311:PX4:H20	0.51	1.82	10	1
4:A:307:PX4:H25	4:A:307:PX4:H59	0.51	1.81	1	1
4:A:326:PX4:H52	4:A:353:PX4:H45	0.51	1.82	5	1
4:A:328:PX4:O7	4:A:347:PX4:H14	0.51	2.05	5	1
4:A:394:PX4:H26	4:A:401:PX4:H55	0.51	1.82	5	1
4:A:396:PX4:H24	4:A:407:PX4:H17	0.51	1.81	13	1
1:A:156:LEU:HD12	1:A:178:TRP:CH2	0.51	2.41	2	1
4:A:335:PX4:H58	4:A:347:PX4:H63	0.51	1.80	2	1
4:A:307:PX4:O2	4:A:332:PX4:H8	0.51	2.05	17	1
4:A:376:PX4:H21	4:A:383:PX4:H27	0.51	1.80	17	1
4:A:386:PX4:H10	4:A:417:PX4:O6	0.51	2.05	8	1
4:A:409:PX4:H36	4:A:425:PX4:H39	0.51	1.82	16	1
4:A:339:PX4:H71	4:A:363:PX4:H35	0.51	1.81	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:323:PX4:H49	4:A:360:PX4:H23	0.51	1.83	9	1
4:A:357:PX4:H17	4:A:363:PX4:H25	0.51	1.82	9	1
4:A:316:PX4:H25	4:A:352:PX4:H27	0.51	1.82	7	1
4:A:387:PX4:H62	4:A:404:PX4:H35	0.51	1.82	6	1
1:A:114:ASN:OD1	4:A:348:PX4:H3	0.51	2.05	19	3
4:A:372:PX4:C2	4:A:410:PX4:H15	0.51	2.36	10	1
4:A:409:PX4:H43	4:A:428:PX4:H53	0.51	1.83	13	1
4:A:333:PX4:H13	4:A:334:PX4:O8	0.51	2.05	15	1
4:A:322:PX4:H67	4:A:369:PX4:H43	0.51	1.81	11	1
4:A:398:PX4:H29	4:A:411:PX4:H53	0.51	1.81	11	1
4:A:307:PX4:H21	4:A:322:PX4:H46	0.51	1.82	4	1
1:A:98:ARG:O	4:A:334:PX4:H6	0.51	2.06	4	1
4:A:321:PX4:H41	4:A:375:PX4:H39	0.51	1.81	10	1
4:A:428:PX4:H28	4:A:429:PX4:H27	0.51	1.83	10	1
4:A:368:PX4:H7	4:A:368:PX4:H14	0.51	1.83	3	1
4:A:385:PX4:H47	4:A:415:PX4:H21	0.51	1.82	6	1
4:A:309:PX4:H39	4:A:323:PX4:H41	0.51	1.82	14	1
4:A:316:PX4:C8	4:A:352:PX4:H19	0.51	2.32	17	1
4:A:306:PX4:H41	4:A:358:PX4:H68	0.51	1.82	18	1
4:A:374:PX4:H36	4:A:418:PX4:H24	0.51	1.82	18	1
4:A:362:PX4:H28	4:A:364:PX4:H57	0.51	1.83	4	1
4:A:322:PX4:H52	4:A:337:PX4:H52	0.51	1.82	9	1
4:A:334:PX4:H65	4:A:426:PX4:H60	0.51	1.81	9	1
4:A:307:PX4:H13	4:A:322:PX4:H15	0.51	1.81	3	1
4:A:386:PX4:H31	4:A:386:PX4:H63	0.51	1.83	7	1
4:A:318:PX4:H23	4:A:339:PX4:H29	0.51	1.82	14	1
4:A:404:PX4:H57	4:A:415:PX4:H53	0.51	1.82	2	1
4:A:325:PX4:H62	4:A:355:PX4:H66	0.51	1.80	17	1
4:A:342:PX4:H40	4:A:345:PX4:H66	0.51	1.82	19	1
4:A:328:PX4:O4	4:A:347:PX4:H14	0.51	2.06	19	1
4:A:334:PX4:H39	4:A:340:PX4:H32	0.51	1.81	7	1
4:A:306:PX4:H31	4:A:358:PX4:H17	0.51	1.82	7	1
4:A:382:PX4:H17	4:A:423:PX4:H25	0.51	1.82	7	1
4:A:428:PX4:H28	4:A:429:PX4:H32	0.51	1.82	13	1
4:A:375:PX4:H26	4:A:392:PX4:H36	0.51	1.82	8	1
4:A:397:PX4:H20	4:A:411:PX4:H70	0.51	1.81	16	1
4:A:340:PX4:H14	4:A:340:PX4:H7	0.51	1.80	1	1
4:A:365:PX4:H17	4:A:383:PX4:H21	0.51	1.82	1	1
4:A:373:PX4:H23	4:A:426:PX4:H47	0.51	1.83	1	1
4:A:382:PX4:H28	4:A:385:PX4:H54	0.51	1.82	7	1
4:A:382:PX4:H20	4:A:398:PX4:H47	0.51	1.81	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:406:PX4:H53	4:A:414:PX4:H21	0.51	1.82	7	1
4:A:381:PX4:H32	4:A:394:PX4:H57	0.51	1.81	14	1
4:A:325:PX4:H23	4:A:355:PX4:H17	0.51	1.82	17	1
4:A:344:PX4:H71	4:A:393:PX4:H63	0.51	1.81	17	1
4:A:375:PX4:H10	4:A:375:PX4:H14	0.51	1.83	15	1
4:A:414:PX4:H46	4:A:426:PX4:H19	0.51	1.81	10	1
4:A:394:PX4:H71	4:A:402:PX4:H72	0.51	1.83	9	1
4:A:348:PX4:H45	4:A:407:PX4:H41	0.51	1.82	1	1
4:A:408:PX4:H57	4:A:414:PX4:H48	0.51	1.83	3	1
4:A:332:PX4:H16	4:A:348:PX4:H11	0.51	1.83	7	1
4:A:348:PX4:H23	4:A:359:PX4:H21	0.51	1.83	2	1
4:A:353:PX4:H49	4:A:361:PX4:H25	0.51	1.82	8	1
4:A:323:PX4:H21	4:A:353:PX4:H20	0.51	1.83	10	1
4:A:324:PX4:H61	4:A:324:PX4:H33	0.51	1.82	9	1
4:A:399:PX4:H35	4:A:424:PX4:H28	0.51	1.83	1	1
4:A:400:PX4:O5	4:A:401:PX4:H49	0.51	2.05	20	1
4:A:400:PX4:H1	4:A:401:PX4:O2	0.51	2.06	20	1
4:A:387:PX4:H57	4:A:418:PX4:H58	0.51	1.83	20	1
4:A:321:PX4:H51	4:A:342:PX4:H28	0.50	1.81	2	1
4:A:327:PX4:H43	4:A:369:PX4:H38	0.50	1.83	12	1
4:A:322:PX4:H17	4:A:344:PX4:H18	0.50	1.82	4	1
4:A:414:PX4:H32	5:A:432:C3S:H693	0.50	1.82	10	1
4:A:374:PX4:H23	4:A:423:PX4:H53	0.50	1.83	14	1
4:A:338:PX4:H33	4:A:344:PX4:H67	0.50	1.82	18	1
4:A:371:PX4:H72	4:A:373:PX4:H45	0.50	1.83	18	1
4:A:412:PX4:H47	4:A:412:PX4:H8	0.50	1.82	20	1
4:A:318:PX4:H50	4:A:363:PX4:H30	0.50	1.84	3	1
4:A:308:PX4:H52	4:A:320:PX4:H25	0.50	1.83	7	1
4:A:343:PX4:H56	4:A:350:PX4:H17	0.50	1.82	13	1
4:A:332:PX4:H4	4:A:348:PX4:H49	0.50	1.84	2	1
4:A:312:PX4:H22	4:A:346:PX4:H52	0.50	1.82	17	1
4:A:354:PX4:H64	4:A:419:PX4:H45	0.50	1.82	17	1
4:A:345:PX4:H32	4:A:349:PX4:H63	0.50	1.83	8	1
4:A:377:PX4:H45	4:A:408:PX4:H61	0.50	1.83	19	1
4:A:387:PX4:O3	4:A:416:PX4:H12	0.50	2.06	15	1
4:A:342:PX4:O1	4:A:358:PX4:H12	0.50	2.06	12	1
4:A:318:PX4:H56	4:A:357:PX4:H23	0.50	1.82	4	1
4:A:327:PX4:H40	4:A:348:PX4:H62	0.50	1.82	7	1
4:A:386:PX4:O8	4:A:402:PX4:H14	0.50	2.05	6	1
4:A:383:PX4:H16	4:A:396:PX4:H46	0.50	1.82	8	1
4:A:305:PX4:H59	4:A:339:PX4:H41	0.50	1.82	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:336:PX4:H26	4:A:360:PX4:H59	0.50	1.82	11	1
4:A:310:PX4:H59	4:A:311:PX4:H33	0.50	1.83	4	1
4:A:386:PX4:O5	4:A:402:PX4:H14	0.50	2.07	9	1
4:A:403:PX4:H26	4:A:421:PX4:H55	0.50	1.82	9	1
4:A:323:PX4:H19	4:A:349:PX4:H16	0.50	1.84	3	1
4:A:420:PX4:O6	4:A:422:PX4:H16	0.50	2.07	5	1
4:A:385:PX4:H17	5:A:433:C3S:C13	0.50	2.37	6	1
4:A:324:PX4:H61	4:A:386:PX4:H70	0.50	1.82	2	1
4:A:336:PX4:H17	4:A:352:PX4:H11	0.50	1.81	8	1
4:A:327:PX4:H69	4:A:348:PX4:H50	0.50	1.82	12	1
4:A:315:PX4:H60	4:A:332:PX4:H17	0.50	1.84	4	1
4:A:336:PX4:H49	4:A:354:PX4:H51	0.50	1.82	4	1
4:A:369:PX4:H57	4:A:419:PX4:H21	0.50	1.83	5	1
4:A:379:PX4:H18	4:A:425:PX4:O6	0.50	2.07	17	1
4:A:404:PX4:H36	4:A:417:PX4:H25	0.50	1.82	8	1
4:A:427:PX4:O6	4:A:427:PX4:H2	0.50	2.06	8	2
4:A:322:PX4:H69	4:A:337:PX4:H39	0.50	1.82	16	1
4:A:346:PX4:H35	4:A:349:PX4:H40	0.50	1.82	16	1
4:A:357:PX4:H72	4:A:363:PX4:H33	0.50	1.82	18	1
4:A:370:PX4:O6	4:A:383:PX4:H9	0.50	2.07	18	1
1:A:156:LEU:HD23	1:A:156:LEU:H	0.50	1.66	4	1
4:A:319:PX4:H25	4:A:341:PX4:H71	0.50	1.84	4	1
4:A:311:PX4:H62	4:A:329:PX4:H64	0.50	1.82	9	1
4:A:350:PX4:H72	4:A:402:PX4:H39	0.50	1.83	20	1
4:A:340:PX4:O6	4:A:350:PX4:H8	0.50	2.06	13	2
4:A:375:PX4:H57	4:A:405:PX4:H25	0.50	1.83	13	1
4:A:323:PX4:H14	4:A:353:PX4:O8	0.50	2.07	6	1
4:A:387:PX4:H3	4:A:416:PX4:O2	0.50	2.07	6	1
4:A:394:PX4:H31	4:A:400:PX4:H52	0.50	1.83	14	1
4:A:367:PX4:H62	4:A:367:PX4:H30	0.50	1.83	2	1
4:A:416:PX4:O6	4:A:416:PX4:H2	0.50	2.07	9	1
4:A:375:PX4:H20	4:A:427:PX4:H17	0.50	1.84	3	1
4:A:404:PX4:H48	4:A:415:PX4:H17	0.50	1.84	2	1
4:A:393:PX4:H2	4:A:416:PX4:H14	0.50	1.82	8	1
4:A:370:PX4:H23	4:A:383:PX4:H48	0.50	1.84	18	1
4:A:307:PX4:H56	4:A:348:PX4:H58	0.50	1.84	10	1
4:A:376:PX4:H61	4:A:390:PX4:H48	0.50	1.83	10	1
4:A:420:PX4:H34	4:A:422:PX4:H61	0.50	1.83	10	1
4:A:409:PX4:O8	4:A:428:PX4:H7	0.50	2.06	9	1
4:A:386:PX4:H49	4:A:421:PX4:H66	0.50	1.84	1	1
4:A:400:PX4:H62	4:A:405:PX4:H53	0.50	1.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:392:PX4:O2	4:A:425:PX4:H14	0.50	2.06	5	1
4:A:309:PX4:H50	4:A:347:PX4:H20	0.50	1.83	13	1
4:A:409:PX4:H29	4:A:428:PX4:H12	0.50	1.82	14	1
4:A:373:PX4:H47	4:A:406:PX4:H53	0.50	1.84	19	1
4:A:388:PX4:H32	4:A:396:PX4:H35	0.50	1.82	15	1
4:A:313:PX4:H15	4:A:355:PX4:H47	0.50	1.84	9	1
4:A:386:PX4:H24	4:A:402:PX4:H16	0.50	1.83	1	1
4:A:323:PX4:H41	4:A:349:PX4:H22	0.50	1.82	3	1
4:A:371:PX4:O3	4:A:373:PX4:H18	0.50	2.06	7	1
4:A:305:PX4:H60	4:A:312:PX4:H63	0.49	1.83	13	1
4:A:312:PX4:H22	4:A:346:PX4:C27	0.49	2.37	17	1
4:A:395:PX4:H48	4:A:401:PX4:H54	0.49	1.83	17	1
4:A:344:PX4:H9	4:A:354:PX4:O6	0.49	2.07	4	1
4:A:365:PX4:H43	4:A:413:PX4:H41	0.49	1.84	4	1
4:A:307:PX4:H21	4:A:307:PX4:H55	0.49	1.83	1	1
4:A:333:PX4:H42	4:A:364:PX4:H39	0.49	1.84	1	1
4:A:393:PX4:O5	4:A:419:PX4:H19	0.49	2.07	1	1
4:A:389:PX4:H16	4:A:399:PX4:H52	0.49	1.83	7	1
4:A:394:PX4:H16	4:A:395:PX4:H49	0.49	1.84	5	1
4:A:378:PX4:H9	4:A:388:PX4:O1	0.49	2.07	6	1
4:A:408:PX4:H55	4:A:427:PX4:H50	0.49	1.82	2	1
4:A:306:PX4:H69	4:A:316:PX4:H28	0.49	1.82	17	1
4:A:366:PX4:H62	4:A:403:PX4:H57	0.49	1.85	8	1
4:A:320:PX4:H56	5:A:432:C3S:H41	0.49	1.84	8	1
4:A:341:PX4:H23	4:A:362:PX4:H26	0.49	1.82	16	1
4:A:341:PX4:H17	4:A:341:PX4:H6	0.49	1.85	12	1
4:A:340:PX4:H17	4:A:356:PX4:H53	0.49	1.83	4	2
4:A:367:PX4:H22	4:A:399:PX4:H15	0.49	1.84	9	1
4:A:365:PX4:H38	4:A:376:PX4:H25	0.49	1.84	9	1
4:A:394:PX4:H53	4:A:395:PX4:H50	0.49	1.84	9	1
1:A:224:PHE:O	4:A:315:PX4:H5	0.49	2.07	1	2
4:A:307:PX4:H54	4:A:344:PX4:H49	0.49	1.84	20	1
4:A:429:PX4:H14	4:A:429:PX4:H13	0.49	1.83	20	1
4:A:308:PX4:H29	4:A:315:PX4:H39	0.49	1.84	13	1
4:A:376:PX4:H60	4:A:390:PX4:H64	0.49	1.83	13	1
4:A:310:PX4:H36	4:A:364:PX4:H38	0.49	1.84	6	1
4:A:322:PX4:H69	4:A:327:PX4:H63	0.49	1.82	14	1
4:A:378:PX4:H38	4:A:426:PX4:H39	0.49	1.83	17	1
4:A:326:PX4:H36	4:A:330:PX4:H32	0.49	1.83	19	1
4:A:337:PX4:H32	4:A:337:PX4:H53	0.49	1.84	19	1
4:A:313:PX4:H65	4:A:325:PX4:H56	0.49	1.82	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:382:PX4:H24	4:A:423:PX4:H31	0.49	1.83	20	1
4:A:314:PX4:H57	4:A:336:PX4:H70	0.49	1.83	6	1
4:A:406:PX4:H20	4:A:410:PX4:H49	0.49	1.83	6	1
4:A:320:PX4:H59	4:A:334:PX4:H51	0.49	1.83	16	1
4:A:370:PX4:H26	4:A:383:PX4:H17	0.49	1.84	18	1
4:A:341:PX4:H7	4:A:364:PX4:O8	0.49	2.07	15	1
4:A:402:PX4:H42	5:A:431:C3S:H502	0.49	1.85	11	1
4:A:368:PX4:H49	4:A:414:PX4:H23	0.49	1.85	9	1
4:A:420:PX4:O8	4:A:420:PX4:H4	0.49	2.08	9	1
4:A:366:PX4:H30	4:A:414:PX4:H70	0.49	1.84	5	1
4:A:369:PX4:H53	4:A:419:PX4:H48	0.49	1.84	5	1
4:A:355:PX4:H16	4:A:362:PX4:H46	0.49	1.84	6	1
4:A:381:PX4:H41	4:A:394:PX4:H69	0.49	1.84	6	1
4:A:309:PX4:H47	4:A:328:PX4:H23	0.49	1.84	2	1
4:A:374:PX4:H29	4:A:418:PX4:H24	0.49	1.84	11	1
4:A:414:PX4:H16	5:A:436:C3S:H652	0.49	1.84	11	1
4:A:397:PX4:H29	4:A:412:PX4:H58	0.49	1.85	4	1
4:A:396:PX4:H19	4:A:407:PX4:C6	0.49	2.37	10	1
4:A:386:PX4:H30	4:A:417:PX4:H50	0.49	1.85	20	1
4:A:390:PX4:H37	4:A:419:PX4:H29	0.49	1.84	20	1
4:A:380:PX4:H25	4:A:385:PX4:H30	0.49	1.83	7	1
4:A:317:PX4:H61	4:A:330:PX4:H39	0.49	1.85	14	1
4:A:307:PX4:H41	4:A:374:PX4:H29	0.49	1.85	16	1
4:A:389:PX4:H46	4:A:400:PX4:H19	0.49	1.85	9	1
4:A:322:PX4:H53	4:A:330:PX4:H30	0.49	1.83	7	1
4:A:375:PX4:H48	4:A:392:PX4:H22	0.49	1.83	13	1
4:A:368:PX4:H69	4:A:368:PX4:H34	0.49	1.85	3	2
4:A:305:PX4:H53	4:A:311:PX4:H26	0.49	1.85	2	1
4:A:308:PX4:H43	4:A:343:PX4:H67	0.49	1.83	16	1
4:A:375:PX4:H67	4:A:379:PX4:H41	0.49	1.83	15	1
4:A:307:PX4:H22	4:A:331:PX4:H27	0.49	1.84	4	1
4:A:330:PX4:H67	4:A:331:PX4:H36	0.49	1.83	1	1
4:A:338:PX4:H15	4:A:351:PX4:H2	0.49	1.84	20	1
4:A:308:PX4:H27	4:A:320:PX4:H17	0.49	1.83	3	1
4:A:320:PX4:H50	4:A:334:PX4:H49	0.49	1.84	3	1
4:A:308:PX4:H3	4:A:334:PX4:O6	0.49	2.08	3	1
4:A:307:PX4:H21	4:A:322:PX4:H17	0.49	1.84	7	1
4:A:428:PX4:H14	4:A:429:PX4:O3	0.49	2.08	7	1
4:A:316:PX4:H25	4:A:321:PX4:H20	0.49	1.84	5	1
4:A:409:PX4:H34	4:A:428:PX4:O6	0.49	2.08	13	1
4:A:370:PX4:H35	4:A:400:PX4:H60	0.49	1.83	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:373:PX4:H47	4:A:406:PX4:H49	0.49	1.85	19	1
4:A:342:PX4:H72	4:A:377:PX4:H44	0.49	1.83	11	1
4:A:343:PX4:H48	4:A:356:PX4:C26	0.49	2.38	4	1
4:A:394:PX4:H40	4:A:407:PX4:H28	0.49	1.85	20	1
4:A:388:PX4:H50	4:A:391:PX4:H47	0.49	1.83	7	1
4:A:308:PX4:H15	4:A:326:PX4:H46	0.49	1.85	2	1
4:A:370:PX4:H69	4:A:374:PX4:H64	0.49	1.84	2	1
4:A:305:PX4:O2	4:A:339:PX4:H2	0.49	2.08	8	1
4:A:373:PX4:H21	4:A:406:PX4:H53	0.49	1.84	18	1
4:A:353:PX4:H19	4:A:361:PX4:H49	0.49	1.84	4	1
4:A:394:PX4:H22	4:A:400:PX4:H46	0.49	1.83	20	2
4:A:308:PX4:H70	4:A:418:PX4:H43	0.49	1.83	1	1
4:A:374:PX4:H36	4:A:382:PX4:H54	0.49	1.82	20	1
4:A:309:PX4:H6	4:A:351:PX4:H20	0.49	1.85	3	1
4:A:310:PX4:H46	4:A:333:PX4:H54	0.49	1.85	3	1
4:A:375:PX4:H68	4:A:392:PX4:H40	0.49	1.85	13	1
1:A:222:GLN:O	4:A:317:PX4:H5	0.49	2.08	2	1
4:A:365:PX4:H40	4:A:430:PX4:H68	0.49	1.85	2	1
4:A:365:PX4:O6	4:A:369:PX4:H13	0.49	2.08	2	1
4:A:322:PX4:H66	4:A:430:PX4:C35	0.49	2.36	17	1
4:A:341:PX4:H40	4:A:362:PX4:H64	0.49	1.85	16	1
4:A:374:PX4:O2	4:A:423:PX4:H3	0.49	2.08	16	1
4:A:343:PX4:H47	4:A:356:PX4:H51	0.49	1.82	18	1
4:A:324:PX4:H66	4:A:373:PX4:H34	0.49	1.85	15	1
4:A:306:PX4:H69	4:A:342:PX4:H35	0.49	1.84	3	1
4:A:346:PX4:H25	5:A:431:C3S:H41	0.49	1.85	7	1
4:A:423:PX4:H69	4:A:428:PX4:H63	0.48	1.85	6	1
4:A:325:PX4:H8	4:A:328:PX4:H49	0.48	1.83	2	1
4:A:322:PX4:O6	4:A:336:PX4:H11	0.48	2.08	16	1
4:A:391:PX4:H49	4:A:427:PX4:H19	0.48	1.85	16	1
4:A:314:PX4:H65	4:A:387:PX4:H42	0.48	1.84	15	1
4:A:411:PX4:H62	4:A:424:PX4:H39	0.48	1.83	15	1
4:A:397:PX4:H16	4:A:411:PX4:H20	0.48	1.85	12	1
4:A:378:PX4:H17	4:A:426:PX4:O6	0.48	2.07	11	1
4:A:383:PX4:H61	4:A:405:PX4:H61	0.48	1.84	1	1
4:A:410:PX4:H22	4:A:414:PX4:H36	0.48	1.84	7	1
4:A:373:PX4:H70	4:A:399:PX4:H44	0.48	1.85	5	1
4:A:325:PX4:H50	4:A:355:PX4:H55	0.48	1.84	17	1
4:A:417:PX4:H16	4:A:418:PX4:H22	0.48	1.85	8	1
4:A:399:PX4:H30	4:A:414:PX4:H36	0.48	1.85	12	1
4:A:397:PX4:H62	4:A:429:PX4:H58	0.48	1.84	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:327:PX4:H22	4:A:348:PX4:H20	0.48	1.84	11	1
4:A:345:PX4:H40	4:A:346:PX4:H38	0.48	1.84	9	1
4:A:317:PX4:H46	4:A:330:PX4:H23	0.48	1.84	20	1
4:A:308:PX4:H44	4:A:343:PX4:H66	0.48	1.85	13	1
4:A:376:PX4:H38	4:A:427:PX4:H24	0.48	1.83	14	1
4:A:411:PX4:H72	4:A:411:PX4:H24	0.48	1.84	16	1
4:A:385:PX4:H49	4:A:415:PX4:H20	0.48	1.83	16	1
4:A:315:PX4:H32	4:A:350:PX4:H42	0.48	1.84	12	1
4:A:326:PX4:H71	4:A:371:PX4:H37	0.48	1.85	11	1
4:A:369:PX4:H36	4:A:374:PX4:H61	0.48	1.85	11	1
4:A:316:PX4:H47	4:A:321:PX4:H33	0.48	1.84	4	1
4:A:341:PX4:H52	4:A:356:PX4:H23	0.48	1.85	9	1
4:A:388:PX4:O2	4:A:391:PX4:H15	0.48	2.07	1	1
4:A:312:PX4:H19	4:A:346:PX4:H17	0.48	1.85	7	1
4:A:403:PX4:H31	4:A:421:PX4:H69	0.48	1.86	5	1
4:A:382:PX4:O4	4:A:398:PX4:H17	0.48	2.07	14	1
4:A:309:PX4:H66	4:A:351:PX4:H34	0.48	1.83	2	1
4:A:327:PX4:H20	4:A:348:PX4:H16	0.48	1.85	8	1
1:A:102:HIS:CE1	4:A:350:PX4:H6	0.48	2.43	8	1
4:A:414:PX4:O2	4:A:426:PX4:H10	0.48	2.07	12	1
4:A:379:PX4:O8	4:A:425:PX4:H3	0.48	2.09	4	1
4:A:382:PX4:H6	4:A:424:PX4:O6	0.48	2.08	4	1
1:A:113:LEU:HD21	1:A:196:LEU:HD22	0.48	1.83	10	1
4:A:377:PX4:H49	4:A:408:PX4:H23	0.48	1.85	10	1
4:A:368:PX4:O6	4:A:414:PX4:H14	0.48	2.08	1	1
4:A:388:PX4:H67	4:A:414:PX4:H63	0.48	1.84	3	1
4:A:328:PX4:H70	4:A:390:PX4:H41	0.48	1.85	5	1
4:A:384:PX4:H34	4:A:389:PX4:H56	0.48	1.85	6	1
4:A:333:PX4:H39	4:A:389:PX4:C36	0.48	2.39	2	1
4:A:395:PX4:H17	4:A:401:PX4:H49	0.48	1.85	2	1
4:A:397:PX4:H64	4:A:423:PX4:H62	0.48	1.85	8	1
4:A:321:PX4:H58	4:A:342:PX4:H37	0.48	1.84	18	1
4:A:321:PX4:H50	4:A:342:PX4:H34	0.48	1.86	19	1
4:A:419:PX4:H31	4:A:429:PX4:H26	0.48	1.84	15	1
4:A:315:PX4:H60	4:A:332:PX4:H69	0.48	1.85	12	1
4:A:338:PX4:H24	4:A:351:PX4:H72	0.48	1.85	12	1
4:A:309:PX4:H24	4:A:345:PX4:H67	0.48	1.84	9	1
4:A:405:PX4:H59	4:A:407:PX4:H60	0.48	1.85	9	1
4:A:374:PX4:H9	4:A:423:PX4:O2	0.48	2.08	1	1
4:A:328:PX4:H64	4:A:360:PX4:H22	0.48	1.86	20	1
4:A:305:PX4:H32	4:A:310:PX4:H57	0.48	1.85	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:393:PX4:H71	4:A:429:PX4:H43	0.48	1.83	5	1
4:A:389:PX4:H37	4:A:399:PX4:H66	0.48	1.84	13	1
4:A:317:PX4:H35	4:A:361:PX4:H29	0.48	1.85	17	1
4:A:337:PX4:H23	4:A:355:PX4:H27	0.48	1.84	17	1
4:A:346:PX4:H45	4:A:402:PX4:H35	0.48	1.83	17	1
4:A:309:PX4:H26	4:A:359:PX4:H22	0.48	1.85	8	1
4:A:327:PX4:H15	4:A:348:PX4:H16	0.48	1.84	16	1
4:A:365:PX4:H67	4:A:407:PX4:H61	0.48	1.86	16	1
4:A:352:PX4:C20	4:A:375:PX4:H44	0.48	2.33	18	1
4:A:374:PX4:H51	4:A:430:PX4:H53	0.48	1.85	19	1
4:A:312:PX4:H69	5:A:431:C3S:H693	0.48	1.85	12	1
4:A:323:PX4:H52	4:A:328:PX4:H16	0.48	1.83	12	1
4:A:324:PX4:H52	5:A:432:C3S:H322	0.48	1.84	1	1
4:A:325:PX4:H63	4:A:329:PX4:H52	0.48	1.84	20	1
4:A:374:PX4:H20	4:A:423:PX4:H49	0.48	1.85	20	1
1:A:128:VAL:HG21	4:A:343:PX4:H63	0.48	1.84	3	1
1:A:158:HIS:CD2	1:A:171:HIS:HB2	0.48	2.43	13	1
4:A:400:PX4:H20	4:A:401:PX4:H47	0.48	1.86	13	1
4:A:343:PX4:H20	4:A:352:PX4:H54	0.48	1.85	6	1
4:A:314:PX4:H14	4:A:336:PX4:O6	0.48	2.08	14	1
4:A:367:PX4:O8	4:A:367:PX4:H17	0.48	2.07	2	1
4:A:379:PX4:H59	4:A:413:PX4:H22	0.48	1.85	8	1
4:A:341:PX4:H3	4:A:341:PX4:O8	0.48	2.09	16	1
4:A:328:PX4:H37	4:A:345:PX4:H27	0.48	1.86	18	1
4:A:391:PX4:H34	4:A:408:PX4:H66	0.48	1.86	15	1
4:A:320:PX4:H42	4:A:350:PX4:H35	0.48	1.85	12	1
4:A:392:PX4:H50	4:A:425:PX4:H49	0.48	1.86	11	1
4:A:322:PX4:H42	4:A:331:PX4:H41	0.48	1.84	4	1
4:A:313:PX4:O7	4:A:329:PX4:H15	0.48	2.09	10	1
1:A:15:ALA:HB1	1:A:39:LEU:HD21	0.48	1.86	9	1
1:A:99:ASP:O	4:A:334:PX4:H11	0.48	2.09	3	1
4:A:376:PX4:H63	4:A:396:PX4:H64	0.48	1.85	3	1
4:A:371:PX4:H20	4:A:400:PX4:H41	0.48	1.84	3	1
4:A:367:PX4:H69	4:A:389:PX4:H31	0.48	1.84	13	1
4:A:338:PX4:C10	4:A:344:PX4:H53	0.48	2.39	17	1
4:A:327:PX4:H32	4:A:332:PX4:H56	0.48	1.85	18	1
4:A:367:PX4:H18	4:A:399:PX4:O7	0.48	2.09	18	1
4:A:340:PX4:H13	5:A:432:C3S:O4	0.48	2.08	19	1
4:A:384:PX4:O8	4:A:405:PX4:H11	0.48	2.08	12	1
4:A:429:PX4:H63	4:A:430:PX4:H33	0.48	1.85	11	1
1:A:156:LEU:CD2	1:A:156:LEU:H	0.48	2.21	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:314:PX4:H19	4:A:336:PX4:H29	0.48	1.86	1	1
4:A:399:PX4:H35	4:A:424:PX4:H31	0.48	1.85	5	1
4:A:327:PX4:H19	4:A:359:PX4:H30	0.48	1.85	13	1
4:A:369:PX4:H23	4:A:374:PX4:H54	0.48	1.86	19	1
4:A:377:PX4:H17	4:A:408:PX4:O1	0.48	2.08	15	1
4:A:392:PX4:H20	4:A:407:PX4:H18	0.48	1.85	15	1
4:A:376:PX4:H21	4:A:383:PX4:H30	0.48	1.86	4	1
4:A:373:PX4:H41	4:A:401:PX4:H34	0.48	1.86	10	1
4:A:377:PX4:H16	5:A:436:C3S:H442	0.48	1.85	9	1
1:A:128:VAL:HG23	4:A:343:PX4:H39	0.48	1.84	1	1
4:A:396:PX4:H19	4:A:407:PX4:H17	0.48	1.85	7	2
4:A:320:PX4:H71	4:A:350:PX4:H46	0.48	1.84	20	1
4:A:378:PX4:H54	4:A:402:PX4:H22	0.48	1.84	20	1
4:A:308:PX4:H59	4:A:417:PX4:H40	0.48	1.84	3	1
4:A:343:PX4:H42	4:A:384:PX4:H43	0.48	1.85	7	1
4:A:381:PX4:H58	4:A:430:PX4:H65	0.48	1.86	7	1
4:A:307:PX4:H36	4:A:331:PX4:H35	0.48	1.86	14	1
4:A:322:PX4:H24	4:A:331:PX4:H51	0.48	1.85	14	1
4:A:316:PX4:H63	4:A:352:PX4:H68	0.48	1.86	17	1
4:A:374:PX4:H23	4:A:397:PX4:H67	0.48	1.84	17	1
4:A:374:PX4:O2	4:A:397:PX4:H15	0.48	2.09	17	1
4:A:367:PX4:H46	4:A:384:PX4:H5	0.48	1.86	17	1
4:A:320:PX4:H8	4:A:326:PX4:H17	0.48	1.86	8	1
4:A:319:PX4:H54	4:A:356:PX4:H16	0.48	1.84	8	1
4:A:342:PX4:H44	4:A:405:PX4:H37	0.48	1.86	16	1
4:A:353:PX4:H20	4:A:361:PX4:H48	0.48	1.84	15	1
4:A:328:PX4:H57	4:A:347:PX4:H22	0.48	1.86	12	1
1:A:15:ALA:HB1	1:A:39:LEU:CD2	0.48	2.39	9	1
4:A:378:PX4:H35	4:A:403:PX4:H39	0.48	1.85	20	1
4:A:326:PX4:H33	4:A:404:PX4:H39	0.48	1.85	3	1
4:A:387:PX4:H6	4:A:415:PX4:O3	0.48	2.08	7	1
4:A:319:PX4:H59	4:A:341:PX4:H57	0.47	1.85	17	1
4:A:375:PX4:H35	4:A:391:PX4:H26	0.47	1.84	8	1
4:A:348:PX4:H63	4:A:350:PX4:H40	0.47	1.85	16	1
4:A:400:PX4:H26	4:A:405:PX4:H26	0.47	1.85	15	1
4:A:334:PX4:H63	5:A:431:C3S:H48	0.47	1.86	12	1
1:A:124:PHE:HB2	4:A:348:PX4:H1	0.47	1.84	12	1
4:A:309:PX4:H46	4:A:349:PX4:H54	0.47	1.84	11	1
4:A:400:PX4:O4	4:A:401:PX4:H1	0.47	2.09	9	1
4:A:398:PX4:H2	5:A:435:C3S:O2	0.47	2.08	1	1
4:A:322:PX4:H50	4:A:331:PX4:H19	0.47	1.85	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:407:PX4:O4	4:A:427:PX4:H1	0.47	2.09	17	1
4:A:321:PX4:H59	4:A:357:PX4:H42	0.47	1.85	8	1
4:A:378:PX4:H63	4:A:426:PX4:H26	0.47	1.84	16	1
4:A:417:PX4:H3	4:A:418:PX4:O6	0.47	2.07	19	1
4:A:305:PX4:O6	4:A:311:PX4:H12	0.47	2.09	12	1
4:A:399:PX4:H18	4:A:424:PX4:H13	0.47	1.86	4	1
4:A:399:PX4:H19	5:A:435:C3S:H42	0.47	1.85	4	1
4:A:383:PX4:H57	4:A:394:PX4:H37	0.47	1.85	1	1
4:A:385:PX4:H15	4:A:415:PX4:H18	0.47	1.86	1	1
4:A:326:PX4:H55	4:A:361:PX4:H57	0.47	1.84	5	1
4:A:366:PX4:H53	4:A:403:PX4:H49	0.47	1.86	14	1
4:A:343:PX4:H28	4:A:352:PX4:H58	0.47	1.86	8	1
4:A:382:PX4:H53	5:A:435:C3S:H601	0.47	1.87	12	1
4:A:310:PX4:H19	4:A:311:PX4:H47	0.47	1.86	4	1
4:A:370:PX4:H56	4:A:381:PX4:H47	0.47	1.84	10	1
4:A:383:PX4:H52	4:A:395:PX4:H59	0.47	1.86	1	1
4:A:385:PX4:H46	4:A:415:PX4:H46	0.47	1.86	1	1
4:A:343:PX4:H19	4:A:352:PX4:H55	0.47	1.86	5	1
4:A:387:PX4:H32	4:A:393:PX4:H50	0.47	1.85	5	1
4:A:346:PX4:H24	4:A:358:PX4:H24	0.47	1.86	14	1
4:A:409:PX4:H6	5:A:434:C3S:H91	0.47	1.84	2	1
4:A:412:PX4:H17	4:A:424:PX4:H53	0.47	1.87	19	1
4:A:340:PX4:H70	4:A:406:PX4:H68	0.47	1.86	12	1
4:A:387:PX4:H32	4:A:416:PX4:H60	0.47	1.86	12	1
4:A:336:PX4:H52	4:A:354:PX4:H21	0.47	1.85	10	1
4:A:368:PX4:H11	4:A:406:PX4:O1	0.47	2.10	9	1
4:A:367:PX4:H64	4:A:412:PX4:H26	0.47	1.86	9	1
4:A:347:PX4:H15	4:A:351:PX4:O8	0.47	2.09	1	1
4:A:397:PX4:H51	4:A:430:PX4:H20	0.47	1.87	20	1
4:A:345:PX4:H65	4:A:359:PX4:H27	0.47	1.87	6	1
4:A:389:PX4:H56	4:A:405:PX4:H27	0.47	1.87	14	1
4:A:371:PX4:H10	4:A:426:PX4:H50	0.47	1.86	17	1
4:A:368:PX4:H69	4:A:372:PX4:H39	0.47	1.85	18	1
4:A:324:PX4:H61	4:A:406:PX4:H72	0.47	1.85	19	1
4:A:412:PX4:H49	4:A:424:PX4:H51	0.47	1.86	19	1
4:A:328:PX4:H21	4:A:347:PX4:H23	0.47	1.86	10	1
4:A:316:PX4:H67	4:A:350:PX4:H55	0.47	1.86	9	1
4:A:368:PX4:C13	4:A:391:PX4:H44	0.47	2.38	1	1
4:A:327:PX4:H27	4:A:351:PX4:H6	0.47	1.85	3	1
4:A:310:PX4:H54	4:A:333:PX4:H48	0.47	1.85	5	1
4:A:384:PX4:H33	4:A:405:PX4:H37	0.47	1.85	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:379:PX4:H24	4:A:384:PX4:H53	0.47	1.84	13	1
4:A:398:PX4:H20	4:A:411:PX4:H46	0.47	1.86	14	1
4:A:338:PX4:H31	4:A:354:PX4:O8	0.47	2.10	17	1
4:A:327:PX4:O2	4:A:351:PX4:H4	0.47	2.10	19	1
4:A:319:PX4:H71	4:A:356:PX4:H32	0.47	1.85	19	1
4:A:370:PX4:H49	4:A:394:PX4:H54	0.47	1.86	19	1
4:A:323:PX4:H63	4:A:328:PX4:C30	0.47	2.40	11	1
4:A:382:PX4:H37	4:A:398:PX4:H39	0.47	1.86	4	1
4:A:376:PX4:H5	4:A:390:PX4:O8	0.47	2.10	4	1
4:A:334:PX4:H29	4:A:334:PX4:H56	0.47	1.84	9	1
4:A:342:PX4:C22	4:A:405:PX4:H69	0.47	2.40	3	1
4:A:316:PX4:H43	4:A:352:PX4:H44	0.47	1.87	6	1
4:A:307:PX4:H31	4:A:344:PX4:H33	0.47	1.86	14	1
1:A:124:PHE:O	4:A:348:PX4:H2	0.47	2.10	18	3
4:A:351:PX4:H43	4:A:392:PX4:H41	0.47	1.87	2	1
4:A:384:PX4:H30	4:A:405:PX4:H41	0.47	1.85	2	1
4:A:407:PX4:H10	4:A:427:PX4:O6	0.47	2.10	2	1
4:A:327:PX4:H66	4:A:347:PX4:H42	0.47	1.86	17	1
4:A:378:PX4:H40	4:A:418:PX4:H72	0.47	1.86	8	1
4:A:387:PX4:H27	4:A:416:PX4:H52	0.47	1.87	8	1
4:A:317:PX4:H30	4:A:326:PX4:H20	0.47	1.84	16	1
4:A:318:PX4:H16	4:A:357:PX4:H35	0.47	1.87	18	1
4:A:309:PX4:H38	4:A:345:PX4:H57	0.47	1.86	12	1
4:A:323:PX4:H67	4:A:328:PX4:H58	0.47	1.85	11	1
4:A:333:PX4:H34	4:A:340:PX4:H40	0.47	1.85	4	1
4:A:423:PX4:H13	4:A:423:PX4:H15	0.47	1.86	4	1
4:A:412:PX4:O2	4:A:412:PX4:H10	0.47	2.10	4	1
4:A:384:PX4:H52	5:A:434:C3S:H261	0.47	1.85	20	1
4:A:398:PX4:H31	5:A:435:C3S:H502	0.47	1.85	7	1
1:A:134:ILE:HG23	1:A:168:GLY:O	0.47	2.09	5	1
4:A:392:PX4:H21	4:A:427:PX4:H60	0.47	1.86	14	1
4:A:374:PX4:H13	4:A:423:PX4:O8	0.47	2.09	14	1
4:A:319:PX4:O1	4:A:352:PX4:H3	0.47	2.09	17	1
1:A:71:ASP:OD1	1:A:198:HIS:CE1	0.47	2.68	8	1
4:A:317:PX4:H43	4:A:361:PX4:H59	0.47	1.86	16	1
4:A:335:PX4:H27	4:A:363:PX4:H57	0.47	1.85	4	1
4:A:419:PX4:H30	4:A:429:PX4:H37	0.47	1.87	4	1
4:A:348:PX4:H27	4:A:359:PX4:H16	0.47	1.87	10	2
4:A:308:PX4:H61	4:A:326:PX4:H57	0.47	1.87	20	1
4:A:325:PX4:H55	4:A:329:PX4:H55	0.47	1.85	7	1
4:A:385:PX4:H19	5:A:433:C3S:H91	0.47	1.85	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:372:PX4:H44	4:A:426:PX4:H70	0.47	1.85	17	1
4:A:390:PX4:H36	4:A:421:PX4:H23	0.47	1.84	18	1
4:A:306:PX4:H20	4:A:358:PX4:H15	0.47	1.87	11	1
4:A:428:PX4:H63	4:A:430:PX4:H32	0.47	1.86	11	1
4:A:312:PX4:H68	4:A:402:PX4:H38	0.47	1.87	10	1
4:A:404:PX4:H35	4:A:418:PX4:H38	0.47	1.84	10	1
4:A:334:PX4:H33	4:A:334:PX4:H60	0.47	1.86	9	1
4:A:343:PX4:H65	4:A:350:PX4:H25	0.47	1.85	1	1
4:A:380:PX4:H50	4:A:420:PX4:H22	0.47	1.87	7	1
4:A:373:PX4:H46	4:A:410:PX4:H10	0.47	1.87	5	1
4:A:327:PX4:H48	4:A:338:PX4:H58	0.47	1.87	8	1
4:A:404:PX4:H36	4:A:417:PX4:C13	0.47	2.39	8	1
4:A:322:PX4:H47	4:A:337:PX4:H17	0.47	1.87	16	1
4:A:377:PX4:H23	4:A:408:PX4:H23	0.47	1.87	18	1
4:A:321:PX4:H71	4:A:357:PX4:H29	0.47	1.86	12	1
4:A:315:PX4:O6	4:A:332:PX4:H2	0.47	2.10	12	1
4:A:368:PX4:H33	4:A:388:PX4:H65	0.47	1.85	9	1
4:A:347:PX4:H36	4:A:413:PX4:H40	0.47	1.85	1	1
4:A:307:PX4:H34	4:A:337:PX4:H36	0.47	1.86	3	1
4:A:307:PX4:H46	4:A:332:PX4:H6	0.47	1.87	7	1
4:A:375:PX4:H64	4:A:384:PX4:H28	0.47	1.85	5	1
4:A:404:PX4:H20	4:A:423:PX4:H27	0.46	1.87	6	1
4:A:317:PX4:H59	4:A:337:PX4:H59	0.46	1.87	14	1
4:A:329:PX4:C17	4:A:360:PX4:H33	0.46	2.40	14	1
4:A:418:PX4:H71	4:A:421:PX4:H23	0.46	1.87	14	1
4:A:325:PX4:H10	4:A:361:PX4:O2	0.46	2.10	8	1
4:A:351:PX4:H66	4:A:387:PX4:H45	0.46	1.86	8	1
4:A:375:PX4:H51	4:A:405:PX4:H17	0.46	1.87	16	1
4:A:345:PX4:H30	4:A:349:PX4:H58	0.46	1.86	18	1
4:A:315:PX4:H70	4:A:321:PX4:H36	0.46	1.87	19	1
4:A:315:PX4:H19	4:A:337:PX4:H62	0.46	1.87	12	1
4:A:372:PX4:H4	4:A:410:PX4:O2	0.46	2.09	10	1
4:A:338:PX4:H43	4:A:411:PX4:H51	0.46	1.87	9	1
4:A:318:PX4:H16	4:A:321:PX4:H51	0.46	1.87	1	1
4:A:404:PX4:H20	4:A:418:PX4:H58	0.46	1.85	1	1
4:A:306:PX4:H15	4:A:306:PX4:O8	0.46	2.09	20	1
4:A:397:PX4:H39	4:A:424:PX4:H42	0.46	1.85	20	1
4:A:395:PX4:H64	4:A:395:PX4:H37	0.46	1.86	7	1
4:A:384:PX4:H56	4:A:392:PX4:H56	0.46	1.87	13	1
4:A:370:PX4:H27	4:A:383:PX4:H51	0.46	1.85	6	1
4:A:413:PX4:H20	4:A:429:PX4:H21	0.46	1.86	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:307:PX4:H39	4:A:338:PX4:H64	0.46	1.87	8	1
4:A:308:PX4:H33	4:A:350:PX4:H58	0.46	1.86	8	1
4:A:309:PX4:H22	4:A:345:PX4:H60	0.46	1.85	16	1
4:A:309:PX4:H29	4:A:359:PX4:H36	0.46	1.86	12	1
1:A:71:ASP:OD1	1:A:204:HIS:CD2	0.46	2.68	4	1
1:A:129:TRP:HB3	4:A:316:PX4:H55	0.46	1.87	9	1
4:A:370:PX4:H38	4:A:394:PX4:H32	0.46	1.85	9	1
4:A:395:PX4:H13	4:A:401:PX4:H49	0.46	1.88	9	1
4:A:330:PX4:H35	4:A:337:PX4:H57	0.46	1.87	3	1
1:A:118:LYS:O	4:A:351:PX4:H3	0.46	2.10	5	1
4:A:340:PX4:H13	5:A:432:C3S:H91	0.46	1.87	13	1
4:A:404:PX4:O3	4:A:404:PX4:H9	0.46	2.10	13	1
4:A:321:PX4:H58	4:A:352:PX4:H38	0.46	1.87	19	1
4:A:308:PX4:H15	4:A:320:PX4:H12	0.46	1.86	4	1
4:A:376:PX4:H17	4:A:388:PX4:C10	0.46	2.40	4	1
4:A:330:PX4:H54	4:A:362:PX4:H30	0.46	1.87	9	1
1:A:36:GLU:OE2	1:A:40:LYS:NZ	0.46	2.48	9	1
4:A:312:PX4:H43	4:A:388:PX4:H54	0.46	1.86	1	1
4:A:399:PX4:H39	4:A:424:PX4:H32	0.46	1.87	1	1
4:A:308:PX4:H41	4:A:350:PX4:H27	0.46	1.87	7	1
4:A:370:PX4:H34	4:A:383:PX4:H33	0.46	1.86	13	1
4:A:371:PX4:H57	4:A:389:PX4:H17	0.46	1.87	2	1
4:A:371:PX4:H47	4:A:389:PX4:H46	0.46	1.87	8	1
4:A:366:PX4:H17	4:A:403:PX4:H28	0.46	1.86	18	1
4:A:328:PX4:H43	4:A:358:PX4:H36	0.46	1.88	19	1
4:A:400:PX4:H21	4:A:405:PX4:H19	0.46	1.87	15	1
4:A:325:PX4:H37	4:A:430:PX4:H43	0.46	1.87	15	1
4:A:325:PX4:H34	4:A:362:PX4:H68	0.46	1.87	9	1
4:A:369:PX4:H52	4:A:419:PX4:H54	0.46	1.87	20	1
4:A:307:PX4:H3	4:A:322:PX4:O3	0.46	2.10	3	1
4:A:409:PX4:H22	4:A:412:PX4:H20	0.46	1.88	3	1
4:A:350:PX4:H44	4:A:395:PX4:H29	0.46	1.86	2	1
4:A:394:PX4:H59	4:A:396:PX4:H67	0.46	1.85	2	1
4:A:417:PX4:H21	4:A:418:PX4:H32	0.46	1.86	17	1
4:A:325:PX4:H19	4:A:355:PX4:H17	0.46	1.86	16	1
4:A:328:PX4:H8	4:A:349:PX4:O8	0.46	2.10	16	1
4:A:328:PX4:H36	4:A:361:PX4:H34	0.46	1.88	16	1
4:A:371:PX4:H3	4:A:373:PX4:O1	0.46	2.10	11	1
4:A:375:PX4:H53	4:A:384:PX4:H55	0.46	1.87	11	1
4:A:376:PX4:H57	4:A:388:PX4:H35	0.46	1.86	4	1
4:A:313:PX4:H55	4:A:325:PX4:H55	0.46	1.86	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:O1	4:A:351:PX4:H7	0.46	2.11	20	1
4:A:371:PX4:H14	4:A:373:PX4:H18	0.46	1.87	20	1
4:A:313:PX4:H68	4:A:323:PX4:H57	0.46	1.85	3	1
1:A:7:MET:SD	1:A:54:LEU:HD22	0.46	2.51	13	1
4:A:327:PX4:H20	4:A:348:PX4:H20	0.46	1.87	2	1
4:A:311:PX4:H40	4:A:339:PX4:H51	0.46	1.88	2	1
4:A:306:PX4:H22	4:A:342:PX4:H15	0.46	1.88	2	1
4:A:370:PX4:H31	4:A:383:PX4:H51	0.46	1.87	16	1
4:A:386:PX4:H27	4:A:402:PX4:H53	0.46	1.88	18	1
4:A:313:PX4:H46	4:A:329:PX4:H17	0.46	1.88	12	1
4:A:398:PX4:H33	4:A:411:PX4:H54	0.46	1.88	20	1
4:A:377:PX4:H54	4:A:422:PX4:H25	0.46	1.86	3	1
4:A:316:PX4:O2	4:A:321:PX4:H11	0.46	2.11	6	1
4:A:404:PX4:O2	4:A:404:PX4:H13	0.46	2.11	6	1
4:A:340:PX4:H12	5:A:432:C3S:H91	0.46	1.88	14	1
4:A:319:PX4:H36	4:A:425:PX4:H70	0.46	1.88	17	1
4:A:336:PX4:H68	4:A:412:PX4:H37	0.46	1.87	17	1
4:A:388:PX4:H47	4:A:391:PX4:H51	0.46	1.88	17	1
4:A:429:PX4:H53	4:A:430:PX4:H20	0.46	1.88	18	1
4:A:384:PX4:O3	4:A:401:PX4:H5	0.46	2.10	12	1
4:A:306:PX4:H58	4:A:342:PX4:H36	0.46	1.88	11	1
4:A:306:PX4:H54	4:A:359:PX4:C27	0.46	2.40	4	1
4:A:366:PX4:H55	4:A:403:PX4:H47	0.46	1.87	20	1
4:A:325:PX4:H39	4:A:326:PX4:H25	0.46	1.88	5	1
4:A:396:PX4:H16	4:A:407:PX4:H52	0.46	1.88	5	1
4:A:366:PX4:H52	4:A:378:PX4:H26	0.46	1.87	6	1
4:A:365:PX4:H30	4:A:430:PX4:H33	0.46	1.87	2	1
4:A:338:PX4:H28	4:A:354:PX4:H48	0.46	1.88	17	1
4:A:324:PX4:H24	4:A:324:PX4:H49	0.46	1.88	16	1
4:A:336:PX4:H14	4:A:336:PX4:H2	0.46	1.87	16	1
4:A:305:PX4:H55	4:A:311:PX4:H39	0.46	1.88	18	1
1:A:222:GLN:O	4:A:317:PX4:H11	0.46	2.10	19	1
4:A:417:PX4:H7	4:A:418:PX4:H21	0.46	1.87	19	1
4:A:400:PX4:H16	4:A:401:PX4:H46	0.46	1.88	10	1
4:A:318:PX4:H28	4:A:321:PX4:H54	0.46	1.87	9	1
4:A:320:PX4:H51	4:A:334:PX4:H15	0.46	1.87	1	1
4:A:386:PX4:O6	4:A:402:PX4:H20	0.46	2.11	7	1
4:A:406:PX4:O1	4:A:410:PX4:H10	0.46	2.11	10	2
4:A:387:PX4:H67	4:A:421:PX4:H35	0.46	1.87	8	1
4:A:413:PX4:H49	4:A:429:PX4:H23	0.46	1.86	16	1
4:A:322:PX4:H8	4:A:337:PX4:H2	0.46	1.88	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:393:PX4:H50	4:A:419:PX4:H19	0.46	1.87	12	1
1:A:111:LYS:HE3	4:A:315:PX4:H15	0.46	1.88	9	1
4:A:305:PX4:H51	4:A:324:PX4:H72	0.46	1.88	7	1
4:A:320:PX4:H59	4:A:334:PX4:H54	0.46	1.87	13	1
4:A:348:PX4:H31	4:A:359:PX4:H31	0.46	1.88	13	1
4:A:357:PX4:H3	4:A:363:PX4:O6	0.46	2.11	2	1
4:A:393:PX4:H27	4:A:419:PX4:H54	0.46	1.87	17	1
4:A:327:PX4:H24	4:A:348:PX4:H26	0.46	1.88	18	1
4:A:370:PX4:H60	4:A:381:PX4:H35	0.46	1.87	18	1
4:A:329:PX4:H51	4:A:355:PX4:H60	0.46	1.88	12	1
4:A:399:PX4:H26	4:A:410:PX4:H32	0.46	1.88	1	1
4:A:406:PX4:H44	4:A:410:PX4:H65	0.46	1.86	20	1
4:A:414:PX4:H9	4:A:426:PX4:O6	0.46	2.11	3	1
4:A:340:PX4:H63	4:A:364:PX4:H38	0.46	1.88	7	1
4:A:424:PX4:H15	4:A:424:PX4:O8	0.46	2.11	5	1
4:A:322:PX4:H50	4:A:331:PX4:H20	0.45	1.86	6	1
4:A:325:PX4:H23	4:A:355:PX4:H48	0.45	1.88	6	1
4:A:389:PX4:H62	4:A:394:PX4:H42	0.45	1.88	6	1
4:A:391:PX4:H60	4:A:427:PX4:H40	0.45	1.88	2	1
4:A:337:PX4:H30	4:A:341:PX4:H25	0.45	1.87	16	1
4:A:308:PX4:H36	4:A:373:PX4:H43	0.45	1.87	16	1
4:A:377:PX4:H27	4:A:408:PX4:H28	0.45	1.87	18	1
4:A:308:PX4:H26	4:A:326:PX4:H58	0.45	1.88	19	1
4:A:384:PX4:O4	4:A:405:PX4:H5	0.45	2.10	19	1
4:A:352:PX4:H35	4:A:392:PX4:H65	0.45	1.87	10	1
1:A:184:LEU:HD21	4:A:349:PX4:H12	0.45	1.87	3	1
4:A:365:PX4:H26	4:A:369:PX4:H23	0.45	1.86	3	1
4:A:311:PX4:H69	4:A:364:PX4:H69	0.45	1.87	7	1
4:A:333:PX4:H27	4:A:340:PX4:H30	0.45	1.89	7	1
4:A:367:PX4:H33	4:A:389:PX4:H30	0.45	1.88	5	1
4:A:377:PX4:H29	4:A:377:PX4:H54	0.45	1.88	5	1
4:A:382:PX4:H62	4:A:397:PX4:H40	0.45	1.88	2	1
4:A:342:PX4:H38	4:A:357:PX4:H37	0.45	1.88	17	1
4:A:392:PX4:H9	4:A:405:PX4:H15	0.45	1.87	17	1
4:A:342:PX4:H54	4:A:357:PX4:H37	0.45	1.89	18	1
4:A:420:PX4:H20	4:A:422:PX4:H16	0.45	1.89	15	1
1:A:90:THR:HG21	4:A:321:PX4:H1	0.45	1.87	20	1
4:A:306:PX4:C9	4:A:342:PX4:H14	0.45	2.41	3	1
4:A:376:PX4:H16	4:A:390:PX4:H47	0.45	1.87	3	1
4:A:379:PX4:H26	5:A:434:C3S:H152	0.45	1.87	14	1
4:A:318:PX4:H11	4:A:321:PX4:O8	0.45	2.12	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:375:PX4:H61	4:A:379:PX4:H42	0.45	1.86	17	1
4:A:316:PX4:H35	4:A:321:PX4:H53	0.45	1.88	16	1
4:A:370:PX4:O1	4:A:383:PX4:H11	0.45	2.12	18	1
4:A:309:PX4:H6	4:A:328:PX4:O6	0.45	2.11	19	2
4:A:320:PX4:H61	4:A:334:PX4:H67	0.45	1.88	15	1
4:A:397:PX4:H21	4:A:411:PX4:H16	0.45	1.88	15	1
4:A:386:PX4:H27	4:A:417:PX4:H55	0.45	1.88	11	1
4:A:312:PX4:H26	4:A:324:PX4:H22	0.45	1.89	4	1
4:A:404:PX4:H26	4:A:418:PX4:H20	0.45	1.89	10	1
4:A:375:PX4:H17	4:A:392:PX4:O1	0.45	2.12	9	1
4:A:375:PX4:H22	4:A:407:PX4:H19	0.45	1.88	7	1
4:A:382:PX4:H17	4:A:423:PX4:H20	0.45	1.88	7	1
4:A:327:PX4:H55	4:A:327:PX4:H35	0.45	1.89	13	1
4:A:336:PX4:H27	4:A:354:PX4:H34	0.45	1.89	13	1
4:A:382:PX4:H64	4:A:415:PX4:H59	0.45	1.88	13	1
4:A:316:PX4:O2	4:A:318:PX4:H4	0.45	2.12	2	1
4:A:375:PX4:H68	4:A:384:PX4:H31	0.45	1.86	2	1
4:A:374:PX4:H34	4:A:397:PX4:H69	0.45	1.88	18	1
4:A:365:PX4:O6	4:A:369:PX4:H10	0.45	2.11	19	1
4:A:345:PX4:H63	4:A:358:PX4:H56	0.45	1.88	11	1
4:A:377:PX4:H23	4:A:408:PX4:H54	0.45	1.87	10	1
4:A:368:PX4:H57	4:A:426:PX4:H55	0.45	1.87	9	1
4:A:371:PX4:H32	4:A:395:PX4:H27	0.45	1.89	1	1
4:A:345:PX4:H71	4:A:419:PX4:H66	0.45	1.87	20	1
4:A:369:PX4:H5	4:A:370:PX4:O6	0.45	2.11	20	1
4:A:368:PX4:H43	4:A:426:PX4:H29	0.45	1.86	5	1
4:A:307:PX4:O2	4:A:322:PX4:H9	0.45	2.12	6	1
4:A:323:PX4:H42	4:A:345:PX4:H37	0.45	1.89	14	1
4:A:384:PX4:O3	4:A:384:PX4:H12	0.45	2.10	14	1
4:A:375:PX4:O2	4:A:427:PX4:H2	0.45	2.12	14	1
1:A:123:HIS:CE1	4:A:348:PX4:H21	0.45	2.46	15	2
4:A:350:PX4:H70	4:A:402:PX4:H70	0.45	1.87	12	1
4:A:391:PX4:H19	4:A:408:PX4:H53	0.45	1.88	12	1
4:A:374:PX4:H25	4:A:423:PX4:H21	0.45	1.88	11	1
4:A:397:PX4:H31	4:A:398:PX4:H36	0.45	1.88	1	1
4:A:383:PX4:H71	4:A:407:PX4:H30	0.45	1.89	1	1
4:A:351:PX4:H67	4:A:429:PX4:H38	0.45	1.89	20	1
4:A:368:PX4:H3	4:A:372:PX4:O1	0.45	2.12	5	2
4:A:350:PX4:H40	4:A:371:PX4:H44	0.45	1.89	7	1
4:A:373:PX4:H59	4:A:414:PX4:H32	0.45	1.89	7	1
4:A:310:PX4:H50	4:A:333:PX4:H53	0.45	1.88	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:373:PX4:H37	4:A:400:PX4:H44	0.45	1.88	2	1
4:A:391:PX4:H27	4:A:407:PX4:H27	0.45	1.89	4	1
4:A:350:PX4:H60	4:A:395:PX4:H44	0.45	1.87	10	1
4:A:409:PX4:H43	4:A:429:PX4:H37	0.45	1.89	9	1
4:A:322:PX4:H29	4:A:322:PX4:H67	0.45	1.88	1	1
4:A:403:PX4:H3	4:A:417:PX4:O6	0.45	2.12	3	1
4:A:370:PX4:H32	4:A:383:PX4:H25	0.45	1.87	5	1
4:A:378:PX4:H53	4:A:426:PX4:H14	0.45	1.89	13	1
4:A:331:PX4:H40	4:A:337:PX4:H17	0.45	1.88	2	1
4:A:401:PX4:H67	4:A:401:PX4:H38	0.45	1.89	8	1
4:A:362:PX4:H41	4:A:424:PX4:H42	0.45	1.88	8	1
4:A:317:PX4:H43	4:A:361:PX4:C30	0.45	2.42	16	1
4:A:366:PX4:H19	4:A:417:PX4:H20	0.45	1.88	16	1
4:A:305:PX4:H42	4:A:372:PX4:H40	0.45	1.88	18	1
4:A:324:PX4:H40	4:A:426:PX4:H31	0.45	1.87	19	1
4:A:326:PX4:H63	5:A:431:C3S:H442	0.45	1.88	11	1
4:A:308:PX4:H17	4:A:326:PX4:H51	0.45	1.88	10	1
4:A:338:PX4:H16	4:A:344:PX4:H48	0.45	1.88	9	1
4:A:316:PX4:H70	4:A:340:PX4:H60	0.45	1.87	1	1
4:A:308:PX4:H61	4:A:326:PX4:C29	0.45	2.41	20	1
4:A:341:PX4:H8	4:A:356:PX4:O6	0.45	2.12	20	1
4:A:335:PX4:H37	4:A:360:PX4:H36	0.45	1.88	20	1
4:A:318:PX4:H24	4:A:342:PX4:H48	0.45	1.89	5	1
4:A:411:PX4:H46	4:A:424:PX4:H47	0.45	1.88	8	1
4:A:365:PX4:H62	4:A:376:PX4:H28	0.45	1.88	16	1
4:A:391:PX4:O2	4:A:414:PX4:H8	0.45	2.11	18	1
4:A:327:PX4:H21	4:A:348:PX4:C11	0.45	2.36	4	1
4:A:333:PX4:O6	4:A:340:PX4:H4	0.45	2.12	4	1
4:A:389:PX4:H45	4:A:405:PX4:H34	0.45	1.88	4	1
4:A:428:PX4:H21	4:A:428:PX4:H54	0.45	1.88	4	1
4:A:323:PX4:H48	4:A:361:PX4:H19	0.45	1.88	10	1
4:A:328:PX4:H40	4:A:360:PX4:H35	0.45	1.89	9	1
4:A:368:PX4:H40	4:A:391:PX4:H35	0.45	1.87	9	1
4:A:326:PX4:H69	4:A:361:PX4:H41	0.45	1.87	3	1
4:A:386:PX4:O6	4:A:417:PX4:H17	0.45	2.12	14	1
4:A:308:PX4:H28	4:A:334:PX4:H34	0.45	1.88	2	1
4:A:346:PX4:H32	4:A:361:PX4:H65	0.45	1.87	18	1
4:A:375:PX4:C11	4:A:400:PX4:H62	0.45	2.42	19	1
4:A:333:PX4:H33	4:A:340:PX4:H34	0.45	1.89	12	1
4:A:386:PX4:H31	4:A:417:PX4:H51	0.45	1.89	12	1
4:A:375:PX4:H17	4:A:405:PX4:H4	0.45	1.89	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:370:PX4:H12	4:A:397:PX4:H46	0.45	1.88	3	1
4:A:367:PX4:H29	4:A:399:PX4:H25	0.45	1.89	13	1
1:A:96:TYR:CD2	1:A:102:HIS:HA	0.45	2.47	6	1
4:A:369:PX4:H58	4:A:428:PX4:H36	0.45	1.89	14	1
4:A:392:PX4:H62	4:A:422:PX4:H56	0.45	1.88	14	1
4:A:366:PX4:H40	4:A:368:PX4:H40	0.45	1.89	8	1
4:A:353:PX4:H56	4:A:378:PX4:C22	0.45	2.42	8	1
4:A:320:PX4:H25	4:A:332:PX4:H42	0.45	1.88	18	1
4:A:305:PX4:H47	4:A:312:PX4:H61	0.45	1.89	15	1
4:A:309:PX4:O6	4:A:351:PX4:H18	0.45	2.11	15	1
4:A:365:PX4:H6	4:A:383:PX4:O2	0.45	2.12	15	1
4:A:315:PX4:H37	4:A:327:PX4:H66	0.45	1.89	12	1
4:A:324:PX4:H55	4:A:334:PX4:H55	0.45	1.88	11	1
4:A:310:PX4:H22	4:A:311:PX4:H17	0.45	1.89	10	1
4:A:420:PX4:O8	4:A:420:PX4:H10	0.45	2.11	9	1
4:A:384:PX4:H47	4:A:389:PX4:H26	0.44	1.89	17	1
4:A:306:PX4:H59	4:A:321:PX4:H17	0.44	1.89	8	1
4:A:316:PX4:H25	4:A:342:PX4:H38	0.44	1.89	16	1
4:A:400:PX4:O6	4:A:405:PX4:H10	0.44	2.13	18	1
4:A:400:PX4:H59	4:A:405:PX4:H21	0.44	1.89	19	1
4:A:308:PX4:H16	4:A:320:PX4:H17	0.44	1.90	15	1
4:A:395:PX4:O4	4:A:401:PX4:H16	0.44	2.12	11	1
4:A:405:PX4:H7	4:A:405:PX4:H17	0.44	1.89	1	1
4:A:369:PX4:H24	4:A:374:PX4:H51	0.44	1.88	20	1
4:A:395:PX4:O1	4:A:402:PX4:H4	0.44	2.12	14	1
4:A:366:PX4:O6	4:A:417:PX4:H5	0.44	2.11	14	1
4:A:317:PX4:H21	4:A:326:PX4:H20	0.44	1.87	17	1
4:A:333:PX4:H51	4:A:333:PX4:H17	0.44	1.89	16	1
4:A:391:PX4:H31	4:A:408:PX4:H61	0.44	1.89	15	1
4:A:328:PX4:H58	4:A:347:PX4:H26	0.44	1.89	12	1
4:A:343:PX4:O6	4:A:343:PX4:H16	0.44	2.12	11	1
4:A:378:PX4:H55	4:A:386:PX4:H30	0.44	1.89	11	1
4:A:338:PX4:H46	4:A:351:PX4:H48	0.44	1.89	10	1
4:A:391:PX4:H35	4:A:427:PX4:H65	0.44	1.89	10	1
4:A:398:PX4:H38	4:A:411:PX4:H67	0.44	1.89	20	1
4:A:307:PX4:H11	4:A:337:PX4:O2	0.44	2.12	3	1
4:A:371:PX4:H23	4:A:402:PX4:H23	0.44	1.89	3	1
4:A:412:PX4:H54	4:A:424:PX4:H51	0.44	1.89	6	1
4:A:318:PX4:H31	4:A:321:PX4:H49	0.44	1.89	14	1
4:A:323:PX4:H21	4:A:328:PX4:H23	0.44	1.88	14	1
4:A:382:PX4:H17	4:A:415:PX4:H46	0.44	1.88	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:361:PX4:H52	4:A:402:PX4:H43	0.44	1.89	17	1
4:A:340:PX4:H62	4:A:356:PX4:H34	0.44	1.89	8	1
4:A:409:PX4:H69	4:A:411:PX4:H27	0.44	1.89	8	1
4:A:411:PX4:H14	4:A:411:PX4:H9	0.44	1.89	8	1
4:A:307:PX4:O2	4:A:322:PX4:H7	0.44	2.12	16	1
4:A:367:PX4:O6	4:A:399:PX4:H17	0.44	2.12	18	1
4:A:320:PX4:H41	4:A:381:PX4:H61	0.44	1.88	18	1
4:A:375:PX4:H19	4:A:392:PX4:H10	0.44	1.90	18	1
4:A:345:PX4:H16	4:A:349:PX4:H51	0.44	1.88	19	1
4:A:369:PX4:O8	4:A:419:PX4:H8	0.44	2.12	4	1
4:A:396:PX4:H20	4:A:407:PX4:H14	0.44	1.89	4	1
4:A:380:PX4:H39	4:A:422:PX4:H66	0.44	1.87	10	1
4:A:309:PX4:H22	4:A:345:PX4:H57	0.44	1.89	9	1
4:A:342:PX4:O4	4:A:358:PX4:H10	0.44	2.12	1	1
4:A:328:PX4:H47	4:A:347:PX4:H14	0.44	1.88	13	2
4:A:331:PX4:O2	4:A:337:PX4:H11	0.44	2.11	13	1
4:A:327:PX4:H25	4:A:338:PX4:H62	0.44	1.89	2	1
4:A:330:PX4:H59	4:A:337:PX4:H31	0.44	1.89	17	1
4:A:404:PX4:H16	4:A:418:PX4:H47	0.44	1.89	15	1
4:A:368:PX4:H54	4:A:406:PX4:H29	0.44	1.90	11	1
4:A:341:PX4:H48	4:A:356:PX4:H23	0.44	1.87	9	1
4:A:393:PX4:H57	4:A:413:PX4:H32	0.44	1.89	1	1
4:A:309:PX4:H59	4:A:359:PX4:H34	0.44	1.89	7	1
4:A:314:PX4:H23	4:A:352:PX4:O6	0.44	2.13	13	1
4:A:308:PX4:H51	4:A:326:PX4:H62	0.44	1.89	13	1
4:A:390:PX4:H49	4:A:403:PX4:H52	0.44	1.89	14	1
4:A:394:PX4:H29	4:A:395:PX4:H54	0.44	1.87	17	1
4:A:307:PX4:H64	4:A:327:PX4:H36	0.44	1.88	16	1
4:A:371:PX4:H48	4:A:373:PX4:H16	0.44	1.87	16	1
4:A:389:PX4:H16	4:A:399:PX4:H50	0.44	1.89	16	1
4:A:408:PX4:H69	4:A:426:PX4:H20	0.44	1.90	16	1
4:A:328:PX4:H26	4:A:347:PX4:H24	0.44	1.90	19	1
4:A:310:PX4:H64	4:A:356:PX4:H44	0.44	1.90	15	1
4:A:372:PX4:H54	4:A:398:PX4:H71	0.44	1.89	12	1
1:A:181:GLY:O	4:A:361:PX4:H10	0.44	2.13	9	1
4:A:334:PX4:H27	4:A:414:PX4:H66	0.44	1.89	9	1
4:A:323:PX4:H58	4:A:347:PX4:H31	0.44	1.90	9	1
4:A:371:PX4:H39	4:A:373:PX4:H32	0.44	1.89	9	1
4:A:411:PX4:H25	4:A:424:PX4:H60	0.44	1.88	9	1
4:A:312:PX4:H66	4:A:363:PX4:H72	0.44	1.90	1	1
4:A:306:PX4:H62	4:A:348:PX4:H37	0.44	1.88	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H34	4:A:423:PX4:H58	0.44	1.90	13	1
4:A:388:PX4:H8	4:A:391:PX4:O6	0.44	2.12	13	1
4:A:385:PX4:H17	4:A:415:PX4:H20	0.44	1.88	13	1
4:A:326:PX4:H62	4:A:361:PX4:H30	0.44	1.88	6	1
4:A:343:PX4:O1	4:A:356:PX4:H5	0.44	2.13	6	1
4:A:371:PX4:H17	4:A:401:PX4:O6	0.44	2.13	6	1
4:A:320:PX4:H36	4:A:334:PX4:H40	0.44	1.88	14	1
4:A:384:PX4:H62	5:A:434:C3S:C60	0.44	2.42	14	1
4:A:400:PX4:H14	4:A:401:PX4:O2	0.44	2.12	14	1
4:A:387:PX4:O6	4:A:421:PX4:H20	0.44	2.13	16	1
4:A:330:PX4:H16	4:A:337:PX4:H19	0.44	1.90	19	1
4:A:428:PX4:H16	4:A:429:PX4:H50	0.44	1.89	19	1
4:A:423:PX4:H72	4:A:429:PX4:H65	0.44	1.88	12	1
4:A:402:PX4:H8	4:A:417:PX4:O1	0.44	2.12	11	1
4:A:305:PX4:H32	4:A:310:PX4:H30	0.44	1.89	4	1
4:A:393:PX4:H22	4:A:416:PX4:H23	0.44	1.89	4	1
4:A:371:PX4:H35	4:A:395:PX4:H35	0.44	1.89	9	1
4:A:338:PX4:H6	4:A:344:PX4:O6	0.44	2.13	20	1
4:A:389:PX4:H66	4:A:400:PX4:H38	0.44	1.88	20	1
4:A:354:PX4:H48	4:A:357:PX4:H49	0.44	1.90	3	1
4:A:387:PX4:H28	4:A:418:PX4:C30	0.44	2.43	3	1
4:A:314:PX4:H27	4:A:352:PX4:H22	0.44	1.90	13	1
4:A:382:PX4:H61	4:A:423:PX4:H36	0.44	1.88	13	1
4:A:428:PX4:H28	4:A:429:PX4:H36	0.44	1.89	14	1
1:A:101:PRO:HG3	4:A:334:PX4:H1	0.44	1.88	2	1
1:A:83:LYS:HG2	1:A:238:TYR:CE1	0.44	2.48	2	1
4:A:381:PX4:H20	4:A:394:PX4:H53	0.44	1.88	17	1
4:A:399:PX4:H22	4:A:399:PX4:H48	0.44	1.88	19	1
4:A:395:PX4:H68	4:A:405:PX4:H37	0.44	1.88	11	1
4:A:383:PX4:H68	4:A:396:PX4:H60	0.44	1.87	4	1
4:A:326:PX4:H72	4:A:417:PX4:H64	0.44	1.90	4	1
4:A:307:PX4:H29	4:A:307:PX4:H62	0.44	1.88	1	1
4:A:397:PX4:H54	4:A:430:PX4:H21	0.44	1.90	1	1
4:A:323:PX4:H46	4:A:325:PX4:H15	0.44	1.88	5	1
4:A:336:PX4:C36	4:A:409:PX4:H31	0.44	2.42	5	1
4:A:404:PX4:O1	4:A:418:PX4:H12	0.44	2.12	6	1
4:A:317:PX4:H65	4:A:330:PX4:H45	0.44	1.89	14	1
4:A:359:PX4:H69	4:A:383:PX4:H61	0.44	1.90	8	1
4:A:332:PX4:H72	4:A:388:PX4:H43	0.44	1.88	8	1
4:A:394:PX4:H21	4:A:401:PX4:H50	0.44	1.90	8	1
4:A:327:PX4:H68	4:A:338:PX4:H24	0.44	1.88	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:337:PX4:H36	4:A:355:PX4:H36	0.44	1.89	12	1
4:A:428:PX4:H33	4:A:429:PX4:H35	0.44	1.88	12	1
4:A:398:PX4:H10	5:A:435:C3S:O2	0.44	2.12	12	1
1:A:128:VAL:CG2	4:A:315:PX4:H72	0.44	2.41	10	1
4:A:322:PX4:H62	4:A:369:PX4:H38	0.44	1.89	10	1
4:A:369:PX4:H65	4:A:429:PX4:H65	0.44	1.90	10	1
4:A:317:PX4:H59	4:A:332:PX4:H25	0.44	1.90	9	1
4:A:343:PX4:H59	4:A:350:PX4:H66	0.44	1.89	9	1
4:A:306:PX4:H34	4:A:358:PX4:H52	0.44	1.89	1	1
4:A:372:PX4:H56	4:A:398:PX4:H57	0.44	1.90	1	1
4:A:397:PX4:H36	4:A:404:PX4:H70	0.44	1.89	3	1
4:A:333:PX4:H34	4:A:340:PX4:H57	0.44	1.89	7	1
4:A:377:PX4:H50	4:A:408:PX4:H23	0.44	1.88	5	1
4:A:312:PX4:H21	4:A:324:PX4:H9	0.44	1.88	13	1
4:A:404:PX4:H32	4:A:423:PX4:H35	0.44	1.89	13	1
4:A:322:PX4:H50	4:A:331:PX4:C10	0.44	2.42	6	1
4:A:349:PX4:H33	4:A:361:PX4:H56	0.44	1.90	14	1
4:A:340:PX4:H32	4:A:389:PX4:H71	0.44	1.90	17	1
4:A:306:PX4:H61	4:A:332:PX4:H61	0.44	1.90	16	1
4:A:365:PX4:H66	4:A:388:PX4:H42	0.44	1.90	18	1
4:A:388:PX4:H47	4:A:390:PX4:H51	0.44	1.89	11	1
4:A:370:PX4:H57	4:A:374:PX4:H48	0.44	1.88	10	1
4:A:389:PX4:H31	4:A:389:PX4:H38	0.44	1.48	10	1
4:A:308:PX4:H32	4:A:315:PX4:H34	0.44	1.89	9	1
4:A:336:PX4:H36	4:A:354:PX4:H64	0.44	1.90	1	1
4:A:328:PX4:H53	4:A:347:PX4:H54	0.43	1.90	6	1
4:A:385:PX4:H63	4:A:415:PX4:H38	0.43	1.88	6	1
4:A:416:PX4:H32	4:A:416:PX4:H25	0.43	1.62	17	1
4:A:368:PX4:H24	5:A:436:C3S:H502	0.43	1.89	8	1
4:A:329:PX4:H31	4:A:355:PX4:H63	0.43	1.88	18	1
4:A:316:PX4:H15	4:A:352:PX4:H20	0.43	1.89	19	1
4:A:367:PX4:H16	4:A:399:PX4:H50	0.43	1.89	19	1
4:A:365:PX4:H48	4:A:370:PX4:H34	0.43	1.89	15	1
4:A:321:PX4:H29	4:A:343:PX4:H40	0.43	1.89	11	1
4:A:314:PX4:H16	4:A:336:PX4:H22	0.43	1.88	11	1
4:A:411:PX4:H7	4:A:411:PX4:H14	0.43	1.90	11	1
4:A:320:PX4:H30	4:A:326:PX4:H41	0.43	1.89	9	1
4:A:386:PX4:H36	4:A:386:PX4:H60	0.43	1.89	9	1
4:A:306:PX4:H57	4:A:342:PX4:H26	0.43	1.90	1	1
4:A:338:PX4:O3	4:A:347:PX4:H5	0.43	2.13	3	1
4:A:343:PX4:O4	4:A:350:PX4:H9	0.43	2.12	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:404:PX4:H69	4:A:423:PX4:H36	0.43	1.90	7	1
4:A:375:PX4:H38	4:A:427:PX4:H50	0.43	1.90	6	1
4:A:346:PX4:O2	4:A:346:PX4:H6	0.43	2.13	17	1
4:A:366:PX4:H13	4:A:403:PX4:H13	0.43	1.90	8	1
1:A:84:TRP:CE2	1:A:162:PRO:HB3	0.43	2.47	16	1
4:A:375:PX4:H39	4:A:427:PX4:H72	0.43	1.90	15	1
4:A:321:PX4:H46	4:A:342:PX4:H23	0.43	1.89	4	1
4:A:305:PX4:H49	4:A:324:PX4:H59	0.43	1.90	1	1
4:A:335:PX4:H8	4:A:360:PX4:H18	0.43	1.90	1	1
4:A:326:PX4:H42	4:A:326:PX4:H68	0.43	1.90	7	1
4:A:305:PX4:H40	5:A:432:C3S:H693	0.43	1.89	5	1
4:A:376:PX4:H14	4:A:396:PX4:O1	0.43	2.13	5	1
4:A:374:PX4:H49	4:A:397:PX4:H50	0.43	1.90	13	1
4:A:423:PX4:O3	4:A:423:PX4:H10	0.43	2.12	2	1
4:A:308:PX4:H68	4:A:397:PX4:H66	0.43	1.90	8	1
4:A:371:PX4:H59	4:A:402:PX4:H45	0.43	1.89	8	1
4:A:343:PX4:H31	4:A:343:PX4:H26	0.43	1.53	18	1
4:A:325:PX4:H16	4:A:355:PX4:H48	0.43	1.90	18	1
4:A:310:PX4:H24	4:A:311:PX4:H17	0.43	1.89	15	1
4:A:328:PX4:H46	4:A:347:PX4:H48	0.43	1.89	15	1
4:A:372:PX4:H3	4:A:410:PX4:H15	0.43	1.89	10	1
4:A:345:PX4:H17	4:A:358:PX4:H20	0.43	1.89	9	1
4:A:374:PX4:H57	4:A:381:PX4:H54	0.43	1.89	20	1
4:A:343:PX4:H31	4:A:352:PX4:H64	0.43	1.90	3	1
4:A:338:PX4:H64	4:A:351:PX4:H51	0.43	1.89	3	1
4:A:322:PX4:H43	4:A:362:PX4:H37	0.43	1.90	7	1
1:A:96:TYR:OH	4:A:340:PX4:H3	0.43	2.13	7	1
4:A:309:PX4:H72	4:A:390:PX4:H40	0.43	1.90	7	1
4:A:385:PX4:C8	4:A:415:PX4:H20	0.43	2.43	13	1
4:A:327:PX4:H55	4:A:348:PX4:H69	0.43	1.89	6	1
4:A:370:PX4:H8	4:A:394:PX4:O2	0.43	2.13	6	1
4:A:383:PX4:H49	4:A:407:PX4:H50	0.43	1.90	14	1
4:A:411:PX4:H28	4:A:423:PX4:H56	0.43	1.90	2	1
4:A:318:PX4:H25	4:A:321:PX4:H55	0.43	1.90	16	1
4:A:351:PX4:H29	4:A:351:PX4:H36	0.43	1.55	16	1
4:A:390:PX4:H33	4:A:390:PX4:H62	0.43	1.90	16	1
4:A:306:PX4:H56	4:A:342:PX4:H23	0.43	1.90	19	1
4:A:313:PX4:O6	4:A:355:PX4:H3	0.43	2.14	12	1
4:A:328:PX4:H30	4:A:328:PX4:H35	0.43	1.50	12	1
4:A:340:PX4:H25	4:A:340:PX4:H20	0.43	1.56	12	1
4:A:314:PX4:H25	4:A:352:PX4:H22	0.43	1.90	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:305:PX4:H39	4:A:368:PX4:H71	0.43	1.90	10	1
4:A:345:PX4:H66	4:A:383:PX4:H45	0.43	1.89	1	1
4:A:334:PX4:H47	5:A:432:C3S:H7	0.43	1.90	1	1
4:A:342:PX4:H30	4:A:358:PX4:H56	0.43	1.89	20	1
4:A:324:PX4:H22	5:A:431:C3S:H262	0.43	1.90	20	1
4:A:383:PX4:H53	4:A:407:PX4:H50	0.43	1.90	3	1
4:A:312:PX4:H19	4:A:346:PX4:H66	0.43	1.89	6	1
4:A:344:PX4:H38	4:A:354:PX4:H41	0.43	1.90	2	1
4:A:335:PX4:O4	4:A:347:PX4:H51	0.43	2.12	17	1
4:A:306:PX4:H52	4:A:359:PX4:H46	0.43	1.89	16	1
4:A:380:PX4:H58	4:A:416:PX4:H51	0.43	1.88	16	1
4:A:369:PX4:H35	4:A:370:PX4:H42	0.43	1.89	18	1
4:A:309:PX4:H7	4:A:328:PX4:O1	0.43	2.13	19	1
4:A:324:PX4:H48	5:A:431:C3S:H501	0.43	1.89	4	1
4:A:320:PX4:H66	4:A:373:PX4:H44	0.43	1.89	4	1
4:A:388:PX4:O6	4:A:407:PX4:H5	0.43	2.14	4	1
4:A:393:PX4:H4	4:A:416:PX4:H16	0.43	1.90	10	1
4:A:382:PX4:H70	4:A:404:PX4:H45	0.43	1.90	9	1
4:A:384:PX4:H15	5:A:434:C3S:H42	0.43	1.89	7	1
4:A:315:PX4:H36	4:A:395:PX4:H45	0.43	1.90	5	1
4:A:403:PX4:H67	4:A:416:PX4:H40	0.43	1.90	6	1
4:A:316:PX4:C13	4:A:321:PX4:H32	0.43	2.43	14	1
4:A:371:PX4:H29	4:A:401:PX4:H41	0.43	1.91	2	1
4:A:312:PX4:H18	4:A:346:PX4:H17	0.43	1.89	17	1
4:A:325:PX4:H32	4:A:353:PX4:H36	0.43	1.89	16	1
4:A:399:PX4:H70	4:A:405:PX4:H45	0.43	1.88	16	1
4:A:340:PX4:H47	4:A:356:PX4:H46	0.43	1.91	18	1
4:A:419:PX4:H66	4:A:419:PX4:H60	0.43	1.64	18	1
1:A:104:THR:C	1:A:108:LEU:HD12	0.43	2.34	19	1
4:A:306:PX4:H21	4:A:342:PX4:H19	0.43	1.89	12	1
4:A:316:PX4:H55	4:A:316:PX4:H48	0.43	1.66	4	1
4:A:398:PX4:H25	4:A:411:PX4:H53	0.43	1.89	4	1
4:A:365:PX4:H17	4:A:383:PX4:H19	0.43	1.90	10	1
4:A:389:PX4:H44	4:A:399:PX4:H72	0.43	1.90	1	1
4:A:335:PX4:H65	4:A:363:PX4:H66	0.43	1.91	20	1
4:A:355:PX4:H71	4:A:421:PX4:H40	0.43	1.89	20	1
4:A:326:PX4:H42	4:A:418:PX4:H33	0.43	1.88	3	1
4:A:389:PX4:H3	4:A:401:PX4:O2	0.43	2.12	7	1
1:A:118:LYS:O	4:A:351:PX4:H4	0.43	2.13	2	1
4:A:328:PX4:H67	4:A:335:PX4:H41	0.43	1.90	2	1
4:A:367:PX4:H14	4:A:389:PX4:O4	0.43	2.13	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:377:PX4:H26	4:A:408:PX4:H24	0.43	1.89	2	1
1:A:114:ASN:ND2	4:A:332:PX4:H1	0.43	2.29	17	1
4:A:365:PX4:O8	4:A:396:PX4:H10	0.43	2.13	16	1
4:A:368:PX4:H56	4:A:426:PX4:H66	0.43	1.89	18	1
4:A:317:PX4:H68	4:A:418:PX4:H42	0.43	1.89	19	1
4:A:382:PX4:H19	4:A:398:PX4:H54	0.43	1.91	19	1
4:A:308:PX4:O6	4:A:308:PX4:H1	0.43	2.14	12	1
4:A:376:PX4:O8	4:A:390:PX4:H7	0.43	2.14	11	1
4:A:368:PX4:H54	4:A:406:PX4:H30	0.43	1.90	10	1
4:A:408:PX4:H63	4:A:408:PX4:H56	0.43	1.50	9	1
4:A:307:PX4:H68	4:A:369:PX4:H70	0.43	1.90	1	1
4:A:308:PX4:H46	4:A:326:PX4:H48	0.43	1.89	20	1
4:A:374:PX4:H3	4:A:397:PX4:H18	0.43	1.91	3	1
4:A:400:PX4:H44	4:A:401:PX4:H18	0.43	1.91	3	1
4:A:370:PX4:H41	4:A:394:PX4:H48	0.43	1.89	7	1
4:A:346:PX4:H42	4:A:376:PX4:H43	0.43	1.90	7	1
4:A:381:PX4:H25	4:A:395:PX4:H24	0.43	1.89	5	1
4:A:379:PX4:H59	4:A:422:PX4:H65	0.43	1.88	13	1
4:A:365:PX4:H22	4:A:419:PX4:H56	0.43	1.91	6	1
4:A:380:PX4:H47	4:A:385:PX4:H23	0.43	1.91	6	1
4:A:371:PX4:H55	4:A:373:PX4:H57	0.43	1.90	14	1
4:A:417:PX4:O6	4:A:418:PX4:H49	0.43	2.14	2	1
4:A:319:PX4:H28	4:A:336:PX4:H18	0.43	1.89	8	1
1:A:223:ASN:O	4:A:315:PX4:H8	0.43	2.13	18	1
4:A:357:PX4:H49	4:A:363:PX4:H24	0.43	1.91	18	1
4:A:382:PX4:H55	4:A:423:PX4:H22	0.43	1.89	18	1
4:A:428:PX4:H24	4:A:429:PX4:H17	0.43	1.91	15	2
4:A:322:PX4:H71	4:A:429:PX4:H56	0.43	1.90	15	1
4:A:371:PX4:H4	4:A:373:PX4:H18	0.43	1.90	12	1
4:A:307:PX4:H53	4:A:338:PX4:H72	0.43	1.89	4	1
4:A:317:PX4:H71	4:A:417:PX4:H45	0.43	1.91	9	1
4:A:307:PX4:H43	4:A:411:PX4:H58	0.43	1.89	9	1
4:A:354:PX4:H8	4:A:360:PX4:O4	0.43	2.14	1	1
4:A:387:PX4:H22	4:A:416:PX4:H17	0.43	1.90	1	1
4:A:371:PX4:H68	4:A:424:PX4:H35	0.43	1.89	3	1
4:A:308:PX4:H36	4:A:332:PX4:H40	0.43	1.90	5	1
4:A:351:PX4:H23	4:A:359:PX4:H25	0.43	1.90	5	1
4:A:389:PX4:H25	4:A:399:PX4:H51	0.43	1.91	13	1
4:A:317:PX4:H22	4:A:326:PX4:H16	0.43	1.91	6	1
4:A:357:PX4:H51	4:A:363:PX4:H49	0.43	1.91	6	1
4:A:331:PX4:H22	4:A:337:PX4:H21	0.43	1.90	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:316:PX4:H67	4:A:401:PX4:H41	0.43	1.91	16	1
4:A:367:PX4:H7	4:A:367:PX4:O2	0.43	2.13	18	1
4:A:416:PX4:H67	4:A:416:PX4:H60	0.43	1.49	18	1
4:A:371:PX4:H57	4:A:389:PX4:H48	0.43	1.91	15	1
4:A:320:PX4:H29	4:A:332:PX4:H28	0.43	1.91	12	1
4:A:404:PX4:H37	4:A:417:PX4:H28	0.43	1.89	11	1
4:A:389:PX4:H64	4:A:389:PX4:H72	0.43	1.46	4	1
4:A:345:PX4:H3	4:A:345:PX4:O6	0.43	2.14	10	1
4:A:320:PX4:H28	4:A:320:PX4:H21	0.43	1.41	3	1
4:A:307:PX4:H46	4:A:332:PX4:C3	0.43	2.44	7	1
4:A:354:PX4:H72	4:A:425:PX4:H37	0.43	1.90	7	1
4:A:315:PX4:H57	4:A:332:PX4:H17	0.43	1.90	13	1
4:A:349:PX4:H24	4:A:361:PX4:H19	0.43	1.90	6	1
4:A:309:PX4:H38	4:A:345:PX4:H38	0.43	1.90	14	1
4:A:410:PX4:H59	5:A:435:C3S:H151	0.43	1.91	14	1
4:A:377:PX4:H57	4:A:377:PX4:H62	0.43	1.60	2	1
4:A:395:PX4:H41	4:A:401:PX4:H65	0.43	1.91	2	1
4:A:313:PX4:H60	4:A:353:PX4:H58	0.43	1.90	16	1
4:A:327:PX4:H25	4:A:332:PX4:H68	0.43	1.90	18	1
4:A:306:PX4:H19	4:A:358:PX4:H47	0.43	1.91	19	1
4:A:416:PX4:O6	4:A:416:PX4:H10	0.43	2.13	19	1
4:A:318:PX4:H28	4:A:357:PX4:C14	0.43	2.42	15	1
4:A:370:PX4:H52	4:A:381:PX4:H50	0.43	1.89	12	1
4:A:385:PX4:H51	4:A:415:PX4:H16	0.43	1.91	11	1
4:A:355:PX4:H45	4:A:412:PX4:H64	0.43	1.90	4	1
4:A:370:PX4:H16	4:A:383:PX4:H49	0.43	1.91	10	1
4:A:403:PX4:H44	4:A:403:PX4:H38	0.43	1.53	10	1
4:A:317:PX4:H36	4:A:361:PX4:H22	0.43	1.91	20	1
4:A:305:PX4:H38	4:A:324:PX4:H70	0.43	1.91	3	1
4:A:344:PX4:H26	4:A:344:PX4:H31	0.43	1.65	3	1
4:A:309:PX4:H48	4:A:347:PX4:H24	0.43	1.90	3	1
4:A:406:PX4:H32	5:A:435:C3S:H443	0.43	1.90	3	1
4:A:344:PX4:H33	4:A:344:PX4:H28	0.43	1.60	7	1
4:A:351:PX4:H40	4:A:393:PX4:H37	0.43	1.90	7	1
4:A:367:PX4:H55	4:A:424:PX4:H50	0.43	1.89	5	1
4:A:378:PX4:H55	4:A:426:PX4:H53	0.43	1.90	5	1
4:A:403:PX4:H17	4:A:421:PX4:H47	0.42	1.90	13	1
4:A:374:PX4:H30	4:A:397:PX4:H69	0.42	1.91	18	1
4:A:400:PX4:H8	4:A:407:PX4:H48	0.42	1.90	18	1
1:A:128:VAL:CG2	4:A:343:PX4:H50	0.42	2.44	19	1
4:A:307:PX4:H26	4:A:374:PX4:H70	0.42	1.90	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:312:PX4:H46	4:A:312:PX4:H53	0.42	1.53	15	1
4:A:316:PX4:O6	4:A:318:PX4:H11	0.42	2.14	15	1
4:A:324:PX4:H42	4:A:346:PX4:H42	0.42	1.90	15	1
4:A:330:PX4:H66	4:A:330:PX4:H61	0.42	1.65	12	1
1:A:156:LEU:CD2	1:A:156:LEU:N	0.42	2.82	4	1
4:A:349:PX4:H57	4:A:349:PX4:H62	0.42	1.49	4	1
4:A:403:PX4:H60	4:A:403:PX4:H67	0.42	1.57	10	1
4:A:318:PX4:H63	4:A:412:PX4:H44	0.42	1.90	9	1
1:A:30:LYS:O	1:A:31:ASN:HB3	0.42	2.13	1	1
4:A:381:PX4:H26	4:A:417:PX4:H58	0.42	1.91	1	1
4:A:322:PX4:H46	4:A:337:PX4:H17	0.42	1.90	20	1
4:A:417:PX4:H19	4:A:418:PX4:H49	0.42	1.91	20	1
4:A:338:PX4:H26	4:A:344:PX4:H17	0.42	1.91	7	1
4:A:414:PX4:H69	4:A:426:PX4:H72	0.42	1.91	6	1
4:A:395:PX4:H66	4:A:402:PX4:H61	0.42	1.90	14	1
4:A:428:PX4:H1	4:A:428:PX4:H10	0.42	1.58	14	1
4:A:325:PX4:H55	4:A:325:PX4:H48	0.42	1.43	16	1
4:A:380:PX4:H49	4:A:385:PX4:H26	0.42	1.91	16	1
4:A:397:PX4:H18	4:A:411:PX4:H1	0.42	1.91	18	1
4:A:384:PX4:H16	4:A:405:PX4:H9	0.42	1.91	18	1
4:A:409:PX4:H55	4:A:409:PX4:H48	0.42	1.59	18	1
4:A:309:PX4:H59	4:A:328:PX4:H45	0.42	1.90	19	1
4:A:330:PX4:H40	4:A:337:PX4:H45	0.42	1.90	19	1
4:A:308:PX4:H52	4:A:326:PX4:H19	0.42	1.91	12	1
4:A:379:PX4:H22	4:A:425:PX4:H25	0.42	1.91	12	1
4:A:334:PX4:H47	5:A:432:C3S:H232	0.42	1.91	11	1
4:A:371:PX4:H46	4:A:389:PX4:H51	0.42	1.90	11	1
1:A:57:ARG:CZ	1:A:217:GLY:HA3	0.42	2.44	10	1
4:A:386:PX4:H22	4:A:402:PX4:H20	0.42	1.91	10	1
4:A:348:PX4:H9	4:A:348:PX4:H15	0.42	1.90	9	1
1:A:71:ASP:OD2	1:A:198:HIS:CE1	0.42	2.72	7	1
4:A:352:PX4:H40	4:A:375:PX4:H63	0.42	1.91	7	1
4:A:369:PX4:H63	4:A:393:PX4:H34	0.42	1.90	7	1
4:A:316:PX4:H15	4:A:352:PX4:O5	0.42	2.14	5	1
4:A:325:PX4:O6	4:A:361:PX4:H6	0.42	2.14	5	1
4:A:393:PX4:H17	4:A:416:PX4:H22	0.42	1.91	5	1
4:A:320:PX4:H54	4:A:334:PX4:H72	0.42	1.91	2	1
4:A:379:PX4:H21	4:A:425:PX4:H20	0.42	1.92	17	1
4:A:313:PX4:H30	4:A:362:PX4:H48	0.42	1.91	18	1
4:A:375:PX4:H70	4:A:405:PX4:H48	0.42	1.90	18	1
4:A:324:PX4:H38	4:A:324:PX4:H31	0.42	1.55	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:340:PX4:O8	4:A:341:PX4:H11	0.42	2.14	15	1
4:A:353:PX4:H59	4:A:361:PX4:H28	0.42	1.90	15	1
4:A:389:PX4:H4	4:A:401:PX4:O1	0.42	2.14	1	1
4:A:372:PX4:H16	4:A:410:PX4:H53	0.42	1.91	20	1
4:A:404:PX4:H23	4:A:418:PX4:H24	0.42	1.90	20	1
4:A:323:PX4:H61	4:A:328:PX4:H61	0.42	1.90	3	1
4:A:383:PX4:H11	4:A:400:PX4:O8	0.42	2.14	7	1
4:A:327:PX4:H41	4:A:338:PX4:H34	0.42	1.92	6	1
4:A:324:PX4:H46	4:A:346:PX4:H67	0.42	1.90	6	1
4:A:354:PX4:H34	4:A:354:PX4:H39	0.42	1.54	14	1
1:A:127:VAL:HG12	1:A:129:TRP:CZ2	0.42	2.49	2	1
4:A:362:PX4:H36	4:A:362:PX4:H29	0.42	1.66	2	1
4:A:376:PX4:H61	4:A:388:PX4:H35	0.42	1.90	2	1
4:A:428:PX4:H39	4:A:429:PX4:H34	0.42	1.91	2	1
4:A:353:PX4:H55	4:A:353:PX4:H60	0.42	1.46	18	1
4:A:308:PX4:H14	4:A:320:PX4:O3	0.42	2.14	19	1
4:A:305:PX4:O6	4:A:311:PX4:H5	0.42	2.14	15	1
4:A:397:PX4:C34	4:A:423:PX4:H68	0.42	2.41	12	1
4:A:331:PX4:H69	4:A:331:PX4:H62	0.42	1.69	11	1
4:A:403:PX4:H18	4:A:403:PX4:H20	0.42	1.47	11	1
4:A:329:PX4:H50	4:A:355:PX4:H61	0.42	1.90	4	1
4:A:411:PX4:H54	4:A:411:PX4:H49	0.42	1.62	1	1
4:A:380:PX4:H44	4:A:420:PX4:H68	0.42	1.91	20	1
4:A:338:PX4:H25	4:A:344:PX4:H21	0.42	1.91	3	1
4:A:369:PX4:H28	4:A:383:PX4:H27	0.42	1.91	3	1
4:A:417:PX4:H33	4:A:418:PX4:H36	0.42	1.91	3	1
4:A:369:PX4:H25	4:A:430:PX4:H25	0.42	1.91	17	1
4:A:339:PX4:H41	4:A:368:PX4:H65	0.42	1.92	8	1
4:A:395:PX4:H47	4:A:401:PX4:H16	0.42	1.91	15	1
1:A:114:ASN:OD1	4:A:348:PX4:H1	0.42	2.14	11	1
4:A:377:PX4:H60	4:A:408:PX4:H31	0.42	1.92	11	1
4:A:334:PX4:H45	4:A:426:PX4:H20	0.42	1.90	9	1
4:A:419:PX4:H37	4:A:419:PX4:H45	0.42	1.48	9	1
4:A:317:PX4:H60	4:A:337:PX4:H60	0.42	1.92	1	1
4:A:353:PX4:O6	4:A:361:PX4:H1	0.42	2.14	3	1
4:A:371:PX4:H60	4:A:399:PX4:H54	0.42	1.89	3	1
4:A:317:PX4:H39	4:A:415:PX4:H43	0.42	1.92	7	1
4:A:317:PX4:H65	4:A:320:PX4:H35	0.42	1.91	5	1
4:A:370:PX4:H7	4:A:430:PX4:H15	0.42	1.91	13	1
4:A:397:PX4:H56	4:A:430:PX4:H23	0.42	1.90	13	1
4:A:338:PX4:C24	4:A:347:PX4:H57	0.42	2.41	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:322:PX4:H39	4:A:322:PX4:H34	0.42	1.53	17	1
4:A:375:PX4:H72	4:A:384:PX4:H26	0.42	1.91	17	1
1:A:120:ILE:O	4:A:327:PX4:H9	0.42	2.14	15	1
4:A:407:PX4:O4	4:A:427:PX4:H3	0.42	2.14	15	1
4:A:351:PX4:H69	4:A:360:PX4:H50	0.42	1.90	11	1
4:A:428:PX4:H28	4:A:428:PX4:H33	0.42	1.60	11	1
4:A:338:PX4:H65	4:A:374:PX4:H72	0.42	1.90	9	1
4:A:391:PX4:H34	4:A:391:PX4:H27	0.42	1.46	20	1
4:A:374:PX4:H63	4:A:430:PX4:H63	0.42	1.90	7	1
4:A:316:PX4:H30	4:A:316:PX4:H35	0.42	1.67	5	1
4:A:314:PX4:H35	4:A:336:PX4:H68	0.42	1.92	14	1
4:A:310:PX4:H28	4:A:364:PX4:H41	0.42	1.90	14	1
4:A:344:PX4:H29	4:A:344:PX4:H24	0.42	1.69	17	1
4:A:393:PX4:H12	4:A:416:PX4:C23	0.42	2.44	17	1
4:A:393:PX4:H65	4:A:393:PX4:H58	0.42	1.53	8	1
4:A:307:PX4:H41	4:A:327:PX4:H26	0.42	1.90	18	1
4:A:397:PX4:H59	4:A:423:PX4:H51	0.42	1.90	15	1
4:A:408:PX4:H28	4:A:422:PX4:H28	0.42	1.91	15	1
4:A:333:PX4:H29	4:A:333:PX4:H24	0.42	1.60	12	1
4:A:347:PX4:H19	4:A:351:PX4:H25	0.42	1.90	12	1
4:A:336:PX4:H55	4:A:344:PX4:C22	0.42	2.43	11	1
4:A:322:PX4:H17	4:A:344:PX4:H24	0.42	1.90	10	1
4:A:399:PX4:H32	4:A:399:PX4:H60	0.42	1.90	10	1
4:A:374:PX4:H29	4:A:397:PX4:H69	0.42	1.90	20	1
4:A:428:PX4:H19	4:A:428:PX4:H26	0.42	1.54	20	1
4:A:340:PX4:H31	4:A:340:PX4:H52	0.42	1.90	3	1
4:A:366:PX4:H56	4:A:421:PX4:H63	0.42	1.91	5	1
4:A:393:PX4:H13	4:A:416:PX4:H16	0.42	1.91	13	1
4:A:383:PX4:H46	4:A:405:PX4:H48	0.42	1.91	6	1
4:A:396:PX4:H63	4:A:396:PX4:H68	0.42	1.64	2	1
1:A:120:ILE:O	4:A:327:PX4:H8	0.42	2.14	17	1
1:A:128:VAL:CG2	4:A:343:PX4:H53	0.42	2.45	17	1
4:A:309:PX4:H37	4:A:309:PX4:H31	0.42	1.57	17	1
4:A:373:PX4:H35	4:A:373:PX4:H41	0.42	1.33	17	1
4:A:327:PX4:H58	4:A:327:PX4:H52	0.42	1.62	8	1
4:A:377:PX4:H46	4:A:377:PX4:H16	0.42	1.57	1	3
4:A:404:PX4:H25	4:A:418:PX4:H58	0.42	1.92	19	1
4:A:425:PX4:H35	4:A:425:PX4:H42	0.42	1.59	19	1
1:A:119:GLU:O	1:A:120:ILE:HG23	0.42	2.14	15	1
4:A:314:PX4:H30	4:A:314:PX4:H24	0.42	1.62	15	1
4:A:332:PX4:H25	4:A:332:PX4:H20	0.42	1.48	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:397:PX4:H33	4:A:412:PX4:H63	0.42	1.92	15	1
4:A:317:PX4:O1	4:A:320:PX4:H11	0.42	2.15	11	1
4:A:416:PX4:H51	5:A:433:C3S:H152	0.42	1.92	11	1
4:A:312:PX4:O6	4:A:324:PX4:H12	0.42	2.15	4	1
4:A:332:PX4:H69	4:A:348:PX4:H33	0.42	1.91	4	1
4:A:402:PX4:H33	4:A:426:PX4:H52	0.42	1.91	10	1
4:A:358:PX4:H72	4:A:383:PX4:H70	0.42	1.92	1	1
4:A:356:PX4:H57	4:A:356:PX4:H62	0.42	1.66	3	1
4:A:410:PX4:H38	5:A:435:C3S:H402	0.42	1.91	5	1
4:A:319:PX4:O2	4:A:341:PX4:H13	0.42	2.15	13	1
4:A:413:PX4:H35	4:A:428:PX4:C17	0.42	2.41	6	1
4:A:387:PX4:H49	4:A:418:PX4:H69	0.42	1.92	6	1
4:A:349:PX4:H63	4:A:349:PX4:H56	0.42	1.68	14	1
4:A:396:PX4:H24	4:A:407:PX4:H48	0.42	1.92	14	1
4:A:411:PX4:H32	4:A:423:PX4:H61	0.42	1.91	2	1
4:A:324:PX4:H52	4:A:324:PX4:H59	0.42	1.72	17	1
4:A:342:PX4:H18	4:A:357:PX4:H43	0.42	1.92	17	1
4:A:367:PX4:H17	4:A:399:PX4:H4	0.42	1.92	17	1
4:A:309:PX4:H60	4:A:309:PX4:H67	0.42	1.62	8	1
4:A:411:PX4:H33	4:A:412:PX4:H62	0.42	1.91	8	1
4:A:323:PX4:H33	4:A:323:PX4:H40	0.42	1.62	16	1
4:A:373:PX4:H17	4:A:406:PX4:H46	0.42	1.92	16	1
4:A:410:PX4:H29	4:A:414:PX4:H26	0.42	1.90	16	1
4:A:347:PX4:H29	4:A:347:PX4:H36	0.42	1.51	18	1
4:A:319:PX4:H62	4:A:321:PX4:H41	0.42	1.92	12	1
4:A:345:PX4:H54	4:A:359:PX4:H15	0.42	1.90	11	1
4:A:332:PX4:H14	4:A:348:PX4:H50	0.42	1.90	11	1
4:A:313:PX4:H39	4:A:362:PX4:H26	0.42	1.92	4	1
4:A:306:PX4:H37	4:A:345:PX4:H30	0.42	1.90	4	1
4:A:364:PX4:H57	4:A:364:PX4:H51	0.42	1.45	10	1
4:A:351:PX4:H36	4:A:419:PX4:H65	0.42	1.90	20	1
4:A:318:PX4:H18	4:A:318:PX4:H13	0.42	1.91	3	1
4:A:407:PX4:H68	4:A:407:PX4:H63	0.42	1.69	3	1
4:A:308:PX4:H48	4:A:320:PX4:H22	0.42	1.92	7	1
4:A:365:PX4:O6	4:A:369:PX4:H3	0.42	2.13	7	1
4:A:313:PX4:H15	4:A:313:PX4:O8	0.42	2.14	5	1
4:A:307:PX4:H18	4:A:331:PX4:H36	0.42	1.92	5	1
4:A:305:PX4:H58	4:A:312:PX4:H56	0.42	1.92	13	1
4:A:335:PX4:H26	4:A:360:PX4:H48	0.42	1.91	13	1
4:A:312:PX4:H33	4:A:346:PX4:H17	0.42	1.92	6	1
4:A:376:PX4:H50	4:A:390:PX4:H15	0.42	1.90	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:376:PX4:H60	4:A:390:PX4:H17	0.42	1.92	17	1
4:A:317:PX4:H20	4:A:326:PX4:H14	0.42	1.91	18	1
4:A:345:PX4:H12	4:A:349:PX4:H17	0.42	1.90	18	1
4:A:367:PX4:H59	4:A:424:PX4:H62	0.42	1.91	18	1
4:A:374:PX4:H20	4:A:423:PX4:H12	0.42	1.91	19	1
4:A:305:PX4:H18	4:A:311:PX4:H2	0.42	1.92	12	1
4:A:398:PX4:H28	4:A:398:PX4:H21	0.42	1.79	11	1
4:A:384:PX4:H20	4:A:405:PX4:H23	0.42	1.92	10	1
4:A:375:PX4:H45	4:A:375:PX4:H37	0.42	1.63	1	1
4:A:381:PX4:H28	4:A:417:PX4:H62	0.42	1.91	1	1
4:A:350:PX4:H62	4:A:426:PX4:H70	0.42	1.90	1	1
4:A:389:PX4:O3	4:A:401:PX4:H6	0.42	2.15	20	1
4:A:318:PX4:H46	4:A:352:PX4:H22	0.42	1.92	5	1
4:A:413:PX4:H25	4:A:413:PX4:H32	0.42	1.48	5	1
4:A:428:PX4:H6	4:A:429:PX4:O4	0.42	2.15	5	1
4:A:395:PX4:H36	4:A:395:PX4:H29	0.41	1.59	6	1
4:A:377:PX4:O2	4:A:408:PX4:H9	0.41	2.15	6	1
4:A:366:PX4:H69	4:A:390:PX4:H66	0.41	1.90	14	1
4:A:331:PX4:H67	4:A:331:PX4:H60	0.41	1.41	2	1
4:A:369:PX4:H24	4:A:430:PX4:H58	0.41	1.91	2	1
4:A:319:PX4:C26	4:A:356:PX4:H16	0.41	2.45	17	1
4:A:416:PX4:H40	4:A:418:PX4:C36	0.41	2.45	16	1
4:A:391:PX4:H49	4:A:427:PX4:H27	0.41	1.91	19	1
4:A:314:PX4:H70	4:A:416:PX4:H72	0.41	1.91	15	1
1:A:161:ALA:HB1	1:A:162:PRO:HD2	0.41	1.92	4	1
4:A:391:PX4:H49	4:A:427:PX4:H40	0.41	1.93	4	1
4:A:315:PX4:H32	4:A:317:PX4:H46	0.41	1.91	10	1
4:A:348:PX4:H44	4:A:348:PX4:H38	0.41	1.58	9	1
4:A:366:PX4:H64	4:A:387:PX4:H55	0.41	1.92	9	1
4:A:404:PX4:H33	4:A:404:PX4:H40	0.41	1.36	9	1
4:A:422:PX4:H10	4:A:425:PX4:O2	0.41	2.15	9	1
4:A:333:PX4:H55	4:A:333:PX4:H24	0.41	1.91	3	1
4:A:374:PX4:H35	4:A:397:PX4:H67	0.41	1.92	7	1
4:A:359:PX4:H59	4:A:407:PX4:H43	0.41	1.91	5	1
4:A:409:PX4:H64	4:A:411:PX4:H32	0.41	1.92	6	1
4:A:359:PX4:H72	4:A:376:PX4:H33	0.41	1.93	8	1
4:A:381:PX4:H44	4:A:402:PX4:H72	0.41	1.92	8	1
4:A:382:PX4:H24	4:A:404:PX4:H56	0.41	1.91	16	1
4:A:369:PX4:H27	4:A:374:PX4:H58	0.41	1.91	18	1
4:A:408:PX4:H11	4:A:414:PX4:O1	0.41	2.15	18	1
4:A:399:PX4:H23	4:A:424:PX4:H28	0.41	1.92	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:345:PX4:H53	4:A:345:PX4:H58	0.41	1.60	12	1
4:A:382:PX4:H54	4:A:404:PX4:C22	0.41	2.42	12	1
4:A:359:PX4:H24	4:A:359:PX4:H30	0.41	1.70	11	1
4:A:348:PX4:H67	4:A:396:PX4:H72	0.41	1.92	11	1
4:A:394:PX4:H8	4:A:395:PX4:O2	0.41	2.15	4	1
4:A:315:PX4:H59	4:A:332:PX4:O8	0.41	2.15	10	1
4:A:379:PX4:H18	4:A:425:PX4:O5	0.41	2.15	9	1
4:A:379:PX4:O4	4:A:425:PX4:H3	0.41	2.15	1	1
4:A:385:PX4:H52	4:A:415:PX4:H58	0.41	1.91	20	1
4:A:313:PX4:H61	4:A:360:PX4:H23	0.41	1.93	3	1
4:A:406:PX4:H67	4:A:406:PX4:H60	0.41	1.46	3	1
1:A:104:THR:CG2	4:A:320:PX4:H46	0.41	2.45	5	1
4:A:362:PX4:H48	4:A:362:PX4:H21	0.41	1.91	5	1
4:A:307:PX4:H39	4:A:344:PX4:H33	0.41	1.92	13	1
4:A:345:PX4:H58	4:A:359:PX4:H17	0.41	1.91	13	1
4:A:312:PX4:H21	4:A:324:PX4:H6	0.41	1.91	6	1
4:A:374:PX4:H5	4:A:411:PX4:O8	0.41	2.14	6	1
4:A:309:PX4:H32	4:A:309:PX4:H63	0.41	1.92	14	1
4:A:403:PX4:H30	4:A:417:PX4:H27	0.41	1.91	14	1
4:A:363:PX4:H58	4:A:363:PX4:H65	0.41	1.62	8	1
4:A:373:PX4:H26	4:A:402:PX4:H25	0.41	1.91	8	1
4:A:390:PX4:H27	4:A:416:PX4:H19	0.41	1.91	8	1
4:A:428:PX4:O5	4:A:429:PX4:H54	0.41	2.15	19	1
4:A:365:PX4:H34	4:A:369:PX4:H28	0.41	1.92	15	1
4:A:408:PX4:H18	4:A:427:PX4:H46	0.41	1.91	15	1
4:A:331:PX4:H53	4:A:331:PX4:H58	0.41	1.52	12	1
4:A:312:PX4:H64	4:A:333:PX4:H55	0.41	1.92	4	1
4:A:339:PX4:H65	4:A:339:PX4:H71	0.41	1.70	9	1
4:A:375:PX4:H34	4:A:396:PX4:H37	0.41	1.91	9	1
4:A:320:PX4:C36	4:A:350:PX4:H46	0.41	2.45	20	1
4:A:309:PX4:H19	4:A:345:PX4:H57	0.41	1.92	3	1
4:A:376:PX4:C12	4:A:396:PX4:H50	0.41	2.44	3	1
4:A:305:PX4:H33	4:A:305:PX4:H68	0.41	1.91	5	1
4:A:338:PX4:H31	4:A:344:PX4:H58	0.41	1.92	14	1
4:A:350:PX4:H7	4:A:356:PX4:H51	0.41	1.92	17	1
4:A:400:PX4:H21	4:A:405:PX4:O6	0.41	2.15	17	1
4:A:308:PX4:H67	4:A:326:PX4:H35	0.41	1.91	8	1
4:A:375:PX4:H20	4:A:392:PX4:H32	0.41	1.92	8	1
4:A:386:PX4:H52	4:A:417:PX4:C16	0.41	2.45	16	1
4:A:324:PX4:H3	5:A:431:C3S:O4	0.41	2.15	15	1
4:A:310:PX4:H41	4:A:313:PX4:H64	0.41	1.92	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:327:PX4:H32	4:A:359:PX4:H60	0.41	1.91	11	1
4:A:372:PX4:H59	4:A:372:PX4:H53	0.41	1.74	11	1
4:A:372:PX4:H72	4:A:410:PX4:H31	0.41	1.92	11	1
4:A:402:PX4:H42	5:A:431:C3S:C50	0.41	2.45	11	1
4:A:322:PX4:H54	4:A:344:PX4:H22	0.41	1.93	4	1
4:A:342:PX4:H40	4:A:358:PX4:H67	0.41	1.91	4	1
4:A:387:PX4:H33	4:A:387:PX4:H40	0.41	1.60	10	1
4:A:400:PX4:H53	4:A:401:PX4:H55	0.41	1.91	10	1
4:A:330:PX4:O8	4:A:337:PX4:H3	0.41	2.15	9	1
4:A:373:PX4:H37	4:A:401:PX4:H33	0.41	1.91	9	1
4:A:332:PX4:H27	4:A:332:PX4:H34	0.41	1.69	20	1
4:A:323:PX4:H60	4:A:360:PX4:H22	0.41	1.92	3	1
4:A:379:PX4:H45	4:A:384:PX4:H35	0.41	1.92	5	1
4:A:400:PX4:H15	4:A:405:PX4:O2	0.41	2.15	5	1
4:A:421:PX4:H31	4:A:421:PX4:H38	0.41	1.64	6	1
4:A:384:PX4:H8	4:A:389:PX4:O6	0.41	2.14	2	1
4:A:392:PX4:H13	4:A:405:PX4:O1	0.41	2.13	2	1
4:A:387:PX4:H62	4:A:421:PX4:H57	0.41	1.92	2	1
4:A:382:PX4:H69	4:A:382:PX4:H63	0.41	1.56	17	1
4:A:336:PX4:H30	4:A:357:PX4:H18	0.41	1.92	8	1
4:A:424:PX4:H23	5:A:435:C3S:C44	0.41	2.45	8	1
4:A:382:PX4:H50	4:A:404:PX4:H17	0.41	1.92	16	1
4:A:375:PX4:H32	4:A:427:PX4:H25	0.41	1.93	16	1
4:A:321:PX4:H35	4:A:332:PX4:H65	0.41	1.92	19	1
4:A:333:PX4:H12	4:A:333:PX4:H15	0.41	1.91	19	1
4:A:353:PX4:H33	4:A:361:PX4:H63	0.41	1.91	19	1
4:A:380:PX4:H20	4:A:420:PX4:H53	0.41	1.92	19	1
4:A:305:PX4:H52	4:A:312:PX4:H56	0.41	1.93	12	1
4:A:387:PX4:C36	4:A:403:PX4:H35	0.41	2.42	12	1
4:A:324:PX4:H17	5:A:431:C3S:H30	0.41	1.91	12	1
4:A:335:PX4:H39	4:A:387:PX4:H41	0.41	1.92	11	1
4:A:395:PX4:H28	4:A:402:PX4:C27	0.41	2.45	10	1
4:A:321:PX4:H38	4:A:367:PX4:H44	0.41	1.92	9	1
4:A:315:PX4:H70	4:A:332:PX4:H63	0.41	1.91	1	1
4:A:349:PX4:H16	4:A:361:PX4:H10	0.41	1.92	20	1
4:A:373:PX4:H62	4:A:414:PX4:H35	0.41	1.91	20	1
4:A:381:PX4:H34	4:A:381:PX4:H27	0.41	1.76	3	1
4:A:329:PX4:H68	4:A:329:PX4:H63	0.41	1.78	5	1
4:A:400:PX4:H18	4:A:405:PX4:O2	0.41	2.16	5	1
4:A:328:PX4:H41	4:A:328:PX4:H36	0.41	1.66	13	1
4:A:313:PX4:H26	4:A:313:PX4:H19	0.41	1.64	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:324:PX4:H47	4:A:333:PX4:H14	0.41	1.93	6	1
4:A:334:PX4:H55	4:A:334:PX4:H48	0.41	1.61	6	1
4:A:406:PX4:H40	4:A:410:PX4:H39	0.41	1.92	2	1
4:A:414:PX4:H33	4:A:414:PX4:H28	0.41	1.71	8	1
1:A:221:PRO:O	4:A:317:PX4:H5	0.41	2.16	18	1
4:A:362:PX4:H14	4:A:362:PX4:H13	0.41	1.91	18	1
4:A:369:PX4:H53	4:A:419:PX4:H47	0.41	1.92	18	1
4:A:342:PX4:H29	4:A:358:PX4:H52	0.41	1.91	15	1
4:A:356:PX4:H28	4:A:356:PX4:H21	0.41	1.60	4	1
4:A:359:PX4:H41	4:A:430:PX4:H42	0.41	1.90	9	1
4:A:307:PX4:O2	4:A:322:PX4:H4	0.41	2.16	1	1
4:A:342:PX4:H35	4:A:342:PX4:H29	0.41	1.72	1	1
4:A:346:PX4:H38	4:A:346:PX4:H31	0.41	1.57	1	1
4:A:311:PX4:H43	4:A:377:PX4:H62	0.41	1.91	1	1
4:A:377:PX4:H17	4:A:408:PX4:H18	0.41	1.91	1	1
4:A:335:PX4:H33	4:A:360:PX4:H31	0.41	1.93	20	1
4:A:308:PX4:O4	4:A:320:PX4:H17	0.41	2.16	5	1
4:A:393:PX4:H52	4:A:419:PX4:H28	0.41	1.92	5	1
4:A:347:PX4:H17	4:A:351:PX4:O6	0.41	2.15	13	1
4:A:382:PX4:H25	4:A:382:PX4:H20	0.41	1.53	13	1
4:A:380:PX4:H60	4:A:416:PX4:H46	0.41	1.92	6	1
4:A:370:PX4:H30	4:A:370:PX4:H35	0.41	1.61	2	1
4:A:406:PX4:H34	4:A:406:PX4:H39	0.41	1.43	8	1
4:A:322:PX4:H41	4:A:331:PX4:C20	0.41	2.46	16	1
4:A:338:PX4:H50	4:A:338:PX4:H57	0.41	1.71	16	1
4:A:315:PX4:H25	4:A:320:PX4:H20	0.41	1.92	19	1
4:A:315:PX4:H43	4:A:423:PX4:H41	0.41	1.91	19	1
4:A:374:PX4:H37	4:A:374:PX4:H32	0.41	1.56	19	2
4:A:318:PX4:H28	4:A:318:PX4:H33	0.41	1.62	12	1
4:A:389:PX4:H51	4:A:400:PX4:H23	0.41	1.93	12	1
4:A:308:PX4:H32	4:A:320:PX4:H17	0.41	1.92	4	1
4:A:306:PX4:H60	4:A:321:PX4:H17	0.41	1.92	4	1
4:A:370:PX4:H22	4:A:394:PX4:O7	0.41	2.16	4	1
4:A:398:PX4:H68	4:A:415:PX4:H51	0.41	1.93	4	1
4:A:379:PX4:H27	4:A:379:PX4:H34	0.41	1.67	10	1
4:A:324:PX4:H41	4:A:414:PX4:H52	0.41	1.93	10	1
4:A:368:PX4:H25	4:A:408:PX4:H52	0.41	1.92	9	1
4:A:334:PX4:H48	5:A:432:C3S:H20	0.41	1.91	1	1
4:A:428:PX4:H35	4:A:428:PX4:H42	0.41	1.35	3	1
4:A:366:PX4:H51	4:A:403:PX4:H53	0.41	1.92	5	1
4:A:372:PX4:H63	4:A:372:PX4:H56	0.41	1.70	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:375:PX4:H34	4:A:427:PX4:H46	0.41	1.92	6	1
4:A:340:PX4:O2	4:A:343:PX4:H12	0.41	2.16	14	1
4:A:307:PX4:H25	4:A:322:PX4:H48	0.41	1.92	8	1
4:A:428:PX4:O3	4:A:429:PX4:H15	0.41	2.15	8	1
4:A:394:PX4:H40	4:A:401:PX4:H61	0.41	1.92	16	1
4:A:400:PX4:H65	4:A:405:PX4:H25	0.41	1.92	16	1
4:A:321:PX4:H66	4:A:342:PX4:H72	0.41	1.91	18	1
4:A:386:PX4:H9	4:A:417:PX4:H49	0.41	1.92	18	1
4:A:415:PX4:H66	4:A:421:PX4:H30	0.41	1.91	12	1
4:A:417:PX4:H16	4:A:418:PX4:H20	0.41	1.92	9	1
4:A:315:PX4:H59	4:A:315:PX4:H52	0.41	1.65	1	1
4:A:316:PX4:H30	4:A:321:PX4:H52	0.41	1.92	1	1
4:A:382:PX4:H27	4:A:415:PX4:H61	0.41	1.92	1	1
4:A:371:PX4:H14	4:A:373:PX4:C8	0.41	2.45	20	1
4:A:400:PX4:H55	4:A:405:PX4:H49	0.41	1.92	20	1
4:A:415:PX4:H44	4:A:421:PX4:H19	0.41	1.93	20	1
4:A:338:PX4:O3	4:A:344:PX4:H4	0.41	2.16	7	1
4:A:429:PX4:H41	4:A:429:PX4:H36	0.41	1.71	7	1
4:A:306:PX4:H19	4:A:306:PX4:H26	0.41	1.60	5	1
4:A:359:PX4:H37	4:A:359:PX4:H32	0.41	1.71	13	1
4:A:412:PX4:H13	4:A:412:PX4:H15	0.41	1.93	13	1
4:A:377:PX4:H45	4:A:391:PX4:H35	0.41	1.92	13	1
4:A:322:PX4:H67	4:A:337:PX4:H40	0.41	1.93	6	1
4:A:374:PX4:O8	4:A:423:PX4:H9	0.41	2.16	6	1
4:A:318:PX4:H19	4:A:321:PX4:H50	0.41	1.93	6	1
4:A:371:PX4:H28	4:A:371:PX4:H21	0.41	1.65	6	1
4:A:402:PX4:H38	4:A:402:PX4:H32	0.41	1.69	6	1
4:A:365:PX4:H53	4:A:383:PX4:H20	0.41	1.92	14	1
4:A:374:PX4:H4	4:A:397:PX4:O6	0.41	2.16	14	1
4:A:319:PX4:O6	4:A:352:PX4:H47	0.41	2.16	2	1
4:A:386:PX4:O3	4:A:402:PX4:H13	0.41	2.15	2	1
4:A:353:PX4:H37	4:A:353:PX4:H32	0.41	1.50	17	1
4:A:310:PX4:H28	4:A:310:PX4:H21	0.41	1.76	17	1
4:A:392:PX4:H29	4:A:405:PX4:H48	0.41	1.93	17	1
4:A:383:PX4:H58	4:A:405:PX4:H50	0.41	1.92	16	1
4:A:316:PX4:H48	4:A:321:PX4:H24	0.41	1.93	18	1
4:A:369:PX4:H21	4:A:429:PX4:H52	0.41	1.92	18	1
4:A:317:PX4:H30	4:A:317:PX4:H35	0.41	1.59	19	1
4:A:318:PX4:H59	4:A:336:PX4:C17	0.41	2.45	19	1
4:A:340:PX4:H6	5:A:432:C3S:O3	0.41	2.16	19	1
4:A:352:PX4:H57	4:A:352:PX4:H62	0.41	1.51	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:368:PX4:H13	4:A:368:PX4:H14	0.41	1.92	19	1
4:A:394:PX4:O6	4:A:400:PX4:H10	0.41	2.16	19	1
4:A:338:PX4:H4	4:A:360:PX4:H46	0.41	1.93	15	1
4:A:400:PX4:O7	4:A:405:PX4:H16	0.41	2.16	15	1
4:A:391:PX4:H55	4:A:391:PX4:H48	0.41	1.60	15	1
4:A:325:PX4:H25	4:A:325:PX4:H20	0.41	1.63	12	1
4:A:326:PX4:H46	4:A:361:PX4:H47	0.41	1.92	12	1
4:A:414:PX4:H46	4:A:414:PX4:H53	0.41	1.65	12	1
4:A:413:PX4:H18	4:A:419:PX4:H22	0.41	1.92	12	1
1:A:126:LYS:NZ	4:A:350:PX4:H17	0.41	2.31	11	1
4:A:313:PX4:H10	4:A:362:PX4:O1	0.41	2.15	4	1
4:A:402:PX4:H6	4:A:402:PX4:O8	0.41	2.15	4	1
4:A:336:PX4:H66	4:A:429:PX4:H43	0.41	1.91	10	1
4:A:393:PX4:H65	4:A:393:PX4:H71	0.41	1.63	10	1
4:A:399:PX4:H55	4:A:424:PX4:H33	0.41	1.92	10	1
4:A:329:PX4:H71	4:A:329:PX4:H65	0.41	1.60	9	1
4:A:354:PX4:H60	4:A:354:PX4:H55	0.41	1.52	9	1
4:A:386:PX4:H60	4:A:386:PX4:H40	0.41	1.92	9	1
4:A:371:PX4:H26	4:A:395:PX4:H27	0.41	1.93	1	1
4:A:413:PX4:H18	4:A:429:PX4:H26	0.41	1.92	1	1
4:A:413:PX4:H33	4:A:419:PX4:H31	0.41	1.93	1	1
4:A:383:PX4:H59	4:A:383:PX4:H53	0.41	1.68	1	1
4:A:373:PX4:H66	4:A:406:PX4:H67	0.41	1.92	1	1
4:A:370:PX4:C22	4:A:383:PX4:H64	0.41	2.45	20	1
4:A:363:PX4:H56	4:A:363:PX4:H63	0.41	1.71	20	1
4:A:392:PX4:H56	4:A:392:PX4:H63	0.41	1.63	20	1
4:A:397:PX4:H38	4:A:397:PX4:H32	0.41	1.69	3	1
1:A:102:HIS:CD2	4:A:350:PX4:H14	0.41	2.51	3	1
4:A:313:PX4:H54	4:A:360:PX4:H45	0.41	1.92	3	1
4:A:406:PX4:H26	4:A:410:PX4:H21	0.41	1.92	3	1
4:A:330:PX4:H52	4:A:330:PX4:H59	0.41	1.40	7	1
4:A:382:PX4:H51	5:A:435:C3S:H653	0.41	1.92	7	1
4:A:316:PX4:H33	4:A:316:PX4:H28	0.41	1.69	7	1
4:A:401:PX4:H65	4:A:405:PX4:H29	0.41	1.93	7	1
4:A:332:PX4:H61	4:A:376:PX4:H36	0.41	1.93	5	1
4:A:306:PX4:H56	4:A:321:PX4:H24	0.41	1.92	6	1
4:A:323:PX4:H32	4:A:323:PX4:H37	0.41	1.50	6	1
4:A:366:PX4:H19	4:A:378:PX4:H20	0.41	1.92	14	1
4:A:369:PX4:H52	4:A:419:PX4:H59	0.41	1.93	14	1
4:A:318:PX4:H27	4:A:342:PX4:H57	0.41	1.92	2	1
4:A:320:PX4:H68	4:A:320:PX4:H63	0.41	1.79	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:397:PX4:H29	4:A:398:PX4:C15	0.41	2.45	2	1
4:A:374:PX4:O2	4:A:423:PX4:H7	0.41	2.16	2	1
4:A:407:PX4:H17	4:A:427:PX4:O4	0.41	2.15	17	1
4:A:366:PX4:H59	4:A:378:PX4:H22	0.41	1.92	16	1
4:A:367:PX4:H56	4:A:412:PX4:H48	0.41	1.93	16	1
4:A:366:PX4:H54	4:A:378:PX4:H27	0.41	1.92	18	1
4:A:379:PX4:H22	5:A:434:C3S:C13	0.41	2.45	19	1
4:A:307:PX4:H65	4:A:348:PX4:H65	0.41	1.92	15	1
4:A:322:PX4:H24	4:A:330:PX4:H60	0.41	1.93	15	1
4:A:409:PX4:H38	4:A:409:PX4:H45	0.41	1.76	15	1
4:A:323:PX4:H41	4:A:325:PX4:H63	0.41	1.92	11	1
4:A:312:PX4:H21	4:A:346:PX4:H47	0.41	1.93	11	1
4:A:308:PX4:H53	4:A:326:PX4:H19	0.41	1.91	4	1
4:A:365:PX4:H30	4:A:369:PX4:H53	0.41	1.93	4	1
4:A:335:PX4:H55	4:A:335:PX4:H48	0.41	1.80	10	1
4:A:406:PX4:H18	4:A:414:PX4:H26	0.41	1.92	9	1
4:A:430:PX4:H66	4:A:430:PX4:H31	0.41	1.93	9	1
4:A:369:PX4:H6	4:A:430:PX4:O8	0.41	2.15	1	1
4:A:330:PX4:H21	4:A:337:PX4:H20	0.41	1.93	20	1
4:A:317:PX4:O2	4:A:330:PX4:H4	0.41	2.15	20	1
4:A:406:PX4:H19	4:A:414:PX4:H33	0.41	1.91	20	1
4:A:325:PX4:O6	4:A:330:PX4:H10	0.41	2.15	3	1
4:A:409:PX4:H29	4:A:409:PX4:H23	0.41	1.67	3	1
4:A:385:PX4:H65	4:A:415:PX4:H55	0.41	1.93	3	1
4:A:403:PX4:H32	4:A:417:PX4:H32	0.40	1.92	13	1
4:A:330:PX4:O8	4:A:337:PX4:H13	0.40	2.16	6	1
4:A:322:PX4:H63	4:A:337:PX4:H36	0.40	1.92	14	1
4:A:369:PX4:H31	4:A:383:PX4:H23	0.40	1.93	14	1
4:A:402:PX4:H63	4:A:402:PX4:H68	0.40	1.76	14	1
4:A:404:PX4:H21	4:A:418:PX4:H22	0.40	1.93	14	1
4:A:363:PX4:H39	4:A:363:PX4:H34	0.40	1.74	2	1
4:A:329:PX4:H59	4:A:329:PX4:H52	0.40	1.68	17	1
4:A:328:PX4:H34	4:A:351:PX4:H31	0.40	1.92	18	1
4:A:429:PX4:O6	4:A:429:PX4:H4	0.40	2.16	18	1
4:A:350:PX4:H54	4:A:350:PX4:H61	0.40	1.48	12	1
4:A:323:PX4:H34	4:A:353:PX4:H25	0.40	1.92	12	1
4:A:311:PX4:H62	4:A:311:PX4:H56	0.40	1.74	11	1
4:A:332:PX4:H55	4:A:332:PX4:H60	0.40	1.72	11	1
4:A:305:PX4:H45	4:A:333:PX4:H63	0.40	1.93	11	1
4:A:383:PX4:H54	4:A:394:PX4:H26	0.40	1.92	4	1
4:A:422:PX4:H50	4:A:425:PX4:H17	0.40	1.92	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:382:PX4:H30	4:A:398:PX4:H59	0.40	1.93	10	1
4:A:394:PX4:H21	4:A:407:PX4:H54	0.40	1.92	10	1
4:A:389:PX4:H24	4:A:389:PX4:H29	0.40	1.67	9	1
4:A:366:PX4:H36	4:A:403:PX4:H25	0.40	1.91	1	1
4:A:375:PX4:H66	4:A:405:PX4:H42	0.40	1.92	1	1
4:A:318:PX4:H19	4:A:342:PX4:H18	0.40	1.91	3	1
4:A:307:PX4:C17	4:A:337:PX4:H36	0.40	2.46	3	1
4:A:338:PX4:C35	4:A:359:PX4:H32	0.40	2.42	3	1
4:A:408:PX4:H19	4:A:408:PX4:H26	0.40	1.68	3	1
4:A:392:PX4:H47	4:A:425:PX4:H50	0.40	1.92	5	1
4:A:397:PX4:H55	4:A:423:PX4:H55	0.40	1.93	6	1
4:A:317:PX4:H52	4:A:326:PX4:H27	0.40	1.93	2	1
4:A:334:PX4:H52	4:A:334:PX4:H59	0.40	1.73	17	1
4:A:374:PX4:H8	4:A:428:PX4:O1	0.40	2.17	17	1
4:A:351:PX4:H30	4:A:359:PX4:H39	0.40	1.93	8	1
4:A:343:PX4:H64	4:A:343:PX4:H72	0.40	1.30	16	1
4:A:370:PX4:H67	4:A:374:PX4:H69	0.40	1.93	18	1
4:A:325:PX4:H70	4:A:403:PX4:H72	0.40	1.92	19	1
4:A:408:PX4:H38	4:A:422:PX4:H44	0.40	1.94	19	1
4:A:307:PX4:H41	4:A:307:PX4:H35	0.40	1.45	15	1
4:A:417:PX4:H64	4:A:418:PX4:H31	0.40	1.93	12	1
4:A:322:PX4:H25	4:A:322:PX4:H20	0.40	1.72	11	1
4:A:388:PX4:H13	4:A:388:PX4:H2	0.40	1.72	11	1
4:A:409:PX4:H27	4:A:412:PX4:H29	0.40	1.93	4	1
4:A:306:PX4:H30	4:A:306:PX4:H35	0.40	1.72	9	1
4:A:361:PX4:H25	4:A:361:PX4:H19	0.40	1.56	9	1
4:A:370:PX4:H45	4:A:383:PX4:H67	0.40	1.93	9	1
4:A:333:PX4:H62	4:A:333:PX4:H68	0.40	1.67	1	1
4:A:324:PX4:H66	4:A:333:PX4:H53	0.40	1.92	20	1
4:A:375:PX4:H51	4:A:384:PX4:C13	0.40	2.46	20	1
4:A:336:PX4:H45	4:A:413:PX4:H63	0.40	1.92	3	1
4:A:343:PX4:H59	4:A:350:PX4:H59	0.40	1.94	7	1
4:A:365:PX4:H29	4:A:419:PX4:H60	0.40	1.92	7	1
4:A:400:PX4:H36	4:A:401:PX4:H62	0.40	1.92	7	1
4:A:404:PX4:H33	4:A:417:PX4:H31	0.40	1.94	7	1
4:A:349:PX4:H26	4:A:353:PX4:H50	0.40	1.93	5	1
4:A:305:PX4:H62	4:A:305:PX4:H57	0.40	1.67	13	1
4:A:323:PX4:H34	4:A:328:PX4:H37	0.40	1.93	13	1
4:A:373:PX4:H57	4:A:406:PX4:H52	0.40	1.93	13	1
4:A:348:PX4:H39	4:A:383:PX4:H42	0.40	1.92	13	1
4:A:305:PX4:H69	4:A:324:PX4:H31	0.40	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:308:PX4:H30	4:A:320:PX4:H17	0.40	1.91	6	1
4:A:370:PX4:O8	4:A:381:PX4:H1	0.40	2.16	2	1
4:A:391:PX4:H71	4:A:414:PX4:H59	0.40	1.92	2	1
4:A:340:PX4:H40	4:A:340:PX4:H33	0.40	1.51	8	1
4:A:314:PX4:H62	4:A:354:PX4:H29	0.40	1.92	16	1
4:A:371:PX4:H27	4:A:395:PX4:H30	0.40	1.92	16	1
4:A:401:PX4:H37	4:A:401:PX4:H32	0.40	1.58	19	1
4:A:373:PX4:H49	4:A:406:PX4:H17	0.40	1.93	15	1
4:A:313:PX4:H27	4:A:362:PX4:H62	0.40	1.93	12	1
4:A:375:PX4:H7	4:A:392:PX4:O6	0.40	2.16	12	1
4:A:417:PX4:H26	4:A:418:PX4:H46	0.40	1.93	12	1
4:A:310:PX4:H57	4:A:310:PX4:H62	0.40	1.66	10	1
4:A:349:PX4:H65	4:A:358:PX4:H36	0.40	1.91	10	1
4:A:355:PX4:H20	4:A:362:PX4:H17	0.40	1.93	9	1
4:A:415:PX4:H46	4:A:415:PX4:H53	0.40	1.69	9	1
4:A:319:PX4:H57	4:A:343:PX4:H19	0.40	1.93	20	1
4:A:351:PX4:H65	4:A:351:PX4:H71	0.40	1.70	20	1
4:A:401:PX4:H25	4:A:401:PX4:H32	0.40	1.64	20	1
4:A:306:PX4:H56	4:A:342:PX4:H24	0.40	1.93	3	1
4:A:386:PX4:H27	4:A:386:PX4:H21	0.40	1.81	7	1
4:A:413:PX4:H58	4:A:413:PX4:H65	0.40	1.65	7	1
4:A:343:PX4:H66	4:A:343:PX4:H61	0.40	1.70	13	1
4:A:354:PX4:H26	4:A:354:PX4:H31	0.40	1.66	6	1
4:A:383:PX4:H38	4:A:383:PX4:H31	0.40	1.80	14	1
1:A:57:ARG:NH2	1:A:60:GLU:OE2	0.40	2.45	14	1
4:A:321:PX4:H72	4:A:321:PX4:H64	0.40	1.78	17	1
4:A:322:PX4:H35	4:A:337:PX4:H42	0.40	1.92	8	1
4:A:306:PX4:H21	4:A:342:PX4:H25	0.40	1.93	16	1
4:A:391:PX4:H6	4:A:391:PX4:H2	0.40	1.82	16	1
4:A:409:PX4:H56	4:A:409:PX4:H51	0.40	1.59	16	1
4:A:328:PX4:H37	4:A:345:PX4:H23	0.40	1.93	18	1
4:A:330:PX4:H31	4:A:330:PX4:H38	0.40	1.56	19	1
1:A:221:PRO:CG	1:A:224:PHE:HB2	0.40	2.46	15	1
4:A:322:PX4:H47	4:A:344:PX4:H19	0.40	1.92	15	1
4:A:391:PX4:H1	4:A:427:PX4:O2	0.40	2.17	15	1
4:A:368:PX4:H33	4:A:368:PX4:H28	0.40	1.69	10	1
4:A:369:PX4:O6	4:A:429:PX4:H49	0.40	2.16	9	1
4:A:374:PX4:H25	4:A:417:PX4:H68	0.40	1.92	9	1
4:A:384:PX4:H38	4:A:405:PX4:H27	0.40	1.92	1	1
4:A:317:PX4:H69	4:A:330:PX4:H44	0.40	1.93	20	1
4:A:411:PX4:H63	4:A:423:PX4:H51	0.40	1.92	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:H55	4:A:359:PX4:H35	0.40	1.93	5	1
4:A:377:PX4:H30	4:A:408:PX4:H30	0.40	1.94	13	1
4:A:345:PX4:H37	4:A:345:PX4:H32	0.40	1.78	2	1
4:A:365:PX4:H21	4:A:365:PX4:H27	0.40	1.69	2	1
4:A:363:PX4:H43	4:A:408:PX4:H43	0.40	1.92	2	1
4:A:331:PX4:H69	4:A:331:PX4:H63	0.40	1.72	17	1
4:A:371:PX4:H62	4:A:402:PX4:H40	0.40	1.93	8	1
4:A:378:PX4:H38	4:A:378:PX4:H44	0.40	1.70	16	1
4:A:395:PX4:H11	4:A:395:PX4:H47	0.40	1.92	16	1
4:A:314:PX4:H19	4:A:336:PX4:H24	0.40	1.94	18	1
4:A:314:PX4:H64	4:A:314:PX4:H72	0.40	1.73	19	1
4:A:344:PX4:H27	4:A:344:PX4:H34	0.40	1.46	19	1
4:A:362:PX4:H29	4:A:364:PX4:H48	0.40	1.92	19	1
4:A:400:PX4:H59	4:A:405:PX4:C11	0.40	2.46	19	1
4:A:379:PX4:O1	4:A:409:PX4:H25	0.40	2.15	12	1
4:A:330:PX4:H53	4:A:330:PX4:H58	0.40	1.70	10	1
4:A:376:PX4:H49	4:A:390:PX4:H4	0.40	1.93	10	1
4:A:409:PX4:H63	4:A:411:PX4:H22	0.40	1.94	9	1
4:A:368:PX4:H47	5:A:436:C3S:H322	0.40	1.92	9	1
4:A:306:PX4:H71	4:A:306:PX4:H65	0.40	1.73	1	1
4:A:324:PX4:H49	4:A:324:PX4:H54	0.40	1.53	20	1
4:A:313:PX4:C28	4:A:325:PX4:H55	0.40	2.46	20	1
4:A:339:PX4:H20	4:A:339:PX4:H26	0.40	1.73	20	1
4:A:366:PX4:H51	4:A:403:PX4:C23	0.40	2.47	20	1
4:A:426:PX4:H7	4:A:426:PX4:H15	0.40	1.94	3	1
4:A:370:PX4:H35	4:A:394:PX4:H20	0.40	1.93	7	1
4:A:367:PX4:H8	4:A:389:PX4:O1	0.40	2.17	5	1
4:A:397:PX4:H31	4:A:397:PX4:H26	0.40	1.65	5	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/250 (95%)	211±3 (89±1%)	20±3 (8±1%)	6±1 (3±1%)	10	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4740/5000 (95%)	4216 (89%)	401 (8%)	123 (3%)	10	46

All 22 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	31	ASN	18
1	A	147	TYR	18
1	A	150	ASP	16
1	A	224	PHE	11
1	A	25	TYR	11
1	A	155	THR	9
1	A	57	ARG	6
1	A	55	ASN	5
1	A	166	LEU	4
1	A	154	ASN	4
1	A	130	GLY	4
1	A	24	LEU	3
1	A	58	VAL	2
1	A	143	HIS	2
1	A	83	LYS	2
1	A	162	PRO	2
1	A	214	PRO	1
1	A	7	MET	1
1	A	49	PRO	1
1	A	117	GLY	1
1	A	141	GLY	1
1	A	183	SER	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/208 (94%)	186±3 (95±2%)	9±3 (5±2%)	34	79
All	All	3900/4160 (94%)	3711 (95%)	189 (5%)	34	79

All 68 unique residues with a non-rotameric sidechain are listed below. They are sorted by the

frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	150	ASP	20
1	A	155	THR	12
1	A	158	HIS	9
1	A	177	ARG	9
1	A	75	TYR	8
1	A	118	LYS	7
1	A	122	LEU	6
1	A	156	LEU	6
1	A	45	PHE	5
1	A	71	ASP	5
1	A	179	THR	5
1	A	26	ASP	5
1	A	97	THR	5
1	A	126	LYS	5
1	A	166	LEU	4
1	A	202	MET	4
1	A	96	TYR	3
1	A	171	HIS	3
1	A	175	ASP	3
1	A	174	GLU	3
1	A	98	ARG	3
1	A	110	SER	3
1	A	129	TRP	2
1	A	116	TRP	2
1	A	224	PHE	2
1	A	143	HIS	2
1	A	38	LYS	2
1	A	16	GLN	2
1	A	63	GLN	2
1	A	180	ASP	2
1	A	3	GLU	2
1	A	2	GLN	2
1	A	30	LYS	1
1	A	184	LEU	1
1	A	67	CYS	1
1	A	182	SER	1
1	A	10	LEU	1
1	A	34	SER	1
1	A	164	THR	1
1	A	72	VAL	1
1	A	94	VAL	1
1	A	114	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	41	GLU	1
1	A	209	ASN	1
1	A	189	LEU	1
1	A	83	LYS	1
1	A	149	PHE	1
1	A	215	THR	1
1	A	162	PRO	1
1	A	127	VAL	1
1	A	107	ARG	1
1	A	14	GLN	1
1	A	128	VAL	1
1	A	100	LEU	1
1	A	198	HIS	1
1	A	115	MET	1
1	A	36	GLU	1
1	A	99	ASP	1
1	A	105	VAL	1
1	A	17	ASP	1
1	A	225	LYS	1
1	A	9	GLU	1
1	A	145	ASP	1
1	A	74	GLU	1
1	A	86	SER	1
1	A	183	SER	1
1	A	235	GLN	1
1	A	120	ILE	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

Of 136 ligands modelled in this entry, 4 are monoatomic - leaving 132 for Mogul analysis.

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
4	PX4	A	305	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	306	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.62±0.01	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.62±0.01	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.62±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	337	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	348	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.62±0.01	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	374	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	376	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.62±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	380	-	45,45,45	0.62±0.01	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.62±0.01	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	388	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.63±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	423	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.62±0.00	0±0 (0±0%)
5	C3S	A	431	-	35,35,35	1.34±0.01	1±0 (2±0%)
5	C3S	A	432	-	35,35,35	1.34±0.01	1±0 (2±0%)
5	C3S	A	433	-	35,35,35	1.34±0.01	1±0 (2±0%)
5	C3S	A	434	-	35,35,35	1.35±0.01	1±0 (2±0%)
5	C3S	A	435	-	35,35,35	1.34±0.01	1±0 (2±0%)
5	C3S	A	436	-	35,35,35	1.34±0.01	1±0 (2±0%)

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
4	PX4	A	305	-	50,53,53	1.44±0.10	0±0 (0±0%)
4	PX4	A	306	-	50,53,53	1.53±0.13	0±0 (0±0%)
4	PX4	A	307	-	50,53,53	1.49±0.15	0±0 (0±0%)
4	PX4	A	308	-	50,53,53	1.48±0.17	0±0 (0±0%)
4	PX4	A	309	-	50,53,53	1.54±0.17	0±1 (0±1%)
4	PX4	A	310	-	50,53,53	1.50±0.17	0±1 (0±1%)
4	PX4	A	311	-	50,53,53	1.49±0.16	0±1 (0±1%)
4	PX4	A	312	-	50,53,53	1.47±0.18	0±1 (0±1%)
4	PX4	A	313	-	50,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	314	-	50,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	315	-	50,53,53	1.43±0.12	0±0 (0±0%)
4	PX4	A	316	-	50,53,53	1.48±0.13	0±1 (0±1%)
4	PX4	A	317	-	50,53,53	1.43±0.17	0±0 (0±0%)
4	PX4	A	318	-	50,53,53	1.50±0.14	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	319	-	50,53,53	1.51±0.18	0±1 (0±1%)
4	PX4	A	320	-	50,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	321	-	50,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	322	-	50,53,53	1.53±0.14	0±0 (0±0%)
4	PX4	A	323	-	50,53,53	1.50±0.11	0±0 (0±0%)
4	PX4	A	324	-	50,53,53	1.50±0.17	0±0 (0±0%)
4	PX4	A	325	-	50,53,53	1.52±0.17	0±0 (0±0%)
4	PX4	A	326	-	50,53,53	1.51±0.15	0±0 (0±0%)
4	PX4	A	327	-	50,53,53	1.40±0.18	0±0 (0±0%)
4	PX4	A	328	-	50,53,53	1.55±0.19	0±0 (0±0%)
4	PX4	A	329	-	50,53,53	1.43±0.14	0±0 (0±0%)
4	PX4	A	330	-	50,53,53	1.55±0.13	0±1 (0±1%)
4	PX4	A	331	-	50,53,53	1.53±0.17	0±0 (0±0%)
4	PX4	A	332	-	50,53,53	1.49±0.15	0±0 (0±0%)
4	PX4	A	333	-	50,53,53	1.47±0.21	0±0 (0±0%)
4	PX4	A	334	-	50,53,53	1.48±0.14	0±0 (0±0%)
4	PX4	A	335	-	50,53,53	1.54±0.15	0±0 (0±0%)
4	PX4	A	336	-	50,53,53	1.55±0.20	0±0 (0±0%)
4	PX4	A	337	-	50,53,53	1.47±0.16	0±0 (0±0%)
4	PX4	A	338	-	50,53,53	1.48±0.20	0±0 (0±0%)
4	PX4	A	339	-	50,53,53	1.41±0.13	0±0 (0±0%)
4	PX4	A	340	-	50,53,53	1.49±0.15	0±0 (0±0%)
4	PX4	A	341	-	50,53,53	1.48±0.20	0±0 (0±0%)
4	PX4	A	342	-	50,53,53	1.49±0.17	0±0 (0±0%)
4	PX4	A	343	-	50,53,53	1.56±0.16	0±0 (0±0%)
4	PX4	A	344	-	50,53,53	1.43±0.19	0±0 (0±0%)
4	PX4	A	345	-	50,53,53	1.49±0.17	0±1 (0±1%)
4	PX4	A	346	-	50,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	347	-	50,53,53	1.52±0.15	0±0 (0±0%)
4	PX4	A	348	-	50,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	349	-	50,53,53	1.47±0.13	0±1 (0±1%)
4	PX4	A	350	-	50,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	351	-	50,53,53	1.44±0.15	0±0 (0±0%)
4	PX4	A	352	-	50,53,53	1.50±0.12	0±0 (0±0%)
4	PX4	A	353	-	50,53,53	1.53±0.20	0±1 (0±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	354	-	50,53,53	1.52±0.20	0±0 (0±0%)
4	PX4	A	355	-	50,53,53	1.48±0.16	0±1 (0±1%)
4	PX4	A	356	-	50,53,53	1.56±0.16	0±0 (0±0%)
4	PX4	A	357	-	50,53,53	1.57±0.16	0±0 (0±0%)
4	PX4	A	358	-	50,53,53	1.45±0.19	0±0 (0±0%)
4	PX4	A	359	-	50,53,53	1.50±0.13	0±0 (0±0%)
4	PX4	A	360	-	50,53,53	1.48±0.17	0±0 (0±0%)
4	PX4	A	361	-	50,53,53	1.47±0.19	0±1 (0±1%)
4	PX4	A	362	-	50,53,53	1.43±0.13	0±0 (0±0%)
4	PX4	A	363	-	50,53,53	1.45±0.17	0±0 (0±0%)
4	PX4	A	364	-	50,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	365	-	50,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	366	-	50,53,53	1.41±0.16	0±0 (0±0%)
4	PX4	A	367	-	50,53,53	1.50±0.14	0±1 (0±1%)
4	PX4	A	368	-	50,53,53	1.47±0.11	0±0 (0±0%)
4	PX4	A	369	-	50,53,53	1.45±0.08	0±0 (0±0%)
4	PX4	A	370	-	50,53,53	1.49±0.15	0±0 (0±0%)
4	PX4	A	371	-	50,53,53	1.51±0.13	0±0 (0±0%)
4	PX4	A	372	-	50,53,53	1.52±0.21	0±1 (0±1%)
4	PX4	A	373	-	50,53,53	1.47±0.18	0±0 (0±0%)
4	PX4	A	374	-	50,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	375	-	50,53,53	1.52±0.16	0±0 (0±0%)
4	PX4	A	376	-	50,53,53	1.55±0.23	0±1 (0±1%)
4	PX4	A	377	-	50,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	378	-	50,53,53	1.49±0.20	0±0 (0±0%)
4	PX4	A	379	-	50,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	380	-	50,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	381	-	50,53,53	1.56±0.18	0±1 (0±1%)
4	PX4	A	382	-	50,53,53	1.49±0.10	0±0 (0±0%)
4	PX4	A	383	-	50,53,53	1.46±0.17	0±0 (0±0%)
4	PX4	A	384	-	50,53,53	1.52±0.17	0±0 (0±0%)
4	PX4	A	385	-	50,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	386	-	50,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	387	-	50,53,53	1.54±0.12	0±0 (0±0%)
4	PX4	A	388	-	50,53,53	1.45±0.11	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	389	-	50,53,53	1.48±0.14	0±0 (0±0%)
4	PX4	A	390	-	50,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	391	-	50,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	392	-	50,53,53	1.50±0.13	0±1 (0±1%)
4	PX4	A	393	-	50,53,53	1.52±0.14	0±1 (0±1%)
4	PX4	A	394	-	50,53,53	1.49±0.16	0±0 (0±0%)
4	PX4	A	395	-	50,53,53	1.52±0.17	0±0 (0±0%)
4	PX4	A	396	-	50,53,53	1.45±0.14	0±0 (0±0%)
4	PX4	A	397	-	50,53,53	1.52±0.13	0±0 (0±0%)
4	PX4	A	398	-	50,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	399	-	50,53,53	1.51±0.16	0±0 (0±0%)
4	PX4	A	400	-	50,53,53	1.46±0.15	0±0 (0±0%)
4	PX4	A	401	-	50,53,53	1.55±0.18	0±1 (0±1%)
4	PX4	A	402	-	50,53,53	1.54±0.16	0±1 (0±1%)
4	PX4	A	403	-	50,53,53	1.47±0.11	0±0 (0±0%)
4	PX4	A	404	-	50,53,53	1.42±0.15	0±0 (0±0%)
4	PX4	A	405	-	50,53,53	1.55±0.15	0±0 (0±0%)
4	PX4	A	406	-	50,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	407	-	50,53,53	1.49±0.16	0±0 (0±0%)
4	PX4	A	408	-	50,53,53	1.48±0.22	0±1 (0±1%)
4	PX4	A	409	-	50,53,53	1.55±0.16	0±0 (0±0%)
4	PX4	A	410	-	50,53,53	1.45±0.10	0±0 (0±0%)
4	PX4	A	411	-	50,53,53	1.50±0.17	0±0 (0±0%)
4	PX4	A	412	-	50,53,53	1.47±0.18	0±0 (0±0%)
4	PX4	A	413	-	50,53,53	1.50±0.16	0±0 (0±0%)
4	PX4	A	414	-	50,53,53	1.49±0.13	0±0 (0±0%)
4	PX4	A	415	-	50,53,53	1.51±0.14	0±0 (0±0%)
4	PX4	A	416	-	50,53,53	1.52±0.16	0±1 (0±1%)
4	PX4	A	417	-	50,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	418	-	50,53,53	1.55±0.17	0±0 (0±0%)
4	PX4	A	419	-	50,53,53	1.55±0.14	0±0 (0±0%)
4	PX4	A	420	-	50,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	421	-	50,53,53	1.51±0.18	0±1 (0±1%)
4	PX4	A	422	-	50,53,53	1.45±0.14	0±0 (0±0%)
4	PX4	A	423	-	50,53,53	1.47±0.16	0±0 (0±0%)



Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	424	-	50,53,53	1.45±0.20	0±0 (0±0%)
4	PX4	A	425	-	50,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	426	-	50,53,53	1.43±0.17	0±0 (0±0%)
4	PX4	A	427	-	50,53,53	1.49±0.19	0±0 (0±0%)
4	PX4	A	428	-	50,53,53	1.43±0.18	0±0 (0±0%)
4	PX4	A	429	-	50,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	430	-	50,53,53	1.40±0.18	0±0 (0±0%)
5	C3S	A	431	-	51,55,55	2.25±0.30	1±1 (2±1%)
5	C3S	A	432	-	51,55,55	2.34±0.21	2±1 (4±2%)
5	C3S	A	433	-	51,55,55	2.24±0.21	1±1 (2±1%)
5	C3S	A	434	-	51,55,55	2.24±0.25	1±1 (2±2%)
5	C3S	A	435	-	51,55,55	2.25±0.20	1±1 (2±2%)
5	C3S	A	436	-	51,55,55	2.28±0.23	2±1 (3±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	PX4	A	305	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	306	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	307	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	308	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	309	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	310	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	311	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	312	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	313	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	314	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	315	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	316	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	317	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	318	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	319	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	320	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	321	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	322	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	323	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	324	-	-	0±0,49,49,49	0±0,0,0,0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	325	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	326	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	327	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	328	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	329	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	330	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	331	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	332	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	333	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	334	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	335	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	336	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	337	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	338	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	339	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	340	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	341	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	342	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	343	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	344	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	345	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	346	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	347	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	348	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	349	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	350	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	351	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	352	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	353	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	354	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	355	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	356	-	-	2±0,49,49,49	0±0,0,0,0
4	PX4	A	357	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	358	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	359	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	360	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	361	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	362	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	363	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	364	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	365	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	366	-	-	0±0,49,49,49	0±0,0,0,0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	367	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	368	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	369	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	370	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	371	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	372	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	373	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	374	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	375	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	376	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	377	-	-	2±0,49,49,49	0±0,0,0,0
4	PX4	A	378	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	379	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	380	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	381	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	382	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	383	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	384	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	385	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	386	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	387	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	388	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	389	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	390	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	391	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	392	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	393	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	394	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	395	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	396	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	397	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	398	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	399	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	400	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	401	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	402	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	403	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	404	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	405	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	406	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	407	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	408	-	-	0±0,49,49,49	0±0,0,0,0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	409	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	410	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	411	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	412	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	413	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	414	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	415	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	416	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	417	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	418	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	419	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	420	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	421	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	422	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	423	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	424	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	425	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	426	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	427	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	428	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	429	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	430	-	-	0±0,49,49,49	0±0,0,0,0
5	C3S	A	431	-	2±0,2,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	432	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	433	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	434	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	435	-	2±0,2,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	436	-	2±0,2,12,12	0±0,15,73,73	0±0,4,4,4

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
5	A	434	C3S	O6-S1	6.81	1.76	1.56	7	20
5	A	435	C3S	O6-S1	6.79	1.76	1.56	14	20
5	A	432	C3S	O6-S1	6.79	1.76	1.56	3	20
5	A	436	C3S	O6-S1	6.79	1.76	1.56	7	20
5	A	433	C3S	O6-S1	6.78	1.76	1.56	12	20
5	A	431	C3S	O6-S1	6.78	1.76	1.56	14	20

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
5	A	432	C3S	C29-C38-C48	10.05	135.60	119.47	14	14
5	A	433	C3S	O6-C7-C4	9.16	121.32	107.54	20	2
5	A	434	C3S	C29-C38-C48	9.13	134.12	119.47	15	5
5	A	436	C3S	C50-C48-C38	8.57	126.36	112.95	16	5
4	A	375	PX4	C8-C7-C6	8.49	92.71	111.86	11	1
5	A	431	C3S	C29-C38-C48	8.46	133.05	119.47	8	7
4	A	308	PX4	C8-C7-C6	8.32	93.09	111.86	4	4
5	A	433	C3S	C29-C38-C48	8.29	132.78	119.47	18	10
5	A	436	C3S	O6-C7-C4	8.23	119.91	107.54	6	4
5	A	431	C3S	C9-C12-C22	8.20	127.67	116.41	1	2
5	A	434	C3S	C40-C29-C30	7.91	126.70	111.73	12	3
4	A	426	PX4	O5-C8-C7	7.83	128.32	108.66	6	1
5	A	436	C3S	C35-C38-C48	7.80	124.63	112.14	8	3
5	A	431	C3S	O6-C7-C4	7.80	119.26	107.54	12	1
5	A	434	C3S	C23-C20-C22	7.78	123.85	113.10	13	1
4	A	376	PX4	O5-C8-C7	7.78	128.20	108.66	7	1
4	A	381	PX4	O7-C23-C24	7.71	127.55	111.55	17	3
4	A	354	PX4	C8-C7-C6	7.59	94.73	111.86	15	4
4	A	391	PX4	C8-C7-C6	7.54	94.84	111.86	3	1
4	A	337	PX4	C8-C7-C6	7.53	94.87	111.86	2	1
4	A	324	PX4	O5-C8-C7	7.47	127.42	108.66	19	1
4	A	423	PX4	O5-C8-C7	7.46	127.39	108.66	4	3
5	A	436	C3S	C29-C38-C48	7.45	131.41	119.47	12	4
4	A	406	PX4	C8-C7-C6	7.42	95.12	111.86	12	1
5	A	435	C3S	C20-C18-C30	7.40	119.12	109.09	10	1
4	A	353	PX4	O7-C23-C24	7.36	126.83	111.55	17	1
5	A	434	C3S	C40-C29-C26	7.36	98.57	110.59	16	2
5	A	434	C3S	O6-C7-C4	7.36	118.60	107.54	2	1
4	A	424	PX4	C7-O7-C23	7.26	135.03	117.88	18	1
5	A	435	C3S	C9-C12-C22	7.25	126.38	116.41	13	5
5	A	434	C3S	C9-C12-C22	7.23	126.34	116.41	15	7
5	A	435	C3S	C29-C38-C48	7.20	131.02	119.47	14	5
5	A	432	C3S	O6-C7-C4	7.15	118.29	107.54	19	3
4	A	328	PX4	O5-C8-C7	7.11	126.53	108.66	1	2
5	A	433	C3S	C54-C48-C38	7.10	125.18	110.26	14	4
4	A	376	PX4	C8-C7-C6	7.09	95.86	111.86	3	1
4	A	325	PX4	O7-C23-C24	7.08	126.24	111.55	8	1
5	A	436	C3S	C50-C48-C54	7.05	99.24	110.35	9	1
5	A	432	C3S	C9-C12-C22	6.99	126.01	116.41	18	7
5	A	432	C3S	C50-C48-C54	6.97	99.36	110.35	12	2
4	A	367	PX4	O7-C23-C24	6.95	125.98	111.55	8	3
4	A	414	PX4	O5-C8-C7	6.94	126.09	108.66	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	407	PX4	C8-C7-C6	6.92	96.25	111.86	3	3
4	A	317	PX4	C8-C7-C6	6.91	96.27	111.86	17	1
4	A	376	PX4	C7-O7-C23	6.88	134.12	117.88	7	1
4	A	389	PX4	C8-C7-C6	6.85	96.40	111.86	6	3
4	A	418	PX4	O5-C8-C7	6.79	125.72	108.66	13	2
4	A	376	PX4	O7-C23-C24	6.78	125.64	111.55	3	3
5	A	435	C3S	C7-C9-C12	6.78	122.30	111.52	11	1
4	A	345	PX4	O7-C23-C24	6.75	125.57	111.55	1	2
5	A	431	C3S	C35-C38-C29	6.74	95.53	103.83	8	3
4	A	401	PX4	O5-C8-C7	6.71	125.53	108.66	17	2
5	A	436	C3S	C9-C12-C22	6.70	125.61	116.41	9	5
4	A	356	PX4	C7-O7-C23	6.69	133.68	117.88	7	1
4	A	311	PX4	O5-C8-C7	6.68	125.45	108.66	6	1
4	A	378	PX4	C8-C7-C6	6.64	96.88	111.86	17	2
4	A	335	PX4	O7-C23-C24	6.63	125.32	111.55	5	3
4	A	336	PX4	O5-C8-C7	6.63	125.31	108.66	16	2
4	A	394	PX4	O5-C8-C7	6.63	125.31	108.66	2	2
4	A	385	PX4	O5-C8-C7	6.63	125.31	108.66	15	1
5	A	435	C3S	C44-C22-C20	6.62	119.87	111.68	1	1
4	A	413	PX4	C8-C7-C6	6.61	96.95	111.86	16	2
5	A	432	C3S	C44-C22-C20	6.61	119.85	111.68	18	1
4	A	365	PX4	O5-C8-C7	6.59	125.22	108.66	4	1
4	A	333	PX4	C8-C7-C6	6.58	97.01	111.86	7	2
4	A	421	PX4	C8-C7-C6	6.55	97.07	111.86	9	2
4	A	421	PX4	O5-C8-C7	6.53	125.08	108.66	3	1
4	A	383	PX4	O5-C8-C7	6.53	125.07	108.66	6	1
4	A	403	PX4	C8-C7-C6	6.52	97.14	111.86	3	1
4	A	405	PX4	C8-C7-C6	6.51	97.17	111.86	10	2
4	A	346	PX4	O5-C8-C7	6.50	124.99	108.66	18	1
5	A	431	C3S	C15-C18-C20	6.48	101.58	109.72	18	1
4	A	345	PX4	C8-C7-C6	6.49	97.23	111.86	10	1
4	A	405	PX4	O5-C8-C7	6.48	124.94	108.66	6	2
4	A	343	PX4	O5-C8-C7	6.47	124.91	108.66	17	1
4	A	411	PX4	C8-C7-C6	6.47	97.27	111.86	17	2
4	A	400	PX4	C8-C7-C6	6.46	97.28	111.86	10	1
4	A	401	PX4	C8-C7-C6	6.45	97.32	111.86	17	2
4	A	392	PX4	C7-O7-C23	6.42	133.05	117.88	16	2
4	A	410	PX4	O5-C8-C7	6.42	124.78	108.66	6	3
4	A	336	PX4	C8-C7-C6	6.41	97.39	111.86	8	2
4	A	417	PX4	C8-C7-C6	6.41	97.40	111.86	5	2
4	A	316	PX4	O5-C8-C7	6.41	124.75	108.66	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	354	PX4	O5-C8-C7	6.40	124.75	108.66	17	2
4	A	370	PX4	O5-C8-C7	6.40	124.73	108.66	19	3
4	A	361	PX4	C8-C7-C6	6.40	97.43	111.86	8	3
5	A	432	C3S	O6-C7-C9	6.38	118.78	107.28	14	2
4	A	372	PX4	C8-C7-C6	6.37	97.48	111.86	13	1
5	A	432	C3S	C40-C29-C30	6.36	123.77	111.73	13	2
4	A	342	PX4	O5-C8-C7	6.35	124.62	108.66	6	2
4	A	309	PX4	O5-C8-C7	6.33	124.56	108.66	19	5
4	A	427	PX4	O5-C8-C7	6.33	124.56	108.66	9	1
4	A	309	PX4	O7-C23-C24	6.30	124.64	111.55	7	1
4	A	347	PX4	C7-O7-C23	6.30	132.76	117.88	18	1
4	A	387	PX4	O5-C8-C7	6.30	124.49	108.66	19	3
4	A	408	PX4	C8-C7-C6	6.30	97.66	111.86	4	4
4	A	336	PX4	O7-C23-C24	6.28	124.59	111.55	5	1
4	A	321	PX4	O5-C8-C7	6.26	124.39	108.66	17	1
4	A	397	PX4	O5-C8-C7	6.25	124.35	108.66	13	2
4	A	368	PX4	O5-C8-C7	6.25	124.35	108.66	1	1
4	A	312	PX4	C7-O7-C23	6.22	132.57	117.88	9	1
4	A	388	PX4	C8-C7-C6	6.21	97.85	111.86	10	2
4	A	343	PX4	O7-C23-C24	6.20	124.42	111.55	6	3
4	A	382	PX4	C8-C7-C6	6.19	97.90	111.86	2	1
5	A	434	C3S	C44-C22-C20	6.19	119.33	111.68	14	1
4	A	310	PX4	C5-N1-C4	6.19	93.31	108.98	5	1
4	A	321	PX4	C8-C7-C6	6.19	97.91	111.86	17	1
4	A	307	PX4	C8-C7-C6	6.18	97.91	111.86	1	2
4	A	371	PX4	C8-C7-C6	6.18	97.93	111.86	2	2
4	A	355	PX4	O7-C23-C24	6.16	124.35	111.55	19	2
4	A	398	PX4	O5-C8-C7	6.16	124.14	108.66	16	3
5	A	436	C3S	O6-C7-C9	6.15	118.37	107.28	18	4
4	A	320	PX4	O5-C8-C7	6.14	124.09	108.66	6	1
4	A	374	PX4	C7-O7-C23	6.08	132.25	117.88	14	2
4	A	421	PX4	C7-O7-C23	6.07	132.22	117.88	17	2
4	A	338	PX4	O5-C8-C7	6.07	123.90	108.66	15	2
4	A	312	PX4	C8-C7-C6	6.06	98.19	111.86	15	1
4	A	362	PX4	O5-C8-C7	6.06	123.87	108.66	1	1
4	A	365	PX4	C8-C7-C6	6.05	98.22	111.86	5	2
4	A	373	PX4	C7-O7-C23	6.04	132.16	117.88	4	1
5	A	435	C3S	C40-C29-C26	6.04	100.72	110.59	7	2
5	A	434	C3S	C4-C7-C9	6.04	101.54	111.02	20	1
4	A	412	PX4	C8-C7-C6	6.02	98.27	111.86	2	1
4	A	310	PX4	C7-O7-C23	6.02	132.10	117.88	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	417	PX4	O5-C8-C7	6.01	123.75	108.66	7	2
5	A	431	C3S	C44-C22-C12	6.01	98.42	108.34	2	3
4	A	404	PX4	O7-C23-C24	6.00	124.02	111.55	18	1
4	A	415	PX4	C5-N1-C4	6.00	93.79	108.98	2	1
4	A	390	PX4	O7-C23-C24	5.98	123.96	111.55	11	1
4	A	378	PX4	C7-O7-C23	5.97	131.99	117.88	9	1
4	A	406	PX4	O5-C8-C7	5.97	123.65	108.66	2	2
4	A	393	PX4	O5-C8-C7	5.97	123.65	108.66	17	1
4	A	330	PX4	C7-O7-C23	5.97	131.97	117.88	7	1
4	A	406	PX4	O7-C23-O8	5.96	108.80	123.68	8	1
5	A	433	C3S	C44-C22-C12	5.96	98.49	108.34	10	1
4	A	324	PX4	C8-C7-C6	5.96	98.41	111.86	10	3
4	A	402	PX4	C8-C7-C6	5.95	98.43	111.86	9	2
4	A	430	PX4	C4-N1-C3	5.96	93.90	108.98	11	1
4	A	337	PX4	O7-C23-C24	5.94	123.89	111.55	14	2
4	A	396	PX4	O5-C8-C7	5.94	123.58	108.66	3	1
4	A	392	PX4	O5-C8-C7	5.94	123.58	108.66	6	2
4	A	427	PX4	O7-C23-C24	5.93	123.87	111.55	18	2
5	A	433	C3S	C1-C4-C7	5.93	120.72	110.30	1	1
4	A	390	PX4	O5-C8-C7	5.92	123.54	108.66	10	1
4	A	352	PX4	O7-C23-C24	5.92	123.84	111.55	12	2
5	A	434	C3S	C20-C18-C30	5.92	117.11	109.09	13	1
4	A	334	PX4	O5-C8-C7	5.92	123.53	108.66	15	1
4	A	344	PX4	O5-C8-C7	5.91	123.51	108.66	1	2
4	A	326	PX4	C8-C7-C6	5.91	98.53	111.86	11	2
4	A	317	PX4	O5-C8-C7	5.91	123.50	108.66	2	3
4	A	394	PX4	C8-C7-C6	5.90	98.54	111.86	9	2
4	A	331	PX4	C8-C7-C6	5.90	98.55	111.86	19	1
4	A	323	PX4	C5-N1-C4	5.89	94.05	108.98	4	1
4	A	324	PX4	C7-O7-C23	5.89	131.80	117.88	15	1
4	A	381	PX4	C5-N1-C4	5.88	94.09	108.98	9	1
4	A	395	PX4	O7-C23-O8	5.87	109.04	123.68	7	1
4	A	388	PX4	C4-N1-C3	5.87	94.12	108.98	1	1
4	A	330	PX4	C8-C7-C6	5.87	98.62	111.86	3	3
4	A	360	PX4	C8-C7-C6	5.86	98.63	111.86	2	2
4	A	408	PX4	O5-C8-C7	5.86	123.38	108.66	7	2
5	A	436	C3S	C40-C29-C26	5.86	101.02	110.59	10	3
4	A	306	PX4	C8-C7-C6	5.85	98.65	111.86	1	3
4	A	418	PX4	O7-C23-C24	5.85	123.69	111.55	14	1
5	A	436	C3S	C20-C18-C30	5.84	117.00	109.09	18	1
4	A	419	PX4	C8-C7-C6	5.84	98.69	111.86	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	434	C3S	C35-C38-C29	5.83	96.65	103.83	11	1
4	A	349	PX4	O7-C23-C24	5.82	123.65	111.55	11	1
4	A	327	PX4	O7-C23-C24	5.82	123.64	111.55	19	1
5	A	434	C3S	C44-C22-C12	5.82	98.73	108.34	7	1
4	A	422	PX4	O5-C8-C7	5.81	123.26	108.66	4	1
4	A	311	PX4	C8-C7-C6	5.81	98.75	111.86	12	1
4	A	312	PX4	O5-C8-C7	5.81	123.25	108.66	5	2
4	A	371	PX4	O7-C23-C24	5.80	123.60	111.55	13	2
4	A	393	PX4	C8-C7-C6	5.80	98.78	111.86	3	2
5	A	431	C3S	C40-C29-C26	5.79	101.12	110.59	17	3
5	A	432	C3S	C54-C48-C38	5.79	122.42	110.26	4	4
5	A	435	C3S	C35-C38-C29	5.79	96.70	103.83	10	1
5	A	431	C3S	C44-C22-C1	5.79	118.72	109.41	13	1
5	A	435	C3S	C4-C7-C9	5.79	120.11	111.02	2	2
4	A	426	PX4	O7-C23-C24	5.78	123.56	111.55	14	1
5	A	436	C3S	C9-C12-C13	5.78	111.77	120.59	9	1
4	A	393	PX4	O7-C23-C24	5.78	123.55	111.55	3	2
4	A	377	PX4	O7-C23-C24	5.77	123.54	111.55	18	2
4	A	413	PX4	O7-C23-C24	5.77	123.53	111.55	1	1
4	A	371	PX4	O5-C8-C7	5.77	123.15	108.66	10	1
5	A	432	C3S	C44-C22-C12	5.76	98.82	108.34	7	2
4	A	419	PX4	O5-C8-C7	5.76	123.13	108.66	20	2
4	A	408	PX4	C7-O7-C23	5.76	131.48	117.88	17	1
4	A	353	PX4	C8-C7-C6	5.76	98.87	111.86	16	1
4	A	313	PX4	O7-C23-C24	5.75	123.50	111.55	17	1
5	A	435	C3S	O6-C7-C9	5.75	117.65	107.28	9	1
4	A	360	PX4	O5-C8-C7	5.75	123.10	108.66	4	1
5	A	436	C3S	C44-C22-C12	5.75	98.85	108.34	13	4
4	A	392	PX4	C8-C7-C6	5.74	98.92	111.86	8	2
5	A	433	C3S	C20-C18-C30	5.72	116.84	109.09	18	2
4	A	357	PX4	C8-C7-C6	5.72	98.96	111.86	9	1
4	A	349	PX4	O3-P1-O2	5.71	86.22	109.25	3	1
4	A	340	PX4	O5-C8-C7	5.70	122.99	108.66	9	1
5	A	436	C3S	C23-C20-C22	5.70	120.97	113.10	7	2
5	A	436	C3S	C44-C22-C20	5.70	118.73	111.68	4	1
4	A	332	PX4	C8-C7-C6	5.69	99.01	111.86	15	3
4	A	325	PX4	O5-C8-C7	5.69	122.96	108.66	20	2
5	A	431	C3S	C50-C48-C38	5.69	121.86	112.95	5	1
4	A	372	PX4	O5-C8-C7	5.69	122.95	108.66	4	1
4	A	332	PX4	O5-C8-C7	5.68	122.94	108.66	3	2
4	A	318	PX4	O5-C8-C7	5.68	122.93	108.66	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	432	C3S	C40-C29-C26	5.68	101.31	110.59	17	2
4	A	401	PX4	O7-C23-C24	5.67	123.32	111.55	1	1
4	A	342	PX4	C8-C7-C6	5.67	99.07	111.86	15	1
4	A	407	PX4	O7-C23-O8	5.67	109.54	123.68	14	1
4	A	309	PX4	C8-C7-C6	5.67	99.08	111.86	13	1
4	A	411	PX4	O5-C8-C7	5.66	122.88	108.66	3	1
4	A	353	PX4	O5-C8-C7	5.65	122.85	108.66	16	2
4	A	328	PX4	C8-C7-C6	5.65	99.12	111.86	3	1
4	A	346	PX4	C7-O7-C23	5.65	131.22	117.88	15	1
4	A	416	PX4	O7-C23-C24	5.64	123.27	111.55	6	2
4	A	404	PX4	C7-O7-C23	5.63	131.19	117.88	13	1
4	A	379	PX4	O5-C8-C7	5.63	122.81	108.66	6	1
4	A	330	PX4	O5-C8-C7	5.63	122.79	108.66	18	4
4	A	399	PX4	C8-C7-C6	5.62	99.17	111.86	1	1
4	A	307	PX4	O5-C8-C7	5.62	122.78	108.66	4	1
4	A	336	PX4	O7-C23-O8	5.62	109.65	123.68	6	1
4	A	327	PX4	C8-C7-C6	5.62	99.18	111.86	15	1
4	A	372	PX4	O7-C23-C24	5.62	123.21	111.55	4	2
4	A	329	PX4	O7-C23-C24	5.61	123.20	111.55	19	1
4	A	386	PX4	C8-C7-C6	5.61	99.21	111.86	8	1
4	A	312	PX4	O7-C23-C24	5.60	123.18	111.55	10	2
4	A	351	PX4	O7-C23-C24	5.60	123.17	111.55	11	1
4	A	334	PX4	C8-C7-C6	5.59	99.25	111.86	18	1
4	A	327	PX4	O5-C8-C7	5.58	122.69	108.66	11	1
4	A	379	PX4	C8-C7-C6	5.58	99.27	111.86	12	1
4	A	306	PX4	O7-C23-C24	5.58	123.13	111.55	14	1
4	A	403	PX4	C7-O7-C23	5.57	131.04	117.88	4	1
4	A	352	PX4	C8-C7-C6	5.57	99.30	111.86	4	1
4	A	366	PX4	O7-C23-C24	5.57	123.11	111.55	7	1
4	A	396	PX4	C8-C7-C6	5.57	99.30	111.86	10	2
4	A	418	PX4	C1-C2-N1	5.57	134.74	115.86	15	1
4	A	389	PX4	O5-C8-C7	5.56	122.62	108.66	19	2
4	A	314	PX4	C8-C7-C6	5.55	99.33	111.86	1	2
5	A	431	C3S	C1-C22-C20	5.55	116.65	108.68	9	1
4	A	316	PX4	O7-C23-C24	5.54	123.05	111.55	12	1
4	A	420	PX4	C8-C7-C6	5.54	99.37	111.86	14	2
5	A	433	C3S	C9-C12-C22	5.54	124.02	116.41	1	1
4	A	352	PX4	O5-C8-C7	5.52	122.54	108.66	18	1
4	A	412	PX4	O5-C8-C7	5.52	122.53	108.66	17	1
4	A	425	PX4	C8-C7-C6	5.52	99.41	111.86	3	2
4	A	374	PX4	C4-N1-C3	5.51	95.01	108.98	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	364	PX4	O7-C23-C24	5.51	123.00	111.55	14	1
4	A	359	PX4	C8-C7-C6	5.51	99.44	111.86	15	3
4	A	357	PX4	C7-O7-C23	5.50	130.88	117.88	10	1
5	A	433	C3S	C40-C29-C30	5.50	122.14	111.73	6	1
4	A	407	PX4	O5-C8-C7	5.50	122.47	108.66	18	1
4	A	344	PX4	C8-C7-C6	5.49	99.47	111.86	15	1
4	A	313	PX4	O7-C23-O8	5.49	109.98	123.68	4	1
4	A	306	PX4	C7-O7-C23	5.48	130.83	117.88	12	1
4	A	417	PX4	O7-C7-C8	5.48	128.35	108.44	1	1
4	A	409	PX4	C8-C7-C6	5.48	99.50	111.86	4	2
4	A	356	PX4	O5-C8-C7	5.47	122.40	108.66	20	1
4	A	428	PX4	C5-N1-C3	5.46	95.14	108.98	8	1
4	A	383	PX4	C8-C7-C6	5.46	99.54	111.86	18	1
4	A	387	PX4	C7-O7-C23	5.46	130.76	117.88	12	1
4	A	356	PX4	C8-C7-C6	5.45	99.56	111.86	13	2
4	A	348	PX4	O7-C23-C24	5.45	122.86	111.55	2	1
4	A	341	PX4	O7-C23-C24	5.44	122.85	111.55	10	2
4	A	413	PX4	C5-N1-C3	5.44	95.19	108.98	9	1
5	A	434	C3S	C50-C48-C54	5.44	101.77	110.35	8	3
4	A	369	PX4	O7-C23-C24	5.44	122.85	111.55	6	1
4	A	335	PX4	C8-C7-C6	5.44	99.59	111.86	8	2
4	A	422	PX4	C8-C7-C6	5.44	99.59	111.86	11	2
4	A	349	PX4	O5-C8-C7	5.44	122.32	108.66	11	1
4	A	358	PX4	C8-C7-C6	5.43	99.60	111.86	12	1
4	A	309	PX4	C5-N1-C4	5.43	95.24	108.98	12	1
5	A	432	C3S	C15-C13-C12	5.42	114.53	125.06	3	1
4	A	308	PX4	C7-O7-C23	5.41	130.66	117.88	20	1
4	A	380	PX4	C5-N1-C4	5.40	95.30	108.98	20	1
4	A	375	PX4	O5-C8-C7	5.40	122.22	108.66	4	1
4	A	419	PX4	O7-C23-C24	5.39	122.75	111.55	14	1
4	A	357	PX4	O5-C8-C7	5.39	122.19	108.66	2	3
5	A	433	C3S	C20-C22-C12	5.38	118.08	109.65	20	1
4	A	327	PX4	C7-O7-C23	5.38	105.16	117.88	5	1
4	A	373	PX4	O5-C8-C7	5.38	122.17	108.66	19	1
4	A	382	PX4	C5-N1-C4	5.37	95.37	108.98	20	1
4	A	329	PX4	C8-C7-C6	5.37	99.74	111.86	12	1
4	A	369	PX4	O5-C8-C7	5.37	122.15	108.66	18	1
4	A	326	PX4	C7-O7-C23	5.37	130.56	117.88	2	1
4	A	319	PX4	O5-C8-C7	5.37	122.14	108.66	8	3
5	A	435	C3S	C9-C12-C13	5.37	112.40	120.59	17	1
4	A	311	PX4	O7-C23-C24	5.36	122.69	111.55	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	432	C3S	C20-C22-C12	5.36	118.05	109.65	8	1
4	A	377	PX4	C8-C7-C6	5.36	99.76	111.86	7	1
4	A	337	PX4	O5-C8-C7	5.36	122.12	108.66	3	1
5	A	432	C3S	C22-C12-C13	5.36	114.27	122.92	17	1
4	A	321	PX4	C7-O7-C23	5.34	130.50	117.88	1	1
4	A	351	PX4	C8-C7-C6	5.33	99.83	111.86	13	2
4	A	370	PX4	C8-C7-C6	5.33	99.84	111.86	16	2
4	A	420	PX4	O7-C23-C24	5.32	122.60	111.55	19	1
4	A	316	PX4	O7-C23-O8	5.32	110.40	123.68	12	1
4	A	375	PX4	O7-C23-C24	5.32	122.59	111.55	18	1
4	A	331	PX4	O7-C23-C24	5.31	122.58	111.55	13	1
4	A	335	PX4	C5-N1-C3	5.31	95.53	108.98	1	1
4	A	349	PX4	O5-C9-O6	5.30	110.39	123.55	15	1
4	A	395	PX4	O3-P1-O2	5.30	87.86	109.25	2	1
4	A	320	PX4	C8-C7-C6	5.30	99.91	111.86	7	1
4	A	404	PX4	O5-C8-C7	5.29	121.96	108.66	9	1
5	A	432	C3S	C23-C20-C22	5.29	120.40	113.10	13	1
4	A	402	PX4	C1-C2-N1	5.29	133.79	115.86	4	1
4	A	361	PX4	O7-C23-C24	5.29	122.53	111.55	8	1
4	A	339	PX4	O7-C23-C24	5.28	122.52	111.55	10	2
4	A	350	PX4	C8-C7-C6	5.28	99.94	111.86	8	1
4	A	402	PX4	O5-C8-C7	5.28	121.92	108.66	9	2
4	A	378	PX4	O3-P1-O2	5.28	87.96	109.25	7	1
5	A	432	C3S	C26-C29-C38	5.28	108.72	116.58	13	1
4	A	404	PX4	C8-C7-C6	5.28	99.96	111.86	8	1
4	A	306	PX4	O7-C7-C6	5.28	127.61	108.44	18	1
4	A	367	PX4	O5-C8-C7	5.27	121.91	108.66	13	3
4	A	358	PX4	O5-C8-C7	5.27	121.91	108.66	4	2
5	A	435	C3S	C40-C29-C30	5.27	121.71	111.73	20	2
4	A	340	PX4	C8-C7-C6	5.27	99.97	111.86	9	1
4	A	305	PX4	C5-N1-C4	5.26	95.66	108.98	2	1
4	A	397	PX4	C7-O7-C23	5.25	130.29	117.88	10	1
5	A	435	C3S	C26-C29-C30	5.25	99.04	107.27	8	1
4	A	412	PX4	O7-C23-C24	5.25	122.45	111.55	1	1
4	A	384	PX4	C8-C7-C6	5.25	100.02	111.86	3	1
4	A	380	PX4	C8-C7-C6	5.25	100.02	111.86	11	1
4	A	417	PX4	O7-C23-C24	5.24	122.44	111.55	16	3
4	A	421	PX4	O5-C9-O6	5.24	110.54	123.55	1	1
4	A	427	PX4	C8-C7-C6	5.23	100.07	111.86	10	1
5	A	434	C3S	C4-C1-C22	5.22	123.76	112.81	7	1
5	A	435	C3S	O6-C7-C4	5.22	99.68	107.54	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	332	PX4	O7-C7-C8	5.22	127.43	108.44	20	1
4	A	326	PX4	O5-C8-C7	5.22	121.77	108.66	4	2
4	A	355	PX4	O5-C9-C10	5.21	127.06	111.90	19	1
4	A	310	PX4	C8-C7-C6	5.21	100.11	111.86	7	1
4	A	366	PX4	C8-C7-C6	5.21	100.11	111.86	7	1
4	A	315	PX4	O5-C8-C7	5.19	121.71	108.66	7	1
4	A	362	PX4	C8-C7-C6	5.19	100.15	111.86	14	1
4	A	359	PX4	O5-C8-C7	5.19	121.69	108.66	17	1
4	A	381	PX4	O5-C8-C7	5.19	121.69	108.66	14	1
4	A	339	PX4	O5-C8-C7	5.19	121.69	108.66	9	2
4	A	387	PX4	C8-C7-C6	5.18	100.16	111.86	15	1
4	A	341	PX4	O5-C8-C7	5.18	121.68	108.66	1	2
4	A	397	PX4	C8-C7-C6	5.18	100.18	111.86	20	1
4	A	428	PX4	C7-O7-C23	5.18	130.11	117.88	7	1
4	A	373	PX4	C8-C7-C6	5.17	100.19	111.86	14	1
4	A	402	PX4	C7-O7-C23	5.17	130.09	117.88	13	1
4	A	345	PX4	O5-C8-C7	5.17	121.64	108.66	10	2
4	A	423	PX4	C8-C7-C6	5.17	100.20	111.86	9	1
4	A	305	PX4	O5-C8-C7	5.16	121.62	108.66	1	1
4	A	385	PX4	P1-O3-C1	5.15	94.64	121.60	16	1
4	A	357	PX4	O7-C23-C24	5.15	122.25	111.55	17	2
4	A	343	PX4	C8-C7-C6	5.15	100.25	111.86	16	1
4	A	430	PX4	O5-C8-C7	5.15	121.59	108.66	7	1
4	A	355	PX4	C7-O7-C23	5.15	130.04	117.88	17	1
4	A	398	PX4	C8-C7-C6	5.14	100.26	111.86	2	1
4	A	381	PX4	C8-C7-C6	5.14	100.26	111.86	9	1
4	A	318	PX4	C8-C7-C6	5.14	100.27	111.86	17	2
4	A	341	PX4	C8-C7-C6	5.14	100.27	111.86	14	1
4	A	325	PX4	C8-C7-C6	5.14	100.27	111.86	10	2
4	A	379	PX4	O7-C7-C8	5.13	127.10	108.44	10	1
4	A	319	PX4	O7-C23-C24	5.12	122.19	111.55	4	1
4	A	386	PX4	P1-O3-C1	5.12	94.84	121.60	20	1
4	A	311	PX4	O7-C7-C6	5.11	127.02	108.44	12	1
4	A	346	PX4	O5-C9-C10	5.11	126.76	111.90	19	1
4	A	401	PX4	C5-N1-C4	5.10	96.06	108.98	18	1
4	A	319	PX4	C8-C7-C6	5.10	100.36	111.86	13	1
4	A	383	PX4	O7-C23-C24	5.09	122.13	111.55	10	1
4	A	368	PX4	O7-C23-C24	5.09	122.12	111.55	4	2
4	A	416	PX4	C8-C7-C6	5.09	100.38	111.86	11	1
5	A	433	C3S	C50-C48-C38	5.09	104.98	112.95	12	1
4	A	364	PX4	O5-C8-C7	5.09	121.44	108.66	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	334	PX4	C4-N1-C3	5.09	96.10	108.98	15	1
4	A	430	PX4	O7-C23-C24	5.08	122.11	111.55	18	1
4	A	379	PX4	C7-O7-C23	5.08	129.89	117.88	7	1
4	A	310	PX4	O7-C23-C24	5.08	122.10	111.55	7	1
4	A	308	PX4	O7-C23-C24	5.08	122.09	111.55	14	1
5	A	432	C3S	C1-C4-C7	5.07	119.22	110.30	20	1
4	A	331	PX4	O5-C8-C7	5.07	121.39	108.66	8	1
4	A	419	PX4	O3-P1-O2	5.07	88.81	109.25	1	1
4	A	386	PX4	O7-C23-C24	5.06	122.07	111.55	2	1
5	A	432	C3S	C29-C30-C18	5.06	122.10	114.39	19	1
4	A	322	PX4	O5-C8-C7	5.06	121.38	108.66	18	1
5	A	435	C3S	C35-C38-C48	5.06	120.23	112.14	20	1
4	A	309	PX4	O7-C23-O8	5.05	111.07	123.68	12	1
4	A	416	PX4	O7-C23-O8	5.05	111.08	123.68	11	1
5	A	434	C3S	O6-C7-C9	5.05	116.38	107.28	10	1
4	A	410	PX4	C8-C7-C6	5.04	100.48	111.86	4	1
4	A	364	PX4	O5-C9-O6	5.04	111.03	123.55	19	1
4	A	384	PX4	O5-C8-C7	5.04	121.32	108.66	2	1
5	A	431	C3S	C20-C18-C30	5.04	115.91	109.09	16	1
4	A	401	PX4	P1-O3-C1	5.03	95.27	121.60	16	1
4	A	428	PX4	C8-O5-C9	5.03	102.00	117.13	3	1
4	A	316	PX4	C7-O7-C23	5.02	129.75	117.88	17	1
4	A	407	PX4	O7-C23-C24	5.02	121.98	111.55	2	1
5	A	436	C3S	C23-C26-C29	5.02	121.54	112.80	7	1
4	A	409	PX4	C5-N1-C3	5.02	96.27	108.98	20	1
4	A	418	PX4	C8-C7-C6	5.02	100.54	111.86	18	1
4	A	360	PX4	O7-C23-C24	5.01	121.96	111.55	20	1
4	A	372	PX4	O5-C9-O6	5.01	111.10	123.55	11	1
4	A	342	PX4	O5-C9-O6	5.01	111.10	123.55	9	1
4	A	333	PX4	O7-C23-C24	5.01	121.95	111.55	12	1
4	A	419	PX4	O1-P1-O3	5.01	84.50	108.14	18	1
4	A	408	PX4	O7-C23-C24	5.00	121.94	111.55	17	1
5	A	433	C3S	C44-C22-C20	5.00	117.86	111.68	5	1
4	A	403	PX4	O5-C8-C7	5.00	121.22	108.66	9	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
5	A	431	C3S	C7	20
5	A	431	C3S	C48	20
5	A	433	C3S	C48	20

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Mol	Chain	Res	Type	Atoms	Models (Total)
5	A	435	C3S	C7	20
5	A	435	C3S	C48	20
5	A	436	C3S	C7	20
5	A	436	C3S	C48	20
5	A	432	C3S	C48	20
5	A	434	C3S	C48	20

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

Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	377	PX4	C7-O7-C23-O8	14
4	A	377	PX4	C7-O7-C23-C24	14
4	A	376	PX4	C7-O7-C23-O8	5
4	A	376	PX4	C7-O7-C23-C24	5
4	A	356	PX4	C7-O7-C23-O8	3
4	A	356	PX4	C7-O7-C23-C24	3
4	A	372	PX4	C7-O7-C23-C24	3
4	A	372	PX4	C7-O7-C23-O8	2
4	A	424	PX4	C7-O7-C23-O8	1
4	A	424	PX4	C7-O7-C23-C24	1

There are no ring outliers.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 21% for the well-defined parts and 20% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2mzi\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	797
Number of shifts mapped to atoms	797
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	188	$0.12 \pm 0.20$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 21%, i.e. 605 atoms were assigned a chemical shift out of a possible 2874. 10 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	417/1161 (36%)	233/462 (50%)	0/474 (0%)	184/225 (82%)
Sidechain	175/1419 (12%)	126/838 (15%)	45/517 (9%)	4/64 (6%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	13/294 (4%)	9/156 (6%)	0/125 (0%)	4/13 (31%)
Overall	605/2874 (21%)	368/1456 (25%)	45/1116 (4%)	192/302 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 20%, i.e. 615 atoms were assigned a chemical shift out of a possible 3030. 10 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	425/1212 (35%)	237/482 (49%)	0/496 (0%)	188/234 (80%)
Sidechain	177/1515 (12%)	127/897 (14%)	46/548 (8%)	4/70 (6%)
Aromatic	13/303 (4%)	9/161 (6%)	0/129 (0%)	4/13 (31%)
Overall	615/3030 (20%)	373/1540 (24%)	46/1173 (4%)	196/317 (62%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

