



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 06:51 AM BST

PDB ID : 2MLR
Title : Membrane Bilayer complex with Matrix Metalloproteinase-12 at its Alpha-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

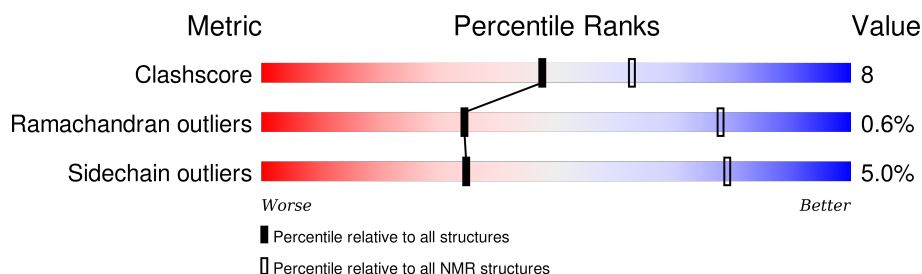
1 Overall quality at a glance

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	 79% 18% ..

2 Ensemble composition and analysis

This entry contains 14 models. Model 3 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:100-A:187, A:192-A:263 (160)	0.38	3

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

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

The models can be grouped into 4 clusters. No single-model clusters were found.

Cluster number	Models
1	8, 9, 10, 11, 13
2	1, 2, 3, 4, 5
3	6, 7
4	12, 14

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

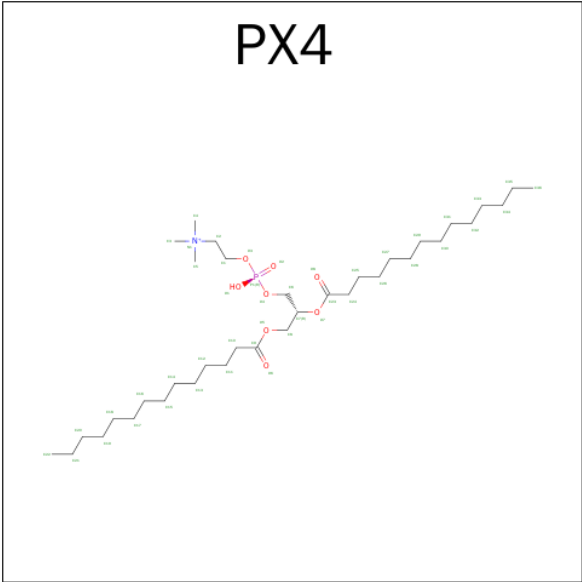
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

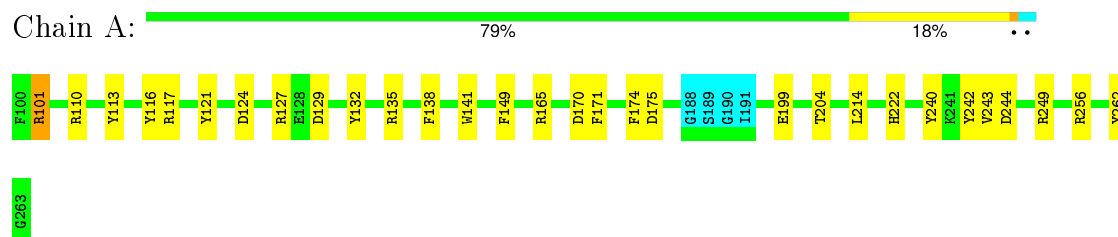
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Macrophage metalloelastase

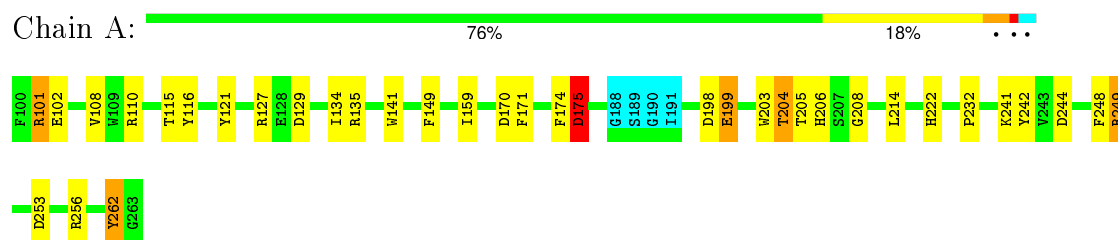


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

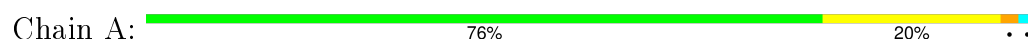
4.2.1 Score per residue for model 1

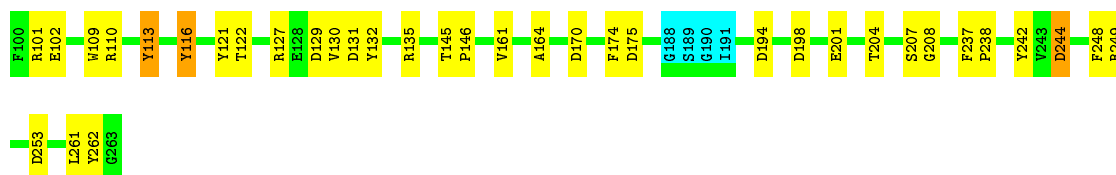
- Molecule 1: Macrophage metalloelastase



4.2.2 Score per residue for model 2

- Molecule 1: Macrophage metalloelastase





4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Macrophage metalloelastase

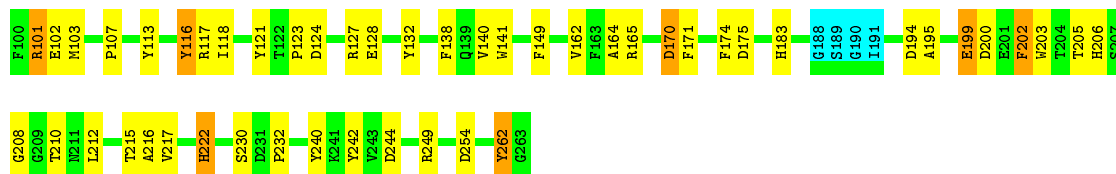
Chain A: 79% 16% ..



4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase

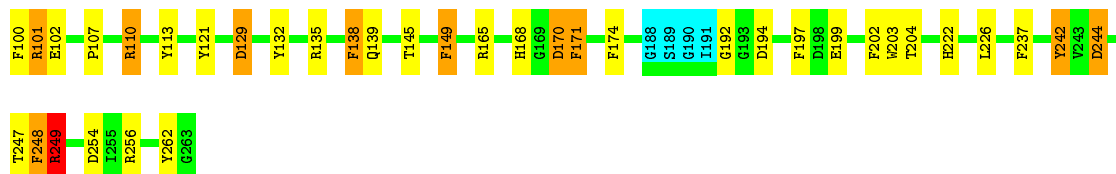
Chain A: 68% 26% ..



4.2.5 Score per residue for model 5

- Molecule 1: Macrophage metalloelastase

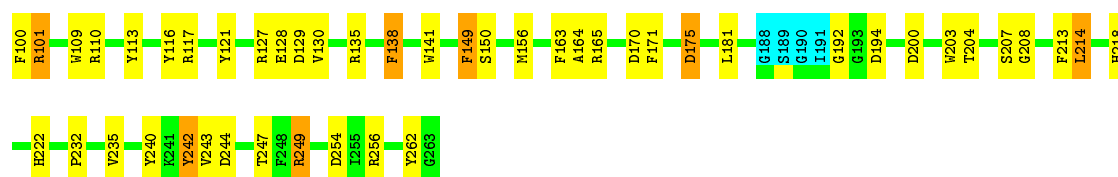
Chain A: 75% 16% 6% ..



4.2.6 Score per residue for model 6

- Molecule 1: Macrophage metalloelastase

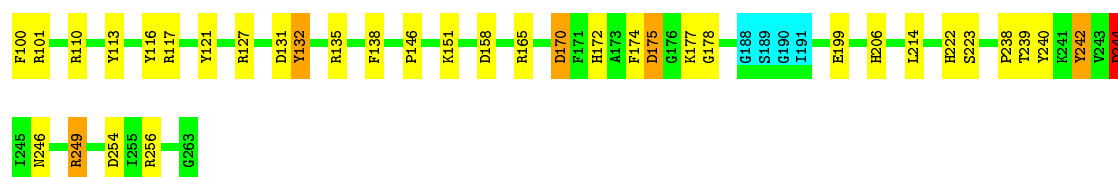
Chain A: 69% 24% ..



4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase

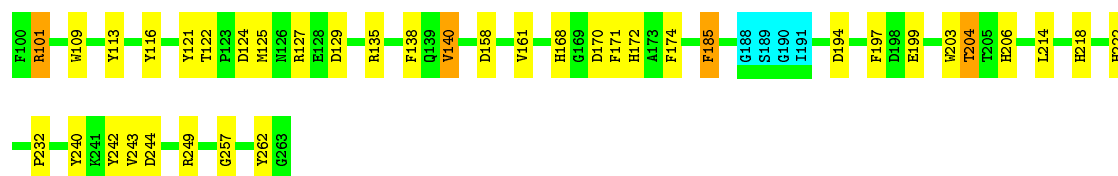
Chain A: 76% 18% ...



4.2.8 Score per residue for model 8

- Molecule 1: Macrophage metalloelastase

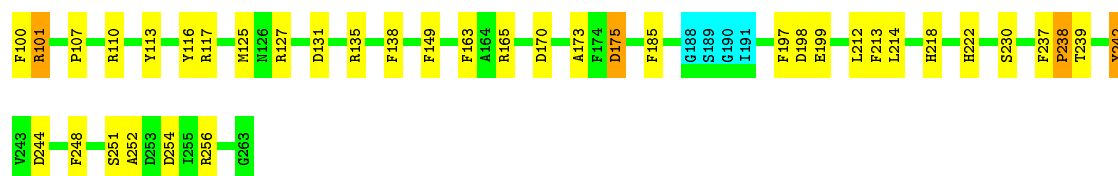
Chain A: 74% 21% ..



4.2.9 Score per residue for model 9

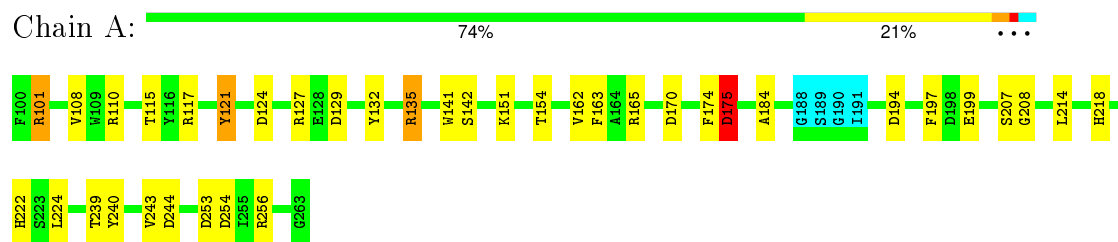
- Molecule 1: Macrophage metalloelastase

Chain A: 74% 21% ..



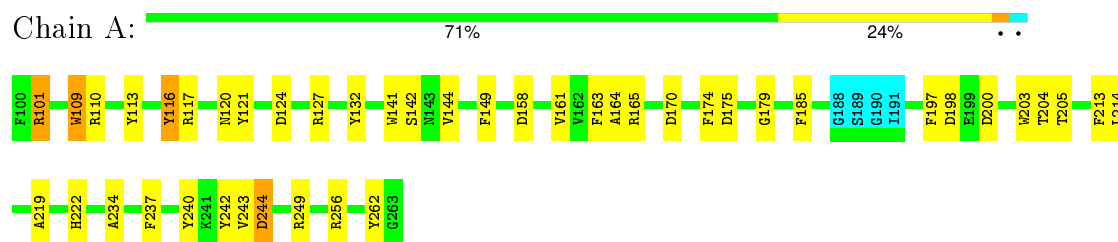
4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase



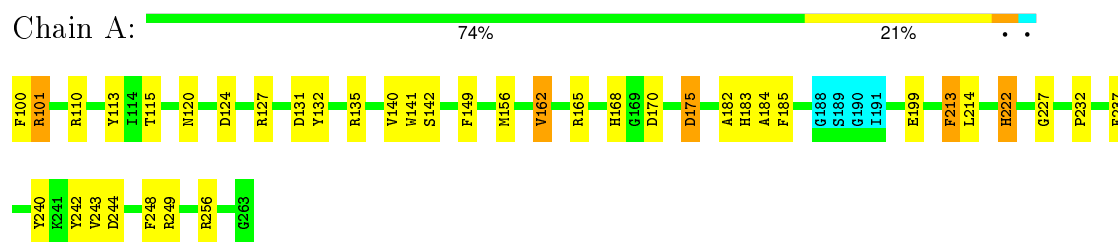
4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



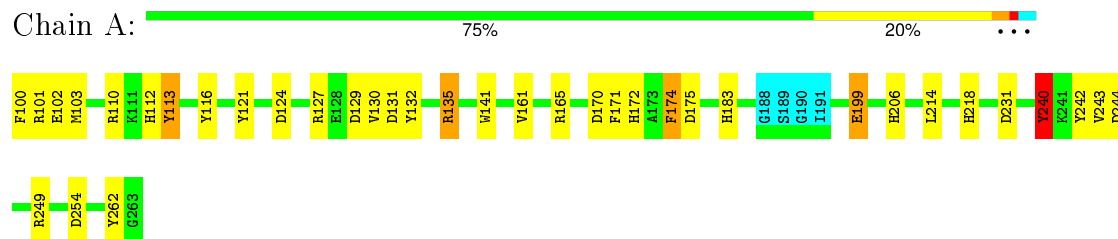
4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



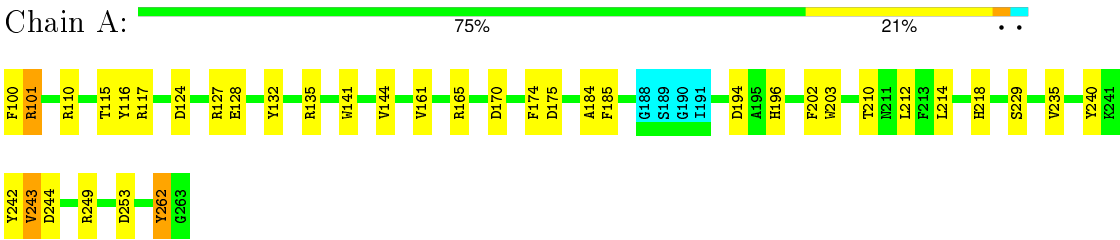
4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase



4.2.14 Score per residue for model 14

● Molecule 1: Macrophage metalloelastase



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)	2mlr_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	0.58±0.01	0±0/1305 (0.0±0.0%)	2.04±0.06	42±6/1768 (2.4±0.4%)
All	All	0.58	0/18270 (0.0%)	2.05	584/24752 (2.4%)

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	5.1±1.9
All	All	0	71

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	249	ARG	NE-CZ-NH1	19.17	129.88	120.30	11	6
1	A	127	ARG	NE-CZ-NH2	-18.79	110.91	120.30	11	8
1	A	165	ARG	NE-CZ-NH2	-18.12	111.24	120.30	5	4
1	A	262	TYR	CB-CG-CD2	-17.25	110.65	121.00	14	4
1	A	240	TYR	CB-CG-CD1	-14.90	112.06	121.00	6	5
1	A	110	ARG	NE-CZ-NH2	-14.86	112.87	120.30	13	6
1	A	174	PHE	CB-CG-CD1	-14.06	110.95	120.80	8	6
1	A	113	TYR	CB-CG-CD2	-14.02	112.59	121.00	2	3
1	A	165	ARG	NE-CZ-NH1	14.01	127.31	120.30	3	8
1	A	101	ARG	NE-CZ-NH2	-13.97	113.31	120.30	12	7
1	A	117	ARG	NE-CZ-NH2	-12.67	113.97	120.30	3	5
1	A	135	ARG	NE-CZ-NH2	-12.59	114.00	120.30	7	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	256	ARG	NE-CZ-NH2	-12.30	114.15	120.30	11	5
1	A	101	ARG	NE-CZ-NH1	12.20	126.40	120.30	4	6
1	A	127	ARG	NE-CZ-NH1	12.07	126.33	120.30	9	6
1	A	110	ARG	NE-CZ-NH1	-11.95	114.33	120.30	12	7
1	A	135	ARG	NE-CZ-NH1	11.80	126.20	120.30	13	6
1	A	248	PHE	CB-CG-CD1	-11.62	112.66	120.80	1	3
1	A	100	PHE	CB-CG-CD2	11.57	128.90	120.80	9	5
1	A	254	ASP	CB-CG-OD2	-11.53	107.92	118.30	10	6
1	A	117	ARG	NE-CZ-NH1	10.99	125.80	120.30	3	3
1	A	132	TYR	CB-CG-CD2	-10.80	114.52	121.00	10	4
1	A	256	ARG	NE-CZ-NH1	10.79	125.69	120.30	11	4
1	A	113	TYR	CG-CD1-CE1	-10.52	112.89	121.30	9	2
1	A	113	TYR	CD1-CE1-CZ	-10.37	110.46	119.80	5	2
1	A	213	PHE	CB-CG-CD1	-10.26	113.62	120.80	6	3
1	A	249	ARG	NE-CZ-NH2	-10.21	115.19	120.30	11	6
1	A	163	PHE	CB-CG-CD2	10.18	127.93	120.80	11	2
1	A	175	ASP	CB-CG-OD1	10.08	127.37	118.30	12	8
1	A	113	TYR	CB-CG-CD1	-10.07	114.96	121.00	9	7
1	A	199	GLU	OE1-CD-OE2	-10.05	111.24	123.30	4	2
1	A	175	ASP	CB-CG-OD2	10.01	127.31	118.30	11	4
1	A	170	ASP	CB-CG-OD1	9.97	127.27	118.30	14	11
1	A	124	ASP	CB-CG-OD1	9.87	127.18	118.30	10	6
1	A	185	PHE	CB-CG-CD2	-9.86	113.90	120.80	14	3
1	A	194	ASP	CB-CG-OD1	9.75	127.08	118.30	2	6
1	A	113	TYR	CG-CD2-CE2	-9.56	113.66	121.30	13	2
1	A	156	MET	CG-SD-CE	9.52	115.43	100.20	6	1
1	A	116	TYR	CB-CG-CD1	-9.48	115.31	121.00	11	4
1	A	262	TYR	CB-CG-CD1	9.38	126.63	121.00	14	4
1	A	121	TYR	CB-CG-CD2	9.29	126.57	121.00	10	5
1	A	100	PHE	CB-CG-CD1	-9.26	114.32	120.80	9	3
1	A	116	TYR	CG-CD1-CE1	-9.17	113.97	121.30	4	1
1	A	170	ASP	OD1-CG-OD2	-9.04	106.13	123.30	8	14
1	A	242	TYR	CB-CG-CD1	-9.02	115.59	121.00	2	5
1	A	132	TYR	CB-CG-CD1	8.98	126.39	121.00	10	4
1	A	204	THR	CA-CB-CG2	8.97	124.96	112.40	8	3
1	A	161	VAL	CA-CB-CG1	8.94	124.31	110.90	14	2
1	A	170	ASP	CB-CG-OD2	8.93	126.34	118.30	11	10
1	A	102	GLU	OE1-CD-OE2	-8.90	112.62	123.30	13	5
1	A	202	PHE	CB-CG-CD2	-8.86	114.60	120.80	5	2
1	A	121	TYR	CB-CG-CD1	-8.83	115.70	121.00	3	4
1	A	253	ASP	CB-CG-OD2	-8.44	110.70	118.30	14	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	163	PHE	CB-CG-CD1	-8.39	114.93	120.80	11	2
1	A	101	ARG	CD-NE-CZ	8.38	135.32	123.60	14	1
1	A	254	ASP	CB-CG-OD1	-8.36	110.78	118.30	5	3
1	A	194	ASP	CB-CG-OD2	8.35	125.82	118.30	8	3
1	A	138	PHE	CB-CG-CD1	8.31	126.62	120.80	5	4
1	A	262	TYR	CZ-CE2-CD2	-8.26	112.37	119.80	4	2
1	A	174	PHE	CB-CG-CD2	-8.15	115.09	120.80	2	4
1	A	248	PHE	CB-CG-CD2	-8.13	115.11	120.80	5	3
1	A	141	TRP	CD1-NE1-CE2	8.13	116.32	109.00	14	4
1	A	115	THR	CA-CB-CG2	8.11	123.76	112.40	1	3
1	A	231	ASP	CB-CG-OD1	-8.08	111.03	118.30	13	1
1	A	141	TRP	NE1-CE2-CD2	-7.98	99.32	107.30	14	3
1	A	203	TRP	CG-CD2-CE3	7.91	141.02	133.90	11	2
1	A	116	TYR	CB-CG-CD2	-7.88	116.27	121.00	3	5
1	A	141	TRP	NE1-CE2-CZ2	7.83	139.01	130.40	14	2
1	A	161	VAL	CA-CB-CG2	7.82	122.62	110.90	13	2
1	A	213	PHE	CB-CG-CD2	-7.77	115.36	120.80	9	3
1	A	238	PRO	N-CA-CB	7.76	112.61	103.30	2	3
1	A	237	PHE	CB-CG-CD2	7.72	126.20	120.80	11	1
1	A	131	ASP	CB-CG-OD2	-7.68	111.39	118.30	13	2
1	A	240	TYR	CB-CG-CD2	-7.67	116.40	121.00	8	3
1	A	140	VAL	CA-CB-CG1	7.62	122.33	110.90	4	3
1	A	185	PHE	CB-CG-CD1	7.59	126.11	120.80	14	2
1	A	116	TYR	CD1-CE1-CZ	7.50	126.55	119.80	4	2
1	A	129	ASP	CB-CG-OD1	7.49	125.04	118.30	5	6
1	A	138	PHE	CB-CG-CD2	-7.48	115.57	120.80	7	3
1	A	109	TRP	CD1-NE1-CE2	7.41	115.66	109.00	11	3
1	A	256	ARG	CD-NE-CZ	7.39	133.95	123.60	9	1
1	A	184	ALA	N-CA-CB	-7.39	99.75	110.10	12	2
1	A	203	TRP	CD1-NE1-CE2	7.39	115.65	109.00	1	3
1	A	232	PRO	N-CA-CB	7.29	112.05	103.30	1	3
1	A	135	ARG	CD-NE-CZ	7.25	133.75	123.60	14	2
1	A	197	PHE	CB-CG-CD2	-7.20	115.76	120.80	8	2
1	A	203	TRP	CD1-CG-CD2	7.18	112.04	106.30	5	2
1	A	210	THR	CA-CB-CG2	7.10	122.34	112.40	14	1
1	A	194	ASP	OD1-CG-OD2	-7.09	109.82	123.30	8	2
1	A	109	TRP	NE1-CE2-CD2	-7.07	100.23	107.30	11	3
1	A	262	TYR	CG-CD1-CE1	-7.07	115.64	121.30	6	1
1	A	253	ASP	CB-CG-OD1	7.06	124.66	118.30	10	3
1	A	197	PHE	CB-CG-CD1	7.04	125.73	120.80	8	3
1	A	149	PHE	CZ-CE2-CD2	-7.00	111.70	120.10	5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	122	THR	CA-CB-CG2	6.95	122.13	112.40	8	1
1	A	127	ARG	NH1-CZ-NH2	6.94	127.04	119.40	11	2
1	A	132	TYR	CG-CD2-CE2	-6.93	115.75	121.30	11	2
1	A	244	ASP	CB-CG-OD1	-6.93	112.06	118.30	7	1
1	A	141	TRP	CB-CG-CD2	6.91	135.58	126.60	11	1
1	A	201	GLU	CB-CA-C	-6.90	96.60	110.40	2	1
1	A	222	HIS	CA-CB-CG	6.90	125.32	113.60	4	2
1	A	149	PHE	CB-CG-CD1	-6.89	115.98	120.80	9	4
1	A	171	PHE	CB-CG-CD2	-6.83	116.02	120.80	1	1
1	A	239	THR	N-CA-CB	-6.81	97.36	110.30	7	1
1	A	172	HIS	CA-CB-CG	6.79	125.15	113.60	7	2
1	A	235	VAL	CA-CB-CG1	6.78	121.06	110.90	14	2
1	A	242	TYR	CB-CG-CD2	-6.73	116.96	121.00	14	5
1	A	141	TRP	CB-CG-CD1	-6.61	118.40	127.00	11	1
1	A	101	ARG	NH1-CZ-NH2	6.58	126.63	119.40	6	2
1	A	158	ASP	CB-CG-OD2	-6.54	112.42	118.30	7	3
1	A	218	HIS	CA-CB-CG	6.54	124.71	113.60	13	5
1	A	239	THR	CA-CB-CG2	6.51	121.52	112.40	10	2
1	A	141	TRP	CZ3-CH2-CZ2	-6.48	113.83	121.60	6	2
1	A	175	ASP	OD1-CG-OD2	-6.47	111.01	123.30	12	6
1	A	131	ASP	CB-CG-OD1	6.45	124.10	118.30	9	3
1	A	240	TYR	CG-CD1-CE1	-6.45	116.14	121.30	6	3
1	A	164	ALA	CB-CA-C	6.43	119.75	110.10	4	2
1	A	168	HIS	C-N-CA	6.41	135.76	122.30	5	2
1	A	110	ARG	CD-NE-CZ	6.41	132.57	123.60	12	2
1	A	262	TYR	CG-CD2-CE2	-6.40	116.18	121.30	3	3
1	A	210	THR	O-C-N	-6.39	112.47	122.70	4	1
1	A	174	PHE	CG-CD2-CE2	-6.35	113.81	120.80	8	1
1	A	174	PHE	CD1-CG-CD2	6.33	126.52	118.30	11	2
1	A	227	GLY	N-CA-C	-6.28	97.41	113.10	12	1
1	A	248	PHE	CG-CD1-CE1	-6.25	113.92	120.80	9	1
1	A	117	ARG	CD-NE-CZ	6.25	132.34	123.60	6	2
1	A	130	VAL	CA-CB-CG1	6.23	120.24	110.90	13	2
1	A	151	LYS	C-N-CA	6.23	137.27	121.70	7	1
1	A	174	PHE	CB-CA-C	6.22	122.84	110.40	14	4
1	A	237	PHE	CB-CG-CD1	6.21	125.15	120.80	2	3
1	A	216	ALA	CB-CA-C	-6.21	100.79	110.10	4	1
1	A	158	ASP	CB-CG-OD1	-6.20	112.72	118.30	3	1
1	A	254	ASP	CA-CB-CG	6.18	126.99	113.40	4	1
1	A	183	HIS	CA-CB-CG	6.17	124.10	113.60	13	1
1	A	113	TYR	CZ-CE2-CD2	6.16	125.35	119.80	13	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	128	GLU	OE1-CD-OE2	-6.14	115.93	123.30	14	2
1	A	212	LEU	CB-CG-CD1	6.14	121.44	111.00	14	2
1	A	243	VAL	CA-CB-CG2	6.13	120.10	110.90	14	1
1	A	162	VAL	CA-CB-CG1	6.13	120.10	110.90	3	3
1	A	247	THR	O-C-N	-6.11	112.92	122.70	6	2
1	A	223	SER	N-CA-CB	-6.10	101.34	110.50	7	1
1	A	202	PHE	CB-CG-CD1	-6.05	116.56	120.80	14	1
1	A	116	TYR	CA-CB-CG	6.04	124.88	113.40	3	1
1	A	200	ASP	CB-CG-OD2	-6.03	112.87	118.30	6	1
1	A	200	ASP	CB-CG-OD1	6.03	123.73	118.30	4	1
1	A	175	ASP	CB-CA-C	6.01	122.42	110.40	4	1
1	A	165	ARG	CB-CA-C	5.97	122.35	110.40	9	2
1	A	116	TYR	CB-CA-C	5.97	122.34	110.40	6	1
1	A	150	SER	N-CA-CB	-5.96	101.56	110.50	6	1
1	A	231	ASP	CB-CG-OD2	5.95	123.65	118.30	13	1
1	A	229	SER	N-CA-CB	-5.91	101.63	110.50	14	1
1	A	135	ARG	NH1-CZ-NH2	5.89	125.89	119.40	12	1
1	A	165	ARG	NH1-CZ-NH2	5.88	125.86	119.40	5	1
1	A	205	THR	CA-CB-OG1	5.84	121.26	109.00	11	1
1	A	141	TRP	CE2-CD2-CG	5.82	111.95	107.30	14	3
1	A	149	PHE	CB-CG-CD2	-5.81	116.73	120.80	6	2
1	A	198	ASP	CB-CG-OD2	-5.80	113.08	118.30	1	2
1	A	132	TYR	CG-CD1-CE1	-5.79	116.67	121.30	2	1
1	A	219	ALA	N-CA-CB	-5.77	102.02	110.10	11	1
1	A	262	TYR	CA-CB-CG	5.77	124.36	113.40	1	1
1	A	102	GLU	N-CA-CB	-5.76	100.24	110.60	13	1
1	A	145	THR	CA-CB-CG2	5.73	120.43	112.40	5	1
1	A	130	VAL	CG1-CB-CG2	-5.71	101.77	110.90	2	1
1	A	124	ASP	CB-CG-OD2	5.68	123.41	118.30	4	2
1	A	109	TRP	CE2-CD2-CG	5.65	111.82	107.30	8	1
1	A	203	TRP	CG-CD1-NE1	-5.63	104.47	110.10	5	2
1	A	103	MET	N-CA-CB	-5.63	100.46	110.60	4	1
1	A	192	GLY	CA-C-N	5.62	127.43	116.20	5	1
1	A	249	ARG	NH1-CZ-NH2	-5.61	113.23	119.40	3	1
1	A	129	ASP	CB-CG-OD2	5.57	123.31	118.30	2	3
1	A	108	VAL	CA-CB-CG2	5.56	119.24	110.90	1	2
1	A	113	TYR	CD1-CG-CD2	5.56	124.01	117.90	9	1
1	A	168	HIS	CB-CA-C	5.56	121.51	110.40	12	1
1	A	171	PHE	CB-CG-CD1	-5.55	116.92	120.80	5	1
1	A	124	ASP	OD1-CG-OD2	-5.55	112.76	123.30	8	1
1	A	257	GLY	O-C-N	5.54	131.57	122.70	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	107	PRO	N-CD-CG	5.53	111.50	103.20	3	1
1	A	112	HIS	C-N-CA	5.52	135.50	121.70	13	1
1	A	226	LEU	CB-CG-CD2	5.51	120.37	111.00	5	1
1	A	163	PHE	CZ-CE2-CD2	-5.49	113.51	120.10	6	1
1	A	132	TYR	CD1-CG-CD2	5.48	123.93	117.90	14	1
1	A	107	PRO	C-N-CA	5.48	135.39	121.70	9	1
1	A	240	TYR	CD1-CG-CD2	5.47	123.92	117.90	6	1
1	A	125	MET	N-CA-CB	5.47	120.45	110.60	9	1
1	A	174	PHE	CG-CD1-CE1	5.44	126.79	120.80	4	2
1	A	150	SER	CB-CA-C	5.42	120.39	110.10	3	1
1	A	230	SER	N-CA-CB	-5.41	102.38	110.50	9	2
1	A	203	TRP	NE1-CE2-CZ2	5.41	136.35	130.40	8	1
1	A	128	GLU	O-C-N	-5.41	114.05	122.70	6	1
1	A	161	VAL	CG1-CB-CG2	-5.39	102.27	110.90	2	1
1	A	208	GLY	CA-C-O	-5.37	110.94	120.60	4	1
1	A	203	TRP	CA-CB-CG	5.37	123.90	113.70	6	1
1	A	123	PRO	C-N-CA	5.35	135.07	121.70	4	1
1	A	162	VAL	CB-CA-C	5.34	121.55	111.40	4	1
1	A	241	LYS	CB-CA-C	5.33	121.06	110.40	1	1
1	A	249	ARG	CD-NE-CZ	5.33	131.06	123.60	12	1
1	A	208	GLY	N-CA-C	-5.32	99.79	113.10	10	1
1	A	232	PRO	N-CD-CG	5.32	111.17	103.20	12	2
1	A	182	ALA	CB-CA-C	5.31	118.07	110.10	12	1
1	A	242	TYR	C-N-CA	5.30	134.95	121.70	13	2
1	A	132	TYR	CZ-CE2-CD2	5.30	124.57	119.80	11	1
1	A	149	PHE	CD1-CG-CD2	5.29	125.18	118.30	9	1
1	A	149	PHE	CG-CD1-CE1	-5.29	114.98	120.80	9	1
1	A	116	TYR	CG-CD2-CE2	-5.29	117.07	121.30	1	1
1	A	118	ILE	N-CA-C	-5.28	96.73	111.00	4	1
1	A	235	VAL	CG1-CB-CG2	-5.28	102.46	110.90	6	1
1	A	202	PHE	CG-CD2-CE2	-5.27	115.00	120.80	14	1
1	A	125	MET	CB-CA-C	5.24	120.88	110.40	8	1
1	A	144	VAL	CA-CB-CG2	5.24	118.76	110.90	14	2
1	A	129	ASP	N-CA-CB	5.24	120.03	110.60	3	1
1	A	240	TYR	CZ-CE2-CD2	-5.24	115.09	119.80	12	1
1	A	109	TRP	CB-CG-CD1	-5.23	120.20	127.00	2	1
1	A	240	TYR	C-N-CA	5.23	134.78	121.70	10	1
1	A	120	ASN	CB-CA-C	5.23	120.86	110.40	11	1
1	A	141	TRP	CH2-CZ2-CE2	5.22	122.62	117.40	6	2
1	A	251	SER	N-CA-CB	-5.21	102.68	110.50	9	1
1	A	165	ARG	CD-NE-CZ	5.20	130.88	123.60	11	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	163	PHE	CG-CD2-CE2	5.19	126.51	120.80	6	1
1	A	130	VAL	CA-CB-CG2	5.18	118.67	110.90	6	1
1	A	212	LEU	O-C-N	-5.17	114.42	122.70	4	1
1	A	215	THR	OG1-CB-CG2	-5.17	98.11	110.00	4	1
1	A	246	ASN	CB-CA-C	-5.15	100.10	110.40	7	1
1	A	256	ARG	C-N-CA	5.15	133.11	122.30	12	1
1	A	244	ASP	CB-CG-OD2	5.14	122.93	118.30	11	1
1	A	240	TYR	CG-CD2-CE2	-5.14	117.19	121.30	10	1
1	A	184	ALA	CB-CA-C	-5.14	102.39	110.10	14	1
1	A	101	ARG	C-N-CA	5.13	134.51	121.70	14	1
1	A	122	THR	N-CA-CB	-5.12	100.58	110.30	8	1
1	A	181	LEU	CB-CG-CD1	5.11	119.68	111.00	6	1
1	A	173	ALA	N-CA-CB	5.11	117.25	110.10	9	1
1	A	109	TRP	NE1-CE2-CZ2	5.11	136.02	130.40	11	2
1	A	154	THR	CA-CB-CG2	5.10	119.54	112.40	10	1
1	A	120	ASN	N-CA-CB	5.10	119.78	110.60	12	1
1	A	192	GLY	C-N-CA	5.09	132.99	122.30	6	1
1	A	242	TYR	CG-CD1-CE1	5.09	125.37	121.30	12	1
1	A	110	ARG	C-N-CA	5.08	134.40	121.70	7	1
1	A	121	TYR	CG-CD1-CE1	-5.08	117.24	121.30	11	1
1	A	164	ALA	O-C-N	-5.08	114.58	122.70	11	1
1	A	222	HIS	CG-ND1-CE1	-5.08	99.10	105.70	12	1
1	A	217	VAL	O-C-N	-5.08	114.58	122.70	4	1
1	A	199	GLU	CA-CB-CG	5.08	124.57	113.40	13	1
1	A	261	LEU	CB-CA-C	-5.06	100.59	110.20	2	1
1	A	206	HIS	CA-CB-CG	5.06	122.20	113.60	8	1
1	A	195	ALA	N-CA-CB	-5.05	103.03	110.10	4	1
1	A	174	PHE	C-N-CA	5.03	134.28	121.70	1	1
1	A	262	TYR	CB-CA-C	5.01	120.42	110.40	2	1
1	A	173	ALA	CB-CA-C	5.00	117.61	110.10	3	1
1	A	185	PHE	C-N-CA	5.00	132.80	122.30	9	1
1	A	234	ALA	C-N-CA	5.00	134.20	121.70	11	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	242	TYR	Peptide,Sidechain	7
1	A	204	THR	Peptide	5
1	A	262	TYR	Sidechain	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	121	TYR	Sidechain	5
1	A	240	TYR	Sidechain,Peptide	4
1	A	132	TYR	Sidechain	3
1	A	116	TYR	Sidechain,Mainchain	3
1	A	113	TYR	Sidechain	3
1	A	248	PHE	Sidechain,Peptide	2
1	A	197	PHE	Sidechain	2
1	A	110	ARG	Sidechain	2
1	A	185	PHE	Sidechain	2
1	A	135	ARG	Sidechain	2
1	A	127	ARG	Mainchain	1
1	A	199	GLU	Sidechain	1
1	A	174	PHE	Peptide	1
1	A	218	HIS	Sidechain	1
1	A	224	LEU	Mainchain	1
1	A	159	ILE	Peptide	1
1	A	249	ARG	Sidechain	1
1	A	252	ALA	Mainchain	1
1	A	101	ARG	Sidechain	1
1	A	183	HIS	Sidechain	1
1	A	172	HIS	Sidechain	1
1	A	117	ARG	Sidechain	1
1	A	151	LYS	Peptide	1
1	A	196	HIS	Sidechain	1
1	A	256	ARG	Sidechain	1
1	A	206	HIS	Sidechain	1
1	A	163	PHE	Sidechain	1
1	A	202	PHE	Sidechain	1
1	A	164	ALA	Peptide	1
1	A	237	PHE	Sidechain	1
1	A	100	PHE	Sidechain	1
1	A	222	HIS	Sidechain	1
1	A	171	PHE	Sidechain	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	1265	1199	1196	2±1
4	A	5750	0	9000	131±13
All	All	98280	16786	142744	1846

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:388:PX4:H39	4:A:411:PX4:H17	0.99	1.35	4	1
4:A:337:PX4:H47	4:A:353:PX4:H15	0.93	1.41	8	2
4:A:413:PX4:H24	4:A:430:PX4:H63	0.92	1.40	10	1
4:A:320:PX4:H20	4:A:359:PX4:H57	0.92	1.42	5	1
4:A:368:PX4:H22	4:A:369:PX4:H51	0.90	1.40	6	1
4:A:342:PX4:H24	4:A:352:PX4:H47	0.88	1.43	11	1
4:A:378:PX4:H16	4:A:417:PX4:H47	0.85	1.46	7	9
4:A:309:PX4:H59	4:A:324:PX4:H57	0.84	1.50	12	1
4:A:355:PX4:H48	4:A:356:PX4:H14	0.83	1.49	4	2
4:A:332:PX4:H61	4:A:349:PX4:H51	0.83	1.51	6	1
4:A:329:PX4:H70	4:A:382:PX4:H26	0.82	1.50	7	1
4:A:316:PX4:H20	4:A:364:PX4:H47	0.82	1.49	9	1
4:A:386:PX4:H28	4:A:394:PX4:H50	0.82	1.50	11	1
4:A:416:PX4:H21	4:A:425:PX4:H46	0.81	1.51	11	1
4:A:313:PX4:H18	4:A:318:PX4:H46	0.81	1.50	9	2
4:A:335:PX4:H21	4:A:343:PX4:H22	0.81	1.52	5	1
4:A:317:PX4:H17	4:A:325:PX4:H52	0.81	1.53	9	1
4:A:384:PX4:H60	4:A:385:PX4:H35	0.80	1.54	2	1
4:A:387:PX4:H47	4:A:411:PX4:H17	0.79	1.54	12	1
4:A:340:PX4:H66	4:A:340:PX4:H31	0.79	1.55	5	1
4:A:387:PX4:H24	4:A:394:PX4:H53	0.78	1.55	1	2
4:A:404:PX4:H34	4:A:419:PX4:H22	0.78	1.55	8	1
4:A:376:PX4:H54	4:A:385:PX4:H17	0.77	1.57	13	1
4:A:317:PX4:H47	4:A:342:PX4:H69	0.77	1.57	12	1
4:A:421:PX4:H31	4:A:422:PX4:H39	0.77	1.55	2	1
4:A:310:PX4:H16	4:A:363:PX4:H20	0.76	1.56	9	2
4:A:368:PX4:H25	4:A:425:PX4:H42	0.76	1.58	4	1
4:A:413:PX4:H50	4:A:422:PX4:H33	0.75	1.58	2	1
4:A:321:PX4:H20	4:A:354:PX4:H48	0.75	1.56	10	1
4:A:393:PX4:H22	4:A:394:PX4:H19	0.75	1.58	7	1
4:A:400:PX4:H51	4:A:409:PX4:H20	0.75	1.57	12	1
4:A:326:PX4:H50	4:A:351:PX4:H18	0.75	1.58	4	1
4:A:321:PX4:H41	4:A:354:PX4:H59	0.75	1.58	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PX4:H31	4:A:426:PX4:H61	0.74	1.58	6	1
4:A:398:PX4:H16	4:A:407:PX4:H49	0.74	1.58	14	1
4:A:330:PX4:H22	4:A:335:PX4:H19	0.74	1.60	2	1
4:A:345:PX4:H48	4:A:353:PX4:H46	0.74	1.59	4	1
4:A:330:PX4:H60	4:A:357:PX4:H24	0.73	1.60	10	2
4:A:306:PX4:H23	4:A:321:PX4:H39	0.73	1.60	5	1
4:A:332:PX4:H31	4:A:332:PX4:H51	0.73	1.58	7	1
4:A:392:PX4:H18	4:A:393:PX4:H50	0.72	1.61	1	1
4:A:395:PX4:H53	4:A:405:PX4:H22	0.72	1.60	4	1
4:A:317:PX4:H17	4:A:325:PX4:H49	0.72	1.60	1	1
4:A:376:PX4:H50	4:A:385:PX4:H17	0.72	1.60	11	2
4:A:383:PX4:H65	4:A:399:PX4:H31	0.72	1.60	8	1
4:A:403:PX4:H10	4:A:427:PX4:H49	0.72	1.61	3	2
4:A:325:PX4:H30	4:A:334:PX4:H18	0.72	1.60	4	1
4:A:317:PX4:H46	4:A:324:PX4:H17	0.72	1.60	8	1
4:A:367:PX4:H28	4:A:424:PX4:H52	0.72	1.62	4	1
4:A:371:PX4:H59	4:A:379:PX4:H33	0.72	1.61	4	1
4:A:378:PX4:H63	4:A:417:PX4:H62	0.72	1.62	11	1
4:A:323:PX4:H68	4:A:367:PX4:H40	0.72	1.62	3	1
4:A:321:PX4:H38	4:A:328:PX4:H57	0.72	1.61	13	1
4:A:385:PX4:H52	4:A:386:PX4:H26	0.71	1.61	14	1
4:A:383:PX4:H61	4:A:399:PX4:H29	0.71	1.60	6	1
4:A:402:PX4:H38	4:A:404:PX4:H62	0.71	1.59	14	1
4:A:376:PX4:H64	4:A:392:PX4:H29	0.71	1.60	5	1
4:A:387:PX4:H65	4:A:411:PX4:H54	0.71	1.63	8	1
4:A:332:PX4:H43	4:A:363:PX4:H72	0.71	1.63	12	1
4:A:409:PX4:H33	4:A:410:PX4:H46	0.71	1.60	2	1
4:A:402:PX4:H60	4:A:413:PX4:H41	0.71	1.63	7	1
4:A:363:PX4:H1	4:A:364:PX4:H20	0.71	1.61	11	1
4:A:391:PX4:H64	4:A:408:PX4:H55	0.71	1.63	7	1
4:A:321:PX4:H38	4:A:412:PX4:H43	0.70	1.62	14	1
4:A:370:PX4:H19	4:A:403:PX4:H17	0.70	1.63	11	2
4:A:419:PX4:H49	4:A:427:PX4:H49	0.70	1.63	13	1
4:A:308:PX4:H62	4:A:311:PX4:H41	0.70	1.64	13	1
4:A:325:PX4:H31	4:A:332:PX4:H25	0.70	1.63	11	1
4:A:306:PX4:H56	4:A:321:PX4:H55	0.69	1.64	13	1
4:A:384:PX4:H42	4:A:385:PX4:H43	0.69	1.62	8	1
4:A:317:PX4:H16	4:A:351:PX4:H24	0.69	1.64	14	1
4:A:408:PX4:H17	4:A:415:PX4:H20	0.69	1.64	8	1
4:A:332:PX4:H33	4:A:347:PX4:H62	0.69	1.64	11	1
4:A:322:PX4:H50	4:A:336:PX4:H27	0.69	1.63	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H49	4:A:382:PX4:H46	0.69	1.62	8	2
4:A:358:PX4:H23	4:A:363:PX4:H53	0.69	1.64	9	1
4:A:315:PX4:H17	4:A:316:PX4:H49	0.69	1.64	13	1
4:A:360:PX4:H70	4:A:419:PX4:H41	0.69	1.62	4	1
4:A:368:PX4:H17	4:A:369:PX4:H53	0.69	1.63	9	1
4:A:399:PX4:H29	4:A:399:PX4:H63	0.69	1.64	2	1
4:A:396:PX4:H38	4:A:402:PX4:H41	0.69	1.64	12	1
4:A:331:PX4:H58	4:A:339:PX4:H22	0.69	1.63	4	1
4:A:422:PX4:H36	4:A:423:PX4:H23	0.68	1.65	5	1
4:A:388:PX4:H54	4:A:395:PX4:H30	0.68	1.65	12	1
4:A:368:PX4:H47	4:A:369:PX4:H56	0.68	1.63	1	1
4:A:429:PX4:H30	4:A:429:PX4:H55	0.68	1.63	11	1
4:A:328:PX4:H70	4:A:412:PX4:H70	0.68	1.65	13	1
4:A:337:PX4:H50	4:A:353:PX4:H21	0.68	1.64	4	1
4:A:416:PX4:H55	4:A:418:PX4:H30	0.68	1.66	12	1
4:A:395:PX4:H55	4:A:404:PX4:H46	0.68	1.66	1	1
4:A:388:PX4:H38	4:A:411:PX4:H46	0.68	1.65	5	1
4:A:306:PX4:H14	4:A:321:PX4:H28	0.68	1.66	12	1
4:A:316:PX4:H14	4:A:320:PX4:H22	0.68	1.64	10	1
4:A:378:PX4:H51	4:A:418:PX4:H50	0.68	1.65	13	1
4:A:376:PX4:H67	4:A:385:PX4:H30	0.68	1.64	2	1
4:A:391:PX4:H40	4:A:408:PX4:H42	0.67	1.66	2	1
4:A:370:PX4:H22	4:A:403:PX4:H17	0.67	1.65	9	2
4:A:306:PX4:H20	4:A:329:PX4:H52	0.67	1.66	9	1
4:A:346:PX4:H22	4:A:354:PX4:H21	0.67	1.65	9	1
4:A:331:PX4:H63	4:A:340:PX4:H71	0.67	1.67	14	1
4:A:330:PX4:H44	4:A:344:PX4:H45	0.67	1.66	12	1
4:A:312:PX4:H16	4:A:359:PX4:H5	0.67	1.64	14	1
4:A:384:PX4:H2	4:A:385:PX4:H18	0.67	1.66	1	4
4:A:331:PX4:H33	4:A:340:PX4:H69	0.67	1.66	3	1
4:A:332:PX4:H25	4:A:390:PX4:H41	0.67	1.67	6	1
4:A:315:PX4:H42	4:A:425:PX4:H31	0.67	1.67	4	1
4:A:308:PX4:H38	4:A:311:PX4:H69	0.67	1.65	12	1
4:A:417:PX4:H19	4:A:426:PX4:H24	0.67	1.66	12	1
4:A:331:PX4:H35	4:A:397:PX4:H44	0.66	1.66	7	1
4:A:424:PX4:H53	4:A:425:PX4:H22	0.66	1.67	2	1
4:A:395:PX4:H49	4:A:396:PX4:H24	0.66	1.67	14	1
4:A:350:PX4:H56	4:A:364:PX4:H37	0.66	1.66	3	1
4:A:371:PX4:H61	4:A:372:PX4:H27	0.66	1.68	4	1
4:A:378:PX4:H56	4:A:417:PX4:H58	0.66	1.68	8	2
4:A:306:PX4:H56	4:A:361:PX4:H59	0.66	1.66	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:311:PX4:H53	4:A:316:PX4:H20	0.66	1.68	6	1
4:A:311:PX4:H65	4:A:359:PX4:H71	0.65	1.66	7	1
4:A:326:PX4:H28	4:A:350:PX4:H24	0.65	1.68	5	1
4:A:391:PX4:H28	4:A:414:PX4:H46	0.65	1.69	5	1
4:A:313:PX4:H49	4:A:328:PX4:H17	0.65	1.65	4	1
4:A:380:PX4:H56	4:A:387:PX4:H50	0.65	1.68	11	1
4:A:383:PX4:H50	4:A:399:PX4:H17	0.65	1.67	8	1
4:A:373:PX4:H26	4:A:381:PX4:H53	0.65	1.68	9	1
4:A:311:PX4:H10	4:A:359:PX4:H51	0.65	1.68	2	1
4:A:321:PX4:H50	4:A:354:PX4:H27	0.65	1.66	6	1
4:A:316:PX4:H51	4:A:320:PX4:H27	0.65	1.69	12	1
4:A:417:PX4:H31	4:A:426:PX4:H37	0.65	1.67	13	1
4:A:345:PX4:H40	4:A:345:PX4:H64	0.65	1.69	4	1
4:A:356:PX4:H16	4:A:356:PX4:H10	0.65	1.68	8	1
4:A:333:PX4:H56	4:A:341:PX4:H54	0.65	1.68	12	1
4:A:387:PX4:H16	4:A:394:PX4:H9	0.65	1.69	2	1
4:A:382:PX4:H19	4:A:428:PX4:H23	0.64	1.69	1	1
4:A:421:PX4:H22	4:A:422:PX4:H26	0.64	1.68	6	1
4:A:317:PX4:H55	4:A:324:PX4:H31	0.64	1.69	14	1
4:A:388:PX4:H20	4:A:411:PX4:H14	0.64	1.70	3	1
4:A:306:PX4:H18	4:A:322:PX4:H51	0.64	1.69	13	1
4:A:371:PX4:H20	4:A:379:PX4:H21	0.64	1.68	14	1
4:A:354:PX4:H50	4:A:360:PX4:H55	0.64	1.69	4	1
4:A:314:PX4:H34	4:A:356:PX4:H33	0.64	1.67	7	1
4:A:385:PX4:H71	4:A:392:PX4:H30	0.64	1.69	5	1
4:A:326:PX4:O8	4:A:351:PX4:H17	0.64	1.91	6	1
4:A:403:PX4:H7	4:A:427:PX4:H52	0.64	1.68	9	1
4:A:418:PX4:H42	4:A:422:PX4:H59	0.64	1.68	1	1
4:A:307:PX4:H60	4:A:349:PX4:H45	0.64	1.69	14	1
4:A:335:PX4:H48	4:A:343:PX4:H21	0.64	1.67	11	1
4:A:406:PX4:H48	4:A:421:PX4:H53	0.64	1.69	12	1
4:A:360:PX4:H44	4:A:412:PX4:H60	0.64	1.69	4	1
4:A:317:PX4:H48	4:A:342:PX4:H54	0.64	1.69	5	1
4:A:311:PX4:H52	4:A:320:PX4:H24	0.64	1.68	5	1
4:A:391:PX4:H43	4:A:394:PX4:H34	0.64	1.70	5	1
4:A:371:PX4:H16	4:A:379:PX4:H20	0.64	1.70	14	2
4:A:306:PX4:H38	4:A:321:PX4:H43	0.64	1.68	12	1
4:A:403:PX4:H47	4:A:427:PX4:H48	0.64	1.68	12	1
4:A:391:PX4:H48	4:A:408:PX4:H16	0.64	1.69	2	3
4:A:387:PX4:H46	4:A:388:PX4:H37	0.64	1.68	6	1
4:A:308:PX4:H34	4:A:314:PX4:H58	0.64	1.70	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:345:PX4:H37	4:A:353:PX4:H64	0.64	1.68	1	1
4:A:395:PX4:H19	4:A:398:PX4:H54	0.64	1.68	4	1
4:A:404:PX4:H39	4:A:419:PX4:H30	0.63	1.68	9	1
4:A:404:PX4:H34	4:A:419:PX4:H48	0.63	1.70	3	1
4:A:409:PX4:H41	4:A:410:PX4:H24	0.63	1.70	4	1
4:A:350:PX4:H50	4:A:363:PX4:H51	0.63	1.68	11	2
4:A:385:PX4:H32	4:A:386:PX4:H32	0.63	1.70	7	1
4:A:421:PX4:H39	4:A:423:PX4:H33	0.63	1.68	11	1
4:A:313:PX4:H22	4:A:318:PX4:H51	0.63	1.70	11	1
4:A:404:PX4:H49	4:A:413:PX4:H21	0.63	1.68	5	1
4:A:424:PX4:H48	4:A:425:PX4:H21	0.63	1.70	9	1
4:A:322:PX4:H17	4:A:336:PX4:H23	0.63	1.70	11	1
4:A:324:PX4:H48	4:A:341:PX4:H3	0.63	1.69	8	1
4:A:428:PX4:H61	4:A:430:PX4:H29	0.63	1.71	7	1
4:A:355:PX4:H72	4:A:356:PX4:H53	0.63	1.70	3	1
4:A:320:PX4:H17	4:A:359:PX4:H56	0.63	1.71	7	1
4:A:382:PX4:H22	4:A:428:PX4:H32	0.63	1.68	5	1
4:A:395:PX4:H47	4:A:396:PX4:H20	0.63	1.71	12	1
4:A:408:PX4:H47	4:A:415:PX4:H21	0.63	1.70	9	1
4:A:410:PX4:H62	4:A:426:PX4:H37	0.63	1.69	4	1
4:A:363:PX4:H20	4:A:364:PX4:H33	0.63	1.69	1	1
4:A:311:PX4:H50	4:A:316:PX4:H19	0.63	1.71	14	1
4:A:372:PX4:H38	4:A:378:PX4:H42	0.63	1.70	13	1
4:A:325:PX4:H24	4:A:340:PX4:H53	0.63	1.70	5	1
4:A:362:PX4:H13	4:A:362:PX4:O2	0.62	1.93	11	1
4:A:370:PX4:H54	4:A:411:PX4:H50	0.62	1.71	12	1
4:A:308:PX4:H22	4:A:364:PX4:H14	0.62	1.71	3	1
4:A:309:PX4:H40	4:A:372:PX4:H45	0.62	1.69	11	1
4:A:375:PX4:H55	4:A:429:PX4:H41	0.62	1.70	5	1
4:A:377:PX4:H4	4:A:418:PX4:H49	0.62	1.71	6	1
4:A:320:PX4:H68	4:A:417:PX4:H72	0.62	1.71	1	1
4:A:353:PX4:H39	4:A:366:PX4:H26	0.62	1.70	1	1
4:A:317:PX4:H55	4:A:324:PX4:H20	0.62	1.70	2	1
4:A:331:PX4:H66	4:A:373:PX4:H45	0.62	1.71	13	1
4:A:330:PX4:H64	4:A:357:PX4:H28	0.62	1.71	10	1
4:A:337:PX4:H58	4:A:353:PX4:H27	0.62	1.69	5	1
4:A:378:PX4:H21	4:A:417:PX4:H48	0.62	1.72	3	1
4:A:395:PX4:H63	4:A:421:PX4:H20	0.62	1.70	9	1
4:A:317:PX4:H63	4:A:325:PX4:H59	0.62	1.71	5	1
4:A:326:PX4:H17	4:A:351:PX4:O8	0.62	1.95	14	2
4:A:389:PX4:H69	4:A:397:PX4:H45	0.62	1.71	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:345:PX4:H29	4:A:362:PX4:H65	0.62	1.71	12	1
4:A:378:PX4:H22	4:A:417:PX4:H48	0.62	1.69	8	1
4:A:354:PX4:H39	4:A:362:PX4:H33	0.62	1.70	8	1
4:A:405:PX4:H17	4:A:406:PX4:H54	0.62	1.70	1	2
4:A:307:PX4:H28	4:A:349:PX4:H23	0.62	1.71	14	1
4:A:331:PX4:H28	4:A:347:PX4:H49	0.62	1.71	4	1
4:A:317:PX4:H16	4:A:342:PX4:H52	0.61	1.70	5	1
4:A:329:PX4:H18	4:A:336:PX4:H53	0.61	1.69	8	1
4:A:426:PX4:H64	4:A:426:PX4:H38	0.61	1.72	1	1
4:A:314:PX4:H57	4:A:364:PX4:H53	0.61	1.71	9	1
4:A:306:PX4:H15	4:A:321:PX4:H42	0.61	1.70	10	1
4:A:417:PX4:O6	4:A:417:PX4:H4	0.61	1.95	5	1
4:A:369:PX4:H38	4:A:378:PX4:H68	0.61	1.72	14	1
4:A:376:PX4:H46	4:A:385:PX4:H17	0.61	1.71	10	1
4:A:380:PX4:H18	4:A:381:PX4:H15	0.61	1.71	4	3
4:A:320:PX4:H54	4:A:359:PX4:H26	0.61	1.70	6	1
4:A:316:PX4:H34	4:A:320:PX4:H37	0.61	1.71	3	1
4:A:307:PX4:H52	4:A:321:PX4:H59	0.61	1.72	13	1
4:A:391:PX4:H62	4:A:408:PX4:H52	0.61	1.72	4	1
4:A:403:PX4:H53	4:A:403:PX4:H32	0.61	1.73	12	1
4:A:376:PX4:H40	4:A:399:PX4:H64	0.61	1.73	1	1
4:A:386:PX4:O6	4:A:394:PX4:H18	0.61	1.94	7	1
4:A:423:PX4:H48	4:A:425:PX4:H18	0.61	1.73	12	1
4:A:398:PX4:H16	4:A:407:PX4:H48	0.61	1.72	9	1
4:A:368:PX4:H52	4:A:369:PX4:H64	0.61	1.73	3	1
4:A:369:PX4:H31	4:A:377:PX4:H62	0.61	1.73	13	1
4:A:360:PX4:H2	4:A:366:PX4:H16	0.61	1.71	6	2
4:A:380:PX4:H67	4:A:387:PX4:H65	0.61	1.73	12	1
4:A:306:PX4:H66	4:A:362:PX4:H45	0.61	1.71	10	1
4:A:347:PX4:H19	4:A:348:PX4:H14	0.61	1.72	13	1
1:A:214:LEU:HD12	1:A:240:TYR:CE1	0.61	2.30	13	1
4:A:371:PX4:H20	4:A:372:PX4:H17	0.60	1.71	7	1
4:A:317:PX4:H17	4:A:325:PX4:H46	0.60	1.73	7	2
4:A:406:PX4:O1	4:A:414:PX4:H9	0.60	1.95	8	1
4:A:367:PX4:H49	4:A:428:PX4:H51	0.60	1.73	1	1
4:A:391:PX4:H55	4:A:408:PX4:H55	0.60	1.72	3	1
4:A:363:PX4:H24	4:A:364:PX4:H37	0.60	1.71	1	1
4:A:329:PX4:H24	4:A:336:PX4:H60	0.60	1.73	3	1
4:A:393:PX4:O2	4:A:394:PX4:H17	0.60	1.96	10	2
4:A:347:PX4:H30	4:A:348:PX4:H19	0.60	1.72	14	1
4:A:404:PX4:H70	4:A:430:PX4:H65	0.60	1.73	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:306:PX4:H23	4:A:328:PX4:H54	0.60	1.73	13	1
4:A:325:PX4:H45	4:A:407:PX4:H29	0.60	1.72	7	1
4:A:371:PX4:H14	4:A:379:PX4:H20	0.60	1.71	11	1
4:A:401:PX4:H46	4:A:426:PX4:H56	0.60	1.72	13	1
4:A:398:PX4:H30	4:A:407:PX4:H18	0.60	1.72	10	1
4:A:378:PX4:H20	4:A:410:PX4:H52	0.60	1.73	12	2
4:A:350:PX4:H67	4:A:358:PX4:H33	0.60	1.71	3	1
1:A:244:ASP:OD2	4:A:349:PX4:H9	0.60	1.96	7	2
4:A:348:PX4:H11	4:A:355:PX4:O2	0.60	1.95	5	2
4:A:395:PX4:H64	4:A:406:PX4:H56	0.60	1.72	1	2
4:A:321:PX4:H26	4:A:360:PX4:H61	0.60	1.72	12	1
4:A:311:PX4:H29	4:A:311:PX4:H60	0.60	1.74	9	1
4:A:327:PX4:H20	4:A:328:PX4:H16	0.60	1.72	7	2
4:A:381:PX4:H51	4:A:396:PX4:H46	0.60	1.73	14	1
4:A:380:PX4:H52	4:A:387:PX4:H49	0.60	1.73	6	1
4:A:328:PX4:H72	4:A:374:PX4:H43	0.59	1.74	5	1
4:A:315:PX4:H55	4:A:323:PX4:H46	0.59	1.74	1	1
4:A:400:PX4:H71	4:A:426:PX4:H43	0.59	1.73	2	1
4:A:347:PX4:H64	4:A:356:PX4:H56	0.59	1.72	3	1
4:A:422:PX4:H35	4:A:423:PX4:H32	0.59	1.74	3	1
4:A:424:PX4:H47	4:A:429:PX4:H21	0.59	1.74	2	1
4:A:403:PX4:H2	4:A:427:PX4:H46	0.59	1.73	14	1
4:A:413:PX4:O2	4:A:430:PX4:H18	0.59	1.96	3	1
4:A:347:PX4:H35	4:A:348:PX4:H24	0.59	1.73	4	1
4:A:371:PX4:H54	4:A:379:PX4:H25	0.59	1.73	11	1
4:A:335:PX4:H28	4:A:343:PX4:H56	0.59	1.74	6	1
4:A:331:PX4:H31	4:A:340:PX4:H56	0.59	1.73	8	1
4:A:316:PX4:O6	4:A:364:PX4:H12	0.59	1.98	3	1
4:A:351:PX4:H50	4:A:358:PX4:H55	0.59	1.74	10	1
4:A:388:PX4:O6	4:A:395:PX4:H5	0.59	1.97	8	2
4:A:416:PX4:H58	4:A:423:PX4:H60	0.59	1.74	6	1
4:A:330:PX4:H25	4:A:343:PX4:H54	0.59	1.75	14	1
4:A:350:PX4:H60	4:A:364:PX4:H41	0.59	1.73	3	1
4:A:306:PX4:H29	4:A:329:PX4:H51	0.59	1.73	3	1
4:A:342:PX4:H24	4:A:352:PX4:C24	0.59	2.24	11	1
4:A:400:PX4:H46	4:A:408:PX4:H64	0.59	1.74	12	1
4:A:345:PX4:H33	4:A:362:PX4:H69	0.59	1.73	12	1
4:A:393:PX4:H45	4:A:394:PX4:H37	0.59	1.72	5	1
4:A:369:PX4:H20	4:A:377:PX4:H51	0.59	1.75	14	1
4:A:371:PX4:H34	4:A:377:PX4:H36	0.59	1.74	5	1
4:A:327:PX4:H26	4:A:327:PX4:H57	0.59	1.73	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:375:PX4:H65	4:A:412:PX4:H38	0.59	1.74	9	1
4:A:421:PX4:H44	4:A:428:PX4:H58	0.59	1.74	2	1
4:A:416:PX4:H49	4:A:425:PX4:H57	0.58	1.75	9	1
4:A:347:PX4:H34	4:A:348:PX4:H22	0.58	1.73	14	1
4:A:334:PX4:H42	4:A:391:PX4:H43	0.58	1.75	2	1
4:A:312:PX4:H61	4:A:359:PX4:H33	0.58	1.73	6	1
4:A:377:PX4:H72	4:A:425:PX4:H68	0.58	1.74	6	1
4:A:409:PX4:H51	4:A:415:PX4:H21	0.58	1.74	8	1
4:A:383:PX4:H63	4:A:399:PX4:H67	0.58	1.74	3	1
4:A:337:PX4:H71	4:A:353:PX4:H62	0.58	1.75	10	1
4:A:350:PX4:H9	4:A:358:PX4:O6	0.58	1.99	12	2
4:A:404:PX4:O2	4:A:413:PX4:H17	0.58	1.97	7	1
4:A:428:PX4:H52	4:A:430:PX4:H53	0.58	1.75	7	1
4:A:377:PX4:H34	4:A:379:PX4:H27	0.58	1.76	7	1
4:A:308:PX4:H24	4:A:364:PX4:H22	0.58	1.74	12	1
4:A:382:PX4:H69	4:A:412:PX4:H71	0.58	1.75	13	1
4:A:354:PX4:H51	4:A:360:PX4:H18	0.58	1.74	4	1
4:A:360:PX4:H62	4:A:360:PX4:H25	0.58	1.73	4	1
4:A:307:PX4:H56	4:A:362:PX4:H23	0.58	1.75	14	1
4:A:395:PX4:H67	4:A:406:PX4:H56	0.58	1.75	2	1
4:A:375:PX4:H42	4:A:424:PX4:H69	0.58	1.76	2	1
4:A:378:PX4:H20	4:A:410:PX4:H48	0.58	1.75	13	1
4:A:374:PX4:H31	4:A:427:PX4:H20	0.58	1.74	10	1
4:A:350:PX4:H54	4:A:415:PX4:H43	0.58	1.76	7	1
4:A:363:PX4:H24	4:A:365:PX4:H22	0.58	1.75	13	2
4:A:392:PX4:H66	4:A:415:PX4:H39	0.58	1.75	8	1
4:A:412:PX4:H55	4:A:427:PX4:H22	0.58	1.75	3	1
4:A:354:PX4:H60	4:A:360:PX4:H63	0.58	1.76	7	1
4:A:314:PX4:H34	4:A:362:PX4:H16	0.58	1.75	3	1
4:A:316:PX4:H61	4:A:323:PX4:H70	0.58	1.76	12	1
4:A:318:PX4:H53	4:A:359:PX4:H25	0.58	1.75	2	1
4:A:329:PX4:H69	4:A:382:PX4:H41	0.58	1.75	8	1
4:A:400:PX4:H17	4:A:408:PX4:H61	0.58	1.76	12	1
4:A:382:PX4:H21	4:A:428:PX4:H29	0.58	1.76	9	1
4:A:410:PX4:H51	4:A:426:PX4:H25	0.58	1.74	3	1
4:A:395:PX4:H49	4:A:396:PX4:H20	0.58	1.74	13	1
4:A:351:PX4:H28	4:A:352:PX4:H26	0.58	1.76	4	1
4:A:314:PX4:H49	4:A:364:PX4:H18	0.58	1.75	10	2
4:A:326:PX4:H16	4:A:351:PX4:H16	0.58	1.76	4	3
4:A:388:PX4:H20	4:A:411:PX4:H19	0.58	1.74	1	1
4:A:317:PX4:H60	4:A:325:PX4:H68	0.58	1.76	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:323:PX4:H34	4:A:323:PX4:H55	0.58	1.74	9	1
4:A:370:PX4:H35	4:A:403:PX4:H67	0.58	1.75	3	1
4:A:348:PX4:H5	4:A:355:PX4:O3	0.58	1.99	3	1
4:A:393:PX4:H11	4:A:401:PX4:H16	0.57	1.75	11	1
4:A:403:PX4:H50	4:A:404:PX4:H28	0.57	1.75	8	1
4:A:409:PX4:H29	4:A:425:PX4:H71	0.57	1.76	8	1
4:A:372:PX4:H62	4:A:379:PX4:H61	0.57	1.75	2	1
4:A:332:PX4:H67	4:A:349:PX4:H57	0.57	1.76	12	1
4:A:340:PX4:H66	4:A:397:PX4:H31	0.57	1.74	11	1
4:A:352:PX4:H20	4:A:358:PX4:H15	0.57	1.75	9	1
4:A:410:PX4:H58	4:A:426:PX4:H32	0.57	1.76	4	1
4:A:349:PX4:H17	4:A:356:PX4:H21	0.57	1.76	7	2
4:A:378:PX4:H30	4:A:417:PX4:H56	0.57	1.76	10	1
4:A:337:PX4:H63	4:A:353:PX4:H56	0.57	1.77	8	1
4:A:420:PX4:H72	4:A:426:PX4:H40	0.57	1.76	8	1
4:A:391:PX4:H62	4:A:400:PX4:H32	0.57	1.76	9	1
4:A:402:PX4:H15	4:A:404:PX4:H14	0.57	1.75	2	1
4:A:400:PX4:H28	4:A:408:PX4:H52	0.57	1.75	7	1
4:A:334:PX4:H69	4:A:352:PX4:H32	0.57	1.77	6	1
4:A:318:PX4:H27	4:A:327:PX4:H56	0.57	1.75	12	1
4:A:319:PX4:H39	4:A:324:PX4:H37	0.57	1.77	14	1
4:A:367:PX4:O2	4:A:424:PX4:H1	0.57	1.99	3	1
4:A:330:PX4:H21	4:A:335:PX4:H22	0.57	1.75	12	1
4:A:333:PX4:H39	4:A:375:PX4:H28	0.57	1.76	1	1
4:A:393:PX4:H46	4:A:401:PX4:H19	0.57	1.75	4	1
4:A:388:PX4:H17	4:A:396:PX4:H22	0.57	1.75	8	1
4:A:334:PX4:H37	4:A:407:PX4:H43	0.57	1.75	12	1
4:A:351:PX4:H62	4:A:358:PX4:H30	0.57	1.76	13	1
4:A:352:PX4:H33	4:A:358:PX4:H64	0.57	1.74	4	1
4:A:314:PX4:H69	4:A:350:PX4:H55	0.57	1.77	5	1
4:A:326:PX4:H47	4:A:334:PX4:H56	0.57	1.77	8	1
4:A:331:PX4:H11	4:A:340:PX4:O1	0.57	1.99	2	1
4:A:376:PX4:H52	4:A:385:PX4:H21	0.57	1.77	8	1
4:A:342:PX4:O2	4:A:352:PX4:H4	0.57	1.99	14	1
4:A:337:PX4:H17	4:A:345:PX4:H46	0.57	1.76	4	2
4:A:320:PX4:H20	4:A:359:PX4:C29	0.57	2.26	5	1
4:A:371:PX4:H56	4:A:378:PX4:H62	0.57	1.75	5	1
4:A:312:PX4:H65	4:A:359:PX4:H37	0.57	1.76	6	1
4:A:344:PX4:H28	4:A:348:PX4:H21	0.57	1.76	3	1
4:A:345:PX4:H15	4:A:353:PX4:H16	0.57	1.76	2	1
4:A:380:PX4:H67	4:A:388:PX4:H62	0.56	1.77	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:367:PX4:H47	4:A:428:PX4:H48	0.56	1.76	11	1
4:A:349:PX4:H56	4:A:350:PX4:H30	0.56	1.77	12	1
4:A:362:PX4:H38	4:A:430:PX4:H69	0.56	1.76	12	1
4:A:375:PX4:H14	4:A:375:PX4:H10	0.56	1.77	14	1
4:A:424:PX4:H17	4:A:429:PX4:O6	0.56	2.00	3	1
4:A:311:PX4:H70	4:A:312:PX4:H69	0.56	1.77	3	1
4:A:317:PX4:H31	4:A:326:PX4:H62	0.56	1.76	5	1
1:A:207:SER:O	4:A:321:PX4:H4	0.56	2.00	2	1
4:A:373:PX4:H31	4:A:381:PX4:H30	0.56	1.77	11	1
4:A:329:PX4:H26	4:A:336:PX4:H60	0.56	1.75	11	1
4:A:393:PX4:H20	4:A:401:PX4:H16	0.56	1.77	5	2
4:A:360:PX4:H33	4:A:366:PX4:H64	0.56	1.76	5	1
4:A:391:PX4:H21	4:A:392:PX4:H47	0.56	1.78	5	1
4:A:400:PX4:H59	4:A:426:PX4:H40	0.56	1.76	6	1
4:A:336:PX4:H70	4:A:382:PX4:H42	0.56	1.76	8	1
4:A:371:PX4:H68	4:A:379:PX4:H41	0.56	1.76	9	1
4:A:309:PX4:H63	4:A:316:PX4:H65	0.56	1.77	14	1
4:A:318:PX4:H27	4:A:359:PX4:H23	0.56	1.76	2	1
4:A:320:PX4:C10	4:A:359:PX4:H57	0.56	2.25	5	1
4:A:388:PX4:H23	4:A:402:PX4:H16	0.56	1.75	3	1
4:A:318:PX4:H64	4:A:318:PX4:H43	0.56	1.78	11	1
4:A:379:PX4:H58	4:A:420:PX4:H31	0.56	1.78	11	1
4:A:429:PX4:H53	4:A:429:PX4:H33	0.56	1.77	9	1
4:A:310:PX4:H20	4:A:365:PX4:H21	0.56	1.76	14	1
4:A:315:PX4:H29	4:A:361:PX4:H24	0.56	1.77	4	1
4:A:320:PX4:H19	4:A:359:PX4:H59	0.56	1.77	14	1
4:A:313:PX4:H58	4:A:327:PX4:H23	0.56	1.78	2	1
4:A:352:PX4:O8	4:A:365:PX4:H11	0.56	2.00	1	1
4:A:316:PX4:H48	4:A:320:PX4:H26	0.56	1.77	3	1
4:A:307:PX4:H65	4:A:349:PX4:H28	0.56	1.76	11	1
4:A:402:PX4:H3	4:A:404:PX4:O1	0.56	2.01	3	1
4:A:332:PX4:H56	4:A:349:PX4:H48	0.56	1.76	3	1
4:A:400:PX4:H53	4:A:410:PX4:H50	0.56	1.78	12	1
4:A:408:PX4:H43	4:A:414:PX4:H64	0.56	1.76	12	1
4:A:369:PX4:H56	4:A:416:PX4:H69	0.56	1.78	9	1
4:A:338:PX4:H71	4:A:395:PX4:H40	0.56	1.78	13	1
4:A:389:PX4:H30	4:A:397:PX4:H54	0.55	1.79	4	1
1:A:177:LYS:O	4:A:354:PX4:H13	0.55	2.01	7	1
4:A:337:PX4:H62	4:A:366:PX4:H53	0.55	1.77	8	1
4:A:377:PX4:H16	4:A:418:PX4:H7	0.55	1.78	8	1
4:A:309:PX4:H55	4:A:324:PX4:H53	0.55	1.77	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:381:PX4:H29	4:A:386:PX4:H58	0.55	1.77	12	1
4:A:358:PX4:H19	4:A:363:PX4:H49	0.55	1.77	3	1
4:A:347:PX4:H69	4:A:407:PX4:H68	0.55	1.77	11	1
4:A:349:PX4:H54	4:A:355:PX4:H34	0.55	1.76	11	1
4:A:412:PX4:H20	4:A:428:PX4:H46	0.55	1.77	11	1
4:A:395:PX4:H36	4:A:397:PX4:H61	0.55	1.76	6	1
4:A:375:PX4:H58	4:A:382:PX4:H71	0.55	1.78	6	1
4:A:330:PX4:H19	4:A:338:PX4:H19	0.55	1.77	1	1
4:A:380:PX4:H66	4:A:411:PX4:H22	0.55	1.77	2	1
4:A:337:PX4:H55	4:A:353:PX4:H47	0.55	1.77	10	1
4:A:326:PX4:H18	4:A:334:PX4:H72	0.55	1.79	11	1
4:A:360:PX4:H47	4:A:366:PX4:H46	0.55	1.77	11	1
4:A:341:PX4:H34	4:A:399:PX4:H69	0.55	1.78	14	1
4:A:392:PX4:H35	4:A:399:PX4:H56	0.55	1.77	10	1
4:A:399:PX4:H25	4:A:399:PX4:H59	0.55	1.77	2	1
4:A:354:PX4:H56	4:A:360:PX4:H59	0.55	1.77	7	1
4:A:412:PX4:H19	4:A:428:PX4:H54	0.55	1.79	5	1
4:A:313:PX4:H64	4:A:328:PX4:H68	0.55	1.77	1	1
4:A:338:PX4:H34	4:A:357:PX4:H27	0.55	1.78	9	1
4:A:357:PX4:H29	4:A:365:PX4:H62	0.55	1.78	14	1
4:A:416:PX4:H25	4:A:422:PX4:H56	0.55	1.77	6	1
4:A:375:PX4:H68	4:A:428:PX4:H54	0.55	1.78	14	1
4:A:367:PX4:H2	4:A:428:PX4:O8	0.55	2.02	14	1
4:A:369:PX4:H38	4:A:416:PX4:H63	0.55	1.78	11	1
4:A:346:PX4:H70	4:A:357:PX4:H31	0.55	1.77	6	1
4:A:329:PX4:H46	4:A:336:PX4:H18	0.55	1.78	2	1
4:A:385:PX4:H45	4:A:386:PX4:H45	0.55	1.78	10	1
4:A:317:PX4:H51	4:A:324:PX4:H17	0.55	1.79	11	1
4:A:314:PX4:H46	4:A:364:PX4:H18	0.55	1.79	11	1
4:A:395:PX4:H19	4:A:396:PX4:H14	0.55	1.79	12	1
4:A:306:PX4:H49	4:A:321:PX4:H22	0.55	1.77	1	1
4:A:373:PX4:H20	4:A:381:PX4:H18	0.55	1.78	1	1
4:A:360:PX4:H45	4:A:404:PX4:H41	0.55	1.78	9	1
4:A:348:PX4:H69	4:A:355:PX4:H27	0.55	1.79	14	1
4:A:316:PX4:H36	4:A:364:PX4:H55	0.55	1.78	3	1
4:A:392:PX4:H60	4:A:408:PX4:H31	0.55	1.78	7	1
4:A:392:PX4:H2	4:A:392:PX4:O6	0.55	2.02	9	1
4:A:416:PX4:H30	4:A:423:PX4:H30	0.55	1.79	2	1
4:A:382:PX4:H45	4:A:428:PX4:H43	0.54	1.78	8	1
4:A:307:PX4:H31	4:A:364:PX4:H57	0.54	1.79	1	1
4:A:339:PX4:H50	4:A:339:PX4:H32	0.54	1.78	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:389:PX4:H63	4:A:397:PX4:H35	0.54	1.78	14	1
4:A:408:PX4:H72	4:A:426:PX4:H69	0.54	1.79	2	1
4:A:332:PX4:H17	4:A:356:PX4:H7	0.54	1.78	2	1
4:A:318:PX4:O2	4:A:359:PX4:H14	0.54	2.03	5	1
4:A:321:PX4:H71	4:A:322:PX4:H33	0.54	1.79	8	1
4:A:355:PX4:H52	4:A:356:PX4:H14	0.54	1.77	1	1
4:A:383:PX4:H57	4:A:407:PX4:H24	0.54	1.80	9	1
4:A:330:PX4:H25	4:A:343:PX4:H51	0.54	1.77	6	1
4:A:380:PX4:H32	4:A:381:PX4:H59	0.54	1.77	3	1
4:A:416:PX4:H20	4:A:422:PX4:H48	0.54	1.80	4	1
4:A:323:PX4:H55	4:A:424:PX4:H70	0.54	1.77	6	1
4:A:307:PX4:H43	4:A:311:PX4:H43	0.54	1.78	12	1
4:A:317:PX4:H21	4:A:342:PX4:H68	0.54	1.78	10	1
4:A:403:PX4:H61	4:A:427:PX4:H62	0.54	1.78	6	1
4:A:404:PX4:H21	4:A:419:PX4:H10	0.54	1.79	9	1
4:A:383:PX4:H54	4:A:407:PX4:H20	0.54	1.78	9	1
4:A:372:PX4:H51	4:A:420:PX4:H19	0.54	1.78	3	1
4:A:308:PX4:H54	4:A:364:PX4:H31	0.54	1.79	4	1
4:A:325:PX4:H53	4:A:334:PX4:H36	0.54	1.78	12	1
4:A:332:PX4:O8	4:A:347:PX4:H52	0.54	2.03	13	1
4:A:354:PX4:H28	4:A:362:PX4:H17	0.54	1.79	5	1
4:A:372:PX4:H58	4:A:379:PX4:H57	0.54	1.80	5	1
4:A:428:PX4:H70	4:A:430:PX4:H32	0.54	1.79	1	1
4:A:351:PX4:H67	4:A:358:PX4:H36	0.54	1.79	2	1
4:A:331:PX4:H56	4:A:339:PX4:H22	0.54	1.80	2	1
4:A:338:PX4:H59	4:A:348:PX4:H57	0.54	1.78	12	1
4:A:386:PX4:H25	4:A:394:PX4:H20	0.54	1.79	9	1
4:A:423:PX4:H13	4:A:430:PX4:H46	0.54	1.80	10	1
4:A:373:PX4:H25	4:A:397:PX4:H15	0.54	1.79	7	1
4:A:327:PX4:H19	4:A:329:PX4:H23	0.54	1.78	5	1
4:A:369:PX4:H21	4:A:377:PX4:H56	0.54	1.78	1	1
4:A:406:PX4:H12	4:A:406:PX4:H15	0.54	1.80	9	1
4:A:416:PX4:H48	4:A:425:PX4:H49	0.54	1.79	14	1
4:A:419:PX4:H63	4:A:427:PX4:H60	0.54	1.80	2	1
4:A:377:PX4:H51	4:A:418:PX4:H52	0.54	1.79	13	1
4:A:384:PX4:O2	4:A:385:PX4:H18	0.54	2.03	8	2
4:A:370:PX4:H23	4:A:427:PX4:H59	0.54	1.80	9	1
4:A:307:PX4:H4	4:A:322:PX4:O8	0.54	2.03	3	1
4:A:308:PX4:H43	4:A:425:PX4:H68	0.54	1.79	13	1
4:A:372:PX4:H52	4:A:420:PX4:H21	0.54	1.80	4	1
4:A:340:PX4:H63	4:A:397:PX4:H30	0.53	1.81	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:367:PX4:H22	4:A:424:PX4:H16	0.53	1.79	7	1
4:A:381:PX4:H35	4:A:381:PX4:H62	0.53	1.79	11	1
4:A:381:PX4:H57	4:A:397:PX4:H46	0.53	1.80	6	1
4:A:412:PX4:H54	4:A:427:PX4:H22	0.53	1.79	6	1
1:A:208:GLY:HA3	4:A:307:PX4:H15	0.53	1.80	2	3
4:A:391:PX4:H23	4:A:414:PX4:H51	0.53	1.80	1	1
4:A:412:PX4:H48	4:A:419:PX4:H22	0.53	1.80	4	2
4:A:409:PX4:H16	4:A:410:PX4:H8	0.53	1.80	4	1
4:A:378:PX4:H49	4:A:410:PX4:H23	0.53	1.80	6	1
4:A:307:PX4:H29	4:A:361:PX4:H28	0.53	1.80	8	1
4:A:393:PX4:H66	4:A:399:PX4:H69	0.53	1.79	12	1
4:A:337:PX4:H64	4:A:345:PX4:H63	0.53	1.78	1	1
4:A:317:PX4:H26	4:A:334:PX4:H40	0.53	1.80	9	1
4:A:400:PX4:H51	4:A:409:PX4:H21	0.53	1.80	9	1
4:A:371:PX4:H21	4:A:379:PX4:H20	0.53	1.80	13	1
4:A:332:PX4:H44	4:A:389:PX4:H57	0.53	1.79	13	1
4:A:406:PX4:H27	4:A:415:PX4:H59	0.53	1.80	7	1
4:A:430:PX4:H28	4:A:430:PX4:H71	0.53	1.79	11	1
4:A:311:PX4:O2	4:A:359:PX4:H13	0.53	2.03	5	1
4:A:328:PX4:H55	4:A:329:PX4:H47	0.53	1.79	1	1
4:A:421:PX4:H4	4:A:422:PX4:O6	0.53	2.03	1	1
4:A:363:PX4:H70	4:A:392:PX4:H66	0.53	1.81	7	1
4:A:311:PX4:H43	4:A:425:PX4:H68	0.53	1.78	5	1
4:A:311:PX4:H17	4:A:359:PX4:H51	0.53	1.79	6	2
4:A:389:PX4:H48	4:A:390:PX4:H49	0.53	1.79	5	2
4:A:329:PX4:H66	4:A:375:PX4:H35	0.53	1.79	1	1
4:A:388:PX4:H58	4:A:397:PX4:H54	0.53	1.78	9	1
4:A:345:PX4:H37	4:A:403:PX4:H45	0.53	1.80	14	1
4:A:352:PX4:H48	4:A:358:PX4:H50	0.53	1.79	3	1
4:A:367:PX4:H59	4:A:424:PX4:H21	0.53	1.81	4	1
4:A:345:PX4:H44	4:A:402:PX4:H67	0.53	1.81	6	1
4:A:388:PX4:H18	4:A:411:PX4:O2	0.53	2.04	6	1
4:A:384:PX4:H19	4:A:385:PX4:H23	0.53	1.79	1	1
4:A:429:PX4:H15	4:A:429:PX4:H10	0.53	1.80	3	1
4:A:386:PX4:H35	4:A:394:PX4:H36	0.53	1.81	3	1
4:A:395:PX4:H44	4:A:398:PX4:H69	0.53	1.81	4	1
4:A:391:PX4:H49	4:A:408:PX4:H16	0.53	1.80	7	1
4:A:317:PX4:H20	4:A:351:PX4:O6	0.53	2.04	11	1
4:A:308:PX4:H16	4:A:311:PX4:H20	0.53	1.78	5	1
4:A:338:PX4:H32	4:A:348:PX4:H33	0.53	1.81	6	1
4:A:395:PX4:H58	4:A:404:PX4:H48	0.53	1.79	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:398:PX4:H38	4:A:414:PX4:H47	0.53	1.80	6	1
4:A:350:PX4:H68	4:A:351:PX4:H58	0.53	1.81	2	1
4:A:358:PX4:H29	4:A:363:PX4:H26	0.53	1.79	10	1
4:A:325:PX4:H15	4:A:341:PX4:H17	0.53	1.79	5	1
4:A:345:PX4:H42	4:A:388:PX4:H40	0.53	1.79	12	1
4:A:351:PX4:H66	4:A:358:PX4:H32	0.53	1.79	3	1
4:A:311:PX4:H48	4:A:320:PX4:H21	0.53	1.79	4	1
4:A:329:PX4:H30	4:A:336:PX4:H68	0.53	1.79	8	1
4:A:410:PX4:H16	4:A:418:PX4:H28	0.53	1.80	12	1
4:A:400:PX4:H28	4:A:426:PX4:H59	0.53	1.81	12	1
4:A:361:PX4:H34	4:A:423:PX4:H35	0.53	1.80	12	1
4:A:310:PX4:H65	4:A:312:PX4:H52	0.53	1.80	9	1
4:A:370:PX4:H69	4:A:411:PX4:H65	0.53	1.80	2	1
4:A:416:PX4:H51	4:A:418:PX4:H26	0.53	1.79	4	1
4:A:307:PX4:H37	4:A:423:PX4:H39	0.53	1.78	4	1
4:A:335:PX4:H31	4:A:343:PX4:H55	0.53	1.79	11	1
4:A:309:PX4:H51	4:A:316:PX4:H48	0.53	1.80	5	1
4:A:405:PX4:H22	4:A:406:PX4:H61	0.53	1.79	13	1
4:A:376:PX4:H26	4:A:399:PX4:H48	0.53	1.81	4	1
4:A:337:PX4:H40	4:A:338:PX4:H47	0.53	1.79	10	1
4:A:311:PX4:H24	4:A:311:PX4:H60	0.53	1.81	6	1
4:A:392:PX4:H68	4:A:400:PX4:H45	0.53	1.80	1	1
4:A:349:PX4:H58	4:A:356:PX4:H42	0.52	1.80	10	1
4:A:398:PX4:H39	4:A:414:PX4:H31	0.52	1.81	10	1
4:A:367:PX4:H64	4:A:375:PX4:H57	0.52	1.80	7	1
4:A:347:PX4:H20	4:A:348:PX4:H14	0.52	1.81	6	1
4:A:412:PX4:H12	4:A:419:PX4:O1	0.52	2.04	12	1
4:A:413:PX4:H61	4:A:430:PX4:H42	0.52	1.81	9	1
4:A:398:PX4:H21	4:A:407:PX4:H49	0.52	1.80	10	1
4:A:306:PX4:H47	4:A:322:PX4:H50	0.52	1.81	7	1
4:A:337:PX4:H56	4:A:345:PX4:H59	0.52	1.81	5	1
4:A:389:PX4:H32	4:A:397:PX4:H22	0.52	1.82	6	1
4:A:314:PX4:H53	4:A:364:PX4:H18	0.52	1.81	1	1
4:A:407:PX4:H30	4:A:414:PX4:H61	0.52	1.81	11	1
4:A:326:PX4:H48	4:A:334:PX4:H35	0.52	1.79	5	1
4:A:346:PX4:H19	4:A:354:PX4:H28	0.52	1.80	1	1
4:A:361:PX4:H26	4:A:364:PX4:H54	0.52	1.81	3	1
4:A:311:PX4:H44	4:A:314:PX4:H65	0.52	1.82	13	1
4:A:315:PX4:O6	4:A:315:PX4:H10	0.52	2.04	4	1
4:A:388:PX4:H49	4:A:396:PX4:H21	0.52	1.81	12	1
4:A:410:PX4:H67	4:A:417:PX4:H37	0.52	1.81	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:PX4:H56	4:A:422:PX4:H53	0.52	1.81	13	1
4:A:313:PX4:H56	4:A:327:PX4:H27	0.52	1.82	13	1
4:A:329:PX4:H56	4:A:336:PX4:H35	0.52	1.82	6	2
4:A:325:PX4:H55	4:A:334:PX4:H40	0.52	1.81	11	1
4:A:314:PX4:H33	4:A:362:PX4:O8	0.52	2.04	9	1
4:A:310:PX4:H34	4:A:365:PX4:H34	0.52	1.81	3	1
4:A:404:PX4:H21	4:A:413:PX4:H30	0.52	1.81	10	1
4:A:308:PX4:H21	4:A:311:PX4:H55	0.52	1.82	7	1
4:A:393:PX4:H71	4:A:414:PX4:H53	0.52	1.81	11	1
4:A:329:PX4:H60	4:A:336:PX4:H40	0.52	1.82	8	1
4:A:340:PX4:H36	4:A:340:PX4:H59	0.52	1.79	12	1
4:A:400:PX4:H46	4:A:409:PX4:H23	0.52	1.81	1	1
4:A:313:PX4:H28	4:A:366:PX4:H21	0.52	1.81	9	1
4:A:405:PX4:H51	4:A:406:PX4:H51	0.52	1.81	3	1
4:A:340:PX4:H22	4:A:341:PX4:H63	0.52	1.81	2	1
4:A:317:PX4:H21	4:A:326:PX4:H53	0.52	1.81	13	1
4:A:307:PX4:H45	4:A:422:PX4:H39	0.52	1.80	13	1
4:A:390:PX4:H1	4:A:399:PX4:O6	0.52	2.05	13	1
4:A:331:PX4:H38	4:A:340:PX4:H40	0.52	1.82	10	1
4:A:380:PX4:H6	4:A:381:PX4:O1	0.52	2.04	11	1
4:A:348:PX4:H52	4:A:355:PX4:H67	0.52	1.81	5	1
4:A:306:PX4:H61	4:A:362:PX4:H37	0.52	1.82	9	1
4:A:342:PX4:H29	4:A:352:PX4:H60	0.52	1.82	9	1
4:A:312:PX4:H29	4:A:365:PX4:H24	0.52	1.82	3	1
4:A:405:PX4:H55	4:A:406:PX4:H51	0.52	1.82	2	1
4:A:354:PX4:H69	4:A:360:PX4:H27	0.52	1.81	2	1
4:A:410:PX4:H16	4:A:418:PX4:H31	0.52	1.81	10	1
4:A:383:PX4:H71	4:A:399:PX4:H67	0.52	1.80	5	1
4:A:419:PX4:H67	4:A:427:PX4:H69	0.52	1.81	5	1
4:A:370:PX4:H19	4:A:427:PX4:H55	0.52	1.82	9	1
4:A:341:PX4:H39	4:A:399:PX4:H72	0.52	1.81	5	1
4:A:306:PX4:H43	4:A:328:PX4:H67	0.52	1.82	8	1
4:A:310:PX4:H60	4:A:312:PX4:H53	0.52	1.82	4	2
4:A:371:PX4:H56	4:A:372:PX4:H23	0.52	1.82	4	1
4:A:327:PX4:H14	4:A:328:PX4:O2	0.52	2.05	7	1
4:A:308:PX4:H27	4:A:316:PX4:H27	0.52	1.81	8	1
4:A:314:PX4:H26	4:A:356:PX4:H25	0.52	1.82	12	1
4:A:361:PX4:H39	4:A:364:PX4:H65	0.52	1.81	9	1
4:A:313:PX4:H61	4:A:329:PX4:H25	0.52	1.81	13	1
4:A:377:PX4:H71	4:A:425:PX4:H19	0.51	1.81	8	1
4:A:354:PX4:H65	4:A:360:PX4:H20	0.51	1.81	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:324:PX4:H66	4:A:341:PX4:H32	0.51	1.82	9	1
4:A:409:PX4:H67	4:A:415:PX4:H33	0.51	1.81	3	1
4:A:338:PX4:H67	4:A:348:PX4:H58	0.51	1.82	10	1
4:A:360:PX4:H31	4:A:419:PX4:H42	0.51	1.80	7	1
4:A:321:PX4:H28	4:A:412:PX4:H41	0.51	1.80	5	1
4:A:387:PX4:H47	4:A:411:PX4:H54	0.51	1.80	5	1
4:A:416:PX4:H45	4:A:422:PX4:H67	0.51	1.81	12	1
4:A:421:PX4:H71	4:A:422:PX4:H32	0.51	1.81	4	1
4:A:393:PX4:H23	4:A:401:PX4:H16	0.51	1.81	4	1
4:A:323:PX4:H38	4:A:361:PX4:H54	0.51	1.82	6	1
4:A:350:PX4:H51	4:A:363:PX4:H62	0.51	1.82	8	1
4:A:380:PX4:H32	4:A:380:PX4:H60	0.51	1.80	12	1
4:A:368:PX4:H10	4:A:369:PX4:O2	0.51	2.05	1	1
4:A:398:PX4:H44	4:A:415:PX4:H27	0.51	1.82	14	1
4:A:360:PX4:H43	4:A:403:PX4:H65	0.51	1.82	3	1
4:A:417:PX4:H31	4:A:426:PX4:H66	0.51	1.83	7	1
4:A:400:PX4:H59	4:A:410:PX4:H62	0.51	1.82	5	1
4:A:347:PX4:H56	4:A:356:PX4:H58	0.51	1.83	4	1
4:A:308:PX4:H27	4:A:311:PX4:H31	0.51	1.81	4	1
4:A:393:PX4:H18	4:A:401:PX4:H20	0.51	1.83	12	1
4:A:404:PX4:H15	4:A:413:PX4:H20	0.51	1.81	1	1
4:A:322:PX4:H49	4:A:336:PX4:H25	0.51	1.83	9	1
4:A:402:PX4:H21	4:A:404:PX4:H67	0.51	1.83	14	1
4:A:378:PX4:H29	4:A:420:PX4:H57	0.51	1.82	4	1
4:A:345:PX4:H15	4:A:353:PX4:H14	0.51	1.81	4	2
4:A:358:PX4:H23	4:A:363:PX4:H55	0.51	1.83	12	1
4:A:349:PX4:H26	4:A:356:PX4:H38	0.51	1.83	11	1
4:A:312:PX4:H31	4:A:365:PX4:H46	0.51	1.82	14	1
4:A:346:PX4:H68	4:A:362:PX4:H72	0.51	1.82	14	1
4:A:372:PX4:H34	4:A:420:PX4:H29	0.51	1.82	14	1
4:A:314:PX4:H47	4:A:350:PX4:H43	0.51	1.82	14	1
4:A:363:PX4:H71	4:A:392:PX4:H66	0.51	1.82	3	1
4:A:392:PX4:H57	4:A:401:PX4:H29	0.51	1.81	13	1
4:A:306:PX4:H60	4:A:362:PX4:H38	0.51	1.83	10	1
4:A:321:PX4:H56	4:A:361:PX4:H54	0.51	1.82	10	1
4:A:333:PX4:H14	4:A:340:PX4:H1	0.51	1.82	11	1
4:A:318:PX4:H53	4:A:328:PX4:H22	0.51	1.81	11	1
4:A:311:PX4:O1	4:A:359:PX4:H3	0.51	2.06	5	2
4:A:372:PX4:H23	4:A:417:PX4:H46	0.51	1.83	8	1
4:A:316:PX4:H20	4:A:364:PX4:H14	0.51	1.81	12	1
4:A:378:PX4:H59	4:A:410:PX4:H26	0.51	1.82	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:343:PX4:H33	4:A:344:PX4:H30	0.51	1.83	12	1
4:A:306:PX4:H22	4:A:321:PX4:H35	0.51	1.82	9	1
4:A:410:PX4:H42	4:A:418:PX4:H42	0.51	1.82	14	1
4:A:346:PX4:H19	4:A:354:PX4:H31	0.51	1.82	3	1
4:A:309:PX4:H3	4:A:320:PX4:O1	0.51	2.05	13	1
4:A:409:PX4:O6	4:A:410:PX4:H5	0.51	2.06	13	1
4:A:355:PX4:H36	4:A:356:PX4:H41	0.51	1.81	4	1
4:A:333:PX4:H54	4:A:341:PX4:H54	0.51	1.83	11	1
4:A:410:PX4:H16	4:A:418:PX4:H29	0.51	1.81	6	1
4:A:354:PX4:H49	4:A:360:PX4:H49	0.51	1.83	4	1
4:A:388:PX4:H51	4:A:396:PX4:H48	0.51	1.81	10	1
4:A:390:PX4:H57	4:A:429:PX4:H60	0.51	1.82	11	1
4:A:320:PX4:H51	4:A:359:PX4:H25	0.51	1.81	8	1
4:A:400:PX4:H20	4:A:426:PX4:H50	0.51	1.82	12	1
4:A:319:PX4:H51	4:A:324:PX4:H16	0.51	1.83	1	1
4:A:395:PX4:H24	4:A:396:PX4:H64	0.51	1.83	4	1
4:A:313:PX4:H20	4:A:360:PX4:H15	0.50	1.82	7	1
4:A:327:PX4:H16	4:A:328:PX4:O6	0.50	2.05	5	1
4:A:363:PX4:H47	4:A:364:PX4:H37	0.50	1.81	14	1
4:A:344:PX4:H60	4:A:344:PX4:H25	0.50	1.83	14	1
4:A:345:PX4:H70	4:A:370:PX4:H39	0.50	1.83	10	1
4:A:369:PX4:H19	4:A:418:PX4:H15	0.50	1.83	10	1
4:A:310:PX4:H48	4:A:365:PX4:H20	0.50	1.81	7	1
4:A:413:PX4:H63	4:A:430:PX4:H36	0.50	1.82	7	1
4:A:308:PX4:H18	4:A:311:PX4:O8	0.50	2.06	14	2
4:A:403:PX4:H3	4:A:427:PX4:H48	0.50	1.83	11	1
4:A:388:PX4:H29	4:A:411:PX4:H24	0.50	1.83	5	1
4:A:412:PX4:H47	4:A:419:PX4:H14	0.50	1.84	12	1
1:A:206:HIS:ND1	4:A:314:PX4:H1	0.50	2.21	13	3
4:A:337:PX4:H39	4:A:338:PX4:H51	0.50	1.83	9	1
4:A:402:PX4:H21	4:A:403:PX4:H21	0.50	1.82	3	1
4:A:307:PX4:H42	4:A:350:PX4:H45	0.50	1.82	2	1
4:A:346:PX4:H12	4:A:360:PX4:H46	0.50	1.82	13	1
4:A:352:PX4:H61	4:A:358:PX4:H57	0.50	1.82	9	1
4:A:311:PX4:O4	4:A:359:PX4:H6	0.50	2.05	13	1
4:A:363:PX4:H25	4:A:365:PX4:H26	0.50	1.83	13	1
4:A:378:PX4:H35	4:A:410:PX4:H60	0.50	1.83	13	1
4:A:416:PX4:H53	4:A:418:PX4:H30	0.50	1.84	13	1
4:A:370:PX4:H17	4:A:403:PX4:O1	0.50	2.06	4	1
4:A:407:PX4:H9	4:A:414:PX4:H48	0.50	1.83	14	1
4:A:394:PX4:H9	4:A:394:PX4:O8	0.50	2.07	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:368:PX4:H32	4:A:425:PX4:H42	0.50	1.81	3	1
4:A:347:PX4:H35	4:A:348:PX4:H28	0.50	1.83	13	1
4:A:388:PX4:H24	4:A:402:PX4:O8	0.50	2.05	11	1
4:A:316:PX4:H65	4:A:320:PX4:H40	0.50	1.83	5	1
4:A:421:PX4:H13	4:A:423:PX4:O6	0.50	2.07	1	1
4:A:378:PX4:H50	4:A:418:PX4:H51	0.50	1.81	9	1
4:A:374:PX4:H22	4:A:428:PX4:H20	0.50	1.82	14	1
4:A:383:PX4:H46	4:A:399:PX4:H50	0.50	1.83	3	1
4:A:402:PX4:H4	4:A:404:PX4:O2	0.50	2.06	11	2
4:A:422:PX4:H38	4:A:423:PX4:H40	0.50	1.83	6	1
4:A:408:PX4:H2	4:A:408:PX4:H18	0.50	1.84	6	1
4:A:392:PX4:H27	4:A:393:PX4:H61	0.50	1.84	9	1
1:A:237:PHE:CD1	1:A:238:PRO:HD2	0.50	2.42	9	1
4:A:409:PX4:H54	4:A:422:PX4:H62	0.50	1.82	3	1
4:A:384:PX4:H56	4:A:385:PX4:H32	0.50	1.82	3	1
4:A:307:PX4:H67	4:A:307:PX4:H34	0.50	1.84	2	1
4:A:395:PX4:H42	4:A:405:PX4:H36	0.50	1.81	13	1
4:A:416:PX4:H24	4:A:422:PX4:H17	0.50	1.83	10	1
4:A:345:PX4:H46	4:A:346:PX4:H56	0.50	1.84	12	1
4:A:371:PX4:H35	4:A:371:PX4:H68	0.50	1.83	12	1
4:A:400:PX4:H30	4:A:401:PX4:H57	0.50	1.83	1	1
4:A:408:PX4:H17	4:A:415:PX4:O6	0.50	2.07	1	1
4:A:322:PX4:O2	4:A:333:PX4:H9	0.50	2.07	13	1
4:A:369:PX4:H18	4:A:425:PX4:H9	0.50	1.82	4	1
4:A:321:PX4:H24	4:A:354:PX4:H53	0.50	1.81	2	2
4:A:306:PX4:H19	4:A:321:PX4:H42	0.50	1.84	6	1
4:A:380:PX4:H49	4:A:381:PX4:H13	0.50	1.83	12	1
4:A:400:PX4:H68	4:A:410:PX4:H67	0.49	1.84	10	1
4:A:428:PX4:H63	4:A:430:PX4:H32	0.49	1.84	8	1
4:A:338:PX4:H17	4:A:348:PX4:H17	0.49	1.84	1	1
4:A:395:PX4:H58	4:A:404:PX4:H50	0.49	1.83	1	1
4:A:356:PX4:H32	4:A:362:PX4:H27	0.49	1.82	1	1
4:A:308:PX4:H40	4:A:316:PX4:H41	0.49	1.84	4	1
4:A:409:PX4:H51	4:A:415:PX4:C11	0.49	2.36	8	1
4:A:347:PX4:H22	4:A:348:PX4:H56	0.49	1.83	5	1
4:A:393:PX4:H3	4:A:401:PX4:O2	0.49	2.08	5	1
4:A:374:PX4:H18	4:A:382:PX4:O7	0.49	2.06	8	1
4:A:312:PX4:H29	4:A:365:PX4:H22	0.49	1.84	12	1
4:A:306:PX4:H22	4:A:322:PX4:H57	0.49	1.84	1	1
4:A:390:PX4:H62	4:A:397:PX4:H42	0.49	1.84	9	1
4:A:393:PX4:H37	4:A:401:PX4:H70	0.49	1.84	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:308:PX4:O6	4:A:364:PX4:H3	0.49	2.07	12	1
4:A:372:PX4:H20	4:A:420:PX4:H16	0.49	1.84	13	2
4:A:421:PX4:H67	4:A:423:PX4:H45	0.49	1.83	3	1
4:A:337:PX4:H9	4:A:357:PX4:H2	0.49	1.84	11	1
4:A:317:PX4:H14	4:A:351:PX4:H20	0.49	1.85	5	1
4:A:316:PX4:H51	4:A:320:PX4:C14	0.49	2.37	12	1
4:A:312:PX4:H35	4:A:365:PX4:H46	0.49	1.83	13	1
4:A:377:PX4:H42	4:A:379:PX4:H56	0.49	1.84	13	1
4:A:326:PX4:O6	4:A:363:PX4:H61	0.49	2.07	8	1
4:A:313:PX4:H65	4:A:360:PX4:H70	0.49	1.85	1	1
4:A:347:PX4:H21	4:A:348:PX4:H55	0.49	1.83	3	1
4:A:316:PX4:H29	4:A:361:PX4:H25	0.49	1.85	2	1
4:A:369:PX4:H20	4:A:377:PX4:H46	0.49	1.85	4	1
4:A:348:PX4:H35	4:A:380:PX4:H42	0.49	1.83	7	1
4:A:419:PX4:H42	4:A:427:PX4:H41	0.49	1.83	5	1
4:A:335:PX4:O6	4:A:343:PX4:H14	0.49	2.08	5	1
4:A:390:PX4:O1	4:A:399:PX4:H12	0.49	2.08	6	1
4:A:306:PX4:H59	4:A:361:PX4:H57	0.49	1.84	8	1
4:A:345:PX4:O1	4:A:346:PX4:H9	0.49	2.08	9	1
4:A:340:PX4:H42	4:A:389:PX4:H27	0.49	1.84	9	1
4:A:326:PX4:H19	4:A:334:PX4:H55	0.49	1.83	4	1
4:A:344:PX4:H56	4:A:347:PX4:H33	0.49	1.84	10	1
4:A:408:PX4:H4	4:A:414:PX4:O2	0.49	2.07	10	2
4:A:392:PX4:H70	4:A:415:PX4:H33	0.49	1.84	7	1
4:A:332:PX4:H53	4:A:356:PX4:H47	0.49	1.84	5	1
4:A:406:PX4:H23	4:A:415:PX4:H22	0.49	1.85	13	1
4:A:337:PX4:H31	4:A:338:PX4:H28	0.49	1.84	10	1
4:A:337:PX4:H42	4:A:347:PX4:H30	0.49	1.84	7	1
4:A:313:PX4:H51	4:A:354:PX4:H66	0.49	1.85	5	1
4:A:395:PX4:H19	4:A:396:PX4:H15	0.49	1.85	8	1
4:A:337:PX4:H48	4:A:345:PX4:H51	0.49	1.82	12	1
4:A:393:PX4:H32	4:A:401:PX4:H53	0.49	1.83	12	1
4:A:313:PX4:H15	4:A:360:PX4:C9	0.49	2.38	14	1
4:A:312:PX4:H25	4:A:365:PX4:H20	0.49	1.84	3	1
4:A:332:PX4:H52	4:A:347:PX4:H65	0.49	1.85	3	1
4:A:421:PX4:H26	4:A:423:PX4:H22	0.49	1.85	7	1
4:A:385:PX4:H49	4:A:393:PX4:H52	0.49	1.84	5	1
4:A:400:PX4:H39	4:A:401:PX4:H35	0.49	1.84	5	1
4:A:319:PX4:H17	4:A:324:PX4:O4	0.49	2.08	8	1
4:A:400:PX4:H57	4:A:408:PX4:H72	0.49	1.85	8	1
4:A:387:PX4:H47	4:A:411:PX4:C8	0.49	2.34	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:361:PX4:H37	4:A:423:PX4:H36	0.49	1.84	9	1
4:A:326:PX4:H69	4:A:393:PX4:H62	0.49	1.83	9	1
4:A:344:PX4:H52	4:A:347:PX4:H27	0.49	1.84	9	1
4:A:405:PX4:H64	4:A:406:PX4:H67	0.49	1.85	3	1
4:A:415:PX4:H56	4:A:421:PX4:H68	0.49	1.83	3	1
4:A:321:PX4:H34	4:A:322:PX4:H58	0.49	1.83	13	1
4:A:385:PX4:H23	4:A:386:PX4:H28	0.48	1.85	5	1
4:A:376:PX4:H59	4:A:385:PX4:H57	0.48	1.84	5	1
4:A:355:PX4:H54	4:A:356:PX4:H47	0.48	1.85	8	1
4:A:367:PX4:H18	4:A:424:PX4:O3	0.48	2.08	8	1
4:A:373:PX4:O2	4:A:382:PX4:H9	0.48	2.08	12	1
4:A:376:PX4:H61	4:A:392:PX4:H32	0.48	1.85	14	1
4:A:316:PX4:H64	4:A:323:PX4:H69	0.48	1.84	14	1
4:A:335:PX4:H1	4:A:344:PX4:O6	0.48	2.08	4	1
4:A:385:PX4:H28	4:A:386:PX4:H28	0.48	1.85	7	1
4:A:406:PX4:H28	4:A:421:PX4:H63	0.48	1.86	5	1
4:A:322:PX4:H56	4:A:336:PX4:H31	0.48	1.85	3	1
4:A:308:PX4:H19	4:A:311:PX4:H52	0.48	1.85	2	1
4:A:404:PX4:H48	4:A:413:PX4:O6	0.48	2.08	4	1
4:A:421:PX4:H40	4:A:423:PX4:H53	0.48	1.85	7	1
4:A:311:PX4:H31	4:A:364:PX4:H27	0.48	1.86	11	1
4:A:332:PX4:H43	4:A:407:PX4:H61	0.48	1.85	3	1
4:A:369:PX4:H32	4:A:410:PX4:H21	0.48	1.83	2	1
4:A:372:PX4:H25	4:A:420:PX4:H50	0.48	1.84	4	1
4:A:357:PX4:H71	4:A:357:PX4:H29	0.48	1.84	10	1
4:A:345:PX4:H20	4:A:346:PX4:H15	0.48	1.85	11	1
4:A:376:PX4:H60	4:A:392:PX4:H25	0.48	1.84	5	1
4:A:320:PX4:H71	4:A:378:PX4:H40	0.48	1.85	8	1
4:A:316:PX4:H24	4:A:364:PX4:H47	0.48	1.86	8	1
4:A:307:PX4:H71	4:A:349:PX4:H45	0.48	1.84	1	1
4:A:378:PX4:H2	4:A:410:PX4:O6	0.48	2.09	13	1
4:A:307:PX4:H22	4:A:321:PX4:H64	0.48	1.83	13	1
4:A:389:PX4:H51	4:A:390:PX4:H24	0.48	1.85	13	1
4:A:349:PX4:H38	4:A:421:PX4:H42	0.48	1.85	10	1
4:A:400:PX4:H46	4:A:409:PX4:H20	0.48	1.85	10	1
4:A:354:PX4:H24	4:A:362:PX4:H17	0.48	1.84	11	1
4:A:346:PX4:H50	4:A:362:PX4:H56	0.48	1.86	11	1
4:A:310:PX4:O6	4:A:365:PX4:H11	0.48	2.08	12	1
4:A:400:PX4:H40	4:A:401:PX4:H45	0.48	1.85	1	1
4:A:326:PX4:H21	4:A:350:PX4:H17	0.48	1.85	9	1
4:A:309:PX4:H65	4:A:320:PX4:H36	0.48	1.85	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:400:PX4:H60	4:A:410:PX4:H54	0.48	1.85	13	1
4:A:388:PX4:H23	4:A:396:PX4:H30	0.48	1.84	11	1
4:A:353:PX4:H70	4:A:412:PX4:H37	0.48	1.86	5	1
4:A:377:PX4:H60	4:A:416:PX4:H62	0.48	1.85	5	1
4:A:392:PX4:H67	4:A:408:PX4:H36	0.48	1.84	12	1
4:A:331:PX4:O6	4:A:340:PX4:H4	0.48	2.08	1	1
4:A:330:PX4:C11	4:A:335:PX4:H19	0.48	2.36	2	1
4:A:393:PX4:H42	4:A:401:PX4:H40	0.48	1.84	2	1
4:A:337:PX4:H50	4:A:353:PX4:H25	0.48	1.84	10	1
4:A:374:PX4:H29	4:A:427:PX4:H31	0.48	1.86	7	1
4:A:337:PX4:H30	4:A:338:PX4:H48	0.48	1.86	5	1
4:A:319:PX4:H21	4:A:324:PX4:H19	0.48	1.84	6	1
4:A:395:PX4:H48	4:A:405:PX4:H19	0.48	1.86	12	2
4:A:369:PX4:H18	4:A:425:PX4:H1	0.48	1.86	1	1
4:A:390:PX4:H62	4:A:397:PX4:C21	0.48	2.38	9	1
4:A:358:PX4:H27	4:A:363:PX4:H26	0.48	1.86	2	1
1:A:242:TYR:CD1	4:A:314:PX4:H19	0.48	2.43	4	1
4:A:406:PX4:H18	4:A:415:PX4:O1	0.48	2.09	11	1
4:A:331:PX4:H18	4:A:340:PX4:H21	0.48	1.84	5	1
4:A:346:PX4:H51	4:A:355:PX4:H14	0.48	1.85	6	1
1:A:145:THR:HB	1:A:146:PRO:HD2	0.48	1.85	2	1
4:A:323:PX4:H26	4:A:333:PX4:H17	0.48	1.85	4	1
4:A:318:PX4:O2	4:A:359:PX4:H18	0.48	2.07	4	1
4:A:315:PX4:H45	4:A:425:PX4:H27	0.48	1.85	7	1
4:A:307:PX4:H49	4:A:321:PX4:H56	0.48	1.86	5	1
4:A:348:PX4:H55	4:A:388:PX4:H71	0.48	1.84	6	1
4:A:326:PX4:H20	4:A:350:PX4:H48	0.48	1.86	8	1
4:A:326:PX4:H49	4:A:351:PX4:H18	0.48	1.84	1	1
4:A:404:PX4:H53	4:A:413:PX4:H24	0.48	1.86	14	1
4:A:347:PX4:H13	4:A:348:PX4:O1	0.48	2.08	6	3
4:A:325:PX4:H62	4:A:334:PX4:H45	0.48	1.86	11	1
4:A:337:PX4:H22	4:A:337:PX4:H8	0.48	1.85	12	1
4:A:321:PX4:H15	4:A:354:PX4:H15	0.48	1.85	12	1
4:A:421:PX4:H30	4:A:423:PX4:H19	0.48	1.86	12	1
4:A:416:PX4:O3	4:A:416:PX4:H10	0.48	2.09	1	1
4:A:351:PX4:C5	4:A:352:PX4:H24	0.48	2.39	9	1
4:A:404:PX4:H59	4:A:430:PX4:H40	0.48	1.86	4	1
4:A:308:PX4:O1	4:A:311:PX4:H14	0.47	2.10	7	1
4:A:349:PX4:H30	4:A:356:PX4:H38	0.47	1.86	7	1
4:A:424:PX4:H69	4:A:429:PX4:H67	0.47	1.86	7	1
4:A:325:PX4:H17	4:A:341:PX4:H47	0.47	1.85	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:373:PX4:H60	4:A:381:PX4:H25	0.47	1.85	3	1
4:A:357:PX4:H39	4:A:402:PX4:H41	0.47	1.84	4	1
4:A:402:PX4:O2	4:A:402:PX4:H10	0.47	2.09	7	1
4:A:413:PX4:H50	4:A:430:PX4:H23	0.47	1.86	7	1
4:A:388:PX4:H17	4:A:396:PX4:O6	0.47	2.09	1	2
4:A:331:PX4:H14	4:A:347:PX4:H14	0.47	1.86	5	1
4:A:421:PX4:H30	4:A:430:PX4:H19	0.47	1.84	5	1
4:A:326:PX4:H35	4:A:350:PX4:H52	0.47	1.86	10	1
4:A:322:PX4:H25	4:A:361:PX4:H48	0.47	1.86	10	2
4:A:314:PX4:H61	4:A:364:PX4:H71	0.47	1.86	7	1
4:A:351:PX4:H55	4:A:358:PX4:H52	0.47	1.86	7	1
4:A:335:PX4:H24	4:A:344:PX4:H24	0.47	1.86	11	1
4:A:332:PX4:H3	4:A:356:PX4:O3	0.47	2.08	14	1
4:A:376:PX4:H68	4:A:385:PX4:H63	0.47	1.87	14	1
4:A:367:PX4:H28	4:A:423:PX4:H50	0.47	1.85	14	1
4:A:338:PX4:H68	4:A:396:PX4:H38	0.47	1.85	2	1
4:A:310:PX4:H48	4:A:312:PX4:H21	0.47	1.86	10	1
4:A:311:PX4:H69	4:A:320:PX4:H44	0.47	1.86	10	1
4:A:342:PX4:H54	4:A:351:PX4:H29	0.47	1.86	11	2
4:A:345:PX4:H19	4:A:346:PX4:H19	0.47	1.86	11	1
4:A:405:PX4:H54	4:A:414:PX4:H30	0.47	1.86	11	1
4:A:398:PX4:H40	4:A:414:PX4:H32	0.47	1.86	6	1
4:A:368:PX4:H1	4:A:369:PX4:O2	0.47	2.09	1	1
4:A:421:PX4:H5	4:A:423:PX4:O1	0.47	2.09	3	2
4:A:355:PX4:H20	4:A:362:PX4:H51	0.47	1.86	14	1
4:A:372:PX4:H55	4:A:379:PX4:H53	0.47	1.86	2	1
4:A:378:PX4:H52	4:A:410:PX4:H26	0.47	1.87	13	1
4:A:412:PX4:H5	4:A:427:PX4:O1	0.47	2.10	7	1
4:A:325:PX4:H12	4:A:325:PX4:H14	0.47	1.87	5	1
4:A:400:PX4:H47	4:A:426:PX4:H26	0.47	1.85	12	1
4:A:325:PX4:H17	4:A:341:PX4:H17	0.47	1.87	1	1
4:A:399:PX4:O1	4:A:407:PX4:H7	0.47	2.10	9	1
4:A:326:PX4:H51	4:A:334:PX4:H40	0.47	1.87	3	1
4:A:351:PX4:H56	4:A:358:PX4:H56	0.47	1.86	3	1
1:A:205:THR:O	4:A:314:PX4:H9	0.47	2.09	4	1
4:A:338:PX4:H70	4:A:362:PX4:H44	0.47	1.86	4	1
4:A:317:PX4:O1	4:A:351:PX4:H20	0.47	2.09	4	1
4:A:405:PX4:O2	4:A:406:PX4:H12	0.47	2.09	7	1
4:A:424:PX4:H48	4:A:425:PX4:H22	0.47	1.86	7	1
4:A:340:PX4:H47	4:A:341:PX4:H61	0.47	1.87	7	1
4:A:358:PX4:H20	4:A:363:PX4:H18	0.47	1.86	14	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:316:PX4:H61	4:A:323:PX4:C36	0.47	2.38	12	1
4:A:361:PX4:H31	4:A:367:PX4:H42	0.47	1.84	1	1
4:A:417:PX4:H64	4:A:420:PX4:H60	0.47	1.86	4	1
4:A:346:PX4:H46	4:A:355:PX4:O1	0.47	2.10	10	1
4:A:390:PX4:H60	4:A:390:PX4:H29	0.47	1.86	7	1
1:A:214:LEU:H	1:A:214:LEU:HD23	0.47	1.69	7	2
4:A:405:PX4:H9	4:A:405:PX4:O6	0.47	2.10	11	1
4:A:388:PX4:H52	4:A:411:PX4:H28	0.47	1.87	11	1
4:A:306:PX4:H70	4:A:349:PX4:H35	0.47	1.86	5	1
4:A:346:PX4:H29	4:A:354:PX4:H19	0.47	1.86	5	1
4:A:322:PX4:H40	4:A:361:PX4:H54	0.47	1.84	5	1
4:A:395:PX4:H59	4:A:405:PX4:H42	0.47	1.84	5	1
4:A:308:PX4:H54	4:A:364:PX4:H30	0.47	1.85	5	1
4:A:310:PX4:H54	4:A:312:PX4:H22	0.47	1.87	5	1
4:A:345:PX4:O1	4:A:346:PX4:H13	0.47	2.08	6	1
4:A:360:PX4:H3	4:A:366:PX4:O4	0.47	2.10	6	1
4:A:403:PX4:H52	4:A:419:PX4:H55	0.47	1.86	6	1
4:A:335:PX4:H48	4:A:343:PX4:H22	0.47	1.86	12	1
4:A:306:PX4:H29	4:A:336:PX4:H31	0.47	1.87	1	1
4:A:319:PX4:H12	4:A:342:PX4:O2	0.47	2.09	1	1
4:A:358:PX4:H38	4:A:365:PX4:H34	0.47	1.86	9	1
4:A:396:PX4:H63	4:A:398:PX4:H50	0.47	1.86	9	1
4:A:400:PX4:O2	4:A:426:PX4:H14	0.47	2.09	9	1
4:A:309:PX4:O6	4:A:320:PX4:H4	0.47	2.09	9	1
4:A:392:PX4:H51	4:A:408:PX4:H24	0.47	1.85	14	1
4:A:331:PX4:H69	4:A:347:PX4:H42	0.47	1.85	14	1
4:A:381:PX4:H52	4:A:388:PX4:H46	0.47	1.86	14	1
4:A:359:PX4:H44	4:A:372:PX4:H40	0.47	1.87	2	1
4:A:391:PX4:H64	4:A:409:PX4:H62	0.47	1.87	13	1
4:A:402:PX4:H37	4:A:413:PX4:H36	0.47	1.86	13	1
4:A:336:PX4:H36	4:A:361:PX4:H67	0.47	1.86	4	1
4:A:349:PX4:H12	4:A:349:PX4:O6	0.47	2.09	4	1
4:A:412:PX4:H27	4:A:413:PX4:H38	0.47	1.84	10	1
4:A:400:PX4:H48	4:A:410:PX4:H46	0.47	1.87	10	1
4:A:376:PX4:H23	4:A:399:PX4:H49	0.47	1.86	11	1
4:A:389:PX4:H21	4:A:396:PX4:H71	0.47	1.87	5	1
4:A:323:PX4:H43	4:A:424:PX4:H27	0.47	1.86	1	1
4:A:413:PX4:H66	4:A:422:PX4:H41	0.47	1.87	1	1
4:A:315:PX4:H28	4:A:322:PX4:H40	0.47	1.87	9	1
4:A:371:PX4:H71	4:A:378:PX4:H62	0.47	1.87	14	1
4:A:391:PX4:H41	4:A:408:PX4:H39	0.47	1.85	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:400:PX4:H17	4:A:408:PX4:H53	0.47	1.85	7	1
4:A:398:PX4:H16	4:A:407:PX4:H46	0.47	1.85	7	1
4:A:371:PX4:H39	4:A:420:PX4:H36	0.47	1.86	11	1
4:A:334:PX4:H41	4:A:408:PX4:H41	0.47	1.87	5	1
4:A:350:PX4:H49	4:A:363:PX4:H50	0.47	1.87	5	1
4:A:312:PX4:H28	4:A:365:PX4:H46	0.47	1.85	8	1
4:A:326:PX4:H36	4:A:349:PX4:H71	0.47	1.87	1	1
4:A:408:PX4:H72	4:A:426:PX4:H57	0.47	1.87	9	1
4:A:355:PX4:H17	4:A:355:PX4:H61	0.47	1.85	9	1
4:A:332:PX4:H37	4:A:390:PX4:H39	0.47	1.86	14	1
4:A:307:PX4:H64	4:A:321:PX4:H67	0.47	1.87	4	1
4:A:369:PX4:H32	4:A:377:PX4:H61	0.47	1.86	4	1
4:A:375:PX4:H68	4:A:419:PX4:H32	0.47	1.86	4	1
4:A:416:PX4:H57	4:A:423:PX4:H64	0.47	1.86	9	1
4:A:402:PX4:H51	4:A:404:PX4:H47	0.47	1.87	3	1
4:A:322:PX4:H25	4:A:361:PX4:H46	0.47	1.85	13	1
4:A:419:PX4:O8	4:A:427:PX4:H17	0.47	2.09	13	1
4:A:388:PX4:H34	4:A:402:PX4:H24	0.47	1.87	4	1
4:A:342:PX4:H19	4:A:352:PX4:H23	0.46	1.87	10	1
4:A:404:PX4:H41	4:A:412:PX4:H64	0.46	1.88	10	1
4:A:349:PX4:H41	4:A:422:PX4:H45	0.46	1.87	7	1
4:A:345:PX4:H20	4:A:346:PX4:H47	0.46	1.86	5	1
4:A:308:PX4:H62	4:A:363:PX4:H21	0.46	1.87	1	1
4:A:372:PX4:H26	4:A:378:PX4:H34	0.46	1.87	9	1
4:A:358:PX4:H31	4:A:364:PX4:H43	0.46	1.85	14	1
4:A:368:PX4:O2	4:A:369:PX4:H4	0.46	2.09	2	1
4:A:370:PX4:H68	4:A:403:PX4:H23	0.46	1.88	13	1
4:A:353:PX4:H27	4:A:366:PX4:H14	0.46	1.86	10	1
4:A:310:PX4:H71	4:A:311:PX4:H20	0.46	1.85	7	1
4:A:380:PX4:H52	4:A:387:PX4:H46	0.46	1.87	11	1
4:A:392:PX4:H18	4:A:393:PX4:H47	0.46	1.87	11	2
4:A:400:PX4:H31	4:A:426:PX4:H58	0.46	1.87	8	1
4:A:386:PX4:H29	4:A:387:PX4:H26	0.46	1.86	12	1
4:A:382:PX4:H59	4:A:428:PX4:H21	0.46	1.88	3	1
4:A:393:PX4:H38	4:A:401:PX4:H36	0.46	1.86	2	1
4:A:325:PX4:H47	4:A:341:PX4:H22	0.46	1.87	2	1
4:A:400:PX4:H29	4:A:401:PX4:H31	0.46	1.87	13	1
4:A:310:PX4:H63	4:A:311:PX4:H21	0.46	1.87	10	1
4:A:310:PX4:H72	4:A:311:PX4:H67	0.46	1.87	6	1
4:A:424:PX4:H40	4:A:429:PX4:H68	0.46	1.88	6	1
4:A:378:PX4:H19	4:A:410:PX4:H27	0.46	1.87	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:404:PX4:H15	4:A:413:PX4:O6	0.46	2.11	9	1
4:A:315:PX4:H5	4:A:361:PX4:O6	0.46	2.11	14	1
4:A:392:PX4:H49	4:A:393:PX4:H50	0.46	1.88	14	1
4:A:355:PX4:H40	4:A:356:PX4:H35	0.46	1.87	3	1
4:A:395:PX4:H35	4:A:397:PX4:H64	0.46	1.86	3	1
4:A:322:PX4:H38	4:A:413:PX4:H68	0.46	1.88	2	1
4:A:330:PX4:H30	4:A:338:PX4:H29	0.46	1.87	10	1
4:A:390:PX4:H61	4:A:397:PX4:H36	0.46	1.87	10	1
4:A:315:PX4:H17	4:A:316:PX4:H54	0.46	1.87	7	1
4:A:371:PX4:H60	4:A:378:PX4:H66	0.46	1.87	5	1
4:A:331:PX4:H42	4:A:397:PX4:H30	0.46	1.88	6	1
4:A:353:PX4:O6	4:A:366:PX4:H3	0.46	2.10	8	1
4:A:315:PX4:H21	4:A:316:PX4:H32	0.46	1.88	12	1
4:A:407:PX4:H18	4:A:414:PX4:H49	0.46	1.85	12	1
4:A:404:PX4:H69	4:A:412:PX4:H45	0.46	1.87	1	1
4:A:383:PX4:H59	4:A:399:PX4:H17	0.46	1.87	9	1
4:A:398:PX4:H19	4:A:407:PX4:H19	0.46	1.86	9	1
4:A:410:PX4:H60	4:A:417:PX4:H62	0.46	1.87	14	1
4:A:349:PX4:H56	4:A:350:PX4:H28	0.46	1.86	10	1
4:A:417:PX4:H20	4:A:426:PX4:H23	0.46	1.87	7	1
4:A:321:PX4:H68	4:A:361:PX4:H49	0.46	1.88	7	1
4:A:378:PX4:H42	4:A:410:PX4:H71	0.46	1.85	5	1
4:A:321:PX4:H70	4:A:423:PX4:H41	0.46	1.88	12	1
4:A:347:PX4:H43	4:A:348:PX4:H31	0.46	1.86	3	1
4:A:378:PX4:H17	4:A:410:PX4:H22	0.46	1.86	3	1
4:A:322:PX4:H24	4:A:361:PX4:H48	0.46	1.85	2	1
4:A:391:PX4:H29	4:A:414:PX4:H46	0.46	1.87	13	1
4:A:307:PX4:H39	4:A:349:PX4:H69	0.46	1.86	13	1
4:A:349:PX4:H64	4:A:405:PX4:H70	0.46	1.87	11	1
4:A:307:PX4:H55	4:A:362:PX4:H27	0.46	1.86	11	1
4:A:369:PX4:H25	4:A:418:PX4:H25	0.46	1.87	11	1
4:A:387:PX4:H6	4:A:387:PX4:H14	0.46	1.86	6	1
4:A:402:PX4:H18	4:A:404:PX4:H20	0.46	1.85	6	1
4:A:367:PX4:H25	4:A:424:PX4:H26	0.46	1.87	1	1
4:A:347:PX4:H72	4:A:356:PX4:H65	0.46	1.87	9	1
4:A:350:PX4:H69	4:A:351:PX4:H69	0.46	1.87	3	1
4:A:346:PX4:H30	4:A:353:PX4:H65	0.46	1.86	13	1
4:A:331:PX4:H28	4:A:347:PX4:C25	0.46	2.40	4	1
4:A:313:PX4:C19	4:A:337:PX4:H64	0.46	2.41	10	1
4:A:423:PX4:H55	4:A:425:PX4:H28	0.46	1.88	10	1
4:A:421:PX4:H43	4:A:423:PX4:H41	0.46	1.87	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:337:PX4:H47	4:A:353:PX4:C6	0.46	2.29	8	1
4:A:331:PX4:H29	4:A:347:PX4:H52	0.46	1.87	8	1
4:A:308:PX4:H52	4:A:363:PX4:H24	0.46	1.86	12	1
4:A:321:PX4:H61	4:A:361:PX4:H46	0.46	1.88	12	1
4:A:340:PX4:H36	4:A:397:PX4:H65	0.46	1.85	9	1
4:A:340:PX4:H65	4:A:340:PX4:H28	0.46	1.86	13	1
4:A:396:PX4:H63	4:A:398:PX4:H51	0.46	1.88	11	1
4:A:383:PX4:H20	4:A:392:PX4:H27	0.46	1.85	12	1
4:A:337:PX4:H65	4:A:353:PX4:H40	0.46	1.86	12	1
4:A:407:PX4:H7	4:A:407:PX4:O6	0.46	2.11	1	1
4:A:390:PX4:H57	4:A:397:PX4:H35	0.46	1.86	13	1
4:A:313:PX4:H60	4:A:327:PX4:H31	0.46	1.87	13	1
4:A:391:PX4:H17	4:A:408:PX4:H2	0.46	1.88	7	1
4:A:392:PX4:H29	4:A:393:PX4:H61	0.46	1.88	11	1
4:A:330:PX4:H13	4:A:338:PX4:O6	0.46	2.11	5	1
4:A:317:PX4:H42	4:A:342:PX4:H72	0.46	1.88	6	1
4:A:344:PX4:H31	4:A:348:PX4:H25	0.46	1.88	8	1
4:A:392:PX4:H68	4:A:408:PX4:H35	0.46	1.88	8	1
4:A:367:PX4:H48	4:A:428:PX4:H50	0.46	1.86	9	1
4:A:325:PX4:H42	4:A:334:PX4:H59	0.46	1.87	14	1
4:A:357:PX4:H43	4:A:358:PX4:H44	0.46	1.86	13	1
4:A:311:PX4:H20	4:A:311:PX4:H55	0.46	1.88	10	1
4:A:311:PX4:H51	4:A:359:PX4:H59	0.46	1.86	7	1
4:A:362:PX4:H26	4:A:413:PX4:H72	0.46	1.88	7	1
4:A:388:PX4:H14	4:A:396:PX4:H18	0.46	1.88	7	1
4:A:332:PX4:H29	4:A:347:PX4:H66	0.46	1.87	5	1
4:A:338:PX4:H47	4:A:348:PX4:C23	0.46	2.41	8	1
4:A:382:PX4:H60	4:A:412:PX4:H64	0.46	1.88	8	1
4:A:398:PX4:H32	4:A:414:PX4:H55	0.46	1.86	8	1
4:A:398:PX4:H48	4:A:407:PX4:H57	0.46	1.86	12	1
4:A:340:PX4:H37	4:A:397:PX4:H29	0.46	1.88	1	1
4:A:402:PX4:H20	4:A:411:PX4:O8	0.46	2.11	1	1
4:A:370:PX4:H42	4:A:403:PX4:H38	0.46	1.86	1	1
4:A:330:PX4:H19	4:A:330:PX4:C4	0.45	2.41	10	1
4:A:410:PX4:O2	4:A:416:PX4:H3	0.45	2.10	14	2
4:A:326:PX4:H55	4:A:408:PX4:H44	0.45	1.87	11	1
4:A:391:PX4:H16	4:A:392:PX4:H46	0.45	1.88	12	1
4:A:334:PX4:H33	4:A:407:PX4:H38	0.45	1.88	9	1
4:A:312:PX4:H32	4:A:357:PX4:H55	0.45	1.88	14	1
4:A:361:PX4:H19	4:A:364:PX4:H46	0.45	1.87	14	1
4:A:404:PX4:H26	4:A:419:PX4:H9	0.45	1.87	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:409:PX4:H64	4:A:415:PX4:H60	0.45	1.88	4	1
4:A:413:PX4:H35	4:A:419:PX4:H27	0.45	1.87	10	1
4:A:308:PX4:H16	4:A:311:PX4:C9	0.45	2.41	7	1
4:A:308:PX4:H21	4:A:311:PX4:H49	0.45	1.88	7	1
4:A:316:PX4:H48	4:A:320:PX4:H21	0.45	1.87	7	1
4:A:333:PX4:H33	4:A:389:PX4:H45	0.45	1.88	11	1
4:A:360:PX4:H43	4:A:382:PX4:H64	0.45	1.88	8	1
4:A:317:PX4:H51	4:A:341:PX4:H19	0.45	1.87	8	1
4:A:380:PX4:H62	4:A:388:PX4:H42	0.45	1.88	9	1
4:A:421:PX4:H7	4:A:422:PX4:O6	0.45	2.11	9	1
4:A:367:PX4:H16	4:A:424:PX4:H14	0.45	1.87	14	1
4:A:323:PX4:H4	4:A:333:PX4:O2	0.45	2.11	3	1
4:A:345:PX4:C36	4:A:370:PX4:H39	0.45	2.41	10	1
4:A:331:PX4:C21	4:A:397:PX4:H30	0.45	2.41	6	1
4:A:391:PX4:H48	4:A:392:PX4:H46	0.45	1.87	8	1
4:A:390:PX4:H1	4:A:399:PX4:H18	0.45	1.88	12	1
4:A:403:PX4:H46	4:A:419:PX4:H51	0.45	1.88	1	1
4:A:351:PX4:H12	4:A:352:PX4:H24	0.45	1.88	9	1
4:A:317:PX4:H59	4:A:319:PX4:H56	0.45	1.88	14	1
4:A:383:PX4:O4	4:A:392:PX4:H1	0.45	2.10	3	1
4:A:393:PX4:H31	4:A:394:PX4:C11	0.45	2.41	3	1
4:A:422:PX4:H3	4:A:423:PX4:O2	0.45	2.10	4	1
4:A:354:PX4:H63	4:A:360:PX4:H63	0.45	1.88	4	1
4:A:307:PX4:H37	4:A:416:PX4:H42	0.45	1.88	5	1
4:A:313:PX4:H21	4:A:366:PX4:H18	0.45	1.88	5	1
4:A:331:PX4:H40	4:A:340:PX4:H63	0.45	1.88	5	1
4:A:310:PX4:H70	4:A:359:PX4:H59	0.45	1.88	5	1
4:A:337:PX4:H48	4:A:345:PX4:H49	0.45	1.88	6	1
4:A:348:PX4:H55	4:A:388:PX4:H70	0.45	1.88	1	1
4:A:328:PX4:H47	4:A:329:PX4:H28	0.45	1.89	9	1
4:A:380:PX4:H20	4:A:381:PX4:H48	0.45	1.89	9	1
4:A:348:PX4:H59	4:A:362:PX4:H54	0.45	1.89	13	1
4:A:405:PX4:H47	4:A:406:PX4:H48	0.45	1.88	4	1
4:A:369:PX4:H21	4:A:377:PX4:H71	0.45	1.87	10	1
4:A:381:PX4:H59	4:A:397:PX4:H47	0.45	1.87	7	1
4:A:338:PX4:H66	4:A:395:PX4:H38	0.45	1.89	4	1
4:A:349:PX4:O1	4:A:350:PX4:H14	0.45	2.11	10	1
4:A:391:PX4:H46	4:A:401:PX4:O6	0.45	2.12	11	1
4:A:313:PX4:H42	4:A:403:PX4:H62	0.45	1.87	5	1
4:A:421:PX4:H24	4:A:423:PX4:H19	0.45	1.87	5	1
4:A:412:PX4:O8	4:A:428:PX4:H17	0.45	2.11	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:307:PX4:H5	4:A:321:PX4:H48	0.45	1.87	8	1
4:A:378:PX4:H19	4:A:410:PX4:C14	0.45	2.42	12	1
4:A:371:PX4:H58	4:A:379:PX4:H32	0.45	1.89	13	1
4:A:375:PX4:H50	4:A:428:PX4:H14	0.45	1.88	13	1
4:A:323:PX4:H36	4:A:424:PX4:H67	0.45	1.87	4	1
4:A:416:PX4:H27	4:A:423:PX4:H24	0.45	1.87	7	1
4:A:373:PX4:O6	4:A:397:PX4:H12	0.45	2.12	11	1
4:A:419:PX4:H18	4:A:419:PX4:H12	0.45	1.87	11	1
4:A:312:PX4:H62	4:A:320:PX4:H67	0.45	1.87	11	1
4:A:393:PX4:H56	4:A:401:PX4:H35	0.45	1.89	1	1
4:A:322:PX4:H22	4:A:323:PX4:H19	0.45	1.89	1	1
1:A:214:LEU:HD11	1:A:243:VAL:H	0.45	1.71	14	1
4:A:313:PX4:H42	4:A:403:PX4:H66	0.45	1.89	2	1
4:A:391:PX4:H40	4:A:392:PX4:H56	0.45	1.88	13	1
4:A:368:PX4:H37	4:A:418:PX4:H72	0.45	1.89	4	1
4:A:330:PX4:H21	4:A:338:PX4:H22	0.45	1.87	10	1
4:A:342:PX4:H27	4:A:358:PX4:H58	0.45	1.89	5	1
4:A:331:PX4:H43	4:A:389:PX4:H29	0.45	1.88	6	1
1:A:243:VAL:HG12	4:A:356:PX4:H23	0.45	1.88	6	1
4:A:367:PX4:H17	4:A:428:PX4:H54	0.45	1.88	9	1
4:A:316:PX4:H25	4:A:320:PX4:H33	0.45	1.88	3	1
4:A:394:PX4:H34	4:A:401:PX4:H39	0.45	1.89	3	1
4:A:373:PX4:H36	4:A:381:PX4:H45	0.45	1.88	2	1
4:A:402:PX4:H57	4:A:404:PX4:H60	0.45	1.88	4	1
4:A:331:PX4:H53	4:A:340:PX4:H34	0.45	1.87	4	1
4:A:378:PX4:H16	4:A:417:PX4:C24	0.45	2.33	7	1
4:A:330:PX4:H19	4:A:330:PX4:H7	0.45	1.87	11	1
4:A:398:PX4:H67	4:A:405:PX4:H57	0.45	1.88	6	1
4:A:370:PX4:H28	4:A:403:PX4:H57	0.45	1.89	1	1
4:A:306:PX4:H14	4:A:321:PX4:O6	0.45	2.12	3	1
4:A:310:PX4:H17	4:A:365:PX4:O5	0.45	2.11	13	1
4:A:392:PX4:H25	4:A:393:PX4:H66	0.45	1.87	13	1
4:A:337:PX4:H53	4:A:353:PX4:H25	0.45	1.89	4	1
4:A:369:PX4:H52	4:A:425:PX4:H21	0.45	1.89	11	1
4:A:383:PX4:H24	4:A:383:PX4:H31	0.45	1.89	5	1
4:A:384:PX4:H34	4:A:384:PX4:H61	0.45	1.89	5	1
4:A:350:PX4:H1	4:A:358:PX4:O2	0.45	2.12	12	1
4:A:389:PX4:O2	4:A:398:PX4:H4	0.45	2.12	14	1
4:A:417:PX4:H24	4:A:426:PX4:H26	0.45	1.89	4	1
4:A:347:PX4:H10	4:A:348:PX4:O1	0.44	2.13	10	1
4:A:352:PX4:H52	4:A:358:PX4:H50	0.44	1.89	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:322:PX4:H62	4:A:412:PX4:H42	0.44	1.88	11	1
4:A:369:PX4:H44	4:A:418:PX4:H68	0.44	1.87	11	1
4:A:398:PX4:H13	4:A:398:PX4:H15	0.44	1.90	11	1
4:A:380:PX4:H26	4:A:381:PX4:H36	0.44	1.87	8	1
4:A:383:PX4:H66	4:A:399:PX4:H69	0.44	1.89	1	1
4:A:412:PX4:H23	4:A:413:PX4:H31	0.44	1.89	9	1
4:A:406:PX4:H25	4:A:415:PX4:H22	0.44	1.88	14	1
4:A:306:PX4:H59	4:A:361:PX4:H54	0.44	1.89	13	1
4:A:353:PX4:H20	4:A:366:PX4:H2	0.44	1.88	10	1
4:A:317:PX4:O2	4:A:325:PX4:H10	0.44	2.12	7	1
4:A:334:PX4:H3	4:A:334:PX4:O6	0.44	2.12	7	1
4:A:313:PX4:H47	4:A:328:PX4:H17	0.44	1.90	11	1
4:A:311:PX4:H53	4:A:359:PX4:H56	0.44	1.89	5	1
4:A:319:PX4:H26	4:A:324:PX4:H24	0.44	1.88	5	1
4:A:347:PX4:H19	4:A:347:PX4:H9	0.44	1.89	6	1
4:A:367:PX4:H48	4:A:424:PX4:H19	0.44	1.88	6	1
4:A:389:PX4:H30	4:A:396:PX4:H60	0.44	1.89	8	1
4:A:410:PX4:H66	4:A:426:PX4:H41	0.44	1.89	12	1
4:A:398:PX4:H45	4:A:414:PX4:H21	0.44	1.89	9	1
4:A:419:PX4:H60	4:A:427:PX4:H58	0.44	1.89	11	1
4:A:318:PX4:H18	4:A:328:PX4:H19	0.44	1.88	11	1
4:A:307:PX4:H51	4:A:362:PX4:H22	0.44	1.90	6	1
4:A:396:PX4:H31	4:A:411:PX4:H34	0.44	1.90	8	1
4:A:375:PX4:H21	4:A:429:PX4:H45	0.44	1.88	1	1
4:A:423:PX4:H16	4:A:425:PX4:O8	0.44	2.12	13	1
4:A:387:PX4:H54	4:A:388:PX4:H38	0.44	1.89	10	1
4:A:402:PX4:H54	4:A:404:PX4:H59	0.44	1.89	11	1
4:A:370:PX4:H26	4:A:427:PX4:H57	0.44	1.89	11	1
4:A:337:PX4:H15	4:A:353:PX4:O1	0.44	2.13	1	2
4:A:422:PX4:H34	4:A:423:PX4:H45	0.44	1.88	6	1
4:A:321:PX4:H68	4:A:322:PX4:H30	0.44	1.90	9	1
4:A:329:PX4:H67	4:A:424:PX4:H40	0.44	1.90	14	1
4:A:400:PX4:H47	4:A:409:PX4:H23	0.44	1.89	3	1
4:A:311:PX4:O3	4:A:311:PX4:H6	0.44	2.10	2	1
4:A:377:PX4:H10	4:A:418:PX4:O8	0.44	2.13	2	1
4:A:337:PX4:H52	4:A:345:PX4:H55	0.44	1.88	7	2
4:A:380:PX4:H46	4:A:387:PX4:H20	0.44	1.89	11	1
4:A:326:PX4:H66	4:A:399:PX4:H65	0.44	1.88	11	1
4:A:389:PX4:H48	4:A:398:PX4:H17	0.44	1.89	12	1
4:A:345:PX4:H35	4:A:346:PX4:H37	0.44	1.89	12	1
4:A:369:PX4:O1	4:A:425:PX4:H4	0.44	2.13	12	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:405:PX4:H53	4:A:414:PX4:H33	0.44	1.89	9	1
4:A:319:PX4:H66	4:A:324:PX4:H58	0.44	1.88	9	1
4:A:412:PX4:H27	4:A:430:PX4:H60	0.44	1.89	14	1
4:A:338:PX4:H55	4:A:348:PX4:H53	0.44	1.90	14	1
4:A:342:PX4:H29	4:A:351:PX4:H30	0.44	1.89	3	1
4:A:320:PX4:H54	4:A:359:PX4:H30	0.44	1.90	13	1
1:A:207:SER:O	4:A:321:PX4:H6	0.44	2.13	10	1
4:A:315:PX4:H5	4:A:364:PX4:O8	0.44	2.11	7	1
4:A:355:PX4:H38	4:A:356:PX4:H44	0.44	1.88	7	1
4:A:390:PX4:H30	4:A:398:PX4:H19	0.44	1.89	8	1
4:A:389:PX4:H30	4:A:396:PX4:C31	0.44	2.42	8	1
4:A:391:PX4:H25	4:A:393:PX4:H64	0.44	1.89	1	1
4:A:310:PX4:O6	4:A:365:PX4:H4	0.44	2.12	1	1
4:A:321:PX4:H37	4:A:354:PX4:H59	0.44	1.90	9	1
4:A:400:PX4:C24	4:A:409:PX4:H23	0.44	2.42	2	1
4:A:346:PX4:H39	4:A:354:PX4:H31	0.44	1.89	5	1
4:A:393:PX4:H14	4:A:394:PX4:C9	0.44	2.43	8	1
4:A:331:PX4:H44	4:A:340:PX4:H71	0.44	1.89	3	1
4:A:391:PX4:H58	4:A:401:PX4:H36	0.44	1.89	13	1
4:A:338:PX4:H64	4:A:411:PX4:H36	0.44	1.89	4	1
4:A:315:PX4:H20	4:A:320:PX4:H28	0.44	1.89	4	1
4:A:333:PX4:H61	4:A:368:PX4:H72	0.44	1.90	4	1
4:A:393:PX4:H41	4:A:394:PX4:H40	0.44	1.89	10	1
4:A:400:PX4:H38	4:A:401:PX4:H38	0.44	1.87	7	1
4:A:322:PX4:H34	4:A:361:PX4:H22	0.44	1.88	6	1
4:A:344:PX4:H37	4:A:347:PX4:H45	0.44	1.90	8	1
4:A:403:PX4:H9	4:A:427:PX4:O8	0.44	2.13	8	1
4:A:377:PX4:H16	4:A:418:PX4:C3	0.44	2.42	8	1
4:A:402:PX4:H36	4:A:403:PX4:H35	0.44	1.89	1	1
4:A:312:PX4:H25	4:A:363:PX4:H32	0.44	1.90	9	1
4:A:310:PX4:H23	4:A:358:PX4:H49	0.44	1.89	14	1
4:A:313:PX4:H57	4:A:327:PX4:H21	0.44	1.87	14	1
4:A:406:PX4:H35	4:A:414:PX4:H32	0.44	1.90	3	1
4:A:393:PX4:O6	4:A:394:PX4:H15	0.44	2.13	2	1
4:A:318:PX4:H24	4:A:320:PX4:H46	0.44	1.90	2	1
4:A:358:PX4:H22	4:A:363:PX4:H53	0.44	1.89	13	1
4:A:338:PX4:H17	4:A:348:PX4:O6	0.44	2.13	13	1
4:A:392:PX4:H35	4:A:399:PX4:H61	0.44	1.89	4	1
4:A:314:PX4:H69	4:A:364:PX4:H45	0.44	1.89	10	1
4:A:367:PX4:H46	4:A:428:PX4:H47	0.44	1.90	7	1
4:A:326:PX4:H57	4:A:334:PX4:H34	0.44	1.90	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:323:PX4:H16	4:A:333:PX4:H51	0.44	1.90	1	1
4:A:352:PX4:H32	4:A:358:PX4:H62	0.44	1.90	14	1
4:A:370:PX4:H34	4:A:403:PX4:H67	0.44	1.90	14	1
4:A:382:PX4:H52	4:A:428:PX4:H28	0.44	1.88	3	1
4:A:413:PX4:H69	4:A:428:PX4:H70	0.44	1.88	4	1
4:A:308:PX4:H44	4:A:311:PX4:H70	0.43	1.90	12	1
4:A:417:PX4:H28	4:A:426:PX4:H32	0.43	1.90	12	1
4:A:330:PX4:H52	4:A:338:PX4:H24	0.43	1.90	12	1
4:A:318:PX4:H35	4:A:327:PX4:H65	0.43	1.89	12	1
4:A:340:PX4:H62	4:A:341:PX4:H66	0.43	1.90	1	1
4:A:374:PX4:H32	4:A:427:PX4:H23	0.43	1.90	14	1
4:A:351:PX4:O7	4:A:352:PX4:H23	0.43	2.13	2	1
4:A:416:PX4:O1	4:A:422:PX4:H10	0.43	2.13	2	1
4:A:312:PX4:H69	4:A:359:PX4:H37	0.43	1.89	13	1
4:A:376:PX4:H66	4:A:385:PX4:H30	0.43	1.90	13	1
4:A:321:PX4:H67	4:A:361:PX4:H24	0.43	1.90	13	1
4:A:351:PX4:H8	4:A:352:PX4:O1	0.43	2.13	4	1
4:A:310:PX4:H43	4:A:365:PX4:H37	0.43	1.90	7	1
4:A:312:PX4:H44	4:A:365:PX4:H68	0.43	1.89	5	1
4:A:393:PX4:H45	4:A:401:PX4:H45	0.43	1.90	6	1
4:A:416:PX4:O8	4:A:418:PX4:H40	0.43	2.13	8	1
4:A:328:PX4:H25	4:A:328:PX4:H20	0.43	1.38	8	1
4:A:346:PX4:H46	4:A:362:PX4:H46	0.43	1.90	12	1
4:A:361:PX4:H40	4:A:423:PX4:H66	0.43	1.90	3	1
4:A:330:PX4:H63	4:A:338:PX4:H42	0.43	1.88	2	1
4:A:311:PX4:H5	4:A:320:PX4:O4	0.43	2.13	13	1
4:A:386:PX4:H38	4:A:394:PX4:H67	0.43	1.89	10	1
4:A:430:PX4:H38	4:A:430:PX4:H44	0.43	1.51	11	1
4:A:347:PX4:O4	4:A:348:PX4:H6	0.43	2.13	5	1
4:A:326:PX4:H37	4:A:350:PX4:H32	0.43	1.89	1	1
4:A:418:PX4:O1	4:A:425:PX4:H5	0.43	2.13	3	1
1:A:244:ASP:OD2	4:A:349:PX4:H3	0.43	2.14	2	1
4:A:378:PX4:H29	4:A:378:PX4:H23	0.43	1.63	2	1
4:A:395:PX4:H43	4:A:405:PX4:H40	0.43	1.89	13	1
4:A:307:PX4:H61	4:A:362:PX4:H27	0.43	1.91	10	1
4:A:378:PX4:O1	4:A:417:PX4:H17	0.43	2.12	10	1
4:A:341:PX4:H58	4:A:390:PX4:H72	0.43	1.89	7	1
4:A:314:PX4:H31	4:A:356:PX4:H28	0.43	1.90	11	1
4:A:418:PX4:H36	4:A:418:PX4:H41	0.43	1.56	5	1
4:A:320:PX4:H32	4:A:359:PX4:H63	0.43	1.90	8	1
4:A:315:PX4:H10	4:A:316:PX4:O6	0.43	2.13	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:334:PX4:H69	4:A:352:PX4:H37	0.43	1.89	2	1
4:A:389:PX4:H33	4:A:397:PX4:H21	0.43	1.90	2	1
4:A:306:PX4:H51	4:A:306:PX4:H56	0.43	1.58	7	1
4:A:363:PX4:H30	4:A:363:PX4:H35	0.43	1.61	6	1
4:A:331:PX4:H51	4:A:347:PX4:H22	0.43	1.91	8	1
4:A:387:PX4:H5	4:A:411:PX4:O3	0.43	2.13	12	1
4:A:410:PX4:O2	4:A:416:PX4:H10	0.43	2.14	9	1
4:A:314:PX4:H71	4:A:409:PX4:H31	0.43	1.90	13	1
4:A:352:PX4:O8	4:A:365:PX4:H3	0.43	2.13	10	1
4:A:338:PX4:H70	4:A:395:PX4:H38	0.43	1.90	10	1
4:A:407:PX4:O6	4:A:414:PX4:H49	0.43	2.13	10	1
1:A:178:GLY:HA3	4:A:354:PX4:H1	0.43	1.89	7	1
4:A:376:PX4:H19	4:A:383:PX4:H19	0.43	1.90	7	1
4:A:342:PX4:C12	4:A:352:PX4:H47	0.43	2.31	11	1
4:A:423:PX4:H55	4:A:425:PX4:H27	0.43	1.90	11	1
4:A:410:PX4:H51	4:A:426:PX4:H33	0.43	1.90	11	1
4:A:374:PX4:H58	4:A:382:PX4:H50	0.43	1.91	11	1
4:A:333:PX4:H53	4:A:341:PX4:H57	0.43	1.89	5	1
4:A:374:PX4:H8	4:A:427:PX4:H20	0.43	1.91	8	1
4:A:316:PX4:H47	4:A:320:PX4:H23	0.43	1.90	12	1
4:A:341:PX4:H72	4:A:397:PX4:H35	0.43	1.89	1	1
4:A:369:PX4:H29	4:A:378:PX4:H51	0.43	1.89	1	1
4:A:393:PX4:H30	4:A:400:PX4:H31	0.43	1.91	13	1
4:A:314:PX4:H37	4:A:362:PX4:H16	0.43	1.90	4	1
4:A:353:PX4:H35	4:A:366:PX4:H22	0.43	1.91	10	1
4:A:395:PX4:O1	4:A:396:PX4:H17	0.43	2.14	7	1
4:A:334:PX4:H51	4:A:334:PX4:H56	0.43	1.42	11	1
4:A:356:PX4:H62	4:A:397:PX4:H71	0.43	1.90	11	1
4:A:349:PX4:H65	4:A:406:PX4:H68	0.43	1.88	5	1
4:A:412:PX4:H58	4:A:427:PX4:H30	0.43	1.90	5	1
4:A:325:PX4:H49	4:A:341:PX4:H19	0.43	1.89	6	1
4:A:345:PX4:H19	4:A:346:PX4:H22	0.43	1.90	6	1
4:A:387:PX4:H56	4:A:387:PX4:H50	0.43	1.43	6	1
4:A:391:PX4:H26	4:A:392:PX4:H46	0.43	1.89	6	1
4:A:333:PX4:H14	4:A:340:PX4:O2	0.43	2.14	9	1
4:A:398:PX4:H21	4:A:407:PX4:H46	0.43	1.91	14	1
4:A:333:PX4:H30	4:A:339:PX4:H28	0.43	1.90	14	1
4:A:331:PX4:H17	4:A:340:PX4:H5	0.43	1.89	3	1
4:A:346:PX4:O6	4:A:362:PX4:H15	0.43	2.14	3	1
4:A:309:PX4:H28	4:A:309:PX4:H62	0.43	1.89	3	1
4:A:412:PX4:H36	4:A:419:PX4:H28	0.43	1.90	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:330:PX4:H31	4:A:348:PX4:H30	0.43	1.89	13	1
4:A:384:PX4:O1	4:A:385:PX4:H10	0.43	2.13	4	1
4:A:326:PX4:H61	4:A:334:PX4:H35	0.43	1.89	10	1
4:A:345:PX4:H71	4:A:403:PX4:H36	0.43	1.91	10	1
4:A:391:PX4:H23	4:A:392:PX4:H14	0.43	1.89	10	1
4:A:314:PX4:H33	4:A:362:PX4:H16	0.43	1.89	7	1
4:A:403:PX4:H3	4:A:427:PX4:H49	0.43	1.90	7	1
4:A:314:PX4:H44	4:A:355:PX4:H46	0.43	1.90	11	1
1:A:116:TYR:CD1	1:A:138:PHE:CE2	0.43	3.06	8	1
4:A:326:PX4:H47	4:A:334:PX4:H60	0.43	1.90	1	1
4:A:373:PX4:H28	4:A:381:PX4:H57	0.43	1.91	1	1
4:A:395:PX4:H9	4:A:411:PX4:O2	0.43	2.14	14	1
4:A:308:PX4:H14	4:A:311:PX4:O8	0.43	2.14	3	1
4:A:350:PX4:H61	4:A:363:PX4:H23	0.43	1.89	3	1
4:A:381:PX4:H16	4:A:388:PX4:H12	0.43	1.90	2	1
4:A:391:PX4:H37	4:A:393:PX4:H72	0.43	1.89	13	1
4:A:339:PX4:H68	4:A:339:PX4:H62	0.43	1.44	13	1
4:A:330:PX4:H5	4:A:344:PX4:H16	0.43	1.91	4	1
4:A:335:PX4:H42	4:A:343:PX4:H64	0.43	1.89	10	1
4:A:403:PX4:H32	4:A:404:PX4:H21	0.43	1.91	7	1
4:A:371:PX4:H46	4:A:371:PX4:H16	0.43	1.75	3	2
4:A:354:PX4:H65	4:A:360:PX4:H24	0.43	1.89	5	1
4:A:386:PX4:H17	4:A:394:PX4:O8	0.43	2.13	6	1
4:A:327:PX4:H10	4:A:327:PX4:O3	0.43	2.14	6	1
4:A:376:PX4:H36	4:A:376:PX4:H42	0.43	1.68	6	1
4:A:337:PX4:H45	4:A:338:PX4:H52	0.43	1.91	8	1
4:A:412:PX4:H51	4:A:419:PX4:H16	0.43	1.91	12	1
4:A:325:PX4:H28	4:A:407:PX4:H41	0.43	1.90	1	1
4:A:325:PX4:H32	4:A:332:PX4:H28	0.43	1.90	9	1
4:A:378:PX4:H19	4:A:426:PX4:H28	0.43	1.90	3	1
4:A:379:PX4:H65	4:A:379:PX4:H71	0.43	1.55	2	1
4:A:404:PX4:H71	4:A:404:PX4:H19	0.43	1.89	13	1
4:A:367:PX4:H20	4:A:424:PX4:H16	0.43	1.91	10	1
4:A:328:PX4:H56	4:A:354:PX4:H72	0.43	1.90	7	1
4:A:353:PX4:H58	4:A:360:PX4:H61	0.43	1.91	11	1
4:A:393:PX4:H17	4:A:401:PX4:H22	0.43	1.91	11	1
4:A:372:PX4:H54	4:A:379:PX4:H53	0.43	1.90	5	1
1:A:207:SER:O	4:A:321:PX4:H9	0.43	2.13	6	1
4:A:377:PX4:H72	4:A:425:PX4:O2	0.43	2.13	8	1
4:A:314:PX4:H47	4:A:349:PX4:H19	0.43	1.91	8	1
4:A:403:PX4:H47	4:A:427:PX4:H47	0.43	1.90	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:314:PX4:H38	4:A:355:PX4:H57	0.43	1.91	3	1
4:A:314:PX4:H71	4:A:364:PX4:H39	0.43	1.91	2	1
4:A:320:PX4:H17	4:A:359:PX4:C29	0.42	2.43	7	1
4:A:335:PX4:H41	4:A:335:PX4:H36	0.42	1.61	7	1
4:A:316:PX4:O2	4:A:364:PX4:H12	0.42	2.13	12	1
4:A:419:PX4:H60	4:A:427:PX4:H25	0.42	1.91	1	1
4:A:348:PX4:H60	4:A:348:PX4:H67	0.42	1.52	9	1
4:A:418:PX4:H40	4:A:418:PX4:H33	0.42	1.61	3	1
4:A:395:PX4:H62	4:A:413:PX4:O8	0.42	2.14	2	1
4:A:388:PX4:H63	4:A:397:PX4:H63	0.42	1.89	4	1
4:A:378:PX4:H23	4:A:378:PX4:H30	0.42	1.54	4	1
4:A:331:PX4:H28	4:A:347:PX4:H51	0.42	1.91	11	1
4:A:412:PX4:H17	4:A:419:PX4:H20	0.42	1.89	5	1
4:A:315:PX4:H3	4:A:361:PX4:O1	0.42	2.14	6	1
4:A:342:PX4:H52	4:A:351:PX4:H27	0.42	1.91	8	1
4:A:308:PX4:H66	4:A:308:PX4:H61	0.42	1.59	12	1
4:A:308:PX4:H34	4:A:311:PX4:H65	0.42	1.89	12	1
4:A:330:PX4:C22	4:A:344:PX4:H45	0.42	2.40	12	1
4:A:376:PX4:H62	4:A:385:PX4:H30	0.42	1.90	12	1
4:A:398:PX4:H41	4:A:415:PX4:H20	0.42	1.90	1	1
4:A:349:PX4:H16	4:A:350:PX4:H30	0.42	1.90	9	1
4:A:344:PX4:H37	4:A:344:PX4:H45	0.42	1.62	3	1
4:A:317:PX4:H55	4:A:324:PX4:C10	0.42	2.42	2	1
4:A:392:PX4:O6	4:A:392:PX4:H10	0.42	2.13	13	1
4:A:354:PX4:H22	4:A:362:PX4:H21	0.42	1.90	13	1
4:A:314:PX4:H26	4:A:314:PX4:H19	0.42	1.66	10	1
4:A:429:PX4:H54	4:A:429:PX4:H27	0.42	1.91	7	1
4:A:361:PX4:C33	4:A:412:PX4:H40	0.42	2.44	11	1
4:A:423:PX4:H26	4:A:423:PX4:H57	0.42	1.91	11	1
4:A:310:PX4:H16	4:A:363:PX4:O6	0.42	2.14	5	1
4:A:314:PX4:O8	4:A:314:PX4:H15	0.42	2.13	5	1
4:A:378:PX4:H60	4:A:410:PX4:H70	0.42	1.90	8	1
4:A:369:PX4:H58	4:A:424:PX4:H50	0.42	1.91	1	1
4:A:351:PX4:H54	4:A:358:PX4:H22	0.42	1.90	9	1
4:A:333:PX4:H16	4:A:340:PX4:H15	0.42	1.90	9	1
4:A:310:PX4:H36	4:A:351:PX4:H65	0.42	1.91	14	1
4:A:332:PX4:H28	4:A:334:PX4:H53	0.42	1.90	14	1
4:A:317:PX4:H1	4:A:317:PX4:O6	0.42	2.14	13	1
4:A:380:PX4:O4	4:A:381:PX4:H15	0.42	2.14	4	1
4:A:358:PX4:H70	4:A:401:PX4:H37	0.42	1.91	10	1
4:A:356:PX4:H42	4:A:356:PX4:H35	0.42	1.71	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:382:PX4:H22	4:A:428:PX4:C16	0.42	2.42	5	1
4:A:416:PX4:H48	4:A:425:PX4:H48	0.42	1.91	5	1
4:A:357:PX4:H61	4:A:357:PX4:H66	0.42	1.65	5	1
4:A:332:PX4:H66	4:A:349:PX4:H67	0.42	1.91	8	1
4:A:346:PX4:H25	4:A:354:PX4:H31	0.42	1.90	12	1
4:A:361:PX4:H29	4:A:361:PX4:H24	0.42	1.61	9	1
4:A:391:PX4:H67	4:A:401:PX4:H33	0.42	1.91	9	1
4:A:320:PX4:H21	4:A:359:PX4:H60	0.42	1.91	9	1
4:A:412:PX4:H20	4:A:428:PX4:H49	0.42	1.90	14	1
4:A:381:PX4:H61	4:A:381:PX4:H40	0.42	1.91	3	1
4:A:316:PX4:H71	4:A:333:PX4:H67	0.42	1.92	2	1
4:A:355:PX4:H55	4:A:355:PX4:H49	0.42	1.69	4	1
4:A:315:PX4:O3	4:A:361:PX4:H4	0.42	2.15	10	1
4:A:387:PX4:H17	4:A:411:PX4:H61	0.42	1.90	10	1
4:A:369:PX4:H48	4:A:377:PX4:H67	0.42	1.91	10	1
4:A:312:PX4:H59	4:A:359:PX4:H30	0.42	1.91	7	1
4:A:325:PX4:H64	4:A:341:PX4:H35	0.42	1.90	7	1
4:A:334:PX4:H22	4:A:334:PX4:H27	0.42	1.65	11	1
4:A:308:PX4:H16	4:A:311:PX4:C10	0.42	2.44	5	1
4:A:356:PX4:H16	4:A:356:PX4:O3	0.42	2.15	5	1
4:A:424:PX4:H17	4:A:429:PX4:H21	0.42	1.92	6	1
4:A:387:PX4:H17	4:A:411:PX4:H57	0.42	1.91	12	1
4:A:307:PX4:H16	4:A:307:PX4:H46	0.42	1.64	4	2
4:A:415:PX4:H11	4:A:422:PX4:H16	0.42	1.91	1	1
4:A:418:PX4:H34	4:A:425:PX4:H56	0.42	1.91	1	1
4:A:412:PX4:H24	4:A:430:PX4:H58	0.42	1.92	9	1
4:A:330:PX4:H49	4:A:343:PX4:H46	0.42	1.91	14	1
4:A:381:PX4:H54	4:A:388:PX4:H57	0.42	1.90	3	1
4:A:356:PX4:H42	4:A:405:PX4:H60	0.42	1.91	3	1
4:A:335:PX4:H6	4:A:344:PX4:O6	0.42	2.13	2	1
4:A:395:PX4:H27	4:A:405:PX4:H28	0.42	1.91	13	1
4:A:406:PX4:O1	4:A:414:PX4:H3	0.42	2.15	4	1
4:A:354:PX4:H50	4:A:360:PX4:H18	0.42	1.90	11	1
4:A:404:PX4:H54	4:A:405:PX4:H39	0.42	1.91	5	1
4:A:367:PX4:O6	4:A:423:PX4:H11	0.42	2.15	6	1
4:A:326:PX4:H44	4:A:416:PX4:H41	0.42	1.91	8	1
4:A:350:PX4:O2	4:A:363:PX4:H7	0.42	2.14	8	1
4:A:337:PX4:H20	4:A:346:PX4:H63	0.42	1.92	12	1
4:A:384:PX4:H3	4:A:385:PX4:H18	0.42	1.91	14	1
4:A:406:PX4:H33	4:A:414:PX4:H34	0.42	1.91	2	1
4:A:317:PX4:H66	4:A:342:PX4:H66	0.42	1.91	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:372:PX4:H29	4:A:420:PX4:H55	0.42	1.92	4	1
4:A:346:PX4:O4	4:A:362:PX4:H11	0.42	2.15	10	1
4:A:382:PX4:H22	4:A:428:PX4:H34	0.42	1.92	10	1
4:A:391:PX4:H71	4:A:415:PX4:H45	0.42	1.92	10	1
4:A:406:PX4:H17	4:A:414:PX4:H22	0.42	1.92	10	1
4:A:381:PX4:H53	4:A:397:PX4:H46	0.42	1.90	10	1
4:A:338:PX4:H68	4:A:348:PX4:H58	0.42	1.90	11	1
4:A:349:PX4:O6	4:A:349:PX4:H7	0.42	2.15	11	1
4:A:334:PX4:H29	4:A:414:PX4:H69	0.42	1.91	11	1
4:A:326:PX4:O6	4:A:350:PX4:H5	0.42	2.14	6	1
4:A:342:PX4:H37	4:A:352:PX4:H33	0.42	1.90	9	1
4:A:332:PX4:H25	4:A:334:PX4:H49	0.42	1.90	14	1
4:A:331:PX4:H62	4:A:397:PX4:H59	0.42	1.92	10	1
4:A:384:PX4:H30	4:A:384:PX4:H57	0.42	1.91	7	1
4:A:333:PX4:O8	4:A:340:PX4:H15	0.42	2.15	11	1
4:A:307:PX4:H58	4:A:314:PX4:H17	0.42	1.92	5	1
4:A:337:PX4:O6	4:A:345:PX4:H49	0.42	2.15	5	1
4:A:347:PX4:H56	4:A:356:PX4:H56	0.42	1.92	5	1
4:A:416:PX4:H17	4:A:425:PX4:O8	0.42	2.14	5	1
4:A:344:PX4:H27	4:A:348:PX4:H21	0.42	1.92	6	1
4:A:398:PX4:H40	4:A:414:PX4:C16	0.42	2.45	6	1
4:A:370:PX4:H36	4:A:402:PX4:H40	0.42	1.92	8	1
4:A:375:PX4:H19	4:A:429:PX4:H45	0.42	1.90	3	1
4:A:371:PX4:H36	4:A:379:PX4:H60	0.42	1.91	3	1
4:A:321:PX4:H47	4:A:354:PX4:H20	0.42	1.91	2	1
4:A:338:PX4:H65	4:A:338:PX4:H58	0.42	1.68	13	1
4:A:402:PX4:H33	4:A:402:PX4:H28	0.42	1.57	4	1
4:A:391:PX4:H66	4:A:408:PX4:H57	0.42	1.92	4	1
4:A:395:PX4:H70	4:A:421:PX4:H58	0.42	1.91	10	1
4:A:388:PX4:H28	4:A:411:PX4:H16	0.42	1.91	7	1
4:A:324:PX4:H23	4:A:342:PX4:H55	0.42	1.91	7	1
4:A:408:PX4:H50	4:A:409:PX4:H19	0.42	1.92	11	1
4:A:403:PX4:H52	4:A:403:PX4:H47	0.42	1.50	11	1
4:A:337:PX4:H43	4:A:380:PX4:H39	0.42	1.91	6	1
4:A:308:PX4:H7	4:A:308:PX4:O3	0.42	2.15	12	1
4:A:335:PX4:H17	4:A:343:PX4:O1	0.42	2.15	12	1
4:A:318:PX4:H56	4:A:328:PX4:H33	0.42	1.90	12	1
4:A:363:PX4:H47	4:A:364:PX4:H33	0.42	1.91	9	1
4:A:354:PX4:H30	4:A:362:PX4:H17	0.42	1.90	3	1
4:A:372:PX4:H61	4:A:379:PX4:H59	0.42	1.91	3	1
4:A:367:PX4:O1	4:A:423:PX4:H3	0.42	2.15	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:317:PX4:H41	4:A:385:PX4:H65	0.42	1.92	13	1
4:A:391:PX4:H17	4:A:408:PX4:O5	0.42	2.15	13	1
4:A:332:PX4:H54	4:A:407:PX4:H70	0.42	1.90	13	1
4:A:325:PX4:H62	4:A:342:PX4:H70	0.42	1.90	13	1
4:A:353:PX4:H35	4:A:353:PX4:H41	0.42	1.58	4	1
4:A:375:PX4:H3	4:A:429:PX4:H17	0.42	1.91	4	1
4:A:382:PX4:H14	4:A:382:PX4:O6	0.42	2.14	4	1
4:A:322:PX4:C27	4:A:336:PX4:H32	0.42	2.45	10	1
4:A:354:PX4:H32	4:A:354:PX4:H25	0.42	1.63	10	1
4:A:373:PX4:H22	4:A:397:PX4:O3	0.42	2.14	7	1
4:A:333:PX4:H23	4:A:340:PX4:H24	0.42	1.91	5	1
4:A:364:PX4:H69	4:A:364:PX4:H62	0.42	1.69	5	1
4:A:383:PX4:H13	4:A:399:PX4:O1	0.42	2.15	6	1
4:A:395:PX4:H40	4:A:397:PX4:H65	0.42	1.92	6	1
4:A:350:PX4:H36	4:A:415:PX4:H71	0.42	1.92	6	1
4:A:334:PX4:C35	4:A:352:PX4:H32	0.42	2.45	6	1
4:A:398:PX4:H48	4:A:405:PX4:H49	0.42	1.92	6	1
4:A:388:PX4:H6	4:A:396:PX4:O8	0.42	2.15	12	1
4:A:413:PX4:H17	4:A:430:PX4:C8	0.42	2.45	12	1
4:A:424:PX4:H47	4:A:429:PX4:H19	0.42	1.91	1	1
4:A:308:PX4:H69	4:A:426:PX4:H70	0.42	1.91	14	1
4:A:316:PX4:H34	4:A:320:PX4:C19	0.42	2.43	3	1
4:A:306:PX4:H40	4:A:329:PX4:H40	0.42	1.91	3	1
4:A:372:PX4:H29	4:A:420:PX4:H26	0.42	1.91	2	1
4:A:424:PX4:H48	4:A:424:PX4:H55	0.42	1.64	13	1
4:A:376:PX4:H26	4:A:399:PX4:C25	0.42	2.45	4	1
4:A:363:PX4:H62	4:A:363:PX4:H57	0.41	1.56	10	1
4:A:389:PX4:H68	4:A:390:PX4:H38	0.41	1.92	10	1
4:A:340:PX4:H35	4:A:397:PX4:H60	0.41	1.91	10	1
4:A:369:PX4:C19	4:A:416:PX4:H63	0.41	2.45	11	1
4:A:410:PX4:H57	4:A:417:PX4:H69	0.41	1.91	11	1
4:A:318:PX4:H39	4:A:359:PX4:H36	0.41	1.92	5	1
4:A:308:PX4:H41	4:A:410:PX4:H45	0.41	1.91	12	1
4:A:423:PX4:H40	4:A:430:PX4:H36	0.41	1.92	12	1
4:A:371:PX4:O8	4:A:377:PX4:H3	0.41	2.15	1	1
4:A:378:PX4:H28	4:A:420:PX4:H57	0.41	1.92	1	1
4:A:393:PX4:H10	4:A:393:PX4:O6	0.41	2.14	9	1
4:A:403:PX4:H48	4:A:419:PX4:H9	0.41	1.91	14	1
4:A:346:PX4:H24	4:A:360:PX4:H55	0.41	1.92	14	1
4:A:322:PX4:H37	4:A:361:PX4:H25	0.41	1.91	13	1
4:A:398:PX4:H51	4:A:405:PX4:C23	0.41	2.45	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:405:PX4:H58	4:A:414:PX4:H26	0.41	1.91	4	1
4:A:378:PX4:H47	4:A:410:PX4:H19	0.41	1.93	7	1
4:A:308:PX4:H63	4:A:308:PX4:H68	0.41	1.64	11	1
4:A:337:PX4:H5	4:A:337:PX4:H25	0.41	1.92	11	1
4:A:335:PX4:H39	4:A:344:PX4:H39	0.41	1.92	11	1
4:A:403:PX4:H49	4:A:404:PX4:H28	0.41	1.90	5	1
4:A:347:PX4:H20	4:A:348:PX4:O3	0.41	2.14	6	1
4:A:421:PX4:H35	4:A:430:PX4:H48	0.41	1.92	6	1
4:A:416:PX4:H22	4:A:425:PX4:H50	0.41	1.92	6	1
4:A:372:PX4:H39	4:A:420:PX4:H34	0.41	1.92	12	1
4:A:309:PX4:H23	4:A:320:PX4:H49	0.41	1.92	1	1
4:A:410:PX4:H14	4:A:418:PX4:H40	0.41	1.92	1	1
4:A:352:PX4:H31	4:A:352:PX4:H38	0.41	1.60	14	1
4:A:398:PX4:H63	4:A:398:PX4:H68	0.41	1.73	14	1
4:A:349:PX4:H27	4:A:356:PX4:H30	0.41	1.92	3	1
4:A:308:PX4:H67	4:A:359:PX4:H70	0.41	1.91	13	1
4:A:308:PX4:H32	4:A:364:PX4:H52	0.41	1.91	4	1
4:A:345:PX4:H68	4:A:345:PX4:H45	0.41	1.91	4	1
4:A:373:PX4:H66	4:A:381:PX4:H44	0.41	1.92	10	1
4:A:314:PX4:H34	4:A:356:PX4:H41	0.41	1.91	8	1
4:A:421:PX4:H34	4:A:423:PX4:H23	0.41	1.93	12	1
4:A:383:PX4:O6	4:A:392:PX4:H3	0.41	2.14	1	1
4:A:313:PX4:H62	4:A:329:PX4:H32	0.41	1.90	1	1
4:A:376:PX4:H65	4:A:392:PX4:H35	0.41	1.92	14	1
4:A:322:PX4:H17	4:A:361:PX4:H56	0.41	1.92	13	1
4:A:341:PX4:H29	4:A:341:PX4:H24	0.41	1.63	10	1
4:A:348:PX4:H37	4:A:357:PX4:H36	0.41	1.92	7	1
4:A:421:PX4:H41	4:A:423:PX4:H35	0.41	1.91	7	1
4:A:393:PX4:H16	4:A:401:PX4:H18	0.41	1.91	5	1
4:A:389:PX4:H60	4:A:398:PX4:H17	0.41	1.93	5	1
4:A:346:PX4:H27	4:A:353:PX4:H58	0.41	1.93	6	1
4:A:337:PX4:H24	4:A:346:PX4:H69	0.41	1.91	6	1
4:A:347:PX4:H68	4:A:390:PX4:H39	0.41	1.92	6	1
4:A:352:PX4:H13	4:A:352:PX4:H2	0.41	1.76	6	1
4:A:403:PX4:H26	4:A:404:PX4:H21	0.41	1.92	8	1
4:A:316:PX4:O2	4:A:364:PX4:H11	0.41	2.15	8	1
4:A:380:PX4:H59	4:A:380:PX4:H25	0.41	1.91	8	1
4:A:368:PX4:H46	4:A:429:PX4:H20	0.41	1.90	1	1
4:A:366:PX4:H60	4:A:366:PX4:H55	0.41	1.70	9	1
4:A:372:PX4:O2	4:A:420:PX4:H9	0.41	2.15	9	1
4:A:420:PX4:H57	4:A:420:PX4:H50	0.41	1.68	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:407:PX4:H29	4:A:408:PX4:H41	0.41	1.90	14	1
4:A:367:PX4:H63	4:A:367:PX4:H68	0.41	1.51	14	1
4:A:331:PX4:H8	4:A:340:PX4:O1	0.41	2.14	3	1
4:A:378:PX4:H35	4:A:378:PX4:H42	0.41	1.61	3	1
4:A:367:PX4:H20	4:A:424:PX4:H22	0.41	1.93	2	1
4:A:406:PX4:H34	4:A:406:PX4:H39	0.41	1.55	7	1
1:A:244:ASP:OD1	4:A:349:PX4:H3	0.41	2.15	5	1
4:A:325:PX4:H27	4:A:334:PX4:H21	0.41	1.93	5	1
4:A:347:PX4:O1	4:A:348:PX4:H3	0.41	2.15	8	1
4:A:362:PX4:H21	4:A:362:PX4:H28	0.41	1.65	8	1
1:A:214:LEU:HD22	1:A:243:VAL:CG2	0.41	2.45	8	1
4:A:340:PX4:H43	4:A:389:PX4:H27	0.41	1.93	12	1
4:A:423:PX4:H36	4:A:423:PX4:H42	0.41	1.54	12	1
4:A:337:PX4:H61	4:A:353:PX4:H48	0.41	1.93	9	1
4:A:392:PX4:H56	4:A:392:PX4:H63	0.41	1.65	14	1
4:A:332:PX4:H38	4:A:407:PX4:H61	0.41	1.93	14	1
4:A:306:PX4:H37	4:A:367:PX4:H72	0.41	1.92	14	1
4:A:314:PX4:H35	4:A:314:PX4:H41	0.41	1.64	3	1
4:A:359:PX4:H47	4:A:359:PX4:H53	0.41	1.64	3	1
4:A:413:PX4:H9	4:A:430:PX4:O1	0.41	2.16	2	1
4:A:405:PX4:H48	4:A:406:PX4:H52	0.41	1.92	4	1
4:A:369:PX4:O1	4:A:425:PX4:H1	0.41	2.15	4	1
4:A:355:PX4:H30	4:A:356:PX4:H51	0.41	1.91	10	1
4:A:350:PX4:H60	4:A:400:PX4:H44	0.41	1.93	11	1
4:A:385:PX4:H67	4:A:392:PX4:H26	0.41	1.90	5	1
1:A:138:PHE:CD1	1:A:149:PHE:CD1	0.41	3.08	6	2
4:A:383:PX4:H65	4:A:407:PX4:H27	0.41	1.92	6	1
4:A:420:PX4:H67	4:A:426:PX4:H38	0.41	1.92	8	1
4:A:367:PX4:H60	4:A:429:PX4:H41	0.41	1.91	8	1
4:A:418:PX4:H72	4:A:418:PX4:H64	0.41	1.59	12	1
4:A:321:PX4:H61	4:A:361:PX4:H57	0.41	1.93	1	1
4:A:360:PX4:H30	4:A:366:PX4:H61	0.41	1.91	9	1
4:A:398:PX4:H42	4:A:408:PX4:H26	0.41	1.92	9	1
4:A:337:PX4:H65	4:A:345:PX4:H71	0.41	1.92	14	1
4:A:338:PX4:H68	4:A:338:PX4:H63	0.41	1.58	14	1
4:A:344:PX4:H49	4:A:344:PX4:H54	0.41	1.71	14	1
4:A:345:PX4:O4	4:A:346:PX4:H10	0.41	2.15	3	1
4:A:408:PX4:H32	4:A:415:PX4:H42	0.41	1.92	2	1
4:A:308:PX4:H14	4:A:311:PX4:H16	0.41	1.92	2	1
4:A:388:PX4:H3	4:A:395:PX4:O1	0.41	2.15	13	1
4:A:308:PX4:H65	4:A:308:PX4:H72	0.41	1.59	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:369:PX4:O1	4:A:425:PX4:H13	0.41	2.16	4	1
4:A:380:PX4:H59	4:A:388:PX4:H40	0.41	1.91	7	1
4:A:319:PX4:H60	4:A:324:PX4:H59	0.41	1.92	7	1
4:A:338:PX4:H45	4:A:338:PX4:H38	0.41	1.58	11	1
4:A:416:PX4:H40	4:A:421:PX4:H70	0.41	1.92	5	1
4:A:395:PX4:H56	4:A:402:PX4:H50	0.41	1.91	6	1
4:A:377:PX4:H44	4:A:377:PX4:H38	0.41	1.75	6	1
4:A:381:PX4:H42	4:A:381:PX4:H60	0.41	1.92	8	1
4:A:308:PX4:H23	4:A:311:PX4:H54	0.41	1.92	1	1
4:A:392:PX4:H65	4:A:392:PX4:H72	0.41	1.73	14	1
4:A:409:PX4:H37	4:A:410:PX4:H53	0.41	1.93	3	1
4:A:311:PX4:H17	4:A:359:PX4:H50	0.41	1.93	2	1
4:A:382:PX4:H29	4:A:382:PX4:H36	0.41	1.73	2	1
4:A:323:PX4:H19	4:A:333:PX4:H47	0.41	1.92	4	1
4:A:363:PX4:H38	4:A:365:PX4:H30	0.41	1.92	4	1
4:A:391:PX4:H48	4:A:391:PX4:H54	0.41	1.60	4	1
4:A:407:PX4:H17	4:A:414:PX4:O8	0.41	2.16	10	1
4:A:332:PX4:H14	4:A:356:PX4:H9	0.41	1.92	7	1
4:A:367:PX4:H42	4:A:423:PX4:H36	0.41	1.90	11	1
4:A:309:PX4:O8	4:A:316:PX4:H46	0.41	2.16	11	1
4:A:395:PX4:H54	4:A:395:PX4:H61	0.41	1.72	5	1
4:A:388:PX4:H34	4:A:388:PX4:H39	0.41	1.63	6	1
4:A:421:PX4:H52	4:A:421:PX4:H59	0.41	1.65	6	1
4:A:352:PX4:H16	4:A:358:PX4:H47	0.41	1.93	8	1
4:A:328:PX4:H20	4:A:328:PX4:H25	0.41	1.67	14	1
4:A:415:PX4:H55	4:A:421:PX4:H56	0.41	1.93	2	1
4:A:400:PX4:H56	4:A:409:PX4:H34	0.41	1.93	13	1
4:A:378:PX4:H63	4:A:418:PX4:H62	0.41	1.93	13	1
4:A:349:PX4:H45	4:A:355:PX4:H45	0.41	1.93	13	1
4:A:398:PX4:H21	4:A:407:PX4:H22	0.41	1.93	13	1
4:A:428:PX4:H38	4:A:428:PX4:H44	0.41	1.78	4	1
4:A:307:PX4:H10	4:A:322:PX4:O8	0.41	2.16	4	1
4:A:366:PX4:H68	4:A:419:PX4:H38	0.41	1.93	10	1
4:A:404:PX4:H63	4:A:404:PX4:H68	0.41	1.65	7	1
4:A:326:PX4:H29	4:A:350:PX4:H51	0.41	1.92	5	1
4:A:415:PX4:H5	4:A:421:PX4:H14	0.41	1.92	5	1
4:A:316:PX4:H26	4:A:364:PX4:H47	0.41	1.92	5	1
4:A:345:PX4:H17	4:A:346:PX4:H6	0.41	1.93	5	1
4:A:375:PX4:H47	4:A:429:PX4:H40	0.41	1.92	6	1
4:A:423:PX4:H4	4:A:430:PX4:O8	0.41	2.16	8	1
4:A:372:PX4:H52	4:A:372:PX4:H47	0.41	1.71	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:383:PX4:H20	4:A:392:PX4:C14	0.41	2.46	12	1
4:A:335:PX4:H23	4:A:343:PX4:H53	0.41	1.91	12	1
4:A:390:PX4:H63	4:A:397:PX4:H40	0.41	1.92	12	1
4:A:330:PX4:H16	4:A:343:PX4:H2	0.41	1.93	1	1
4:A:345:PX4:H69	4:A:388:PX4:H35	0.41	1.92	1	1
4:A:306:PX4:H56	4:A:354:PX4:C13	0.41	2.46	1	1
4:A:348:PX4:H68	4:A:348:PX4:H63	0.41	1.63	1	1
4:A:315:PX4:H24	4:A:322:PX4:H36	0.41	1.92	9	1
4:A:416:PX4:H48	4:A:425:PX4:H53	0.41	1.92	9	1
4:A:363:PX4:H28	4:A:365:PX4:H21	0.41	1.92	9	1
4:A:391:PX4:H47	4:A:408:PX4:H16	0.41	1.93	9	1
4:A:429:PX4:H33	4:A:429:PX4:C27	0.41	2.46	9	1
4:A:424:PX4:H25	4:A:424:PX4:H32	0.41	1.37	14	1
4:A:331:PX4:O6	4:A:331:PX4:H7	0.41	2.16	14	1
4:A:375:PX4:H18	4:A:382:PX4:O6	0.41	2.16	3	1
4:A:312:PX4:H39	4:A:365:PX4:H37	0.41	1.93	3	1
4:A:363:PX4:H60	4:A:363:PX4:H55	0.41	1.65	3	1
4:A:358:PX4:H35	4:A:365:PX4:H31	0.41	1.91	3	1
4:A:376:PX4:H46	4:A:384:PX4:H3	0.41	1.93	2	1
4:A:314:PX4:H47	4:A:350:PX4:H37	0.41	1.91	2	1
4:A:375:PX4:H67	4:A:375:PX4:H60	0.41	1.66	2	1
4:A:337:PX4:H45	4:A:338:PX4:H56	0.41	1.93	2	1
4:A:404:PX4:H52	4:A:404:PX4:H59	0.41	1.53	2	1
4:A:307:PX4:H41	4:A:361:PX4:H42	0.41	1.92	13	1
4:A:338:PX4:H62	4:A:362:PX4:H62	0.41	1.93	13	1
4:A:325:PX4:H9	4:A:341:PX4:O6	0.41	2.15	13	1
4:A:314:PX4:H42	4:A:362:PX4:H21	0.41	1.91	4	1
4:A:306:PX4:O2	4:A:329:PX4:H12	0.41	2.15	4	1
4:A:349:PX4:H60	4:A:349:PX4:H66	0.41	1.58	10	1
4:A:388:PX4:H51	4:A:396:PX4:C25	0.41	2.45	10	1
4:A:354:PX4:H21	4:A:362:PX4:C5	0.41	2.46	7	1
4:A:332:PX4:O3	4:A:356:PX4:H4	0.41	2.16	7	1
4:A:330:PX4:H19	4:A:330:PX4:C3	0.41	2.46	7	1
4:A:353:PX4:H31	4:A:366:PX4:H25	0.41	1.93	11	1
4:A:341:PX4:H32	4:A:383:PX4:H70	0.41	1.93	6	1
4:A:309:PX4:H27	4:A:318:PX4:H28	0.41	1.93	8	1
4:A:311:PX4:H71	4:A:316:PX4:H38	0.41	1.93	12	1
4:A:369:PX4:H71	4:A:369:PX4:H65	0.41	1.47	12	1
4:A:424:PX4:H56	4:A:425:PX4:H31	0.41	1.93	9	1
4:A:388:PX4:H15	4:A:396:PX4:H18	0.41	1.92	9	1
4:A:382:PX4:H67	4:A:428:PX4:H20	0.41	1.93	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:326:PX4:H64	4:A:391:PX4:H43	0.41	1.92	14	1
4:A:319:PX4:H19	4:A:342:PX4:H50	0.41	1.92	14	1
4:A:345:PX4:H4	4:A:353:PX4:O4	0.41	2.16	14	1
4:A:405:PX4:H45	4:A:405:PX4:H37	0.41	1.61	14	1
4:A:326:PX4:H27	4:A:350:PX4:H21	0.41	1.92	3	1
4:A:325:PX4:H45	4:A:334:PX4:H40	0.41	1.93	4	1
4:A:389:PX4:H61	4:A:389:PX4:H66	0.40	1.60	10	1
4:A:366:PX4:H41	4:A:366:PX4:H36	0.40	1.64	7	1
4:A:384:PX4:H46	4:A:386:PX4:H49	0.40	1.93	11	1
4:A:358:PX4:H27	4:A:364:PX4:H42	0.40	1.92	6	1
4:A:416:PX4:H35	4:A:421:PX4:H66	0.40	1.92	8	1
4:A:380:PX4:H31	4:A:381:PX4:H60	0.40	1.92	12	1
4:A:427:PX4:H37	4:A:427:PX4:H32	0.40	1.63	12	1
4:A:326:PX4:H55	4:A:326:PX4:H60	0.40	1.78	12	1
4:A:387:PX4:H38	4:A:387:PX4:H31	0.40	1.72	1	1
4:A:403:PX4:O8	4:A:419:PX4:H8	0.40	2.15	1	1
4:A:313:PX4:H18	4:A:318:PX4:C24	0.40	2.36	9	1
4:A:404:PX4:H8	4:A:412:PX4:O6	0.40	2.17	14	1
4:A:313:PX4:H15	4:A:360:PX4:O6	0.40	2.16	14	1
4:A:316:PX4:O4	4:A:364:PX4:H5	0.40	2.16	2	1
4:A:378:PX4:H17	4:A:410:PX4:O6	0.40	2.15	13	1
4:A:384:PX4:H17	4:A:385:PX4:H20	0.40	1.93	13	1
4:A:322:PX4:H69	4:A:322:PX4:H62	0.40	1.62	13	1
4:A:314:PX4:H64	4:A:314:PX4:H59	0.40	1.39	4	1
4:A:350:PX4:H56	4:A:363:PX4:H52	0.40	1.92	4	1
4:A:334:PX4:H65	4:A:363:PX4:H69	0.40	1.93	4	1
4:A:371:PX4:H65	4:A:417:PX4:H65	0.40	1.92	4	1
4:A:308:PX4:H25	4:A:311:PX4:H23	0.40	1.93	10	1
4:A:308:PX4:H51	4:A:363:PX4:H19	0.40	1.92	10	1
4:A:330:PX4:H14	4:A:338:PX4:H19	0.40	1.91	7	1
4:A:428:PX4:H65	4:A:430:PX4:H48	0.40	1.93	11	1
4:A:368:PX4:H20	4:A:377:PX4:H57	0.40	1.92	11	1
4:A:323:PX4:H58	4:A:323:PX4:H65	0.40	1.68	5	1
4:A:377:PX4:H62	4:A:416:PX4:H55	0.40	1.92	6	1
4:A:334:PX4:H64	4:A:334:PX4:H59	0.40	1.36	8	1
4:A:327:PX4:H43	4:A:374:PX4:H66	0.40	1.93	12	1
4:A:352:PX4:H7	4:A:352:PX4:H15	0.40	1.93	14	1
4:A:419:PX4:H71	4:A:427:PX4:H64	0.40	1.93	3	1
4:A:308:PX4:H41	4:A:316:PX4:H39	0.40	1.92	3	1
4:A:315:PX4:H43	4:A:425:PX4:H32	0.40	1.92	2	1
4:A:391:PX4:H31	4:A:408:PX4:H23	0.40	1.91	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:332:PX4:H45	4:A:407:PX4:H53	0.40	1.93	13	1
4:A:389:PX4:H52	4:A:389:PX4:H59	0.40	1.59	13	1
4:A:319:PX4:O2	4:A:324:PX4:H4	0.40	2.16	7	1
4:A:348:PX4:H56	4:A:355:PX4:H72	0.40	1.93	11	1
1:A:109:TRP:CH2	1:A:158:ASP:HB3	0.40	2.51	11	1
4:A:372:PX4:H38	4:A:372:PX4:H32	0.40	1.63	5	1
4:A:401:PX4:H38	4:A:401:PX4:H44	0.40	1.72	6	1
4:A:317:PX4:O5	4:A:351:PX4:H23	0.40	2.17	8	1
4:A:405:PX4:H58	4:A:414:PX4:H30	0.40	1.93	8	1
4:A:321:PX4:H45	4:A:360:PX4:H69	0.40	1.93	1	1
4:A:417:PX4:H65	4:A:417:PX4:H58	0.40	1.62	14	1
4:A:383:PX4:H55	4:A:399:PX4:H17	0.40	1.92	13	1
4:A:404:PX4:H2	4:A:412:PX4:O1	0.40	2.16	13	1
4:A:323:PX4:H14	4:A:323:PX4:H9	0.40	1.92	4	1
4:A:412:PX4:H16	4:A:428:PX4:H16	0.40	1.93	10	1
4:A:375:PX4:H37	4:A:375:PX4:H32	0.40	1.68	10	1
4:A:307:PX4:C12	4:A:314:PX4:H16	0.40	2.47	11	1
4:A:362:PX4:H54	4:A:362:PX4:H60	0.40	1.39	11	1
4:A:381:PX4:H10	4:A:381:PX4:H14	0.40	1.93	11	1
4:A:345:PX4:H33	4:A:353:PX4:H61	0.40	1.94	5	1
4:A:416:PX4:H47	4:A:416:PX4:H52	0.40	1.75	5	1
4:A:410:PX4:O2	4:A:416:PX4:H4	0.40	2.17	8	1
4:A:321:PX4:H63	4:A:321:PX4:H68	0.40	1.68	12	1
4:A:402:PX4:H39	4:A:402:PX4:H34	0.40	1.45	12	1
4:A:388:PX4:H25	4:A:388:PX4:H32	0.40	1.65	9	1
4:A:394:PX4:H65	4:A:394:PX4:H71	0.40	1.66	14	1
4:A:326:PX4:H34	4:A:406:PX4:H36	0.40	1.93	3	1
4:A:410:PX4:H40	4:A:410:PX4:H61	0.40	1.92	2	1
4:A:378:PX4:H67	4:A:418:PX4:H66	0.40	1.93	13	1
4:A:378:PX4:H47	4:A:418:PX4:H46	0.40	1.92	13	1
4:A:336:PX4:H28	4:A:361:PX4:H63	0.40	1.93	13	1
4:A:395:PX4:H15	4:A:396:PX4:H15	0.40	1.93	13	1
4:A:380:PX4:H20	4:A:381:PX4:H6	0.40	1.93	13	1
4:A:353:PX4:H35	4:A:353:PX4:H30	0.40	1.62	7	1
4:A:319:PX4:H58	4:A:324:PX4:H30	0.40	1.94	11	1
4:A:332:PX4:H39	4:A:334:PX4:H57	0.40	1.92	11	1
4:A:316:PX4:H60	4:A:320:PX4:H36	0.40	1.93	5	1
4:A:344:PX4:H38	4:A:347:PX4:H38	0.40	1.93	5	1
4:A:429:PX4:H53	4:A:429:PX4:H29	0.40	1.93	5	1
4:A:319:PX4:H38	4:A:319:PX4:H44	0.40	1.70	6	1
4:A:385:PX4:O1	4:A:392:PX4:H8	0.40	2.17	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:364:PX4:H32	4:A:364:PX4:H25	0.40	1.68	1	1
4:A:380:PX4:H28	4:A:380:PX4:H33	0.40	1.75	1	1
4:A:374:PX4:H20	4:A:374:PX4:H25	0.40	1.49	14	1
4:A:355:PX4:C10	4:A:362:PX4:H51	0.40	2.47	14	1
4:A:374:PX4:H34	4:A:374:PX4:H27	0.40	1.72	3	1
4:A:345:PX4:H17	4:A:346:PX4:H10	0.40	1.91	2	1
4:A:398:PX4:H60	4:A:405:PX4:H29	0.40	1.94	13	1
4:A:320:PX4:H20	4:A:359:PX4:H58	0.40	1.94	4	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/164 (96%)	145±3 (92±2%)	12±3 (8±2%)	1±1 (1±0%)	34	78
All	All	2212/2296 (96%)	2030 (92%)	168 (8%)	14 (1%)	34	78

All 7 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	171	PHE	5
1	A	175	ASP	3
1	A	107	PRO	2
1	A	213	PHE	1
1	A	179	GLY	1
1	A	146	PRO	1
1	A	183	HIS	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/131 (98%)	123±2 (95±2%)	6±2 (5±2%)	35	79
All	All	1806/1834 (98%)	1716 (95%)	90 (5%)	35	79

All 25 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	244	ASP	14
1	A	101	ARG	14
1	A	199	GLU	9
1	A	222	HIS	8
1	A	249	ARG	7
1	A	214	LEU	6
1	A	175	ASP	5
1	A	243	VAL	4
1	A	142	SER	3
1	A	170	ASP	3
1	A	198	ASP	2
1	A	129	ASP	2
1	A	122	THR	1
1	A	200	ASP	1
1	A	139	GLN	1
1	A	115	THR	1
1	A	140	VAL	1
1	A	168	HIS	1
1	A	205	THR	1
1	A	156	MET	1
1	A	146	PRO	1
1	A	162	VAL	1
1	A	134	ILE	1
1	A	108	VAL	1
1	A	103	MET	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [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±0.01	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.66±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±0.02	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.65±0.02	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	0.65±0.02	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.64±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	0.65±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±0.01	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.65±0.02	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	0.64±0.01	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.64±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	0.64±0.02	0±0 (0±0%)
4	PX4	A	332	-	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	333	-	45,45,45	0.65±0.01	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	0.65±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	0.65±0.02	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.66±0.01	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.65±0.01	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%)
4	PX4	A	342	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.66±0.01	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.65±0.01	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	0.64±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	0.65±0.01	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.64±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	0.65±0.01	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.65±0.01	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	0.65±0.02	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.64±0.01	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	0.65±0.02	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.64±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	0.66±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	0.64±0.02	0±0 (0±0%)
4	PX4	A	375	-	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	376	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.64±0.01	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	0.64±0.03	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.65±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±0.01	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.65±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	0.65±0.01	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	0.64±0.02	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.64±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	0.64±0.01	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.65±0.01	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	0.65±0.02	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.64±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	419	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.64±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	0.64±0.01	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.65±0.01	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	1.47±0.07	0±0 (0±0%)
4	PX4	A	307	-	49,53,53	1.55±0.19	0±0 (0±0%)
4	PX4	A	308	-	49,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	309	-	49,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	310	-	49,53,53	1.44±0.16	0±0 (0±0%)
4	PX4	A	311	-	49,53,53	1.52±0.20	0±1 (0±1%)
4	PX4	A	312	-	49,53,53	1.45±0.18	0±1 (0±1%)
4	PX4	A	313	-	49,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	314	-	49,53,53	1.46±0.16	0±0 (0±0%)
4	PX4	A	315	-	49,53,53	1.40±0.13	0±0 (0±0%)
4	PX4	A	316	-	49,53,53	1.41±0.11	0±0 (0±0%)
4	PX4	A	317	-	49,53,53	1.41±0.14	0±0 (0±0%)
4	PX4	A	318	-	49,53,53	1.42±0.15	0±0 (0±0%)
4	PX4	A	319	-	49,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	320	-	49,53,53	1.44±0.16	0±1 (0±1%)
4	PX4	A	321	-	49,53,53	1.42±0.14	0±0 (0±0%)
4	PX4	A	322	-	49,53,53	1.48±0.17	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	323	-	49,53,53	1.39±0.17	0±0 (0±0%)
4	PX4	A	324	-	49,53,53	1.41±0.16	0±0 (0±0%)
4	PX4	A	325	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	326	-	49,53,53	1.42±0.19	0±0 (0±0%)
4	PX4	A	327	-	49,53,53	1.53±0.12	0±0 (0±1%)
4	PX4	A	328	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	329	-	49,53,53	1.48±0.12	0±0 (0±0%)
4	PX4	A	330	-	49,53,53	1.44±0.13	0±0 (0±0%)
4	PX4	A	331	-	49,53,53	1.49±0.13	0±0 (0±0%)
4	PX4	A	332	-	49,53,53	1.44±0.14	0±0 (0±0%)
4	PX4	A	333	-	49,53,53	1.48±0.16	0±0 (0±0%)
4	PX4	A	334	-	49,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	335	-	49,53,53	1.45±0.14	0±0 (0±0%)
4	PX4	A	336	-	49,53,53	1.46±0.19	0±0 (0±0%)
4	PX4	A	337	-	49,53,53	1.42±0.19	0±0 (0±0%)
4	PX4	A	338	-	49,53,53	1.50±0.16	0±0 (0±0%)
4	PX4	A	339	-	49,53,53	1.42±0.23	0±1 (0±1%)
4	PX4	A	340	-	49,53,53	1.53±0.10	0±0 (0±0%)
4	PX4	A	341	-	49,53,53	1.46±0.14	0±0 (0±0%)
4	PX4	A	342	-	49,53,53	1.48±0.14	0±0 (0±0%)
4	PX4	A	343	-	49,53,53	1.43±0.19	0±0 (0±0%)
4	PX4	A	344	-	49,53,53	1.49±0.16	0±0 (0±0%)
4	PX4	A	345	-	49,53,53	1.41±0.17	0±0 (0±0%)
4	PX4	A	346	-	49,53,53	1.44±0.15	0±0 (0±0%)
4	PX4	A	347	-	49,53,53	1.45±0.20	0±0 (0±0%)
4	PX4	A	348	-	49,53,53	1.46±0.16	0±1 (0±1%)
4	PX4	A	349	-	49,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	350	-	49,53,53	1.40±0.11	0±0 (0±0%)
4	PX4	A	351	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	352	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	353	-	49,53,53	1.47±0.11	0±0 (0±1%)
4	PX4	A	354	-	49,53,53	1.53±0.15	0±0 (0±0%)
4	PX4	A	355	-	49,53,53	1.44±0.13	0±0 (0±0%)
4	PX4	A	356	-	49,53,53	1.48±0.19	0±0 (0±0%)
4	PX4	A	357	-	49,53,53	1.45±0.13	0±0 (0±0%)
4	PX4	A	358	-	49,53,53	1.42±0.14	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	359	-	49,53,53	1.50±0.15	0±1 (0±1%)
4	PX4	A	360	-	49,53,53	1.47±0.12	0±1 (0±1%)
4	PX4	A	361	-	49,53,53	1.50±0.12	0±0 (0±0%)
4	PX4	A	362	-	49,53,53	1.47±0.07	0±0 (0±0%)
4	PX4	A	363	-	49,53,53	1.42±0.16	0±0 (0±0%)
4	PX4	A	364	-	49,53,53	1.51±0.20	0±0 (0±0%)
4	PX4	A	365	-	49,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	366	-	49,53,53	1.48±0.12	0±0 (0±0%)
4	PX4	A	367	-	49,53,53	1.46±0.17	0±0 (0±0%)
4	PX4	A	368	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	369	-	49,53,53	1.36±0.14	0±0 (0±0%)
4	PX4	A	370	-	49,53,53	1.45±0.12	0±0 (0±0%)
4	PX4	A	371	-	49,53,53	1.65±0.16	0±0 (0±0%)
4	PX4	A	372	-	49,53,53	1.43±0.16	0±0 (0±0%)
4	PX4	A	373	-	49,53,53	1.56±0.16	0±0 (0±0%)
4	PX4	A	374	-	49,53,53	1.43±0.15	0±0 (0±0%)
4	PX4	A	375	-	49,53,53	1.48±0.16	0±0 (0±0%)
4	PX4	A	376	-	49,53,53	1.47±0.18	0±0 (0±0%)
4	PX4	A	377	-	49,53,53	1.50±0.19	0±1 (0±1%)
4	PX4	A	378	-	49,53,53	1.41±0.16	0±0 (0±0%)
4	PX4	A	379	-	49,53,53	1.50±0.13	0±0 (0±0%)
4	PX4	A	380	-	49,53,53	1.44±0.16	0±1 (0±1%)
4	PX4	A	381	-	49,53,53	1.54±0.14	0±1 (0±1%)
4	PX4	A	382	-	49,53,53	1.42±0.16	0±0 (0±0%)
4	PX4	A	383	-	49,53,53	1.40±0.11	0±0 (0±0%)
4	PX4	A	384	-	49,53,53	1.46±0.22	0±0 (0±0%)
4	PX4	A	385	-	49,53,53	1.49±0.17	0±0 (0±0%)
4	PX4	A	386	-	49,53,53	1.44±0.16	0±0 (0±0%)
4	PX4	A	387	-	49,53,53	1.50±0.16	0±0 (0±0%)
4	PX4	A	388	-	49,53,53	1.41±0.14	0±0 (0±0%)
4	PX4	A	389	-	49,53,53	1.50±0.16	0±0 (0±0%)
4	PX4	A	390	-	49,53,53	1.44±0.13	0±0 (0±0%)
4	PX4	A	391	-	49,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	392	-	49,53,53	1.51±0.13	0±0 (0±0%)
4	PX4	A	393	-	49,53,53	1.52±0.13	0±0 (0±0%)
4	PX4	A	394	-	49,53,53	1.48±0.15	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	395	-	49,53,53	1.47±0.13	0±0 (0±0%)
4	PX4	A	396	-	49,53,53	1.51±0.18	1±1 (1±1%)
4	PX4	A	397	-	49,53,53	1.49±0.19	0±0 (0±0%)
4	PX4	A	398	-	49,53,53	1.44±0.16	0±0 (0±0%)
4	PX4	A	399	-	49,53,53	1.44±0.16	0±0 (0±0%)
4	PX4	A	400	-	49,53,53	1.46±0.19	0±1 (0±1%)
4	PX4	A	401	-	49,53,53	1.54±0.15	0±1 (0±1%)
4	PX4	A	402	-	49,53,53	1.40±0.15	0±0 (0±0%)
4	PX4	A	403	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	404	-	49,53,53	1.51±0.16	0±0 (0±0%)
4	PX4	A	405	-	49,53,53	1.45±0.14	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	1.42±0.18	0±0 (0±0%)
4	PX4	A	408	-	49,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	409	-	49,53,53	1.48±0.10	0±0 (0±0%)
4	PX4	A	410	-	49,53,53	1.46±0.18	0±0 (0±0%)
4	PX4	A	411	-	49,53,53	1.44±0.11	0±0 (0±0%)
4	PX4	A	412	-	49,53,53	1.39±0.13	0±0 (0±0%)
4	PX4	A	413	-	49,53,53	1.47±0.13	0±0 (0±0%)
4	PX4	A	414	-	49,53,53	1.50±0.14	0±0 (0±0%)
4	PX4	A	415	-	49,53,53	1.53±0.17	0±1 (0±1%)
4	PX4	A	416	-	49,53,53	1.44±0.17	0±0 (0±0%)
4	PX4	A	417	-	49,53,53	1.51±0.16	0±0 (0±0%)
4	PX4	A	418	-	49,53,53	1.45±0.15	0±0 (0±0%)
4	PX4	A	419	-	49,53,53	1.48±0.12	0±0 (0±0%)
4	PX4	A	420	-	49,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	421	-	49,53,53	1.45±0.13	0±1 (0±1%)
4	PX4	A	422	-	49,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	423	-	49,53,53	1.44±0.12	0±0 (0±0%)
4	PX4	A	424	-	49,53,53	1.39±0.18	0±0 (0±0%)
4	PX4	A	425	-	49,53,53	1.42±0.11	0±0 (0±0%)
4	PX4	A	426	-	49,53,53	1.43±0.14	0±1 (0±1%)
4	PX4	A	427	-	49,53,53	1.59±0.18	0±0 (0±0%)
4	PX4	A	428	-	49,53,53	1.50±0.10	0±0 (0±0%)
4	PX4	A	429	-	49,53,53	1.45±0.18	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	430	-	49,53,53	1.55±0.14	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
4	PX4	A	307	-	-	2±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	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	336	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	337	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	338	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	339	-	-	0±0,49,49,49	0±0,0,0,0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	340	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	341	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	342	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	343	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	344	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	345	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	346	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	347	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	348	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	349	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	350	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	351	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	352	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	353	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	354	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	355	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	356	-	-	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	-	-	2±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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	382	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	383	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	384	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	385	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	386	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	387	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	388	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	389	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	390	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	391	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	392	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	393	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	394	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	395	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	396	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	397	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	398	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	399	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	400	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	401	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	402	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	403	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	404	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	405	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	406	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	407	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	408	-	-	0±0,49,49,49	0±0,0,0,0
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	417	PX4	O7-C23-C24	7.71	127.78	111.53	6	2
4	A	413	PX4	C8-C7-C6	7.21	95.29	112.08	8	1
4	A	396	PX4	C8-C7-C6	7.14	95.44	112.08	3	6
4	A	426	PX4	O7-C23-C24	7.00	126.28	111.53	7	1
4	A	385	PX4	O7-C23-C24	6.99	126.27	111.53	6	1
4	A	427	PX4	C8-C7-C6	6.99	95.79	112.08	14	1
4	A	427	PX4	O5-C8-C7	6.87	127.26	108.70	6	2
4	A	353	PX4	C8-C7-C6	6.86	96.10	112.08	11	4
4	A	376	PX4	C8-C7-C6	6.83	96.16	112.08	2	1
4	A	349	PX4	O7-C23-C24	6.82	125.89	111.53	8	3
4	A	389	PX4	C8-C7-C6	6.80	96.24	112.08	10	1
4	A	424	PX4	O7-C23-C24	6.78	125.82	111.53	7	1
4	A	397	PX4	O7-C23-C24	6.78	125.81	111.53	13	1
4	A	371	PX4	O7-C23-C24	6.71	125.67	111.53	3	4
4	A	367	PX4	O7-C23-C24	6.66	125.56	111.53	5	2
4	A	310	PX4	C8-C7-C6	6.64	96.60	112.08	3	1
4	A	428	PX4	C8-C7-C6	6.58	96.74	112.08	6	1
4	A	331	PX4	C8-C7-C6	6.55	96.81	112.08	12	2
4	A	401	PX4	C8-C7-C6	6.54	96.84	112.08	13	1
4	A	380	PX4	C8-C7-C6	6.51	96.92	112.08	14	1
4	A	370	PX4	O5-C8-C7	6.48	126.20	108.70	1	1
4	A	388	PX4	O5-C8-C7	6.44	126.09	108.70	7	1
4	A	320	PX4	O5-C8-C7	6.44	126.09	108.70	7	1
4	A	397	PX4	C8-C7-C6	6.42	97.12	112.08	3	1
4	A	312	PX4	O5-C8-C7	6.41	126.00	108.70	5	1
4	A	334	PX4	O5-C8-C7	6.38	125.92	108.70	4	1
4	A	361	PX4	C8-C7-C6	6.30	97.41	112.08	3	2
4	A	321	PX4	C8-C7-C6	6.27	97.48	112.08	13	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	359	PX4	O7-C23-C24	6.23	124.65	111.53	7	2
4	A	345	PX4	O5-C8-C7	6.23	125.52	108.70	7	1
4	A	337	PX4	C7-O7-C23	6.22	133.29	117.91	12	1
4	A	348	PX4	O7-C7-C8	6.22	130.20	108.36	6	1
4	A	380	PX4	O5-C8-C7	6.21	125.48	108.70	11	1
4	A	382	PX4	C8-C7-C6	6.21	97.61	112.08	8	1
4	A	377	PX4	C8-C7-C6	6.21	97.62	112.08	14	2
4	A	345	PX4	C8-C7-C6	6.20	97.63	112.08	6	2
4	A	399	PX4	O7-C23-C24	6.17	124.53	111.53	10	1
4	A	389	PX4	O7-C23-C24	6.17	124.53	111.53	11	1
4	A	339	PX4	O7-C23-C24	6.16	124.50	111.53	3	2
4	A	427	PX4	O7-C23-C24	6.14	124.47	111.53	1	1
4	A	429	PX4	O5-C8-C7	6.14	125.26	108.70	5	1
4	A	403	PX4	O3-P1-O2	6.13	84.12	109.21	2	1
4	A	326	PX4	O5-C8-C7	6.10	125.18	108.70	6	1
4	A	425	PX4	C8-C7-C6	6.10	97.86	112.08	14	1
4	A	414	PX4	C8-C7-C6	6.09	97.88	112.08	6	1
4	A	403	PX4	C5-N1-C3	6.07	93.24	108.96	7	1
4	A	405	PX4	O5-C8-C7	6.07	125.09	108.70	11	1
4	A	335	PX4	O5-C8-C7	6.07	125.09	108.70	8	2
4	A	318	PX4	C8-C7-C6	6.03	98.02	112.08	3	3
4	A	333	PX4	O5-C8-C7	5.98	124.85	108.70	13	2
4	A	311	PX4	C8-C7-C6	5.97	98.17	112.08	8	1
4	A	317	PX4	C7-O7-C23	5.97	132.66	117.91	5	1
4	A	365	PX4	O5-C8-C7	5.97	124.81	108.70	6	1
4	A	363	PX4	O5-C8-C7	5.96	124.80	108.70	9	1
4	A	415	PX4	C4-N1-C3	5.94	93.59	108.96	14	1
4	A	430	PX4	C8-C7-C6	5.94	98.24	112.08	10	1
4	A	386	PX4	O7-C23-C24	5.94	124.04	111.53	8	2
4	A	341	PX4	O7-C23-C24	5.93	124.03	111.53	5	1
4	A	401	PX4	C5-N1-C3	5.93	93.61	108.96	13	1
4	A	413	PX4	O5-C8-C7	5.91	124.65	108.70	10	1
4	A	339	PX4	O5-C8-C7	5.90	124.64	108.70	5	2
4	A	375	PX4	C8-C7-C6	5.90	98.33	112.08	1	1
4	A	390	PX4	O5-C8-C7	5.89	124.61	108.70	6	1
4	A	418	PX4	O7-C23-C24	5.89	123.95	111.53	4	1
4	A	390	PX4	O7-C23-C24	5.88	123.91	111.53	7	2
4	A	327	PX4	O7-C23-C24	5.87	123.89	111.53	11	2
4	A	323	PX4	O7-C23-C24	5.86	123.88	111.53	8	1
4	A	415	PX4	C8-C7-C6	5.84	98.48	112.08	3	2
4	A	356	PX4	O7-C23-C24	5.84	123.83	111.53	3	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	360	PX4	O5-C8-C7	5.82	124.41	108.70	12	1
4	A	311	PX4	C5-N1-C3	5.79	93.99	108.96	10	1
4	A	363	PX4	C8-C7-C6	5.77	98.63	112.08	11	3
4	A	401	PX4	O5-C8-C7	5.76	124.25	108.70	7	1
4	A	307	PX4	O7-C23-C24	5.75	123.64	111.53	9	1
4	A	314	PX4	O5-C8-C7	5.73	124.16	108.70	11	1
4	A	353	PX4	O5-C8-C7	5.72	124.15	108.70	14	2
4	A	377	PX4	O5-C8-C7	5.72	124.14	108.70	11	1
4	A	370	PX4	C8-C7-C6	5.69	98.82	112.08	7	2
4	A	359	PX4	C8-C7-C6	5.68	98.83	112.08	5	2
4	A	319	PX4	C8-C7-C6	5.68	98.85	112.08	6	1
4	A	350	PX4	C8-C7-C6	5.67	98.88	112.08	10	2
4	A	327	PX4	C8-C7-C6	5.66	98.89	112.08	4	3
4	A	421	PX4	O5-C8-C7	5.66	123.98	108.70	9	2
4	A	331	PX4	O7-C23-C24	5.66	123.46	111.53	8	1
4	A	306	PX4	O7-C23-C24	5.66	123.46	111.53	5	1
4	A	406	PX4	O7-C23-C24	5.65	123.44	111.53	6	1
4	A	342	PX4	O7-C23-C24	5.65	123.43	111.53	14	1
4	A	400	PX4	C8-C7-C6	5.64	98.95	112.08	8	2
4	A	408	PX4	C4-N1-C3	5.63	123.53	108.96	14	1
4	A	377	PX4	C7-O7-C23	5.63	131.83	117.91	4	1
4	A	351	PX4	C8-C7-C6	5.63	98.96	112.08	4	2
4	A	378	PX4	O3-P1-O2	5.63	86.18	109.21	4	1
4	A	416	PX4	O7-C23-C24	5.63	123.38	111.53	13	1
4	A	407	PX4	C8-C7-C6	5.62	98.97	112.08	11	1
4	A	428	PX4	O5-C8-C7	5.62	123.88	108.70	1	2
4	A	312	PX4	C8-C7-C6	5.61	99.00	112.08	5	1
4	A	385	PX4	C8-C7-C6	5.60	99.03	112.08	8	2
4	A	330	PX4	C8-C7-C6	5.59	99.06	112.08	13	1
4	A	334	PX4	C8-C7-C6	5.59	99.06	112.08	9	1
4	A	367	PX4	C8-C7-C6	5.58	99.08	112.08	13	1
4	A	422	PX4	O7-C23-C24	5.57	123.27	111.53	10	2
4	A	430	PX4	O5-C8-C7	5.56	123.71	108.70	8	2
4	A	394	PX4	C8-C7-C6	5.56	99.13	112.08	10	2
4	A	375	PX4	O7-C23-C24	5.55	123.23	111.53	3	1
4	A	371	PX4	C8-C7-C6	5.55	99.15	112.08	9	1
4	A	429	PX4	C8-C7-C6	5.53	99.18	112.08	14	1
4	A	398	PX4	O5-C8-C7	5.53	123.62	108.70	11	1
4	A	320	PX4	C8-C7-C6	5.52	99.21	112.08	7	1
4	A	387	PX4	P1-O3-C1	5.52	92.70	121.60	5	1
4	A	343	PX4	O7-C23-C24	5.52	123.15	111.53	14	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	362	PX4	C8-C7-C6	5.51	99.23	112.08	10	1
4	A	333	PX4	C8-C7-C6	5.51	99.25	112.08	7	3
4	A	379	PX4	C7-O7-C23	5.50	131.51	117.91	2	1
4	A	368	PX4	C8-C7-C6	5.49	99.28	112.08	11	1
4	A	368	PX4	O5-C8-C7	5.48	123.49	108.70	13	1
4	A	374	PX4	O5-C8-C7	5.48	123.49	108.70	10	1
4	A	346	PX4	C8-C7-C6	5.46	99.35	112.08	9	1
4	A	311	PX4	O5-C8-C7	5.46	123.44	108.70	8	1
4	A	355	PX4	O5-C8-C7	5.46	123.44	108.70	7	1
4	A	338	PX4	C8-C7-C6	5.46	99.36	112.08	14	1
4	A	387	PX4	C8-C7-C6	5.45	99.38	112.08	4	3
4	A	423	PX4	O5-C9-O6	5.45	109.23	123.51	4	1
4	A	422	PX4	C4-N1-C3	5.45	94.87	108.96	9	1
4	A	346	PX4	O7-C23-C24	5.44	122.99	111.53	6	1
4	A	324	PX4	C8-C7-C6	5.43	99.43	112.08	9	1
4	A	381	PX4	C7-O7-C23	5.43	104.49	117.91	8	1
4	A	397	PX4	O5-C8-C7	5.43	123.35	108.70	11	1
4	A	418	PX4	O5-C8-C7	5.42	123.33	108.70	13	1
4	A	380	PX4	O7-C23-C24	5.42	122.95	111.53	6	2
4	A	373	PX4	O5-C8-C7	5.42	123.33	108.70	4	1
4	A	340	PX4	C8-C7-C6	5.41	99.47	112.08	11	1
4	A	339	PX4	C8-C7-C6	5.40	99.49	112.08	11	1
4	A	422	PX4	O5-C8-C7	5.40	123.29	108.70	6	1
4	A	327	PX4	C7-O7-C23	5.40	131.26	117.91	6	1
4	A	348	PX4	C8-C7-C6	5.37	99.57	112.08	6	3
4	A	313	PX4	O7-C23-C24	5.37	122.83	111.53	7	1
4	A	307	PX4	C7-O7-C23	5.36	131.16	117.91	3	1
4	A	329	PX4	O5-C8-C7	5.36	123.17	108.70	1	1
4	A	394	PX4	O5-C8-C7	5.36	123.17	108.70	6	1
4	A	317	PX4	C8-C7-C6	5.36	99.59	112.08	11	1
4	A	393	PX4	C8-C7-C6	5.34	99.64	112.08	2	1
4	A	341	PX4	O7-C7-C8	5.32	127.06	108.36	7	1
4	A	417	PX4	O5-C8-C7	5.32	123.06	108.70	14	1
4	A	408	PX4	C8-C7-C6	5.31	99.70	112.08	11	1
4	A	360	PX4	C8-C7-C6	5.31	99.70	112.08	12	1
4	A	328	PX4	O7-C23-C24	5.31	122.72	111.53	10	1
4	A	354	PX4	O5-C8-C7	5.28	122.96	108.70	1	1
4	A	392	PX4	O5-C8-C7	5.27	122.93	108.70	2	2
4	A	381	PX4	O7-C23-C24	5.27	122.63	111.53	12	1
4	A	411	PX4	O5-C8-C7	5.26	122.89	108.70	12	1
4	A	342	PX4	C8-C7-C6	5.25	99.84	112.08	6	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	309	PX4	O7-C23-C24	5.23	122.56	111.53	13	1
4	A	388	PX4	C5-N1-C4	5.23	95.42	108.96	3	1
4	A	352	PX4	C8-C7-C6	5.23	99.89	112.08	6	1
4	A	335	PX4	C8-C7-C6	5.23	99.90	112.08	11	2
4	A	384	PX4	O5-C8-C7	5.22	122.81	108.70	13	1
4	A	417	PX4	C8-C7-C6	5.22	99.91	112.08	1	1
4	A	392	PX4	C8-C7-C6	5.22	99.93	112.08	12	1
4	A	410	PX4	C8-C7-C6	5.20	99.95	112.08	8	2
4	A	415	PX4	O5-C8-C7	5.20	122.75	108.70	14	1
4	A	420	PX4	O7-C23-C24	5.19	122.46	111.53	13	1
4	A	365	PX4	C8-C7-C6	5.18	100.00	112.08	5	1
4	A	411	PX4	C4-N1-C3	5.18	122.35	108.96	1	1
4	A	344	PX4	C8-C7-C6	5.17	100.03	112.08	7	1
4	A	402	PX4	P1-O3-C1	5.17	94.57	121.60	10	1
4	A	313	PX4	O5-C8-C7	5.16	122.62	108.70	14	1
4	A	391	PX4	C8-C7-C6	5.16	100.07	112.08	14	1
4	A	412	PX4	O7-C23-C24	5.15	122.39	111.53	7	1
4	A	400	PX4	O5-C8-C7	5.15	122.61	108.70	7	1
4	A	421	PX4	C8-C7-C6	5.15	100.09	112.08	8	1
4	A	386	PX4	O5-C8-C7	5.14	122.58	108.70	10	1
4	A	423	PX4	O5-C8-C7	5.14	122.57	108.70	5	1
4	A	387	PX4	O7-C23-C24	5.13	122.33	111.53	12	1
4	A	396	PX4	O7-C7-C6	5.13	126.38	108.36	10	1
4	A	316	PX4	O5-C8-C7	5.12	122.53	108.70	12	1
4	A	378	PX4	O5-C8-C7	5.12	122.53	108.70	12	1
4	A	313	PX4	O3-P1-O2	5.12	88.25	109.21	13	1
4	A	328	PX4	C5-N1-C4	5.12	95.72	108.96	5	1
4	A	425	PX4	O7-C23-C24	5.12	122.31	111.53	13	1
4	A	344	PX4	C5-N1-C4	5.12	95.72	108.96	6	1
4	A	410	PX4	O3-P1-O2	5.11	88.28	109.21	13	1
4	A	394	PX4	P1-O3-C1	5.11	94.87	121.60	12	1
4	A	316	PX4	C8-C7-C6	5.10	100.21	112.08	9	1
4	A	389	PX4	P1-O3-C1	5.09	94.98	121.60	6	1
4	A	388	PX4	C8-C7-C6	5.08	100.23	112.08	1	1
4	A	426	PX4	O7-C23-O8	5.07	109.89	123.67	7	1
4	A	384	PX4	O7-C23-C24	5.06	122.19	111.53	3	1
4	A	421	PX4	O7-C23-C24	5.04	122.16	111.53	9	1
4	A	359	PX4	O5-C8-C7	5.04	122.30	108.70	5	1
4	A	395	PX4	C8-C7-C6	5.03	100.35	112.08	8	1
4	A	347	PX4	O5-C8-C7	5.03	122.28	108.70	1	1
4	A	381	PX4	C8-C7-C6	5.03	100.37	112.08	12	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	400	PX4	O7-C23-C24	5.03	122.12	111.53	8	1
4	A	308	PX4	O5-C8-C7	5.02	122.26	108.70	10	1
4	A	310	PX4	O7-C23-C24	5.02	122.10	111.53	14	1
4	A	404	PX4	O5-C8-C7	5.02	122.24	108.70	13	1
4	A	311	PX4	O7-C23-C24	5.01	122.09	111.53	7	1
4	A	322	PX4	O7-C23-C24	5.00	122.07	111.53	1	1
4	A	404	PX4	C8-C7-C6	5.00	100.42	112.08	10	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	371	PX4	C7-O7-C23-O8	14
4	A	371	PX4	C7-O7-C23-C24	14
4	A	307	PX4	C7-O7-C23-C24	12
4	A	307	PX4	C7-O7-C23-O8	11

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: 2mlr_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. 1600 atoms were assigned a chemical shift out of a possible 1936. 15 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	740/786 (94%)	306/313 (98%)	284/320 (89%)	150/153 (98%)
Sidechain	712/887 (80%)	443/521 (85%)	260/326 (80%)	9/40 (22%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	148/263 (56%)	79/142 (56%)	66/109 (61%)	3/12 (25%)
Overall	1600/1936 (83%)	828/976 (85%)	610/755 (81%)	162/205 (79%)

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:

