



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 07:07 AM BST

PDB ID : 2MLS
Title : Membrane Bilayer complex with Matrix Metalloproteinase-12 at its Beta-face
Authors : Koppiseti, R.K.; Fulcher, Y.G.; Prior, S.H.; Lenoir, M.; Overduin, M.; Van Doren, S.R.
Deposited on : 2014-03-04

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

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

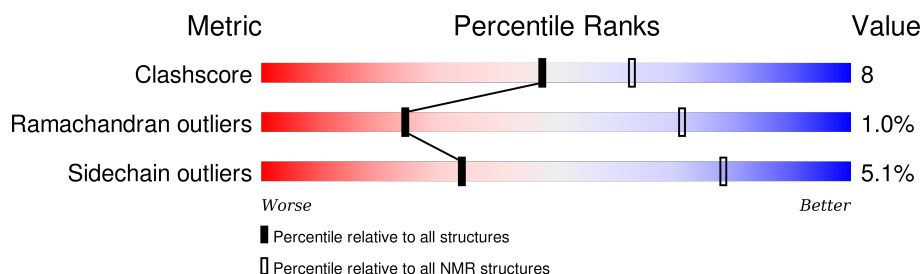
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 83%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	164	

2 Ensemble composition and analysis

This entry contains 14 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:101-A:262 (162)	0.40	8

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 and 5 single-model clusters were found.

Cluster number	Models
1	5, 8, 10, 13
2	11, 12, 14
3	1, 2
Single-model clusters	3; 4; 6; 7; 9

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8263 atoms, of which 1221 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
1	A	164	Total	C	H	N	O	S	0
			2508	824	1221	225	234	4	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	ALA	GLU	ENGINEERED MUTATION	UNP P39900

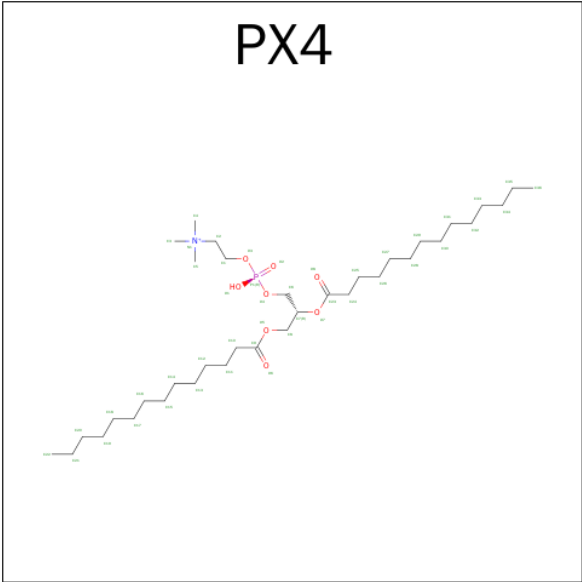
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
3	A	3	Total	Ca
			3	3

- Molecule 4 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C₃₆H₇₃NO₈P).



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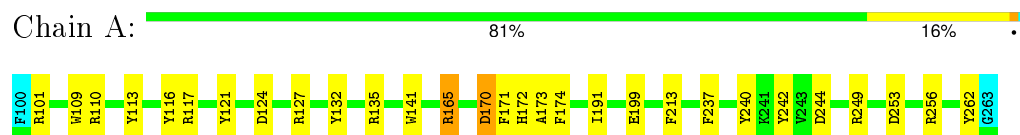
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Macrophage metalloelastase

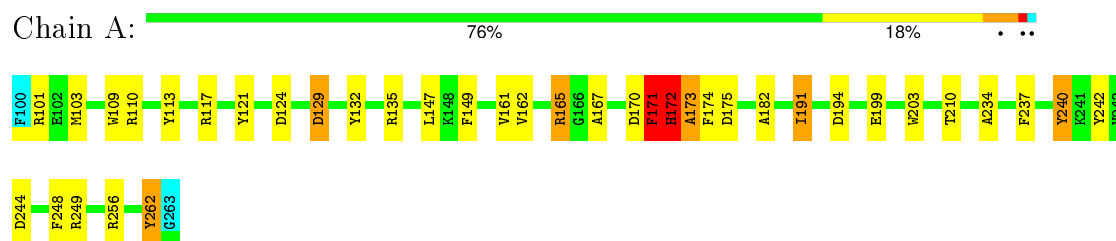


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

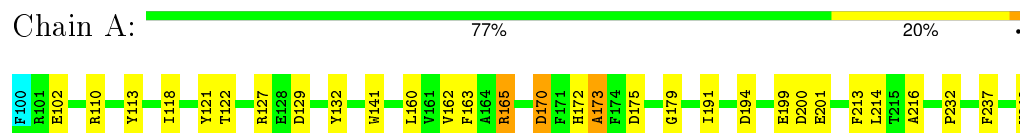
4.2.1 Score per residue for model 1

- Molecule 1: Macrophage metalloelastase



4.2.2 Score per residue for model 2

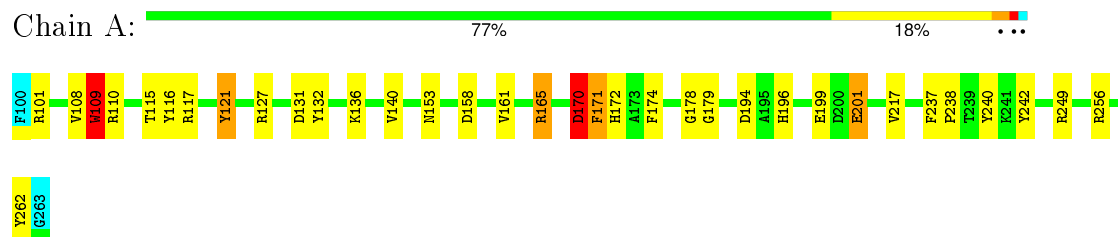
- Molecule 1: Macrophage metalloelastase





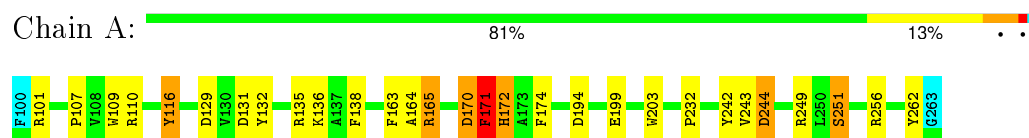
4.2.3 Score per residue for model 3

- Molecule 1: Macrophage metalloelastase



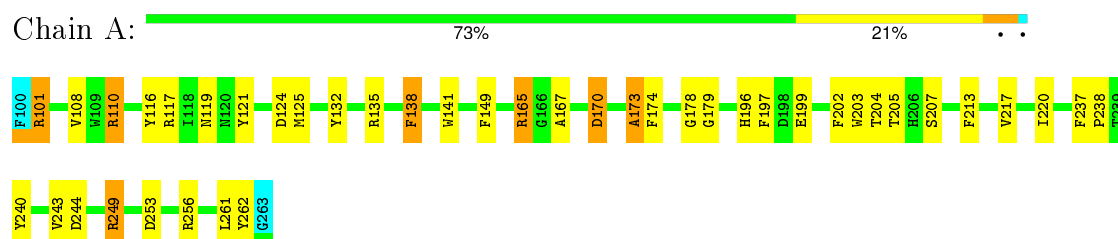
4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase



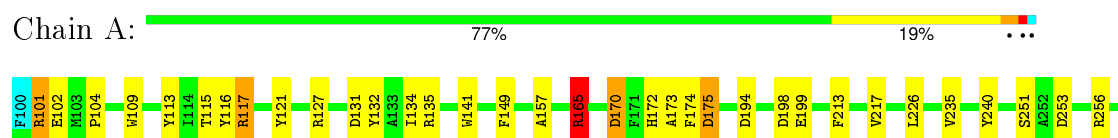
4.2.5 Score per residue for model 5

- Molecule 1: Macrophage metalloelastase



4.2.6 Score per residue for model 6

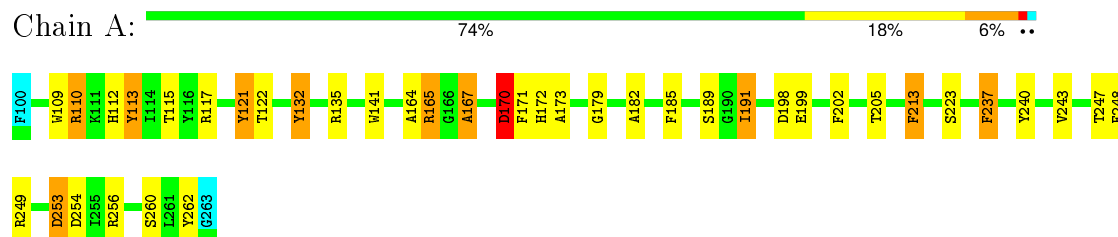
- Molecule 1: Macrophage metalloelastase





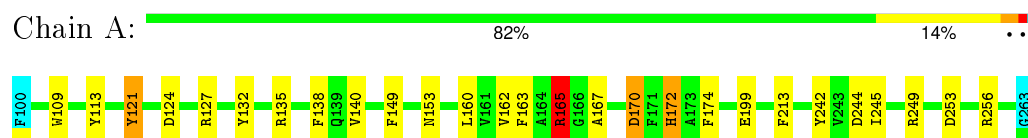
4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



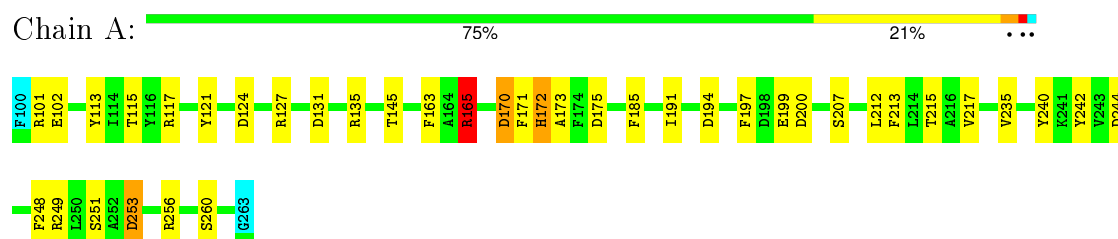
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Macrophage metalloelastase



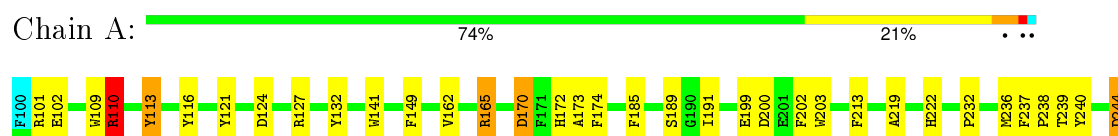
4.2.9 Score per residue for model 9

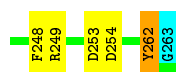
- Molecule 1: Macrophage metalloelastase



4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase

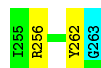
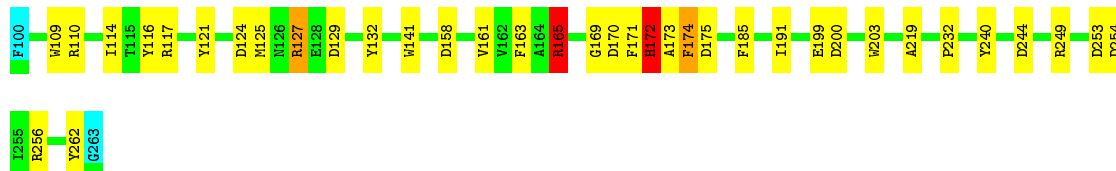




4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase

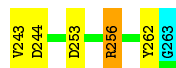
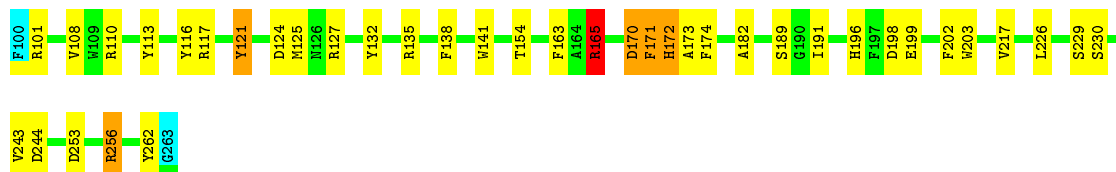
Chain A: 76% 20% ...



4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase

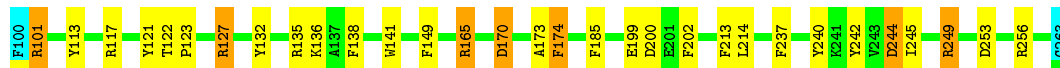
Chain A: 75% 20% ...



4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase

Chain A: 80% 15% ..



4.2.14 Score per residue for model 14

- Molecule 1: Macrophage metalloelastase

Chain A: 79% 16% ..



5 Refinement protocol and experimental data overview

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

Of the 14 calculated structures, 14 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
GROMACS	refinement	

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)	2mls_cs.str
Number of chemical shift lists	1
Total number of shifts	1762
Number of shifts mapped to atoms	1762
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, 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	0.57±0.00	0±0/1311 (0.0±0.0%)	2.03±0.06	38±6/1779 (2.2±0.4%)
All	All	0.57	0/18354 (0.0%)	2.03	537/24906 (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	4.9±2.3
All	All	0	68

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	110	ARG	NE-CZ-NH1	19.82	130.21	120.30	10	5
1	A	170	ASP	CB-CG-OD1	16.29	132.96	118.30	7	14
1	A	256	ARG	NE-CZ-NH1	16.04	128.32	120.30	5	9
1	A	101	ARG	NE-CZ-NH1	-15.89	112.36	120.30	6	7
1	A	197	PHE	CB-CG-CD1	15.56	131.69	120.80	5	3
1	A	197	PHE	CB-CG-CD2	-15.03	110.28	120.80	5	1
1	A	113	TYR	CB-CG-CD1	-13.32	113.01	121.00	12	3
1	A	262	TYR	CB-CG-CD1	-13.06	113.16	121.00	1	5
1	A	127	ARG	NE-CZ-NH1	13.03	126.81	120.30	13	6
1	A	165	ARG	NE-CZ-NH2	-12.96	113.82	120.30	11	6
1	A	121	TYR	CB-CG-CD1	-12.83	113.30	121.00	12	6
1	A	121	TYR	CB-CG-CD2	-12.73	113.36	121.00	2	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	249	ARG	NE-CZ-NH2	-12.54	114.03	120.30	11	6
1	A	262	TYR	CB-CG-CD2	-12.52	113.49	121.00	14	5
1	A	101	ARG	NE-CZ-NH2	-12.21	114.20	120.30	12	7
1	A	165	ARG	NE-CZ-NH1	12.20	126.40	120.30	8	10
1	A	127	ARG	NE-CZ-NH2	-12.02	114.29	120.30	12	8
1	A	198	ASP	CB-CG-OD1	11.77	128.90	118.30	7	1
1	A	194	ASP	CB-CG-OD2	11.54	128.69	118.30	3	5
1	A	171	PHE	CB-CG-CD1	-11.41	112.81	120.80	7	2
1	A	124	ASP	CB-CG-OD1	11.08	128.27	118.30	1	5
1	A	256	ARG	NE-CZ-NH2	-10.71	114.94	120.30	6	6
1	A	171	PHE	CB-CG-CD2	-10.53	113.43	120.80	4	4
1	A	135	ARG	NE-CZ-NH1	10.40	125.50	120.30	12	4
1	A	149	PHE	CB-CG-CD1	10.19	127.94	120.80	13	4
1	A	170	ASP	CB-CG-OD2	10.17	127.45	118.30	1	2
1	A	110	ARG	NE-CZ-NH2	-10.04	115.28	120.30	4	9
1	A	129	ASP	CB-CG-OD1	9.94	127.24	118.30	4	2
1	A	249	ARG	NE-CZ-NH1	9.44	125.02	120.30	8	8
1	A	248	PHE	CB-CG-CD2	-9.41	114.22	120.80	10	1
1	A	175	ASP	CB-CG-OD2	9.36	126.72	118.30	2	4
1	A	117	ARG	NE-CZ-NH1	9.30	124.95	120.30	7	6
1	A	240	TYR	CB-CG-CD1	-9.16	115.50	121.00	6	5
1	A	185	PHE	CB-CG-CD1	9.11	127.18	120.80	7	3
1	A	132	TYR	CB-CG-CD2	9.07	126.44	121.00	1	6
1	A	165	ARG	NH1-CZ-NH2	-9.03	109.46	119.40	8	2
1	A	135	ARG	NE-CZ-NH2	-9.00	115.80	120.30	9	4
1	A	194	ASP	CB-CG-OD1	8.99	126.39	118.30	2	3
1	A	213	PHE	CB-CG-CD1	-8.99	114.51	120.80	2	4
1	A	244	ASP	CB-CG-OD1	-8.78	110.40	118.30	14	6
1	A	244	ASP	CB-CG-OD2	8.69	126.12	118.30	4	4
1	A	170	ASP	OD1-CG-OD2	-8.68	106.81	123.30	6	13
1	A	132	TYR	CB-CG-CD1	-8.66	115.80	121.00	1	7
1	A	163	PHE	CB-CG-CD1	-8.56	114.81	120.80	8	1
1	A	237	PHE	CB-CG-CD1	-8.52	114.84	120.80	5	6
1	A	254	ASP	CB-CG-OD1	8.40	125.86	118.30	7	3
1	A	149	PHE	CB-CG-CD2	-8.40	114.92	120.80	13	2
1	A	141	TRP	CD1-NE1-CE2	8.27	116.45	109.00	7	5
1	A	113	TYR	CB-CG-CD2	-8.13	116.12	121.00	2	3
1	A	253	ASP	CB-CG-OD2	8.13	125.62	118.30	5	7
1	A	164	ALA	CB-CA-C	8.11	122.26	110.10	7	3
1	A	189	SER	N-CA-CB	-8.04	98.45	110.50	12	3
1	A	108	VAL	CA-CB-CG2	8.01	122.91	110.90	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	161	VAL	CA-CB-CG1	7.86	122.69	110.90	3	2
1	A	117	ARG	NE-CZ-NH2	7.82	124.21	120.30	11	4
1	A	262	TYR	CG-CD1-CE1	-7.73	115.11	121.30	14	3
1	A	202	PHE	CB-CG-CD2	-7.63	115.46	120.80	12	2
1	A	173	ALA	N-CA-CB	7.62	120.77	110.10	5	2
1	A	131	ASP	CB-CG-OD1	7.58	125.12	118.30	9	4
1	A	116	TYR	CB-CG-CD2	-7.58	116.45	121.00	5	2
1	A	200	ASP	CB-CG-OD1	7.54	125.09	118.30	10	2
1	A	157	ALA	N-CA-CB	-7.53	99.56	110.10	6	1
1	A	248	PHE	CB-CG-CD1	-7.51	115.54	120.80	2	2
1	A	163	PHE	CB-CG-CD2	7.51	126.06	120.80	2	5
1	A	222	HIS	CA-CB-CG	7.49	126.33	113.60	10	1
1	A	124	ASP	CB-CG-OD2	7.48	125.03	118.30	14	2
1	A	115	THR	CA-CB-CG2	7.47	122.86	112.40	3	2
1	A	141	TRP	CH2-CZ2-CE2	7.44	124.84	117.40	2	3
1	A	185	PHE	CB-CG-CD2	-7.43	115.60	120.80	9	3
1	A	240	TYR	CB-CG-CD2	-7.39	116.56	121.00	10	4
1	A	122	THR	CA-CB-CG2	7.36	122.70	112.40	13	3
1	A	242	TYR	CZ-CE2-CD2	-7.31	113.22	119.80	1	1
1	A	127	ARG	CD-NE-CZ	7.27	133.77	123.60	3	3
1	A	135	ARG	CD-NE-CZ	7.23	133.72	123.60	6	2
1	A	109	TRP	CA-CB-CG	7.20	127.37	113.70	3	2
1	A	219	ALA	N-CA-CB	7.19	120.17	110.10	11	1
1	A	182	ALA	N-CA-CB	7.17	120.14	110.10	12	2
1	A	140	VAL	CA-CB-CG1	7.14	121.61	110.90	3	1
1	A	220	ILE	CA-CB-CG2	7.09	125.09	110.90	5	1
1	A	253	ASP	CB-CG-OD1	-7.08	111.93	118.30	8	1
1	A	175	ASP	CB-CG-OD1	7.06	124.65	118.30	6	2
1	A	113	TYR	CG-CD1-CE1	-7.05	115.66	121.30	12	1
1	A	158	ASP	CB-CG-OD2	-6.99	112.01	118.30	3	1
1	A	116	TYR	CB-CG-CD1	-6.99	116.81	121.00	10	2
1	A	173	ALA	CB-CA-C	6.92	120.48	110.10	1	1
1	A	110	ARG	NH1-CZ-NH2	6.89	126.98	119.40	1	2
1	A	198	ASP	CB-CG-OD2	-6.84	112.15	118.30	12	3
1	A	124	ASP	OD1-CG-OD2	-6.83	110.32	123.30	14	1
1	A	138	PHE	CB-CG-CD1	6.79	125.56	120.80	12	3
1	A	262	TYR	CD1-CE1-CZ	6.76	125.88	119.80	2	1
1	A	121	TYR	CG-CD1-CE1	-6.74	115.91	121.30	11	2
1	A	141	TRP	CD1-CG-CD2	-6.74	100.91	106.30	2	1
1	A	254	ASP	CB-CG-OD2	-6.73	112.24	118.30	11	1
1	A	194	ASP	OD1-CG-OD2	-6.71	110.56	123.30	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	109	TRP	CE2-CD2-CG	6.69	112.66	107.30	4	1
1	A	167	ALA	CB-CA-C	6.69	120.14	110.10	7	1
1	A	232	PRO	N-CD-CG	6.68	113.23	103.20	2	1
1	A	109	TRP	NE1-CE2-CD2	-6.67	100.63	107.30	4	1
1	A	101	ARG	NH1-CZ-NH2	-6.67	112.06	119.40	4	1
1	A	256	ARG	CD-NE-CZ	6.61	132.86	123.60	14	3
1	A	174	PHE	CB-CG-CD2	-6.61	116.17	120.80	11	3
1	A	127	ARG	NH1-CZ-NH2	-6.60	112.14	119.40	13	1
1	A	242	TYR	CB-CG-CD2	-6.58	117.05	121.00	9	4
1	A	113	TYR	CG-CD2-CE2	-6.57	116.04	121.30	8	1
1	A	138	PHE	CB-CG-CD2	-6.57	116.20	120.80	12	1
1	A	101	ARG	CD-NE-CZ	6.56	132.78	123.60	14	2
1	A	232	PRO	N-CA-CB	6.49	111.08	103.30	10	4
1	A	162	VAL	CA-CB-CG2	6.47	120.61	110.90	10	1
1	A	125	MET	CA-CB-CG	6.43	124.22	113.30	11	2
1	A	178	GLY	C-N-CA	6.38	135.69	122.30	5	2
1	A	238	PRO	N-CA-CB	6.37	110.94	103.30	5	2
1	A	165	ARG	CD-NE-CZ	6.37	132.51	123.60	9	2
1	A	172	HIS	CA-CB-CG	6.34	124.37	113.60	11	3
1	A	215	THR	CA-CB-CG2	6.33	121.27	112.40	9	1
1	A	109	TRP	CD1-NE1-CE2	6.31	114.68	109.00	8	3
1	A	235	VAL	O-C-N	-6.30	112.62	122.70	6	1
1	A	104	PRO	N-CD-CG	6.30	112.65	103.20	14	2
1	A	247	THR	CA-CB-CG2	6.29	121.21	112.40	7	2
1	A	167	ALA	N-CA-CB	6.29	118.90	110.10	1	2
1	A	141	TRP	NE1-CE2-CZ2	6.29	137.31	130.40	12	1
1	A	213	PHE	CB-CG-CD2	-6.26	116.41	120.80	13	5
1	A	214	LEU	CB-CG-CD2	6.22	121.57	111.00	2	1
1	A	132	TYR	CA-CB-CG	6.15	125.09	113.40	4	2
1	A	248	PHE	C-N-CA	6.13	137.02	121.70	9	2
1	A	196	HIS	CA-CB-CG	6.07	123.92	113.60	5	2
1	A	243	VAL	CA-CB-CG2	6.05	119.98	110.90	4	2
1	A	116	TYR	CG-CD1-CE1	-6.05	116.46	121.30	6	1
1	A	200	ASP	CB-CG-OD2	6.04	123.74	118.30	14	3
1	A	109	TRP	NE1-CE2-CZ2	6.04	137.04	130.40	11	2
1	A	170	ASP	N-CA-CB	6.03	121.45	110.60	3	1
1	A	240	TYR	CZ-CE2-CD2	6.01	125.21	119.80	9	2
1	A	249	ARG	CD-NE-CZ	6.01	132.02	123.60	13	1
1	A	113	TYR	C-N-CA	5.98	136.65	121.70	10	2
1	A	175	ASP	OD1-CG-OD2	-5.97	111.96	123.30	6	1
1	A	153	ASN	O-C-N	-5.94	113.20	122.70	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	162	VAL	CB-CA-C	5.94	122.68	111.40	1	1
1	A	243	VAL	CG1-CB-CG2	-5.91	101.44	110.90	5	2
1	A	191	ILE	CA-CB-CG2	5.91	122.72	110.90	9	1
1	A	110	ARG	CD-NE-CZ	5.89	131.84	123.60	1	2
1	A	242	TYR	CG-CD1-CE1	-5.89	116.59	121.30	1	1
1	A	217	VAL	CA-CB-CG1	5.88	119.73	110.90	5	4
1	A	141	TRP	CZ3-CH2-CZ2	-5.87	114.56	121.60	2	1
1	A	158	ASP	C-N-CA	5.86	136.36	121.70	11	1
1	A	219	ALA	CB-CA-C	-5.84	101.34	110.10	11	1
1	A	237	PHE	CB-CG-CD2	5.83	124.88	120.80	1	1
1	A	124	ASP	CB-CA-C	-5.80	98.79	110.40	14	2
1	A	234	ALA	N-CA-CB	-5.80	101.98	110.10	1	1
1	A	138	PHE	CG-CD2-CE2	-5.78	114.44	120.80	5	1
1	A	217	VAL	CA-CB-CG2	5.78	119.56	110.90	9	1
1	A	147	LEU	CB-CG-CD2	-5.77	101.20	111.00	1	1
1	A	230	SER	CB-CA-C	5.75	121.03	110.10	12	1
1	A	161	VAL	CA-CB-CG2	5.75	119.53	110.90	11	1
1	A	207	SER	C-N-CA	5.74	134.36	122.30	9	1
1	A	141	TRP	NE1-CE2-CD2	-5.74	101.56	107.30	5	4
1	A	108	VAL	CB-CA-C	5.72	122.27	111.40	3	1
1	A	251	SER	N-CA-CB	-5.70	101.94	110.50	4	3
1	A	102	GLU	OE1-CD-OE2	-5.68	116.49	123.30	9	2
1	A	131	ASP	CB-CG-OD2	5.68	123.41	118.30	4	1
1	A	141	TRP	CG-CD1-NE1	-5.66	104.44	110.10	7	3
1	A	145	THR	CA-CB-CG2	5.64	120.30	112.40	9	1
1	A	240	TYR	CG-CD2-CE2	-5.63	116.80	121.30	9	1
1	A	226	LEU	CB-CG-CD2	5.61	120.53	111.00	12	1
1	A	114	ILE	CA-CB-CG1	5.59	121.62	111.00	11	1
1	A	170	ASP	CB-CA-C	5.56	121.51	110.40	7	2
1	A	260	SER	CA-C-O	-5.54	108.47	120.10	6	1
1	A	175	ASP	CA-CB-CG	5.53	125.57	113.40	14	1
1	A	203	TRP	CD1-NE1-CE2	5.53	113.97	109.00	1	2
1	A	115	THR	CA-CB-OG1	5.52	120.59	109.00	7	1
1	A	165	ARG	N-CA-CB	5.51	120.52	110.60	10	1
1	A	121	TYR	CZ-CE2-CD2	5.51	124.75	119.80	2	1
1	A	202	PHE	CB-CA-C	5.50	121.39	110.40	10	1
1	A	262	TYR	N-CA-CB	5.49	120.48	110.60	4	1
1	A	210	THR	OG1-CB-CG2	-5.49	97.38	110.00	1	1
1	A	226	LEU	C-N-CA	5.48	133.80	122.30	6	1
1	A	116	TYR	CB-CA-C	5.47	121.34	110.40	12	1
1	A	117	ARG	NH1-CZ-NH2	5.44	125.39	119.40	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	163	PHE	O-C-N	-5.44	114.00	122.70	2	1
1	A	171	PHE	N-CA-CB	5.43	120.38	110.60	1	1
1	A	216	ALA	CB-CA-C	-5.43	101.95	110.10	2	1
1	A	170	ASP	C-N-CA	5.43	135.28	121.70	5	2
1	A	203	TRP	CZ3-CH2-CZ2	-5.42	115.09	121.60	12	1
1	A	171	PHE	O-C-N	-5.42	114.03	122.70	12	1
1	A	140	VAL	CA-CB-CG2	5.41	119.02	110.90	14	1
1	A	132	TYR	CZ-CE2-CD2	5.41	124.67	119.80	2	1
1	A	134	ILE	CA-CB-CG1	5.40	121.26	111.00	6	1
1	A	260	SER	N-CA-CB	-5.40	102.41	110.50	9	1
1	A	121	TYR	C-N-CA	5.39	135.18	121.70	7	1
1	A	202	PHE	CG-CD1-CE1	-5.39	114.87	120.80	7	1
1	A	239	THR	N-CA-CB	-5.39	100.06	110.30	10	1
1	A	163	PHE	N-CA-CB	-5.35	100.96	110.60	11	1
1	A	201	GLU	OE1-CD-OE2	-5.35	116.88	123.30	3	1
1	A	141	TRP	CD2-CE3-CZ3	5.34	125.75	118.80	13	1
1	A	125	MET	CB-CA-C	5.34	121.08	110.40	5	1
1	A	129	ASP	CB-CG-OD2	5.32	123.09	118.30	1	1
1	A	101	ARG	CB-CA-C	-5.30	99.80	110.40	9	1
1	A	245	ILE	CB-CA-C	5.28	122.16	111.60	13	1
1	A	102	GLU	O-C-N	-5.26	114.29	122.70	10	1
1	A	118	ILE	CA-CB-CG2	5.24	121.39	110.90	2	1
1	A	259	GLN	N-CA-CB	-5.24	101.17	110.60	14	1
1	A	154	THR	C-N-CA	5.23	133.28	122.30	12	1
1	A	205	THR	CA-CB-CG2	5.22	119.70	112.40	7	1
1	A	240	TYR	CG-CD1-CE1	-5.21	117.13	121.30	7	1
1	A	153	ASN	CB-CA-C	5.19	120.79	110.40	3	1
1	A	238	PRO	N-CD-CG	5.19	110.98	103.20	5	1
1	A	207	SER	N-CA-CB	-5.18	102.72	110.50	5	1
1	A	207	SER	CA-CB-OG	5.16	125.13	111.20	5	1
1	A	262	TYR	CZ-CE2-CD2	-5.15	115.16	119.80	14	1
1	A	203	TRP	CD2-CE3-CZ3	5.13	125.47	118.80	4	1
1	A	203	TRP	CH2-CZ2-CE2	5.12	122.52	117.40	4	2
1	A	204	THR	CA-CB-CG2	5.12	119.57	112.40	5	1
1	A	240	TYR	CD1-CE1-CZ	-5.12	115.19	119.80	5	1
1	A	121	TYR	CG-CD2-CE2	-5.11	117.21	121.30	1	1
1	A	229	SER	N-CA-CB	-5.10	102.85	110.50	12	1
1	A	124	ASP	CA-CB-CG	5.10	124.62	113.40	11	1
1	A	205	THR	C-N-CA	5.09	134.43	121.70	5	1
1	A	112	HIS	N-CA-CB	-5.09	101.44	110.60	7	1
1	A	235	VAL	CA-CB-CG1	5.08	118.53	110.90	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	160	LEU	CB-CG-CD1	5.08	119.64	111.00	2	1
1	A	132	TYR	CG-CD2-CE2	-5.08	117.24	121.30	2	1
1	A	191	ILE	CB-CA-C	5.08	121.76	111.60	7	1
1	A	203	TRP	NE1-CE2-CD2	-5.08	102.22	107.30	5	1
1	A	136	LYS	N-CA-CB	-5.07	101.47	110.60	3	1
1	A	116	TYR	CZ-CE2-CD2	-5.07	115.24	119.80	4	1
1	A	245	ILE	CA-CB-CG1	5.06	120.61	111.00	8	1
1	A	214	LEU	CB-CG-CD1	5.05	119.59	111.00	13	1
1	A	101	ARG	C-N-CA	5.04	134.31	121.70	14	1
1	A	103	MET	N-CA-CB	-5.04	101.52	110.60	1	1
1	A	169	GLY	C-N-CA	5.04	134.29	121.70	11	1
1	A	172	HIS	N-CA-CB	-5.03	101.55	110.60	12	1
1	A	253	ASP	O-C-N	-5.02	114.67	122.70	5	1
1	A	115	THR	N-CA-CB	-5.01	100.78	110.30	9	1
1	A	170	ASP	O-C-N	-5.01	114.69	122.70	9	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	174	PHE	Peptide,Sidechain	11
1	A	121	TYR	Sidechain	6
1	A	262	TYR	Sidechain	5
1	A	171	PHE	Sidechain	4
1	A	132	TYR	Sidechain,Mainchain	4
1	A	242	TYR	Sidechain	3
1	A	113	TYR	Sidechain	3
1	A	135	ARG	Sidechain	2
1	A	110	ARG	Sidechain	2
1	A	172	HIS	Sidechain	2
1	A	117	ARG	Sidechain	2
1	A	256	ARG	Sidechain	2
1	A	101	ARG	Sidechain	2
1	A	127	ARG	Sidechain,Mainchain	2
1	A	249	ARG	Sidechain,Peptide	2
1	A	213	PHE	Sidechain	1
1	A	138	PHE	Sidechain	1
1	A	116	TYR	Sidechain	1
1	A	191	ILE	Peptide	1
1	A	182	ALA	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	196	HIS	Sidechain	1
1	A	149	PHE	Sidechain	1
1	A	251	SER	Mainchain	1
1	A	248	PHE	Sidechain	1
1	A	237	PHE	Sidechain	1
1	A	185	PHE	Sidechain	1
1	A	240	TYR	Sidechain	1
1	A	175	ASP	Sidechain	1
1	A	165	ARG	Sidechain	1
1	A	167	ALA	Peptide	1
1	A	219	ALA	Mainchain	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	1271	1207	1207	2±1
4	A	5750	0	9000	132±12
All	All	98364	16898	142898	1849

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:423:PX4:H16	4:A:424:PX4:H24	1.02	1.23	7	1
4:A:347:PX4:H56	4:A:355:PX4:H25	0.99	1.33	11	1
4:A:321:PX4:H51	4:A:354:PX4:H34	0.93	1.41	10	1
4:A:306:PX4:H23	4:A:360:PX4:H44	0.91	1.42	1	1
4:A:408:PX4:H15	4:A:409:PX4:H2	0.90	1.44	10	2
4:A:361:PX4:H68	4:A:369:PX4:H36	0.84	1.49	12	1
4:A:404:PX4:H34	4:A:412:PX4:H37	0.84	1.49	11	1
4:A:347:PX4:H37	4:A:348:PX4:H64	0.84	1.49	8	1
4:A:313:PX4:H26	4:A:366:PX4:H22	0.84	1.47	13	1
4:A:308:PX4:H30	4:A:308:PX4:H67	0.83	1.50	3	1
4:A:422:PX4:H17	4:A:425:PX4:H56	0.83	1.48	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:PX4:H53	4:A:422:PX4:H28	0.83	1.50	4	1
4:A:350:PX4:H59	4:A:350:PX4:H30	0.83	1.49	14	1
4:A:389:PX4:H15	4:A:398:PX4:H15	0.83	1.49	12	2
4:A:399:PX4:H62	4:A:407:PX4:H36	0.82	1.49	2	1
4:A:314:PX4:H39	4:A:362:PX4:H16	0.82	1.48	4	4
4:A:396:PX4:H57	4:A:398:PX4:H28	0.82	1.49	4	1
4:A:313:PX4:H47	4:A:328:PX4:H16	0.81	1.50	12	4
4:A:312:PX4:H51	4:A:359:PX4:H46	0.81	1.51	2	1
4:A:396:PX4:H19	4:A:397:PX4:H22	0.81	1.50	12	1
4:A:345:PX4:H22	4:A:353:PX4:H17	0.80	1.54	11	1
4:A:315:PX4:H52	4:A:323:PX4:H49	0.80	1.54	7	1
4:A:313:PX4:H27	4:A:359:PX4:H25	0.80	1.53	6	1
4:A:353:PX4:H50	4:A:354:PX4:H61	0.79	1.52	4	1
4:A:388:PX4:H49	4:A:397:PX4:H60	0.79	1.52	7	1
4:A:317:PX4:H55	4:A:342:PX4:H19	0.79	1.55	4	1
4:A:345:PX4:H20	4:A:345:PX4:H54	0.78	1.54	10	1
4:A:368:PX4:H37	4:A:418:PX4:H29	0.78	1.56	2	1
4:A:375:PX4:H49	4:A:429:PX4:H19	0.77	1.54	8	1
4:A:338:PX4:H35	4:A:343:PX4:H58	0.77	1.55	11	1
4:A:338:PX4:H49	4:A:355:PX4:H16	0.77	1.54	10	1
4:A:323:PX4:H60	4:A:368:PX4:H42	0.76	1.57	11	1
4:A:325:PX4:H22	4:A:341:PX4:H56	0.76	1.55	4	1
4:A:405:PX4:H25	4:A:423:PX4:H70	0.76	1.58	12	1
4:A:310:PX4:H50	4:A:311:PX4:H46	0.76	1.57	2	1
4:A:387:PX4:H65	4:A:402:PX4:H25	0.76	1.58	3	1
4:A:406:PX4:H37	4:A:422:PX4:H30	0.76	1.58	3	1
4:A:383:PX4:H35	4:A:390:PX4:H39	0.76	1.58	6	1
4:A:400:PX4:H30	4:A:417:PX4:H28	0.75	1.56	8	1
4:A:307:PX4:H48	4:A:314:PX4:H22	0.75	1.57	2	1
4:A:381:PX4:H51	4:A:397:PX4:H47	0.75	1.57	8	1
4:A:340:PX4:H60	4:A:341:PX4:H24	0.75	1.57	12	1
4:A:321:PX4:H62	4:A:425:PX4:H41	0.75	1.59	14	1
4:A:389:PX4:H37	4:A:397:PX4:H41	0.75	1.59	14	1
4:A:345:PX4:H28	4:A:345:PX4:H61	0.75	1.55	7	1
4:A:378:PX4:H49	4:A:410:PX4:H17	0.75	1.59	12	1
4:A:323:PX4:H42	4:A:333:PX4:H68	0.74	1.58	13	1
4:A:374:PX4:H24	4:A:427:PX4:H19	0.74	1.58	6	1
4:A:310:PX4:H57	4:A:364:PX4:H27	0.74	1.57	1	1
4:A:388:PX4:H24	4:A:396:PX4:H47	0.74	1.58	14	1
4:A:385:PX4:H45	4:A:394:PX4:H65	0.74	1.59	9	1
4:A:307:PX4:H46	4:A:314:PX4:H19	0.74	1.58	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:H16	4:A:345:PX4:H52	0.74	1.59	10	1
4:A:373:PX4:H32	4:A:381:PX4:H47	0.74	1.58	14	1
4:A:412:PX4:H56	4:A:419:PX4:H25	0.73	1.59	14	1
4:A:358:PX4:H52	4:A:358:PX4:H32	0.73	1.58	7	1
4:A:391:PX4:H39	4:A:405:PX4:H69	0.73	1.61	9	1
4:A:406:PX4:H31	4:A:424:PX4:H37	0.73	1.58	4	1
4:A:322:PX4:H49	4:A:361:PX4:H51	0.73	1.61	3	1
4:A:327:PX4:H72	4:A:328:PX4:H33	0.73	1.60	9	1
4:A:422:PX4:H26	4:A:425:PX4:H63	0.73	1.58	2	1
4:A:367:PX4:H50	4:A:412:PX4:H18	0.73	1.60	4	1
4:A:420:PX4:H42	4:A:427:PX4:H38	0.72	1.61	6	1
4:A:367:PX4:H21	4:A:428:PX4:H18	0.72	1.60	1	1
4:A:368:PX4:H51	4:A:424:PX4:H58	0.72	1.58	3	1
4:A:317:PX4:H39	4:A:363:PX4:H62	0.72	1.61	10	1
4:A:334:PX4:H36	4:A:334:PX4:H69	0.72	1.62	4	1
4:A:400:PX4:H39	4:A:401:PX4:H72	0.72	1.61	4	1
4:A:346:PX4:H49	4:A:362:PX4:H50	0.71	1.62	5	3
4:A:415:PX4:H49	4:A:422:PX4:H24	0.71	1.59	4	1
4:A:327:PX4:H65	4:A:327:PX4:H39	0.71	1.62	6	1
4:A:409:PX4:H68	4:A:422:PX4:H68	0.71	1.63	1	1
4:A:318:PX4:H17	4:A:327:PX4:H48	0.71	1.61	2	1
4:A:328:PX4:H17	4:A:360:PX4:H45	0.71	1.61	5	1
4:A:403:PX4:H12	4:A:404:PX4:H16	0.71	1.63	7	1
4:A:397:PX4:H27	4:A:398:PX4:H58	0.71	1.62	2	1
4:A:412:PX4:H35	4:A:419:PX4:H51	0.71	1.63	4	1
4:A:400:PX4:H5	4:A:408:PX4:H49	0.71	1.61	1	1
4:A:335:PX4:H23	4:A:343:PX4:H26	0.71	1.60	5	1
4:A:331:PX4:H49	4:A:331:PX4:H21	0.71	1.61	3	1
4:A:419:PX4:H64	4:A:427:PX4:H58	0.71	1.63	10	1
4:A:328:PX4:H56	4:A:329:PX4:H58	0.70	1.62	2	1
4:A:398:PX4:H24	4:A:407:PX4:H46	0.70	1.63	8	1
4:A:390:PX4:H14	4:A:399:PX4:H20	0.70	1.60	11	1
4:A:369:PX4:H17	4:A:425:PX4:H22	0.70	1.60	6	1
4:A:317:PX4:H48	4:A:324:PX4:H19	0.70	1.63	8	1
4:A:423:PX4:H48	4:A:424:PX4:H24	0.70	1.60	12	1
4:A:380:PX4:H48	4:A:402:PX4:H25	0.70	1.62	11	1
4:A:409:PX4:H16	4:A:416:PX4:H53	0.70	1.63	8	1
4:A:313:PX4:H21	4:A:360:PX4:H17	0.70	1.64	10	1
4:A:374:PX4:H41	4:A:412:PX4:H31	0.70	1.63	7	1
4:A:308:PX4:H58	4:A:311:PX4:H54	0.70	1.61	1	1
4:A:329:PX4:H55	4:A:333:PX4:H45	0.70	1.63	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H37	4:A:419:PX4:H21	0.70	1.62	2	2
4:A:361:PX4:H25	4:A:362:PX4:H31	0.70	1.64	14	2
4:A:317:PX4:H52	4:A:324:PX4:H54	0.70	1.64	11	1
4:A:317:PX4:H17	4:A:324:PX4:H53	0.70	1.64	2	1
4:A:338:PX4:O8	4:A:348:PX4:H4	0.69	1.87	9	2
4:A:311:PX4:H58	4:A:363:PX4:H44	0.69	1.61	14	1
4:A:372:PX4:H51	4:A:384:PX4:H51	0.69	1.63	12	1
4:A:410:PX4:H49	4:A:426:PX4:H19	0.69	1.63	8	1
4:A:353:PX4:H72	4:A:354:PX4:H29	0.69	1.62	7	1
4:A:307:PX4:H4	4:A:361:PX4:H17	0.69	1.64	7	2
4:A:368:PX4:H34	4:A:429:PX4:H67	0.69	1.65	5	1
4:A:326:PX4:H25	4:A:341:PX4:H62	0.69	1.64	6	1
4:A:350:PX4:H45	4:A:363:PX4:H56	0.69	1.62	1	1
4:A:398:PX4:H30	4:A:407:PX4:H54	0.69	1.63	10	1
4:A:360:PX4:H50	4:A:366:PX4:H18	0.69	1.65	8	1
4:A:418:PX4:H26	4:A:425:PX4:H24	0.69	1.65	4	1
4:A:353:PX4:H70	4:A:413:PX4:H43	0.69	1.63	4	1
4:A:322:PX4:H28	4:A:323:PX4:H25	0.69	1.65	14	1
4:A:350:PX4:H72	4:A:365:PX4:H35	0.68	1.65	1	1
4:A:343:PX4:H64	4:A:347:PX4:H27	0.68	1.62	2	1
4:A:391:PX4:H24	4:A:393:PX4:H58	0.68	1.65	13	1
4:A:392:PX4:H52	4:A:393:PX4:H54	0.68	1.64	4	1
4:A:377:PX4:H13	4:A:377:PX4:H15	0.68	1.65	8	1
4:A:367:PX4:H55	4:A:430:PX4:H22	0.68	1.63	6	2
4:A:335:PX4:H16	4:A:344:PX4:H20	0.68	1.64	14	1
4:A:340:PX4:H30	4:A:347:PX4:H72	0.68	1.64	5	1
4:A:360:PX4:H68	4:A:419:PX4:H67	0.68	1.65	2	1
4:A:323:PX4:H14	4:A:333:PX4:H47	0.68	1.64	10	1
4:A:405:PX4:H41	4:A:414:PX4:H42	0.68	1.64	14	1
4:A:332:PX4:H28	4:A:340:PX4:H31	0.68	1.66	2	1
4:A:314:PX4:H38	4:A:355:PX4:H8	0.68	1.64	8	1
4:A:385:PX4:H23	4:A:393:PX4:H22	0.68	1.64	3	1
4:A:345:PX4:H34	4:A:353:PX4:H46	0.68	1.64	14	1
4:A:346:PX4:H40	4:A:355:PX4:H68	0.68	1.64	6	1
4:A:370:PX4:H42	4:A:403:PX4:H33	0.67	1.64	5	1
4:A:313:PX4:H26	4:A:366:PX4:H21	0.67	1.64	7	1
4:A:316:PX4:H47	4:A:319:PX4:H46	0.67	1.67	6	1
4:A:308:PX4:H47	4:A:310:PX4:H60	0.67	1.65	14	1
4:A:315:PX4:H52	4:A:316:PX4:H23	0.67	1.65	14	1
4:A:306:PX4:H57	4:A:423:PX4:H42	0.67	1.65	4	1
4:A:405:PX4:H17	4:A:414:PX4:H19	0.67	1.67	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:409:PX4:H55	4:A:415:PX4:H27	0.66	1.67	1	1
4:A:353:PX4:H69	4:A:362:PX4:H72	0.66	1.65	14	1
4:A:416:PX4:H48	4:A:422:PX4:H59	0.66	1.67	14	1
4:A:340:PX4:H43	4:A:407:PX4:H66	0.66	1.67	1	1
4:A:314:PX4:H58	4:A:364:PX4:H54	0.66	1.66	8	1
4:A:387:PX4:H15	4:A:411:PX4:H49	0.66	1.66	8	1
4:A:388:PX4:H16	4:A:395:PX4:H15	0.66	1.66	5	1
4:A:314:PX4:H64	4:A:422:PX4:H68	0.66	1.65	2	1
4:A:386:PX4:H17	4:A:387:PX4:H24	0.66	1.68	10	1
4:A:347:PX4:H16	4:A:348:PX4:H46	0.66	1.67	4	1
4:A:340:PX4:H58	4:A:341:PX4:H16	0.66	1.68	14	1
4:A:403:PX4:H56	4:A:404:PX4:H39	0.66	1.67	12	1
4:A:339:PX4:H30	4:A:355:PX4:H40	0.66	1.67	10	1
4:A:306:PX4:H16	4:A:322:PX4:H9	0.66	1.68	13	1
4:A:356:PX4:H32	4:A:362:PX4:H24	0.66	1.66	2	2
4:A:336:PX4:H27	4:A:344:PX4:H62	0.66	1.67	6	1
4:A:331:PX4:H21	4:A:340:PX4:H17	0.66	1.66	5	1
4:A:385:PX4:H71	4:A:399:PX4:H61	0.66	1.67	14	1
4:A:357:PX4:H58	4:A:357:PX4:H31	0.66	1.66	8	1
4:A:336:PX4:H65	4:A:344:PX4:H71	0.66	1.68	9	1
4:A:400:PX4:H17	4:A:401:PX4:H3	0.66	1.65	10	1
4:A:335:PX4:H42	4:A:337:PX4:H38	0.66	1.65	10	1
4:A:408:PX4:H50	4:A:409:PX4:H17	0.66	1.66	10	1
4:A:349:PX4:H36	4:A:350:PX4:H40	0.65	1.68	2	1
4:A:391:PX4:H19	4:A:414:PX4:H17	0.65	1.67	8	1
4:A:389:PX4:H42	4:A:389:PX4:H71	0.65	1.66	1	1
4:A:413:PX4:H41	4:A:421:PX4:H67	0.65	1.69	3	1
4:A:308:PX4:H66	4:A:410:PX4:H68	0.65	1.68	10	1
4:A:420:PX4:H51	4:A:427:PX4:H49	0.65	1.68	7	1
4:A:373:PX4:H21	4:A:381:PX4:H32	0.65	1.68	11	1
4:A:359:PX4:H37	4:A:412:PX4:H64	0.65	1.67	8	1
4:A:332:PX4:H37	4:A:340:PX4:H35	0.65	1.68	7	1
4:A:358:PX4:H71	4:A:358:PX4:H39	0.65	1.69	11	1
4:A:393:PX4:H18	4:A:394:PX4:H18	0.65	1.67	9	1
4:A:403:PX4:H16	4:A:404:PX4:H24	0.65	1.69	12	1
4:A:391:PX4:H53	4:A:408:PX4:H20	0.65	1.68	9	1
4:A:373:PX4:H46	4:A:382:PX4:H46	0.65	1.67	5	1
4:A:306:PX4:H54	4:A:321:PX4:H48	0.65	1.68	7	2
4:A:368:PX4:H25	4:A:429:PX4:H66	0.65	1.69	9	1
4:A:419:PX4:H46	4:A:427:PX4:H50	0.65	1.68	1	1
4:A:322:PX4:H62	4:A:361:PX4:H71	0.65	1.69	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:405:PX4:H21	4:A:415:PX4:H50	0.65	1.68	4	1
4:A:312:PX4:H38	4:A:366:PX4:H48	0.65	1.69	3	1
4:A:335:PX4:H16	4:A:344:PX4:H19	0.65	1.67	10	2
4:A:406:PX4:H37	4:A:423:PX4:H28	0.65	1.69	4	1
4:A:390:PX4:H44	4:A:407:PX4:H17	0.65	1.67	14	1
4:A:402:PX4:H52	4:A:403:PX4:H27	0.65	1.69	1	1
4:A:335:PX4:H34	4:A:343:PX4:H65	0.65	1.69	11	1
4:A:400:PX4:H20	4:A:401:PX4:H17	0.65	1.68	6	1
4:A:391:PX4:H47	4:A:394:PX4:H28	0.65	1.67	2	1
4:A:348:PX4:H26	4:A:355:PX4:H25	0.65	1.69	12	1
4:A:406:PX4:H46	4:A:421:PX4:H50	0.65	1.68	7	1
4:A:308:PX4:H19	4:A:364:PX4:H22	0.64	1.68	9	1
4:A:400:PX4:H28	4:A:401:PX4:H46	0.64	1.67	2	1
4:A:391:PX4:H50	4:A:393:PX4:H60	0.64	1.69	10	1
4:A:376:PX4:H20	4:A:377:PX4:H16	0.64	1.67	14	2
4:A:397:PX4:H53	4:A:402:PX4:H21	0.64	1.68	6	1
4:A:404:PX4:O1	4:A:419:PX4:H13	0.64	1.93	2	1
4:A:339:PX4:H23	4:A:347:PX4:H29	0.64	1.69	1	1
4:A:317:PX4:H40	4:A:342:PX4:H38	0.64	1.68	1	1
4:A:379:PX4:H19	4:A:384:PX4:H20	0.64	1.70	4	1
4:A:359:PX4:H36	4:A:366:PX4:H40	0.64	1.69	6	1
4:A:312:PX4:H55	4:A:359:PX4:H56	0.64	1.70	9	1
4:A:316:PX4:H56	4:A:316:PX4:H25	0.64	1.69	9	1
4:A:353:PX4:H46	4:A:354:PX4:H64	0.64	1.68	7	1
4:A:376:PX4:H35	4:A:383:PX4:H60	0.64	1.67	7	1
4:A:397:PX4:H28	4:A:398:PX4:H58	0.64	1.68	1	1
4:A:405:PX4:H4	4:A:414:PX4:H22	0.64	1.67	1	1
4:A:350:PX4:H51	4:A:363:PX4:H59	0.64	1.69	1	1
4:A:313:PX4:H53	4:A:359:PX4:H23	0.64	1.68	10	1
4:A:371:PX4:H31	4:A:376:PX4:H23	0.64	1.70	14	1
4:A:403:PX4:H24	4:A:404:PX4:H53	0.64	1.68	5	1
4:A:357:PX4:H45	4:A:365:PX4:H72	0.64	1.70	10	1
4:A:378:PX4:H63	4:A:418:PX4:H66	0.64	1.69	4	1
4:A:368:PX4:H4	4:A:418:PX4:H2	0.63	1.70	1	1
4:A:369:PX4:H25	4:A:429:PX4:H64	0.63	1.68	2	2
4:A:317:PX4:H55	4:A:342:PX4:H53	0.63	1.68	2	1
4:A:370:PX4:H46	4:A:411:PX4:H53	0.63	1.70	13	1
4:A:320:PX4:H36	4:A:418:PX4:H66	0.63	1.70	9	1
4:A:417:PX4:H50	4:A:426:PX4:H47	0.63	1.70	8	1
4:A:386:PX4:H17	4:A:387:PX4:H21	0.63	1.69	9	1
4:A:405:PX4:H3	4:A:414:PX4:O6	0.63	1.94	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:332:PX4:H41	4:A:407:PX4:H66	0.63	1.68	6	1
4:A:416:PX4:H23	4:A:422:PX4:H52	0.63	1.70	2	1
4:A:355:PX4:H46	4:A:355:PX4:H10	0.63	1.70	8	1
4:A:375:PX4:H36	4:A:375:PX4:H67	0.63	1.71	14	1
4:A:428:PX4:H19	4:A:429:PX4:H37	0.63	1.69	7	2
4:A:312:PX4:H21	4:A:366:PX4:H17	0.63	1.70	2	2
4:A:370:PX4:H46	4:A:411:PX4:H49	0.63	1.69	14	1
4:A:386:PX4:H64	4:A:387:PX4:H34	0.63	1.69	2	1
4:A:367:PX4:H45	4:A:429:PX4:H31	0.63	1.70	3	1
4:A:376:PX4:H21	4:A:377:PX4:H20	0.63	1.71	5	1
4:A:406:PX4:H35	4:A:425:PX4:H68	0.63	1.70	10	1
4:A:314:PX4:H57	4:A:361:PX4:H27	0.63	1.70	9	1
4:A:314:PX4:H34	4:A:362:PX4:H14	0.63	1.70	9	1
4:A:398:PX4:H30	4:A:407:PX4:H53	0.63	1.71	14	1
4:A:355:PX4:H49	4:A:355:PX4:H10	0.63	1.68	12	1
4:A:355:PX4:H68	4:A:415:PX4:H64	0.63	1.71	13	1
4:A:332:PX4:H72	4:A:391:PX4:H25	0.63	1.70	14	1
4:A:407:PX4:H22	4:A:414:PX4:H50	0.63	1.69	12	1
4:A:378:PX4:H15	4:A:410:PX4:H47	0.62	1.69	3	1
4:A:406:PX4:H34	4:A:424:PX4:H35	0.62	1.71	5	1
4:A:378:PX4:H46	4:A:410:PX4:H17	0.62	1.70	10	1
4:A:307:PX4:H65	4:A:349:PX4:H22	0.62	1.71	14	1
4:A:329:PX4:H12	4:A:333:PX4:H41	0.62	1.71	12	1
4:A:393:PX4:H21	4:A:394:PX4:H29	0.62	1.69	11	1
4:A:309:PX4:H56	4:A:319:PX4:H48	0.62	1.70	13	1
4:A:313:PX4:H70	4:A:375:PX4:H69	0.62	1.71	6	1
4:A:338:PX4:H16	4:A:345:PX4:H49	0.62	1.71	7	1
4:A:308:PX4:H22	4:A:310:PX4:H65	0.62	1.70	3	1
4:A:313:PX4:H60	4:A:327:PX4:H32	0.62	1.70	9	1
4:A:419:PX4:H36	4:A:430:PX4:H27	0.62	1.71	1	1
4:A:334:PX4:H54	4:A:356:PX4:H8	0.61	1.69	9	1
4:A:375:PX4:H54	4:A:389:PX4:H60	0.61	1.70	3	1
4:A:339:PX4:H26	4:A:347:PX4:H54	0.61	1.71	12	1
4:A:310:PX4:H53	4:A:364:PX4:H31	0.61	1.70	13	1
4:A:345:PX4:H22	4:A:345:PX4:H59	0.61	1.72	3	1
4:A:353:PX4:H19	4:A:357:PX4:H46	0.61	1.72	5	1
4:A:347:PX4:H54	4:A:355:PX4:H22	0.61	1.71	10	1
4:A:315:PX4:H43	4:A:369:PX4:H28	0.61	1.70	7	1
4:A:317:PX4:H26	4:A:342:PX4:H19	0.61	1.73	8	1
4:A:373:PX4:H39	4:A:402:PX4:H38	0.61	1.72	10	1
4:A:326:PX4:H42	4:A:332:PX4:H51	0.61	1.70	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:355:PX4:H66	4:A:362:PX4:H64	0.61	1.73	4	1
4:A:387:PX4:H47	4:A:411:PX4:H48	0.61	1.71	14	1
4:A:375:PX4:H18	4:A:429:PX4:H24	0.61	1.71	7	1
4:A:392:PX4:H7	4:A:392:PX4:H15	0.61	1.71	13	1
4:A:397:PX4:H31	4:A:398:PX4:H63	0.61	1.73	2	1
4:A:335:PX4:H31	4:A:337:PX4:H33	0.61	1.71	8	1
4:A:410:PX4:H59	4:A:417:PX4:H54	0.61	1.72	12	1
4:A:338:PX4:H25	4:A:347:PX4:H23	0.61	1.72	7	1
4:A:423:PX4:H16	4:A:424:PX4:H19	0.61	1.70	13	1
4:A:331:PX4:H14	4:A:347:PX4:H50	0.61	1.71	10	2
4:A:315:PX4:H43	4:A:424:PX4:H71	0.61	1.72	10	1
1:A:191:ILE:HD13	4:A:314:PX4:H21	0.61	1.72	14	3
4:A:350:PX4:H37	4:A:408:PX4:H39	0.61	1.73	4	1
4:A:380:PX4:H39	4:A:386:PX4:H38	0.61	1.73	12	1
4:A:325:PX4:H61	4:A:341:PX4:H60	0.61	1.72	10	1
4:A:396:PX4:H37	4:A:397:PX4:H42	0.61	1.72	12	1
4:A:395:PX4:H52	4:A:421:PX4:H50	0.61	1.73	2	1
4:A:306:PX4:H58	4:A:321:PX4:H21	0.61	1.72	10	1
4:A:337:PX4:H58	4:A:348:PX4:H32	0.61	1.73	12	1
4:A:330:PX4:H64	4:A:338:PX4:H39	0.61	1.72	1	1
4:A:407:PX4:H32	4:A:414:PX4:H55	0.61	1.72	4	1
4:A:360:PX4:H57	4:A:366:PX4:H56	0.61	1.73	12	1
4:A:319:PX4:H29	4:A:320:PX4:H28	0.61	1.72	6	1
4:A:368:PX4:H17	4:A:390:PX4:H50	0.61	1.73	1	1
4:A:407:PX4:H34	4:A:414:PX4:H65	0.61	1.73	1	1
4:A:331:PX4:H22	4:A:340:PX4:H17	0.61	1.73	13	1
4:A:421:PX4:H47	4:A:423:PX4:H66	0.61	1.73	11	1
4:A:349:PX4:H36	4:A:350:PX4:H37	0.61	1.71	11	1
4:A:355:PX4:H43	4:A:398:PX4:H70	0.60	1.71	3	1
4:A:316:PX4:H37	4:A:316:PX4:H72	0.60	1.72	6	1
4:A:407:PX4:H16	4:A:414:PX4:H49	0.60	1.73	10	3
4:A:334:PX4:H48	4:A:349:PX4:H20	0.60	1.71	11	1
4:A:335:PX4:H34	4:A:337:PX4:H34	0.60	1.74	2	1
4:A:345:PX4:H19	4:A:353:PX4:H47	0.60	1.71	12	1
4:A:387:PX4:H47	4:A:411:PX4:H52	0.60	1.73	13	1
4:A:387:PX4:H53	4:A:411:PX4:H50	0.60	1.72	9	1
4:A:331:PX4:H69	4:A:331:PX4:H40	0.60	1.73	1	1
4:A:357:PX4:H24	4:A:358:PX4:H22	0.60	1.73	6	1
4:A:338:PX4:H28	4:A:348:PX4:H57	0.60	1.72	11	1
4:A:428:PX4:H62	4:A:429:PX4:H50	0.60	1.73	1	1
4:A:314:PX4:H36	4:A:362:PX4:H16	0.60	1.72	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:360:PX4:H70	4:A:404:PX4:H42	0.60	1.74	14	1
4:A:307:PX4:H19	4:A:361:PX4:H15	0.60	1.73	14	4
4:A:376:PX4:H52	4:A:377:PX4:H19	0.60	1.72	8	1
4:A:331:PX4:H54	4:A:339:PX4:H35	0.60	1.72	13	1
4:A:392:PX4:H20	4:A:399:PX4:H48	0.60	1.74	1	1
4:A:368:PX4:H67	4:A:424:PX4:H17	0.60	1.72	8	1
4:A:327:PX4:H37	4:A:328:PX4:H53	0.60	1.72	12	1
4:A:410:PX4:H46	4:A:426:PX4:H15	0.60	1.72	13	2
4:A:335:PX4:H16	4:A:344:PX4:H22	0.60	1.72	7	1
4:A:332:PX4:H55	4:A:334:PX4:H36	0.60	1.74	11	1
4:A:350:PX4:H34	4:A:394:PX4:H43	0.59	1.73	2	1
1:A:191:ILE:HD12	4:A:314:PX4:H21	0.59	1.73	11	1
4:A:370:PX4:H70	4:A:402:PX4:H34	0.59	1.74	9	1
4:A:396:PX4:H55	4:A:396:PX4:H20	0.59	1.73	2	1
4:A:307:PX4:H43	4:A:410:PX4:H29	0.59	1.74	5	1
4:A:406:PX4:H21	4:A:423:PX4:H65	0.59	1.74	7	1
4:A:369:PX4:H61	4:A:425:PX4:H47	0.59	1.73	1	1
4:A:313:PX4:H63	4:A:328:PX4:H66	0.59	1.73	2	1
4:A:400:PX4:H11	4:A:401:PX4:O6	0.59	1.97	10	1
4:A:396:PX4:H53	4:A:398:PX4:H24	0.59	1.75	4	1
4:A:391:PX4:H25	4:A:392:PX4:H62	0.59	1.73	4	1
4:A:389:PX4:H53	4:A:398:PX4:H55	0.59	1.73	11	1
4:A:308:PX4:H23	4:A:364:PX4:H26	0.59	1.73	6	2
4:A:330:PX4:C9	4:A:344:PX4:H49	0.59	2.28	2	1
4:A:317:PX4:H53	4:A:342:PX4:H17	0.59	1.75	10	1
4:A:408:PX4:H40	4:A:422:PX4:H40	0.59	1.75	14	1
4:A:368:PX4:H62	4:A:424:PX4:H23	0.59	1.73	13	1
4:A:338:PX4:H53	4:A:346:PX4:H53	0.59	1.73	11	1
4:A:374:PX4:H30	4:A:427:PX4:H26	0.59	1.73	11	1
4:A:428:PX4:H23	4:A:429:PX4:H42	0.59	1.73	8	1
4:A:322:PX4:H64	4:A:361:PX4:H64	0.59	1.74	4	1
4:A:330:PX4:H52	4:A:338:PX4:H36	0.59	1.73	11	1
4:A:391:PX4:H20	4:A:392:PX4:H61	0.59	1.75	11	1
4:A:428:PX4:H56	4:A:429:PX4:H46	0.59	1.74	6	1
4:A:338:PX4:H60	4:A:355:PX4:H63	0.59	1.75	9	1
4:A:396:PX4:H69	4:A:398:PX4:H43	0.58	1.75	8	1
4:A:334:PX4:H69	4:A:349:PX4:H66	0.58	1.73	5	1
4:A:306:PX4:O8	4:A:322:PX4:H13	0.58	1.98	14	1
4:A:331:PX4:H10	4:A:347:PX4:H49	0.58	1.75	14	1
4:A:400:PX4:H47	4:A:409:PX4:H20	0.58	1.74	9	1
4:A:329:PX4:H42	4:A:336:PX4:H62	0.58	1.74	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:342:PX4:H16	4:A:351:PX4:H20	0.58	1.75	8	1
4:A:395:PX4:H33	4:A:405:PX4:H34	0.58	1.74	10	1
4:A:330:PX4:H50	4:A:337:PX4:H48	0.58	1.74	7	1
4:A:356:PX4:H16	4:A:356:PX4:H12	0.58	1.75	8	1
4:A:381:PX4:H50	4:A:397:PX4:H47	0.58	1.74	4	2
4:A:400:PX4:H22	4:A:408:PX4:H67	0.58	1.75	14	1
4:A:403:PX4:H29	4:A:404:PX4:H35	0.58	1.76	13	1
4:A:331:PX4:H65	4:A:339:PX4:H69	0.58	1.74	11	1
4:A:405:PX4:H4	4:A:414:PX4:H23	0.58	1.74	2	1
4:A:315:PX4:H35	4:A:322:PX4:H49	0.58	1.74	10	1
4:A:393:PX4:H23	4:A:394:PX4:H29	0.58	1.74	12	1
4:A:314:PX4:H45	4:A:346:PX4:H38	0.58	1.76	7	1
4:A:339:PX4:H21	4:A:347:PX4:H50	0.58	1.74	13	1
4:A:410:PX4:H48	4:A:426:PX4:H22	0.58	1.74	13	1
4:A:348:PX4:H27	4:A:348:PX4:H60	0.58	1.74	11	1
4:A:324:PX4:H61	4:A:341:PX4:H24	0.58	1.74	2	1
4:A:370:PX4:H35	4:A:427:PX4:H71	0.58	1.74	2	1
4:A:366:PX4:H27	4:A:427:PX4:H68	0.58	1.74	8	1
4:A:349:PX4:H15	4:A:356:PX4:H28	0.58	1.75	12	2
4:A:330:PX4:H41	4:A:336:PX4:H35	0.58	1.75	6	1
4:A:392:PX4:H48	4:A:393:PX4:H57	0.58	1.73	1	1
4:A:366:PX4:H38	4:A:412:PX4:H41	0.58	1.76	1	1
4:A:343:PX4:H9	4:A:344:PX4:H16	0.58	1.75	3	1
4:A:318:PX4:H47	4:A:327:PX4:H15	0.58	1.74	10	1
4:A:391:PX4:H16	4:A:393:PX4:H65	0.58	1.76	3	1
4:A:318:PX4:H18	4:A:327:PX4:H47	0.58	1.76	3	1
4:A:346:PX4:H43	4:A:356:PX4:H31	0.58	1.74	7	1
4:A:373:PX4:H29	4:A:384:PX4:H59	0.58	1.73	13	1
4:A:341:PX4:H40	4:A:385:PX4:H64	0.58	1.75	6	1
4:A:338:PX4:H46	4:A:355:PX4:H16	0.58	1.75	5	4
4:A:326:PX4:H50	4:A:351:PX4:H49	0.58	1.75	1	1
4:A:332:PX4:H10	4:A:356:PX4:O1	0.58	1.98	2	1
4:A:400:PX4:H22	4:A:408:PX4:H63	0.58	1.74	1	1
4:A:421:PX4:H4	4:A:423:PX4:H51	0.58	1.76	2	1
4:A:330:PX4:H63	4:A:337:PX4:H61	0.58	1.74	8	1
4:A:420:PX4:H47	4:A:427:PX4:H16	0.58	1.75	3	1
4:A:389:PX4:H25	4:A:398:PX4:H58	0.58	1.75	5	1
4:A:332:PX4:H70	4:A:425:PX4:H62	0.58	1.74	7	1
4:A:316:PX4:C24	4:A:319:PX4:H46	0.58	2.29	6	1
4:A:326:PX4:H60	4:A:350:PX4:H71	0.58	1.74	8	1
4:A:383:PX4:H35	4:A:407:PX4:H26	0.58	1.74	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:378:PX4:H69	4:A:410:PX4:H42	0.58	1.74	4	1
4:A:413:PX4:H64	4:A:421:PX4:H62	0.58	1.76	4	1
4:A:390:PX4:H47	4:A:399:PX4:H24	0.58	1.76	14	1
4:A:383:PX4:H17	4:A:392:PX4:H26	0.58	1.75	14	1
4:A:310:PX4:H43	4:A:351:PX4:H66	0.58	1.74	12	1
4:A:310:PX4:H53	4:A:364:PX4:H25	0.58	1.76	12	1
4:A:404:PX4:H50	4:A:413:PX4:H26	0.58	1.75	12	1
4:A:310:PX4:H35	4:A:417:PX4:H31	0.57	1.75	2	1
4:A:372:PX4:H72	4:A:384:PX4:H38	0.57	1.75	11	1
4:A:383:PX4:H40	4:A:390:PX4:H41	0.57	1.76	8	1
4:A:380:PX4:H51	4:A:402:PX4:H24	0.57	1.74	7	1
4:A:378:PX4:H48	4:A:417:PX4:H72	0.57	1.74	7	1
4:A:332:PX4:H32	4:A:339:PX4:H44	0.57	1.76	13	1
4:A:310:PX4:H61	4:A:426:PX4:H44	0.57	1.76	1	1
4:A:338:PX4:H14	4:A:348:PX4:H4	0.57	1.75	2	1
4:A:368:PX4:H51	4:A:424:PX4:C30	0.57	2.29	3	1
4:A:345:PX4:H20	4:A:353:PX4:H52	0.57	1.75	3	1
4:A:330:PX4:H7	4:A:344:PX4:H49	0.57	1.75	5	1
4:A:331:PX4:H27	4:A:340:PX4:H53	0.57	1.76	14	1
4:A:389:PX4:H60	4:A:407:PX4:H55	0.57	1.75	12	1
4:A:326:PX4:H49	4:A:363:PX4:H55	0.57	1.75	7	1
4:A:355:PX4:H18	4:A:356:PX4:H15	0.57	1.75	13	1
4:A:331:PX4:H4	4:A:347:PX4:H50	0.57	1.74	9	1
4:A:368:PX4:H46	4:A:369:PX4:H22	0.57	1.74	8	1
4:A:393:PX4:H29	4:A:394:PX4:H56	0.57	1.75	5	1
4:A:395:PX4:H21	4:A:406:PX4:H51	0.57	1.77	10	1
4:A:316:PX4:H20	4:A:316:PX4:H49	0.57	1.74	10	1
4:A:423:PX4:H67	4:A:424:PX4:H37	0.57	1.75	14	1
4:A:370:PX4:H23	4:A:403:PX4:H17	0.57	1.75	10	1
4:A:378:PX4:H23	4:A:417:PX4:H64	0.57	1.75	10	1
4:A:337:PX4:H58	4:A:357:PX4:H56	0.57	1.75	8	1
4:A:404:PX4:H8	4:A:430:PX4:O6	0.57	2.00	6	2
4:A:412:PX4:H56	4:A:419:PX4:H35	0.57	1.76	13	1
4:A:396:PX4:H61	4:A:396:PX4:H29	0.57	1.77	11	1
4:A:376:PX4:H30	4:A:383:PX4:H64	0.57	1.76	2	1
4:A:423:PX4:H16	4:A:424:PX4:H26	0.57	1.74	2	1
4:A:403:PX4:H2	4:A:411:PX4:O3	0.57	1.99	2	1
4:A:307:PX4:H37	4:A:410:PX4:H44	0.57	1.75	12	1
4:A:378:PX4:H48	4:A:417:PX4:H67	0.57	1.77	13	1
4:A:317:PX4:H58	4:A:342:PX4:H24	0.57	1.76	3	1
4:A:332:PX4:H5	4:A:347:PX4:H61	0.57	1.75	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:335:PX4:H51	4:A:344:PX4:H24	0.57	1.77	6	1
4:A:346:PX4:H35	4:A:354:PX4:H34	0.57	1.75	9	1
1:A:165:ARG:NH1	4:A:362:PX4:H7	0.57	2.14	6	2
4:A:337:PX4:H61	4:A:345:PX4:H36	0.57	1.76	9	1
4:A:330:PX4:H22	4:A:344:PX4:H48	0.57	1.77	4	1
4:A:316:PX4:H45	4:A:418:PX4:H57	0.57	1.77	14	1
4:A:391:PX4:H22	4:A:414:PX4:H17	0.56	1.77	12	3
4:A:378:PX4:H51	4:A:418:PX4:H49	0.56	1.77	2	1
4:A:320:PX4:H34	4:A:378:PX4:H42	0.56	1.75	8	1
4:A:307:PX4:H67	4:A:314:PX4:H67	0.56	1.77	4	1
4:A:371:PX4:H8	4:A:377:PX4:O6	0.56	1.99	1	1
4:A:367:PX4:H17	4:A:430:PX4:H49	0.56	1.76	1	1
4:A:346:PX4:H16	4:A:346:PX4:O6	0.56	1.99	1	1
4:A:329:PX4:O6	4:A:336:PX4:H3	0.56	2.00	2	1
4:A:331:PX4:O1	4:A:332:PX4:H3	0.56	2.00	8	1
4:A:349:PX4:H70	4:A:422:PX4:H32	0.56	1.77	4	1
4:A:361:PX4:H64	4:A:425:PX4:H24	0.56	1.75	13	1
4:A:345:PX4:H65	4:A:348:PX4:H19	0.56	1.76	13	1
4:A:338:PX4:H57	4:A:346:PX4:H57	0.56	1.77	11	1
4:A:400:PX4:H1	4:A:409:PX4:H18	0.56	1.75	6	1
4:A:371:PX4:H52	4:A:377:PX4:H54	0.56	1.77	8	1
4:A:325:PX4:H47	4:A:341:PX4:H49	0.56	1.77	4	1
4:A:357:PX4:H29	4:A:357:PX4:H53	0.56	1.75	7	1
4:A:423:PX4:H49	4:A:424:PX4:H21	0.56	1.76	13	1
4:A:380:PX4:H21	4:A:381:PX4:H53	0.56	1.76	11	1
4:A:395:PX4:H50	4:A:402:PX4:H62	0.56	1.77	11	1
4:A:367:PX4:H23	4:A:368:PX4:H66	0.56	1.76	6	1
4:A:311:PX4:H22	4:A:311:PX4:H52	0.56	1.77	6	1
4:A:316:PX4:H68	4:A:368:PX4:H38	0.56	1.77	6	1
1:A:171:PHE:CZ	4:A:307:PX4:H17	0.56	2.36	1	2
4:A:400:PX4:H33	4:A:401:PX4:H60	0.56	1.77	4	1
4:A:368:PX4:H50	4:A:369:PX4:H25	0.56	1.76	9	1
4:A:376:PX4:H64	4:A:393:PX4:H50	0.56	1.77	2	1
4:A:403:PX4:H55	4:A:419:PX4:H59	0.56	1.77	4	1
4:A:393:PX4:H68	4:A:399:PX4:H68	0.56	1.78	14	1
4:A:306:PX4:H19	4:A:321:PX4:H23	0.56	1.76	12	2
4:A:312:PX4:H30	4:A:360:PX4:H53	0.56	1.76	1	1
4:A:306:PX4:H27	4:A:328:PX4:H41	0.56	1.78	8	1
4:A:329:PX4:H58	4:A:333:PX4:H43	0.56	1.78	3	1
4:A:321:PX4:H48	4:A:354:PX4:H23	0.56	1.77	3	1
4:A:370:PX4:H28	4:A:403:PX4:H17	0.56	1.77	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:396:PX4:H11	4:A:405:PX4:O8	0.56	2.00	13	1
4:A:345:PX4:H71	4:A:357:PX4:H57	0.56	1.78	1	1
4:A:339:PX4:H70	4:A:355:PX4:H43	0.56	1.78	8	1
4:A:354:PX4:H44	4:A:423:PX4:H36	0.56	1.78	14	1
4:A:370:PX4:H37	4:A:404:PX4:H29	0.56	1.76	11	1
4:A:314:PX4:C35	4:A:364:PX4:H29	0.56	2.30	6	1
4:A:342:PX4:H38	4:A:394:PX4:H70	0.56	1.78	9	1
4:A:332:PX4:H12	4:A:332:PX4:H16	0.56	1.77	1	1
4:A:371:PX4:H19	4:A:377:PX4:H17	0.56	1.77	1	1
4:A:380:PX4:H56	4:A:387:PX4:H64	0.56	1.78	2	1
4:A:316:PX4:H25	4:A:320:PX4:H30	0.56	1.78	3	1
4:A:325:PX4:H20	4:A:326:PX4:H22	0.56	1.75	10	1
4:A:314:PX4:H69	4:A:364:PX4:H29	0.56	1.77	6	1
4:A:355:PX4:H68	4:A:422:PX4:H37	0.56	1.77	1	1
4:A:330:PX4:H53	4:A:338:PX4:H21	0.56	1.76	4	1
4:A:412:PX4:H29	4:A:419:PX4:H49	0.56	1.78	12	1
4:A:322:PX4:H67	4:A:367:PX4:H30	0.56	1.77	13	1
4:A:406:PX4:H48	4:A:421:PX4:H53	0.56	1.78	11	1
4:A:359:PX4:H41	4:A:366:PX4:H44	0.56	1.78	1	1
4:A:343:PX4:H31	4:A:344:PX4:H32	0.56	1.78	3	1
4:A:374:PX4:H15	4:A:420:PX4:H19	0.56	1.76	12	2
4:A:306:PX4:H64	4:A:354:PX4:H19	0.56	1.76	10	1
4:A:311:PX4:H56	4:A:311:PX4:H25	0.56	1.75	14	1
4:A:348:PX4:H57	4:A:355:PX4:H32	0.55	1.77	3	1
4:A:313:PX4:H10	4:A:359:PX4:O2	0.55	2.01	14	1
4:A:412:PX4:H44	4:A:419:PX4:H39	0.55	1.79	12	1
4:A:421:PX4:H17	4:A:423:PX4:H52	0.55	1.77	7	2
4:A:374:PX4:H44	4:A:427:PX4:H17	0.55	1.76	7	1
4:A:388:PX4:H63	4:A:406:PX4:H62	0.55	1.78	13	1
4:A:329:PX4:H70	4:A:369:PX4:H41	0.55	1.78	6	1
4:A:309:PX4:H54	4:A:319:PX4:H53	0.55	1.78	12	1
4:A:331:PX4:H24	4:A:340:PX4:H17	0.55	1.78	7	1
4:A:391:PX4:H17	4:A:408:PX4:H20	0.55	1.78	6	1
4:A:308:PX4:H68	4:A:426:PX4:H51	0.55	1.78	7	1
4:A:422:PX4:H17	4:A:425:PX4:C29	0.55	2.30	13	1
4:A:349:PX4:H47	4:A:356:PX4:H38	0.55	1.79	11	1
4:A:336:PX4:H21	4:A:344:PX4:H56	0.55	1.77	9	1
4:A:406:PX4:H53	4:A:423:PX4:H61	0.55	1.77	2	1
4:A:308:PX4:H18	4:A:426:PX4:H43	0.55	1.79	2	1
4:A:349:PX4:H6	4:A:349:PX4:O6	0.55	2.02	5	2
4:A:423:PX4:H16	4:A:424:PX4:H23	0.55	1.79	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:420:PX4:H25	4:A:427:PX4:H31	0.55	1.77	12	1
4:A:421:PX4:H36	4:A:424:PX4:H37	0.55	1.77	7	1
4:A:341:PX4:H72	4:A:407:PX4:H40	0.55	1.78	1	1
4:A:371:PX4:H25	4:A:377:PX4:H21	0.55	1.79	8	1
4:A:342:PX4:H67	4:A:385:PX4:H43	0.55	1.77	10	1
4:A:405:PX4:H71	4:A:407:PX4:H54	0.55	1.78	12	1
4:A:309:PX4:H30	4:A:377:PX4:H70	0.55	1.78	1	1
4:A:363:PX4:H30	4:A:364:PX4:H32	0.55	1.79	10	1
4:A:400:PX4:H61	4:A:417:PX4:H25	0.55	1.78	4	1
4:A:404:PX4:H57	4:A:430:PX4:H27	0.55	1.78	12	1
4:A:310:PX4:H71	4:A:316:PX4:H22	0.55	1.78	13	1
4:A:417:PX4:H47	4:A:426:PX4:H51	0.55	1.77	6	1
4:A:388:PX4:H62	4:A:395:PX4:H55	0.55	1.79	6	1
4:A:348:PX4:H34	4:A:407:PX4:H70	0.55	1.79	1	1
4:A:342:PX4:H57	4:A:351:PX4:H36	0.55	1.78	8	1
4:A:338:PX4:H26	4:A:348:PX4:H22	0.55	1.78	12	1
4:A:404:PX4:H33	4:A:412:PX4:H35	0.55	1.77	7	1
4:A:312:PX4:H56	4:A:359:PX4:H50	0.55	1.79	1	1
4:A:349:PX4:H34	4:A:415:PX4:H45	0.55	1.79	2	1
4:A:391:PX4:H17	4:A:408:PX4:H19	0.55	1.78	8	1
4:A:371:PX4:H16	4:A:377:PX4:H47	0.55	1.79	5	2
4:A:327:PX4:H24	4:A:329:PX4:H31	0.55	1.79	5	1
4:A:412:PX4:H31	4:A:419:PX4:H47	0.55	1.77	4	1
4:A:339:PX4:H25	4:A:347:PX4:H53	0.55	1.79	1	1
4:A:308:PX4:O6	4:A:315:PX4:H11	0.55	2.02	3	1
4:A:325:PX4:H67	4:A:325:PX4:H37	0.55	1.79	10	1
4:A:374:PX4:H68	4:A:420:PX4:H41	0.55	1.77	4	1
4:A:372:PX4:H71	4:A:386:PX4:H37	0.55	1.78	4	1
4:A:391:PX4:H18	4:A:414:PX4:O2	0.55	2.02	7	1
4:A:400:PX4:H59	4:A:400:PX4:H30	0.55	1.77	7	1
4:A:386:PX4:H50	4:A:387:PX4:H58	0.55	1.77	9	1
4:A:306:PX4:H54	4:A:321:PX4:H49	0.55	1.78	5	1
4:A:423:PX4:H14	4:A:424:PX4:H19	0.55	1.78	7	1
4:A:313:PX4:H23	4:A:359:PX4:H21	0.55	1.78	6	1
4:A:366:PX4:H29	4:A:427:PX4:H67	0.54	1.77	9	1
4:A:321:PX4:H5	4:A:362:PX4:O1	0.54	2.02	4	2
4:A:335:PX4:H66	4:A:343:PX4:H45	0.54	1.80	8	1
4:A:359:PX4:H44	4:A:366:PX4:H30	0.54	1.78	8	1
4:A:317:PX4:H68	4:A:317:PX4:H39	0.54	1.79	3	1
4:A:343:PX4:H34	4:A:344:PX4:H37	0.54	1.76	10	1
4:A:380:PX4:H62	4:A:387:PX4:H30	0.54	1.79	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H27	4:A:412:PX4:H46	0.54	1.78	9	1
4:A:392:PX4:H62	4:A:407:PX4:H33	0.54	1.79	2	1
4:A:338:PX4:H32	4:A:347:PX4:H28	0.54	1.79	8	1
4:A:309:PX4:H33	4:A:319:PX4:H37	0.54	1.78	13	1
4:A:357:PX4:H15	4:A:358:PX4:O1	0.54	2.02	11	1
4:A:392:PX4:H63	4:A:393:PX4:H57	0.54	1.78	11	1
4:A:404:PX4:H28	4:A:413:PX4:H32	0.54	1.79	5	1
4:A:327:PX4:H56	4:A:327:PX4:H19	0.54	1.80	5	1
4:A:405:PX4:H25	4:A:415:PX4:H54	0.54	1.80	4	1
4:A:357:PX4:H70	4:A:411:PX4:H42	0.54	1.78	4	1
4:A:421:PX4:H69	4:A:430:PX4:H44	0.54	1.78	4	1
4:A:342:PX4:H30	4:A:351:PX4:H33	0.54	1.78	7	1
4:A:306:PX4:H71	4:A:360:PX4:H30	0.54	1.79	13	1
4:A:338:PX4:H27	4:A:345:PX4:H63	0.54	1.80	13	1
4:A:369:PX4:H31	4:A:424:PX4:H71	0.54	1.77	11	1
4:A:395:PX4:H38	4:A:415:PX4:H62	0.54	1.77	9	1
4:A:348:PX4:H53	4:A:355:PX4:H28	0.54	1.79	3	1
4:A:332:PX4:H48	4:A:334:PX4:H38	0.54	1.80	5	1
4:A:381:PX4:H59	4:A:402:PX4:H27	0.54	1.79	10	1
4:A:370:PX4:H63	4:A:403:PX4:H33	0.54	1.80	7	1
4:A:367:PX4:H11	4:A:424:PX4:H18	0.54	1.78	2	1
4:A:383:PX4:H57	4:A:392:PX4:H31	0.54	1.80	2	1
1:A:119:ASN:OD1	4:A:355:PX4:H7	0.54	2.01	5	2
4:A:324:PX4:H67	4:A:341:PX4:H36	0.54	1.79	11	1
4:A:424:PX4:H60	4:A:429:PX4:H55	0.54	1.79	9	1
4:A:382:PX4:H57	4:A:427:PX4:H42	0.54	1.79	1	1
4:A:397:PX4:H39	4:A:398:PX4:H66	0.54	1.78	1	1
4:A:376:PX4:H17	4:A:383:PX4:H51	0.54	1.80	2	1
4:A:336:PX4:H28	4:A:339:PX4:H29	0.54	1.80	8	1
4:A:327:PX4:H21	4:A:329:PX4:H41	0.54	1.80	4	1
4:A:409:PX4:H50	4:A:422:PX4:H47	0.54	1.79	6	1
4:A:306:PX4:H14	4:A:321:PX4:C10	0.54	2.33	8	1
4:A:317:PX4:H52	4:A:324:PX4:H24	0.54	1.79	8	1
4:A:388:PX4:H18	4:A:396:PX4:H2	0.54	1.79	14	1
4:A:333:PX4:H53	4:A:341:PX4:H16	0.54	1.78	7	1
4:A:416:PX4:H47	4:A:422:PX4:H51	0.54	1.79	7	1
4:A:330:PX4:H30	4:A:336:PX4:H56	0.54	1.80	6	1
1:A:162:VAL:HG11	4:A:314:PX4:H34	0.54	1.80	2	1
4:A:400:PX4:H34	4:A:417:PX4:H32	0.54	1.79	8	1
4:A:380:PX4:H25	4:A:381:PX4:H56	0.54	1.80	11	1
4:A:400:PX4:H64	4:A:417:PX4:H27	0.54	1.78	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:337:PX4:H46	4:A:345:PX4:H56	0.54	1.79	3	1
4:A:420:PX4:H58	4:A:427:PX4:H52	0.54	1.78	3	1
4:A:326:PX4:H37	4:A:334:PX4:H24	0.54	1.79	12	1
4:A:391:PX4:H24	4:A:392:PX4:H61	0.54	1.79	7	1
4:A:332:PX4:H39	4:A:339:PX4:H39	0.54	1.78	1	1
4:A:320:PX4:H69	4:A:378:PX4:H33	0.54	1.79	3	1
4:A:326:PX4:H8	4:A:351:PX4:H22	0.54	1.80	5	1
4:A:328:PX4:H62	4:A:329:PX4:H25	0.54	1.80	4	1
4:A:313:PX4:H42	4:A:430:PX4:H41	0.54	1.79	7	1
4:A:358:PX4:H20	4:A:365:PX4:H17	0.54	1.78	11	1
4:A:393:PX4:H16	4:A:394:PX4:H24	0.54	1.79	6	1
4:A:389:PX4:H25	4:A:389:PX4:H59	0.53	1.81	3	1
4:A:388:PX4:H63	4:A:402:PX4:H72	0.53	1.79	5	1
4:A:415:PX4:H53	4:A:422:PX4:H25	0.53	1.79	9	1
4:A:349:PX4:H50	4:A:356:PX4:H5	0.53	1.79	2	1
4:A:367:PX4:H66	4:A:428:PX4:H27	0.53	1.80	5	1
4:A:339:PX4:H31	4:A:347:PX4:H56	0.53	1.81	9	1
4:A:388:PX4:H7	4:A:397:PX4:H49	0.53	1.80	9	1
4:A:391:PX4:H58	4:A:401:PX4:H26	0.53	1.80	4	1
4:A:363:PX4:H44	4:A:426:PX4:H70	0.53	1.78	12	1
4:A:373:PX4:H52	4:A:381:PX4:H33	0.53	1.79	12	1
4:A:377:PX4:H54	4:A:378:PX4:H25	0.53	1.80	13	1
4:A:374:PX4:H43	4:A:412:PX4:H32	0.53	1.79	11	1
1:A:165:ARG:CZ	4:A:362:PX4:H7	0.53	2.33	13	4
4:A:361:PX4:H26	4:A:362:PX4:H31	0.53	1.80	8	1
4:A:420:PX4:H30	4:A:427:PX4:H33	0.53	1.80	8	1
4:A:388:PX4:H59	4:A:402:PX4:H27	0.53	1.79	5	1
4:A:383:PX4:H27	4:A:399:PX4:H21	0.53	1.81	10	1
4:A:348:PX4:H16	4:A:355:PX4:H20	0.53	1.79	12	1
4:A:389:PX4:H53	4:A:398:PX4:H52	0.53	1.81	13	1
4:A:388:PX4:O1	4:A:396:PX4:H4	0.53	2.03	9	1
4:A:389:PX4:O2	4:A:398:PX4:H15	0.53	2.02	9	1
4:A:392:PX4:H24	4:A:399:PX4:H49	0.53	1.81	2	1
4:A:345:PX4:H16	4:A:346:PX4:O8	0.53	2.04	12	1
4:A:380:PX4:O2	4:A:381:PX4:H15	0.53	2.03	9	1
4:A:395:PX4:H42	4:A:415:PX4:H69	0.53	1.81	9	1
4:A:343:PX4:H69	4:A:344:PX4:H65	0.53	1.79	1	1
4:A:342:PX4:H49	4:A:351:PX4:H25	0.53	1.80	2	1
4:A:337:PX4:H54	4:A:345:PX4:H63	0.53	1.79	5	1
4:A:312:PX4:H17	4:A:359:PX4:H8	0.53	1.80	7	1
4:A:394:PX4:H53	4:A:401:PX4:H25	0.53	1.79	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:369:PX4:H44	4:A:430:PX4:H72	0.53	1.80	6	1
4:A:326:PX4:O2	4:A:350:PX4:H6	0.53	2.03	3	1
4:A:368:PX4:O1	4:A:418:PX4:H7	0.53	2.04	10	1
4:A:328:PX4:H54	4:A:329:PX4:H22	0.53	1.80	13	1
4:A:367:PX4:H26	4:A:430:PX4:H69	0.53	1.78	6	1
4:A:316:PX4:H64	4:A:368:PX4:H42	0.53	1.81	6	1
4:A:313:PX4:H45	4:A:354:PX4:H58	0.53	1.79	9	1
4:A:412:PX4:H63	4:A:421:PX4:H45	0.53	1.79	9	1
4:A:395:PX4:H39	4:A:415:PX4:H59	0.53	1.80	5	1
4:A:389:PX4:H34	4:A:397:PX4:H34	0.53	1.79	10	1
4:A:339:PX4:H19	4:A:347:PX4:H22	0.53	1.80	14	1
4:A:350:PX4:H66	4:A:350:PX4:H33	0.53	1.81	13	1
4:A:366:PX4:H32	4:A:427:PX4:H64	0.53	1.81	11	1
4:A:393:PX4:H68	4:A:394:PX4:H41	0.53	1.80	6	1
4:A:326:PX4:H44	4:A:350:PX4:H28	0.53	1.79	1	1
4:A:340:PX4:H49	4:A:341:PX4:H46	0.53	1.81	7	1
4:A:317:PX4:H20	4:A:342:PX4:H22	0.53	1.80	5	1
4:A:397:PX4:H23	4:A:398:PX4:H53	0.53	1.81	5	1
4:A:421:PX4:H33	4:A:430:PX4:H63	0.53	1.81	12	1
4:A:325:PX4:H29	4:A:325:PX4:H58	0.52	1.80	9	1
4:A:306:PX4:H24	4:A:360:PX4:H43	0.52	1.80	4	1
4:A:308:PX4:H51	4:A:311:PX4:H14	0.52	1.82	9	1
4:A:346:PX4:H44	4:A:362:PX4:H67	0.52	1.81	8	1
4:A:385:PX4:H60	4:A:399:PX4:H62	0.52	1.82	5	1
4:A:351:PX4:H66	4:A:409:PX4:H42	0.52	1.80	4	1
4:A:332:PX4:H47	4:A:347:PX4:H66	0.52	1.80	14	1
4:A:355:PX4:H5	4:A:362:PX4:H46	0.52	1.81	9	1
4:A:388:PX4:H19	4:A:396:PX4:H48	0.52	1.80	8	1
4:A:311:PX4:H71	4:A:426:PX4:H59	0.52	1.82	12	1
4:A:406:PX4:H34	4:A:424:PX4:H38	0.52	1.81	6	1
4:A:337:PX4:H18	4:A:337:PX4:O3	0.52	2.03	6	1
4:A:358:PX4:H16	4:A:358:PX4:H9	0.52	1.81	2	1
4:A:310:PX4:H35	4:A:409:PX4:H38	0.52	1.80	9	1
4:A:380:PX4:H31	4:A:381:PX4:H65	0.52	1.81	2	1
4:A:367:PX4:H24	4:A:424:PX4:H50	0.52	1.82	3	1
4:A:319:PX4:H58	4:A:319:PX4:H19	0.52	1.82	7	1
4:A:390:PX4:H24	4:A:428:PX4:H53	0.52	1.82	9	1
4:A:315:PX4:H58	4:A:322:PX4:H24	0.52	1.80	9	1
4:A:307:PX4:H53	4:A:361:PX4:H24	0.52	1.80	8	1
4:A:337:PX4:H50	4:A:345:PX4:H34	0.52	1.81	12	1
4:A:404:PX4:H9	4:A:419:PX4:O1	0.52	2.05	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:424:PX4:H50	4:A:429:PX4:H51	0.52	1.80	8	1
4:A:322:PX4:H26	4:A:333:PX4:H38	0.52	1.80	5	1
4:A:309:PX4:H16	4:A:320:PX4:H23	0.52	1.82	5	1
4:A:400:PX4:O1	4:A:401:PX4:H2	0.52	2.05	5	1
4:A:307:PX4:H52	4:A:356:PX4:H42	0.52	1.81	10	1
4:A:330:PX4:H26	4:A:344:PX4:H52	0.52	1.81	4	1
4:A:396:PX4:O2	4:A:396:PX4:H16	0.52	2.05	12	1
4:A:310:PX4:H25	4:A:363:PX4:H42	0.52	1.82	7	1
4:A:368:PX4:H58	4:A:424:PX4:H48	0.52	1.82	7	1
4:A:408:PX4:H67	4:A:409:PX4:H32	0.52	1.81	7	1
4:A:404:PX4:H53	4:A:413:PX4:H26	0.52	1.81	13	1
4:A:331:PX4:H56	4:A:339:PX4:H59	0.52	1.82	9	1
4:A:350:PX4:H45	4:A:363:PX4:C29	0.52	2.33	1	1
4:A:400:PX4:C14	4:A:401:PX4:H46	0.52	2.34	2	1
4:A:418:PX4:H26	4:A:425:PX4:C12	0.52	2.33	4	1
4:A:369:PX4:H56	4:A:425:PX4:H29	0.52	1.81	13	1
4:A:361:PX4:H44	4:A:415:PX4:H42	0.52	1.81	6	1
4:A:350:PX4:H22	4:A:363:PX4:H57	0.52	1.82	9	1
4:A:383:PX4:O6	4:A:399:PX4:H16	0.52	2.05	1	1
4:A:405:PX4:H10	4:A:414:PX4:H27	0.52	1.80	2	1
4:A:337:PX4:O1	4:A:357:PX4:H15	0.52	2.04	3	1
4:A:325:PX4:H41	4:A:394:PX4:H41	0.51	1.80	1	1
4:A:348:PX4:H32	4:A:355:PX4:H35	0.51	1.83	14	1
4:A:428:PX4:H52	4:A:429:PX4:H46	0.51	1.81	12	1
4:A:380:PX4:H39	4:A:402:PX4:H35	0.51	1.82	9	1
4:A:388:PX4:H57	4:A:411:PX4:H41	0.51	1.80	8	1
4:A:400:PX4:H20	4:A:409:PX4:H23	0.51	1.81	3	1
4:A:330:PX4:H41	4:A:344:PX4:H64	0.51	1.82	8	1
4:A:380:PX4:H20	4:A:381:PX4:H48	0.51	1.82	3	1
4:A:362:PX4:H44	4:A:409:PX4:H70	0.51	1.81	5	1
4:A:306:PX4:H41	4:A:329:PX4:H70	0.51	1.81	5	1
4:A:364:PX4:H60	4:A:426:PX4:H37	0.51	1.82	5	1
4:A:367:PX4:H48	4:A:430:PX4:H49	0.51	1.81	10	1
4:A:340:PX4:H37	4:A:350:PX4:H42	0.51	1.80	10	1
4:A:388:PX4:H35	4:A:405:PX4:H61	0.51	1.81	14	1
4:A:338:PX4:C6	4:A:348:PX4:H15	0.51	2.35	13	1
4:A:331:PX4:O1	4:A:332:PX4:H7	0.51	2.05	5	2
4:A:375:PX4:H51	4:A:389:PX4:H49	0.51	1.83	5	1
4:A:316:PX4:H27	4:A:368:PX4:H42	0.51	1.82	10	1
4:A:408:PX4:H51	4:A:409:PX4:H48	0.51	1.81	4	1
4:A:356:PX4:H35	4:A:362:PX4:H28	0.51	1.81	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:419:PX4:H31	4:A:430:PX4:H29	0.51	1.82	14	1
4:A:367:PX4:H41	4:A:375:PX4:H64	0.51	1.81	11	1
4:A:315:PX4:H36	4:A:361:PX4:H61	0.51	1.82	11	1
4:A:314:PX4:H54	4:A:361:PX4:H30	0.51	1.82	6	1
4:A:313:PX4:H49	4:A:327:PX4:H25	0.51	1.81	6	1
4:A:326:PX4:H47	4:A:363:PX4:H67	0.51	1.82	1	1
4:A:387:PX4:H47	4:A:411:PX4:H47	0.51	1.82	8	1
4:A:369:PX4:H50	4:A:424:PX4:H20	0.51	1.83	4	2
4:A:355:PX4:H17	4:A:356:PX4:H15	0.51	1.82	5	1
4:A:349:PX4:H43	4:A:415:PX4:H32	0.51	1.82	11	1
4:A:317:PX4:H45	4:A:326:PX4:H52	0.51	1.81	12	1
4:A:330:PX4:H35	4:A:336:PX4:H52	0.51	1.83	11	1
4:A:385:PX4:H62	4:A:392:PX4:H34	0.51	1.82	9	1
4:A:406:PX4:H27	4:A:423:PX4:H62	0.51	1.83	1	1
4:A:348:PX4:H16	4:A:355:PX4:H19	0.51	1.82	8	1
4:A:326:PX4:H21	4:A:363:PX4:H63	0.51	1.83	8	1
4:A:326:PX4:H17	4:A:363:PX4:H61	0.51	1.82	4	1
4:A:313:PX4:H50	4:A:327:PX4:H34	0.51	1.81	12	1
4:A:321:PX4:H42	4:A:367:PX4:H68	0.51	1.81	6	1
4:A:317:PX4:H29	4:A:363:PX4:H71	0.51	1.82	5	1
4:A:403:PX4:H10	4:A:411:PX4:O2	0.51	2.05	4	1
4:A:392:PX4:H58	4:A:414:PX4:H51	0.51	1.83	12	1
4:A:308:PX4:H53	4:A:311:PX4:H19	0.51	1.83	6	1
4:A:388:PX4:H35	4:A:395:PX4:H34	0.51	1.82	1	1
4:A:405:PX4:H6	4:A:414:PX4:H26	0.51	1.82	1	1
4:A:324:PX4:H59	4:A:342:PX4:H26	0.51	1.82	3	1
4:A:402:PX4:H55	4:A:404:PX4:H49	0.51	1.82	10	1
4:A:348:PX4:H71	4:A:348:PX4:H44	0.51	1.83	12	1
4:A:330:PX4:H60	4:A:337:PX4:H29	0.51	1.82	9	1
4:A:306:PX4:H14	4:A:321:PX4:H19	0.51	1.82	8	1
4:A:307:PX4:H64	4:A:314:PX4:H67	0.51	1.83	8	1
4:A:344:PX4:H62	4:A:347:PX4:H36	0.51	1.82	12	1
4:A:309:PX4:H39	4:A:319:PX4:H35	0.50	1.83	9	1
4:A:346:PX4:H7	4:A:353:PX4:H48	0.50	1.84	8	1
4:A:391:PX4:H34	4:A:407:PX4:H46	0.50	1.82	10	1
4:A:342:PX4:H39	4:A:394:PX4:H39	0.50	1.81	10	1
4:A:413:PX4:H60	4:A:421:PX4:H57	0.50	1.83	4	1
4:A:314:PX4:H51	4:A:364:PX4:H46	0.50	1.82	14	1
4:A:390:PX4:H63	4:A:429:PX4:H68	0.50	1.81	7	1
4:A:334:PX4:H47	4:A:350:PX4:H16	0.50	1.83	6	1
4:A:313:PX4:H68	4:A:328:PX4:H44	0.50	1.82	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:317:PX4:H20	4:A:324:PX4:H56	0.50	1.83	10	1
4:A:428:PX4:H14	4:A:429:PX4:H22	0.50	1.83	4	1
4:A:337:PX4:H26	4:A:357:PX4:H35	0.50	1.83	12	1
4:A:310:PX4:H30	4:A:364:PX4:H39	0.50	1.83	2	1
4:A:331:PX4:H61	4:A:333:PX4:H21	0.50	1.81	8	1
4:A:332:PX4:H30	4:A:339:PX4:H39	0.50	1.82	5	1
4:A:408:PX4:H15	4:A:409:PX4:C1	0.50	2.28	10	1
4:A:331:PX4:H59	4:A:339:PX4:H38	0.50	1.84	14	1
4:A:368:PX4:H4	4:A:418:PX4:O1	0.50	2.06	12	1
4:A:367:PX4:H21	4:A:424:PX4:H55	0.50	1.82	7	1
4:A:331:PX4:H47	4:A:347:PX4:H54	0.50	1.83	13	1
4:A:307:PX4:H36	4:A:361:PX4:H54	0.50	1.83	11	1
4:A:317:PX4:O8	4:A:342:PX4:H17	0.50	2.06	6	1
4:A:411:PX4:H45	4:A:421:PX4:H53	0.50	1.84	9	1
4:A:374:PX4:H36	4:A:427:PX4:H21	0.50	1.84	1	1
4:A:412:PX4:H26	4:A:419:PX4:H26	0.50	1.81	1	1
4:A:380:PX4:H16	4:A:381:PX4:H47	0.50	1.83	1	2
4:A:306:PX4:H52	4:A:322:PX4:H61	0.50	1.84	8	1
4:A:330:PX4:H12	4:A:344:PX4:H46	0.50	1.84	3	1
4:A:387:PX4:H72	4:A:402:PX4:H38	0.50	1.82	12	1
4:A:400:PX4:O4	4:A:401:PX4:H3	0.50	2.07	12	1
4:A:410:PX4:H62	4:A:417:PX4:H58	0.50	1.82	12	1
4:A:373:PX4:H28	4:A:381:PX4:H46	0.50	1.82	13	1
4:A:400:PX4:C10	4:A:401:PX4:H17	0.50	2.35	6	1
4:A:420:PX4:H17	4:A:427:PX4:H19	0.50	1.83	1	1
4:A:309:PX4:H16	4:A:320:PX4:H22	0.50	1.83	2	1
4:A:386:PX4:O1	4:A:387:PX4:H13	0.50	2.07	2	1
4:A:365:PX4:C23	4:A:366:PX4:H51	0.50	2.36	8	1
4:A:379:PX4:H56	4:A:379:PX4:H26	0.50	1.82	3	1
4:A:389:PX4:H67	4:A:398:PX4:H37	0.50	1.84	5	1
4:A:318:PX4:H17	4:A:327:PX4:H49	0.50	1.82	13	2
4:A:359:PX4:H63	4:A:420:PX4:H64	0.50	1.83	7	1
4:A:338:PX4:H55	4:A:356:PX4:H55	0.50	1.82	6	1
4:A:408:PX4:O3	4:A:409:PX4:H1	0.50	2.05	1	1
4:A:367:PX4:H68	4:A:421:PX4:H29	0.50	1.83	1	1
4:A:355:PX4:O4	4:A:356:PX4:H15	0.50	2.06	14	2
4:A:350:PX4:H19	4:A:363:PX4:H64	0.50	1.84	1	1
4:A:370:PX4:H13	4:A:411:PX4:O8	0.50	2.07	2	1
4:A:383:PX4:H24	4:A:390:PX4:H56	0.50	1.84	8	1
4:A:380:PX4:H35	4:A:380:PX4:H64	0.50	1.84	12	1
4:A:337:PX4:H16	4:A:357:PX4:H47	0.50	1.84	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:379:PX4:H47	4:A:384:PX4:H16	0.50	1.83	9	1
4:A:321:PX4:H11	4:A:362:PX4:O1	0.50	2.07	8	1
4:A:368:PX4:H11	4:A:369:PX4:O6	0.50	2.07	3	1
4:A:317:PX4:H40	4:A:326:PX4:H61	0.50	1.83	5	1
4:A:378:PX4:H39	4:A:418:PX4:H67	0.50	1.83	4	1
4:A:378:PX4:H28	4:A:417:PX4:H63	0.50	1.83	12	1
4:A:348:PX4:H36	4:A:396:PX4:H43	0.50	1.82	13	1
4:A:309:PX4:H48	4:A:319:PX4:H26	0.50	1.83	9	1
4:A:336:PX4:H33	4:A:339:PX4:H67	0.50	1.84	1	1
4:A:339:PX4:H57	4:A:339:PX4:H41	0.50	1.84	2	1
4:A:395:PX4:H57	4:A:421:PX4:H67	0.50	1.82	5	1
4:A:384:PX4:H21	4:A:385:PX4:H20	0.50	1.82	5	1
4:A:393:PX4:H3	4:A:394:PX4:O4	0.50	2.07	5	1
4:A:383:PX4:H40	4:A:390:PX4:H39	0.50	1.82	13	2
4:A:348:PX4:H40	4:A:395:PX4:H64	0.50	1.83	7	1
4:A:410:PX4:H46	4:A:426:PX4:C6	0.50	2.37	13	1
4:A:404:PX4:H26	4:A:413:PX4:H24	0.50	1.82	13	1
4:A:398:PX4:H20	4:A:407:PX4:H15	0.50	1.84	13	1
4:A:346:PX4:O8	4:A:362:PX4:H13	0.50	2.07	11	2
4:A:307:PX4:H45	4:A:425:PX4:H23	0.50	1.84	10	1
4:A:342:PX4:H14	4:A:351:PX4:H20	0.50	1.83	12	1
4:A:387:PX4:H67	4:A:402:PX4:H34	0.50	1.83	12	1
4:A:388:PX4:H32	4:A:397:PX4:H64	0.49	1.83	1	1
4:A:395:PX4:H40	4:A:405:PX4:H36	0.49	1.83	2	1
4:A:374:PX4:H30	4:A:412:PX4:H52	0.49	1.83	5	1
4:A:380:PX4:H34	4:A:387:PX4:H70	0.49	1.84	7	1
4:A:370:PX4:H19	4:A:403:PX4:O7	0.49	2.07	13	1
4:A:306:PX4:H34	4:A:328:PX4:H36	0.49	1.84	1	1
4:A:335:PX4:H17	4:A:343:PX4:O1	0.49	2.07	1	1
4:A:338:PX4:H16	4:A:345:PX4:H53	0.49	1.82	2	1
4:A:405:PX4:H40	4:A:422:PX4:H38	0.49	1.82	8	1
4:A:402:PX4:H62	4:A:404:PX4:H58	0.49	1.83	3	1
4:A:317:PX4:H46	4:A:342:PX4:H12	0.49	1.84	10	1
4:A:349:PX4:H33	4:A:363:PX4:H17	0.49	1.84	14	1
4:A:404:PX4:H6	4:A:430:PX4:O6	0.49	2.07	12	1
4:A:313:PX4:O2	4:A:360:PX4:H12	0.49	2.07	12	1
4:A:340:PX4:H16	4:A:341:PX4:H50	0.49	1.82	12	1
4:A:371:PX4:H34	4:A:377:PX4:H30	0.49	1.83	12	1
4:A:326:PX4:H36	4:A:332:PX4:H46	0.49	1.83	13	1
4:A:399:PX4:H58	4:A:407:PX4:H32	0.49	1.84	1	1
4:A:400:PX4:H54	4:A:416:PX4:H39	0.49	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:378:PX4:H46	4:A:418:PX4:H47	0.49	1.83	4	1
4:A:323:PX4:H26	4:A:333:PX4:H30	0.49	1.84	14	1
4:A:376:PX4:H35	4:A:418:PX4:H72	0.49	1.84	11	1
4:A:369:PX4:H56	4:A:423:PX4:H25	0.49	1.84	2	1
4:A:413:PX4:H21	4:A:430:PX4:H23	0.49	1.84	14	1
4:A:367:PX4:H54	4:A:412:PX4:H19	0.49	1.83	6	1
4:A:317:PX4:O7	4:A:324:PX4:H14	0.49	2.07	5	1
4:A:408:PX4:H32	4:A:425:PX4:H68	0.49	1.82	5	1
4:A:374:PX4:H45	4:A:419:PX4:H24	0.49	1.85	4	1
4:A:376:PX4:H44	4:A:377:PX4:H61	0.49	1.83	4	1
4:A:377:PX4:H55	4:A:378:PX4:H26	0.49	1.84	7	1
4:A:353:PX4:H20	4:A:366:PX4:H53	0.49	1.83	11	1
4:A:361:PX4:H59	4:A:425:PX4:H31	0.49	1.83	11	1
4:A:409:PX4:H13	4:A:409:PX4:H15	0.49	1.84	9	1
4:A:328:PX4:H24	4:A:360:PX4:H41	0.49	1.84	3	1
4:A:391:PX4:H42	4:A:414:PX4:H19	0.49	1.84	3	1
4:A:331:PX4:H15	4:A:332:PX4:H19	0.49	1.83	5	1
4:A:316:PX4:H58	4:A:316:PX4:H21	0.49	1.85	4	1
4:A:307:PX4:H48	4:A:361:PX4:H24	0.49	1.83	12	1
4:A:334:PX4:H48	4:A:349:PX4:O5	0.49	2.06	12	1
4:A:331:PX4:H29	4:A:340:PX4:H17	0.49	1.83	7	1
4:A:388:PX4:O2	4:A:395:PX4:H4	0.49	2.08	3	2
4:A:307:PX4:H46	4:A:314:PX4:H22	0.49	1.85	10	1
4:A:319:PX4:H39	4:A:377:PX4:H70	0.49	1.84	6	1
4:A:373:PX4:H15	4:A:373:PX4:H13	0.49	1.84	1	1
4:A:313:PX4:H54	4:A:327:PX4:H27	0.49	1.85	10	1
4:A:348:PX4:H26	4:A:355:PX4:C13	0.49	2.37	12	1
4:A:410:PX4:H54	4:A:417:PX4:H54	0.49	1.83	13	1
4:A:327:PX4:H32	4:A:329:PX4:H27	0.49	1.83	11	1
4:A:309:PX4:H15	4:A:319:PX4:O5	0.49	2.08	6	1
4:A:317:PX4:H55	4:A:342:PX4:H48	0.49	1.84	1	1
4:A:400:PX4:H1	4:A:401:PX4:O1	0.49	2.08	2	1
4:A:353:PX4:H28	4:A:366:PX4:H55	0.49	1.85	2	1
4:A:385:PX4:H55	4:A:393:PX4:H54	0.49	1.84	8	1
4:A:367:PX4:H28	4:A:424:PX4:H56	0.49	1.85	10	1
4:A:332:PX4:H62	4:A:415:PX4:H60	0.49	1.84	4	1
4:A:370:PX4:H30	4:A:403:PX4:H26	0.49	1.85	14	1
1:A:191:ILE:HG22	4:A:349:PX4:H3	0.49	1.85	12	1
4:A:306:PX4:H72	4:A:354:PX4:H51	0.49	1.84	6	1
4:A:318:PX4:H63	4:A:329:PX4:H44	0.49	1.85	6	1
4:A:325:PX4:H51	4:A:341:PX4:H49	0.49	1.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:348:PX4:H9	4:A:355:PX4:O2	0.49	2.08	3	2
4:A:371:PX4:H37	4:A:376:PX4:H42	0.49	1.84	5	1
4:A:405:PX4:H17	4:A:414:PX4:H22	0.49	1.85	14	1
4:A:354:PX4:H27	4:A:362:PX4:H60	0.49	1.85	11	1
4:A:355:PX4:H54	4:A:362:PX4:H53	0.49	1.84	11	1
4:A:376:PX4:H40	4:A:377:PX4:H57	0.49	1.83	11	1
4:A:403:PX4:H1	4:A:403:PX4:O6	0.48	2.08	10	1
4:A:315:PX4:H56	4:A:323:PX4:H16	0.48	1.85	4	1
4:A:391:PX4:H48	4:A:408:PX4:H20	0.48	1.83	14	1
4:A:418:PX4:H31	4:A:425:PX4:H22	0.48	1.85	13	1
4:A:346:PX4:H66	4:A:353:PX4:H66	0.48	1.83	6	1
4:A:315:PX4:H32	4:A:322:PX4:H48	0.48	1.83	9	1
4:A:306:PX4:H67	4:A:360:PX4:H30	0.48	1.86	8	1
4:A:306:PX4:H27	4:A:328:PX4:H53	0.48	1.84	3	1
4:A:388:PX4:H14	4:A:395:PX4:O3	0.48	2.08	13	3
4:A:306:PX4:H65	4:A:321:PX4:H17	0.48	1.84	10	1
4:A:310:PX4:H59	4:A:364:PX4:H30	0.48	1.83	7	1
4:A:321:PX4:H27	4:A:322:PX4:H59	0.48	1.84	13	1
4:A:331:PX4:H57	4:A:332:PX4:H29	0.48	1.85	5	1
4:A:353:PX4:H48	4:A:354:PX4:H62	0.48	1.84	12	1
4:A:313:PX4:H63	4:A:328:PX4:H38	0.48	1.84	10	1
4:A:346:PX4:H48	4:A:362:PX4:H50	0.48	1.85	4	1
4:A:328:PX4:H23	4:A:360:PX4:H33	0.48	1.85	14	1
4:A:380:PX4:H63	4:A:386:PX4:H20	0.48	1.85	7	1
4:A:370:PX4:H72	4:A:387:PX4:H71	0.48	1.84	9	1
1:A:163:PHE:CZ	1:A:212:LEU:HD11	0.48	2.43	9	1
4:A:318:PX4:H57	4:A:327:PX4:H54	0.48	1.84	10	1
4:A:322:PX4:H32	4:A:333:PX4:H55	0.48	1.86	14	1
4:A:306:PX4:H37	4:A:360:PX4:H38	0.48	1.83	2	1
4:A:316:PX4:H20	4:A:316:PX4:C25	0.48	2.38	10	1
4:A:322:PX4:H45	4:A:323:PX4:H65	0.48	1.84	4	1
4:A:358:PX4:H60	4:A:358:PX4:H36	0.48	1.86	4	1
4:A:417:PX4:H51	4:A:426:PX4:H46	0.48	1.85	4	1
4:A:343:PX4:H35	4:A:344:PX4:H28	0.48	1.84	13	1
4:A:328:PX4:H27	4:A:360:PX4:H36	0.48	1.85	13	1
4:A:368:PX4:H21	4:A:429:PX4:H62	0.48	1.84	9	1
4:A:332:PX4:O1	4:A:332:PX4:H7	0.48	2.09	2	1
4:A:393:PX4:H72	4:A:394:PX4:H32	0.48	1.84	2	1
4:A:323:PX4:H22	4:A:333:PX4:H49	0.48	1.86	12	1
4:A:405:PX4:H5	4:A:415:PX4:H17	0.48	1.85	7	1
4:A:336:PX4:H23	4:A:339:PX4:H57	0.48	1.86	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:350:PX4:H44	4:A:414:PX4:H42	0.48	1.84	9	1
4:A:309:PX4:H56	4:A:316:PX4:H50	0.48	1.84	8	1
4:A:333:PX4:H49	4:A:341:PX4:H14	0.48	1.85	8	1
4:A:351:PX4:H47	4:A:352:PX4:H19	0.48	1.86	3	1
4:A:358:PX4:H38	4:A:417:PX4:H45	0.48	1.84	12	1
4:A:400:PX4:H8	4:A:401:PX4:O6	0.48	2.09	13	1
4:A:343:PX4:H47	4:A:352:PX4:H53	0.48	1.84	11	1
4:A:345:PX4:H60	4:A:348:PX4:H22	0.48	1.85	11	1
4:A:400:PX4:H1	4:A:409:PX4:O1	0.48	2.09	9	1
4:A:336:PX4:H14	4:A:344:PX4:H51	0.48	1.86	5	1
4:A:349:PX4:H46	4:A:356:PX4:H11	0.48	1.86	4	1
4:A:392:PX4:H51	4:A:407:PX4:H23	0.48	1.86	4	1
4:A:377:PX4:H54	4:A:378:PX4:H30	0.48	1.85	6	1
4:A:396:PX4:H50	4:A:398:PX4:H28	0.48	1.85	1	1
4:A:393:PX4:H19	4:A:394:PX4:H48	0.48	1.85	8	1
4:A:388:PX4:H21	4:A:406:PX4:H70	0.48	1.85	5	1
4:A:388:PX4:H51	4:A:402:PX4:H19	0.48	1.85	5	1
4:A:318:PX4:H47	4:A:327:PX4:H46	0.48	1.85	14	1
4:A:382:PX4:H54	4:A:428:PX4:H27	0.48	1.84	12	1
4:A:381:PX4:H27	4:A:384:PX4:H54	0.48	1.84	13	1
4:A:393:PX4:H67	4:A:394:PX4:H33	0.47	1.84	1	1
4:A:387:PX4:H68	4:A:403:PX4:H36	0.47	1.86	10	1
4:A:392:PX4:H58	4:A:414:PX4:H50	0.47	1.86	4	1
4:A:319:PX4:H33	4:A:320:PX4:H29	0.47	1.85	14	1
4:A:330:PX4:H67	4:A:337:PX4:H36	0.47	1.86	12	1
4:A:308:PX4:H49	4:A:311:PX4:H4	0.47	1.85	13	1
4:A:422:PX4:H47	4:A:425:PX4:H50	0.47	1.86	9	1
4:A:317:PX4:H25	4:A:342:PX4:H28	0.47	1.83	1	1
4:A:314:PX4:H68	4:A:422:PX4:H64	0.47	1.85	2	1
4:A:309:PX4:H17	4:A:319:PX4:H25	0.47	1.87	8	1
4:A:336:PX4:H52	4:A:344:PX4:H57	0.47	1.86	8	1
1:A:138:PHE:CD1	1:A:149:PHE:CG	0.47	3.01	5	1
4:A:336:PX4:H38	4:A:344:PX4:H69	0.47	1.85	14	1
4:A:312:PX4:H48	4:A:359:PX4:H50	0.47	1.85	14	1
4:A:368:PX4:H8	4:A:369:PX4:O6	0.47	2.09	12	1
4:A:403:PX4:H8	4:A:411:PX4:O6	0.47	2.09	13	1
4:A:391:PX4:H44	4:A:395:PX4:H28	0.47	1.86	2	1
4:A:331:PX4:H5	4:A:348:PX4:O4	0.47	2.08	3	1
4:A:420:PX4:H27	4:A:427:PX4:H30	0.47	1.85	3	1
4:A:315:PX4:H65	4:A:323:PX4:H23	0.47	1.85	10	1
4:A:366:PX4:H44	4:A:374:PX4:H42	0.47	1.87	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:386:PX4:H46	4:A:387:PX4:H49	0.47	1.87	12	1
4:A:391:PX4:H62	4:A:415:PX4:H23	0.47	1.86	7	1
4:A:373:PX4:H28	4:A:381:PX4:C24	0.47	2.39	13	1
4:A:396:PX4:H34	4:A:396:PX4:H65	0.47	1.87	11	1
4:A:408:PX4:H17	4:A:415:PX4:O6	0.47	2.09	13	3
4:A:370:PX4:H23	4:A:403:PX4:H47	0.47	1.85	3	1
4:A:317:PX4:H32	4:A:363:PX4:H65	0.47	1.86	4	1
4:A:348:PX4:H44	4:A:405:PX4:H72	0.47	1.86	14	1
4:A:373:PX4:O2	4:A:381:PX4:H8	0.47	2.08	12	1
4:A:331:PX4:H27	4:A:331:PX4:H63	0.47	1.85	13	1
4:A:409:PX4:H55	4:A:416:PX4:H56	0.47	1.87	13	1
4:A:377:PX4:H46	4:A:378:PX4:H21	0.47	1.85	11	1
4:A:364:PX4:H68	4:A:422:PX4:H63	0.47	1.86	6	1
4:A:370:PX4:H20	4:A:403:PX4:H51	0.47	1.86	5	1
4:A:413:PX4:H56	4:A:430:PX4:H31	0.47	1.86	4	1
4:A:391:PX4:H39	4:A:414:PX4:H32	0.47	1.85	12	1
4:A:332:PX4:H60	4:A:393:PX4:H72	0.47	1.86	13	1
4:A:378:PX4:H47	4:A:410:PX4:H19	0.47	1.85	13	1
4:A:314:PX4:H68	4:A:361:PX4:H39	0.47	1.86	9	1
4:A:338:PX4:O7	4:A:348:PX4:H18	0.47	2.09	9	3
4:A:308:PX4:H13	4:A:310:PX4:H51	0.47	1.86	9	1
4:A:325:PX4:H57	4:A:341:PX4:H60	0.47	1.87	9	1
4:A:332:PX4:O1	4:A:356:PX4:H4	0.47	2.09	1	1
4:A:409:PX4:H52	4:A:415:PX4:H23	0.47	1.85	1	1
4:A:354:PX4:H65	4:A:366:PX4:H48	0.47	1.85	2	1
4:A:380:PX4:H51	4:A:381:PX4:H55	0.47	1.86	2	1
4:A:306:PX4:H23	4:A:360:PX4:H39	0.47	1.87	3	1
4:A:308:PX4:H57	4:A:310:PX4:H64	0.47	1.87	5	1
4:A:357:PX4:H69	4:A:357:PX4:H40	0.47	1.86	4	1
4:A:421:PX4:P1	4:A:423:PX4:H4	0.47	2.50	7	1
4:A:391:PX4:H71	4:A:408:PX4:H37	0.47	1.86	13	1
4:A:338:PX4:H30	4:A:348:PX4:H28	0.47	1.87	11	1
4:A:331:PX4:O1	4:A:332:PX4:H10	0.47	2.10	10	3
4:A:306:PX4:H58	4:A:321:PX4:H22	0.47	1.86	1	1
4:A:398:PX4:H19	4:A:407:PX4:H15	0.47	1.87	1	1
4:A:373:PX4:H54	4:A:375:PX4:H33	0.47	1.85	2	1
4:A:314:PX4:H70	4:A:349:PX4:H34	0.47	1.86	8	1
4:A:413:PX4:H54	4:A:423:PX4:H54	0.47	1.87	3	1
4:A:389:PX4:H63	4:A:389:PX4:H27	0.47	1.86	3	1
4:A:400:PX4:C11	4:A:408:PX4:H67	0.47	2.39	14	1
4:A:325:PX4:H22	4:A:326:PX4:H21	0.47	1.86	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:422:PX4:H67	4:A:426:PX4:H31	0.47	1.86	12	1
4:A:391:PX4:O2	4:A:414:PX4:H2	0.47	2.10	12	1
4:A:316:PX4:H36	4:A:378:PX4:H64	0.47	1.85	7	1
4:A:306:PX4:H38	4:A:329:PX4:H51	0.47	1.87	13	1
4:A:375:PX4:H48	4:A:382:PX4:H68	0.47	1.87	11	1
4:A:346:PX4:H60	4:A:362:PX4:H58	0.47	1.87	11	1
4:A:326:PX4:H40	4:A:350:PX4:H28	0.47	1.86	6	1
4:A:367:PX4:H65	4:A:421:PX4:H25	0.47	1.86	1	1
4:A:373:PX4:H36	4:A:397:PX4:H67	0.47	1.87	5	1
4:A:307:PX4:H50	4:A:314:PX4:H19	0.47	1.86	10	1
4:A:314:PX4:H71	4:A:409:PX4:H63	0.47	1.87	10	1
4:A:337:PX4:H31	4:A:343:PX4:H50	0.47	1.86	7	1
4:A:396:PX4:H30	4:A:397:PX4:H67	0.47	1.86	13	1
4:A:322:PX4:H17	4:A:333:PX4:H41	0.47	1.87	6	1
4:A:393:PX4:H13	4:A:394:PX4:O2	0.47	2.10	6	1
4:A:338:PX4:H62	4:A:356:PX4:H59	0.47	1.87	6	1
4:A:364:PX4:H45	4:A:426:PX4:H69	0.47	1.86	1	1
4:A:306:PX4:H3	4:A:329:PX4:O2	0.47	2.10	3	1
4:A:423:PX4:C7	4:A:424:PX4:H24	0.47	2.17	7	1
4:A:315:PX4:H2	4:A:316:PX4:H2	0.47	1.87	6	1
4:A:331:PX4:H57	4:A:332:PX4:H26	0.47	1.87	9	1
4:A:369:PX4:O1	4:A:425:PX4:H18	0.47	2.10	5	1
4:A:344:PX4:H50	4:A:347:PX4:H21	0.47	1.86	13	1
4:A:374:PX4:O2	4:A:420:PX4:H4	0.47	2.10	6	1
4:A:416:PX4:H5	4:A:426:PX4:O3	0.47	2.10	6	1
4:A:315:PX4:H7	4:A:316:PX4:O6	0.46	2.10	1	1
4:A:399:PX4:H54	4:A:407:PX4:H28	0.46	1.86	1	1
4:A:391:PX4:H33	4:A:407:PX4:H61	0.46	1.86	3	1
4:A:380:PX4:H68	4:A:386:PX4:H59	0.46	1.85	3	1
4:A:316:PX4:H72	4:A:316:PX4:H44	0.46	1.85	5	1
4:A:398:PX4:H21	4:A:407:PX4:H47	0.46	1.88	10	1
4:A:370:PX4:H22	4:A:403:PX4:H17	0.46	1.87	14	1
4:A:403:PX4:H29	4:A:413:PX4:H32	0.46	1.87	12	1
4:A:328:PX4:H11	4:A:360:PX4:H29	0.46	1.86	6	1
4:A:320:PX4:H40	4:A:418:PX4:H63	0.46	1.87	2	1
4:A:420:PX4:H40	4:A:427:PX4:H34	0.46	1.87	5	1
4:A:306:PX4:H70	4:A:328:PX4:H5	0.46	1.86	12	1
4:A:340:PX4:H44	4:A:399:PX4:H69	0.46	1.87	11	1
4:A:391:PX4:H17	4:A:408:PX4:H22	0.46	1.87	11	1
4:A:416:PX4:H63	4:A:416:PX4:H44	0.46	1.87	9	1
4:A:388:PX4:H51	4:A:406:PX4:H66	0.46	1.87	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:348:PX4:H50	4:A:355:PX4:H27	0.46	1.87	8	1
4:A:345:PX4:O6	4:A:353:PX4:H15	0.46	2.10	13	2
4:A:389:PX4:H21	4:A:398:PX4:H54	0.46	1.87	5	1
4:A:374:PX4:H39	4:A:427:PX4:H17	0.46	1.86	5	1
4:A:388:PX4:H39	4:A:405:PX4:H65	0.46	1.86	14	1
4:A:325:PX4:H15	4:A:325:PX4:H7	0.46	1.86	13	1
4:A:406:PX4:O2	4:A:415:PX4:H2	0.46	2.10	6	1
4:A:335:PX4:H59	4:A:344:PX4:H37	0.46	1.86	2	1
4:A:401:PX4:H22	4:A:408:PX4:H66	0.46	1.87	3	1
4:A:399:PX4:O7	4:A:407:PX4:H19	0.46	2.11	3	1
4:A:329:PX4:H5	4:A:333:PX4:H30	0.46	1.86	10	1
4:A:315:PX4:H46	4:A:316:PX4:H59	0.46	1.88	4	1
4:A:372:PX4:H59	4:A:384:PX4:H25	0.46	1.86	12	1
4:A:353:PX4:H43	4:A:413:PX4:H37	0.46	1.86	7	1
4:A:353:PX4:H23	4:A:357:PX4:H27	0.46	1.86	7	1
4:A:335:PX4:O1	4:A:343:PX4:H4	0.46	2.10	7	1
4:A:317:PX4:H35	4:A:342:PX4:H33	0.46	1.86	1	1
4:A:307:PX4:H27	4:A:361:PX4:H23	0.46	1.87	2	1
4:A:378:PX4:C6	4:A:410:PX4:H47	0.46	2.39	3	1
4:A:400:PX4:H22	4:A:401:PX4:O7	0.46	2.11	3	1
4:A:330:PX4:H21	4:A:343:PX4:H61	0.46	1.86	4	1
4:A:397:PX4:H40	4:A:398:PX4:H71	0.46	1.86	4	1
4:A:355:PX4:H68	4:A:422:PX4:H42	0.46	1.88	9	1
4:A:311:PX4:O6	4:A:311:PX4:H48	0.46	2.11	2	1
4:A:331:PX4:H14	4:A:347:PX4:H51	0.46	1.87	8	1
4:A:393:PX4:H33	4:A:394:PX4:H34	0.46	1.88	10	1
4:A:380:PX4:H62	4:A:387:PX4:H66	0.46	1.88	14	1
4:A:367:PX4:H28	4:A:424:PX4:H52	0.46	1.88	12	1
4:A:388:PX4:H44	4:A:405:PX4:H72	0.46	1.87	7	1
1:A:167:ALA:O	4:A:307:PX4:H6	0.46	2.10	8	2
4:A:325:PX4:H66	4:A:340:PX4:H66	0.46	1.87	8	1
4:A:330:PX4:H17	4:A:348:PX4:C27	0.46	2.41	14	1
1:A:153:ASN:O	4:A:331:PX4:H11	0.46	2.11	8	1
4:A:367:PX4:H48	4:A:412:PX4:H18	0.46	1.87	8	1
4:A:409:PX4:H51	4:A:415:PX4:H29	0.46	1.87	8	1
4:A:376:PX4:H53	4:A:377:PX4:H25	0.46	1.87	5	1
4:A:399:PX4:O2	4:A:399:PX4:H10	0.46	2.11	5	1
4:A:362:PX4:H64	4:A:413:PX4:H69	0.46	1.85	10	1
4:A:407:PX4:C7	4:A:414:PX4:H49	0.46	2.40	10	1
4:A:422:PX4:H22	4:A:425:PX4:H69	0.46	1.88	10	1
4:A:405:PX4:H22	4:A:406:PX4:H22	0.46	1.86	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:412:PX4:H64	4:A:428:PX4:H45	0.46	1.87	12	1
4:A:374:PX4:H29	4:A:427:PX4:H45	0.46	1.88	3	1
4:A:378:PX4:H9	4:A:417:PX4:H53	0.46	1.88	5	1
4:A:400:PX4:H59	4:A:400:PX4:H24	0.46	1.87	5	1
4:A:322:PX4:H33	4:A:424:PX4:H69	0.46	1.88	4	1
4:A:312:PX4:H19	4:A:366:PX4:H17	0.46	1.88	4	1
4:A:387:PX4:H17	4:A:411:PX4:H55	0.46	1.88	12	2
4:A:332:PX4:H4	4:A:356:PX4:O3	0.46	2.11	7	1
4:A:377:PX4:H46	4:A:378:PX4:H24	0.46	1.87	13	1
4:A:388:PX4:H23	4:A:396:PX4:H9	0.46	1.86	13	1
4:A:316:PX4:H52	4:A:333:PX4:H63	0.46	1.87	1	1
4:A:366:PX4:H34	4:A:427:PX4:H60	0.46	1.89	5	1
4:A:400:PX4:H60	4:A:422:PX4:H71	0.46	1.87	12	1
4:A:354:PX4:H47	4:A:360:PX4:H21	0.46	1.87	7	1
4:A:367:PX4:H47	4:A:412:PX4:H53	0.46	1.87	7	1
4:A:400:PX4:H10	4:A:409:PX4:O6	0.46	2.10	7	1
4:A:373:PX4:H21	4:A:381:PX4:H21	0.46	1.86	13	1
4:A:388:PX4:H51	4:A:411:PX4:H31	0.45	1.88	9	1
4:A:307:PX4:H34	4:A:321:PX4:H68	0.45	1.88	2	1
4:A:416:PX4:H63	4:A:422:PX4:H65	0.45	1.88	8	1
4:A:392:PX4:H35	4:A:399:PX4:H61	0.45	1.87	5	1
4:A:315:PX4:H41	4:A:323:PX4:H65	0.45	1.88	10	1
4:A:361:PX4:H38	4:A:362:PX4:H40	0.45	1.88	10	1
4:A:422:PX4:H17	4:A:425:PX4:H64	0.45	1.88	10	1
4:A:321:PX4:H55	4:A:354:PX4:H34	0.45	1.87	4	1
4:A:353:PX4:H29	4:A:357:PX4:H57	0.45	1.85	4	1
4:A:378:PX4:O3	4:A:378:PX4:H18	0.45	2.11	4	1
4:A:334:PX4:H61	4:A:356:PX4:H39	0.45	1.88	7	1
4:A:348:PX4:H43	4:A:402:PX4:H41	0.45	1.88	7	1
4:A:371:PX4:O6	4:A:371:PX4:H10	0.45	2.11	13	1
4:A:413:PX4:H57	4:A:430:PX4:H32	0.45	1.88	11	1
4:A:378:PX4:H18	4:A:378:PX4:H1	0.45	1.88	11	1
4:A:408:PX4:O3	4:A:409:PX4:H2	0.45	2.11	8	1
4:A:322:PX4:H71	4:A:430:PX4:H65	0.45	1.89	8	1
4:A:361:PX4:H37	4:A:409:PX4:H68	0.45	1.89	3	1
4:A:329:PX4:H46	4:A:336:PX4:H20	0.45	1.88	3	1
4:A:339:PX4:C11	4:A:347:PX4:H53	0.45	2.42	3	1
4:A:385:PX4:H66	4:A:399:PX4:H63	0.45	1.89	10	1
4:A:328:PX4:H33	4:A:359:PX4:H40	0.45	1.87	10	1
4:A:421:PX4:H45	4:A:430:PX4:H40	0.45	1.86	14	1
4:A:337:PX4:O1	4:A:338:PX4:H8	0.45	2.11	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:330:PX4:H34	4:A:343:PX4:H60	0.45	1.88	12	1
4:A:332:PX4:H1	4:A:332:PX4:O6	0.45	2.11	7	1
4:A:338:PX4:H52	4:A:345:PX4:H59	0.45	1.88	11	1
4:A:325:PX4:H18	4:A:334:PX4:H11	0.45	1.88	6	1
4:A:367:PX4:H34	4:A:428:PX4:H48	0.45	1.88	9	1
4:A:379:PX4:H24	4:A:384:PX4:H21	0.45	1.86	9	1
4:A:377:PX4:H51	4:A:378:PX4:H23	0.45	1.89	5	1
4:A:316:PX4:H41	4:A:368:PX4:H25	0.45	1.88	10	1
4:A:399:PX4:H39	4:A:407:PX4:H31	0.45	1.89	7	1
4:A:321:PX4:H8	4:A:362:PX4:O1	0.45	2.12	13	1
4:A:322:PX4:H69	4:A:413:PX4:H58	0.45	1.89	1	1
4:A:403:PX4:H54	4:A:419:PX4:H59	0.45	1.88	8	1
4:A:370:PX4:H40	4:A:404:PX4:H41	0.45	1.87	4	1
4:A:406:PX4:H31	4:A:424:PX4:H45	0.45	1.89	4	1
4:A:368:PX4:H50	4:A:369:PX4:H22	0.45	1.89	14	1
4:A:336:PX4:H34	4:A:339:PX4:H36	0.45	1.87	12	1
4:A:331:PX4:H61	4:A:339:PX4:H62	0.45	1.87	12	1
4:A:357:PX4:H28	4:A:357:PX4:H49	0.45	1.88	7	1
4:A:338:PX4:H23	4:A:348:PX4:H53	0.45	1.88	11	1
4:A:375:PX4:H27	4:A:382:PX4:H28	0.45	1.89	6	1
4:A:399:PX4:H10	4:A:399:PX4:H14	0.45	1.88	1	1
4:A:413:PX4:H70	4:A:430:PX4:H60	0.45	1.89	8	1
4:A:307:PX4:H12	4:A:361:PX4:O6	0.45	2.12	3	1
4:A:317:PX4:H54	4:A:342:PX4:H19	0.45	1.88	3	1
4:A:338:PX4:H69	4:A:346:PX4:H61	0.45	1.89	10	1
4:A:396:PX4:H52	4:A:398:PX4:H56	0.45	1.88	4	1
4:A:321:PX4:H47	4:A:354:PX4:H20	0.45	1.88	14	1
4:A:408:PX4:H29	4:A:415:PX4:H48	0.45	1.89	7	1
4:A:368:PX4:H51	4:A:369:PX4:H16	0.45	1.86	13	1
4:A:380:PX4:O8	4:A:381:PX4:H51	0.45	2.11	6	1
4:A:355:PX4:H61	4:A:405:PX4:H41	0.45	1.88	6	1
4:A:386:PX4:H58	4:A:411:PX4:H60	0.45	1.88	6	1
4:A:408:PX4:H51	4:A:415:PX4:H23	0.45	1.88	2	1
4:A:318:PX4:H53	4:A:336:PX4:H54	0.45	1.88	2	1
4:A:349:PX4:H71	4:A:356:PX4:H65	0.45	1.88	3	1
4:A:328:PX4:O6	4:A:328:PX4:H9	0.45	2.11	5	1
4:A:420:PX4:H48	4:A:427:PX4:H19	0.45	1.88	5	1
4:A:316:PX4:H46	4:A:319:PX4:H46	0.45	1.89	5	1
4:A:326:PX4:H40	4:A:350:PX4:H32	0.45	1.89	4	1
4:A:395:PX4:H59	4:A:406:PX4:H58	0.45	1.87	9	1
4:A:340:PX4:H54	4:A:341:PX4:H51	0.45	1.88	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:363:PX4:H23	4:A:364:PX4:H24	0.45	1.88	10	1
1:A:237:PHE:CD1	1:A:238:PRO:HD2	0.45	2.46	10	1
4:A:322:PX4:H68	4:A:430:PX4:H67	0.45	1.89	13	1
4:A:384:PX4:H7	4:A:386:PX4:O2	0.45	2.12	13	1
4:A:317:PX4:H54	4:A:324:PX4:H24	0.45	1.88	13	1
4:A:367:PX4:H23	4:A:368:PX4:H72	0.45	1.89	1	1
4:A:400:PX4:O2	4:A:409:PX4:H14	0.45	2.12	1	1
4:A:393:PX4:H32	4:A:394:PX4:H67	0.45	1.87	2	1
4:A:321:PX4:H25	4:A:322:PX4:H54	0.45	1.89	2	1
4:A:330:PX4:H28	4:A:344:PX4:H25	0.45	1.89	2	1
4:A:332:PX4:H35	4:A:355:PX4:H39	0.45	1.89	3	1
4:A:404:PX4:H10	4:A:430:PX4:O6	0.45	2.11	10	1
4:A:334:PX4:H70	4:A:406:PX4:H43	0.45	1.89	10	1
4:A:421:PX4:H42	4:A:423:PX4:H44	0.45	1.89	7	1
4:A:396:PX4:H45	4:A:398:PX4:H34	0.45	1.89	7	1
4:A:315:PX4:H29	4:A:425:PX4:H37	0.45	1.88	2	1
4:A:380:PX4:H19	4:A:381:PX4:H20	0.45	1.88	2	1
4:A:313:PX4:H52	4:A:328:PX4:H48	0.45	1.89	8	1
4:A:347:PX4:H41	4:A:348:PX4:H68	0.45	1.87	8	1
4:A:361:PX4:H29	4:A:362:PX4:H35	0.45	1.89	8	1
4:A:315:PX4:H64	4:A:316:PX4:H62	0.45	1.88	3	1
4:A:338:PX4:H59	4:A:345:PX4:H61	0.45	1.87	4	1
4:A:400:PX4:H26	4:A:400:PX4:H59	0.45	1.88	4	1
4:A:367:PX4:O5	4:A:428:PX4:H17	0.45	2.11	7	1
4:A:368:PX4:H24	4:A:390:PX4:H56	0.45	1.87	7	1
4:A:413:PX4:H22	4:A:430:PX4:H19	0.45	1.88	7	1
4:A:383:PX4:H22	4:A:399:PX4:H48	0.45	1.89	13	1
4:A:307:PX4:H13	4:A:361:PX4:O6	0.45	2.12	11	1
4:A:380:PX4:H52	4:A:386:PX4:H49	0.45	1.88	6	1
4:A:358:PX4:H22	4:A:365:PX4:H26	0.45	1.89	9	1
4:A:378:PX4:H3	4:A:410:PX4:O8	0.45	2.12	1	1
4:A:346:PX4:H14	4:A:362:PX4:H3	0.45	1.88	3	1
4:A:348:PX4:H1	4:A:355:PX4:H14	0.45	1.88	3	1
4:A:307:PX4:H42	4:A:364:PX4:H68	0.45	1.87	10	1
4:A:402:PX4:H67	4:A:421:PX4:H55	0.45	1.88	12	1
4:A:366:PX4:H43	4:A:412:PX4:H40	0.45	1.87	11	1
4:A:374:PX4:H17	4:A:382:PX4:H51	0.45	1.89	6	1
4:A:366:PX4:H34	4:A:427:PX4:H72	0.45	1.87	6	1
4:A:357:PX4:H20	4:A:358:PX4:H16	0.44	1.88	4	2
4:A:330:PX4:H53	4:A:338:PX4:C11	0.44	2.42	4	1
4:A:394:PX4:H19	4:A:401:PX4:H23	0.44	1.89	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:334:PX4:H52	4:A:349:PX4:H20	0.44	1.88	7	1
4:A:350:PX4:H22	4:A:363:PX4:H55	0.44	1.89	13	1
4:A:380:PX4:H16	4:A:381:PX4:H48	0.44	1.90	6	1
4:A:374:PX4:H17	4:A:382:PX4:H50	0.44	1.90	1	1
4:A:317:PX4:H19	4:A:325:PX4:H46	0.44	1.87	2	1
4:A:341:PX4:H70	4:A:407:PX4:H41	0.44	1.88	2	1
4:A:391:PX4:H35	4:A:415:PX4:H65	0.44	1.88	2	1
4:A:321:PX4:H59	4:A:354:PX4:H35	0.44	1.90	4	1
4:A:373:PX4:H36	4:A:396:PX4:H30	0.44	1.89	4	1
4:A:361:PX4:H30	4:A:362:PX4:H39	0.44	1.88	12	1
4:A:313:PX4:H31	4:A:360:PX4:H26	0.44	1.88	13	1
4:A:367:PX4:H68	4:A:428:PX4:H21	0.44	1.88	8	1
4:A:346:PX4:H21	4:A:362:PX4:H51	0.44	1.90	4	1
4:A:346:PX4:H20	4:A:362:PX4:H2	0.44	1.89	7	1
4:A:308:PX4:H41	4:A:310:PX4:H41	0.44	1.89	3	1
4:A:331:PX4:H58	4:A:331:PX4:H24	0.44	1.88	5	1
4:A:357:PX4:H35	4:A:358:PX4:H33	0.44	1.89	5	1
4:A:328:PX4:H17	4:A:360:PX4:H39	0.44	1.88	10	1
4:A:311:PX4:H10	4:A:320:PX4:H22	0.44	1.89	10	1
4:A:419:PX4:H56	4:A:427:PX4:H51	0.44	1.88	13	1
4:A:421:PX4:H19	4:A:430:PX4:H16	0.44	1.88	6	1
4:A:340:PX4:H2	4:A:340:PX4:O6	0.44	2.13	6	1
4:A:400:PX4:H22	4:A:408:PX4:H66	0.44	1.89	2	1
4:A:389:PX4:H57	4:A:390:PX4:H35	0.44	1.88	3	1
4:A:368:PX4:H52	4:A:369:PX4:H28	0.44	1.90	12	1
4:A:398:PX4:H52	4:A:398:PX4:H32	0.44	1.88	12	1
4:A:371:PX4:H14	4:A:377:PX4:H4	0.44	1.89	12	1
4:A:367:PX4:H62	4:A:430:PX4:H34	0.44	1.89	6	1
4:A:357:PX4:H23	4:A:358:PX4:H23	0.44	1.89	9	1
4:A:322:PX4:H70	4:A:421:PX4:H69	0.44	1.90	1	1
4:A:358:PX4:H40	4:A:366:PX4:H70	0.44	1.88	8	1
4:A:395:PX4:H62	4:A:406:PX4:H71	0.44	1.89	8	1
4:A:355:PX4:H17	4:A:356:PX4:H49	0.44	1.89	10	1
4:A:308:PX4:H24	4:A:364:PX4:H52	0.44	1.89	4	1
4:A:374:PX4:H27	4:A:428:PX4:H35	0.44	1.90	14	1
4:A:336:PX4:H39	4:A:389:PX4:H68	0.44	1.89	12	1
4:A:373:PX4:H38	4:A:402:PX4:H33	0.44	1.89	6	1
4:A:374:PX4:H27	4:A:427:PX4:H22	0.44	1.90	6	1
4:A:367:PX4:H19	4:A:368:PX4:H67	0.44	1.88	2	1
4:A:328:PX4:H28	4:A:360:PX4:H40	0.44	1.89	2	1
4:A:366:PX4:H43	4:A:419:PX4:H30	0.44	1.90	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:402:PX4:H17	4:A:411:PX4:H22	0.44	1.90	2	1
4:A:366:PX4:H37	4:A:412:PX4:H35	0.44	1.90	3	1
4:A:332:PX4:H1	4:A:356:PX4:O3	0.44	2.12	10	1
4:A:353:PX4:H57	4:A:354:PX4:H56	0.44	1.89	6	1
4:A:412:PX4:H27	4:A:419:PX4:H47	0.44	1.89	6	1
4:A:307:PX4:H52	4:A:314:PX4:H17	0.44	1.90	1	1
4:A:377:PX4:H60	4:A:418:PX4:H66	0.44	1.89	1	1
4:A:321:PX4:H7	4:A:354:PX4:O4	0.44	2.12	2	1
4:A:396:PX4:H62	4:A:398:PX4:H45	0.44	1.88	8	1
4:A:317:PX4:H26	4:A:325:PX4:H52	0.44	1.90	3	1
4:A:341:PX4:H70	4:A:393:PX4:H70	0.44	1.90	5	1
4:A:418:PX4:C13	4:A:425:PX4:H24	0.44	2.38	4	1
4:A:373:PX4:H27	4:A:396:PX4:H22	0.44	1.89	14	1
4:A:313:PX4:H6	4:A:359:PX4:O2	0.44	2.13	13	1
4:A:346:PX4:H39	4:A:355:PX4:H59	0.44	1.90	11	1
4:A:402:PX4:H59	4:A:404:PX4:H54	0.44	1.88	11	1
4:A:322:PX4:H36	4:A:333:PX4:H36	0.44	1.90	9	1
4:A:316:PX4:H25	4:A:320:PX4:H33	0.44	1.90	1	1
4:A:409:PX4:H60	4:A:409:PX4:H66	0.44	1.45	14	1
4:A:410:PX4:H31	4:A:416:PX4:H39	0.44	1.89	12	1
4:A:345:PX4:H46	4:A:348:PX4:H7	0.44	1.89	13	1
4:A:322:PX4:H19	4:A:323:PX4:H21	0.44	1.89	6	1
4:A:355:PX4:H68	4:A:422:PX4:C21	0.43	2.42	9	1
4:A:338:PX4:H62	4:A:345:PX4:H65	0.43	1.89	2	1
4:A:371:PX4:H10	4:A:377:PX4:O6	0.43	2.13	2	1
4:A:337:PX4:H27	4:A:357:PX4:H37	0.43	1.88	8	1
4:A:402:PX4:H67	4:A:411:PX4:H44	0.43	1.90	8	1
4:A:326:PX4:H37	4:A:414:PX4:H38	0.43	1.88	3	1
4:A:324:PX4:H68	4:A:325:PX4:H34	0.43	1.90	5	1
4:A:368:PX4:C27	4:A:424:PX4:H48	0.43	2.43	5	1
4:A:306:PX4:H69	4:A:354:PX4:H22	0.43	1.90	10	1
4:A:399:PX4:H51	4:A:407:PX4:H31	0.43	1.89	10	1
4:A:308:PX4:H53	4:A:311:PX4:H14	0.43	1.90	10	1
4:A:331:PX4:H24	4:A:340:PX4:C8	0.43	2.43	7	1
4:A:360:PX4:H62	4:A:366:PX4:H68	0.43	1.89	11	1
4:A:314:PX4:H50	4:A:361:PX4:H26	0.43	1.89	6	1
4:A:360:PX4:H57	4:A:366:PX4:H20	0.43	1.90	9	1
4:A:424:PX4:H58	4:A:428:PX4:C31	0.43	2.43	1	1
4:A:317:PX4:H65	4:A:342:PX4:H62	0.43	1.90	2	1
4:A:383:PX4:C18	4:A:407:PX4:H26	0.43	2.42	3	1
4:A:337:PX4:H22	4:A:337:PX4:H27	0.43	1.55	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:322:PX4:H17	4:A:333:PX4:H44	0.43	1.89	10	1
4:A:403:PX4:O6	4:A:403:PX4:H12	0.43	2.13	4	1
4:A:334:PX4:H44	4:A:347:PX4:H65	0.43	1.89	14	1
4:A:420:PX4:H22	4:A:427:PX4:H27	0.43	1.90	12	1
1:A:165:ARG:NH1	4:A:354:PX4:O1	0.43	2.52	6	2
4:A:334:PX4:H21	4:A:356:PX4:H10	0.43	1.89	12	2
4:A:308:PX4:H17	4:A:364:PX4:O1	0.43	2.12	1	1
4:A:335:PX4:H35	4:A:337:PX4:H37	0.43	1.91	8	1
4:A:316:PX4:H38	4:A:368:PX4:H30	0.43	1.89	8	1
4:A:421:PX4:H19	4:A:430:PX4:H21	0.43	1.90	5	1
4:A:370:PX4:H54	4:A:403:PX4:H26	0.43	1.90	10	1
4:A:343:PX4:H18	4:A:352:PX4:H57	0.43	1.91	10	1
4:A:353:PX4:O6	4:A:357:PX4:H46	0.43	2.13	14	1
4:A:325:PX4:H58	4:A:325:PX4:H26	0.43	1.90	12	1
4:A:385:PX4:H49	4:A:385:PX4:H54	0.43	1.54	12	1
4:A:314:PX4:O8	4:A:364:PX4:H4	0.43	2.13	11	1
4:A:424:PX4:H66	4:A:424:PX4:H61	0.43	1.54	9	1
4:A:311:PX4:H27	4:A:311:PX4:H60	0.43	1.89	2	1
4:A:405:PX4:H23	4:A:406:PX4:H17	0.43	1.89	8	1
4:A:370:PX4:H35	4:A:404:PX4:H27	0.43	1.89	8	1
4:A:331:PX4:H45	4:A:341:PX4:H68	0.43	1.90	10	1
4:A:326:PX4:H68	4:A:415:PX4:H42	0.43	1.90	10	1
4:A:380:PX4:H53	4:A:387:PX4:H57	0.43	1.91	10	1
4:A:370:PX4:H61	4:A:411:PX4:H54	0.43	1.90	4	1
4:A:392:PX4:H54	4:A:414:PX4:H47	0.43	1.89	4	1
4:A:308:PX4:H63	4:A:308:PX4:H56	0.43	1.47	4	1
4:A:315:PX4:H29	4:A:418:PX4:H42	0.43	1.91	14	1
4:A:422:PX4:C8	4:A:425:PX4:H56	0.43	2.33	13	1
4:A:336:PX4:H22	4:A:344:PX4:H55	0.43	1.90	11	1
4:A:400:PX4:H1	4:A:409:PX4:O4	0.43	2.13	11	1
4:A:315:PX4:H40	4:A:368:PX4:H45	0.43	1.91	6	1
4:A:316:PX4:H65	4:A:333:PX4:H72	0.43	1.90	6	1
4:A:409:PX4:H59	4:A:415:PX4:H34	0.43	1.91	1	1
4:A:314:PX4:H71	4:A:416:PX4:H38	0.43	1.90	1	1
4:A:318:PX4:H15	4:A:327:PX4:H15	0.43	1.91	3	1
4:A:330:PX4:H45	4:A:347:PX4:H38	0.43	1.90	5	1
4:A:400:PX4:H13	4:A:401:PX4:O1	0.43	2.13	10	1
4:A:348:PX4:H10	4:A:355:PX4:O2	0.43	2.13	4	1
4:A:310:PX4:C22	4:A:351:PX4:H66	0.43	2.43	12	1
4:A:356:PX4:H61	4:A:356:PX4:H66	0.43	1.59	12	1
4:A:330:PX4:H68	4:A:380:PX4:H44	0.43	1.90	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:354:PX4:H67	4:A:366:PX4:C27	0.43	2.43	13	1
4:A:349:PX4:H71	4:A:356:PX4:H55	0.43	1.88	13	1
4:A:360:PX4:H51	4:A:366:PX4:H18	0.43	1.89	11	1
4:A:361:PX4:H63	4:A:369:PX4:H34	0.43	1.90	11	1
4:A:428:PX4:H12	4:A:428:PX4:O2	0.43	2.14	6	1
4:A:367:PX4:H58	4:A:430:PX4:H26	0.43	1.90	6	1
4:A:380:PX4:C26	4:A:381:PX4:H55	0.43	2.44	2	1
4:A:338:PX4:O8	4:A:345:PX4:H49	0.43	2.13	2	1
4:A:410:PX4:H34	4:A:410:PX4:H27	0.43	1.58	14	2
4:A:378:PX4:H53	4:A:410:PX4:H58	0.43	1.90	3	1
4:A:372:PX4:C35	4:A:393:PX4:H41	0.43	2.44	3	1
4:A:331:PX4:H51	4:A:332:PX4:H21	0.43	1.89	10	1
4:A:351:PX4:H23	4:A:352:PX4:H17	0.43	1.91	12	1
4:A:417:PX4:H47	4:A:426:PX4:H52	0.43	1.89	13	1
4:A:406:PX4:H49	4:A:421:PX4:H49	0.43	1.91	13	1
4:A:334:PX4:H53	4:A:334:PX4:H21	0.43	1.91	11	1
4:A:375:PX4:H23	4:A:382:PX4:H24	0.43	1.89	6	1
4:A:369:PX4:H30	4:A:429:PX4:H57	0.43	1.91	6	1
4:A:337:PX4:H31	4:A:352:PX4:H54	0.43	1.89	9	1
4:A:391:PX4:C20	4:A:405:PX4:H69	0.43	2.40	9	1
4:A:326:PX4:H65	4:A:350:PX4:H37	0.43	1.91	1	1
4:A:388:PX4:H46	4:A:395:PX4:H47	0.43	1.90	8	1
4:A:373:PX4:H25	4:A:397:PX4:H23	0.43	1.90	8	1
4:A:392:PX4:H48	4:A:399:PX4:H56	0.43	1.89	8	1
4:A:321:PX4:H28	4:A:329:PX4:H72	0.43	1.89	10	1
4:A:388:PX4:H38	4:A:388:PX4:H66	0.43	1.91	4	1
4:A:404:PX4:H55	4:A:413:PX4:H25	0.43	1.90	4	1
4:A:375:PX4:H55	4:A:382:PX4:H71	0.43	1.89	14	1
4:A:317:PX4:H65	4:A:342:PX4:H60	0.43	1.89	14	1
4:A:385:PX4:H50	4:A:392:PX4:H16	0.43	1.90	13	1
4:A:330:PX4:H65	4:A:343:PX4:H65	0.43	1.90	6	1
4:A:317:PX4:H50	4:A:342:PX4:H47	0.43	1.90	9	1
4:A:327:PX4:H23	4:A:329:PX4:H36	0.43	1.91	9	1
4:A:318:PX4:H63	4:A:318:PX4:H56	0.43	1.60	1	1
4:A:403:PX4:H20	4:A:404:PX4:H22	0.43	1.89	2	1
4:A:422:PX4:H52	4:A:425:PX4:H48	0.43	1.90	8	1
4:A:370:PX4:H50	4:A:411:PX4:H59	0.43	1.90	7	1
4:A:306:PX4:H45	4:A:329:PX4:H55	0.43	1.91	13	1
4:A:367:PX4:H66	4:A:412:PX4:H63	0.43	1.91	11	1
4:A:406:PX4:H28	4:A:423:PX4:H58	0.43	1.89	9	1
4:A:316:PX4:H23	4:A:418:PX4:H36	0.43	1.91	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:369:PX4:O2	4:A:425:PX4:H10	0.43	2.14	1	1
4:A:322:PX4:H41	4:A:323:PX4:H71	0.43	1.89	8	1
4:A:411:PX4:H62	4:A:411:PX4:H69	0.43	1.47	3	1
4:A:395:PX4:H41	4:A:406:PX4:H67	0.43	1.91	14	1
4:A:331:PX4:H49	4:A:336:PX4:H28	0.43	1.91	12	1
4:A:389:PX4:H26	4:A:397:PX4:H31	0.43	1.90	12	1
4:A:394:PX4:H15	4:A:401:PX4:H20	0.43	1.91	7	1
4:A:378:PX4:C25	4:A:417:PX4:H67	0.43	2.43	13	1
4:A:370:PX4:H19	4:A:370:PX4:H25	0.43	1.59	11	1
4:A:310:PX4:H54	4:A:364:PX4:H23	0.43	1.91	6	1
4:A:306:PX4:H31	4:A:329:PX4:H60	0.43	1.90	6	1
4:A:307:PX4:H56	4:A:349:PX4:H7	0.43	1.90	9	1
4:A:325:PX4:H38	4:A:326:PX4:H30	0.43	1.91	2	1
4:A:346:PX4:H16	4:A:362:PX4:H4	0.43	1.89	8	1
4:A:381:PX4:H61	4:A:396:PX4:H27	0.43	1.90	3	1
4:A:332:PX4:H62	4:A:414:PX4:H36	0.43	1.90	5	1
4:A:315:PX4:H60	4:A:323:PX4:H59	0.43	1.91	14	1
4:A:346:PX4:H52	4:A:362:PX4:H54	0.43	1.91	12	1
4:A:350:PX4:H41	4:A:414:PX4:H39	0.43	1.89	7	1
4:A:332:PX4:H15	4:A:334:PX4:H19	0.43	1.91	13	1
4:A:395:PX4:H61	4:A:406:PX4:H67	0.43	1.90	11	1
4:A:368:PX4:H53	4:A:424:PX4:H48	0.43	1.91	11	1
4:A:330:PX4:H39	4:A:344:PX4:H72	0.42	1.91	9	1
4:A:324:PX4:H42	4:A:372:PX4:H70	0.42	1.91	3	1
4:A:404:PX4:H28	4:A:419:PX4:H48	0.42	1.91	10	1
4:A:345:PX4:H31	4:A:357:PX4:H54	0.42	1.90	12	1
4:A:390:PX4:H45	4:A:407:PX4:H27	0.42	1.90	12	1
4:A:423:PX4:H19	4:A:425:PX4:H48	0.42	1.91	7	1
4:A:405:PX4:H48	4:A:414:PX4:H20	0.42	1.90	11	1
4:A:401:PX4:H61	4:A:401:PX4:H66	0.42	1.44	6	1
4:A:404:PX4:H13	4:A:430:PX4:O6	0.42	2.14	9	1
4:A:345:PX4:H33	4:A:354:PX4:H66	0.42	1.90	1	1
4:A:325:PX4:H35	4:A:341:PX4:H72	0.42	1.91	8	1
4:A:345:PX4:H53	4:A:346:PX4:H51	0.42	1.91	5	1
4:A:367:PX4:H50	4:A:419:PX4:H26	0.42	1.91	10	1
4:A:307:PX4:H22	4:A:361:PX4:H19	0.42	1.91	4	1
4:A:330:PX4:H56	4:A:357:PX4:H64	0.42	1.90	12	1
4:A:400:PX4:C31	4:A:422:PX4:H71	0.42	2.44	12	1
4:A:394:PX4:H2	4:A:401:PX4:O2	0.42	2.14	6	1
4:A:421:PX4:H23	4:A:430:PX4:H48	0.42	1.91	6	1
4:A:395:PX4:H36	4:A:406:PX4:H60	0.42	1.91	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:308:PX4:H29	4:A:416:PX4:H33	0.42	1.92	9	1
4:A:312:PX4:H31	4:A:366:PX4:H46	0.42	1.89	1	1
4:A:400:PX4:H38	4:A:400:PX4:H44	0.42	1.77	8	1
4:A:368:PX4:C34	4:A:424:PX4:H17	0.42	2.44	8	1
4:A:345:PX4:H9	4:A:353:PX4:O2	0.42	2.14	5	1
4:A:382:PX4:H45	4:A:397:PX4:H44	0.42	1.91	5	1
4:A:306:PX4:H44	4:A:367:PX4:C22	0.42	2.45	5	1
4:A:332:PX4:H44	4:A:340:PX4:H45	0.42	1.91	4	1
4:A:327:PX4:H30	4:A:359:PX4:H25	0.42	1.91	4	1
4:A:307:PX4:H18	4:A:314:PX4:H49	0.42	1.91	14	1
4:A:314:PX4:H36	4:A:356:PX4:H25	0.42	1.91	14	1
4:A:355:PX4:H30	4:A:356:PX4:H62	0.42	1.91	7	1
4:A:370:PX4:H67	4:A:403:PX4:H38	0.42	1.92	7	1
4:A:407:PX4:H22	4:A:407:PX4:H27	0.42	1.63	13	1
4:A:400:PX4:H69	4:A:400:PX4:H62	0.42	1.51	13	1
4:A:350:PX4:H54	4:A:363:PX4:H50	0.42	1.91	13	1
4:A:329:PX4:H72	4:A:329:PX4:H64	0.42	1.41	11	1
4:A:390:PX4:H64	4:A:390:PX4:H59	0.42	1.59	1	1
4:A:392:PX4:H59	4:A:407:PX4:H29	0.42	1.91	2	1
4:A:386:PX4:H59	4:A:387:PX4:H72	0.42	1.92	2	1
4:A:389:PX4:H47	4:A:398:PX4:H17	0.42	1.90	5	2
4:A:353:PX4:H70	4:A:424:PX4:H43	0.42	1.92	10	1
4:A:322:PX4:C18	4:A:424:PX4:H69	0.42	2.44	4	1
4:A:359:PX4:H10	4:A:359:PX4:O8	0.42	2.15	4	1
4:A:417:PX4:H46	4:A:426:PX4:H58	0.42	1.91	12	1
4:A:340:PX4:H56	4:A:341:PX4:H20	0.42	1.91	12	1
4:A:355:PX4:H5	4:A:362:PX4:O8	0.42	2.14	13	1
4:A:386:PX4:H48	4:A:387:PX4:H48	0.42	1.92	13	1
4:A:336:PX4:H25	4:A:344:PX4:H60	0.42	1.90	9	1
4:A:330:PX4:H46	4:A:337:PX4:H17	0.42	1.90	5	2
1:A:163:PHE:HZ	1:A:212:LEU:HD11	0.42	1.74	9	1
4:A:317:PX4:H36	4:A:317:PX4:H29	0.42	1.50	8	1
4:A:410:PX4:H30	4:A:410:PX4:H23	0.42	1.48	3	1
4:A:357:PX4:H39	4:A:358:PX4:H37	0.42	1.90	5	1
4:A:370:PX4:H32	4:A:404:PX4:H27	0.42	1.90	5	1
4:A:391:PX4:H26	4:A:414:PX4:H17	0.42	1.90	10	1
4:A:422:PX4:H22	4:A:425:PX4:H66	0.42	1.92	4	1
4:A:330:PX4:H16	4:A:343:PX4:H5	0.42	1.90	14	1
4:A:353:PX4:H36	4:A:413:PX4:H43	0.42	1.89	14	1
4:A:320:PX4:H43	4:A:376:PX4:H31	0.42	1.90	13	1
4:A:376:PX4:H14	4:A:377:PX4:O2	0.42	2.15	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:422:PX4:H20	4:A:422:PX4:H26	0.42	1.69	3	1
4:A:424:PX4:H64	4:A:429:PX4:H59	0.42	1.92	3	1
4:A:330:PX4:H51	4:A:337:PX4:H53	0.42	1.91	3	1
4:A:335:PX4:H42	4:A:344:PX4:H37	0.42	1.92	5	1
4:A:328:PX4:H19	4:A:360:PX4:H21	0.42	1.92	10	1
4:A:332:PX4:H49	4:A:334:PX4:H32	0.42	1.92	11	1
4:A:306:PX4:H58	4:A:306:PX4:H65	0.42	1.65	11	1
4:A:334:PX4:H70	4:A:349:PX4:H61	0.42	1.92	1	1
4:A:388:PX4:H50	4:A:397:PX4:H58	0.42	1.91	1	1
4:A:346:PX4:H22	4:A:354:PX4:H20	0.42	1.91	8	1
4:A:315:PX4:H64	4:A:315:PX4:H44	0.42	1.91	8	1
4:A:384:PX4:H23	4:A:385:PX4:H24	0.42	1.91	3	1
4:A:322:PX4:H17	4:A:333:PX4:C22	0.42	2.44	10	1
4:A:322:PX4:H36	4:A:323:PX4:H57	0.42	1.91	4	1
1:A:116:TYR:CD2	1:A:138:PHE:CE2	0.42	3.07	4	1
1:A:165:ARG:NH1	4:A:354:PX4:H10	0.42	2.30	12	1
4:A:395:PX4:H19	4:A:405:PX4:H16	0.42	1.92	9	1
4:A:332:PX4:H63	4:A:415:PX4:H63	0.42	1.91	9	1
4:A:320:PX4:H37	4:A:378:PX4:H39	0.42	1.91	9	1
4:A:314:PX4:H63	4:A:314:PX4:H56	0.42	1.62	1	1
4:A:388:PX4:H56	4:A:402:PX4:H57	0.42	1.91	1	1
4:A:424:PX4:H54	4:A:428:PX4:H61	0.42	1.92	1	1
4:A:391:PX4:H63	4:A:391:PX4:H56	0.42	1.60	2	1
4:A:319:PX4:H31	4:A:319:PX4:H37	0.42	1.73	2	1
4:A:349:PX4:H37	4:A:349:PX4:H32	0.42	1.60	8	1
4:A:395:PX4:H58	4:A:406:PX4:H66	0.42	1.90	8	1
4:A:315:PX4:H29	4:A:425:PX4:H44	0.42	1.92	3	1
4:A:340:PX4:H49	4:A:340:PX4:H54	0.42	1.70	5	1
4:A:309:PX4:H54	4:A:316:PX4:H57	0.42	1.92	4	1
4:A:370:PX4:H36	4:A:404:PX4:H37	0.42	1.91	4	1
4:A:368:PX4:H10	4:A:418:PX4:O1	0.42	2.15	12	1
4:A:346:PX4:H6	4:A:360:PX4:O8	0.42	2.15	7	1
4:A:312:PX4:H58	4:A:312:PX4:H65	0.42	1.68	13	1
4:A:331:PX4:C21	4:A:332:PX4:H42	0.42	2.45	11	1
4:A:396:PX4:H47	4:A:405:PX4:H47	0.42	1.91	2	1
4:A:417:PX4:H34	4:A:426:PX4:H65	0.42	1.92	2	1
4:A:408:PX4:H65	4:A:409:PX4:H28	0.42	1.91	8	1
4:A:404:PX4:H12	4:A:419:PX4:O1	0.42	2.15	3	1
4:A:355:PX4:H3	4:A:355:PX4:O8	0.42	2.14	5	1
4:A:400:PX4:H28	4:A:400:PX4:H63	0.42	1.92	5	1
4:A:333:PX4:H21	4:A:333:PX4:H27	0.42	1.45	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:380:PX4:H8	4:A:402:PX4:O6	0.42	2.15	14	1
4:A:329:PX4:H53	4:A:329:PX4:H59	0.42	1.62	12	1
4:A:363:PX4:H19	4:A:364:PX4:H36	0.42	1.90	7	1
4:A:415:PX4:H24	4:A:425:PX4:H66	0.42	1.91	11	1
4:A:328:PX4:H7	4:A:354:PX4:O8	0.42	2.15	6	1
4:A:429:PX4:H51	4:A:429:PX4:H56	0.42	1.63	6	1
4:A:417:PX4:H20	4:A:417:PX4:H25	0.42	1.48	9	1
4:A:315:PX4:H40	4:A:361:PX4:C3	0.42	2.44	1	1
4:A:346:PX4:O8	4:A:362:PX4:H9	0.42	2.14	3	1
4:A:306:PX4:H38	4:A:328:PX4:H37	0.42	1.92	3	1
4:A:306:PX4:H18	4:A:322:PX4:H50	0.42	1.92	5	1
4:A:321:PX4:H48	4:A:354:PX4:H30	0.42	1.91	5	1
4:A:321:PX4:H68	4:A:425:PX4:H37	0.42	1.90	4	1
4:A:420:PX4:H17	4:A:427:PX4:H22	0.42	1.90	4	1
4:A:394:PX4:H55	4:A:394:PX4:H49	0.42	1.73	4	1
4:A:307:PX4:H38	4:A:364:PX4:H58	0.42	1.91	12	1
4:A:416:PX4:H12	4:A:426:PX4:O2	0.42	2.15	12	1
4:A:355:PX4:H11	4:A:362:PX4:O8	0.42	2.15	7	1
4:A:374:PX4:H25	4:A:412:PX4:H56	0.42	1.91	7	1
4:A:421:PX4:H24	4:A:430:PX4:H21	0.42	1.91	11	1
4:A:333:PX4:H52	4:A:333:PX4:H59	0.42	1.57	11	1
4:A:339:PX4:H20	4:A:347:PX4:H48	0.41	1.90	9	1
4:A:421:PX4:O6	4:A:423:PX4:H46	0.41	2.15	9	1
4:A:337:PX4:H59	4:A:338:PX4:H58	0.41	1.92	1	1
4:A:307:PX4:H60	4:A:349:PX4:H5	0.41	1.92	1	1
4:A:370:PX4:H64	4:A:370:PX4:H59	0.41	1.59	3	1
4:A:313:PX4:H53	4:A:359:PX4:C12	0.41	2.42	10	1
4:A:313:PX4:H57	4:A:359:PX4:H26	0.41	1.92	10	1
4:A:335:PX4:H26	4:A:335:PX4:H19	0.41	1.54	10	1
4:A:345:PX4:H35	4:A:353:PX4:H32	0.41	1.92	4	1
4:A:425:PX4:H38	4:A:425:PX4:H32	0.41	1.56	4	1
1:A:191:ILE:O	4:A:314:PX4:H7	0.41	2.16	14	1
4:A:331:PX4:H31	4:A:331:PX4:H37	0.41	1.55	12	1
4:A:391:PX4:H62	4:A:391:PX4:H57	0.41	1.65	12	1
4:A:319:PX4:H23	4:A:320:PX4:H43	0.41	1.91	12	1
4:A:320:PX4:H70	4:A:371:PX4:H67	0.41	1.92	12	1
4:A:347:PX4:H24	4:A:348:PX4:H51	0.41	1.92	7	1
4:A:326:PX4:H35	4:A:340:PX4:H38	0.41	1.91	13	1
4:A:354:PX4:H36	4:A:355:PX4:H72	0.41	1.92	6	1
4:A:380:PX4:H23	4:A:381:PX4:H21	0.41	1.92	6	1
4:A:307:PX4:H70	4:A:350:PX4:H58	0.41	1.91	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:325:PX4:H32	4:A:341:PX4:H67	0.41	1.91	8	1
4:A:426:PX4:H39	4:A:426:PX4:H34	0.41	1.75	10	1
4:A:388:PX4:H33	4:A:406:PX4:H64	0.41	1.93	4	1
4:A:308:PX4:H59	4:A:308:PX4:H52	0.41	1.72	4	1
4:A:402:PX4:H48	4:A:411:PX4:H25	0.41	1.92	14	1
4:A:366:PX4:H53	4:A:366:PX4:H47	0.41	1.69	14	1
4:A:307:PX4:H51	4:A:356:PX4:H37	0.41	1.92	12	1
4:A:314:PX4:H42	4:A:355:PX4:H11	0.41	1.91	7	1
4:A:322:PX4:H11	4:A:361:PX4:O8	0.41	2.15	7	1
4:A:330:PX4:H55	4:A:337:PX4:H52	0.41	1.91	7	1
4:A:319:PX4:H55	4:A:319:PX4:H22	0.41	1.92	13	1
4:A:347:PX4:C29	4:A:355:PX4:H25	0.41	2.24	11	1
4:A:379:PX4:H28	4:A:379:PX4:H33	0.41	1.60	11	1
4:A:312:PX4:H48	4:A:312:PX4:H55	0.41	1.65	6	1
4:A:389:PX4:H52	4:A:398:PX4:H65	0.41	1.91	9	1
1:A:191:ILE:O	4:A:314:PX4:H3	0.41	2.15	1	1
4:A:367:PX4:H52	4:A:430:PX4:H50	0.41	1.90	2	1
4:A:369:PX4:H21	4:A:369:PX4:H27	0.41	1.70	2	1
4:A:314:PX4:H43	4:A:349:PX4:H47	0.41	1.92	8	1
4:A:367:PX4:H46	4:A:367:PX4:H53	0.41	1.55	8	1
4:A:388:PX4:H36	4:A:406:PX4:H60	0.41	1.91	3	1
4:A:336:PX4:H39	4:A:428:PX4:H42	0.41	1.92	3	1
4:A:330:PX4:H22	4:A:343:PX4:H8	0.41	1.91	3	1
4:A:401:PX4:H63	4:A:401:PX4:H56	0.41	1.53	5	1
4:A:405:PX4:H30	4:A:422:PX4:H33	0.41	1.93	10	1
4:A:405:PX4:H33	4:A:415:PX4:H64	0.41	1.91	4	1
4:A:400:PX4:H64	4:A:417:PX4:H29	0.41	1.90	4	1
4:A:388:PX4:H55	4:A:402:PX4:H28	0.41	1.91	12	1
4:A:404:PX4:H23	4:A:419:PX4:H46	0.41	1.90	12	1
4:A:392:PX4:H54	4:A:407:PX4:H21	0.41	1.91	12	1
4:A:387:PX4:H55	4:A:411:PX4:H50	0.41	1.92	7	1
4:A:409:PX4:H52	4:A:409:PX4:H59	0.41	1.60	7	1
4:A:307:PX4:H25	4:A:307:PX4:H20	0.41	1.66	13	1
4:A:405:PX4:H59	4:A:405:PX4:H52	0.41	1.69	11	1
4:A:360:PX4:H47	4:A:366:PX4:H18	0.41	1.93	6	1
4:A:349:PX4:H71	4:A:355:PX4:H71	0.41	1.91	1	1
4:A:329:PX4:H45	4:A:359:PX4:H23	0.41	1.92	1	1
4:A:346:PX4:H33	4:A:362:PX4:H25	0.41	1.92	2	1
4:A:368:PX4:H17	4:A:390:PX4:H48	0.41	1.92	2	1
4:A:395:PX4:H21	4:A:406:PX4:C26	0.41	2.43	10	1
4:A:417:PX4:H47	4:A:417:PX4:H52	0.41	1.67	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:318:PX4:H65	4:A:318:PX4:H71	0.41	1.56	14	1
4:A:410:PX4:H54	4:A:426:PX4:H51	0.41	1.91	12	1
4:A:408:PX4:H24	4:A:415:PX4:H17	0.41	1.92	12	1
4:A:309:PX4:O1	4:A:319:PX4:H18	0.41	2.15	7	1
4:A:368:PX4:H3	4:A:369:PX4:O3	0.41	2.14	11	1
4:A:398:PX4:H52	4:A:398:PX4:H27	0.41	1.92	11	1
4:A:311:PX4:H56	4:A:311:PX4:H26	0.41	1.91	6	1
4:A:307:PX4:H41	4:A:425:PX4:H30	0.41	1.91	9	1
4:A:428:PX4:H49	4:A:429:PX4:H21	0.41	1.92	1	1
4:A:368:PX4:H50	4:A:369:PX4:H30	0.41	1.92	2	1
4:A:391:PX4:H53	4:A:391:PX4:H47	0.41	1.60	2	1
4:A:306:PX4:O8	4:A:322:PX4:H9	0.41	2.15	2	1
4:A:322:PX4:H19	4:A:333:PX4:H37	0.41	1.91	2	1
4:A:384:PX4:H22	4:A:385:PX4:H24	0.41	1.92	8	1
4:A:339:PX4:H65	4:A:339:PX4:H58	0.41	1.68	3	1
4:A:346:PX4:H26	4:A:354:PX4:H25	0.41	1.90	4	1
4:A:390:PX4:H19	4:A:390:PX4:H25	0.41	1.64	12	1
4:A:334:PX4:H26	4:A:334:PX4:H59	0.41	1.91	13	1
4:A:356:PX4:H31	4:A:356:PX4:H25	0.41	1.78	13	1
4:A:319:PX4:H46	4:A:333:PX4:H54	0.41	1.92	13	1
4:A:336:PX4:H30	4:A:336:PX4:H35	0.41	1.62	11	1
4:A:365:PX4:H16	4:A:366:PX4:H5	0.41	1.93	8	2
4:A:312:PX4:O1	4:A:366:PX4:H18	0.41	2.16	1	1
4:A:353:PX4:H57	4:A:353:PX4:H50	0.41	1.62	1	1
4:A:325:PX4:H49	4:A:325:PX4:H55	0.41	1.66	2	1
4:A:371:PX4:H25	4:A:377:PX4:C11	0.41	2.45	8	1
4:A:385:PX4:H8	4:A:393:PX4:O1	0.41	2.16	5	1
4:A:325:PX4:H62	4:A:325:PX4:H33	0.41	1.91	10	1
4:A:351:PX4:H19	4:A:351:PX4:H26	0.41	1.66	4	1
4:A:353:PX4:H27	4:A:365:PX4:H51	0.41	1.92	4	1
4:A:373:PX4:O6	4:A:397:PX4:H1	0.41	2.16	14	1
4:A:307:PX4:H18	4:A:314:PX4:O8	0.41	2.15	12	1
4:A:406:PX4:H61	4:A:421:PX4:H71	0.41	1.93	12	1
4:A:315:PX4:H59	4:A:368:PX4:H44	0.41	1.93	13	1
4:A:322:PX4:H16	4:A:323:PX4:H49	0.41	1.91	1	1
4:A:408:PX4:H37	4:A:425:PX4:H62	0.41	1.93	1	1
4:A:321:PX4:H61	4:A:361:PX4:H30	0.41	1.91	2	1
4:A:321:PX4:O1	4:A:328:PX4:H10	0.41	2.15	2	1
4:A:360:PX4:H68	4:A:413:PX4:H35	0.41	1.91	8	1
4:A:336:PX4:C36	4:A:344:PX4:H35	0.41	2.46	5	1
4:A:379:PX4:H46	4:A:379:PX4:H53	0.41	1.60	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:331:PX4:H15	4:A:332:PX4:O6	0.41	2.15	14	1
4:A:310:PX4:H70	4:A:364:PX4:H52	0.41	1.92	12	1
4:A:406:PX4:H33	4:A:425:PX4:H63	0.41	1.92	12	1
4:A:405:PX4:H17	4:A:414:PX4:H24	0.41	1.93	12	1
4:A:330:PX4:H36	4:A:347:PX4:H37	0.41	1.92	13	1
4:A:314:PX4:H55	4:A:364:PX4:H46	0.41	1.92	13	1
4:A:421:PX4:H35	4:A:421:PX4:H30	0.41	1.67	11	1
4:A:360:PX4:H17	4:A:366:PX4:O6	0.41	2.16	6	1
4:A:321:PX4:H62	4:A:425:PX4:H43	0.41	1.92	6	1
4:A:388:PX4:H14	4:A:395:PX4:O1	0.41	2.15	6	1
4:A:348:PX4:H42	4:A:388:PX4:H69	0.41	1.93	9	1
4:A:343:PX4:H38	4:A:343:PX4:H44	0.41	1.73	1	1
4:A:317:PX4:H56	4:A:324:PX4:H40	0.41	1.93	2	1
4:A:383:PX4:H49	4:A:392:PX4:H26	0.41	1.93	2	1
4:A:353:PX4:H56	4:A:353:PX4:H50	0.41	1.67	8	1
4:A:339:PX4:H21	4:A:348:PX4:H50	0.41	1.91	3	1
4:A:379:PX4:H68	4:A:379:PX4:H41	0.41	1.91	3	1
4:A:430:PX4:H52	4:A:430:PX4:H47	0.41	1.63	3	1
4:A:325:PX4:O6	4:A:334:PX4:H7	0.41	2.16	5	1
4:A:390:PX4:H38	4:A:390:PX4:H44	0.41	1.48	10	1
4:A:334:PX4:H52	4:A:349:PX4:H21	0.41	1.93	4	1
4:A:316:PX4:H69	4:A:368:PX4:H30	0.41	1.91	4	1
4:A:400:PX4:H50	4:A:416:PX4:H34	0.41	1.91	4	1
4:A:376:PX4:H39	4:A:377:PX4:H61	0.41	1.93	4	1
4:A:384:PX4:H19	4:A:386:PX4:O6	0.41	2.16	12	1
4:A:374:PX4:H33	4:A:428:PX4:H44	0.41	1.93	12	1
4:A:359:PX4:H54	4:A:359:PX4:H48	0.41	1.49	13	1
4:A:343:PX4:C24	4:A:352:PX4:H56	0.41	2.45	11	1
4:A:354:PX4:H39	4:A:423:PX4:H41	0.41	1.92	11	1
4:A:332:PX4:H4	4:A:356:PX4:O1	0.41	2.16	11	1
4:A:325:PX4:H43	4:A:393:PX4:H63	0.41	1.92	11	1
4:A:347:PX4:H58	4:A:355:PX4:H23	0.41	1.91	6	1
4:A:388:PX4:H64	4:A:402:PX4:H36	0.41	1.93	9	1
4:A:329:PX4:H62	4:A:428:PX4:H62	0.41	1.93	9	1
4:A:330:PX4:H58	4:A:357:PX4:H61	0.41	1.93	1	1
4:A:416:PX4:H18	4:A:425:PX4:H15	0.41	1.93	1	1
4:A:317:PX4:H16	4:A:342:PX4:O6	0.41	2.16	2	1
4:A:325:PX4:H7	4:A:325:PX4:H15	0.41	1.93	8	1
4:A:421:PX4:H20	4:A:430:PX4:H16	0.41	1.92	8	1
4:A:369:PX4:O1	4:A:425:PX4:H2	0.41	2.16	8	1
4:A:316:PX4:H69	4:A:377:PX4:H38	0.41	1.92	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:413:PX4:H71	4:A:424:PX4:H33	0.41	1.92	8	1
4:A:392:PX4:H47	4:A:392:PX4:H52	0.41	1.69	3	1
4:A:392:PX4:H12	4:A:392:PX4:H15	0.41	1.92	3	1
4:A:335:PX4:H46	4:A:343:PX4:H23	0.41	1.91	5	1
4:A:313:PX4:H47	4:A:327:PX4:H25	0.41	1.93	5	1
4:A:317:PX4:O8	4:A:342:PX4:H4	0.41	2.16	10	1
4:A:378:PX4:H56	4:A:378:PX4:H63	0.41	1.50	10	1
4:A:374:PX4:H28	4:A:427:PX4:H25	0.41	1.92	14	1
4:A:416:PX4:H21	4:A:425:PX4:O7	0.41	2.16	12	1
4:A:383:PX4:H17	4:A:392:PX4:H22	0.41	1.92	12	1
4:A:306:PX4:H19	4:A:360:PX4:H42	0.41	1.93	7	1
4:A:312:PX4:O2	4:A:312:PX4:H9	0.41	2.16	7	1
4:A:361:PX4:H30	4:A:364:PX4:H72	0.41	1.92	13	1
4:A:373:PX4:H38	4:A:373:PX4:H44	0.41	1.55	13	1
4:A:390:PX4:H5	4:A:407:PX4:O1	0.41	2.16	13	1
4:A:337:PX4:H69	4:A:395:PX4:H67	0.41	1.90	11	1
4:A:315:PX4:O7	4:A:316:PX4:H16	0.41	2.15	11	1
4:A:372:PX4:H36	4:A:372:PX4:H41	0.41	1.73	11	1
4:A:310:PX4:H37	4:A:364:PX4:H36	0.41	1.92	6	1
4:A:397:PX4:H60	4:A:406:PX4:H71	0.41	1.92	6	1
4:A:411:PX4:H31	4:A:411:PX4:H26	0.41	1.67	6	1
4:A:395:PX4:C19	4:A:415:PX4:H62	0.41	2.45	9	1
4:A:314:PX4:H67	4:A:314:PX4:H60	0.41	1.70	8	1
4:A:428:PX4:H51	4:A:429:PX4:H22	0.41	1.92	3	1
4:A:393:PX4:H55	4:A:399:PX4:H63	0.41	1.93	3	1
4:A:360:PX4:H49	4:A:360:PX4:H22	0.41	1.93	5	1
4:A:326:PX4:H55	4:A:363:PX4:H48	0.41	1.91	10	1
4:A:306:PX4:H22	4:A:322:PX4:H57	0.41	1.90	14	1
1:A:153:ASN:O	4:A:331:PX4:H12	0.41	2.16	14	1
4:A:416:PX4:H17	4:A:426:PX4:H25	0.41	1.91	14	1
4:A:384:PX4:H40	4:A:384:PX4:H34	0.41	1.72	14	1
4:A:392:PX4:H60	4:A:393:PX4:H63	0.41	1.92	7	1
4:A:410:PX4:H58	4:A:426:PX4:H51	0.41	1.91	11	1
4:A:316:PX4:C19	4:A:316:PX4:H72	0.41	2.43	6	1
4:A:350:PX4:H63	4:A:363:PX4:H58	0.41	1.92	6	1
4:A:416:PX4:H27	4:A:426:PX4:H21	0.41	1.91	6	1
4:A:396:PX4:H67	4:A:398:PX4:H65	0.40	1.93	1	1
4:A:330:PX4:H31	4:A:330:PX4:H26	0.40	1.59	8	1
4:A:333:PX4:H60	4:A:340:PX4:H60	0.40	1.92	8	1
4:A:348:PX4:H42	4:A:398:PX4:H45	0.40	1.91	3	1
4:A:330:PX4:O8	4:A:337:PX4:H10	0.40	2.16	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:306:PX4:H22	4:A:329:PX4:H63	0.40	1.92	10	1
4:A:349:PX4:H24	4:A:350:PX4:H52	0.40	1.93	10	1
4:A:393:PX4:H3	4:A:394:PX4:P1	0.40	2.56	4	1
4:A:428:PX4:H54	4:A:429:PX4:H48	0.40	1.93	4	1
4:A:389:PX4:H56	4:A:389:PX4:H51	0.40	1.63	14	1
4:A:367:PX4:H17	4:A:430:PX4:H50	0.40	1.91	14	1
4:A:355:PX4:H9	4:A:356:PX4:O6	0.40	2.16	12	1
4:A:378:PX4:H47	4:A:378:PX4:H52	0.40	1.76	12	1
4:A:334:PX4:H58	4:A:349:PX4:H48	0.40	1.92	7	1
4:A:322:PX4:H60	4:A:361:PX4:H52	0.40	1.92	7	1
4:A:337:PX4:O6	4:A:337:PX4:H4	0.40	2.16	7	1
4:A:389:PX4:O6	4:A:397:PX4:H8	0.40	2.16	13	1
4:A:325:PX4:H61	4:A:341:PX4:H29	0.40	1.93	13	1
4:A:423:PX4:H52	4:A:423:PX4:H47	0.40	1.69	11	1
4:A:385:PX4:H48	4:A:385:PX4:H54	0.40	1.59	11	1
4:A:327:PX4:H55	4:A:327:PX4:H48	0.40	1.54	9	1
4:A:328:PX4:H62	4:A:328:PX4:H68	0.40	1.73	9	1
4:A:325:PX4:H30	4:A:325:PX4:H23	0.40	1.29	2	1
4:A:315:PX4:H27	4:A:315:PX4:H21	0.40	1.73	3	1
4:A:399:PX4:H14	4:A:399:PX4:H6	0.40	1.94	3	1
4:A:379:PX4:H12	4:A:385:PX4:O1	0.40	2.16	14	1
4:A:395:PX4:H22	4:A:395:PX4:H27	0.40	1.68	14	1
4:A:317:PX4:H17	4:A:324:PX4:H52	0.40	1.93	14	1
4:A:313:PX4:H27	4:A:360:PX4:H21	0.40	1.93	12	1
4:A:307:PX4:H37	4:A:361:PX4:H55	0.40	1.92	13	1
4:A:345:PX4:H23	4:A:345:PX4:H30	0.40	1.74	11	1
4:A:321:PX4:H60	4:A:321:PX4:H67	0.40	1.45	6	1
4:A:392:PX4:H35	4:A:392:PX4:H30	0.40	1.73	6	1
4:A:307:PX4:H41	4:A:315:PX4:H28	0.40	1.93	1	1
4:A:322:PX4:H72	4:A:413:PX4:H63	0.40	1.92	2	1
4:A:331:PX4:H3	4:A:347:PX4:H46	0.40	1.93	2	1
1:A:160:LEU:CD2	4:A:356:PX4:H23	0.40	2.47	8	1
4:A:422:PX4:H40	4:A:423:PX4:H69	0.40	1.93	5	1
4:A:340:PX4:H20	4:A:341:PX4:H55	0.40	1.92	10	1
4:A:370:PX4:H66	4:A:411:PX4:H31	0.40	1.93	4	1
4:A:375:PX4:H47	4:A:389:PX4:H21	0.40	1.93	4	1
4:A:359:PX4:H29	4:A:359:PX4:H24	0.40	1.64	14	1
4:A:346:PX4:H46	4:A:355:PX4:C4	0.40	2.46	13	1
4:A:369:PX4:O2	4:A:425:PX4:H2	0.40	2.16	13	1
1:A:123:PRO:HB3	4:A:345:PX4:H4	0.40	1.93	13	1
4:A:346:PX4:H67	4:A:362:PX4:H68	0.40	1.92	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:386:PX4:H55	4:A:387:PX4:H22	0.40	1.92	9	1
4:A:345:PX4:H46	4:A:348:PX4:H6	0.40	1.94	1	1
4:A:349:PX4:H32	4:A:350:PX4:H35	0.40	1.92	2	1
4:A:422:PX4:H30	4:A:425:PX4:H67	0.40	1.93	2	1
4:A:371:PX4:H33	4:A:377:PX4:H26	0.40	1.93	3	1
4:A:391:PX4:H18	4:A:405:PX4:H3	0.40	1.94	10	1
4:A:387:PX4:H53	4:A:387:PX4:H46	0.40	1.81	10	1
4:A:356:PX4:H53	4:A:356:PX4:H59	0.40	1.60	4	1
4:A:374:PX4:H30	4:A:428:PX4:H39	0.40	1.92	12	1
4:A:313:PX4:H47	4:A:328:PX4:C7	0.40	2.35	12	1
4:A:370:PX4:H36	4:A:413:PX4:H36	0.40	1.92	7	1
4:A:406:PX4:H19	4:A:422:PX4:H19	0.40	1.92	7	1
4:A:334:PX4:H31	4:A:349:PX4:H57	0.40	1.91	13	1
4:A:347:PX4:H55	4:A:355:PX4:H27	0.40	1.92	13	1
4:A:378:PX4:O1	4:A:410:PX4:H7	0.40	2.15	13	1
4:A:373:PX4:H19	4:A:397:PX4:H15	0.40	1.93	13	1
4:A:403:PX4:H1	4:A:403:PX4:H18	0.40	1.94	9	1
4:A:316:PX4:C14	4:A:320:PX4:H40	0.40	2.47	8	1
4:A:328:PX4:H55	4:A:328:PX4:H60	0.40	1.62	8	1
4:A:375:PX4:H48	4:A:375:PX4:H55	0.40	1.63	8	1
4:A:380:PX4:H42	4:A:380:PX4:H35	0.40	1.60	8	1
4:A:315:PX4:H65	4:A:323:PX4:H35	0.40	1.92	3	1
4:A:403:PX4:H27	4:A:411:PX4:H28	0.40	1.94	3	1
4:A:403:PX4:H49	4:A:419:PX4:H51	0.40	1.94	3	1
4:A:330:PX4:H11	4:A:336:PX4:O1	0.40	2.17	5	1
4:A:391:PX4:H26	4:A:391:PX4:H19	0.40	1.43	10	1
4:A:411:PX4:H26	4:A:411:PX4:H19	0.40	1.65	10	1
4:A:374:PX4:H13	4:A:374:PX4:H21	0.40	1.93	4	1
4:A:419:PX4:H17	4:A:427:PX4:H15	0.40	1.92	4	1
4:A:319:PX4:H48	4:A:319:PX4:H55	0.40	1.79	4	1
4:A:421:PX4:H17	4:A:423:PX4:H55	0.40	1.93	14	1
4:A:383:PX4:H29	4:A:399:PX4:H25	0.40	1.93	12	1
4:A:390:PX4:H50	4:A:399:PX4:H34	0.40	1.93	13	1
4:A:401:PX4:H58	4:A:401:PX4:H53	0.40	1.81	13	1
4:A:316:PX4:H68	4:A:368:PX4:H32	0.40	1.93	11	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	151±2 (93±1%)	10±2 (6±1%)	2±1 (1±1%)	24	71
All	All	2268/2296 (99%)	2109 (93%)	136 (6%)	23 (1%)	24	71

All 8 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	173	ALA	11
1	A	179	GLY	4
1	A	172	HIS	2
1	A	170	ASP	2
1	A	171	PHE	1
1	A	107	PRO	1
1	A	109	TRP	1
1	A	110	ARG	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/131 (99%)	123±1 (95±1%)	7±1 (5±1%)	34	78
All	All	1820/1834 (99%)	1728 (95%)	92 (5%)	34	78

All 26 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	199	GLU	14
1	A	165	ARG	14

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Mol	Chain	Res	Type	Models (Total)
1	A	170	ASP	12
1	A	172	HIS	11
1	A	244	ASP	6
1	A	253	ASP	5
1	A	109	TRP	4
1	A	101	ARG	3
1	A	201	GLU	2
1	A	136	LYS	2
1	A	129	ASP	2
1	A	251	SER	2
1	A	260	SER	2
1	A	171	PHE	1
1	A	261	LEU	1
1	A	131	ASP	1
1	A	162	VAL	1
1	A	202	PHE	1
1	A	140	VAL	1
1	A	223	SER	1
1	A	200	ASP	1
1	A	191	ILE	1
1	A	102	GLU	1
1	A	110	ARG	1
1	A	236	MET	1
1	A	108	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 5 are monoatomic - leaving 125 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	306	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.65±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	342	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	348	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	374	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.65±0.03	0±0 (0±0%)
4	PX4	A	376	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.65±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	385	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	388	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.66±0.01	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.65±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	428	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.66±0.02	0±0 (0±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	306	-	49,53,53	1.38±0.12	0±0 (0±0%)
4	PX4	A	307	-	49,53,53	1.42±0.19	0±0 (0±0%)
4	PX4	A	308	-	49,53,53	1.50±0.12	0±0 (0±0%)
4	PX4	A	309	-	49,53,53	1.51±0.14	0±0 (0±0%)
4	PX4	A	310	-	49,53,53	1.45±0.14	0±0 (0±0%)
4	PX4	A	311	-	49,53,53	1.50±0.14	0±0 (0±0%)
4	PX4	A	312	-	49,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	313	-	49,53,53	1.45±0.15	0±0 (0±0%)
4	PX4	A	314	-	49,53,53	1.52±0.13	0±0 (0±0%)
4	PX4	A	315	-	49,53,53	1.38±0.10	0±0 (0±0%)
4	PX4	A	316	-	49,53,53	1.35±0.12	0±0 (0±0%)
4	PX4	A	317	-	49,53,53	1.44±0.11	0±0 (0±0%)
4	PX4	A	318	-	49,53,53	1.41±0.15	0±0 (0±0%)
4	PX4	A	319	-	49,53,53	1.39±0.11	0±0 (0±0%)
4	PX4	A	320	-	49,53,53	1.48±0.12	0±0 (0±0%)
4	PX4	A	321	-	49,53,53	1.53±0.15	0±0 (0±0%)
4	PX4	A	322	-	49,53,53	1.44±0.12	0±0 (0±0%)
4	PX4	A	323	-	49,53,53	1.46±0.14	0±0 (0±0%)
4	PX4	A	324	-	49,53,53	1.38±0.12	0±1 (0±1%)
4	PX4	A	325	-	49,53,53	1.45±0.14	0±0 (0±0%)
4	PX4	A	326	-	49,53,53	1.42±0.14	0±0 (0±0%)
4	PX4	A	327	-	49,53,53	1.45±0.16	0±0 (0±0%)
4	PX4	A	328	-	49,53,53	1.45±0.14	0±0 (0±0%)
4	PX4	A	329	-	49,53,53	1.44±0.15	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	330	-	49,53,53	1.40±0.16	0±0 (0±0%)
4	PX4	A	331	-	49,53,53	1.43±0.14	0±0 (0±0%)
4	PX4	A	332	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	333	-	49,53,53	1.45±0.17	0±0 (0±0%)
4	PX4	A	334	-	49,53,53	1.43±0.13	0±0 (0±0%)
4	PX4	A	335	-	49,53,53	1.50±0.16	0±1 (0±1%)
4	PX4	A	336	-	49,53,53	1.37±0.10	0±0 (0±0%)
4	PX4	A	337	-	49,53,53	1.40±0.14	0±0 (0±0%)
4	PX4	A	338	-	49,53,53	1.44±0.12	0±0 (0±0%)
4	PX4	A	339	-	49,53,53	1.51±0.16	0±0 (0±0%)
4	PX4	A	340	-	49,53,53	1.41±0.14	0±0 (0±0%)
4	PX4	A	341	-	49,53,53	1.41±0.11	0±0 (0±0%)
4	PX4	A	342	-	49,53,53	1.44±0.14	0±0 (0±0%)
4	PX4	A	343	-	49,53,53	1.46±0.15	0±0 (0±0%)
4	PX4	A	344	-	49,53,53	1.51±0.13	0±0 (0±0%)
4	PX4	A	345	-	49,53,53	1.31±0.10	0±0 (0±0%)
4	PX4	A	346	-	49,53,53	1.42±0.14	0±0 (0±0%)
4	PX4	A	347	-	49,53,53	1.48±0.20	0±1 (0±1%)
4	PX4	A	348	-	49,53,53	1.40±0.17	0±0 (0±0%)
4	PX4	A	349	-	49,53,53	1.47±0.12	0±0 (0±0%)
4	PX4	A	350	-	49,53,53	1.42±0.13	0±0 (0±0%)
4	PX4	A	351	-	49,53,53	1.41±0.13	0±0 (0±0%)
4	PX4	A	352	-	49,53,53	1.47±0.16	0±0 (0±0%)
4	PX4	A	353	-	49,53,53	1.47±0.13	0±1 (0±1%)
4	PX4	A	354	-	49,53,53	1.57±0.12	0±0 (0±0%)
4	PX4	A	355	-	49,53,53	1.45±0.19	0±0 (0±0%)
4	PX4	A	356	-	49,53,53	1.42±0.14	0±0 (0±0%)
4	PX4	A	357	-	49,53,53	1.49±0.09	0±0 (0±0%)
4	PX4	A	358	-	49,53,53	1.33±0.10	0±0 (0±0%)
4	PX4	A	359	-	49,53,53	1.45±0.13	0±0 (0±0%)
4	PX4	A	360	-	49,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	361	-	49,53,53	1.56±0.14	0±0 (0±0%)
4	PX4	A	362	-	49,53,53	1.45±0.13	0±0 (0±0%)
4	PX4	A	363	-	49,53,53	1.53±0.08	0±0 (0±0%)
4	PX4	A	364	-	49,53,53	1.45±0.12	0±0 (0±0%)
4	PX4	A	365	-	49,53,53	1.36±0.09	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	366	-	49,53,53	1.54±0.16	0±1 (0±1%)
4	PX4	A	367	-	49,53,53	1.45±0.12	0±0 (0±0%)
4	PX4	A	368	-	49,53,53	1.45±0.15	0±0 (0±0%)
4	PX4	A	369	-	49,53,53	1.49±0.10	0±0 (0±0%)
4	PX4	A	370	-	49,53,53	1.49±0.17	0±0 (0±0%)
4	PX4	A	371	-	49,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	372	-	49,53,53	1.41±0.20	0±0 (0±0%)
4	PX4	A	373	-	49,53,53	1.45±0.11	0±0 (0±0%)
4	PX4	A	374	-	49,53,53	1.42±0.14	0±0 (0±0%)
4	PX4	A	375	-	49,53,53	1.50±0.22	0±0 (0±0%)
4	PX4	A	376	-	49,53,53	1.45±0.15	0±0 (0±0%)
4	PX4	A	377	-	49,53,53	1.38±0.15	0±0 (0±0%)
4	PX4	A	378	-	49,53,53	1.52±0.14	0±0 (0±0%)
4	PX4	A	379	-	49,53,53	1.58±0.19	0±0 (0±0%)
4	PX4	A	380	-	49,53,53	1.47±0.17	0±0 (0±0%)
4	PX4	A	381	-	49,53,53	1.47±0.17	0±0 (0±0%)
4	PX4	A	382	-	49,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	383	-	49,53,53	1.40±0.13	0±0 (0±0%)
4	PX4	A	384	-	49,53,53	1.42±0.15	0±0 (0±0%)
4	PX4	A	385	-	49,53,53	1.45±0.13	0±0 (0±0%)
4	PX4	A	386	-	49,53,53	1.48±0.14	0±0 (0±0%)
4	PX4	A	387	-	49,53,53	1.42±0.18	0±0 (0±0%)
4	PX4	A	388	-	49,53,53	1.50±0.12	0±0 (0±0%)
4	PX4	A	389	-	49,53,53	1.46±0.09	0±0 (0±0%)
4	PX4	A	390	-	49,53,53	1.43±0.11	0±0 (0±0%)
4	PX4	A	391	-	49,53,53	1.46±0.14	0±0 (0±0%)
4	PX4	A	392	-	49,53,53	1.42±0.10	0±0 (0±0%)
4	PX4	A	393	-	49,53,53	1.40±0.13	0±0 (0±0%)
4	PX4	A	394	-	49,53,53	1.38±0.15	0±0 (0±0%)
4	PX4	A	395	-	49,53,53	1.39±0.11	0±0 (0±0%)
4	PX4	A	396	-	49,53,53	1.41±0.15	0±0 (0±0%)
4	PX4	A	397	-	49,53,53	1.43±0.16	0±0 (0±0%)
4	PX4	A	398	-	49,53,53	1.51±0.17	0±0 (0±0%)
4	PX4	A	399	-	49,53,53	1.42±0.11	0±0 (0±0%)
4	PX4	A	400	-	49,53,53	1.43±0.17	0±0 (0±0%)
4	PX4	A	401	-	49,53,53	1.41±0.17	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	402	-	49,53,53	1.56±0.17	0±0 (0±1%)
4	PX4	A	403	-	49,53,53	1.46±0.16	0±0 (0±0%)
4	PX4	A	404	-	49,53,53	1.47±0.16	0±0 (0±0%)
4	PX4	A	405	-	49,53,53	1.36±0.16	0±0 (0±0%)
4	PX4	A	406	-	49,53,53	1.42±0.14	0±0 (0±0%)
4	PX4	A	407	-	49,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	408	-	49,53,53	1.51±0.15	0±0 (0±0%)
4	PX4	A	409	-	49,53,53	1.41±0.18	0±0 (0±0%)
4	PX4	A	410	-	49,53,53	1.42±0.17	0±0 (0±0%)
4	PX4	A	411	-	49,53,53	1.52±0.24	0±1 (0±1%)
4	PX4	A	412	-	49,53,53	1.51±0.17	0±0 (0±0%)
4	PX4	A	413	-	49,53,53	1.52±0.15	0±0 (0±0%)
4	PX4	A	414	-	49,53,53	1.48±0.17	0±0 (0±0%)
4	PX4	A	415	-	49,53,53	1.49±0.15	0±0 (0±0%)
4	PX4	A	416	-	49,53,53	1.53±0.16	0±0 (0±0%)
4	PX4	A	417	-	49,53,53	1.48±0.16	0±0 (0±0%)
4	PX4	A	418	-	49,53,53	1.44±0.13	0±0 (0±0%)
4	PX4	A	419	-	49,53,53	1.42±0.11	0±0 (0±0%)
4	PX4	A	420	-	49,53,53	1.50±0.17	0±0 (0±0%)
4	PX4	A	421	-	49,53,53	1.47±0.17	0±1 (0±1%)
4	PX4	A	422	-	49,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	423	-	49,53,53	1.48±0.10	0±0 (0±0%)
4	PX4	A	424	-	49,53,53	1.43±0.16	0±0 (0±0%)
4	PX4	A	425	-	49,53,53	1.43±0.16	0±0 (0±0%)
4	PX4	A	426	-	49,53,53	1.45±0.16	0±0 (0±0%)
4	PX4	A	427	-	49,53,53	1.53±0.15	0±0 (0±0%)
4	PX4	A	428	-	49,53,53	1.46±0.16	0±0 (0±0%)
4	PX4	A	429	-	49,53,53	1.43±0.15	0±0 (0±0%)
4	PX4	A	430	-	49,53,53	1.46±0.11	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	306	-	-	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	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
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	-	-	1±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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0±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
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	-	-	0±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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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
4	A	307	PX4	C8-C7-C6	7.98	93.49	112.08	5	1
4	A	314	PX4	C8-C7-C6	7.78	93.95	112.08	11	4
4	A	378	PX4	C8-C7-C6	7.73	94.07	112.08	2	2
4	A	371	PX4	C8-C7-C6	7.58	94.42	112.08	3	2
4	A	416	PX4	C8-C7-C6	7.57	94.43	112.08	6	2
4	A	323	PX4	C8-C7-C6	7.46	94.70	112.08	12	1
4	A	341	PX4	C7-O7-C23	7.40	136.20	117.91	2	2
4	A	380	PX4	O7-C23-C24	7.32	126.95	111.53	10	1
4	A	400	PX4	C8-C7-C6	7.21	95.28	112.08	6	2
4	A	350	PX4	O5-C8-C7	7.05	127.73	108.70	4	1
4	A	427	PX4	C8-C7-C6	6.82	96.20	112.08	3	2
4	A	338	PX4	O5-C8-C7	6.71	126.83	108.70	4	1
4	A	313	PX4	C8-C7-C6	6.70	96.47	112.08	8	1
4	A	379	PX4	O3-P1-O2	6.68	81.85	109.21	3	1
4	A	372	PX4	O7-C23-C24	6.68	125.60	111.53	3	1
4	A	420	PX4	C8-C7-C6	6.63	96.63	112.08	1	1
4	A	318	PX4	C8-C7-C6	6.63	96.64	112.08	5	1
4	A	405	PX4	O7-C23-C24	6.61	125.46	111.53	9	1
4	A	376	PX4	C8-C7-C6	6.59	96.72	112.08	3	1
4	A	333	PX4	C8-C7-C6	6.56	96.80	112.08	1	1
4	A	321	PX4	O5-C8-C7	6.50	126.24	108.70	13	1
4	A	413	PX4	C8-C7-C6	6.47	97.01	112.08	3	2
4	A	353	PX4	O7-C23-C24	6.34	124.88	111.53	13	1
4	A	402	PX4	C8-C7-C6	6.33	97.34	112.08	6	4
4	A	337	PX4	C8-C7-C6	6.29	97.43	112.08	7	1
4	A	331	PX4	O5-C8-C7	6.29	125.67	108.70	14	1
4	A	326	PX4	O7-C23-C24	6.27	124.73	111.53	11	1
4	A	355	PX4	C8-C7-C6	6.23	97.56	112.08	14	2
4	A	335	PX4	O7-C23-C24	6.22	124.63	111.53	3	1
4	A	416	PX4	O5-C8-C7	6.21	125.48	108.70	8	1
4	A	414	PX4	C8-C7-C6	6.20	97.64	112.08	4	2
4	A	347	PX4	O5-C8-C7	6.18	125.40	108.70	14	2
4	A	342	PX4	O7-C23-C24	6.18	124.54	111.53	8	1
4	A	347	PX4	C8-C7-C6	6.10	97.86	112.08	9	3
4	A	396	PX4	C8-C7-C6	6.07	97.95	112.08	13	2
4	A	408	PX4	O3-P1-O2	6.05	84.43	109.21	2	2
4	A	414	PX4	O7-C23-C24	6.03	124.23	111.53	5	1
4	A	399	PX4	C8-C7-C6	5.99	98.13	112.08	11	2
4	A	361	PX4	O5-C8-C7	5.96	124.79	108.70	3	1
4	A	426	PX4	C7-O7-C23	5.94	132.58	117.91	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	332	PX4	O7-C23-C24	5.93	124.02	111.53	9	1
4	A	381	PX4	O7-C23-C24	5.86	123.87	111.53	5	1
4	A	312	PX4	O5-C8-C7	5.85	124.49	108.70	3	3
4	A	317	PX4	C8-C7-C6	5.84	98.48	112.08	9	2
4	A	368	PX4	O5-C8-C7	5.84	124.46	108.70	3	2
4	A	325	PX4	C8-C7-C6	5.82	98.52	112.08	14	1
4	A	313	PX4	O5-C8-C7	5.82	124.40	108.70	7	2
4	A	401	PX4	O7-C23-C24	5.78	123.70	111.53	6	1
4	A	389	PX4	O7-C23-C24	5.77	123.69	111.53	10	1
4	A	393	PX4	C8-C7-C6	5.75	98.67	112.08	13	1
4	A	344	PX4	C8-C7-C6	5.75	98.68	112.08	1	1
4	A	320	PX4	O7-C23-C24	5.75	123.64	111.53	3	1
4	A	410	PX4	C8-C7-C6	5.72	98.74	112.08	9	1
4	A	379	PX4	C8-C7-C6	5.72	98.75	112.08	9	2
4	A	412	PX4	C8-C7-C6	5.71	98.77	112.08	4	1
4	A	367	PX4	O5-C8-C7	5.71	124.12	108.70	1	1
4	A	398	PX4	O7-C23-C24	5.69	123.51	111.53	2	1
4	A	418	PX4	O7-C23-C24	5.69	123.51	111.53	13	1
4	A	309	PX4	C8-C7-C6	5.67	98.88	112.08	9	2
4	A	404	PX4	C8-C7-C6	5.65	98.91	112.08	3	3
4	A	415	PX4	O3-P1-O2	5.65	86.07	109.21	13	1
4	A	424	PX4	O7-C23-C24	5.64	123.41	111.53	9	3
4	A	376	PX4	C8-O5-C9	5.64	100.21	117.00	11	1
4	A	355	PX4	C4-N1-C3	5.63	94.39	108.96	2	1
4	A	309	PX4	O7-C23-C24	5.62	123.38	111.53	4	1
4	A	316	PX4	O7-C7-C8	5.62	128.12	108.36	4	1
4	A	334	PX4	C8-C7-C6	5.61	99.00	112.08	3	1
4	A	386	PX4	O3-P1-O2	5.61	86.26	109.21	13	1
4	A	308	PX4	C8-C7-C6	5.61	99.02	112.08	10	1
4	A	366	PX4	C8-C7-C6	5.59	99.05	112.08	8	1
4	A	330	PX4	O5-C8-C7	5.59	123.81	108.70	9	1
4	A	327	PX4	C8-C7-C6	5.58	99.07	112.08	8	1
4	A	354	PX4	C7-O7-C23	5.58	131.70	117.91	13	2
4	A	344	PX4	O5-C8-C7	5.57	123.73	108.70	6	1
4	A	360	PX4	O5-C8-C7	5.57	123.73	108.70	5	1
4	A	386	PX4	C5-N1-C3	5.56	94.57	108.96	5	1
4	A	415	PX4	C8-C7-C6	5.56	99.13	112.08	7	1
4	A	341	PX4	O7-C7-C8	5.55	127.88	108.36	3	1
4	A	348	PX4	O7-C23-C24	5.55	123.22	111.53	3	1
4	A	363	PX4	O7-C23-C24	5.55	123.21	111.53	5	1
4	A	357	PX4	C8-C7-C6	5.53	99.19	112.08	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	373	PX4	O5-C8-C7	5.53	123.63	108.70	7	2
4	A	390	PX4	C7-O7-C23	5.51	131.53	117.91	10	1
4	A	376	PX4	O3-P1-O2	5.51	86.67	109.21	13	1
4	A	321	PX4	C8-C7-C6	5.49	99.29	112.08	3	1
4	A	430	PX4	O7-C23-C24	5.48	123.08	111.53	7	1
4	A	366	PX4	O5-C8-C7	5.48	123.48	108.70	2	1
4	A	413	PX4	C7-O7-C23	5.47	104.39	117.91	5	1
4	A	312	PX4	C8-C7-C6	5.46	99.36	112.08	4	1
4	A	400	PX4	O5-C8-C7	5.46	123.43	108.70	5	1
4	A	369	PX4	O1-P1-O3	5.45	82.28	108.24	13	1
4	A	421	PX4	O7-C23-C24	5.45	123.00	111.53	14	1
4	A	332	PX4	C8-C7-C6	5.44	99.41	112.08	4	1
4	A	359	PX4	O5-C9-O6	5.43	109.26	123.51	13	1
4	A	367	PX4	C8-C7-C6	5.43	99.42	112.08	6	1
4	A	418	PX4	O5-C8-C7	5.43	123.37	108.70	1	1
4	A	403	PX4	C8-C7-C6	5.43	99.44	112.08	11	1
4	A	375	PX4	C8-C7-C6	5.41	99.47	112.08	4	2
4	A	306	PX4	C8-C7-C6	5.41	99.48	112.08	14	1
4	A	411	PX4	C8-C7-C6	5.41	99.49	112.08	1	2
4	A	332	PX4	O5-C8-C7	5.41	123.30	108.70	6	1
4	A	371	PX4	C4-N1-C3	5.40	94.99	108.96	6	1
4	A	356	PX4	O7-C23-C24	5.39	122.88	111.53	10	1
4	A	409	PX4	C8-C7-C6	5.38	99.54	112.08	1	2
4	A	395	PX4	C8-C7-C6	5.38	99.55	112.08	4	1
4	A	409	PX4	O5-C8-C7	5.38	123.23	108.70	9	1
4	A	397	PX4	O5-C8-C7	5.37	123.21	108.70	10	1
4	A	327	PX4	O7-C23-C24	5.37	122.84	111.53	11	1
4	A	311	PX4	C8-C7-C6	5.36	99.59	112.08	8	1
4	A	422	PX4	O3-P1-O2	5.36	87.27	109.21	1	1
4	A	380	PX4	C8-C7-C6	5.36	99.60	112.08	9	1
4	A	320	PX4	C8-C7-C6	5.35	99.61	112.08	11	2
4	A	360	PX4	O7-C23-C24	5.34	122.79	111.53	11	2
4	A	333	PX4	O5-C8-C7	5.34	123.11	108.70	11	1
4	A	375	PX4	O3-P1-O2	5.33	87.39	109.21	8	1
4	A	324	PX4	C8-C7-C6	5.33	99.67	112.08	14	1
4	A	417	PX4	C8-C7-C6	5.33	99.67	112.08	4	1
4	A	343	PX4	O5-C8-C7	5.32	123.07	108.70	11	1
4	A	387	PX4	C8-C7-C6	5.32	99.69	112.08	6	1
4	A	329	PX4	O7-C23-C24	5.32	122.73	111.53	2	1
4	A	390	PX4	C8-C7-C6	5.31	99.72	112.08	8	1
4	A	306	PX4	C7-O7-C23	5.30	131.02	117.91	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	366	PX4	O7-C23-C24	5.29	122.68	111.53	12	2
4	A	331	PX4	O7-C7-C8	5.29	126.95	108.36	3	1
4	A	353	PX4	O7-C23-O8	5.29	109.28	123.67	13	1
4	A	394	PX4	O5-C8-C7	5.29	122.98	108.70	3	1
4	A	421	PX4	O5-C8-C7	5.28	122.96	108.70	13	1
4	A	387	PX4	O1-P1-O3	5.27	83.11	108.24	12	1
4	A	352	PX4	C8-C7-C6	5.27	99.80	112.08	2	1
4	A	368	PX4	C8-C7-C6	5.27	99.80	112.08	6	2
4	A	424	PX4	O5-C8-C7	5.27	122.93	108.70	13	1
4	A	319	PX4	O5-C8-C7	5.25	122.88	108.70	6	1
4	A	389	PX4	C8-C7-C6	5.25	99.84	112.08	5	1
4	A	334	PX4	O5-C8-C7	5.25	122.88	108.70	13	1
4	A	378	PX4	O7-C23-C24	5.25	122.59	111.53	13	1
4	A	328	PX4	C8-C7-C6	5.25	99.86	112.08	2	1
4	A	310	PX4	O5-C9-O6	5.24	109.77	123.51	5	1
4	A	309	PX4	O5-C8-C7	5.24	122.84	108.70	7	1
4	A	337	PX4	O5-C8-C7	5.23	122.83	108.70	12	1
4	A	402	PX4	C8-O5-C9	5.22	132.54	117.00	1	1
4	A	406	PX4	C8-C7-C6	5.22	99.92	112.08	1	1
4	A	423	PX4	O7-C23-O8	5.21	109.49	123.67	3	1
4	A	324	PX4	O5-C8-C7	5.21	122.77	108.70	14	1
4	A	346	PX4	O5-C8-C7	5.21	122.77	108.70	3	1
4	A	311	PX4	O7-C23-O8	5.20	109.52	123.67	3	1
4	A	410	PX4	O7-C23-C24	5.20	122.48	111.53	4	1
4	A	349	PX4	O7-C23-C24	5.19	122.47	111.53	2	1
4	A	370	PX4	C8-C7-C6	5.19	99.98	112.08	4	1
4	A	394	PX4	O7-C23-C24	5.19	122.46	111.53	6	1
4	A	411	PX4	C5-N1-C3	5.18	95.56	108.96	1	1
4	A	331	PX4	O7-C23-C24	5.17	122.42	111.53	8	1
4	A	322	PX4	C8-C7-C6	5.16	100.05	112.08	9	1
4	A	417	PX4	O1-P1-O3	5.15	83.69	108.24	14	1
4	A	363	PX4	O5-C8-C7	5.15	122.60	108.70	11	1
4	A	342	PX4	C8-C7-C6	5.14	100.09	112.08	2	1
4	A	414	PX4	O5-C8-C7	5.14	122.59	108.70	6	1
4	A	389	PX4	O5-C8-C7	5.14	122.58	108.70	13	2
4	A	354	PX4	C8-C7-C6	5.13	100.13	112.08	11	1
4	A	330	PX4	O7-C23-C24	5.13	122.33	111.53	11	1
4	A	398	PX4	C5-N1-C4	5.12	95.71	108.96	9	1
4	A	351	PX4	C8-C7-C6	5.12	100.14	112.08	6	1
4	A	391	PX4	O5-C8-C7	5.12	122.53	108.70	4	1
4	A	386	PX4	C8-C7-C6	5.12	100.16	112.08	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	340	PX4	C8-C7-C6	5.12	100.16	112.08	2	1
4	A	412	PX4	O7-C23-C24	5.10	122.28	111.53	7	1
4	A	359	PX4	C8-C7-C6	5.10	100.19	112.08	14	1
4	A	328	PX4	O5-C8-C7	5.09	122.43	108.70	9	1
4	A	385	PX4	O5-C8-C7	5.08	122.43	108.70	12	1
4	A	370	PX4	O5-C8-C7	5.08	122.42	108.70	2	2
4	A	402	PX4	O5-C8-C7	5.08	122.42	108.70	7	1
4	A	344	PX4	O7-C23-C24	5.06	122.20	111.53	8	1
4	A	421	PX4	C8-C7-C6	5.06	100.28	112.08	14	1
4	A	397	PX4	O7-C23-C24	5.06	122.19	111.53	14	1
4	A	382	PX4	O7-C23-C24	5.06	122.18	111.53	3	1
4	A	422	PX4	O7-C23-C24	5.05	122.17	111.53	5	1
4	A	362	PX4	C8-C7-C6	5.05	100.32	112.08	2	1
4	A	423	PX4	C8-C7-C6	5.05	100.32	112.08	13	1
4	A	405	PX4	C8-O5-C9	5.05	101.96	117.00	13	1
4	A	392	PX4	C5-N1-C4	5.05	95.90	108.96	8	1
4	A	335	PX4	O5-C8-C7	5.04	122.31	108.70	3	1
4	A	422	PX4	C8-C7-C6	5.04	100.35	112.08	13	1
4	A	407	PX4	C8-C7-C6	5.02	100.38	112.08	4	1
4	A	369	PX4	C7-O7-C23	5.02	130.32	117.91	7	1
4	A	420	PX4	C5-N1-C3	5.01	95.99	108.96	7	1
4	A	413	PX4	O5-C8-C7	5.01	122.23	108.70	8	1
4	A	401	PX4	O5-C8-C7	5.01	122.23	108.70	12	1
4	A	381	PX4	O7-C7-C8	5.01	125.95	108.36	2	1
4	A	419	PX4	C8-C7-C6	5.00	100.42	112.08	8	1

There are no chirality outliers.

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	335	PX4	C7-O7-C23-C24	6
4	A	335	PX4	C7-O7-C23-O8	4

There are no ring outliers.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: 2mls_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	1762
Number of shifts mapped to atoms	1762
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	160	-0.25 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	138	0.11 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	129	-0.17 ± 0.15	None needed (< 0.5 ppm)
^{15}N	154	-0.70 ± 0.49	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 1624 atoms were assigned a chemical shift out of a possible 1946. 15 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	752/796 (94%)	312/317 (98%)	287/324 (89%)	153/155 (99%)
Sidechain	724/896 (81%)	450/526 (86%)	265/330 (80%)	9/40 (22%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	148/254 (58%)	79/137 (58%)	66/105 (63%)	3/12 (25%)
Overall	1624/1946 (83%)	841/980 (86%)	618/759 (81%)	165/207 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1629 atoms were assigned a chemical shift out of a possible 1968. 15 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	757/806 (94%)	314/321 (98%)	289/328 (88%)	154/157 (98%)
Sidechain	724/899 (81%)	450/528 (85%)	265/331 (80%)	9/40 (22%)
Aromatic	148/263 (56%)	79/142 (56%)	66/109 (61%)	3/12 (25%)
Overall	1629/1968 (83%)	843/991 (85%)	620/768 (81%)	166/209 (79%)

7.1.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	226	LEU	CG	33.00	32.55 – 21.05	5.4
1	A	214	LEU	CG	33.00	32.55 – 21.05	5.4

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

