



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2019 – 02:41 AM EDT

PDB ID : 6CCX
Title : NMR data-driven model of GTPase KRas-GMPPNP:Cmpd2 complex tethered to a nanodisc
Authors : Fang, Z.; Marshall, C.B.; Nishikawa, T.; Gossert, A.D.; Jansen, J.M.; Jahnke, W.; Ikura, M.
Deposited on : 2018-02-07

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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	:	1.8.0 (224370), CSD as540be (2019)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20031633
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

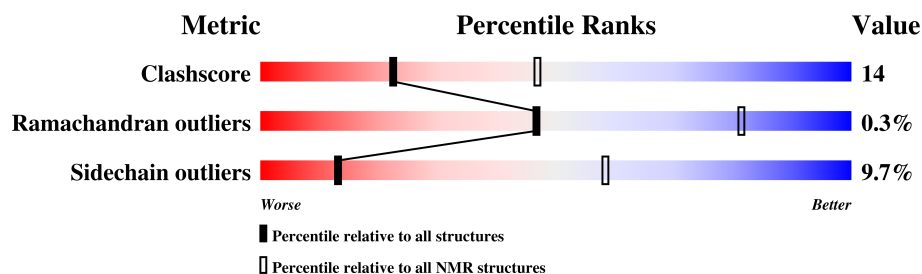
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 3%.

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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	10811

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	200	80% 17% ...
1	C	200	78% 20% ...
2	B	187	76% 15% 7% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 10 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:201-A:396, C:401-C:596 (392)	0.26	10
2	B:2-B:172 (171)	0.41	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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4
2	5, 6, 8, 9
3	7, 10

3 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9535 atoms, of which 429 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
1	A	198	Total	C	H	N	O	S	0
			1645	1019	22	287	314	3	
1	C	198	Total	C	H	N	O	S	0
			1646	1019	22	287	315	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	expression tag	UNP P02647
A	200	PRO	-	expression tag	UNP P02647
C	397	GLY	-	expression tag	UNP P02647
C	398	PRO	-	expression tag	UNP P02647

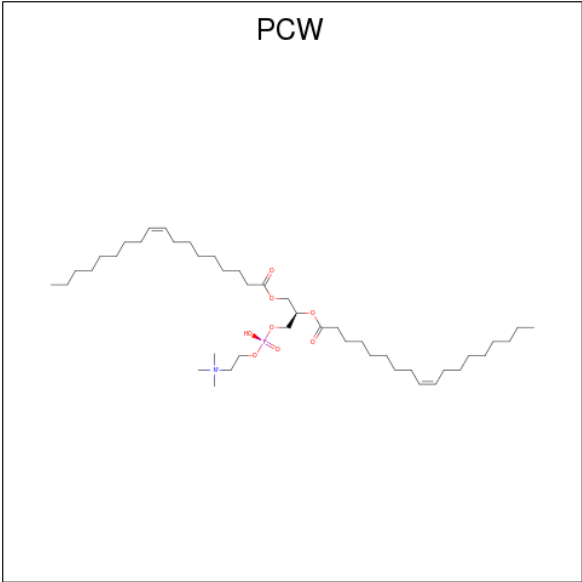
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
2	B	185	Total	C	H	N	O	S	0
			1842	926	363	257	287	9	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P01116
B	0	SER	-	expression tag	UNP P01116
B	12	VAL	GLY	engineered mutation	UNP P01116

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms				
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1

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Mol	Chain	Residues	Atoms				
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1
3	B	1	Total	C	N	O	P
			54	44	1	8	1

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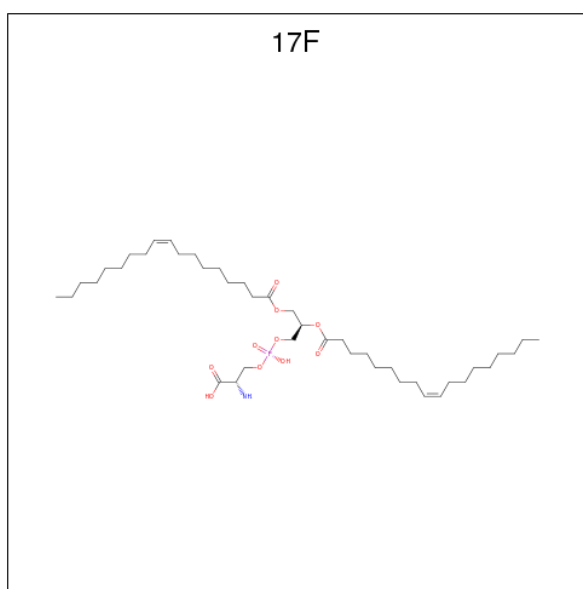
Mol	Chain	Residues	Atoms				
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1

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Mol	Chain	Residues	Atoms				
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1
3	C	1	Total	C	N	O	P
			54	44	1	8	1

- Molecule 4 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: C₄₂H₇₈NO₁₀P).



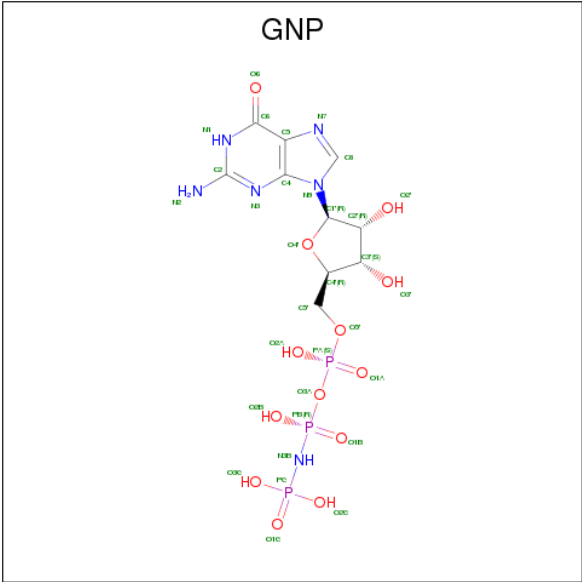
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1

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Mol	Chain	Residues	Atoms				
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	B	1	Total	C	N	O	P
			54	42	1	10	1
4	C	1	Total	C	N	O	P
			54	42	1	10	1
4	C	1	Total	C	N	O	P
			54	42	1	10	1
4	C	1	Total	C	N	O	P
			54	42	1	10	1
4	C	1	Total	C	N	O	P
			54	42	1	10	1
4	C	1	Total	C	N	O	P
			54	42	1	10	1

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

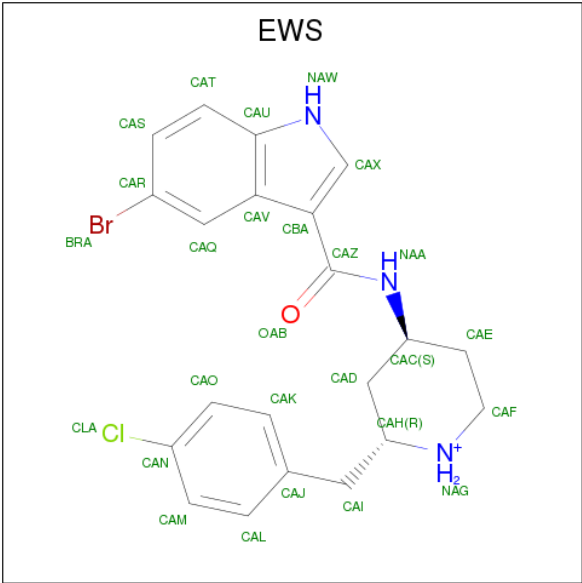


Mol	Chain	Residues	Atoms				
5	B	1	Total	C	N	O	P
			32	10	6	13	3

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
6	B	1	Total	Mg
			1	1

- Molecule 7 is (2R,4S)-4-[(5-bromo-1H-indole-3-carbonyl)amino]-2-[(4-chlorophenyl)methyl]piperidin-1-ium (three-letter code: EWS) (formula: C₂₁H₂₂BrClN₃O).



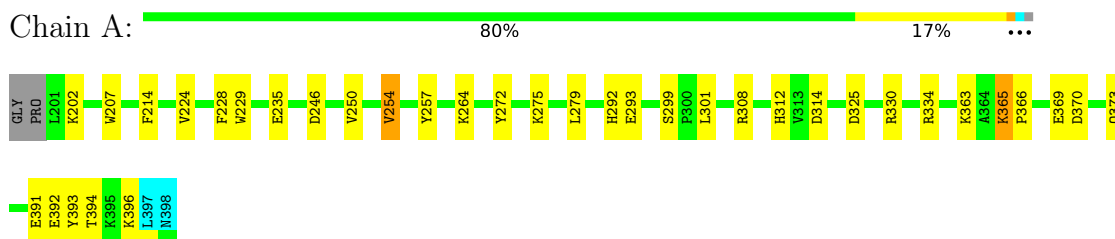
Mol	Chain	Residues	Atoms						
			Total	Br	C	Cl	H	N	O
7	B	1	49	1	21	1	22	3	1

4 Residue-property plots [i](#)

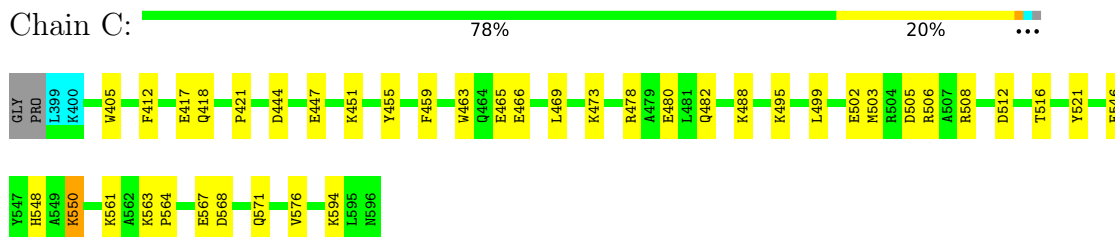
4.1 Average score per residue in the NMR ensemble

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.

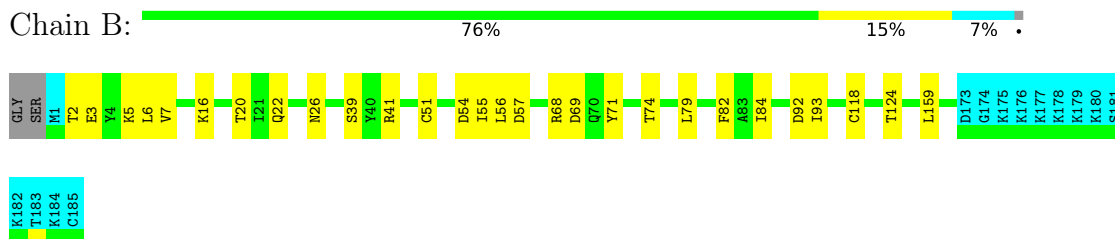
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas




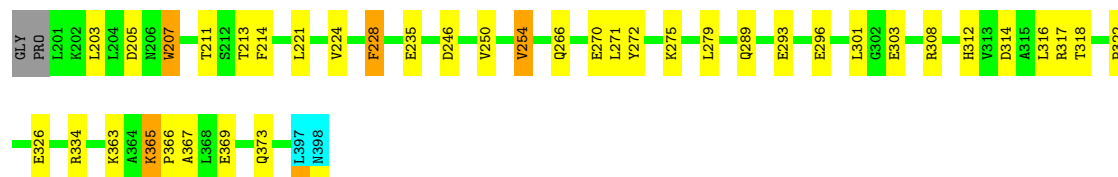
4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.


4.2.1 Score per residue for model 1

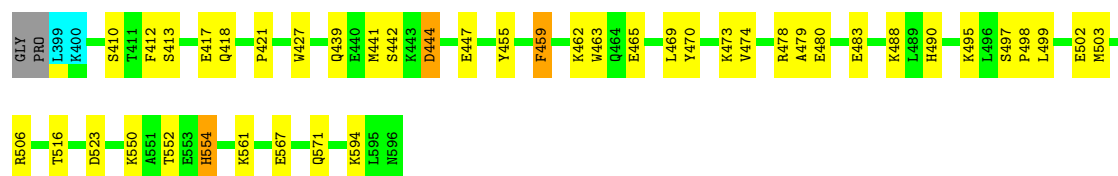
• Molecule 1: Apolipoprotein A-I

Chain A:  79% 18% ...



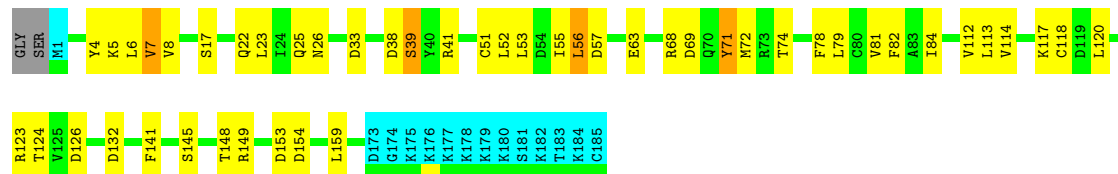
• Molecule 1: Apolipoprotein A-I

Chain C:  77% 20% ...




• Molecule 2: GTPase KRas

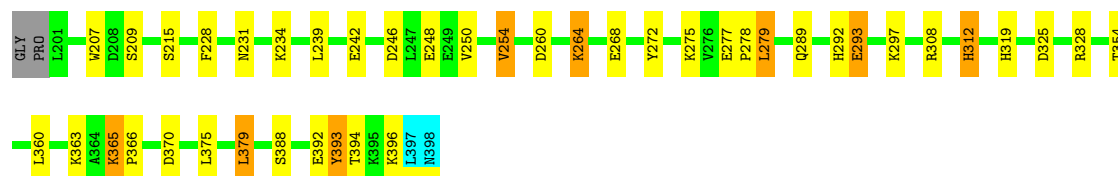
Chain B:  66% 24% 7% ...



4.2.2 Score per residue for model 2

• Molecule 1: Apolipoprotein A-I

Chain A:  77% 17% ...



• Molecule 1: Apolipoprotein A-I

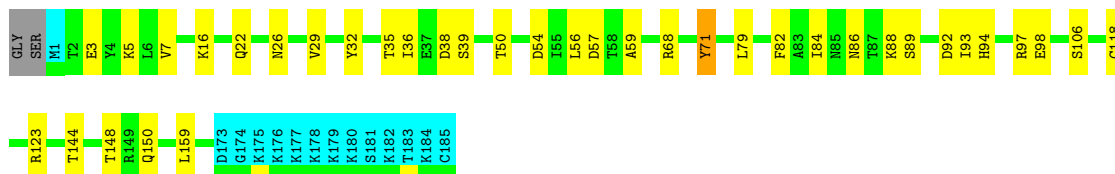
Chain C:  77% 21% ...





• Molecule 2: GTPase KRas

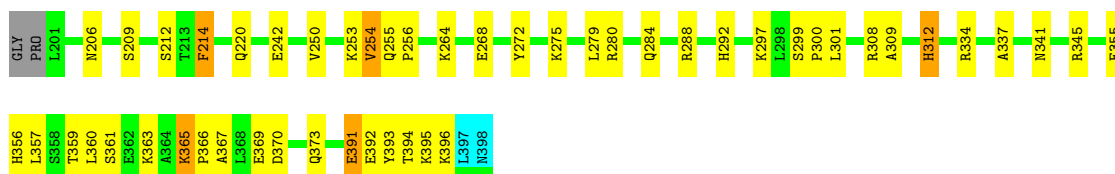
Chain B: 72% 19% 7%



4.2.3 Score per residue for model 3

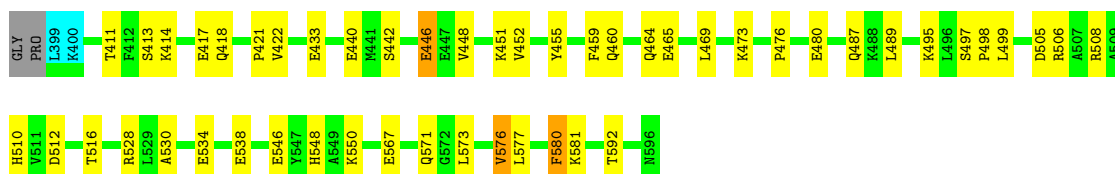
• Molecule 1: Apolipoprotein A-I

Chain A: 73% 23%



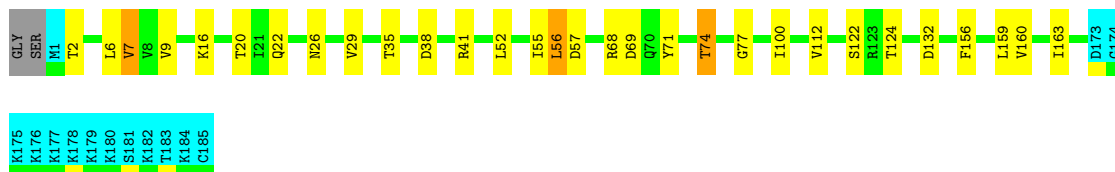
• Molecule 1: Apolipoprotein A-I

Chain C: 73% 24%



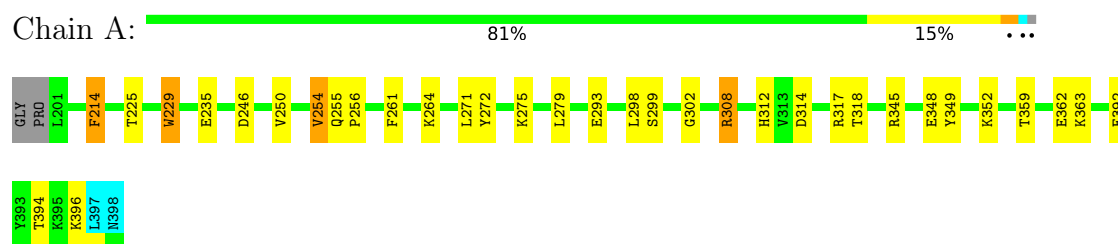
• Molecule 2: GTPase KRas

Chain B: 75% 14% 7%

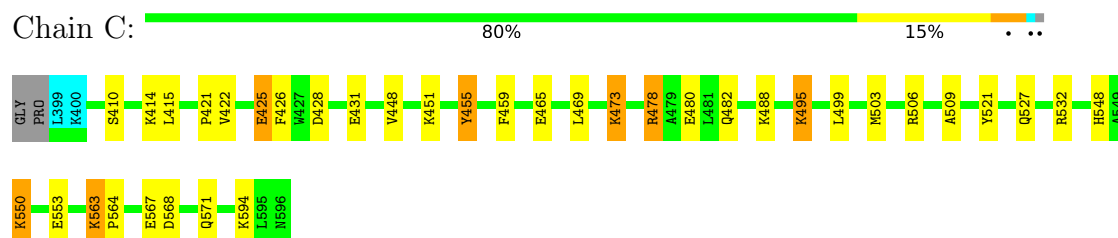


4.2.4 Score per residue for model 4

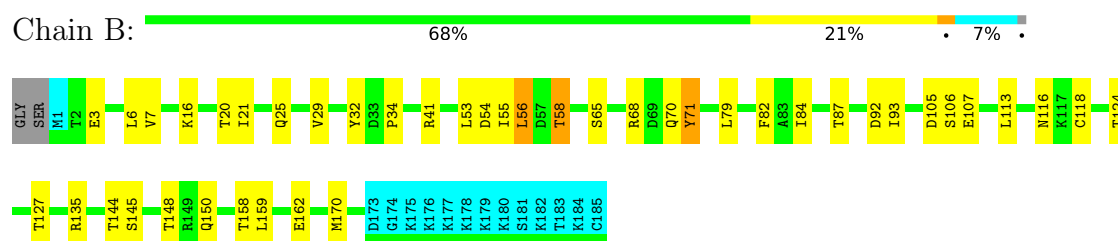
• Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

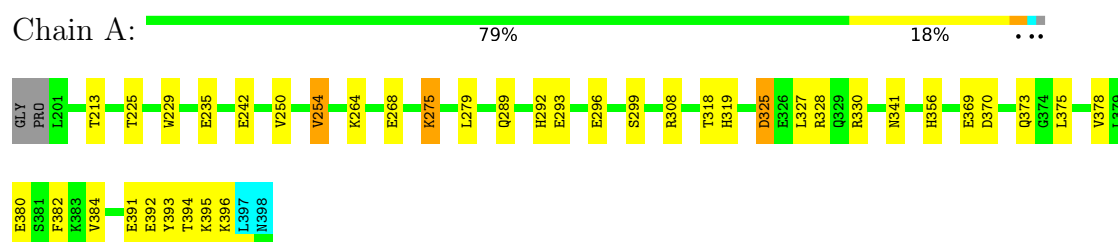


- Molecule 2: GTPase KRas

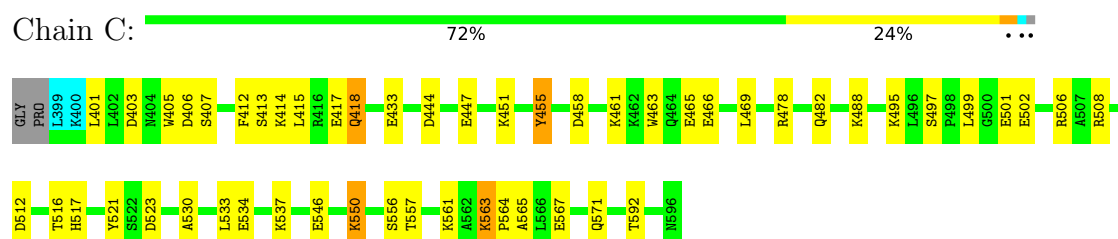


4.2.5 Score per residue for model 5

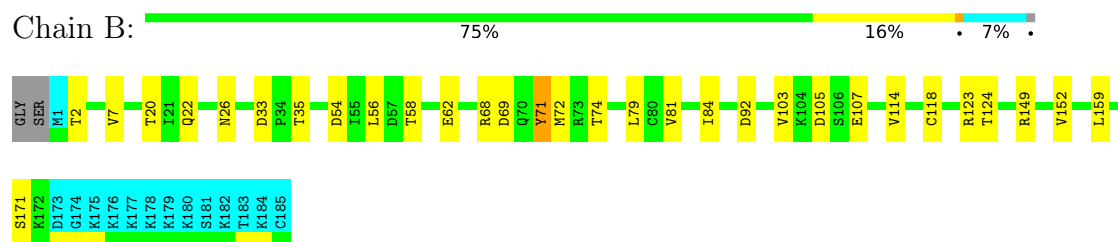
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

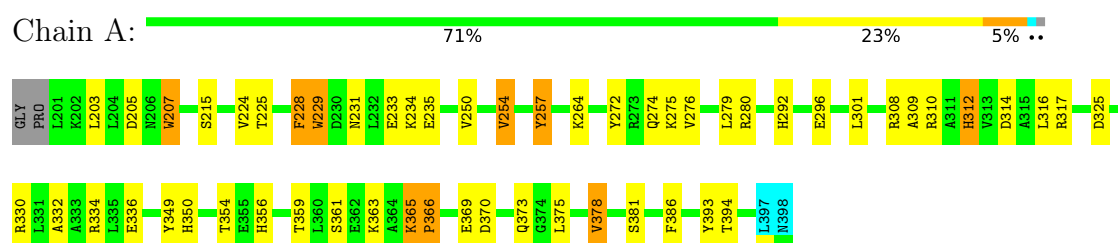


- Molecule 2: GTPase KRas

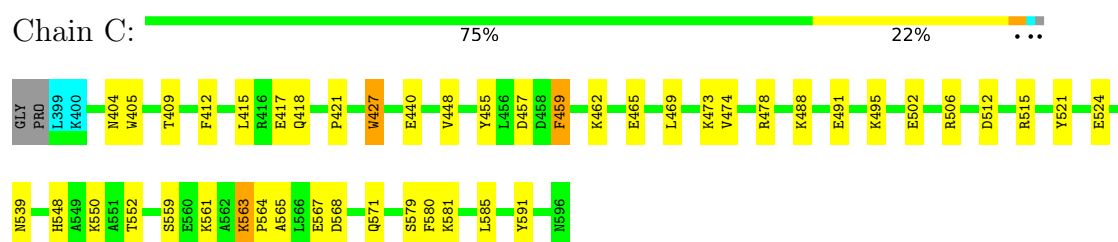


4.2.6 Score per residue for model 6

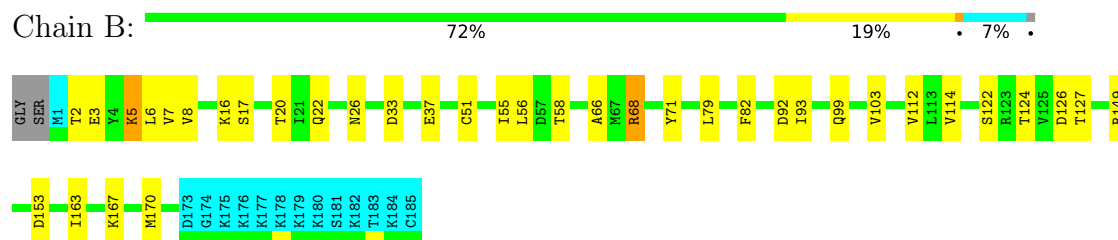
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



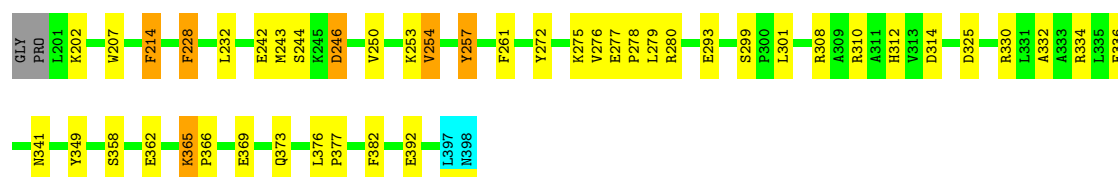
- Molecule 2: GTPase KRas



4.2.7 Score per residue for model 7

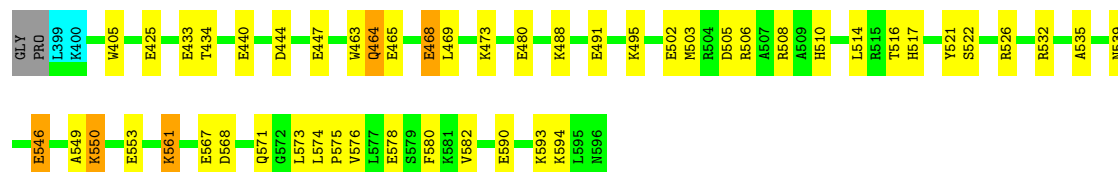
- Molecule 1: Apolipoprotein A-I





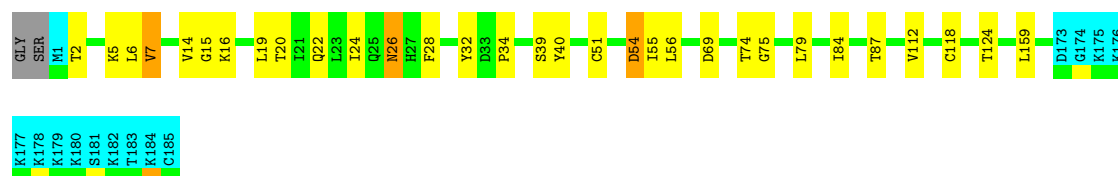
• Molecule 1: Apolipoprotein A-I

Chain C: 73% 23% ..



• Molecule 2: GTPase KRas

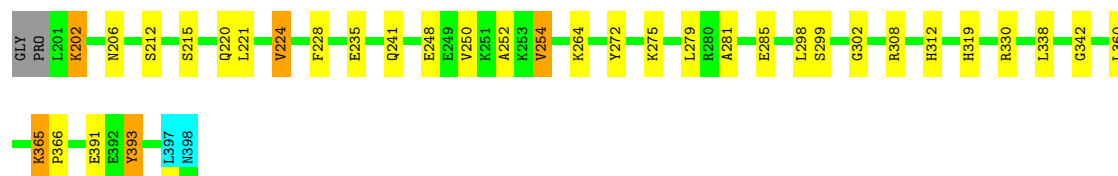
Chain B: 75% 15% 7% ..



4.2.8 Score per residue for model 8

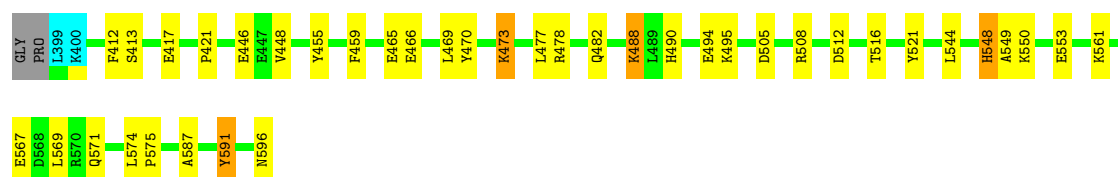
• Molecule 1: Apolipoprotein A-I

Chain A: 81% 15% ..

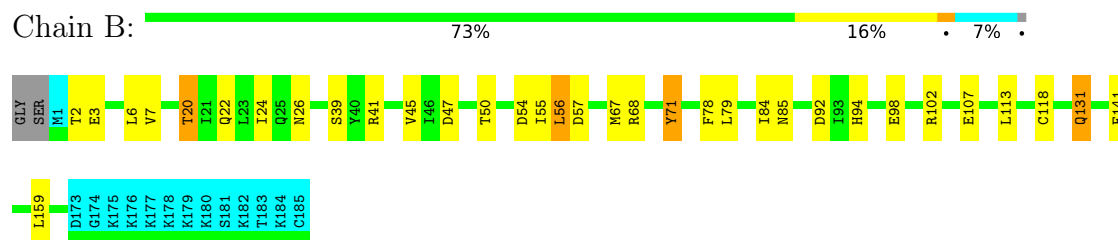


• Molecule 1: Apolipoprotein A-I

Chain C: 79% 18% ..

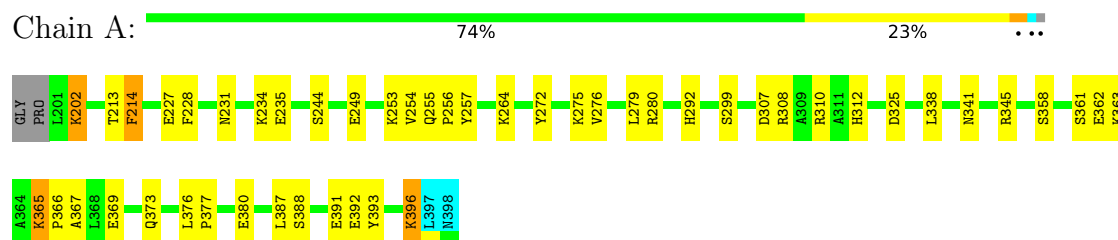


• Molecule 2: GTPase KRas

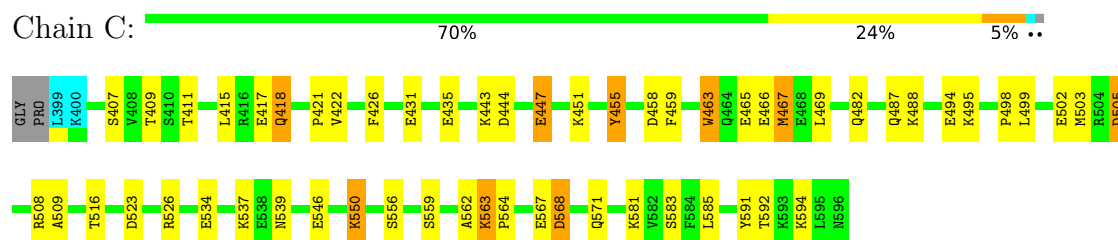


4.2.9 Score per residue for model 9

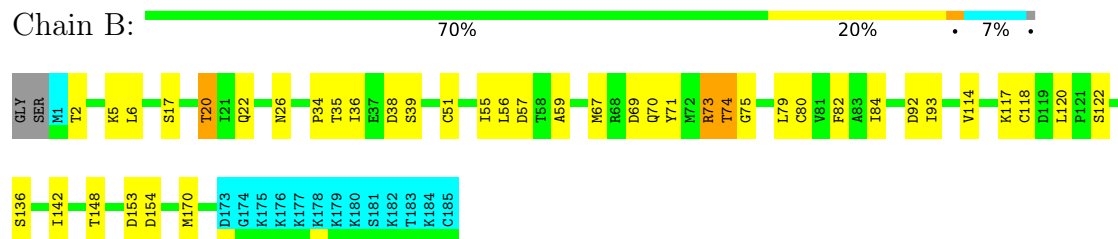
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

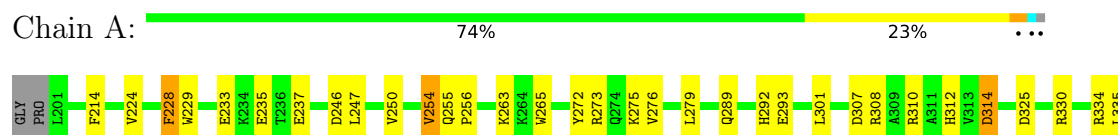


- Molecule 2: GTPase KRas



4.2.10 Score per residue for model 10 (medoid)

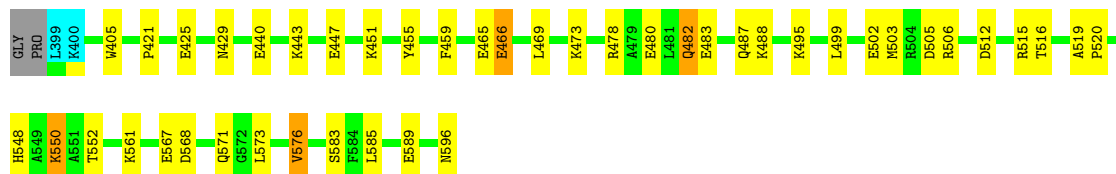
- Molecule 1: Apolipoprotein A-I





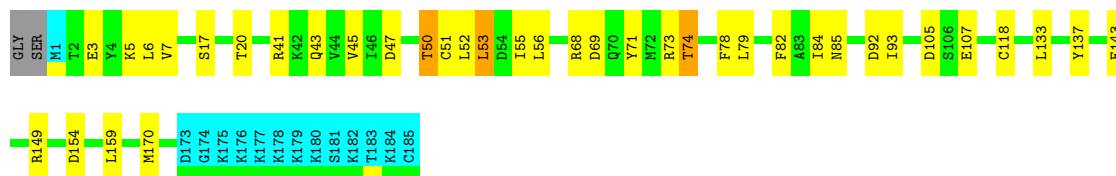
• Molecule 1: Apolipoprotein A-I

Chain C: 76% 20% ...



• Molecule 2: GTPase KRas

Chain B: 71% 19% 7%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 3000 calculated structures, 10 were deposited, based on the following criterion: *10 structures for lowest energy*.

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

Software name	Classification	Version
HADDOCK	structure calculation	
HADDOCK	refinement	
CNS	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)	6ccx_cs.cif
Number of chemical shift lists	1
Total number of shifts	268
Number of shifts mapped to atoms	268
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

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: EWS, 17F, MG, GNP, PCW

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	0.26±0.00	0±0/1635 (0.0±0.0%)	0.40±0.01	0±0/2199 (0.0±0.0%)
1	C	0.26±0.00	0±0/1634 (0.0±0.0%)	0.41±0.01	0±0/2196 (0.0±0.0%)
2	B	0.27±0.00	0±0/1390 (0.0±0.0%)	0.42±0.04	0±1/1875 (0.0±0.0%)
All	All	0.26	0/46590 (0.0%)	0.41	3/62700 (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
2	B	74	THR	CA-CB-OG1	-9.87	88.28	109.00	10	1
2	B	74	THR	CB-CA-C	-7.53	91.26	111.60	10	1
2	B	74	THR	N-CA-CB	7.44	124.44	110.30	10	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1607	22	1609	34±7
1	C	1607	22	1603	35±9
2	B	1368	322	1354	25±5

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
3	A	540	0	840	45±4
3	B	1350	0	2100	97±6
3	C	1566	0	2436	89±10
4	A	54	0	76	4±1
4	B	486	0	684	50±8
4	C	324	0	456	21±4
5	B	32	0	13	1±1
7	B	27	22	0	17±4
All	All	89620	3880	111707	2751

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:393:TYR:CE1	3:A:407:PCW:C28	1.61	1.83	8	2
1:A:393:TYR:CE1	3:A:407:PCW:C27	1.59	1.82	8	2
1:C:488:LYS:CE	3:C:623:PCW:C28	1.54	1.81	4	2
1:C:488:LYS:CE	3:C:623:PCW:H283	1.54	1.15	4	1
1:C:488:LYS:HD3	3:C:623:PCW:C27	1.53	1.04	4	2
1:C:488:LYS:HE2	3:C:623:PCW:C28	1.51	1.27	4	1
1:C:488:LYS:CD	3:C:623:PCW:H271	1.46	1.38	4	1
1:C:488:LYS:HD3	3:C:623:PCW:C28	1.46	1.36	5	7
1:A:308:ARG:CG	1:C:469:LEU:HD11	1.45	1.42	4	2
1:A:393:TYR:CZ	3:A:407:PCW:H271	1.42	1.48	6	4
1:A:393:TYR:CE1	3:A:407:PCW:H271	1.42	1.46	3	3
1:A:396:LYS:NZ	3:A:407:PCW:H271	1.41	1.22	5	1
1:C:488:LYS:CD	3:C:623:PCW:C28	1.39	1.95	4	4
1:C:488:LYS:CD	3:C:623:PCW:C27	1.38	1.92	4	1
3:B:207:PCW:H72	7:B:237:EWS:BRA	1.38	1.73	10	1
1:C:488:LYS:CD	3:C:623:PCW:H281	1.37	1.48	5	5
1:A:393:TYR:CZ	3:A:407:PCW:C27	1.35	1.97	3	3
2:B:75:GLY:N	7:B:237:EWS:BRA	1.35	2.14	9	1
1:A:393:TYR:CD1	3:A:407:PCW:C28	1.33	2.12	8	2
1:A:393:TYR:CD1	3:A:407:PCW:C27	1.32	2.11	8	2
1:A:393:TYR:CE1	3:A:407:PCW:H281	1.32	1.44	8	1
3:B:201:PCW:H32	7:B:237:EWS:CLA	1.31	1.60	5	1
1:A:393:TYR:CD1	3:A:407:PCW:H281	1.31	1.58	8	2
3:B:207:PCW:C7	7:B:237:EWS:BRA	1.31	2.32	10	1
1:A:393:TYR:OH	3:A:407:PCW:H271	1.30	1.14	2	2
1:A:393:TYR:CZ	3:A:407:PCW:H272	1.29	1.53	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:465:GLU:O	1:C:469:LEU:CG	1.27	1.82	10	8
1:A:308:ARG:HG2	1:C:469:LEU:CD1	1.25	1.60	4	1
1:A:396:LYS:CD	3:A:407:PCW:H281	1.25	1.61	5	1
1:A:396:LYS:HD3	3:A:407:PCW:C28	1.24	1.63	5	1
2:B:56:LEU:HD22	7:B:237:EWS:OAB	1.22	1.28	1	7
1:C:465:GLU:O	1:C:469:LEU:HG	1.22	1.00	10	10
2:B:74:THR:HB	7:B:237:EWS:BRA	1.21	1.90	9	1
1:A:396:LYS:NZ	3:A:407:PCW:C27	1.19	2.06	5	1
1:A:393:TYR:OH	3:A:407:PCW:C27	1.19	1.91	2	2
1:A:393:TYR:OH	3:A:407:PCW:C26	1.19	1.91	6	1
3:B:220:PCW:H52	7:B:237:EWS:BRA	1.19	1.93	8	1
3:B:208:PCW:H81	7:B:237:EWS:BRA	1.17	1.93	4	1
3:B:220:PCW:H42	7:B:237:EWS:BRA	1.17	1.93	8	1
3:B:220:PCW:C4	7:B:237:EWS:BRA	1.15	2.49	8	1
3:B:207:PCW:C6	7:B:237:EWS:BRA	1.14	2.50	10	1
1:C:488:LYS:CG	3:C:623:PCW:H281	1.13	1.73	4	2
1:A:393:TYR:HE1	3:A:407:PCW:C28	1.13	1.25	8	1
3:B:207:PCW:H63	7:B:237:EWS:BRA	1.12	1.99	10	1
2:B:56:LEU:CD2	7:B:237:EWS:OAB	1.12	1.96	1	7
1:A:214:PHE:CZ	3:A:404:PCW:H162	1.12	1.79	4	2
1:A:393:TYR:OH	3:A:407:PCW:H262	1.12	1.43	6	1
3:B:220:PCW:C5	7:B:237:EWS:BRA	1.11	2.53	8	1
1:A:391:GLU:O	1:A:395:LYS:HG3	1.09	1.46	5	1
1:A:393:TYR:CD1	3:A:407:PCW:H272	1.08	1.79	8	1
1:C:488:LYS:HG2	3:C:623:PCW:H281	1.07	1.23	4	1
2:B:56:LEU:HD13	7:B:237:EWS:CAZ	1.07	1.79	1	1
1:C:455:TYR:OH	3:C:601:PCW:C21	1.07	2.03	3	4
2:B:56:LEU:HD13	7:B:237:EWS:OAB	1.04	1.49	9	5
1:C:567:GLU:O	1:C:571:GLN:HG3	1.04	1.50	8	10
1:C:488:LYS:CE	3:C:623:PCW:H281	1.03	1.83	9	3
2:B:5:LYS:HB3	7:B:237:EWS:CAT	1.03	1.84	1	3
3:A:408:PCW:H341	3:B:231:PCW:H39	1.02	1.30	4	7
1:A:396:LYS:HZ2	3:A:407:PCW:C27	1.02	1.63	5	1
2:B:71:TYR:HB3	7:B:237:EWS:CAF	1.02	1.84	5	1
2:B:74:THR:C	7:B:237:EWS:BRA	1.02	2.53	9	1
3:B:221:PCW:H51	7:B:237:EWS:BRA	1.01	2.10	1	1
1:C:455:TYR:OH	3:C:601:PCW:H211	1.01	1.56	4	4
2:B:56:LEU:CD1	7:B:237:EWS:OAB	1.01	2.08	9	5
1:A:308:ARG:CD	1:C:469:LEU:HD21	1.00	1.86	6	2
2:B:71:TYR:HA	7:B:237:EWS:CAC	1.00	1.86	1	1
4:B:228:17F:H4	4:B:228:17F:H1	0.99	1.29	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:HG3	1:C:469:LEU:HD21	0.99	1.32	9	7
3:B:221:PCW:C5	7:B:237:EWS:BRA	0.99	2.65	1	1
1:A:393:TYR:HD1	3:A:407:PCW:H281	0.99	1.18	10	1
3:B:201:PCW:C3	7:B:237:EWS:CLA	0.98	2.47	5	1
1:C:488:LYS:HD3	3:C:623:PCW:H281	0.98	1.01	10	7
1:A:396:LYS:HD3	3:A:407:PCW:H281	0.98	1.01	5	1
3:B:201:PCW:O3P	7:B:237:EWS:CAO	0.97	2.13	5	1
3:B:202:PCW:H31	3:B:212:PCW:H322	0.97	1.34	10	2
2:B:56:LEU:HD23	7:B:237:EWS:OAB	0.97	1.59	5	1
1:A:214:PHE:CZ	3:A:404:PCW:H171	0.97	1.94	1	2
3:B:221:PCW:H32	7:B:237:EWS:CLA	0.96	1.96	9	1
1:A:392:GLU:OE1	1:A:395:LYS:HD2	0.94	1.62	5	1
1:C:488:LYS:HD3	3:C:623:PCW:H283	0.93	1.39	5	1
2:B:7:VAL:HG13	7:B:237:EWS:NAW	0.92	1.79	7	2
1:C:455:TYR:OH	3:C:601:PCW:C22	0.92	2.18	9	2
1:C:455:TYR:OH	3:C:601:PCW:H232	0.92	1.65	8	2
1:C:567:GLU:O	1:C:571:GLN:CG	0.91	2.17	8	3
1:A:369:GLU:OE1	1:A:373:GLN:NE2	0.91	2.02	1	1
2:B:74:THR:CB	7:B:237:EWS:BRA	0.91	2.73	9	1
4:B:228:17F:H1	4:B:228:17F:H4	0.91	1.39	2	2
1:A:393:TYR:HE1	3:A:407:PCW:H271	0.90	1.16	3	1
1:A:396:LYS:CE	3:A:407:PCW:H281	0.90	1.98	5	1
3:B:208:PCW:H71	7:B:237:EWS:BRA	0.89	2.22	4	1
1:A:308:ARG:HD2	1:C:469:LEU:HD21	0.89	1.43	6	1
1:A:369:GLU:O	1:A:373:GLN:HG3	0.89	1.67	9	7
1:C:488:LYS:NZ	3:C:623:PCW:H281	0.89	1.82	9	2
3:B:210:PCW:H162	4:B:227:17F:H11A	0.88	1.43	8	1
3:B:210:PCW:H332	4:B:224:17F:H19	0.88	1.45	9	1
1:C:455:TYR:OH	3:C:601:PCW:C20	0.88	2.22	3	3
3:C:607:PCW:H412	3:C:611:PCW:H31	0.88	1.45	9	3
2:B:75:GLY:CA	7:B:237:EWS:BRA	0.88	2.76	9	1
1:C:488:LYS:HD3	3:C:623:PCW:H272	0.87	1.41	9	1
3:B:217:PCW:H11	7:B:237:EWS:CAM	0.87	2.00	7	1
3:A:407:PCW:H342	4:B:225:17F:H9	0.87	1.44	6	5
3:A:410:PCW:H372	4:C:633:17F:H36	0.87	1.46	4	1
3:B:221:PCW:H63	7:B:237:EWS:BRA	0.86	2.25	1	2
3:B:210:PCW:C7	7:B:237:EWS:CAO	0.86	2.53	10	1
1:A:396:LYS:HZ3	3:A:407:PCW:H271	0.86	1.04	5	1
1:A:214:PHE:HZ	3:A:404:PCW:H162	0.85	1.12	4	1
3:C:618:PCW:H121	3:C:620:PCW:H381	0.85	1.47	10	1
3:A:410:PCW:H331	4:C:633:17F:H37	0.85	1.49	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:214:PHE:HZ	3:A:404:PCW:H171	0.85	1.27	1	2
4:B:223:17F:H35	4:B:225:17F:H20A	0.84	1.46	6	1
1:A:308:ARG:HG3	1:C:469:LEU:CD2	0.84	2.01	9	3
3:B:219:PCW:O2P	7:B:237:EWS:CAI	0.84	2.25	9	1
1:A:392:GLU:CD	1:A:395:LYS:HD2	0.84	1.93	5	1
3:C:621:PCW:H361	3:C:629:PCW:H212	0.84	1.50	10	3
4:A:411:17F:H35	3:C:624:PCW:H482	0.84	1.47	3	2
3:B:208:PCW:H61	7:B:237:EWS:BRA	0.84	2.28	4	1
3:B:207:PCW:H71	7:B:237:EWS:BRA	0.84	2.28	10	1
1:A:392:GLU:OE1	1:A:395:LYS:CD	0.83	2.25	5	1
3:A:410:PCW:H121	4:C:633:17F:H30	0.83	1.47	8	8
3:B:207:PCW:O3P	7:B:237:EWS:CAK	0.83	2.26	6	1
3:B:231:PCW:H341	3:C:604:PCW:H322	0.83	1.50	6	7
3:A:407:PCW:H122	4:B:223:17F:H20	0.83	1.48	3	2
1:C:488:LYS:NZ	3:C:623:PCW:H283	0.83	1.87	4	1
2:B:56:LEU:HD22	7:B:237:EWS:CAZ	0.82	2.03	8	4
1:C:465:GLU:O	1:C:469:LEU:CB	0.82	2.27	6	3
3:A:407:PCW:H342	4:B:225:17F:H8A	0.82	1.49	9	1
2:B:70:GLN:HG3	3:B:220:PCW:H41	0.82	1.51	9	1
4:B:234:17F:H57	3:C:625:PCW:H141	0.82	1.52	1	6
4:C:633:17F:H4A	4:C:633:17F:H2	0.82	1.49	2	2
1:A:393:TYR:HD1	3:A:407:PCW:C28	0.82	1.86	8	2
1:A:314:ASP:HA	1:A:317:ARG:HD2	0.81	1.52	1	3
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.81	1.49	4	6
3:B:201:PCW:H411	3:B:219:PCW:H452	0.81	1.50	5	3
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.81	1.52	1	8
3:B:208:PCW:H371	4:B:226:17F:H18A	0.81	1.48	10	1
2:B:7:VAL:CG2	7:B:237:EWS:CAX	0.81	2.58	8	3
3:A:410:PCW:H362	4:C:633:17F:H36	0.80	1.53	6	2
3:A:407:PCW:H331	4:B:223:17F:H20	0.80	1.52	10	1
3:B:208:PCW:H321	7:B:237:EWS:CAO	0.80	2.05	4	1
1:A:214:PHE:CZ	3:A:404:PCW:H161	0.80	2.11	10	1
3:B:207:PCW:H12	7:B:237:EWS:CAO	0.80	2.06	6	1
3:C:617:PCW:H212	4:C:632:17F:H41	0.80	1.50	6	2
3:C:607:PCW:H252	4:C:631:17F:H39	0.80	1.53	3	3
3:B:219:PCW:H73	7:B:237:EWS:NAA	0.80	1.91	9	1
3:B:221:PCW:C4	7:B:237:EWS:BRA	0.80	2.84	1	1
1:A:308:ARG:CB	1:C:469:LEU:HD11	0.80	2.06	4	2
3:B:202:PCW:H12	3:B:212:PCW:H322	0.80	1.52	8	1
3:A:401:PCW:H40	3:C:613:PCW:H251	0.79	1.52	1	1
3:B:232:PCW:H122	3:C:625:PCW:H171	0.79	1.54	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:411:17F:H47	3:C:617:PCW:H422	0.79	1.52	8	1
3:C:618:PCW:H122	3:C:620:PCW:H381	0.79	1.52	1	3
1:A:279:LEU:HD22	1:C:495:LYS:HG2	0.79	1.51	6	2
3:C:617:PCW:H222	4:C:635:17F:H39	0.79	1.54	10	3
3:C:618:PCW:H381	3:C:619:PCW:H121	0.79	1.54	4	1
1:A:393:TYR:HE1	3:A:407:PCW:H283	0.79	1.35	8	1
1:A:396:LYS:HZ2	3:A:407:PCW:H271	0.79	1.00	5	1
3:A:410:PCW:H352	4:C:633:17F:H36	0.78	1.54	3	5
3:B:202:PCW:H442	4:B:226:17F:H12A	0.78	1.53	6	4
2:B:71:TYR:CB	7:B:237:EWS:CAF	0.78	2.60	5	1
3:A:408:PCW:H422	3:B:204:PCW:H451	0.78	1.54	3	1
3:B:205:PCW:H83	7:B:237:EWS:BRA	0.78	2.33	6	2
3:B:208:PCW:H31	3:B:221:PCW:H141	0.78	1.56	8	2
3:A:402:PCW:H39	3:B:214:PCW:H232	0.78	1.54	2	1
3:B:217:PCW:H152	3:B:218:PCW:H141	0.77	1.55	10	2
1:C:455:TYR:OH	3:C:601:PCW:H222	0.77	1.78	9	1
3:B:221:PCW:C3	7:B:237:EWS:CLA	0.77	2.69	9	1
3:B:210:PCW:H52	7:B:237:EWS:CAK	0.77	2.10	10	1
1:A:391:GLU:O	1:A:395:LYS:CG	0.77	2.31	5	1
3:B:211:PCW:H382	4:B:229:17F:H10A	0.77	1.55	3	4
1:A:393:TYR:CE1	3:A:407:PCW:H272	0.77	2.14	2	2
3:C:605:PCW:H182	3:C:626:PCW:H151	0.77	1.56	2	3
1:A:393:TYR:HH	3:A:407:PCW:H271	0.77	0.97	2	1
1:C:465:GLU:O	1:C:469:LEU:CD1	0.76	2.32	6	3
1:A:393:TYR:HD1	1:A:396:LYS:HE3	0.76	1.39	5	1
2:B:54:ASP:OD2	7:B:237:EWS:BRA	0.76	2.58	7	1
2:B:56:LEU:HD22	7:B:237:EWS:CAX	0.76	2.10	9	2
2:B:38:ASP:HB3	2:B:57:ASP:HB3	0.76	1.58	2	2
1:A:392:GLU:O	1:A:396:LYS:HG3	0.76	1.80	5	1
1:A:308:ARG:HD3	1:C:469:LEU:HD21	0.76	1.57	6	1
3:B:221:PCW:H72	7:B:237:EWS:BRA	0.76	2.36	1	1
3:B:203:PCW:H11	3:B:220:PCW:H81	0.76	1.57	9	1
3:A:410:PCW:H381	4:C:633:17F:H36	0.76	1.58	10	3
3:A:406:PCW:H182	3:A:409:PCW:H261	0.76	1.55	7	1
3:A:406:PCW:H152	4:B:226:17F:H34	0.75	1.55	5	1
3:A:406:PCW:H40	4:B:226:17F:H69	0.75	1.59	10	1
3:B:202:PCW:H421	4:B:226:17F:H40	0.75	1.57	7	4
1:A:297:LYS:HE2	1:C:476:PRO:HB2	0.75	1.56	3	2
3:A:408:PCW:H422	3:B:204:PCW:H472	0.75	1.58	9	1
3:A:410:PCW:H331	4:C:633:17F:H12A	0.75	1.59	10	6
3:B:201:PCW:H251	4:B:228:17F:H64	0.75	1.57	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:210:PCW:H161	4:B:224:17F:H18A	0.75	1.58	8	1
3:C:611:PCW:H242	3:C:617:PCW:H421	0.75	1.58	9	1
3:B:208:PCW:C8	7:B:237:EWS:BRA	0.75	2.83	4	1
4:B:226:17F:HN1	7:B:237:EWS:CAL	0.75	1.93	4	1
1:C:563:LYS:HB2	1:C:564:PRO:HD3	0.75	1.55	4	4
3:A:410:PCW:H332	4:C:633:17F:H12A	0.75	1.56	1	2
4:B:226:17F:H12	4:B:230:17F:H11	0.75	1.58	5	1
3:C:611:PCW:H381	3:C:617:PCW:H412	0.74	1.58	2	3
1:A:396:LYS:CE	3:A:407:PCW:C28	0.74	2.63	5	1
3:C:611:PCW:H482	4:C:635:17F:H42	0.74	1.59	1	3
4:B:234:17F:H56	3:C:625:PCW:H19	0.74	1.59	10	1
1:A:308:ARG:CG	1:C:469:LEU:CD1	0.74	2.39	4	1
3:B:217:PCW:H2	7:B:237:EWS:CLA	0.74	2.18	7	1
1:A:214:PHE:CZ	3:A:404:PCW:C16	0.74	2.69	4	3
4:A:411:17F:H29	4:C:631:17F:H65	0.74	1.59	1	1
3:C:618:PCW:H121	3:C:620:PCW:H382	0.74	1.57	5	3
1:A:393:TYR:CD1	1:A:396:LYS:HE3	0.73	2.18	5	1
2:B:7:VAL:HG21	7:B:237:EWS:CAX	0.73	2.13	6	2
4:B:223:17F:H1	4:B:223:17F:H4	0.73	1.58	3	1
2:B:71:TYR:HB2	7:B:237:EWS:CAC	0.73	2.12	8	1
3:A:407:PCW:H121	4:B:223:17F:H20A	0.73	1.59	10	2
4:B:234:17F:H31	3:C:625:PCW:H19	0.73	1.60	8	1
3:C:619:PCW:H322	3:C:621:PCW:H172	0.73	1.60	3	1
3:C:621:PCW:H31	3:C:629:PCW:H151	0.73	1.59	3	1
2:B:56:LEU:CD2	7:B:237:EWS:CAZ	0.73	2.65	5	1
3:C:606:PCW:H471	3:C:622:PCW:H39	0.73	1.58	6	1
3:B:215:PCW:H221	3:C:609:PCW:H483	0.73	1.58	8	1
3:C:617:PCW:H241	4:C:635:17F:H44	0.73	1.57	10	1
4:B:228:17F:C4	4:B:228:17F:H1	0.73	2.12	10	1
4:B:225:17F:H63	3:C:626:PCW:H262	0.73	1.61	2	1
1:C:455:TYR:HE2	3:C:601:PCW:H231	0.73	1.43	3	1
3:A:407:PCW:H331	4:B:223:17F:H31	0.73	1.60	9	3
1:A:393:TYR:HD1	1:A:396:LYS:CE	0.73	1.96	5	1
3:B:219:PCW:H212	3:C:605:PCW:H281	0.73	1.58	10	1
3:A:410:PCW:H121	4:C:633:17F:H29	0.73	1.61	1	2
4:C:631:17F:H60	4:C:631:17F:H37	0.73	1.60	2	1
3:C:608:PCW:H31	3:C:628:PCW:H332	0.73	1.58	8	3
3:B:220:PCW:H62	3:B:220:PCW:H2	0.73	1.60	9	1
3:B:210:PCW:H72	7:B:237:EWS:CAO	0.73	2.13	10	1
3:B:209:PCW:H252	3:B:213:PCW:H431	0.72	1.61	9	2
3:B:231:PCW:H341	3:C:604:PCW:H331	0.72	1.60	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H182	3:A:409:PCW:H242	0.72	1.61	5	2
3:A:410:PCW:H132	4:C:633:17F:H11A	0.72	1.60	2	4
3:C:613:PCW:H162	3:C:626:PCW:H451	0.72	1.60	7	4
4:B:234:17F:H9A	4:B:234:17F:H20A	0.72	1.62	5	2
3:C:613:PCW:H162	3:C:622:PCW:H161	0.72	1.59	9	3
3:B:209:PCW:H122	3:B:213:PCW:H122	0.72	1.61	3	3
3:B:217:PCW:H42	3:B:217:PCW:H321	0.72	1.61	5	2
3:C:617:PCW:H211	4:C:632:17F:H41	0.72	1.58	5	1
3:C:611:PCW:H372	3:C:617:PCW:H412	0.72	1.62	4	1
3:A:409:PCW:H481	3:B:208:PCW:H462	0.72	1.62	6	1
3:B:207:PCW:H20	3:B:232:PCW:H483	0.72	1.60	1	1
3:C:610:PCW:H341	3:C:614:PCW:H121	0.72	1.60	1	2
2:B:7:VAL:CG1	7:B:237:EWS:NAW	0.71	2.53	7	2
4:B:223:17F:H1	4:B:223:17F:C4	0.71	2.15	3	3
3:B:210:PCW:H172	4:B:224:17F:H18	0.71	1.60	5	3
1:A:308:ARG:CG	1:C:469:LEU:HD21	0.71	2.14	9	2
3:A:403:PCW:H332	3:B:204:PCW:H32	0.71	1.62	10	2
4:B:234:17F:H9	4:B:234:17F:H20	0.71	1.60	9	1
3:A:408:PCW:H342	3:C:604:PCW:H232	0.71	1.61	4	1
3:C:618:PCW:H122	3:C:620:PCW:H382	0.71	1.63	7	2
4:B:234:17F:H12	4:C:631:17F:H38	0.71	1.61	6	1
3:A:403:PCW:H351	3:A:403:PCW:H161	0.71	1.62	2	1
3:B:210:PCW:H361	4:B:224:17F:H19A	0.71	1.63	8	1
3:C:607:PCW:H332	3:C:611:PCW:H131	0.71	1.61	3	1
3:A:407:PCW:H352	4:B:223:17F:H56	0.71	1.61	10	3
3:C:613:PCW:H151	3:C:626:PCW:H431	0.71	1.63	7	4
2:B:74:THR:HB	4:B:230:17F:H1A	0.70	1.61	1	1
3:A:407:PCW:H331	4:B:223:17F:H32	0.70	1.62	8	4
3:C:627:PCW:H331	3:C:628:PCW:H121	0.70	1.63	6	7
4:A:411:17F:H1A	4:C:631:17F:H6A	0.70	1.63	4	6
3:B:217:PCW:C2	7:B:237:EWS:CLA	0.70	2.76	7	1
3:B:220:PCW:H122	3:B:220:PCW:H361	0.70	1.63	8	1
4:B:228:17F:H4	4:B:228:17F:C1	0.70	2.17	2	2
3:B:210:PCW:H372	4:B:224:17F:H20A	0.70	1.62	7	2
3:B:210:PCW:H73	7:B:237:EWS:CAO	0.70	2.15	10	1
3:B:233:PCW:H411	3:C:604:PCW:H39	0.70	1.63	2	2
2:B:39:SER:HB2	7:B:237:EWS:BRA	0.70	2.42	7	1
3:B:209:PCW:H331	3:B:213:PCW:H121	0.70	1.63	3	1
3:A:407:PCW:H151	4:B:223:17F:H33	0.70	1.63	9	2
3:B:210:PCW:H331	4:B:224:17F:H19	0.70	1.62	7	1
3:B:217:PCW:C1	7:B:237:EWS:CLA	0.70	2.77	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:56:LEU:HD13	7:B:237:EWS:CBA	0.70	2.16	1	1
3:B:231:PCW:H371	3:C:604:PCW:H212	0.70	1.64	10	4
4:B:223:17F:H51	3:C:626:PCW:H231	0.70	1.64	7	1
3:B:208:PCW:H331	3:B:221:PCW:H19	0.70	1.63	7	2
3:A:402:PCW:H341	3:B:213:PCW:H321	0.70	1.62	3	1
3:B:212:PCW:H131	3:B:212:PCW:H332	0.70	1.63	4	1
3:B:201:PCW:H371	4:B:226:17F:H42	0.70	1.63	9	1
3:C:609:PCW:H162	4:C:632:17F:H18	0.69	1.62	8	2
3:C:615:PCW:H132	3:C:622:PCW:H382	0.69	1.63	3	3
3:B:202:PCW:H331	4:B:228:17F:H4A	0.69	1.62	8	1
3:B:205:PCW:H232	3:B:220:PCW:H412	0.69	1.64	8	1
2:B:7:VAL:HG22	7:B:237:EWS:NAW	0.69	2.03	1	2
1:A:396:LYS:CD	3:A:407:PCW:C28	0.69	2.41	5	1
2:B:71:TYR:HB2	7:B:237:EWS:CAE	0.69	2.17	5	2
3:B:207:PCW:H162	3:B:232:PCW:H281	0.69	1.63	10	1
3:B:210:PCW:H131	3:B:216:PCW:H2	0.69	1.63	2	2
3:B:217:PCW:H11	7:B:237:EWS:CLA	0.69	2.24	7	1
3:B:211:PCW:H412	4:B:229:17F:H60	0.69	1.65	2	1
3:B:209:PCW:H181	3:B:213:PCW:H19	0.69	1.64	3	2
3:C:611:PCW:H341	3:C:617:PCW:H341	0.69	1.64	4	1
3:A:407:PCW:H121	4:B:223:17F:H33	0.69	1.65	5	4
1:C:458:ASP:HA	1:C:461:LYS:HE2	0.69	1.63	5	1
3:C:611:PCW:H171	3:C:617:PCW:H352	0.69	1.65	5	1
2:B:7:VAL:HG23	7:B:237:EWS:NAW	0.69	2.03	8	1
3:C:611:PCW:H181	3:C:617:PCW:H351	0.69	1.63	9	1
1:A:308:ARG:HG2	1:C:469:LEU:HD11	0.69	0.70	4	1
4:B:228:17F:H63	3:C:615:PCW:H472	0.69	1.64	5	1
3:B:231:PCW:H472	3:C:604:PCW:H271	0.69	1.63	10	1
1:A:255:GLN:HB2	1:A:256:PRO:HD3	0.68	1.65	3	3
3:B:202:PCW:H451	4:B:226:17F:H10A	0.68	1.64	5	1
3:B:219:PCW:H342	4:B:226:17F:H37	0.68	1.63	1	1
3:B:218:PCW:H262	3:C:625:PCW:H421	0.68	1.63	4	1
3:A:406:PCW:H151	4:B:226:17F:H34	0.68	1.64	8	1
4:B:234:17F:H69	4:C:631:17F:H77	0.68	1.65	2	1
3:A:408:PCW:H372	3:B:204:PCW:H481	0.68	1.64	10	1
3:C:621:PCW:H412	3:C:629:PCW:H19	0.68	1.62	3	1
3:B:202:PCW:H483	3:B:208:PCW:H411	0.68	1.64	5	2
2:B:79:LEU:HG	2:B:159:LEU:HD22	0.68	1.65	7	7
3:B:207:PCW:H321	3:B:220:PCW:H372	0.68	1.64	4	1
1:A:396:LYS:HD3	3:A:407:PCW:C27	0.68	2.17	5	1
4:B:234:17F:H10	4:C:631:17F:H41	0.68	1.64	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:407:PCW:H131	4:B:223:17F:H33	0.68	1.65	6	2
3:B:205:PCW:H62	7:B:237:EWS:BRA	0.68	2.43	6	1
3:C:619:PCW:H411	3:C:621:PCW:H472	0.68	1.64	3	1
3:B:211:PCW:H121	4:B:229:17F:H9A	0.68	1.66	9	3
3:B:209:PCW:H351	3:B:213:PCW:H132	0.68	1.65	7	1
3:A:406:PCW:H441	3:A:409:PCW:H20	0.68	1.64	2	2
1:A:392:GLU:OE2	1:A:395:LYS:NZ	0.68	2.24	5	1
1:A:308:ARG:HD3	1:C:469:LEU:HD11	0.68	1.65	6	2
1:C:590:GLU:HA	1:C:593:LYS:HE3	0.68	1.62	7	2
1:C:488:LYS:CE	3:C:623:PCW:C27	0.68	2.52	4	1
3:B:209:PCW:H141	3:B:213:PCW:H332	0.67	1.65	10	1
3:B:201:PCW:H242	4:B:228:17F:H59	0.67	1.65	4	1
3:C:611:PCW:H152	3:C:617:PCW:H321	0.67	1.66	5	6
3:B:202:PCW:H422	4:B:226:17F:H12A	0.67	1.63	9	1
3:B:233:PCW:H32	3:C:604:PCW:H11	0.67	1.65	9	3
1:A:276:VAL:O	1:A:280:ARG:HB2	0.67	1.88	7	3
2:B:5:LYS:CB	7:B:237:EWS:CAT	0.67	2.69	1	2
3:B:203:PCW:H142	4:B:229:17F:H20	0.67	1.66	5	1
3:B:216:PCW:H73	4:B:224:17F:HN1A	0.67	1.49	6	1
3:A:406:PCW:H431	3:A:409:PCW:H241	0.67	1.65	7	1
3:C:627:PCW:H351	3:C:628:PCW:H121	0.67	1.66	1	7
1:A:279:LEU:HB3	1:C:495:LYS:HE3	0.67	1.65	9	3
3:B:203:PCW:H142	3:B:211:PCW:H39	0.67	1.67	7	1
3:C:607:PCW:H332	3:C:611:PCW:H122	0.67	1.67	10	1
1:A:388:SER:HB2	1:C:594:LYS:HE2	0.67	1.66	2	1
1:C:455:TYR:OH	3:C:601:PCW:C23	0.67	2.40	8	2
1:A:396:LYS:CD	3:A:407:PCW:C27	0.67	2.72	5	1
3:A:403:PCW:H332	3:B:204:PCW:H31	0.67	1.66	8	1
3:B:213:PCW:H332	3:B:216:PCW:H122	0.67	1.67	9	1
2:B:56:LEU:CG	7:B:237:EWS:OAB	0.67	2.43	1	2
4:B:229:17F:H4	4:B:229:17F:H1	0.67	1.65	6	1
3:B:215:PCW:H252	3:C:609:PCW:H472	0.67	1.66	3	1
3:B:207:PCW:H39	3:B:211:PCW:H381	0.67	1.66	6	1
1:A:393:TYR:CD1	1:A:396:LYS:NZ	0.66	2.62	5	1
4:B:224:17F:H11	4:B:230:17F:H59	0.66	1.67	5	1
4:B:229:17F:H45	3:C:604:PCW:H481	0.66	1.66	5	1
4:B:234:17F:H10A	4:B:234:17F:H34	0.66	1.66	7	1
3:B:201:PCW:H222	4:B:225:17F:H65	0.66	1.65	8	1
1:C:503:MET:HA	1:C:506:ARG:HD2	0.66	1.67	1	4
3:A:409:PCW:H441	3:C:627:PCW:H441	0.66	1.65	2	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.66	1.90	5	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:218:PCW:H261	3:C:629:PCW:H283	0.66	1.66	3	1
3:B:202:PCW:H361	3:B:212:PCW:H331	0.66	1.67	5	1
3:B:220:PCW:H472	3:B:233:PCW:H283	0.66	1.67	6	1
3:B:207:PCW:C1	7:B:237:EWS:CAK	0.66	2.72	6	1
2:B:54:ASP:CG	7:B:237:EWS:BRA	0.66	2.89	7	1
3:C:619:PCW:H40	3:C:629:PCW:H252	0.66	1.67	8	2
3:C:606:PCW:H232	3:C:615:PCW:H181	0.66	1.65	5	1
3:A:408:PCW:H451	3:B:204:PCW:H452	0.66	1.68	6	1
3:C:613:PCW:H351	3:C:626:PCW:H411	0.66	1.65	8	3
1:A:214:PHE:CE1	3:A:404:PCW:H162	0.66	2.25	4	1
3:C:611:PCW:H161	3:C:617:PCW:H351	0.66	1.67	4	2
3:C:621:PCW:H381	3:C:629:PCW:H171	0.66	1.66	9	6
3:C:614:PCW:H63	3:C:629:PCW:H32	0.66	1.67	9	1
1:A:369:GLU:OE1	1:A:373:GLN:CD	0.65	2.34	1	1
3:B:210:PCW:H483	4:B:224:17F:H49	0.65	1.68	4	1
3:A:402:PCW:H341	3:B:213:PCW:H322	0.65	1.67	4	1
3:B:233:PCW:H172	3:C:625:PCW:H232	0.65	1.66	5	1
3:B:210:PCW:H331	4:B:224:17F:H5	0.65	1.65	6	2
3:B:201:PCW:H42	3:B:219:PCW:H322	0.65	1.66	7	1
3:B:220:PCW:H52	7:B:237:EWS:CAR	0.65	2.22	8	1
3:B:210:PCW:H121	4:B:224:17F:H18A	0.65	1.66	10	1
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.65	1.68	3	2
1:C:455:TYR:HH	3:C:601:PCW:H211	0.65	1.50	4	2
1:A:396:LYS:CE	3:A:407:PCW:C27	0.65	2.74	5	1
4:B:234:17F:H40	4:B:234:17F:H64	0.65	1.68	5	1
1:A:214:PHE:HZ	3:A:404:PCW:C17	0.65	2.04	1	1
3:C:611:PCW:H411	3:C:617:PCW:H432	0.65	1.68	1	1
3:C:616:PCW:H412	3:C:622:PCW:H221	0.65	1.66	4	1
3:B:212:PCW:H121	4:B:226:17F:H6	0.65	1.68	3	1
3:B:221:PCW:C6	7:B:237:EWS:BRA	0.65	2.98	1	1
4:B:226:17F:H6A	7:B:237:EWS:CAM	0.65	2.22	2	1
3:A:402:PCW:H362	3:B:214:PCW:H161	0.65	1.68	1	1
3:C:611:PCW:H32	3:C:617:PCW:H62	0.65	1.68	5	3
4:B:225:17F:H12A	4:B:225:17F:H62	0.65	1.68	3	1
2:B:35:THR:HG21	2:B:57:ASP:HB3	0.65	1.68	3	1
3:C:611:PCW:H442	4:C:635:17F:H43	0.65	1.66	7	2
3:C:617:PCW:H221	4:C:635:17F:H44	0.65	1.67	9	1
3:B:209:PCW:H282	3:B:213:PCW:H431	0.65	1.69	5	1
1:A:393:TYR:OH	3:A:403:PCW:H281	0.65	1.91	2	1
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.65	1.68	6	2
3:A:403:PCW:H431	3:C:618:PCW:H482	0.65	1.68	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:401:PCW:H472	3:C:626:PCW:H482	0.65	1.67	1	2
3:C:608:PCW:H31	3:C:628:PCW:H331	0.65	1.68	6	1
2:B:7:VAL:HB	2:B:78:PHE:CD1	0.65	2.26	8	2
3:B:207:PCW:H381	3:B:232:PCW:H242	0.64	1.69	3	1
3:C:628:PCW:H362	3:C:628:PCW:H142	0.64	1.68	7	1
3:B:203:PCW:H371	3:B:220:PCW:H151	0.64	1.68	8	1
3:B:207:PCW:H61	7:B:237:EWS:BRA	0.64	2.44	10	1
3:B:231:PCW:H362	3:C:604:PCW:H181	0.64	1.70	8	4
3:A:407:PCW:H341	4:B:225:17F:H11	0.64	1.69	9	2
3:B:203:PCW:H141	3:B:207:PCW:H351	0.64	1.68	1	1
4:B:230:17F:H76	4:C:631:17F:H54	0.64	1.70	3	2
4:C:633:17F:C4	4:C:633:17F:H2	0.64	2.23	2	1
3:C:601:PCW:H421	4:C:630:17F:H54	0.64	1.67	4	1
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.64	1.69	7	3
3:B:205:PCW:H211	3:B:219:PCW:H141	0.64	1.69	1	1
3:C:611:PCW:H151	3:C:617:PCW:H352	0.64	1.67	2	1
1:A:308:ARG:CD	1:C:469:LEU:HD11	0.64	2.23	7	1
3:B:205:PCW:H161	3:B:219:PCW:H122	0.64	1.68	5	1
3:A:409:PCW:H481	3:B:208:PCW:H441	0.63	1.68	1	1
2:B:84:ILE:HD12	2:B:123:ARG:HG3	0.63	1.68	2	3
2:B:71:TYR:CB	7:B:237:EWS:CAE	0.63	2.76	5	1
3:A:406:PCW:H231	3:A:409:PCW:H261	0.63	1.69	1	1
3:B:213:PCW:H232	3:C:611:PCW:H422	0.63	1.67	9	1
3:C:621:PCW:H372	3:C:629:PCW:H152	0.63	1.69	10	5
3:B:202:PCW:H431	3:B:212:PCW:H172	0.63	1.69	2	1
3:C:613:PCW:H161	3:C:622:PCW:H19	0.63	1.71	5	2
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.63	1.68	9	1
3:B:204:PCW:H483	3:B:231:PCW:H422	0.63	1.70	6	1
1:A:264:LYS:HE2	1:C:509:ALA:HB1	0.63	1.69	9	1
3:B:231:PCW:H412	3:C:604:PCW:H432	0.63	1.69	1	1
3:B:204:PCW:H232	3:C:618:PCW:H481	0.63	1.69	1	1
3:B:207:PCW:H20	3:B:232:PCW:H481	0.63	1.69	2	1
4:B:228:17F:H1	4:B:228:17F:C4	0.63	2.19	2	2
3:C:606:PCW:H182	3:C:615:PCW:H142	0.63	1.70	2	1
3:B:213:PCW:H441	3:B:216:PCW:H251	0.63	1.70	5	1
3:B:209:PCW:H171	3:B:216:PCW:H162	0.63	1.70	7	1
4:B:227:17F:H75	3:C:602:PCW:H431	0.63	1.71	1	1
3:B:203:PCW:H322	3:B:220:PCW:H121	0.63	1.70	6	3
3:A:408:PCW:H371	3:A:410:PCW:H361	0.63	1.69	6	1
1:C:470:TYR:CE1	4:C:632:17F:H76	0.63	2.28	1	2
3:B:209:PCW:H251	3:C:611:PCW:H483	0.63	1.69	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:209:PCW:H382	3:B:213:PCW:H152	0.63	1.71	6	2
4:B:227:17F:H29	4:B:227:17F:H39	0.63	1.70	8	1
1:A:393:TYR:CD1	1:A:396:LYS:CE	0.62	2.80	5	1
1:A:301:LEU:HD22	1:C:473:LYS:HG2	0.62	1.69	7	2
3:B:219:PCW:H232	4:B:230:17F:H73	0.62	1.69	1	1
3:C:611:PCW:H182	3:C:617:PCW:H351	0.62	1.71	3	3
3:B:205:PCW:H251	3:B:219:PCW:H422	0.62	1.69	7	1
3:B:203:PCW:H481	3:B:233:PCW:H481	0.62	1.72	8	1
3:C:617:PCW:H221	4:C:635:17F:H40	0.62	1.70	2	1
3:A:403:PCW:H352	3:A:403:PCW:H122	0.62	1.71	5	1
3:C:608:PCW:H361	3:C:628:PCW:H212	0.62	1.71	7	2
1:C:505:ASP:HA	1:C:508:ARG:HD2	0.62	1.71	7	3
3:B:201:PCW:H483	3:C:627:PCW:H252	0.62	1.71	10	1
4:B:234:17F:H10	4:C:631:17F:H38	0.62	1.71	4	2
1:A:392:GLU:HA	1:A:395:LYS:HB2	0.62	1.71	5	1
2:B:56:LEU:HD11	3:B:219:PCW:H61	0.62	1.68	6	1
3:B:233:PCW:H171	3:C:625:PCW:H232	0.62	1.70	6	1
3:C:615:PCW:H372	3:C:622:PCW:H351	0.62	1.71	10	1
1:A:308:ARG:CB	1:C:469:LEU:CD1	0.62	2.76	4	1
2:B:54:ASP:HB3	7:B:237:EWS:BRA	0.62	2.49	2	1
1:A:393:TYR:CE2	3:A:407:PCW:H272	0.62	2.25	3	1
3:B:232:PCW:H371	3:B:232:PCW:H152	0.62	1.70	3	1
3:A:407:PCW:H152	4:B:223:17F:H33	0.62	1.72	5	3
3:A:406:PCW:H431	3:A:409:PCW:H251	0.62	1.71	8	1
3:A:407:PCW:C34	4:B:225:17F:H11	0.62	2.25	9	1
3:B:202:PCW:H341	3:B:212:PCW:H351	0.62	1.71	1	1
4:C:631:17F:C21	4:C:631:17F:H60	0.62	2.25	2	1
3:C:608:PCW:H352	3:C:609:PCW:H352	0.62	1.72	6	1
3:B:221:PCW:H2	4:B:230:17F:H18A	0.62	1.71	7	1
3:A:409:PCW:H371	3:C:627:PCW:H341	0.61	1.72	5	3
3:B:232:PCW:H331	3:C:619:PCW:H341	0.61	1.71	3	2
3:C:611:PCW:H181	3:C:617:PCW:H341	0.61	1.70	10	1
3:B:220:PCW:H142	3:B:220:PCW:H39	0.61	1.73	1	1
3:B:210:PCW:H352	4:B:224:17F:H19	0.61	1.71	6	2
3:C:605:PCW:H122	3:C:605:PCW:H351	0.61	1.69	2	1
3:C:610:PCW:H461	3:C:614:PCW:H19	0.61	1.70	5	1
3:B:202:PCW:H322	3:B:212:PCW:H371	0.61	1.71	8	1
3:B:210:PCW:H362	4:B:224:17F:H8	0.61	1.71	9	1
4:B:230:17F:H49	3:C:613:PCW:H452	0.61	1.70	2	2
3:B:205:PCW:H231	3:B:219:PCW:H412	0.61	1.71	4	1
3:B:201:PCW:H342	3:B:219:PCW:H362	0.61	1.72	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:226:17F:H6A	7:B:237:EWS:CLA	0.61	2.32	1	1
3:B:208:PCW:H151	3:B:215:PCW:H171	0.61	1.73	2	1
1:C:418:GLN:O	1:C:422:VAL:HB	0.61	1.95	9	2
1:A:334:ARG:HD2	1:C:440:GLU:OE1	0.61	1.96	6	2
3:A:401:PCW:H61	4:B:226:17F:H1A	0.61	1.72	8	1
1:A:330:ARG:HH21	1:C:447:GLU:HB2	0.61	1.56	5	1
3:B:218:PCW:H482	3:C:629:PCW:H281	0.61	1.72	9	2
3:B:217:PCW:H172	3:B:218:PCW:H161	0.61	1.70	6	1
3:B:203:PCW:H232	3:C:621:PCW:H481	0.61	1.72	9	1
3:B:219:PCW:H341	4:B:226:17F:H37	0.61	1.73	10	1
2:B:6:LEU:HB2	2:B:55:ILE:HG13	0.61	1.71	1	1
3:A:409:PCW:H442	3:C:605:PCW:H231	0.61	1.70	8	1
3:B:209:PCW:H241	3:C:611:PCW:H461	0.61	1.71	5	1
3:B:219:PCW:H422	3:B:220:PCW:H182	0.61	1.72	3	1
3:B:202:PCW:H122	4:B:228:17F:H9	0.61	1.72	10	3
3:B:218:PCW:H372	3:C:603:PCW:H372	0.61	1.71	8	1
3:B:209:PCW:H161	3:B:216:PCW:H182	0.61	1.71	10	1
3:B:201:PCW:H362	3:B:219:PCW:H351	0.60	1.71	4	1
3:A:401:PCW:H462	3:C:613:PCW:H251	0.60	1.71	7	1
4:B:225:17F:H75	3:C:615:PCW:H242	0.60	1.71	8	1
3:B:210:PCW:H472	4:B:227:17F:H44	0.60	1.73	9	1
3:B:220:PCW:H371	3:B:220:PCW:H122	0.60	1.73	1	1
3:A:410:PCW:H121	4:C:633:17F:C1X	0.60	2.25	1	4
3:B:205:PCW:H39	4:B:224:17F:H59	0.60	1.73	3	1
3:C:607:PCW:H242	4:C:631:17F:H39	0.60	1.73	6	1
3:A:407:PCW:H331	4:B:223:17F:C1Y	0.60	2.27	3	4
3:A:408:PCW:H322	3:B:231:PCW:H372	0.60	1.72	3	1
3:B:210:PCW:H231	4:B:227:17F:H44	0.60	1.74	4	1
3:A:407:PCW:H451	4:B:223:17F:H71	0.60	1.73	5	2
3:B:201:PCW:O2P	7:B:237:EWS:CAK	0.60	2.49	5	1
3:B:219:PCW:N	7:B:237:EWS:BRA	0.60	2.89	6	1
3:B:210:PCW:H332	4:B:224:17F:H5	0.60	1.74	7	1
1:C:561:LYS:HA	1:C:565:ALA:HB3	0.60	1.73	6	2
3:B:232:PCW:H151	3:C:625:PCW:H171	0.60	1.73	3	2
3:B:206:PCW:H372	3:B:215:PCW:H412	0.60	1.72	3	1
3:B:209:PCW:H122	3:B:213:PCW:H132	0.60	1.74	8	1
1:A:365:LYS:O	1:A:369:GLU:HB2	0.60	1.97	1	2
3:B:207:PCW:H471	3:B:232:PCW:H39	0.60	1.71	2	1
3:B:211:PCW:H342	4:B:229:17F:H11	0.60	1.73	9	3
3:B:203:PCW:H162	3:B:211:PCW:H39	0.60	1.73	1	1
3:B:231:PCW:C34	3:C:604:PCW:H322	0.60	2.25	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:621:PCW:H352	3:C:629:PCW:H162	0.60	1.72	8	1
3:B:219:PCW:H221	3:B:233:PCW:H272	0.60	1.71	10	1
3:C:629:PCW:H242	4:C:634:17F:H45	0.60	1.72	10	1
3:B:211:PCW:H212	3:B:217:PCW:H411	0.60	1.73	2	1
4:B:223:17F:H43	3:C:626:PCW:H271	0.60	1.72	2	1
2:B:144:THR:HA	2:B:150:GLN:O	0.60	1.97	4	2
2:B:38:ASP:HB2	2:B:57:ASP:HB3	0.60	1.73	1	1
3:B:213:PCW:H231	4:C:635:17F:H47	0.60	1.73	1	1
3:C:613:PCW:H73	3:C:627:PCW:H61	0.60	1.74	2	1
3:C:602:PCW:H271	4:C:630:17F:H52	0.60	1.74	3	1
3:B:201:PCW:P	7:B:237:EWS:CAK	0.60	2.90	5	1
2:B:56:LEU:HD22	7:B:237:EWS:CBA	0.60	2.27	9	2
3:C:610:PCW:H372	3:C:614:PCW:H221	0.60	1.73	10	1
3:B:209:PCW:H171	3:B:213:PCW:H171	0.60	1.73	5	1
4:A:411:17F:H54	3:C:607:PCW:H222	0.60	1.71	7	2
3:B:205:PCW:H171	4:B:224:17F:H37	0.60	1.73	6	1
3:B:231:PCW:H461	3:C:604:PCW:H461	0.60	1.72	6	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.59	1.97	1	9
3:B:233:PCW:H351	3:C:626:PCW:H121	0.59	1.74	8	3
3:B:233:PCW:H12	3:C:605:PCW:H71	0.59	1.72	2	1
3:B:220:PCW:H442	3:B:232:PCW:H251	0.59	1.71	4	1
4:B:234:17F:H34	4:B:234:17F:H10A	0.59	1.74	4	1
3:C:615:PCW:H382	3:C:615:PCW:H151	0.59	1.74	5	1
3:B:208:PCW:H372	4:B:226:17F:H20A	0.59	1.72	9	1
2:B:8:VAL:HG12	2:B:79:LEU:HB2	0.59	1.74	1	1
3:B:201:PCW:H221	4:B:225:17F:H68	0.59	1.73	7	1
3:A:405:PCW:H19	3:B:222:PCW:H242	0.59	1.72	8	1
3:C:619:PCW:H352	3:C:621:PCW:H141	0.59	1.73	8	1
3:C:619:PCW:H411	3:C:621:PCW:H461	0.59	1.74	8	1
3:B:210:PCW:H412	4:B:224:17F:H8	0.59	1.73	10	1
4:B:234:17F:H73	4:C:631:17F:H68	0.59	1.73	3	3
2:B:6:LEU:O	2:B:55:ILE:HA	0.59	1.96	9	6
3:B:202:PCW:H331	4:B:228:17F:H6	0.59	1.75	4	2
1:A:214:PHE:HZ	3:A:404:PCW:C16	0.59	2.10	3	1
3:C:606:PCW:H412	3:C:622:PCW:H412	0.59	1.73	3	1
3:A:407:PCW:H361	4:B:225:17F:H11	0.59	1.73	5	1
3:B:218:PCW:H242	3:C:629:PCW:H283	0.59	1.72	10	1
1:C:451:LYS:O	1:C:455:TYR:HB2	0.59	1.98	4	6
3:C:627:PCW:H39	3:C:628:PCW:H382	0.59	1.72	5	1
1:A:393:TYR:HH	3:A:407:PCW:H262	0.59	1.54	6	1
2:B:39:SER:CB	7:B:237:EWS:BRA	0.59	3.06	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:609:PCW:H272	4:C:632:17F:H48	0.59	1.75	8	1
3:B:233:PCW:H371	3:C:606:PCW:H351	0.59	1.75	2	1
2:B:32:TYR:HD1	5:B:235:GNP:H5'1	0.59	1.58	4	2
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.59	1.74	4	5
3:C:619:PCW:H381	3:C:629:PCW:H20	0.59	1.73	4	1
3:C:610:PCW:H362	3:C:614:PCW:H351	0.59	1.74	7	1
3:C:611:PCW:H341	3:C:617:PCW:H352	0.59	1.74	10	1
1:A:231:ASN:HA	1:A:234:LYS:HE2	0.59	1.73	2	3
4:A:411:17F:H58	3:C:624:PCW:H431	0.59	1.74	2	3
3:B:205:PCW:H11	3:B:207:PCW:H82	0.59	1.73	7	1
3:B:210:PCW:H341	4:B:224:17F:H5	0.59	1.75	8	2
3:C:601:PCW:H411	3:C:602:PCW:H212	0.59	1.72	8	1
3:B:220:PCW:H451	3:B:233:PCW:H271	0.59	1.75	9	1
3:C:617:PCW:H211	4:C:632:17F:H42	0.59	1.74	9	1
2:B:45:VAL:HG22	2:B:50:THR:HB	0.59	1.73	10	1
3:B:218:PCW:H411	3:C:603:PCW:H421	0.59	1.74	10	1
3:A:407:PCW:H341	4:B:225:17F:H9	0.59	1.73	1	1
3:B:201:PCW:O3P	7:B:237:EWS:CAN	0.59	2.50	5	1
3:B:203:PCW:H451	3:B:220:PCW:H20	0.59	1.74	6	1
3:B:209:PCW:H261	3:B:213:PCW:H461	0.59	1.74	7	1
3:C:609:PCW:H371	4:C:630:17F:H56	0.59	1.73	10	1
3:B:211:PCW:H132	4:B:229:17F:H6A	0.59	1.75	9	4
3:B:201:PCW:H352	4:B:225:17F:H31	0.59	1.73	2	1
3:A:404:PCW:H411	3:B:217:PCW:H421	0.59	1.75	10	4
3:A:403:PCW:H483	4:B:229:17F:H71	0.59	1.75	4	1
1:A:375:LEU:HA	1:A:378:VAL:HG12	0.59	1.75	5	2
1:C:466:GLU:HA	1:C:469:LEU:HD12	0.59	1.73	5	2
3:C:617:PCW:H232	4:C:632:17F:H45	0.59	1.75	5	1
3:B:232:PCW:H181	3:C:625:PCW:H182	0.59	1.74	6	1
1:A:345:ARG:HG2	1:C:429:ASN:OD1	0.59	1.97	10	1
3:C:614:PCW:H72	3:C:629:PCW:H32	0.59	1.74	10	1
3:B:211:PCW:H351	4:B:229:17F:H8A	0.58	1.73	10	4
3:B:202:PCW:H172	3:B:202:PCW:H121	0.58	1.74	3	1
3:C:621:PCW:H331	3:C:629:PCW:H172	0.58	1.73	3	1
4:B:229:17F:H64	3:C:619:PCW:H281	0.58	1.75	4	1
3:B:205:PCW:H172	3:B:219:PCW:H122	0.58	1.74	6	1
3:B:211:PCW:H331	4:B:229:17F:H8A	0.58	1.74	2	2
4:B:223:17F:H75	3:C:606:PCW:H252	0.58	1.75	5	1
3:B:231:PCW:H412	3:C:604:PCW:H422	0.58	1.75	8	1
3:B:201:PCW:H252	4:B:228:17F:H64	0.58	1.75	3	1
3:A:407:PCW:H351	4:B:223:17F:H56	0.58	1.74	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H412	4:B:226:17F:H62	0.58	1.74	6	1
3:B:205:PCW:C8	7:B:237:EWS:BRA	0.58	3.07	6	2
4:C:633:17F:H4A	4:C:633:17F:N1	0.58	2.13	6	2
2:B:74:THR:CA	7:B:237:EWS:BRA	0.58	3.06	9	1
1:A:214:PHE:CZ	3:A:404:PCW:C17	0.58	2.80	1	1
3:B:233:PCW:H212	3:C:625:PCW:H251	0.58	1.74	1	1
3:B:219:PCW:H232	4:B:230:17F:H74	0.58	1.75	8	1
3:B:212:PCW:H472	3:C:613:PCW:H451	0.58	1.76	6	1
3:A:410:PCW:H351	4:C:633:17F:H12A	0.58	1.73	6	1
3:B:205:PCW:H371	4:B:224:17F:H34	0.58	1.74	9	1
3:B:220:PCW:H161	3:B:220:PCW:H39	0.58	1.73	2	1
3:B:231:PCW:H39	3:C:604:PCW:H232	0.58	1.76	5	1
3:B:218:PCW:H452	3:C:603:PCW:H451	0.58	1.74	6	1
3:B:210:PCW:H361	4:B:224:17F:H18A	0.58	1.73	9	2
3:B:209:PCW:H121	3:B:213:PCW:H321	0.58	1.76	8	1
4:B:234:17F:H71	4:B:234:17F:H41	0.58	1.74	8	1
4:B:234:17F:H71	4:C:631:17F:H68	0.58	1.75	1	2
3:C:606:PCW:H39	3:C:613:PCW:H361	0.58	1.74	2	4
2:B:6:LEU:HB2	2:B:55:ILE:HG12	0.58	1.75	3	2
3:B:221:PCW:H132	4:B:230:17F:H6	0.58	1.74	7	1
3:B:210:PCW:H371	4:B:224:17F:H11A	0.58	1.75	9	2
3:B:205:PCW:H461	4:B:224:17F:H73	0.58	1.75	9	1
3:A:401:PCW:H482	3:C:616:PCW:H20	0.58	1.76	10	1
3:B:221:PCW:C7	7:B:237:EWS:BRA	0.58	3.07	1	1
2:B:38:ASP:O	2:B:56:LEU:HG	0.58	1.97	1	1
3:B:209:PCW:H221	3:C:611:PCW:H483	0.58	1.75	1	1
4:A:411:17F:H53	3:C:607:PCW:H222	0.58	1.74	2	1
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.58	1.74	9	2
4:B:228:17F:H66	3:C:615:PCW:H452	0.58	1.74	3	2
3:B:202:PCW:H451	4:B:230:17F:H48	0.58	1.75	4	1
3:C:624:PCW:H212	4:C:634:17F:H19	0.58	1.76	4	1
4:A:411:17F:H6	3:C:624:PCW:H152	0.58	1.75	5	3
3:B:233:PCW:H421	3:C:604:PCW:H39	0.58	1.76	6	1
2:B:7:VAL:HG13	7:B:237:EWS:CAU	0.58	2.29	7	1
3:C:621:PCW:H331	3:C:629:PCW:H182	0.58	1.76	7	1
3:B:203:PCW:H151	3:B:211:PCW:H39	0.58	1.73	8	1
3:C:611:PCW:H341	3:C:617:PCW:H362	0.58	1.75	2	3
3:B:231:PCW:H421	3:C:604:PCW:H261	0.58	1.74	6	2
3:B:203:PCW:H142	3:B:207:PCW:H351	0.58	1.76	10	3
3:C:613:PCW:H382	3:C:626:PCW:H422	0.58	1.76	1	2
3:A:402:PCW:H212	3:B:214:PCW:H242	0.58	1.75	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:607:PCW:H222	4:C:631:17F:H35	0.58	1.75	8	1
3:B:202:PCW:H482	3:B:212:PCW:H212	0.58	1.75	10	1
3:A:410:PCW:C33	4:C:633:17F:H12A	0.57	2.29	1	1
3:B:208:PCW:C7	7:B:237:EWS:BRA	0.57	3.05	4	1
3:B:205:PCW:H172	3:B:219:PCW:H142	0.57	1.73	1	1
4:B:223:17F:C4	4:B:223:17F:H1	0.57	2.29	9	3
1:A:308:ARG:HG3	1:C:469:LEU:HD11	0.57	1.72	7	2
3:A:403:PCW:H431	4:B:229:17F:H73	0.57	1.76	10	1
3:B:205:PCW:H121	3:B:220:PCW:H342	0.57	1.77	1	1
2:B:7:VAL:CG2	7:B:237:EWS:NAW	0.57	2.67	6	4
4:B:226:17F:N1	7:B:237:EWS:CAL	0.57	2.65	4	1
3:B:202:PCW:H122	4:B:228:17F:H9A	0.57	1.76	2	1
3:A:408:PCW:H332	3:A:410:PCW:H341	0.57	1.75	7	2
3:B:207:PCW:H12	7:B:237:EWS:CAK	0.57	2.27	6	1
3:A:408:PCW:H341	3:B:231:PCW:H371	0.57	1.76	8	2
2:B:80:CYS:HB3	2:B:93:ILE:HD12	0.57	1.76	9	1
3:B:209:PCW:H122	3:B:213:PCW:H131	0.57	1.74	10	1
3:B:221:PCW:H281	4:B:226:17F:H72	0.57	1.76	1	1
3:B:207:PCW:H481	3:B:232:PCW:H141	0.57	1.76	3	1
1:C:478:ARG:O	1:C:482:GLN:HB2	0.57	1.99	10	4
3:A:401:PCW:H411	3:B:212:PCW:H471	0.57	1.75	6	2
3:A:403:PCW:H461	3:C:618:PCW:H452	0.57	1.76	8	1
3:A:402:PCW:H122	3:A:402:PCW:H341	0.57	1.75	10	2
3:A:401:PCW:H42	4:B:226:17F:O2	0.57	2.00	3	1
3:B:207:PCW:H212	4:C:631:17F:H76	0.57	1.76	9	2
3:B:203:PCW:H39	3:B:220:PCW:H172	0.57	1.76	7	1
3:B:203:PCW:H121	3:B:207:PCW:H342	0.57	1.77	10	1
3:B:208:PCW:H471	3:C:627:PCW:H471	0.57	1.76	2	1
3:B:205:PCW:H281	3:B:233:PCW:H232	0.57	1.77	3	1
3:C:614:PCW:H341	3:C:614:PCW:H132	0.57	1.75	6	1
3:C:611:PCW:H411	3:C:617:PCW:H442	0.57	1.76	9	1
3:A:408:PCW:H39	3:A:410:PCW:H412	0.57	1.74	2	1
3:C:607:PCW:H262	4:C:631:17F:H39	0.57	1.76	5	2
3:C:613:PCW:H132	3:C:622:PCW:H151	0.57	1.76	7	1
3:A:406:PCW:H352	3:B:215:PCW:H412	0.57	1.75	8	1
3:B:217:PCW:H262	3:C:619:PCW:H461	0.57	1.76	8	3
3:A:407:PCW:H481	3:A:410:PCW:H211	0.57	1.75	5	1
3:C:611:PCW:H121	3:C:617:PCW:H342	0.57	1.76	8	1
3:C:617:PCW:H231	4:C:635:17F:H44	0.57	1.75	4	2
3:C:614:PCW:H132	3:C:614:PCW:H331	0.57	1.75	5	1
3:A:401:PCW:H462	3:C:613:PCW:H241	0.57	1.77	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:214:PHE:HE1	3:A:404:PCW:H171	0.57	1.60	10	1
3:B:209:PCW:H242	3:C:611:PCW:H481	0.56	1.78	2	1
1:A:327:LEU:HD23	1:A:330:ARG:HD2	0.56	1.77	5	1
3:B:201:PCW:O3P	7:B:237:EWS:CAK	0.56	2.52	5	1
3:B:203:PCW:H40	3:B:231:PCW:H281	0.56	1.76	6	1
3:C:607:PCW:H231	4:C:631:17F:H39	0.56	1.76	2	1
3:B:207:PCW:H182	3:B:232:PCW:H283	0.56	1.77	5	1
3:B:203:PCW:H261	3:B:217:PCW:H442	0.56	1.77	1	1
4:B:228:17F:H61	3:C:615:PCW:H462	0.56	1.77	1	1
3:B:218:PCW:H461	3:C:629:PCW:H281	0.56	1.77	2	2
3:B:210:PCW:H351	4:B:224:17F:H19	0.56	1.78	3	1
3:B:219:PCW:H331	3:B:219:PCW:H132	0.56	1.77	6	1
3:B:208:PCW:H31	3:B:221:PCW:H131	0.56	1.78	7	1
4:B:227:17F:O2	3:C:602:PCW:H73	0.56	2.00	7	1
3:A:402:PCW:H342	3:B:214:PCW:H152	0.56	1.77	1	1
3:A:408:PCW:H11	3:B:231:PCW:H321	0.56	1.77	3	3
3:A:408:PCW:H141	3:C:620:PCW:H141	0.56	1.77	6	1
2:B:45:VAL:HA	2:B:50:THR:HA	0.56	1.78	8	2
3:C:610:PCW:H182	3:C:614:PCW:H171	0.56	1.78	9	2
3:B:202:PCW:H483	3:B:208:PCW:H381	0.56	1.76	1	1
3:B:216:PCW:H481	3:C:603:PCW:H412	0.56	1.76	2	1
3:C:602:PCW:H462	3:C:609:PCW:H252	0.56	1.76	2	1
3:C:610:PCW:H382	3:C:614:PCW:H371	0.56	1.77	2	2
3:B:217:PCW:H282	3:C:619:PCW:H482	0.56	1.78	5	3
1:C:414:LYS:O	1:C:418:GLN:HG3	0.56	2.00	3	2
3:B:213:PCW:H482	4:C:635:17F:H66	0.56	1.77	3	1
3:A:409:PCW:H431	3:C:627:PCW:H231	0.56	1.77	6	1
3:C:613:PCW:H39	3:C:627:PCW:H242	0.56	1.76	8	1
3:B:206:PCW:H262	3:C:602:PCW:H411	0.56	1.78	3	1
3:B:207:PCW:H19	4:B:234:17F:H45	0.56	1.77	5	1
3:B:232:PCW:H341	3:C:625:PCW:H151	0.56	1.78	7	1
3:B:203:PCW:H212	3:B:217:PCW:H211	0.56	1.78	9	1
3:C:611:PCW:H162	3:C:628:PCW:H271	0.56	1.76	4	1
1:A:396:LYS:HZ3	3:A:407:PCW:C27	0.56	1.90	5	1
1:A:242:GLU:HB3	1:C:532:ARG:HH21	0.56	1.61	7	1
3:A:402:PCW:H272	3:B:209:PCW:H283	0.56	1.76	10	1
3:C:609:PCW:H161	4:C:630:17F:H34	0.56	1.76	2	1
3:B:201:PCW:H221	4:B:225:17F:H69	0.56	1.75	3	1
2:B:7:VAL:HG13	7:B:237:EWS:CAX	0.56	2.31	3	1
3:C:605:PCW:H62	3:C:605:PCW:H331	0.56	1.78	3	1
3:A:406:PCW:H341	3:B:206:PCW:H342	0.56	1.76	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:402:PCW:H322	3:A:402:PCW:H83	0.56	1.78	9	1
3:C:615:PCW:H132	3:C:622:PCW:H371	0.56	1.77	5	1
3:B:210:PCW:H222	4:B:227:17F:H43	0.56	1.76	6	1
1:A:279:LEU:HB3	1:C:495:LYS:HD3	0.56	1.78	7	1
4:B:230:17F:H38	3:C:605:PCW:H282	0.56	1.77	7	1
3:B:220:PCW:H271	3:B:231:PCW:H452	0.56	1.78	8	1
3:B:213:PCW:H272	4:C:630:17F:H74	0.56	1.78	9	1
3:B:202:PCW:H342	3:B:202:PCW:H131	0.56	1.77	1	1
3:C:618:PCW:H142	3:C:620:PCW:H431	0.56	1.77	1	1
3:A:408:PCW:H381	3:A:408:PCW:H171	0.56	1.77	2	1
4:B:228:17F:H9	4:B:228:17F:H19	0.56	1.78	4	1
3:B:217:PCW:H261	3:C:619:PCW:H461	0.56	1.76	4	1
3:A:408:PCW:H40	3:A:410:PCW:H441	0.56	1.78	8	1
3:A:401:PCW:H261	3:C:622:PCW:H281	0.56	1.77	8	1
3:B:209:PCW:H351	3:B:213:PCW:H141	0.56	1.76	10	2
4:A:411:17F:H37	3:C:624:PCW:H461	0.55	1.77	1	2
1:A:308:ARG:HG2	1:C:469:LEU:CG	0.55	2.29	4	1
3:A:407:PCW:H121	4:B:223:17F:H57	0.55	1.78	4	1
3:C:622:PCW:H381	3:C:622:PCW:H151	0.55	1.76	5	2
3:C:621:PCW:H352	3:C:629:PCW:H172	0.55	1.76	6	1
4:B:225:17F:H10	3:C:626:PCW:H281	0.55	1.78	9	1
3:B:207:PCW:N	7:B:237:EWS:BRA	0.55	2.94	10	1
3:C:607:PCW:H161	3:C:607:PCW:H342	0.55	1.77	10	1
3:B:213:PCW:H221	4:B:227:17F:H46	0.55	1.78	5	2
1:C:455:TYR:HH	3:C:601:PCW:C20	0.55	2.12	3	1
3:A:407:PCW:H2	4:B:223:17F:H18	0.55	1.78	4	1
2:B:7:VAL:HG23	7:B:237:EWS:CAX	0.55	2.29	8	1
3:A:408:PCW:H181	3:C:604:PCW:H252	0.55	1.78	10	1
3:B:212:PCW:H40	3:C:613:PCW:H482	0.55	1.77	3	1
3:C:610:PCW:H122	3:C:614:PCW:H212	0.55	1.79	3	1
1:C:488:LYS:HE2	3:C:623:PCW:H283	0.55	0.58	4	1
3:B:217:PCW:H11	7:B:237:EWS:CAN	0.55	2.31	7	1
3:A:401:PCW:H411	3:B:212:PCW:H452	0.55	1.79	2	1
2:B:116:ASN:HA	2:B:144:THR:O	0.55	2.02	4	1
3:B:203:PCW:H352	3:B:220:PCW:H132	0.55	1.78	4	1
3:B:205:PCW:H231	3:B:219:PCW:H411	0.55	1.77	6	1
3:C:622:PCW:H381	3:C:622:PCW:H142	0.55	1.79	6	1
2:B:70:GLN:CG	3:B:220:PCW:H41	0.55	2.29	9	1
1:C:466:GLU:OE1	1:C:469:LEU:HD12	0.55	2.01	10	1
4:B:234:17F:H70	3:C:607:PCW:H262	0.55	1.79	1	1
3:C:618:PCW:H2	3:C:620:PCW:H352	0.55	1.79	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:621:PCW:H122	3:C:629:PCW:H181	0.55	1.78	8	4
2:B:5:LYS:HG3	7:B:237:EWS:CAT	0.55	2.31	6	1
3:A:401:PCW:H341	3:B:212:PCW:H371	0.55	1.78	3	1
1:A:214:PHE:CE1	3:A:404:PCW:C16	0.55	2.88	4	2
3:C:624:PCW:H421	4:C:634:17F:H60	0.55	1.78	5	1
3:A:406:PCW:H432	4:B:226:17F:H70	0.55	1.78	7	1
3:B:210:PCW:H152	4:B:224:17F:H4	0.55	1.78	8	1
3:A:407:PCW:H472	4:B:223:17F:H72	0.55	1.79	9	1
3:B:201:PCW:H351	4:B:226:17F:H38	0.55	1.79	9	1
3:B:202:PCW:H272	3:C:622:PCW:H262	0.55	1.77	10	1
4:B:225:17F:H59	3:C:626:PCW:H282	0.55	1.79	2	2
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.55	1.78	7	2
3:A:409:PCW:H412	3:C:627:PCW:H432	0.55	1.77	4	1
4:B:226:17F:H10	4:B:230:17F:H8	0.55	1.77	8	3
3:B:210:PCW:H121	4:B:224:17F:H19A	0.55	1.79	9	1
3:B:207:PCW:C1	7:B:237:EWS:CAO	0.55	2.83	6	1
3:B:219:PCW:H20	3:B:233:PCW:H272	0.55	1.78	8	1
3:A:408:PCW:H352	3:A:410:PCW:H341	0.55	1.79	3	1
3:C:613:PCW:H322	3:C:622:PCW:H122	0.55	1.78	6	2
1:C:447:GLU:OE1	1:C:451:LYS:HE2	0.55	2.01	9	2
3:B:211:PCW:H151	4:B:229:17F:C6	0.55	2.32	2	1
4:A:411:17F:H31	4:A:411:17F:H10	0.55	1.78	3	1
3:A:401:PCW:H83	4:B:226:17F:O2	0.55	2.01	4	1
4:B:234:17F:H77	4:B:234:17F:H48	0.55	1.78	4	1
4:B:229:17F:H1	4:B:229:17F:C4	0.55	2.32	6	1
3:B:209:PCW:H271	3:C:611:PCW:H483	0.55	1.78	7	1
3:A:409:PCW:H351	3:C:627:PCW:H341	0.55	1.78	9	1
3:B:201:PCW:H342	3:B:219:PCW:H351	0.54	1.79	1	1
3:B:217:PCW:C1	7:B:237:EWS:CAM	0.54	2.83	7	1
4:B:229:17F:H58	4:B:229:17F:H10A	0.54	1.79	9	1
2:B:41:ARG:HD2	2:B:52:LEU:HG	0.54	1.78	3	1
1:C:455:TYR:OH	3:C:601:PCW:H20	0.54	2.00	3	2
3:C:621:PCW:H331	3:C:629:PCW:H181	0.54	1.79	5	1
3:B:220:PCW:H281	3:C:625:PCW:H222	0.54	1.79	4	1
3:C:609:PCW:H181	4:C:630:17F:H34	0.54	1.79	4	1
3:B:209:PCW:H142	3:B:213:PCW:H151	0.54	1.79	6	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.54	2.03	5	8
3:B:215:PCW:H481	4:B:226:17F:H75	0.54	1.78	3	1
1:A:330:ARG:NH2	1:C:444:ASP:HA	0.54	2.17	5	1
3:B:220:PCW:H452	3:B:233:PCW:H252	0.54	1.80	7	1
3:B:203:PCW:P	7:B:237:EWS:CAO	0.54	2.96	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:609:PCW:H171	4:C:632:17F:H20A	0.54	1.79	8	1
4:B:234:17F:H34	3:C:625:PCW:H141	0.54	1.79	10	1
1:A:239:LEU:HA	1:A:242:GLU:HB2	0.54	1.79	2	1
3:B:202:PCW:H152	3:B:212:PCW:H412	0.54	1.78	2	1
3:B:211:PCW:H362	4:B:229:17F:H10A	0.54	1.78	2	1
1:A:288:ARG:O	1:A:292:HIS:HB2	0.54	2.03	3	1
3:A:407:PCW:H122	4:B:223:17F:C20	0.54	2.33	6	2
3:A:402:PCW:H372	3:B:214:PCW:H182	0.54	1.78	7	1
3:B:219:PCW:H231	4:B:224:17F:H43	0.54	1.80	8	1
3:B:232:PCW:H351	3:C:619:PCW:H341	0.54	1.80	9	2
3:A:406:PCW:H441	3:A:409:PCW:H231	0.54	1.80	1	1
4:B:234:17F:H40	4:B:234:17F:H69	0.54	1.77	10	2
3:B:205:PCW:H122	3:B:207:PCW:H131	0.54	1.79	6	3
3:C:628:PCW:H142	3:C:628:PCW:H362	0.54	1.79	5	2
3:A:408:PCW:H351	3:A:410:PCW:H351	0.54	1.80	1	1
3:C:611:PCW:H461	4:C:635:17F:H41	0.54	1.78	4	1
3:C:611:PCW:H252	3:C:617:PCW:H441	0.54	1.80	6	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.54	1.80	9	2
3:A:407:PCW:H371	4:B:223:17F:H56	0.54	1.80	9	1
3:C:607:PCW:H483	3:C:611:PCW:H371	0.54	1.79	4	1
2:B:39:SER:HA	2:B:56:LEU:HG	0.54	1.79	9	1
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.54	1.63	2	3
2:B:163:ILE:HG22	2:B:167:LYS:HE3	0.54	1.80	6	1
3:B:209:PCW:H122	3:B:213:PCW:C13	0.54	2.32	8	1
3:B:217:PCW:H283	3:B:218:PCW:H272	0.54	1.77	8	1
3:B:201:PCW:H211	4:B:225:17F:H61	0.54	1.79	10	1
1:C:519:ALA:HB3	1:C:520:PRO:HD3	0.54	1.79	10	1
2:B:117:LYS:HB3	2:B:120:LEU:HD13	0.53	1.81	1	1
2:B:41:ARG:HD2	2:B:52:LEU:HD21	0.53	1.80	1	1
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.53	1.79	10	2
1:C:401:LEU:O	1:C:405:TRP:HB2	0.53	2.03	5	1
3:C:614:PCW:C13	3:C:614:PCW:H331	0.53	2.33	5	1
3:C:617:PCW:H212	4:C:632:17F:H42	0.53	1.79	7	1
4:A:411:17F:H4A	3:C:624:PCW:H132	0.53	1.78	8	2
3:B:212:PCW:H422	3:C:613:PCW:H481	0.53	1.80	9	1
3:B:212:PCW:H181	4:B:226:17F:H10A	0.53	1.80	9	1
2:B:4:TYR:HB2	2:B:53:LEU:HD23	0.53	1.79	1	1
3:B:208:PCW:H31	3:B:221:PCW:H121	0.53	1.79	2	1
3:C:611:PCW:H161	3:C:628:PCW:H282	0.53	1.79	2	1
3:B:218:PCW:H441	3:C:629:PCW:H281	0.53	1.81	3	1
3:A:405:PCW:H251	4:C:634:17F:H55	0.53	1.79	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:231:PCW:H361	3:C:604:PCW:H352	0.53	1.81	9	3
1:C:469:LEU:HD22	1:C:473:LYS:NZ	0.53	2.18	2	1
3:B:220:PCW:H483	3:B:232:PCW:H442	0.53	1.80	3	1
1:C:491:GLU:O	1:C:495:LYS:HG3	0.53	2.03	6	2
3:B:203:PCW:H321	3:B:211:PCW:H332	0.53	1.80	10	1
2:B:71:TYR:CA	7:B:237:EWS:CAC	0.53	2.76	1	1
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.53	2.32	2	3
3:B:208:PCW:C6	7:B:237:EWS:BRA	0.53	3.09	4	1
3:B:208:PCW:H142	3:B:221:PCW:H212	0.53	1.81	6	1
1:C:474:VAL:O	1:C:478:ARG:HB2	0.53	2.04	1	2
3:B:204:PCW:H352	4:B:223:17F:H29	0.53	1.81	6	1
3:B:231:PCW:H482	3:C:604:PCW:H482	0.53	1.78	6	1
3:A:402:PCW:H351	3:B:213:PCW:H322	0.53	1.80	7	1
3:B:207:PCW:O4P	7:B:237:EWS:CAL	0.53	2.57	7	1
3:C:606:PCW:H211	3:C:615:PCW:H142	0.53	1.80	7	1
1:C:567:GLU:O	1:C:571:GLN:CB	0.53	2.57	8	1
1:A:369:GLU:O	1:A:373:GLN:CG	0.53	2.50	9	1
3:A:401:PCW:H73	3:B:212:PCW:H12	0.53	1.78	10	1
3:B:206:PCW:H71	3:B:215:PCW:H12	0.53	1.78	2	1
4:B:223:17F:H46	3:C:626:PCW:H252	0.53	1.80	2	1
3:B:212:PCW:H432	3:B:212:PCW:H20	0.53	1.79	7	2
1:C:544:LEU:O	1:C:548:HIS:HB2	0.53	2.03	8	1
3:C:612:PCW:H31	4:C:634:17F:H6	0.53	1.79	8	2
2:B:74:THR:HG23	7:B:237:EWS:CAD	0.53	2.34	10	1
1:A:301:LEU:HB3	1:C:473:LYS:HE3	0.53	1.81	3	1
3:B:203:PCW:H331	3:B:211:PCW:H322	0.53	1.80	3	1
3:A:404:PCW:H381	3:B:217:PCW:H432	0.53	1.81	9	1
3:C:613:PCW:H141	3:C:622:PCW:H19	0.53	1.78	9	1
3:A:406:PCW:H212	3:A:409:PCW:H241	0.53	1.81	1	1
2:B:82:PHE:HE2	2:B:113:LEU:HG	0.53	1.64	1	2
3:A:402:PCW:H181	3:B:214:PCW:H231	0.53	1.81	6	1
3:B:217:PCW:H221	4:C:634:17F:H54	0.53	1.81	6	1
3:C:607:PCW:H421	3:C:611:PCW:H11	0.53	1.80	6	1
3:B:213:PCW:H342	3:B:216:PCW:H122	0.53	1.80	7	1
3:C:613:PCW:H411	3:C:613:PCW:H19	0.53	1.79	1	1
3:A:409:PCW:O31	3:C:627:PCW:H362	0.53	2.04	1	1
4:B:234:17F:H56	3:C:625:PCW:H181	0.53	1.81	3	1
3:C:618:PCW:H322	3:C:620:PCW:H39	0.53	1.79	4	1
1:A:243:MET:HA	1:A:246:ASP:HB2	0.53	1.79	7	1
3:B:218:PCW:H232	3:B:218:PCW:H432	0.53	1.79	8	1
2:B:84:ILE:HD13	2:B:118:CYS:HA	0.53	1.81	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:627:PCW:H371	3:C:628:PCW:H382	0.53	1.81	8	1
3:B:213:PCW:H283	3:C:611:PCW:H412	0.53	1.81	9	1
3:A:403:PCW:H172	3:A:403:PCW:H351	0.53	1.79	1	1
3:B:209:PCW:H232	3:B:213:PCW:H421	0.53	1.81	3	1
3:B:215:PCW:H251	3:C:609:PCW:H482	0.53	1.81	4	1
3:C:606:PCW:H461	3:C:615:PCW:H172	0.53	1.80	5	1
1:C:465:GLU:O	1:C:469:LEU:HD12	0.53	2.02	6	1
3:A:406:PCW:H162	3:A:409:PCW:H271	0.53	1.80	8	1
3:C:611:PCW:H182	3:C:617:PCW:H362	0.53	1.81	10	1
4:B:234:17F:H33	3:C:625:PCW:H19	0.52	1.80	1	1
3:C:607:PCW:H172	3:C:607:PCW:H342	0.52	1.80	1	1
1:C:455:TYR:HE2	3:C:601:PCW:C23	0.52	2.16	3	1
2:B:68:ARG:HA	2:B:71:TYR:CE2	0.52	2.39	8	4
3:A:406:PCW:H232	3:A:409:PCW:H262	0.52	1.80	7	1
3:A:408:PCW:H422	3:A:410:PCW:H441	0.52	1.81	10	1
3:C:611:PCW:H252	3:C:617:PCW:H431	0.52	1.80	10	1
3:B:220:PCW:H251	3:C:604:PCW:H471	0.52	1.81	2	1
3:C:619:PCW:H411	3:C:621:PCW:H211	0.52	1.81	2	1
3:B:205:PCW:H251	3:B:220:PCW:H211	0.52	1.80	3	1
3:B:219:PCW:O31	4:B:230:17F:H20	0.52	2.04	4	1
3:C:609:PCW:H283	4:C:632:17F:H48	0.52	1.80	6	2
3:B:201:PCW:H232	3:C:613:PCW:H483	0.52	1.81	7	1
3:B:208:PCW:H472	4:B:226:17F:H65	0.52	1.80	8	1
3:C:610:PCW:H372	3:C:614:PCW:H211	0.52	1.81	1	2
3:B:201:PCW:H182	4:B:228:17F:H18	0.52	1.80	3	1
3:B:209:PCW:H81	4:B:227:17F:H1	0.52	1.82	3	1
3:B:216:PCW:H171	4:B:227:17F:H37	0.52	1.80	3	1
3:B:208:PCW:H121	3:B:221:PCW:H162	0.52	1.82	4	1
3:B:212:PCW:H483	3:C:613:PCW:H451	0.52	1.80	4	1
3:A:408:PCW:H331	3:A:408:PCW:H131	0.52	1.79	8	2
3:B:218:PCW:H362	3:B:218:PCW:H162	0.52	1.80	5	1
3:B:203:PCW:H262	3:B:217:PCW:H161	0.52	1.80	7	1
3:A:406:PCW:H141	3:A:406:PCW:H361	0.52	1.82	10	1
3:B:213:PCW:H483	4:C:635:17F:H66	0.52	1.82	4	2
3:B:220:PCW:H251	3:B:232:PCW:H211	0.52	1.81	4	1
3:B:214:PCW:O3P	3:C:603:PCW:H71	0.52	2.05	5	1
3:A:406:PCW:H12	4:B:226:17F:O1	0.52	2.05	10	2
3:B:203:PCW:H481	3:B:233:PCW:H483	0.52	1.80	7	1
3:B:205:PCW:C1	3:B:207:PCW:H82	0.52	2.34	7	1
3:B:232:PCW:H151	3:C:625:PCW:H182	0.52	1.81	8	1
3:A:406:PCW:H242	3:A:409:PCW:H241	0.52	1.82	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:212:PCW:H461	3:C:613:PCW:H462	0.52	1.80	1	1
3:B:222:PCW:H461	4:C:634:17F:H47	0.52	1.81	1	2
1:C:417:GLU:O	1:C:421:PRO:HD2	0.52	2.04	8	5
3:C:619:PCW:H39	3:C:629:PCW:H221	0.52	1.81	2	2
3:C:621:PCW:H382	3:C:629:PCW:H161	0.52	1.79	3	1
3:B:221:PCW:H52	3:B:221:PCW:H31	0.52	1.82	4	1
3:B:209:PCW:H182	3:B:213:PCW:H361	0.52	1.81	5	1
3:B:203:PCW:O3P	3:B:220:PCW:H81	0.52	2.04	5	1
3:C:609:PCW:H83	3:C:611:PCW:H141	0.52	1.82	6	1
3:C:627:PCW:H372	3:C:628:PCW:H141	0.52	1.80	9	5
3:A:410:PCW:H251	4:C:633:17F:H53	0.52	1.80	7	1
1:A:363:LYS:HE2	1:C:411:THR:HB	0.52	1.80	2	1
1:C:510:HIS:O	1:C:514:LEU:HG	0.52	2.04	7	1
3:B:215:PCW:H271	3:C:608:PCW:H451	0.52	1.81	8	1
2:B:7:VAL:CG1	7:B:237:EWS:CAX	0.52	2.88	3	2
3:B:211:PCW:H271	3:C:619:PCW:H272	0.52	1.81	4	2
3:A:405:PCW:H352	3:A:405:PCW:H122	0.52	1.81	5	1
3:C:618:PCW:H181	3:C:620:PCW:H451	0.52	1.82	5	1
4:B:223:17F:H50	3:C:626:PCW:H251	0.52	1.81	6	1
3:A:407:PCW:H121	4:B:223:17F:H20	0.52	1.80	7	1
3:B:221:PCW:H283	4:B:226:17F:H69	0.52	1.82	7	1
3:C:613:PCW:H83	3:C:626:PCW:H322	0.52	1.82	7	1
3:B:213:PCW:H462	4:C:635:17F:H69	0.52	1.82	10	1
3:C:611:PCW:H151	3:C:617:PCW:H321	0.52	1.82	7	1
3:B:210:PCW:H151	4:B:227:17F:H10	0.52	1.81	2	3
1:C:589:GLU:HG2	1:C:593:LYS:HE2	0.52	1.80	2	1
3:A:405:PCW:H332	3:B:222:PCW:H122	0.52	1.81	4	1
2:B:105:ASP:HB3	3:B:203:PCW:H72	0.52	1.82	5	1
1:C:465:GLU:O	1:C:469:LEU:HB2	0.52	2.01	6	1
4:B:228:17F:H70	3:C:622:PCW:H451	0.52	1.81	7	1
2:B:24:ILE:HG13	2:B:40:TYR:HB3	0.52	1.82	7	1
3:A:409:PCW:H422	3:C:605:PCW:H20	0.52	1.82	8	1
1:C:568:ASP:OD1	1:C:571:GLN:OE1	0.52	2.28	9	1
3:C:607:PCW:H231	4:C:631:17F:H35	0.52	1.80	9	1
3:B:205:PCW:H252	3:B:220:PCW:H171	0.52	1.80	10	1
3:B:219:PCW:H31	3:B:220:PCW:H12	0.51	1.81	2	1
2:B:74:THR:HA	4:B:230:17F:HN1A	0.51	1.65	3	1
2:B:41:ARG:HA	2:B:53:LEU:O	0.51	2.04	4	1
1:C:488:LYS:HD3	3:C:623:PCW:H271	0.51	0.52	4	1
3:B:205:PCW:C6	7:B:237:EWS:BRA	0.51	3.12	6	1
3:B:209:PCW:H162	3:B:213:PCW:H161	0.51	1.83	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:207:PCW:H281	3:C:625:PCW:H461	0.51	1.82	6	2
3:B:210:PCW:H182	4:B:227:17F:H30	0.51	1.82	3	1
3:B:204:PCW:H361	4:B:223:17F:H10A	0.51	1.82	4	1
3:B:213:PCW:H39	3:B:214:PCW:H212	0.51	1.82	5	1
3:B:203:PCW:H452	4:B:223:17F:H44	0.51	1.81	5	1
3:C:613:PCW:H162	3:C:626:PCW:H452	0.51	1.81	5	1
3:C:606:PCW:H222	3:C:615:PCW:H172	0.51	1.82	6	1
3:B:201:PCW:H261	3:B:212:PCW:H452	0.51	1.80	8	1
1:A:214:PHE:CZ	3:A:404:PCW:H172	0.51	2.41	9	1
3:B:206:PCW:H282	3:B:215:PCW:H161	0.51	1.81	3	1
3:C:621:PCW:H352	3:C:629:PCW:H182	0.51	1.82	4	1
3:B:219:PCW:H331	3:B:219:PCW:H152	0.51	1.82	9	1
3:A:410:PCW:H331	4:C:633:17F:C12	0.51	2.35	10	1
4:B:228:17F:C4	4:B:228:17F:C1	0.51	2.87	2	2
2:B:79:LEU:HD23	2:B:112:VAL:HB	0.51	1.81	7	2
1:C:559:SER:HA	1:C:562:ALA:HB3	0.51	1.82	9	1
4:B:234:17F:H62	4:C:631:17F:H63	0.51	1.81	10	1
3:A:408:PCW:H32	3:C:620:PCW:H63	0.51	1.82	5	5
3:C:616:PCW:H172	3:C:616:PCW:H411	0.51	1.81	5	1
3:B:211:PCW:H61	4:B:229:17F:O2	0.51	2.06	3	2
3:B:203:PCW:H212	3:B:217:PCW:H181	0.51	1.82	2	1
3:B:233:PCW:H382	3:C:606:PCW:H351	0.51	1.80	3	1
3:B:216:PCW:H19	3:C:617:PCW:H481	0.51	1.82	5	1
3:B:206:PCW:H242	3:B:215:PCW:H20	0.51	1.83	10	1
3:A:409:PCW:H451	3:C:605:PCW:H231	0.51	1.82	10	1
3:B:231:PCW:H412	3:C:604:PCW:H421	0.51	1.82	2	3
1:C:469:LEU:O	1:C:473:LYS:HB2	0.51	2.05	4	2
3:A:407:PCW:H121	4:B:223:17F:C1Z	0.51	2.34	9	3
3:A:406:PCW:H432	3:A:409:PCW:H251	0.51	1.80	6	1
1:A:308:ARG:HD3	1:C:469:LEU:CD2	0.51	2.32	6	1
3:B:203:PCW:H483	4:B:223:17F:H48	0.51	1.83	7	1
1:A:338:LEU:HA	1:A:341:ASN:HB3	0.51	1.82	9	1
3:B:211:PCW:H332	4:B:229:17F:H8A	0.51	1.83	1	2
1:A:221:LEU:HA	1:A:224:VAL:HG12	0.51	1.83	8	2
3:B:210:PCW:H382	4:B:224:17F:H10	0.51	1.81	5	1
4:B:227:17F:H66	3:C:602:PCW:H421	0.51	1.82	7	1
3:C:611:PCW:H461	4:C:635:17F:H39	0.51	1.81	8	1
3:A:407:PCW:C34	4:B:225:17F:H9	0.51	2.28	6	3
3:C:610:PCW:H351	3:C:614:PCW:H382	0.51	1.83	10	3
2:B:3:GLU:OE2	3:B:221:PCW:H63	0.51	2.05	4	1
3:B:219:PCW:H20	3:C:605:PCW:H281	0.51	1.81	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:206:PCW:H351	3:B:215:PCW:H412	0.51	1.81	5	1
1:C:491:GLU:HB3	1:C:495:LYS:HE2	0.51	1.83	7	1
3:B:206:PCW:H142	3:B:208:PCW:H181	0.51	1.83	8	1
3:C:613:PCW:H362	3:C:613:PCW:H171	0.51	1.82	8	1
3:A:408:PCW:H351	3:A:410:PCW:H362	0.51	1.82	9	1
3:B:205:PCW:H31	3:B:205:PCW:H41	0.51	1.82	9	1
4:B:225:17F:H59	3:C:626:PCW:H283	0.51	1.82	5	1
4:C:635:17F:H57	4:C:635:17F:H30	0.51	1.82	5	1
3:B:221:PCW:H281	3:C:627:PCW:H482	0.51	1.83	7	1
3:B:202:PCW:H261	4:B:228:17F:H65	0.50	1.82	3	1
3:A:405:PCW:H372	3:A:405:PCW:H141	0.50	1.83	5	1
4:A:411:17F:H49	3:C:607:PCW:H242	0.50	1.82	7	1
3:C:615:PCW:H281	3:C:626:PCW:H251	0.50	1.81	9	1
3:B:211:PCW:H262	3:B:217:PCW:H451	0.50	1.83	1	1
3:A:406:PCW:H142	3:A:409:PCW:H252	0.50	1.82	3	1
3:B:201:PCW:H171	4:B:225:17F:H60	0.50	1.83	3	1
3:A:402:PCW:H81	3:B:214:PCW:H132	0.50	1.83	4	1
3:C:615:PCW:O1P	3:C:622:PCW:H11	0.50	2.06	6	2
4:B:223:17F:H55	3:C:626:PCW:H232	0.50	1.83	6	1
3:B:220:PCW:H482	3:C:625:PCW:H232	0.50	1.83	7	1
1:A:310:ARG:O	1:A:314:ASP:HB2	0.50	2.07	10	2
3:B:202:PCW:H362	3:B:212:PCW:H372	0.50	1.82	9	1
4:B:234:17F:H35	3:C:625:PCW:H272	0.50	1.83	9	1
3:B:203:PCW:H242	3:B:211:PCW:H451	0.50	1.83	1	1
3:B:211:PCW:H151	4:B:229:17F:H6A	0.50	1.82	2	1
3:B:207:PCW:H362	3:B:211:PCW:H372	0.50	1.83	7	1
1:A:330:ARG:HH21	1:C:447:GLU:HB3	0.50	1.67	10	2
1:A:202:LYS:HZ3	1:A:202:LYS:HB3	0.50	1.66	9	1
3:B:213:PCW:H232	4:B:227:17F:H51	0.50	1.82	2	1
3:A:407:PCW:H122	4:B:223:17F:H33	0.50	1.82	3	1
3:A:408:PCW:H372	3:A:410:PCW:H351	0.50	1.83	3	1
3:B:219:PCW:H461	4:B:223:17F:H45	0.50	1.82	3	1
3:B:211:PCW:H421	4:B:229:17F:H60	0.50	1.83	3	1
3:A:406:PCW:H172	4:B:226:17F:H64	0.50	1.83	4	1
3:B:211:PCW:H171	4:B:229:17F:H33	0.50	1.83	8	1
4:B:223:17F:H43	3:C:626:PCW:H272	0.50	1.84	8	2
3:B:220:PCW:H462	3:B:232:PCW:H481	0.50	1.83	10	1
3:B:208:PCW:H141	3:B:215:PCW:H372	0.50	1.83	3	1
3:B:218:PCW:H182	3:B:218:PCW:H362	0.50	1.83	4	2
4:B:223:17F:H46	3:C:626:PCW:H251	0.50	1.82	4	1
3:B:202:PCW:H321	3:B:212:PCW:H81	0.50	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:406:PCW:H2	4:B:226:17F:O10	0.50	2.07	10	1
3:B:221:PCW:H42	7:B:237:EWS:BRA	0.50	2.59	1	1
3:C:611:PCW:C15	3:C:617:PCW:H321	0.50	2.36	3	1
3:B:202:PCW:H362	3:B:212:PCW:H381	0.50	1.83	7	3
3:B:221:PCW:H39	4:B:230:17F:H71	0.50	1.83	5	1
3:B:203:PCW:H362	3:B:204:PCW:H122	0.50	1.83	7	1
3:A:407:PCW:C15	4:B:223:17F:H33	0.50	2.35	7	1
3:C:621:PCW:H342	3:C:629:PCW:H371	0.50	1.82	7	1
1:C:443:LYS:O	1:C:447:GLU:HB2	0.50	2.07	9	2
4:B:226:17F:H72	3:C:628:PCW:H451	0.50	1.82	9	1
3:A:407:PCW:H152	4:B:223:17F:H20	0.50	1.84	1	1
3:A:406:PCW:H382	3:A:406:PCW:H141	0.50	1.84	2	1
3:B:212:PCW:H171	3:B:212:PCW:H371	0.50	1.84	2	1
3:C:621:PCW:H122	3:C:629:PCW:H182	0.50	1.82	2	1
1:C:442:SER:O	1:C:446:GLU:HB2	0.50	2.07	3	1
1:C:427:TRP:HA	1:C:427:TRP:CE3	0.50	2.40	6	1
3:C:603:PCW:H483	3:C:624:PCW:H252	0.50	1.84	6	1
3:C:607:PCW:H342	3:C:607:PCW:H161	0.50	1.82	6	1
3:B:219:PCW:H221	3:B:233:PCW:H282	0.50	1.84	9	1
4:B:225:17F:H76	3:C:606:PCW:C48	0.50	2.37	9	1
3:B:205:PCW:H161	3:B:207:PCW:H171	0.50	1.82	10	1
3:B:209:PCW:H161	3:B:216:PCW:H181	0.50	1.83	6	1
3:B:220:PCW:H142	3:B:220:PCW:H382	0.50	1.84	9	1
4:B:228:17F:H11A	4:B:228:17F:H31	0.50	1.83	1	1
4:B:234:17F:H70	3:C:607:PCW:H283	0.50	1.83	2	1
3:B:231:PCW:H141	3:C:604:PCW:H19	0.50	1.83	5	2
3:B:220:PCW:H472	3:B:233:PCW:H282	0.50	1.83	10	2
3:B:205:PCW:H83	7:B:237:EWS:CAR	0.50	2.36	6	1
3:B:217:PCW:H261	3:B:218:PCW:H241	0.50	1.84	10	1
3:B:219:PCW:H421	4:B:223:17F:H38	0.50	1.84	10	1
1:A:275:LYS:O	1:A:279:LEU:HB2	0.49	2.06	2	1
3:B:201:PCW:H20	4:B:228:17F:H34	0.49	1.83	4	1
3:C:613:PCW:H222	3:C:622:PCW:H242	0.49	1.83	5	1
3:A:406:PCW:H432	3:A:409:PCW:H221	0.49	1.82	8	1
2:B:7:VAL:HB	2:B:78:PHE:CE1	0.49	2.41	8	1
3:A:406:PCW:H382	4:B:226:17F:H60	0.49	1.83	9	1
3:C:611:PCW:H152	3:C:617:PCW:H332	0.49	1.84	10	1
1:A:214:PHE:CE2	3:A:404:PCW:H171	0.49	2.39	1	1
3:B:218:PCW:H432	3:B:222:PCW:H421	0.49	1.84	1	1
2:B:63:GLU:O	2:B:68:ARG:HG2	0.49	2.06	1	1
1:C:470:TYR:CD1	4:C:632:17F:H76	0.49	2.41	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:229:17F:H55	3:B:231:PCW:H182	0.49	1.83	3	1
1:C:421:PRO:O	1:C:425:GLU:HG3	0.49	2.07	4	1
3:A:409:PCW:H441	3:C:605:PCW:H222	0.49	1.83	1	1
3:B:217:PCW:H321	3:B:217:PCW:H41	0.49	1.83	1	1
3:A:405:PCW:H42	3:B:222:PCW:H32	0.49	1.84	4	1
1:A:253:LYS:O	1:A:257:TYR:HB2	0.49	2.07	7	1
3:B:209:PCW:H432	3:C:617:PCW:H252	0.49	1.84	9	1
3:C:608:PCW:H62	4:C:630:17F:H2	0.49	1.83	10	1
3:C:616:PCW:H412	3:C:622:PCW:H212	0.49	1.83	1	3
2:B:56:LEU:HD23	2:B:58:THR:HG23	0.49	1.83	4	1
1:A:393:TYR:OH	3:A:407:PCW:C25	0.49	2.57	6	1
4:A:411:17F:H69	3:C:624:PCW:H421	0.49	1.85	9	1
1:C:441:MET:HA	1:C:444:ASP:HB2	0.49	1.84	1	1
3:A:408:PCW:H12	3:B:231:PCW:H352	0.49	1.84	3	1
1:C:489:LEU:CD2	3:C:623:PCW:H261	0.49	2.37	3	1
2:B:149:ARG:HG2	2:B:152:VAL:HB	0.49	1.82	5	1
2:B:74:THR:HG21	7:B:237:EWS:NAA	0.49	2.23	7	1
1:A:334:ARG:HD2	1:C:440:GLU:OE2	0.49	2.07	7	1
3:A:402:PCW:H39	3:B:214:PCW:H262	0.49	1.83	8	1
3:B:211:PCW:H241	3:B:217:PCW:H431	0.49	1.84	9	1
1:A:224:VAL:O	1:A:228:PHE:HB2	0.49	2.08	1	3
3:C:608:PCW:H63	4:C:630:17F:H2	0.49	1.85	1	1
3:A:408:PCW:H242	3:C:618:PCW:H483	0.49	1.83	2	1
3:C:617:PCW:H232	4:C:632:17F:H42	0.49	1.83	3	1
3:B:208:PCW:H181	3:B:215:PCW:H411	0.49	1.84	4	1
4:B:228:17F:H72	3:C:622:PCW:H252	0.49	1.85	4	1
1:A:298:LEU:O	1:A:302:GLY:HA3	0.49	2.07	8	2
3:C:610:PCW:H431	3:C:614:PCW:H172	0.49	1.84	5	1
3:C:610:PCW:H161	3:C:619:PCW:H172	0.49	1.82	5	1
1:A:341:ASN:ND2	1:C:433:GLU:HA	0.49	2.22	7	2
2:B:66:ALA:HB3	4:B:229:17F:HN1	0.49	1.68	6	1
4:B:223:17F:H1	4:B:223:17F:H4A	0.49	1.85	9	2
3:A:401:PCW:H452	3:C:616:PCW:H272	0.49	1.84	1	1
2:B:113:LEU:HB3	2:B:141:PHE:HD1	0.49	1.67	1	1
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.49	1.84	5	2
3:A:407:PCW:C12	4:B:223:17F:H20A	0.49	2.38	4	2
3:B:231:PCW:H361	3:C:604:PCW:H382	0.49	1.83	5	2
1:A:332:ALA:O	1:A:336:GLU:HG2	0.49	2.07	7	1
3:B:220:PCW:H382	3:B:220:PCW:H142	0.49	1.85	8	1
3:A:407:PCW:H132	4:B:223:17F:H20	0.49	1.83	9	1
3:B:202:PCW:H471	4:B:226:17F:H10A	0.49	1.84	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:209:PCW:H171	3:B:216:PCW:H181	0.49	1.85	4	1
3:B:231:PCW:H252	3:C:604:PCW:H271	0.49	1.83	4	1
4:B:225:17F:H71	3:C:615:PCW:H242	0.49	1.85	9	2
3:B:204:PCW:H483	3:C:604:PCW:H261	0.49	1.85	5	1
3:B:215:PCW:H451	3:B:221:PCW:H252	0.49	1.85	6	1
3:B:218:PCW:H472	3:C:603:PCW:H471	0.49	1.84	7	1
3:B:219:PCW:H131	4:B:230:17F:H34	0.49	1.85	7	1
3:B:209:PCW:H132	3:B:216:PCW:H122	0.49	1.84	8	1
3:B:232:PCW:H352	3:B:232:PCW:H122	0.49	1.85	10	1
3:C:603:PCW:H441	3:C:625:PCW:H472	0.49	1.83	3	1
3:B:205:PCW:H242	3:B:219:PCW:H431	0.49	1.85	4	1
3:C:621:PCW:H471	4:C:634:17F:H53	0.49	1.85	6	1
1:A:388:SER:HB2	1:C:594:LYS:CE	0.49	2.38	9	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.49	1.84	9	1
1:A:363:LYS:HA	1:A:367:ALA:HB3	0.49	1.84	10	1
3:A:409:PCW:H372	3:C:627:PCW:H361	0.49	1.83	10	1
3:B:221:PCW:N	7:B:237:EWS:BRA	0.49	3.00	1	1
1:C:508:ARG:O	1:C:512:ASP:HB2	0.49	2.07	2	3
1:C:455:TYR:CE2	3:C:601:PCW:H231	0.49	2.34	3	1
4:B:226:17F:H51	4:B:230:17F:H50	0.49	1.85	4	1
3:B:209:PCW:H261	3:C:611:PCW:H482	0.49	1.83	5	1
3:B:201:PCW:H62	3:B:220:PCW:O2P	0.49	2.08	6	1
3:C:606:PCW:H462	3:C:615:PCW:H171	0.49	1.85	6	1
3:B:202:PCW:H20	4:B:228:17F:H12	0.49	1.83	7	1
3:B:212:PCW:H141	4:B:226:17F:H18	0.49	1.84	7	1
3:C:611:PCW:H472	4:C:635:17F:H45	0.49	1.85	10	1
3:B:214:PCW:H461	3:C:612:PCW:H283	0.48	1.85	1	1
2:B:72:MET:HG2	2:B:78:PHE:CE1	0.48	2.43	1	1
1:C:455:TYR:O	1:C:459:PHE:HB2	0.48	2.07	9	3
3:B:203:PCW:H31	3:B:211:PCW:H321	0.48	1.85	3	1
3:B:231:PCW:H362	3:C:604:PCW:H171	0.48	1.84	4	1
3:A:403:PCW:H461	3:C:618:PCW:H461	0.48	1.85	5	1
3:C:611:PCW:H361	3:C:617:PCW:H381	0.48	1.85	5	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.48	1.68	7	2
3:C:612:PCW:H12	4:C:634:17F:H6	0.48	1.85	7	1
3:C:605:PCW:H182	3:C:626:PCW:H132	0.48	1.84	7	1
1:C:534:GLU:HA	1:C:537:LYS:HE3	0.48	1.85	9	1
3:C:616:PCW:H171	3:C:616:PCW:H412	0.48	1.83	9	1
3:C:615:PCW:H132	3:C:622:PCW:H362	0.48	1.85	10	2
1:A:392:GLU:O	1:A:396:LYS:HG2	0.48	2.07	9	2
1:A:327:LEU:HA	1:A:330:ARG:HG2	0.48	1.84	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:H471	4:B:223:17F:H48	0.48	1.84	5	2
3:B:201:PCW:H441	4:B:226:17F:H55	0.48	1.85	5	1
1:C:546:GLU:O	1:C:550:LYS:HD2	0.48	2.08	5	3
3:B:201:PCW:H72	7:B:237:EWS:BRA	0.48	2.63	8	1
3:A:410:PCW:O2P	3:C:620:PCW:H52	0.48	2.08	8	1
4:A:411:17F:H75	4:C:634:17F:H71	0.48	1.83	8	1
3:B:219:PCW:H283	4:C:631:17F:H52	0.48	1.84	1	1
4:B:229:17F:H47	3:B:231:PCW:H212	0.48	1.85	1	1
4:B:227:17F:O2	3:C:602:PCW:H82	0.48	2.07	9	2
3:B:231:PCW:H19	3:C:618:PCW:H39	0.48	1.85	10	3
3:B:203:PCW:H141	3:B:207:PCW:H322	0.48	1.84	7	1
3:B:204:PCW:H81	3:B:220:PCW:H52	0.48	1.85	9	1
4:B:225:17F:H72	4:B:228:17F:H68	0.48	1.84	6	1
3:C:626:PCW:H19	3:C:627:PCW:H282	0.48	1.86	6	1
3:B:205:PCW:H171	3:B:207:PCW:H141	0.48	1.85	7	1
4:B:225:17F:H74	4:B:228:17F:H62	0.48	1.86	2	1
2:B:94:HIS:O	2:B:98:GLU:HG2	0.48	2.07	2	2
3:C:607:PCW:H481	3:C:611:PCW:H372	0.48	1.84	2	1
3:B:209:PCW:H282	3:B:209:PCW:H20	0.48	1.85	4	1
3:B:201:PCW:C1	7:B:237:EWS:CAN	0.48	2.91	5	1
3:B:203:PCW:H20	3:B:217:PCW:H252	0.48	1.86	5	1
3:C:615:PCW:H381	3:C:622:PCW:H371	0.48	1.84	7	1
3:A:402:PCW:H361	3:A:402:PCW:H141	0.48	1.86	9	1
3:B:209:PCW:H483	3:C:617:PCW:H232	0.48	1.85	10	1
4:C:631:17F:H4	4:C:631:17F:H1A	0.48	1.86	10	1
1:A:322:PRO:O	1:A:326:GLU:HG3	0.48	2.09	1	1
3:A:408:PCW:H172	3:A:408:PCW:H362	0.48	1.84	1	2
1:C:455:TYR:HH	3:C:601:PCW:C21	0.48	2.15	3	1
3:C:614:PCW:H342	3:C:614:PCW:H132	0.48	1.85	3	1
4:A:411:17F:H61	4:C:635:17F:H68	0.48	1.84	7	2
3:A:402:PCW:H382	3:B:213:PCW:H372	0.48	1.86	4	1
1:C:488:LYS:CG	3:C:623:PCW:C28	0.48	2.51	4	1
1:A:396:LYS:NZ	3:A:407:PCW:C28	0.48	2.70	5	1
3:A:407:PCW:H342	4:B:225:17F:C9	0.48	2.31	6	1
4:B:234:17F:H58	4:B:234:17F:H12A	0.48	1.84	6	1
3:C:621:PCW:H362	3:C:629:PCW:H411	0.48	1.84	6	1
3:B:219:PCW:H261	3:C:625:PCW:H281	0.48	1.85	7	1
3:C:618:PCW:H182	3:C:620:PCW:H452	0.48	1.84	9	1
3:C:622:PCW:H361	3:C:622:PCW:H152	0.48	1.84	9	1
1:A:214:PHE:CE1	3:A:404:PCW:H171	0.48	2.43	10	1
1:C:479:ALA:O	1:C:483:GLU:HG2	0.48	2.09	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.48	2.35	3	4
3:A:408:PCW:H352	3:A:410:PCW:C34	0.48	2.38	3	1
3:B:216:PCW:H172	4:B:224:17F:H61	0.48	1.86	3	1
2:B:65:SER:HB3	2:B:68:ARG:HB3	0.48	1.86	4	1
3:B:203:PCW:H482	3:B:231:PCW:H452	0.48	1.86	5	1
3:B:219:PCW:H251	3:C:605:PCW:H271	0.48	1.85	7	1
3:B:211:PCW:H442	3:C:621:PCW:H232	0.48	1.86	8	1
1:C:411:THR:O	1:C:415:LEU:HG	0.48	2.09	9	1
1:A:214:PHE:HZ	3:A:404:PCW:H161	0.48	1.62	10	1
3:B:213:PCW:H241	3:C:611:PCW:H422	0.48	1.86	10	1
3:B:205:PCW:O2P	3:B:210:PCW:H51	0.48	2.09	1	1
4:B:230:17F:H37	3:C:605:PCW:H282	0.48	1.84	1	1
3:C:621:PCW:H431	3:C:621:PCW:H162	0.48	1.85	1	1
3:A:406:PCW:H12	3:B:206:PCW:H322	0.48	1.84	2	1
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.48	1.84	3	1
4:B:224:17F:H77	4:C:631:17F:H73	0.48	1.85	5	1
3:B:220:PCW:H232	3:C:604:PCW:H482	0.48	1.85	8	1
3:C:607:PCW:H19	3:C:628:PCW:H272	0.48	1.85	9	1
3:B:206:PCW:H251	3:C:601:PCW:H39	0.48	1.86	10	1
1:A:231:ASN:HA	1:A:234:LYS:CE	0.48	2.38	9	2
3:B:219:PCW:H32	3:B:220:PCW:H322	0.48	1.85	7	1
3:C:613:PCW:H12	3:C:613:PCW:H52	0.48	1.84	7	1
3:B:208:PCW:C3	3:B:221:PCW:H141	0.48	2.39	1	1
3:B:209:PCW:H152	3:B:216:PCW:H162	0.48	1.85	1	1
1:C:495:LYS:O	1:C:499:LEU:HB2	0.48	2.09	5	7
2:B:54:ASP:CB	7:B:237:EWS:BRA	0.48	3.15	2	1
3:B:201:PCW:H39	3:C:626:PCW:H251	0.48	1.86	2	1
3:B:207:PCW:H83	3:B:217:PCW:O1P	0.48	2.09	3	1
3:B:208:PCW:H361	4:B:226:17F:H8A	0.48	1.86	3	1
3:B:219:PCW:C6	7:B:237:EWS:BRA	0.48	3.17	6	1
3:B:209:PCW:H151	4:B:227:17F:H12A	0.48	1.85	9	1
2:B:133:LEU:HG	2:B:137:TYR:CE2	0.48	2.44	10	1
3:B:205:PCW:H171	4:B:224:17F:H29	0.48	1.85	10	1
3:C:606:PCW:H211	3:C:615:PCW:H171	0.48	1.86	10	1
1:A:355:GLU:HA	1:A:355:GLU:OE1	0.47	2.08	3	1
3:A:401:PCW:H372	3:B:202:PCW:H171	0.47	1.84	3	1
3:C:615:PCW:H31	3:C:615:PCW:O31	0.47	2.08	3	2
3:B:211:PCW:H472	3:C:621:PCW:H471	0.47	1.85	3	1
3:B:222:PCW:H472	4:C:634:17F:H47	0.47	1.86	4	1
3:B:209:PCW:H442	3:C:617:PCW:H252	0.47	1.85	4	1
3:C:610:PCW:H162	3:C:614:PCW:H171	0.47	1.85	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:234:17F:H35	3:C:625:PCW:H283	0.47	1.84	7	2
4:B:234:17F:H74	4:B:234:17F:H45	0.47	1.85	7	1
3:C:611:PCW:H182	3:C:617:PCW:H361	0.47	1.85	1	1
3:B:205:PCW:H272	3:B:220:PCW:H241	0.47	1.86	4	1
4:A:411:17F:H34	3:C:624:PCW:H422	0.47	1.86	6	1
3:B:206:PCW:H172	3:B:208:PCW:H232	0.47	1.86	6	1
3:B:211:PCW:H172	4:B:229:17F:H19	0.47	1.85	6	1
3:C:601:PCW:H422	4:C:630:17F:H54	0.47	1.86	10	1
3:C:615:PCW:O31	3:C:615:PCW:H31	0.47	2.08	1	5
3:C:617:PCW:H252	4:C:635:17F:H41	0.47	1.85	1	1
3:C:616:PCW:H412	3:C:622:PCW:H20	0.47	1.84	2	1
3:A:401:PCW:H73	2:B:70:GLN:OE1	0.47	2.09	4	1
3:B:219:PCW:C34	4:B:226:17F:H37	0.47	2.38	10	2
3:B:210:PCW:C37	4:B:224:17F:H11A	0.47	2.39	8	2
3:B:204:PCW:H62	3:B:211:PCW:O2P	0.47	2.08	10	1
3:B:205:PCW:H32	3:B:207:PCW:O1P	0.47	2.10	10	1
4:B:227:17F:H70	3:C:602:PCW:H422	0.47	1.86	10	1
2:B:79:LEU:CD2	2:B:112:VAL:HB	0.47	2.40	1	1
4:B:225:17F:H40	3:C:615:PCW:H232	0.47	1.87	1	1
2:B:72:MET:HG2	2:B:78:PHE:HE1	0.47	1.69	1	1
4:A:411:17F:H53	3:C:607:PCW:H242	0.47	1.85	2	1
3:B:205:PCW:H31	3:B:205:PCW:H42	0.47	1.84	2	1
3:C:610:PCW:H481	3:C:614:PCW:H282	0.47	1.85	3	1
2:B:67:MET:SD	3:B:211:PCW:H63	0.47	2.49	8	1
3:B:201:PCW:H63	3:B:219:PCW:O2P	0.47	2.09	1	1
2:B:39:SER:HA	2:B:55:ILE:O	0.47	2.09	1	1
1:A:316:LEU:HG	1:C:462:LYS:HE3	0.47	1.86	6	2
3:A:410:PCW:H51	3:A:410:PCW:H11	0.47	1.87	2	2
3:B:215:PCW:H282	3:C:609:PCW:H421	0.47	1.87	4	1
1:A:225:THR:O	1:A:229:TRP:HB2	0.47	2.09	5	3
3:A:406:PCW:H472	3:A:409:PCW:H242	0.47	1.84	8	3
3:A:401:PCW:H41	3:B:212:PCW:O11	0.47	2.10	7	1
3:B:212:PCW:H41	3:B:212:PCW:H31	0.47	1.86	1	1
1:A:363:LYS:O	1:A:367:ALA:HB3	0.47	2.10	3	3
3:B:202:PCW:H322	3:B:212:PCW:H331	0.47	1.87	2	1
4:B:223:17F:H4A	4:B:223:17F:H1	0.47	1.86	2	1
3:B:212:PCW:H361	3:B:212:PCW:H161	0.47	1.86	3	1
3:C:628:PCW:O11	3:C:628:PCW:H52	0.47	2.10	3	1
3:A:403:PCW:H451	3:C:618:PCW:H461	0.47	1.86	4	1
3:C:616:PCW:H171	3:C:616:PCW:H351	0.47	1.87	5	1
3:B:231:PCW:H411	3:C:604:PCW:H421	0.47	1.87	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:216:PCW:H232	3:C:611:PCW:H451	0.47	1.85	8	1
3:A:408:PCW:H171	3:A:408:PCW:H362	0.47	1.85	9	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.47	2.10	10	1
3:C:601:PCW:H381	3:C:602:PCW:H141	0.47	1.84	10	1
3:A:401:PCW:H39	3:B:202:PCW:H242	0.47	1.87	1	1
3:A:403:PCW:H82	4:B:223:17F:O4	0.47	2.09	2	1
2:B:32:TYR:CD1	5:B:235:GNP:H5'1	0.47	2.45	2	1
1:C:570:ARG:O	1:C:574:LEU:HG	0.47	2.09	2	1
1:A:391:GLU:O	1:A:395:LYS:HB2	0.47	2.09	3	1
3:B:208:PCW:H31	3:B:221:PCW:H152	0.47	1.86	3	1
3:C:625:PCW:H331	3:C:625:PCW:H73	0.47	1.87	3	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.47	1.85	6	2
3:B:206:PCW:H221	3:C:601:PCW:H371	0.47	1.85	5	1
3:A:402:PCW:H283	3:B:209:PCW:H272	0.47	1.85	6	1
3:A:405:PCW:H83	3:B:222:PCW:H32	0.47	1.87	6	1
3:B:205:PCW:H161	3:B:207:PCW:H162	0.47	1.86	6	1
3:A:409:PCW:H382	3:C:627:PCW:H382	0.47	1.86	6	1
3:A:406:PCW:H212	3:A:409:PCW:H232	0.47	1.86	7	1
3:C:609:PCW:H172	4:C:632:17F:H20A	0.47	1.85	7	1
3:A:401:PCW:H382	3:B:212:PCW:H451	0.47	1.86	8	1
3:B:231:PCW:H131	3:C:619:PCW:H11	0.47	1.85	8	1
3:B:231:PCW:H121	3:C:604:PCW:H19	0.47	1.86	8	1
4:A:411:17F:H55	3:C:617:PCW:H39	0.47	1.85	9	1
3:B:202:PCW:H471	4:B:230:17F:H12A	0.47	1.87	9	1
4:B:224:17F:H29	4:B:230:17F:H59	0.47	1.85	2	1
3:B:203:PCW:H482	3:B:231:PCW:H451	0.47	1.85	7	2
1:C:534:GLU:O	1:C:538:GLU:HG2	0.47	2.10	3	1
3:C:609:PCW:H172	4:C:632:17F:H18	0.47	1.86	3	1
3:B:232:PCW:C48	4:B:234:17F:H42	0.47	2.40	4	1
3:C:606:PCW:H181	3:C:615:PCW:H122	0.47	1.85	4	1
3:C:614:PCW:C34	3:C:614:PCW:H132	0.47	2.40	6	1
2:B:68:ARG:HA	2:B:71:TYR:CD2	0.47	2.44	8	2
4:C:630:17F:H71	4:C:632:17F:H53	0.47	1.87	7	1
3:C:610:PCW:H362	3:C:614:PCW:H362	0.47	1.87	9	1
3:A:406:PCW:H222	3:A:409:PCW:H241	0.47	1.85	10	1
4:B:226:17F:H78	3:C:628:PCW:H451	0.47	1.87	4	1
3:A:407:PCW:C33	4:B:223:17F:H31	0.47	2.38	5	1
4:B:234:17F:H70	3:C:607:PCW:H261	0.47	1.87	9	2
1:C:466:GLU:HA	1:C:469:LEU:HB2	0.47	1.87	9	1
3:B:202:PCW:H452	4:B:226:17F:H12A	0.47	1.86	1	1
3:C:621:PCW:H371	3:C:629:PCW:H412	0.47	1.86	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:201:PCW:H341	3:B:219:PCW:H361	0.47	1.87	3	2
4:B:234:17F:H70	3:C:607:PCW:H271	0.47	1.87	3	2
3:A:407:PCW:C35	4:B:223:17F:H56	0.47	2.38	10	3
3:B:205:PCW:H452	3:B:207:PCW:H241	0.47	1.85	4	1
3:C:617:PCW:C22	4:C:632:17F:H42	0.47	2.40	4	1
3:B:232:PCW:H40	3:C:619:PCW:H452	0.47	1.87	4	1
3:C:617:PCW:H222	4:C:635:17F:H35	0.47	1.86	4	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.47	2.39	10	3
3:B:210:PCW:H352	4:B:224:17F:H31	0.46	1.87	1	1
3:C:609:PCW:H211	4:C:630:17F:H37	0.46	1.86	1	1
3:C:606:PCW:H62	4:C:633:17F:O5	0.46	2.10	1	1
4:B:224:17F:H44	4:B:234:17F:H43	0.46	1.86	2	1
2:B:6:LEU:HD23	2:B:159:LEU:HD23	0.46	1.87	3	1
3:B:201:PCW:H232	3:C:613:PCW:H471	0.46	1.87	3	1
3:C:606:PCW:H181	3:C:615:PCW:H341	0.46	1.87	5	1
3:B:202:PCW:H481	4:B:226:17F:H20	0.46	1.85	6	1
4:B:227:17F:H30	4:B:227:17F:H41	0.46	1.87	6	1
3:C:629:PCW:H231	4:C:634:17F:H40	0.46	1.86	6	1
3:B:213:PCW:H462	4:C:635:17F:H70	0.46	1.87	7	1
3:A:410:PCW:H332	4:C:633:17F:C12	0.46	2.36	8	1
4:C:635:17F:H9A	4:C:635:17F:H18	0.46	1.86	10	1
3:B:205:PCW:H251	3:B:220:PCW:H181	0.46	1.87	2	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.46	2.39	3	1
3:A:406:PCW:H182	3:A:409:PCW:H252	0.46	1.87	8	1
2:B:113:LEU:O	2:B:141:PHE:HA	0.46	2.10	8	1
3:B:201:PCW:H151	4:B:225:17F:O8	0.46	2.11	9	1
2:B:118:CYS:HB3	2:B:143:GLU:HG2	0.46	1.86	10	1
3:B:207:PCW:H341	3:B:220:PCW:H372	0.46	1.86	2	1
3:C:608:PCW:H63	4:C:630:17F:HN1A	0.46	1.70	2	1
3:B:231:PCW:H461	3:C:604:PCW:H271	0.46	1.87	3	1
3:C:613:PCW:H411	3:C:622:PCW:H441	0.46	1.87	4	1
3:A:401:PCW:H62	3:B:212:PCW:H11	0.46	1.86	5	1
4:A:411:17F:H53	3:C:607:PCW:H221	0.46	1.85	6	1
4:B:225:17F:H71	3:C:615:PCW:H222	0.46	1.86	6	1
3:C:611:PCW:C37	4:C:635:17F:H34	0.46	2.40	6	1
3:B:209:PCW:H61	4:B:224:17F:O1	0.46	2.10	9	1
3:C:619:PCW:H39	3:C:629:PCW:H232	0.46	1.87	3	2
1:A:234:LYS:HE3	1:C:539:ASN:OD1	0.46	2.11	2	3
1:A:293:GLU:O	1:A:297:LYS:HB2	0.46	2.09	2	1
3:C:626:PCW:H131	3:C:626:PCW:H39	0.46	1.86	3	1
3:A:409:PCW:H483	3:B:208:PCW:H471	0.46	1.86	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:405:PCW:H261	3:C:621:PCW:H412	0.46	1.87	5	1
3:B:219:PCW:H432	3:B:219:PCW:H381	0.46	1.86	5	1
3:C:621:PCW:H42	3:C:629:PCW:H41	0.46	1.88	5	1
3:B:205:PCW:H282	3:B:220:PCW:H241	0.46	1.86	6	1
3:B:207:PCW:H142	3:B:232:PCW:H281	0.46	1.85	6	1
3:B:212:PCW:H261	4:B:226:17F:H59	0.46	1.87	7	1
1:A:358:SER:O	1:A:362:GLU:HG3	0.46	2.09	9	2
1:C:470:TYR:CE1	4:C:632:17F:C42	0.46	2.98	1	1
4:B:226:17F:H49	3:C:626:PCW:H241	0.46	1.86	3	1
3:B:232:PCW:H411	3:B:232:PCW:H372	0.46	1.86	3	1
1:C:422:VAL:HA	1:C:425:GLU:OE2	0.46	2.11	4	1
3:B:203:PCW:H442	3:B:204:PCW:H39	0.46	1.86	8	1
3:C:606:PCW:H262	3:C:615:PCW:H181	0.46	1.86	8	1
3:A:404:PCW:O2P	3:B:211:PCW:H141	0.46	2.10	9	1
3:B:215:PCW:H2	3:B:215:PCW:H52	0.46	1.86	9	1
3:A:401:PCW:H483	3:C:613:PCW:H271	0.46	1.86	10	1
1:A:203:LEU:O	1:A:207:TRP:HB2	0.46	2.10	6	2
3:B:216:PCW:H221	3:C:611:PCW:H452	0.46	1.86	5	1
1:A:330:ARG:O	1:A:334:ARG:HG2	0.46	2.11	6	2
3:B:217:PCW:H283	3:B:218:PCW:H262	0.46	1.87	6	1
3:B:221:PCW:H81	4:B:224:17F:O2	0.46	2.10	6	1
3:B:218:PCW:H261	3:C:625:PCW:H40	0.46	1.87	7	1
4:B:234:17F:H41	4:B:234:17F:H69	0.46	1.87	9	1
1:C:456:LEU:O	1:C:460:GLN:HB2	0.46	2.10	2	1
3:B:232:PCW:H122	3:C:625:PCW:C17	0.46	2.41	3	1
1:C:563:LYS:HB2	1:C:564:PRO:CD	0.46	2.41	5	2
3:C:627:PCW:H351	3:C:628:PCW:C12	0.46	2.41	5	1
3:C:607:PCW:H371	4:C:631:17F:H6	0.46	1.87	7	1
3:B:212:PCW:H152	3:B:212:PCW:H341	0.46	1.88	10	2
3:A:410:PCW:H382	4:C:633:17F:H36	0.46	1.87	1	1
3:A:405:PCW:H83	3:B:222:PCW:H11	0.46	1.87	1	1
3:C:613:PCW:H382	3:C:613:PCW:H171	0.46	1.88	2	1
4:B:226:17F:H10	4:B:230:17F:H10A	0.46	1.86	3	1
1:C:530:ALA:O	1:C:534:GLU:HG3	0.46	2.11	3	2
3:C:619:PCW:H271	3:C:621:PCW:H242	0.46	1.88	4	1
1:A:308:ARG:HD3	1:C:469:LEU:CD1	0.46	2.38	6	1
4:B:234:17F:H66	4:C:631:17F:H63	0.46	1.88	6	1
3:B:221:PCW:H12	3:B:221:PCW:H52	0.46	1.87	3	1
2:B:41:ARG:HD3	2:B:54:ASP:OD2	0.46	2.11	4	2
2:B:5:LYS:HE3	3:B:219:PCW:H72	0.46	1.87	7	1
3:A:410:PCW:H121	4:C:633:17F:H11A	0.46	1.86	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:499:LEU:O	1:C:503:MET:HB2	0.46	2.11	9	1
3:C:623:PCW:H131	4:C:635:17F:H18A	0.46	1.88	10	1
3:A:406:PCW:H172	4:B:226:17F:H59	0.46	1.87	1	1
3:C:626:PCW:H31	3:C:627:PCW:H161	0.46	1.87	1	3
3:B:203:PCW:H162	3:B:207:PCW:H351	0.46	1.87	4	1
3:C:611:PCW:H482	4:C:635:17F:H45	0.46	1.88	4	1
3:B:213:PCW:H421	3:B:216:PCW:H272	0.46	1.87	5	1
4:B:234:17F:H43	4:B:234:17F:H73	0.46	1.87	6	1
3:A:408:PCW:H431	3:C:604:PCW:H281	0.46	1.86	7	1
3:C:628:PCW:O11	3:C:628:PCW:H83	0.46	2.11	8	1
3:B:213:PCW:H242	3:C:611:PCW:H422	0.45	1.88	1	1
3:C:611:PCW:H172	3:C:617:PCW:H331	0.45	1.88	2	1
3:B:231:PCW:H382	3:C:604:PCW:H432	0.45	1.87	3	1
3:B:219:PCW:H222	4:B:224:17F:H42	0.45	1.87	4	1
3:B:206:PCW:H461	3:B:208:PCW:H271	0.45	1.87	5	1
4:B:226:17F:H43	4:B:230:17F:H42	0.45	1.87	6	1
3:B:210:PCW:H121	4:B:224:17F:H32	0.45	1.87	9	2
2:B:131:GLN:HG2	2:B:141:PHE:CD2	0.45	2.45	8	1
3:C:602:PCW:H283	4:C:630:17F:H52	0.45	1.88	8	1
3:C:616:PCW:H482	3:C:616:PCW:H222	0.45	1.87	8	1
3:A:408:PCW:C33	3:A:410:PCW:H341	0.45	2.41	9	1
1:A:387:LEU:O	1:A:391:GLU:HG3	0.45	2.09	10	2
3:B:203:PCW:H271	4:C:634:17F:H55	0.45	1.87	2	1
1:A:363:LYS:HG2	1:C:411:THR:HG22	0.45	1.88	3	1
1:C:460:GLN:O	1:C:464:GLN:HG3	0.45	2.11	3	1
3:C:605:PCW:H31	3:C:605:PCW:O1P	0.45	2.11	6	1
3:B:210:PCW:H422	3:B:210:PCW:H242	0.45	1.88	8	1
3:B:203:PCW:P	7:B:237:EWS:CAK	0.45	3.04	8	1
3:C:611:PCW:H282	3:C:617:PCW:H452	0.45	1.87	9	2
4:B:227:17F:H39	4:B:227:17F:H30	0.45	1.89	9	1
3:C:628:PCW:H83	3:C:628:PCW:O11	0.45	2.11	9	1
3:B:211:PCW:H221	3:B:217:PCW:H412	0.45	1.87	10	1
1:A:268:GLU:OE1	1:C:506:ARG:HD3	0.45	2.12	3	1
3:B:205:PCW:H221	3:B:233:PCW:H283	0.45	1.87	4	1
1:C:561:LYS:O	1:C:565:ALA:HB3	0.45	2.11	5	1
3:A:406:PCW:H331	3:B:208:PCW:H352	0.45	1.87	7	1
3:B:209:PCW:H131	4:B:227:17F:H10A	0.45	1.89	9	1
1:C:488:LYS:CD	3:C:623:PCW:H272	0.45	2.29	9	1
1:A:335:LEU:O	1:A:339:LYS:HB2	0.45	2.12	10	1
2:B:71:TYR:HB2	7:B:237:EWS:OAB	0.45	2.11	6	2
1:A:264:LYS:CE	1:C:509:ALA:HB1	0.45	2.41	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:411:17F:H32	4:A:411:17F:H8A	0.45	1.87	6	1
3:B:204:PCW:H251	3:C:618:PCW:H483	0.45	1.87	6	1
3:B:216:PCW:H451	4:C:634:17F:H74	0.45	1.87	6	1
3:A:407:PCW:H342	4:B:225:17F:H11A	0.45	1.88	7	1
3:B:201:PCW:H212	4:B:228:17F:H34	0.45	1.88	9	1
3:B:211:PCW:H171	4:B:229:17F:H59	0.45	1.87	1	1
3:A:406:PCW:H372	3:B:208:PCW:H39	0.45	1.89	2	2
3:C:611:PCW:H63	4:C:635:17F:HN1	0.45	1.71	2	1
1:A:345:ARG:O	1:A:349:TYR:HB2	0.45	2.12	4	1
3:A:410:PCW:H412	3:A:410:PCW:H371	0.45	1.87	4	1
3:C:621:PCW:H361	3:C:629:PCW:H221	0.45	1.87	4	1
3:B:209:PCW:H251	4:C:635:17F:H38	0.45	1.87	4	1
3:C:613:PCW:H171	3:C:613:PCW:H381	0.45	1.89	5	1
3:B:207:PCW:H442	3:C:621:PCW:H222	0.45	1.89	6	1
3:A:403:PCW:H332	3:B:204:PCW:C3	0.45	2.39	8	1
3:B:205:PCW:H172	3:B:220:PCW:H352	0.45	1.89	9	1
1:A:393:TYR:OH	3:A:403:PCW:C28	0.45	2.64	2	1
3:C:626:PCW:H19	3:C:627:PCW:H271	0.45	1.87	2	1
2:B:77:GLY:HA3	2:B:163:ILE:HD11	0.45	1.89	3	1
1:A:308:ARG:HG3	1:C:465:GLU:HB3	0.45	1.88	4	1
3:C:615:PCW:H151	3:C:615:PCW:C38	0.45	2.41	5	1
4:B:228:17F:H55	3:C:615:PCW:H483	0.45	1.89	5	1
3:A:408:PCW:H422	3:B:204:PCW:H461	0.45	1.87	7	1
4:B:224:17F:H51	4:B:230:17F:H74	0.45	1.87	7	1
3:C:619:PCW:H282	3:C:621:PCW:H252	0.45	1.88	7	1
1:C:550:LYS:O	1:C:554:HIS:HB2	0.45	2.12	1	1
3:C:607:PCW:H20	4:C:631:17F:H44	0.45	1.88	3	1
4:A:411:17F:H54	3:C:607:PCW:H241	0.45	1.88	4	1
4:B:229:17F:H50	3:B:231:PCW:H181	0.45	1.89	4	1
3:A:401:PCW:H41	3:B:212:PCW:H2	0.45	1.88	6	1
3:B:219:PCW:H482	4:B:223:17F:H49	0.45	1.89	6	2
3:B:201:PCW:H172	4:B:225:17F:H60	0.45	1.88	7	1
1:C:549:ALA:O	1:C:553:GLU:HG3	0.45	2.12	7	2
3:B:231:PCW:H441	3:C:604:PCW:H261	0.45	1.87	7	1
3:B:202:PCW:H271	4:B:228:17F:H66	0.45	1.89	10	1
2:B:118:CYS:SG	2:B:145:SER:HB2	0.45	2.52	4	2
3:C:609:PCW:H211	4:C:630:17F:H58	0.45	1.89	2	1
4:C:631:17F:H57	4:C:631:17F:H37	0.45	1.87	2	1
3:B:219:PCW:H283	3:C:625:PCW:H252	0.45	1.87	4	1
3:B:203:PCW:H483	3:B:220:PCW:H262	0.45	1.88	5	1
1:A:310:ARG:O	1:A:314:ASP:HB3	0.45	2.11	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:607:PCW:C24	4:C:631:17F:H39	0.45	2.41	6	1
3:B:201:PCW:H381	3:B:219:PCW:H441	0.45	1.88	7	1
3:B:219:PCW:H483	3:B:233:PCW:H241	0.45	1.89	10	1
3:C:611:PCW:H282	3:C:617:PCW:H422	0.45	1.88	10	1
3:B:201:PCW:H342	3:B:219:PCW:H361	0.45	1.88	2	1
3:A:410:PCW:H461	3:C:620:PCW:H283	0.45	1.88	2	1
3:B:202:PCW:H432	4:B:226:17F:H43	0.45	1.89	10	2
3:C:615:PCW:H132	3:C:622:PCW:C38	0.45	2.40	3	1
3:B:216:PCW:H73	4:B:224:17F:N1	0.45	2.24	6	1
1:A:202:LYS:HE3	1:C:576:VAL:HG21	0.45	1.89	7	1
3:A:406:PCW:H371	4:B:226:17F:H60	0.45	1.89	7	1
3:B:205:PCW:H272	3:B:233:PCW:H262	0.45	1.89	8	1
3:B:221:PCW:H121	3:B:221:PCW:H341	0.45	1.87	9	1
1:A:247:LEU:HA	1:A:250:VAL:HG12	0.45	1.87	10	1
3:B:205:PCW:H212	3:B:220:PCW:H412	0.45	1.88	10	1
3:B:203:PCW:H171	3:B:217:PCW:H132	0.45	1.89	2	1
3:C:621:PCW:O3	3:C:629:PCW:H171	0.45	2.12	3	1
4:C:630:17F:H35	4:C:630:17F:H42	0.45	1.89	4	1
3:B:215:PCW:H471	3:C:608:PCW:H482	0.45	1.89	5	1
4:A:411:17F:H63	3:B:216:PCW:H251	0.45	1.87	6	1
1:C:415:LEU:HA	1:C:418:GLN:NE2	0.45	2.27	6	1
3:A:401:PCW:H51	3:B:212:PCW:H2	0.45	1.88	8	1
3:B:201:PCW:H242	3:B:212:PCW:H422	0.45	1.88	8	1
3:A:401:PCW:H411	3:B:212:PCW:H472	0.44	1.89	1	1
3:B:202:PCW:H122	4:B:228:17F:C9	0.44	2.41	2	1
3:B:204:PCW:H482	3:B:231:PCW:H422	0.44	1.89	3	1
3:C:609:PCW:H483	4:C:630:17F:H55	0.44	1.89	3	1
3:A:402:PCW:H341	3:A:402:PCW:H122	0.44	1.89	5	1
4:A:411:17F:H61	4:C:635:17F:H72	0.44	1.89	5	1
2:B:56:LEU:HD12	7:B:237:EWS:CAQ	0.44	2.42	7	1
3:B:201:PCW:C22	4:B:225:17F:H65	0.44	2.37	8	1
3:B:203:PCW:O11	4:B:229:17F:H18A	0.44	2.11	8	1
1:A:376:LEU:O	1:A:380:GLU:HG3	0.44	2.12	9	1
1:C:585:LEU:O	1:C:589:GLU:HB2	0.44	2.12	10	1
1:A:268:GLU:O	1:A:272:TYR:HB2	0.44	2.13	2	1
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.44	2.47	2	1
3:C:629:PCW:O31	3:C:629:PCW:H41	0.44	2.12	2	1
3:A:403:PCW:H251	3:A:407:PCW:H231	0.44	1.88	3	1
3:B:202:PCW:O31	3:B:202:PCW:H52	0.44	2.12	3	1
4:B:234:17F:C1Z	4:B:234:17F:H10A	0.44	2.42	4	1
3:B:205:PCW:H40	3:B:216:PCW:H372	0.44	1.88	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:B:226:17F:H49	3:C:613:PCW:H462	0.44	1.88	6	1
4:B:227:17F:O2	3:C:602:PCW:H81	0.44	2.13	6	1
3:A:405:PCW:H162	3:B:222:PCW:H372	0.44	1.88	7	1
3:B:201:PCW:H442	4:B:230:17F:H77	0.44	1.89	8	1
3:B:207:PCW:H341	3:B:232:PCW:H282	0.44	1.89	9	1
3:B:203:PCW:H341	3:B:220:PCW:H132	0.44	1.88	10	1
3:C:603:PCW:H471	3:C:625:PCW:H452	0.44	1.88	10	1
4:B:223:17F:H50	3:C:626:PCW:H232	0.44	1.90	10	1
3:A:409:PCW:H432	3:C:605:PCW:H20	0.44	1.89	3	1
3:B:212:PCW:H421	3:B:212:PCW:H20	0.44	1.88	3	1
3:A:407:PCW:H442	3:C:606:PCW:H271	0.44	1.89	8	1
3:C:607:PCW:H321	3:C:609:PCW:C8	0.44	2.43	8	1
1:A:249:GLU:O	1:A:253:LYS:HB2	0.44	2.12	9	1
3:A:407:PCW:H442	4:B:223:17F:H71	0.44	1.89	1	1
3:B:201:PCW:H483	3:C:605:PCW:H222	0.44	1.88	2	1
3:B:220:PCW:H272	3:B:233:PCW:H212	0.44	1.89	2	1
3:C:607:PCW:H451	3:C:611:PCW:H321	0.44	1.88	4	1
1:A:359:THR:O	1:A:363:LYS:HG3	0.44	2.12	6	2
3:B:209:PCW:H31	4:B:227:17F:H10A	0.44	1.88	5	1
1:A:292:HIS:O	1:A:296:GLU:HG2	0.44	2.13	6	1
3:B:203:PCW:H442	3:B:231:PCW:H451	0.44	1.89	6	1
3:B:203:PCW:H41	4:B:229:17F:O1	0.44	2.13	2	1
3:C:611:PCW:H262	3:C:617:PCW:H441	0.44	1.87	3	1
3:C:606:PCW:H283	3:C:615:PCW:H182	0.44	1.90	5	1
3:C:613:PCW:H151	3:C:626:PCW:H432	0.44	1.89	10	1
3:C:602:PCW:H452	4:C:630:17F:H40	0.44	1.89	1	1
3:C:614:PCW:H83	3:C:629:PCW:H32	0.44	1.88	2	1
1:A:242:GLU:OE1	1:C:528:ARG:HB3	0.44	2.12	3	1
3:B:218:PCW:H442	3:B:222:PCW:H441	0.44	1.90	8	2
3:B:203:PCW:H381	3:B:204:PCW:H142	0.44	1.88	4	1
3:B:201:PCW:H82	3:B:219:PCW:C1	0.44	2.43	5	1
2:B:62:GLU:HB3	2:B:68:ARG:NH1	0.44	2.28	5	1
3:B:207:PCW:H472	4:B:229:17F:H51	0.44	1.88	6	1
3:B:201:PCW:H39	3:C:626:PCW:H242	0.44	1.88	7	1
3:B:212:PCW:H422	3:C:613:PCW:H482	0.44	1.90	7	1
3:A:401:PCW:H471	3:C:613:PCW:H232	0.44	1.90	8	1
3:B:203:PCW:H483	3:B:231:PCW:H432	0.44	1.89	10	1
3:B:209:PCW:H161	3:B:213:PCW:H361	0.44	1.90	1	1
3:B:201:PCW:H422	3:B:219:PCW:H472	0.44	1.88	2	1
4:B:229:17F:H43	3:C:621:PCW:H252	0.44	1.89	6	1
3:B:203:PCW:H481	3:B:233:PCW:C48	0.44	2.43	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:LYS:O	1:A:206:ASN:HB2	0.44	2.13	8	1
3:C:607:PCW:H241	3:C:611:PCW:H283	0.44	1.88	10	1
3:B:209:PCW:H182	3:C:611:PCW:H471	0.44	1.89	1	1
3:B:213:PCW:H20	3:C:611:PCW:H441	0.44	1.90	2	1
3:C:613:PCW:C38	3:C:613:PCW:H171	0.44	2.43	5	2
1:C:448:VAL:O	1:C:452:VAL:HB	0.44	2.12	3	1
3:A:409:PCW:H371	3:C:627:PCW:C34	0.44	2.42	5	1
3:B:205:PCW:H272	3:B:219:PCW:H482	0.44	1.88	5	1
4:B:234:17F:H64	4:B:234:17F:C23	0.44	2.42	5	1
3:C:608:PCW:C3	3:C:628:PCW:H331	0.44	2.41	6	1
3:B:205:PCW:H252	3:B:220:PCW:H421	0.44	1.87	7	1
3:C:626:PCW:H161	3:C:627:PCW:H252	0.44	1.89	7	1
4:B:234:17F:C1Y	3:C:625:PCW:H172	0.44	2.43	9	1
3:B:219:PCW:H261	3:C:625:PCW:H282	0.44	1.90	1	1
3:C:618:PCW:H121	3:C:620:PCW:H412	0.44	1.89	2	2
4:B:223:17F:P1	4:B:223:17F:HN1	0.44	2.36	4	1
3:B:202:PCW:H452	3:B:212:PCW:H162	0.44	1.88	5	1
1:C:533:LEU:O	1:C:537:LYS:HG3	0.44	2.13	5	1
3:B:205:PCW:H181	3:B:219:PCW:H122	0.44	1.89	7	1
3:A:407:PCW:H63	4:B:228:17F:N1	0.44	2.27	7	1
3:A:401:PCW:H472	3:C:626:PCW:H483	0.44	1.89	7	1
3:B:208:PCW:H452	4:B:226:17F:H61	0.44	1.88	8	1
3:C:609:PCW:H83	3:C:611:PCW:H142	0.44	1.89	10	1
1:A:271:LEU:O	1:A:275:LYS:HG2	0.43	2.13	1	2
3:A:410:PCW:H352	4:C:633:17F:C2X	0.43	2.40	5	2
3:A:406:PCW:H362	3:A:406:PCW:H152	0.43	1.87	3	1
3:C:618:PCW:H122	3:C:620:PCW:C38	0.43	2.43	6	2
3:B:207:PCW:H182	3:B:232:PCW:C28	0.43	2.41	5	1
2:B:72:MET:HB3	2:B:103:VAL:HG21	0.43	1.91	5	1
1:C:517:HIS:O	1:C:521:TYR:HB2	0.43	2.13	5	2
3:A:408:PCW:H151	3:C:604:PCW:H221	0.43	1.91	6	1
3:B:210:PCW:H482	4:B:227:17F:H41	0.43	1.89	8	1
3:B:212:PCW:H171	3:B:212:PCW:H362	0.43	1.90	10	1
2:B:53:LEU:HD12	2:B:55:ILE:HD11	0.43	1.90	10	1
3:B:209:PCW:H20	3:C:611:PCW:H471	0.43	1.90	10	1
3:C:613:PCW:H62	3:C:627:PCW:C7	0.43	2.43	1	1
1:C:563:LYS:CB	1:C:564:PRO:HD3	0.43	2.39	9	2
1:A:337:ALA:O	1:A:341:ASN:HB2	0.43	2.12	3	1
3:C:613:PCW:H332	3:C:626:PCW:H411	0.43	1.90	3	1
2:B:8:VAL:HG12	2:B:16:LYS:HD2	0.43	1.88	6	1
3:C:602:PCW:H231	4:C:630:17F:H49	0.43	1.89	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:209:PCW:H151	3:B:213:PCW:H171	0.43	1.90	8	1
3:B:201:PCW:H251	3:C:613:PCW:H482	0.43	1.89	1	1
3:C:611:PCW:H63	4:C:635:17F:N1	0.43	2.28	2	1
3:A:406:PCW:H11	4:B:226:17F:O1	0.43	2.13	3	1
3:A:402:PCW:H331	3:A:402:PCW:H83	0.43	1.90	4	1
3:B:212:PCW:O11	4:B:226:17F:H6	0.43	2.14	4	1
1:C:550:LYS:HA	1:C:553:GLU:OE1	0.43	2.13	4	1
1:C:412:PHE:HA	1:C:415:LEU:HD12	0.43	1.90	5	1
3:A:408:PCW:H341	3:B:231:PCW:C39	0.43	2.44	7	1
3:B:202:PCW:H451	4:B:230:17F:H10A	0.43	1.90	7	1
3:B:219:PCW:H11	3:B:220:PCW:O1P	0.43	2.14	8	1
2:B:114:VAL:HG12	2:B:142:ILE:HB	0.43	1.91	9	1
3:A:406:PCW:H211	3:A:409:PCW:H282	0.43	1.91	10	1
3:B:208:PCW:H152	3:B:215:PCW:H372	0.43	1.90	1	1
3:B:205:PCW:H422	4:B:224:17F:H70	0.43	1.91	2	1
2:B:54:ASP:OD1	3:B:208:PCW:H73	0.43	2.12	2	1
1:A:280:ARG:O	1:A:284:GLN:HB2	0.43	2.13	3	1
3:B:233:PCW:H351	3:C:626:PCW:C12	0.43	2.42	5	1
3:B:205:PCW:H251	3:B:220:PCW:H171	0.43	1.91	6	2
3:A:403:PCW:H142	3:A:403:PCW:H382	0.43	1.89	7	1
3:B:212:PCW:C42	3:C:613:PCW:H482	0.43	2.43	7	1
3:B:211:PCW:C34	4:B:229:17F:H11	0.43	2.44	9	1
3:B:231:PCW:H441	3:C:604:PCW:H452	0.43	1.89	9	1
3:B:210:PCW:H481	3:C:617:PCW:H461	0.43	1.88	9	1
1:C:488:LYS:HZ2	3:C:623:PCW:H281	0.43	1.68	9	1
3:B:210:PCW:H73	7:B:237:EWS:CAN	0.43	2.43	10	1
3:C:606:PCW:H282	3:C:615:PCW:H211	0.43	1.90	10	1
3:B:202:PCW:H141	4:B:228:17F:H9A	0.43	1.89	4	1
3:C:606:PCW:H283	3:C:615:PCW:H181	0.43	1.89	4	1
1:A:393:TYR:HD1	1:A:396:LYS:NZ	0.43	2.03	5	1
3:C:619:PCW:H362	3:C:621:PCW:H142	0.43	1.90	5	1
1:A:229:TRP:O	1:A:233:GLU:HG3	0.43	2.13	6	1
3:B:213:PCW:H39	3:B:214:PCW:H221	0.43	1.90	7	1
3:C:618:PCW:H211	3:C:620:PCW:H471	0.43	1.90	7	1
3:B:215:PCW:H252	3:C:609:PCW:H432	0.43	1.90	8	1
1:C:473:LYS:O	1:C:477:LEU:HB2	0.43	2.12	8	1
3:C:601:PCW:H362	3:C:602:PCW:H121	0.43	1.89	8	1
4:B:225:17F:H44	3:C:615:PCW:H20	0.43	1.90	1	1
3:A:403:PCW:O3P	3:B:204:PCW:H12	0.43	2.12	2	1
4:B:224:17F:H42	4:B:230:17F:H66	0.43	1.91	3	1
1:C:577:LEU:O	1:C:581:LYS:HB2	0.43	2.14	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:232:PCW:H481	4:B:234:17F:H41	0.43	1.90	5	1
3:C:607:PCW:H262	4:C:631:17F:C23	0.43	2.43	5	1
3:C:622:PCW:H361	3:C:622:PCW:H142	0.43	1.90	6	1
1:C:587:ALA:O	1:C:591:TYR:HB2	0.43	2.14	8	1
3:B:231:PCW:H471	3:C:604:PCW:H283	0.43	1.91	8	1
3:B:211:PCW:H151	4:B:229:17F:H8	0.43	1.91	9	1
3:B:205:PCW:H162	3:B:219:PCW:H122	0.43	1.91	9	1
3:A:405:PCW:H481	3:C:629:PCW:H481	0.43	1.89	9	1
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.43	1.91	10	1
4:A:411:17F:H31	4:A:411:17F:H8A	0.43	1.90	10	1
3:B:207:PCW:C16	3:B:232:PCW:H281	0.43	2.41	10	1
4:B:234:17F:H34	3:C:625:PCW:H162	0.43	1.90	10	1
3:A:408:PCW:H351	3:A:410:PCW:C35	0.43	2.43	1	1
1:A:301:LEU:HD13	1:C:473:LYS:HG3	0.43	1.91	3	1
3:B:213:PCW:H212	4:B:227:17F:H42	0.43	1.90	3	1
3:B:201:PCW:H51	3:B:220:PCW:O2P	0.43	2.13	4	1
2:B:171:SER:HA	3:B:218:PCW:H82	0.43	1.90	5	1
3:C:624:PCW:H341	4:C:635:17F:H76	0.43	1.91	5	1
3:B:207:PCW:H282	3:B:218:PCW:H212	0.43	1.90	6	1
3:B:207:PCW:H212	4:C:631:17F:H78	0.43	1.90	8	1
4:B:234:17F:O8	3:C:605:PCW:H342	0.43	2.12	10	1
3:B:215:PCW:H241	3:C:609:PCW:H472	0.43	1.89	10	1
1:A:266:GLN:O	1:A:270:GLU:HG3	0.43	2.13	1	1
1:A:393:TYR:CZ	3:A:403:PCW:H281	0.43	2.48	2	1
3:B:213:PCW:H482	3:C:611:PCW:H483	0.43	1.91	2	1
3:A:406:PCW:H162	3:A:409:PCW:H252	0.43	1.89	4	1
3:B:208:PCW:C32	7:B:237:EWS:CAO	0.43	2.90	4	1
3:C:626:PCW:H421	3:C:627:PCW:H20	0.43	1.90	5	1
3:C:617:PCW:H221	4:C:635:17F:H36	0.43	1.90	6	1
3:A:406:PCW:H12	4:B:226:17F:P1	0.43	2.53	10	2
1:C:522:SER:O	1:C:526:ARG:HG3	0.43	2.13	7	1
1:C:561:LYS:HE3	1:C:561:LYS:HA	0.43	1.90	7	1
3:B:211:PCW:H132	4:B:229:17F:C6	0.43	2.42	9	1
3:C:602:PCW:H211	4:C:630:17F:H49	0.43	1.91	9	1
4:B:229:17F:H20A	4:B:229:17F:H8	0.43	1.90	10	1
3:A:406:PCW:H52	3:B:206:PCW:O2P	0.43	2.14	2	1
3:B:211:PCW:H482	3:C:621:PCW:H451	0.43	1.91	2	1
3:B:219:PCW:H241	3:B:233:PCW:H262	0.43	1.91	2	1
3:C:601:PCW:H372	3:C:602:PCW:H141	0.43	1.91	3	1
3:A:408:PCW:H382	3:A:408:PCW:H172	0.43	1.91	4	1
2:B:68:ARG:HA	2:B:71:TYR:CE1	0.43	2.48	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:212:PCW:H121	4:B:226:17F:O9	0.43	2.14	10	2
3:B:210:PCW:H352	4:B:224:17F:C19	0.43	2.40	6	1
3:C:606:PCW:H2	3:C:606:PCW:O1P	0.43	2.14	6	1
3:B:205:PCW:H251	3:B:220:PCW:H431	0.43	1.91	8	1
2:B:20:THR:O	2:B:24:ILE:HG12	0.43	2.13	8	1
3:A:408:PCW:H332	3:A:410:PCW:C34	0.43	2.43	4	1
2:B:171:SER:HA	3:B:218:PCW:H63	0.43	1.90	5	1
3:B:221:PCW:H83	4:B:224:17F:H6	0.43	1.91	5	1
3:B:220:PCW:H232	3:C:604:PCW:H483	0.43	1.91	7	1
1:A:248:GLU:O	1:A:252:ALA:HB3	0.43	2.14	8	1
3:A:406:PCW:H182	3:A:409:PCW:H232	0.43	1.90	9	1
3:B:219:PCW:H322	4:B:226:17F:H37	0.43	1.91	9	1
1:A:362:GLU:HB3	1:C:414:LYS:HD3	0.42	1.90	4	1
3:B:203:PCW:H462	3:B:205:PCW:H282	0.42	1.91	6	1
3:B:207:PCW:H341	3:B:220:PCW:H39	0.42	1.91	7	1
3:B:212:PCW:H362	3:B:212:PCW:H171	0.42	1.91	8	1
1:C:498:PRO:O	1:C:502:GLU:HB2	0.42	2.14	9	1
4:A:411:17F:C1Y	4:A:411:17F:H8A	0.42	2.44	10	1
2:B:112:VAL:HG23	2:B:159:LEU:HD13	0.42	1.90	3	1
1:C:508:ARG:O	1:C:512:ASP:HB3	0.42	2.14	3	1
3:A:404:PCW:H222	3:C:610:PCW:H261	0.42	1.91	4	1
4:B:234:17F:H65	4:C:631:17F:H77	0.42	1.92	4	1
1:C:422:VAL:O	1:C:426:PHE:HB2	0.42	2.14	4	1
3:A:406:PCW:H172	4:B:226:17F:H58	0.42	1.90	5	1
3:B:219:PCW:H222	4:B:230:17F:H73	0.42	1.90	5	1
3:B:211:PCW:H282	3:C:619:PCW:H251	0.42	1.90	6	1
3:A:402:PCW:C35	3:B:213:PCW:H322	0.42	2.44	7	1
1:C:578:GLU:O	1:C:582:VAL:HG23	0.42	2.14	7	1
3:B:219:PCW:H411	3:B:220:PCW:H172	0.42	1.92	9	1
4:B:224:17F:H46	4:B:230:17F:H70	0.42	1.90	1	1
2:B:74:THR:HB	3:B:201:PCW:H71	0.42	1.90	1	1
2:B:81:VAL:HA	2:B:114:VAL:HB	0.42	1.91	1	1
3:B:203:PCW:H121	3:B:207:PCW:H322	0.42	1.91	3	1
1:C:576:VAL:O	1:C:580:PHE:HB2	0.42	2.14	3	1
3:B:217:PCW:H262	3:C:619:PCW:H472	0.42	1.91	3	1
3:B:209:PCW:H152	3:B:216:PCW:H142	0.42	1.91	4	1
3:C:607:PCW:H331	3:C:611:PCW:H131	0.42	1.91	4	1
3:B:202:PCW:H211	3:B:202:PCW:H242	0.42	1.67	5	1
4:B:234:17F:H57	3:C:625:PCW:H161	0.42	1.91	5	1
3:B:210:PCW:C33	4:B:224:17F:H5	0.42	2.42	7	1
1:C:464:GLN:O	1:C:468:GLU:HB2	0.42	2.13	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:613:PCW:H152	3:C:613:PCW:H331	0.42	1.91	8	1
3:B:208:PCW:O2P	3:B:208:PCW:H2	0.42	2.14	9	1
3:B:210:PCW:H42	7:B:237:EWS:CAJ	0.42	2.44	10	1
3:C:601:PCW:H422	4:C:630:17F:C30	0.42	2.44	10	1
3:C:607:PCW:H411	4:C:631:17F:H9A	0.42	1.90	5	2
3:B:214:PCW:H421	4:C:634:17F:H76	0.42	1.91	2	1
3:B:219:PCW:H232	3:C:605:PCW:H271	0.42	1.90	2	1
3:B:219:PCW:H252	3:C:605:PCW:H271	0.42	1.90	4	1
3:B:221:PCW:H2	4:B:230:17F:H19	0.42	1.91	4	1
3:C:603:PCW:H451	3:C:625:PCW:H472	0.42	1.92	4	1
3:C:626:PCW:H40	3:C:627:PCW:H241	0.42	1.92	5	1
3:C:610:PCW:H411	3:C:614:PCW:H181	0.42	1.90	6	1
3:B:203:PCW:H321	3:B:211:PCW:H341	0.42	1.91	7	1
3:B:220:PCW:H251	3:C:604:PCW:H461	0.42	1.90	8	1
4:B:225:17F:H76	3:C:606:PCW:H483	0.42	1.91	9	1
3:B:209:PCW:H272	3:C:611:PCW:H483	0.42	1.91	9	1
3:A:406:PCW:H2	4:B:226:17F:O1	0.42	2.15	1	1
4:B:234:17F:H72	4:C:631:17F:H72	0.42	1.89	1	2
4:B:225:17F:H63	3:C:626:PCW:C26	0.42	2.39	2	1
3:B:233:PCW:H61	3:C:604:PCW:H332	0.42	1.90	4	1
3:C:619:PCW:H342	3:C:621:PCW:H141	0.42	1.91	4	1
1:C:413:SER:O	1:C:417:GLU:HG3	0.42	2.15	5	1
3:B:216:PCW:C24	4:C:635:17F:H65	0.42	2.45	5	1
1:C:581:LYS:O	1:C:585:LEU:HG	0.42	2.14	9	2
2:B:7:VAL:HB	2:B:78:PHE:HD1	0.42	1.73	10	2
1:A:253:LYS:HE2	1:A:257:TYR:OH	0.42	2.15	9	1
1:A:224:VAL:HG22	1:C:550:LYS:HD3	0.42	1.90	10	1
3:B:202:PCW:C15	3:B:212:PCW:H412	0.42	2.44	2	1
3:A:403:PCW:H31	3:A:403:PCW:O1P	0.42	2.14	4	1
3:B:208:PCW:H161	3:B:215:PCW:H372	0.42	1.91	4	1
3:B:203:PCW:N	3:B:203:PCW:O2P	0.42	2.52	5	1
2:B:22:GLN:CG	2:B:149:ARG:HG3	0.42	2.44	6	1
3:B:205:PCW:H451	3:B:207:PCW:H283	0.42	1.90	6	1
3:A:410:PCW:H251	4:C:633:17F:C30	0.42	2.45	7	1
3:B:211:PCW:H172	4:B:229:17F:H33	0.42	1.92	7	1
1:A:393:TYR:HE1	3:A:407:PCW:C27	0.42	1.61	8	1
3:A:406:PCW:H151	3:A:409:PCW:H252	0.42	1.91	9	1
3:A:408:PCW:H441	3:B:204:PCW:H451	0.42	1.92	9	1
3:B:202:PCW:H321	3:B:212:PCW:H83	0.42	1.90	10	1
3:B:219:PCW:H262	4:C:631:17F:H54	0.42	1.90	1	1
1:A:357:LEU:HA	1:A:360:LEU:HB2	0.42	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:455:TYR:CE2	3:C:601:PCW:C23	0.42	3.00	3	1
1:A:348:GLU:O	1:A:352:LYS:HG3	0.42	2.13	4	1
3:C:601:PCW:H441	3:C:602:PCW:H211	0.42	1.92	4	1
4:B:223:17F:H50	3:C:626:PCW:H231	0.42	1.91	5	1
3:B:232:PCW:H412	3:C:619:PCW:H441	0.42	1.90	7	1
3:B:220:PCW:H422	3:B:232:PCW:H251	0.42	1.91	9	1
1:C:431:GLU:O	1:C:435:GLU:HG3	0.42	2.14	9	1
3:B:203:PCW:H481	4:B:223:17F:H48	0.42	1.91	3	1
3:B:231:PCW:H483	3:B:231:PCW:H232	0.42	1.90	4	1
3:B:231:PCW:H461	3:C:604:PCW:C46	0.42	2.45	4	1
1:A:312:HIS:HA	1:C:462:LYS:HD3	0.42	1.91	6	1
4:B:234:17F:H33	3:C:625:PCW:C19	0.42	2.44	6	1
3:A:408:PCW:H441	3:B:204:PCW:H432	0.42	1.91	7	1
3:B:203:PCW:H412	3:B:204:PCW:H371	0.42	1.92	10	1
2:B:74:THR:CB	3:B:201:PCW:H71	0.42	2.45	1	1
3:B:208:PCW:C34	7:B:237:EWS:CLA	0.42	3.05	2	1
3:C:626:PCW:H40	3:C:627:PCW:H231	0.42	1.90	2	1
3:C:601:PCW:H262	3:C:602:PCW:H282	0.42	1.91	3	1
3:C:610:PCW:H121	3:C:614:PCW:H212	0.42	1.89	4	1
2:B:81:VAL:HG12	2:B:114:VAL:HB	0.42	1.91	5	1
3:B:212:PCW:H332	3:B:212:PCW:H131	0.42	1.91	9	1
1:A:307:ASP:O	1:A:310:ARG:HB2	0.42	2.14	10	1
3:A:402:PCW:H211	3:B:214:PCW:H232	0.42	1.91	1	1
3:B:205:PCW:H272	3:B:220:PCW:H261	0.42	1.90	1	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.42	2.15	10	3
3:B:202:PCW:H222	4:B:228:17F:H59	0.42	1.92	3	1
2:B:34:PRO:HA	5:B:235:GNP:O3G	0.42	2.15	7	2
3:B:201:PCW:H141	4:B:225:17F:H56	0.42	1.91	5	1
3:B:211:PCW:H20	3:B:217:PCW:H361	0.42	1.92	5	1
4:B:226:17F:H12	4:B:230:17F:H8	0.42	1.92	7	1
3:B:231:PCW:C12	3:C:604:PCW:H19	0.42	2.45	8	1
3:C:606:PCW:H211	3:C:615:PCW:H161	0.42	1.92	8	1
3:B:207:PCW:H442	3:C:619:PCW:H452	0.42	1.91	9	1
3:C:620:PCW:H41	3:C:620:PCW:O11	0.42	2.15	10	1
2:B:71:TYR:HA	7:B:237:EWS:CAD	0.41	2.42	1	1
3:B:202:PCW:H52	3:B:202:PCW:O31	0.41	2.14	2	1
3:B:203:PCW:C40	3:B:204:PCW:H151	0.41	2.45	2	1
3:B:231:PCW:H442	3:B:233:PCW:H483	0.41	1.92	2	1
3:C:616:PCW:H181	3:C:616:PCW:H411	0.41	1.92	2	1
3:B:232:PCW:H241	3:C:619:PCW:H482	0.41	1.92	3	1
3:B:222:PCW:H19	3:C:603:PCW:H142	0.41	1.92	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:621:PCW:H122	3:C:629:PCW:C18	0.41	2.44	6	1
3:C:618:PCW:H182	3:C:620:PCW:H451	0.41	1.92	7	1
1:A:376:LEU:CB	1:A:377:PRO:HD3	0.41	2.44	9	1
3:C:606:PCW:H471	3:C:615:PCW:H182	0.41	1.91	9	1
3:B:202:PCW:H321	3:B:212:PCW:C8	0.41	2.45	10	1
3:B:232:PCW:H142	3:C:625:PCW:H181	0.41	1.92	10	1
3:B:208:PCW:H342	7:B:237:EWS:CLA	0.41	2.52	2	1
3:B:202:PCW:H72	4:B:228:17F:H9A	0.41	1.92	3	1
3:C:601:PCW:H451	3:C:601:PCW:H152	0.41	1.92	3	1
3:A:407:PCW:H121	4:B:223:17F:C31	0.41	2.45	4	1
3:C:617:PCW:H221	4:C:632:17F:H42	0.41	1.91	4	1
3:B:216:PCW:H171	4:B:224:17F:H61	0.41	1.92	6	1
1:A:308:ARG:HG3	1:C:469:LEU:CD1	0.41	2.41	7	1
3:B:203:PCW:H151	4:B:229:17F:H20	0.41	1.92	7	1
2:B:32:TYR:HA	5:B:235:GNP:H5'1	0.41	1.91	7	1
3:C:610:PCW:H372	3:C:614:PCW:H241	0.41	1.92	7	1
4:B:229:17F:H55	3:B:231:PCW:H162	0.41	1.90	8	1
3:A:401:PCW:H41	3:B:212:PCW:H11	0.41	1.93	10	1
4:B:229:17F:H51	3:B:231:PCW:H181	0.41	1.92	1	1
1:A:253:LYS:C	1:A:256:PRO:HD2	0.41	2.36	3	1
3:B:205:PCW:H262	3:B:220:PCW:H421	0.41	1.92	3	1
1:A:268:GLU:OE2	1:C:510:HIS:NE2	0.41	2.53	3	1
1:A:264:LYS:HE3	1:C:509:ALA:HB1	0.41	1.92	4	1
4:B:224:17F:H41	4:B:230:17F:H66	0.41	1.90	4	1
3:B:233:PCW:H351	3:C:626:PCW:H331	0.41	1.90	4	1
2:B:21:ILE:HG23	2:B:25:GLN:HE21	0.41	1.75	4	1
3:B:201:PCW:H282	3:C:613:PCW:H221	0.41	1.92	5	1
2:B:37:GLU:OE2	3:B:220:PCW:H83	0.41	2.15	6	1
3:B:218:PCW:H412	3:B:222:PCW:H421	0.41	1.91	7	1
3:C:610:PCW:H431	3:C:614:PCW:H181	0.41	1.91	7	1
4:B:223:17F:H35	4:B:225:17F:H19	0.41	1.90	8	1
3:B:209:PCW:H172	3:B:213:PCW:H151	0.41	1.93	10	1
1:A:334:ARG:HD3	1:C:440:GLU:OE1	0.41	2.15	10	1
3:A:402:PCW:H381	3:B:213:PCW:H351	0.41	1.91	1	1
3:B:211:PCW:H81	4:B:229:17F:O2	0.41	2.16	2	1
3:B:231:PCW:H461	3:C:604:PCW:H462	0.41	1.92	4	1
3:B:232:PCW:H31	3:C:604:PCW:H122	0.41	1.92	5	1
4:B:234:17F:C31	3:C:625:PCW:H141	0.41	2.42	5	1
1:C:521:TYR:HA	1:C:524:GLU:OE1	0.41	2.16	6	1
3:C:617:PCW:H171	4:C:635:17F:H12	0.41	1.90	6	1
3:B:219:PCW:O2	3:B:219:PCW:H352	0.41	2.16	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:611:PCW:C44	4:C:635:17F:H43	0.41	2.46	8	1
3:B:203:PCW:H161	3:B:207:PCW:H372	0.41	1.91	9	1
3:B:216:PCW:H221	3:C:611:PCW:H421	0.41	1.92	9	1
2:B:5:LYS:HD2	2:B:74:THR:O	0.41	2.16	10	1
3:B:207:PCW:H83	3:B:217:PCW:O2P	0.41	2.15	1	1
3:B:220:PCW:H452	3:B:233:PCW:H251	0.41	1.92	1	1
1:A:393:TYR:HE1	3:A:407:PCW:H272	0.41	1.69	2	1
3:B:208:PCW:H131	3:B:215:PCW:H122	0.41	1.92	2	1
2:B:86:ASN:OD1	2:B:88:LYS:HB3	0.41	2.15	2	1
4:B:228:17F:C1	4:B:228:17F:H4	0.41	2.43	3	1
3:B:233:PCW:C34	3:C:626:PCW:H331	0.41	2.45	3	1
3:A:401:PCW:H442	3:C:613:PCW:H251	0.41	1.92	3	1
3:B:217:PCW:H251	3:C:619:PCW:H442	0.41	1.92	3	1
3:A:406:PCW:H362	3:A:406:PCW:H122	0.41	1.92	4	1
4:B:234:17F:H9A	4:B:234:17F:C20	0.41	2.41	5	1
1:A:330:ARG:NH2	1:C:447:GLU:HB2	0.41	2.27	5	1
3:A:402:PCW:H142	3:B:214:PCW:H172	0.41	1.93	7	1
3:A:403:PCW:H282	3:A:407:PCW:H252	0.41	1.91	2	1
3:B:201:PCW:H232	3:C:613:PCW:H482	0.41	1.93	4	1
3:B:212:PCW:H422	3:C:613:PCW:H483	0.41	1.90	4	1
3:C:618:PCW:H122	3:C:620:PCW:H361	0.41	1.92	4	1
1:C:427:TRP:HA	1:C:427:TRP:HE3	0.41	1.74	6	1
3:B:203:PCW:H371	3:B:220:PCW:H181	0.41	1.92	9	1
3:C:608:PCW:H172	3:C:608:PCW:H142	0.41	1.71	10	1
3:B:217:PCW:H252	3:B:218:PCW:H282	0.41	1.92	1	1
1:A:375:LEU:O	1:A:379:LEU:HB2	0.41	2.16	2	1
1:A:341:ASN:O	1:A:345:ARG:HG3	0.41	2.16	3	1
3:A:408:PCW:C1	3:B:231:PCW:H321	0.41	2.44	3	1
1:C:521:TYR:CE2	3:C:603:PCW:H281	0.41	2.51	4	1
3:A:407:PCW:C13	4:B:223:17F:H33	0.41	2.44	6	1
3:B:201:PCW:H422	3:C:626:PCW:H231	0.41	1.91	6	1
3:B:204:PCW:H482	3:C:604:PCW:H282	0.41	1.93	7	1
4:B:224:17F:H46	4:B:230:17F:H71	0.41	1.93	7	1
1:C:469:LEU:O	1:C:473:LYS:HE2	0.41	2.16	8	1
2:B:117:LYS:HB3	2:B:120:LEU:HD12	0.41	1.92	9	1
2:B:3:GLU:HA	2:B:52:LEU:O	0.41	2.15	10	1
3:B:203:PCW:H421	3:B:204:PCW:H19	0.41	1.91	1	1
1:A:388:SER:O	1:A:392:GLU:HG2	0.41	2.16	2	1
3:B:210:PCW:H442	3:B:221:PCW:H381	0.41	1.93	2	1
3:C:614:PCW:H222	3:C:614:PCW:H261	0.41	1.91	2	1
1:C:574:LEU:HB2	1:C:575:PRO:CD	0.41	2.46	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:203:PCW:H182	3:B:211:PCW:H40	0.41	1.91	4	1
2:B:54:ASP:HB3	7:B:237:EWS:CAS	0.41	2.45	5	1
3:B:209:PCW:H73	4:B:224:17F:O1	0.41	2.15	6	1
3:B:213:PCW:H212	4:B:227:17F:H40	0.41	1.92	6	1
2:B:3:GLU:OE2	3:B:205:PCW:H71	0.41	2.16	6	1
1:C:574:LEU:HB2	1:C:575:PRO:HD3	0.41	1.93	7	2
3:C:607:PCW:H482	3:C:611:PCW:H371	0.41	1.92	8	1
3:B:214:PCW:H40	4:C:634:17F:H76	0.41	1.93	8	1
2:B:67:MET:SD	3:B:204:PCW:H63	0.41	2.56	9	1
3:B:233:PCW:H39	3:C:606:PCW:H372	0.41	1.92	9	1
3:B:219:PCW:H52	3:B:220:PCW:O1P	0.41	2.15	1	1
3:A:406:PCW:H171	3:A:406:PCW:H141	0.41	1.81	1	1
3:B:208:PCW:H451	3:C:627:PCW:H483	0.41	1.93	1	1
3:C:602:PCW:H482	3:C:609:PCW:H241	0.41	1.92	1	1
4:B:226:17F:H73	3:C:628:PCW:H451	0.41	1.93	2	1
2:B:5:LYS:NZ	4:B:230:17F:H1	0.41	2.31	2	1
4:B:234:17F:H48	4:B:234:17F:H76	0.41	1.93	2	1
3:C:607:PCW:O1P	3:C:609:PCW:H73	0.41	2.16	2	1
2:B:156:PHE:O	2:B:160:VAL:HG23	0.41	2.16	3	1
3:A:408:PCW:C34	3:B:231:PCW:H39	0.41	2.40	3	1
3:A:410:PCW:H132	4:C:633:17F:H8A	0.41	1.93	3	1
3:B:201:PCW:C41	3:B:219:PCW:H20	0.41	2.46	3	1
1:A:348:GLU:HB3	1:A:352:LYS:HE2	0.41	1.91	4	1
1:A:264:LYS:O	1:A:268:GLU:HG3	0.41	2.14	5	1
3:B:201:PCW:H152	4:B:225:17F:H8	0.41	1.92	5	1
4:B:234:17F:H65	4:B:234:17F:H59	0.41	1.93	5	1
2:B:99:GLN:O	2:B:103:VAL:HG13	0.41	2.16	6	1
3:C:615:PCW:H162	3:C:615:PCW:H422	0.41	1.93	6	1
1:A:228:PHE:O	1:A:232:LEU:HG	0.41	2.16	7	1
1:A:376:LEU:HB2	1:A:377:PRO:CD	0.41	2.46	7	1
3:C:607:PCW:C43	3:C:611:PCW:H11	0.41	2.46	7	1
3:C:613:PCW:H19	3:C:622:PCW:H432	0.41	1.91	7	1
1:A:281:ALA:O	1:A:285:GLU:HG2	0.41	2.16	8	1
3:B:202:PCW:C33	4:B:228:17F:H4A	0.41	2.40	8	1
2:B:17:SER:HA	2:B:20:THR:OG1	0.41	2.16	9	1
2:B:84:ILE:HG12	2:B:118:CYS:HA	0.41	1.91	9	1
3:C:611:PCW:H152	3:C:617:PCW:H342	0.41	1.92	9	1
3:B:203:PCW:O1P	3:B:211:PCW:H12	0.41	2.16	10	1
3:B:231:PCW:H382	3:C:604:PCW:H421	0.41	1.93	10	1
3:B:209:PCW:H441	4:B:227:17F:H72	0.41	1.92	1	1
3:C:625:PCW:H322	3:C:625:PCW:H352	0.41	1.72	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:217:PCW:H283	3:B:218:PCW:H251	0.41	1.93	5	1
2:B:7:VAL:HG22	2:B:56:LEU:HB3	0.41	1.92	5	1
1:A:254:VAL:HA	1:A:257:TYR:HB2	0.41	1.93	6	1
3:A:408:PCW:H322	3:B:231:PCW:H371	0.41	1.93	7	1
3:C:618:PCW:H122	3:C:620:PCW:H412	0.41	1.93	7	1
3:C:609:PCW:H451	4:C:630:17F:H53	0.41	1.92	8	1
3:A:406:PCW:H231	3:A:409:PCW:H262	0.41	1.93	9	1
2:B:34:PRO:HA	5:B:235:GNP:O1G	0.41	2.16	9	1
3:C:622:PCW:H151	3:C:622:PCW:H381	0.41	1.92	9	1
3:A:409:PCW:H171	3:C:616:PCW:H251	0.41	1.93	10	1
3:C:624:PCW:H211	4:C:634:17F:H31	0.41	1.91	10	1
3:B:202:PCW:H282	4:B:228:17F:H66	0.40	1.93	1	1
1:A:253:LYS:O	1:A:256:PRO:HD2	0.40	2.17	3	1
3:A:408:PCW:H322	3:B:231:PCW:C37	0.40	2.46	4	1
3:B:205:PCW:H51	3:B:210:PCW:H341	0.40	1.92	4	1
1:C:561:LYS:HA	1:C:565:ALA:CB	0.40	2.45	6	1
3:C:601:PCW:H351	3:C:602:PCW:H152	0.40	1.93	7	1
1:A:330:ARG:HH22	1:C:448:VAL:HG23	0.40	1.76	8	1
4:B:227:17F:H73	3:C:602:PCW:H371	0.40	1.92	8	1
3:A:408:PCW:H242	3:C:618:PCW:H461	0.40	1.92	9	1
3:B:202:PCW:H412	4:B:226:17F:H40	0.40	1.93	10	1
4:B:234:17F:H73	4:C:631:17F:H72	0.40	1.93	10	1
4:C:630:17F:H42	4:C:630:17F:H35	0.40	1.91	10	1
3:A:410:PCW:H331	4:C:633:17F:C21	0.40	2.33	1	1
3:B:217:PCW:H251	3:C:619:PCW:H441	0.40	1.92	2	1
3:B:218:PCW:H441	3:B:218:PCW:H241	0.40	1.93	2	1
1:C:491:GLU:HB3	1:C:495:LYS:HZ2	0.40	1.76	2	1
3:A:407:PCW:H322	3:A:407:PCW:H351	0.40	1.48	4	1
2:B:158:THR:O	2:B:162:GLU:HG2	0.40	2.16	4	1
3:C:610:PCW:H361	3:C:614:PCW:H132	0.40	1.92	4	1
3:B:201:PCW:H283	3:C:613:PCW:H241	0.40	1.93	6	1
3:B:202:PCW:H241	4:B:228:17F:H62	0.40	1.92	7	1
3:A:403:PCW:C33	3:B:204:PCW:H31	0.40	2.43	8	1
3:C:601:PCW:H452	3:C:602:PCW:H262	0.40	1.93	8	1
3:B:231:PCW:H482	3:B:231:PCW:H261	0.40	1.94	9	1
3:C:605:PCW:H351	3:C:605:PCW:H122	0.40	1.93	9	1
3:C:613:PCW:H62	3:C:627:PCW:H71	0.40	1.92	1	1
1:A:260:ASP:O	1:A:264:LYS:HD3	0.40	2.16	2	1
3:A:406:PCW:H421	4:B:226:17F:H71	0.40	1.94	2	1
3:C:611:PCW:H172	3:C:617:PCW:C33	0.40	2.46	2	1
4:B:234:17F:H35	3:C:625:PCW:H282	0.40	1.92	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:9:VAL:HG21	2:B:100:ILE:HD11	0.40	1.93	3	1
3:C:601:PCW:H411	3:C:602:PCW:H181	0.40	1.93	3	1
4:B:224:17F:H44	4:B:234:17F:H47	0.40	1.93	4	1
3:B:220:PCW:H483	4:B:234:17F:H38	0.40	1.93	6	1
3:A:402:PCW:H39	3:B:213:PCW:H372	0.40	1.92	7	1
4:B:230:17F:H19	4:B:230:17F:H33	0.40	1.71	7	1
1:A:279:LEU:HD22	1:C:495:LYS:HE3	0.40	1.93	10	1
3:B:203:PCW:H222	3:B:211:PCW:H441	0.40	1.92	2	1
3:B:201:PCW:H382	4:B:226:17F:H42	0.40	1.92	3	1
3:A:402:PCW:H362	3:B:214:PCW:C16	0.40	2.46	4	1
1:C:428:ASP:O	1:C:431:GLU:HB2	0.40	2.17	4	1
3:C:602:PCW:H271	4:C:630:17F:H47	0.40	1.93	4	1
1:A:380:GLU:O	1:A:384:VAL:HG23	0.40	2.16	5	1
3:B:201:PCW:H251	4:B:228:17F:C36	0.40	2.38	5	1
3:B:221:PCW:C3	4:B:230:17F:H4A	0.40	2.46	5	1
3:B:232:PCW:H452	3:C:619:PCW:H481	0.40	1.92	6	1
3:C:626:PCW:H371	3:C:627:PCW:H182	0.40	1.93	6	1
2:B:22:GLN:NE2	2:B:28:PHE:HB2	0.40	2.30	7	1
2:B:7:VAL:CG2	2:B:75:GLY:HA3	0.40	2.46	7	1
1:C:535:ALA:O	1:C:539:ASN:HB2	0.40	2.16	7	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.40	2.15	8	1
1:A:233:GLU:O	1:A:237:GLU:HB2	0.40	2.15	10	1
3:B:209:PCW:H332	3:B:213:PCW:H122	0.40	1.93	1	1
3:A:402:PCW:H342	3:B:213:PCW:H322	0.40	1.93	2	1
3:B:218:PCW:H483	3:C:624:PCW:H283	0.40	1.92	2	1
3:B:217:PCW:H232	3:B:218:PCW:H241	0.40	1.93	3	1
3:B:221:PCW:H71	4:B:227:17F:O5	0.40	2.16	3	1
3:B:233:PCW:H231	3:C:625:PCW:H251	0.40	1.94	5	1
1:A:332:ALA:O	1:A:336:GLU:HG3	0.40	2.16	6	1
3:B:203:PCW:H262	3:B:217:PCW:H442	0.40	1.94	6	1
3:B:207:PCW:H272	3:B:218:PCW:H252	0.40	1.92	6	1
3:B:218:PCW:H272	3:C:629:PCW:H262	0.40	1.92	6	1
2:B:15:GLY:O	2:B:19:LEU:HG	0.40	2.15	7	1
3:B:202:PCW:H332	4:B:228:17F:O1	0.40	2.17	7	1
3:B:212:PCW:H182	3:B:212:PCW:H152	0.40	1.71	7	1
1:C:463:TRP:O	1:C:467:MET:HB2	0.40	2.17	9	1
3:B:211:PCW:H241	3:B:217:PCW:H432	0.40	1.92	10	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/200 (98%)	191±2 (98±1%)	4±1 (2±1%)	1±1 (0±0%)	35	77
1	C	195/200 (98%)	191±2 (98±1%)	4±2 (2±1%)	1±1 (0±0%)	47	81
2	B	171/187 (91%)	162±3 (95±2%)	8±3 (5±2%)	0±0 (0±0%)	56	86
All	All	5610/5870 (96%)	5439 (97%)	155 (3%)	16 (0%)	47	81

All 4 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	365	LYS	8
1	C	563	LYS	5
2	B	73	ARG	2
1	A	366	PRO	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/175 (98%)	155±2 (90±1%)	17±2 (10±1%)	12	57
1	C	172/175 (98%)	156±2 (90±1%)	16±2 (10±1%)	13	59
2	B	152/166 (92%)	138±2 (91±2%)	14±2 (9±2%)	14	59
All	All	4960/5160 (96%)	4480 (90%)	480 (10%)	13	58

All 187 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	254	VAL	10
1	C	550	LYS	9
1	A	312	HIS	8
1	C	516	THR	8
1	A	272	TYR	8
2	B	20	THR	8
1	A	228	PHE	7
2	B	92	ASP	7
1	A	235	GLU	7
1	C	459	PHE	6
2	B	71	TYR	6
1	A	293	GLU	6
2	B	2	THR	6
1	C	480	GLU	6
2	B	124	THR	6
2	B	69	ASP	6
1	C	548	HIS	5
1	A	299	SER	5
1	A	325	ASP	5
2	B	51	CYS	5
1	A	394	THR	5
1	A	370	ASP	5
1	C	568	ASP	5
1	A	246	ASP	5
2	B	148	THR	4
1	C	412	PHE	4
1	C	561	LYS	4
1	A	264	LYS	4
1	A	396	LYS	4
2	B	56	LEU	4
2	B	170	MET	4
1	C	455	TYR	4
2	B	107	GLU	4
1	C	487	GLN	4
2	B	16	LYS	4
1	C	444	ASP	4
1	A	292	HIS	4
1	A	207	TRP	4
1	A	214	PHE	4
1	C	405	TRP	4
1	A	289	GLN	4
2	B	7	VAL	4
1	C	505	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	C	463	TRP	4
1	A	319	HIS	3
2	B	153	ASP	3
1	C	594	LYS	3
2	B	17	SER	3
1	A	361	SER	3
2	B	74	THR	3
2	B	58	THR	3
1	A	213	THR	3
2	B	154	ASP	3
1	A	215	SER	3
2	B	39	SER	3
1	A	382	PHE	3
1	C	413	SER	3
1	A	318	THR	3
1	C	552	THR	3
1	C	592	THR	3
1	C	409	THR	3
2	B	33	ASP	3
1	C	580	PHE	3
1	C	418	GLN	3
1	C	427	TRP	3
1	C	591	TYR	3
2	B	122	SER	3
1	A	356	HIS	3
1	A	229	TRP	3
2	B	29	VAL	3
2	B	35	THR	3
1	A	209	SER	2
1	C	490	HIS	2
1	A	296	GLU	2
1	C	447	GLU	2
1	C	532	ARG	2
2	B	149	ARG	2
1	C	546	GLU	2
1	C	554	HIS	2
1	A	261	PHE	2
1	C	425	GLU	2
1	A	257	TYR	2
1	A	349	TYR	2
1	C	556	SER	2
2	B	50	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	C	467	MET	2
1	C	448	VAL	2
1	A	392	GLU	2
1	C	596	ASN	2
2	B	47	ASP	2
1	C	410	SER	2
1	A	381	SER	2
1	A	212	SER	2
1	A	220	GLN	2
2	B	126	ASP	2
1	A	360	LEU	2
2	B	105	ASP	2
1	C	583	SER	2
1	A	391	GLU	2
1	C	576	VAL	2
1	C	494	GLU	2
1	C	466	GLU	2
2	B	5	LYS	2
1	C	559	SER	2
2	B	3	GLU	2
1	C	446	GLU	2
2	B	87	THR	2
2	B	132	ASP	2
1	A	354	THR	2
1	A	393	TYR	2
1	C	523	ASP	2
2	B	85	ASN	2
1	C	473	LYS	2
1	A	244	SER	2
1	C	482	GLN	2
1	A	205	ASP	2
2	B	127	THR	2
2	B	106	SER	2
1	A	202	LYS	2
1	C	407	SER	2
2	B	25	GLN	1
1	C	468	GLU	1
2	B	53	LEU	1
1	A	274	GLN	1
2	B	54	ASP	1
2	B	136	SER	1
1	A	345	ARG	1

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Mol	Chain	Res	Type	Models (Total)
2	B	41	ARG	1
1	A	224	VAL	1
2	B	89	SER	1
2	B	135	ARG	1
2	B	14	VAL	1
1	C	579	SER	1
1	A	359	THR	1
1	C	457	ASP	1
1	A	248	GLU	1
1	C	426	PHE	1
1	C	415	LEU	1
1	C	521	TYR	1
2	B	57	ASP	1
1	C	403	ASP	1
1	C	404	ASN	1
2	B	73	ARG	1
1	A	385	SER	1
1	C	464	GLN	1
1	C	495	LYS	1
1	C	439	GLN	1
1	C	569	LEU	1
1	A	265	TRP	1
2	B	38	ASP	1
1	A	279	LEU	1
1	A	334	ARG	1
1	C	497	SER	1
1	C	527	GLN	1
1	A	242	GLU	1
1	A	263	LYS	1
1	A	386	PHE	1
2	B	43	GLN	1
2	B	97	ARG	1
1	C	488	LYS	1
1	A	308	ARG	1
2	B	23	LEU	1
1	C	434	THR	1
1	C	442	SER	1
1	C	557	THR	1
1	A	350	HIS	1
1	A	314	ASP	1
1	A	378	VAL	1
1	A	241	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	275	LYS	1
1	C	501	GLU	1
2	B	102	ARG	1
1	A	379	LEU	1
2	B	79	LEU	1
2	B	68	ARG	1
1	A	211	THR	1
1	C	483	GLU	1
1	A	303	GLU	1
1	A	227	GLU	1
1	C	478	ARG	1
2	B	114	VAL	1
1	C	406	ASP	1
1	C	433	GLU	1
2	B	131	GLN	1
1	C	458	ASP	1
2	B	26	ASN	1
1	A	206	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 1 is monoatomic - leaving 82 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
3	PCW	A	401	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	402	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	403	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	404	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	405	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	406	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	A	407	-	53,53,53	1.05±0.01	0±0 (0±0%)
3	PCW	A	408	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	A	409	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	410	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	17F	A	411	-	50,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	B	201	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	B	202	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	203	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	204	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	205	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	B	206	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	207	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	208	-	53,53,53	1.03±0.02	0±0 (0±0%)
3	PCW	B	209	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	210	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	B	211	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	B	212	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	213	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	B	214	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	B	215	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	216	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	217	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	B	218	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	B	219	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	220	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	B	221	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	222	-	53,53,53	1.02±0.01	0±0 (0±0%)
4	17F	B	223	-	50,53,53	0.91±0.01	0±0 (0±0%)
4	17F	B	224	-	50,53,53	0.91±0.01	0±0 (0±0%)
4	17F	B	225	-	50,53,53	0.91±0.01	0±0 (0±0%)
4	17F	B	226	-	50,53,53	0.91±0.01	0±0 (0±0%)
4	17F	B	227	-	50,53,53	0.91±0.01	0±0 (0±0%)
4	17F	B	228	-	50,53,53	0.90±0.01	0±0 (0±0%)
4	17F	B	229	-	50,53,53	0.91±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	17F	B	230	-	50,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	B	231	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	232	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	B	233	-	53,53,53	1.02±0.01	0±0 (0±0%)
4	17F	B	234	-	50,53,53	0.92±0.00	0±0 (0±0%)
5	GNP	B	235	-	28,34,34	2.42±0.02	3±0 (10±0%)
7	EWS	B	237	-	30,30,30	3.51±0.01	3±0 (10±0%)
3	PCW	C	601	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	602	-	53,53,53	1.05±0.01	0±0 (0±0%)
3	PCW	C	603	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	604	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	C	605	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	606	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	607	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	C	608	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	609	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	610	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	C	611	-	53,53,53	1.03±0.02	0±0 (0±0%)
3	PCW	C	612	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	613	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	C	614	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	615	-	53,53,53	1.06±0.01	0±0 (0±0%)
3	PCW	C	616	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	C	617	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	C	618	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	C	619	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	C	620	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	C	621	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	622	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	C	623	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	C	624	-	53,53,53	1.03±0.02	0±0 (0±0%)
3	PCW	C	625	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	626	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	627	-	53,53,53	1.02±0.01	0±0 (0±0%)
3	PCW	C	628	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	C	629	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	17F	C	630	-	50,53,53	0.91±0.01	0±0 (0±0%)
4	17F	C	631	-	50,53,53	0.89±0.01	0±0 (0±0%)
4	17F	C	632	-	50,53,53	0.91±0.01	0±0 (0±0%)
4	17F	C	633	-	50,53,53	0.90±0.01	0±0 (0±0%)
4	17F	C	634	-	50,53,53	0.90±0.01	0±0 (0±0%)
4	17F	C	635	-	50,53,53	0.90±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	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	A	401	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	A	402	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	A	403	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	A	404	-	59,61,61	0.85±0.01	0±0 (0±0%)
3	PCW	A	405	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	A	406	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	A	407	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	A	408	-	59,61,61	2.34±0.01	3±0 (4±0%)
3	PCW	A	409	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	A	410	-	59,61,61	2.33±0.01	3±0 (5±0%)
4	17F	A	411	-	52,60,60	0.97±0.02	0±0 (0±0%)
3	PCW	B	201	-	59,61,61	2.34±0.01	3±0 (5±0%)
3	PCW	B	202	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	B	203	-	59,61,61	2.77±0.01	6±0 (10±0%)
3	PCW	B	204	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	B	205	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	B	206	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	B	207	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	B	208	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	B	209	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	B	210	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	B	211	-	59,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	B	212	-	59,61,61	2.34±0.01	3±0 (5±0%)
3	PCW	B	213	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	B	214	-	59,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	B	215	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	B	216	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	B	217	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	B	218	-	59,61,61	2.34±0.00	3±0 (5±0%)
3	PCW	B	219	-	59,61,61	2.33±0.01	3±0 (5±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	B	220	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	B	221	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	B	222	-	59,61,61	2.34±0.01	3±0 (4±0%)
4	17F	B	223	-	52,60,60	1.71±0.02	2±0 (3±0%)
4	17F	B	224	-	52,60,60	0.95±0.02	0±0 (0±0%)
4	17F	B	225	-	52,60,60	0.96±0.02	0±0 (0±0%)
4	17F	B	226	-	52,60,60	1.00±0.03	0±0 (0±0%)
4	17F	B	227	-	52,60,60	0.96±0.03	0±0 (0±0%)
4	17F	B	228	-	52,60,60	0.97±0.03	0±0 (0±0%)
4	17F	B	229	-	52,60,60	0.99±0.02	0±0 (0±0%)
4	17F	B	230	-	52,60,60	0.96±0.02	0±0 (0±0%)
3	PCW	B	231	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	B	232	-	59,61,61	2.77±0.00	6±0 (10±0%)
3	PCW	B	233	-	59,61,61	2.33±0.01	3±0 (5±0%)
4	17F	B	234	-	52,60,60	0.94±0.02	0±0 (0±0%)
5	GNP	B	235	-	30,54,54	1.97±0.01	1±0 (3±0%)
7	EWS	B	237	-	34,42,42	0.90±0.01	0±0 (0±0%)
3	PCW	C	601	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	C	602	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	C	603	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	604	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	605	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	606	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	607	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	608	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	609	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	C	610	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	C	611	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	C	612	-	59,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	C	613	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	C	614	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	615	-	59,61,61	0.82±0.01	0±0 (0±0%)
3	PCW	C	616	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	617	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	C	618	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	619	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	C	620	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	621	-	59,61,61	2.33±0.00	3±0 (5±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	C	622	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	623	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	C	624	-	59,61,61	0.84±0.01	0±0 (0±0%)
3	PCW	C	625	-	59,61,61	2.33±0.01	3±0 (5±0%)
3	PCW	C	626	-	59,61,61	2.34±0.00	3±0 (5±0%)
3	PCW	C	627	-	59,61,61	2.33±0.01	3±0 (4±0%)
3	PCW	C	628	-	59,61,61	2.33±0.00	3±0 (5±0%)
3	PCW	C	629	-	59,61,61	0.83±0.01	0±0 (0±0%)
4	17F	C	630	-	52,60,60	0.97±0.04	0±0 (0±0%)
4	17F	C	631	-	52,60,60	1.02±0.03	0±0 (0±0%)
4	17F	C	632	-	52,60,60	0.94±0.01	0±0 (0±0%)
4	17F	C	633	-	52,60,60	1.74±0.03	2±0 (4±0%)
4	17F	C	634	-	52,60,60	0.97±0.02	0±0 (0±0%)
4	17F	C	635	-	52,60,60	0.94±0.01	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
3	PCW	A	401	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	402	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	403	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	404	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	405	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	406	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	407	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	408	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	409	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	410	-	-	0±0,57,57,57	0±0,0,0,0
4	17F	A	411	-	-	0±0,55,59,59	0±0,0,0,0
3	PCW	B	201	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	202	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	203	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	204	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	205	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	206	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	207	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	208	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	209	-	-	0±0,57,57,57	0±0,0,0,0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	B	210	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	211	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	212	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	213	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	214	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	215	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	216	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	217	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	218	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	219	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	220	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	221	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	222	-	-	0±0,57,57,57	0±0,0,0,0
4	17F	B	223	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	B	224	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	B	225	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	B	226	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	B	227	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	B	228	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	B	229	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	B	230	-	-	0±0,55,59,59	0±0,0,0,0
3	PCW	B	231	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	232	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	B	233	-	-	0±0,57,57,57	0±0,0,0,0
4	17F	B	234	-	-	0±0,55,59,59	0±0,0,0,0
5	GNP	B	235	-	-	1±0,16,38,38	0±0,3,3,3
7	EWS	B	237	-	-	0±0,10,22,22	0±0,4,4,4
3	PCW	C	601	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	602	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	603	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	604	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	605	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	606	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	607	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	608	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	609	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	610	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	611	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	612	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	613	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	614	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	615	-	-	0±0,57,57,57	0±0,0,0,0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	C	616	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	617	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	618	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	619	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	620	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	621	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	622	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	623	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	624	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	625	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	626	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	627	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	628	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	C	629	-	-	0±0,57,57,57	0±0,0,0,0
4	17F	C	630	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	C	631	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	C	632	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	C	633	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	C	634	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	C	635	-	-	0±0,55,59,59	0±0,0,0,0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
7	B	237	EWS	CAX-CBA	9.92	1.33	1.39	5	10
7	B	237	EWS	CBA-CAV	9.81	1.34	1.42	4	10
7	B	237	EWS	CBA-CAZ	9.05	1.34	1.50	5	10
5	B	235	GNP	PG-O1G	6.21	1.53	1.46	7	10
5	B	235	GNP	C4-N9	5.67	1.40	1.47	5	10
5	B	235	GNP	C5-C6	5.36	1.43	1.52	10	10

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
3	B	222	PCW	C8-N-C7	12.22	77.21	108.97	1	10
3	B	219	PCW	C8-N-C7	12.21	77.23	108.97	1	10
3	C	618	PCW	C8-N-C7	12.17	77.35	108.97	9	10
3	C	616	PCW	C8-N-C7	12.16	77.36	108.97	3	10
3	C	625	PCW	C8-N-C7	12.16	77.38	108.97	5	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	408	PCW	C8-N-C7	12.15	77.39	108.97	6	10
3	A	410	PCW	C8-N-C7	12.14	77.42	108.97	8	10
3	C	627	PCW	C8-N-C7	12.14	77.42	108.97	6	10
3	B	232	PCW	C8-N-C7	12.14	77.42	108.97	1	10
3	B	212	PCW	C8-N-C7	12.14	77.42	108.97	1	10
3	B	206	PCW	C8-N-C7	12.13	77.43	108.97	1	10
3	C	606	PCW	C8-N-C7	12.12	77.46	108.97	6	10
3	C	608	PCW	C8-N-C7	12.12	77.48	108.97	5	10
3	A	401	PCW	C8-N-C7	12.11	77.49	108.97	7	10
3	B	217	PCW	C8-N-C7	12.11	77.51	108.97	9	10
3	B	218	PCW	C8-N-C7	12.10	77.52	108.97	6	10
3	C	620	PCW	C8-N-C7	12.09	77.54	108.97	10	10
3	B	231	PCW	C8-N-C7	12.09	77.55	108.97	9	10
3	B	220	PCW	C8-N-C7	12.09	77.56	108.97	7	10
3	B	202	PCW	C8-N-C7	12.09	77.56	108.97	10	10
3	A	403	PCW	C8-N-C7	12.08	77.57	108.97	4	10
3	C	614	PCW	C8-N-C7	12.07	77.59	108.97	10	10
3	C	605	PCW	C8-N-C7	12.07	77.59	108.97	2	10
3	B	233	PCW	C8-N-C7	12.07	77.60	108.97	1	10
3	C	611	PCW	C8-N-C7	12.07	77.60	108.97	2	10
3	C	622	PCW	C8-N-C7	12.07	77.60	108.97	7	10
3	A	406	PCW	C8-N-C7	12.07	77.61	108.97	7	10
3	B	209	PCW	C8-N-C7	12.06	77.62	108.97	3	10
3	C	619	PCW	C8-N-C7	12.06	77.62	108.97	5	10
3	A	402	PCW	C8-N-C7	12.06	77.62	108.97	2	10
3	C	604	PCW	C8-N-C7	12.06	77.63	108.97	10	10
3	B	216	PCW	C8-N-C7	12.06	77.64	108.97	8	10
3	C	617	PCW	C8-N-C7	12.05	77.65	108.97	9	10
3	B	213	PCW	C8-N-C7	12.05	77.66	108.97	5	10
3	B	203	PCW	C8-N-C7	12.04	77.67	108.97	5	10
3	C	628	PCW	C8-N-C7	12.05	77.67	108.97	5	10
3	B	210	PCW	C8-N-C7	12.04	77.68	108.97	7	10
3	B	201	PCW	C8-N-C7	12.04	77.68	108.97	5	10
3	A	405	PCW	C8-N-C7	12.04	77.69	108.97	3	10
3	C	607	PCW	C8-N-C7	12.03	77.70	108.97	4	10
3	C	626	PCW	C8-N-C7	12.03	77.70	108.97	9	10
3	B	215	PCW	C8-N-C7	12.03	77.71	108.97	9	10
3	C	613	PCW	C8-N-C7	12.02	77.73	108.97	2	10
3	C	621	PCW	C8-N-C7	12.02	77.74	108.97	5	10
3	C	603	PCW	C8-N-C7	11.99	77.81	108.97	9	10
3	A	409	PCW	C8-N-C7	11.99	77.81	108.97	5	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	212	PCW	C8-N-C6	10.32	82.16	108.97	9	10
3	C	608	PCW	C8-N-C6	10.31	82.19	108.97	3	10
3	C	606	PCW	C8-N-C6	10.30	82.19	108.97	1	10
3	B	218	PCW	C8-N-C6	10.28	82.24	108.97	1	10
3	C	604	PCW	C8-N-C6	10.26	82.30	108.97	5	10
3	C	625	PCW	C8-N-C6	10.26	82.32	108.97	2	10
3	C	607	PCW	C8-N-C6	10.23	82.38	108.97	6	10
3	B	217	PCW	C8-N-C6	10.23	82.39	108.97	3	10
3	B	209	PCW	C8-N-C6	10.22	82.41	108.97	7	10
3	C	626	PCW	C8-N-C6	10.22	82.42	108.97	8	10
3	B	215	PCW	C8-N-C6	10.21	82.44	108.97	10	10
3	B	233	PCW	C8-N-C6	10.21	82.45	108.97	3	10
3	C	605	PCW	C8-N-C6	10.20	82.46	108.97	1	10
3	A	409	PCW	C8-N-C6	10.20	82.47	108.97	5	10
3	C	622	PCW	C8-N-C6	10.18	82.52	108.97	4	10
3	B	219	PCW	C8-N-C6	10.18	82.52	108.97	4	10
3	C	627	PCW	C8-N-C6	10.18	82.53	108.97	2	10
3	C	628	PCW	C8-N-C6	10.17	82.53	108.97	9	10
3	B	206	PCW	C8-N-C6	10.17	82.53	108.97	5	10
3	A	410	PCW	C8-N-C6	10.17	82.54	108.97	7	10
3	B	220	PCW	C8-N-C6	10.17	82.55	108.97	5	10
3	B	213	PCW	C8-N-C6	10.16	82.56	108.97	6	10
3	C	603	PCW	C8-N-C6	10.16	82.57	108.97	8	10
3	C	613	PCW	C8-N-C6	10.16	82.57	108.97	7	10
3	C	620	PCW	C8-N-C6	10.16	82.57	108.97	2	10
3	C	616	PCW	C8-N-C6	10.16	82.58	108.97	6	10
3	B	222	PCW	C8-N-C6	10.16	82.58	108.97	9	10
3	B	210	PCW	C8-N-C6	10.15	82.58	108.97	6	10
3	B	216	PCW	C8-N-C6	10.15	82.59	108.97	6	10
3	A	401	PCW	C8-N-C6	10.15	82.59	108.97	9	10
3	C	614	PCW	C8-N-C6	10.15	82.59	108.97	2	10
3	C	621	PCW	C8-N-C6	10.15	82.59	108.97	10	10
3	A	408	PCW	C8-N-C6	10.13	82.64	108.97	1	10
3	A	406	PCW	C8-N-C6	10.13	82.64	108.97	6	10
3	B	232	PCW	C8-N-C6	10.12	82.66	108.97	6	10
3	C	618	PCW	C8-N-C6	10.12	82.67	108.97	1	10
3	B	231	PCW	C8-N-C6	10.12	82.67	108.97	1	10
3	B	201	PCW	C8-N-C6	10.12	82.67	108.97	8	10
3	A	403	PCW	C8-N-C6	10.11	82.69	108.97	5	10
3	C	619	PCW	C8-N-C6	10.11	82.69	108.97	9	10
3	C	617	PCW	C8-N-C6	10.11	82.69	108.97	7	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	202	PCW	C8-N-C6	10.11	82.70	108.97	8	10
3	B	203	PCW	C8-N-C6	10.10	82.73	108.97	1	10
3	C	611	PCW	C8-N-C6	10.09	82.75	108.97	8	10
3	A	405	PCW	C8-N-C6	10.09	82.75	108.97	1	10
3	A	402	PCW	C8-N-C6	10.08	82.77	108.97	7	10
3	B	203	PCW	O4P-P-O2P	7.85	78.39	109.07	6	10
3	B	232	PCW	O4P-P-O2P	7.71	78.94	109.07	6	10
4	B	223	17F	O2-P1-O6	6.23	78.83	107.75	5	10
4	B	223	17F	O2-P1-O3	6.17	79.10	107.75	3	10
4	C	633	17F	O2-P1-O6	6.13	79.29	107.75	1	10
5	B	235	GNP	C4-C5-N7	6.11	110.56	102.46	2	10
4	C	633	17F	O2-P1-O3	6.00	79.87	107.75	5	10
3	B	232	PCW	O3P-P-O2P	5.92	85.93	109.07	4	10
3	B	203	PCW	O3P-P-O2P	5.89	86.07	109.07	8	10
4	C	633	17F	O3-C1-C2	5.72	113.05	108.06	1	1
3	A	403	PCW	C8-N-C5	5.42	87.94	109.91	7	10
3	B	232	PCW	O1P-P-O2P	5.40	85.12	112.21	7	10
3	B	203	PCW	O1P-P-O2P	5.40	85.16	112.21	2	10
3	B	203	PCW	C8-N-C5	5.37	88.15	109.91	6	10
3	C	608	PCW	C8-N-C5	5.37	88.15	109.91	8	10
3	C	614	PCW	C8-N-C5	5.36	88.18	109.91	4	10
3	B	231	PCW	C8-N-C5	5.34	88.26	109.91	5	10
3	B	219	PCW	C8-N-C5	5.33	88.32	109.91	10	10
3	C	621	PCW	C8-N-C5	5.32	88.35	109.91	6	10
3	C	618	PCW	C8-N-C5	5.32	88.37	109.91	10	10
3	B	201	PCW	C8-N-C5	5.31	88.38	109.91	6	10
3	A	401	PCW	C8-N-C5	5.31	88.38	109.91	10	10
3	C	606	PCW	C8-N-C5	5.31	88.41	109.91	8	10
3	B	210	PCW	C8-N-C5	5.31	88.41	109.91	9	10
3	A	405	PCW	C8-N-C5	5.30	88.42	109.91	2	10
3	B	216	PCW	C8-N-C5	5.30	88.42	109.91	7	10
3	C	605	PCW	C8-N-C5	5.31	88.42	109.91	7	10
3	C	626	PCW	C8-N-C5	5.30	88.42	109.91	3	10
3	C	607	PCW	C8-N-C5	5.30	88.43	109.91	3	10
3	C	625	PCW	C8-N-C5	5.30	88.43	109.91	7	10
3	C	619	PCW	C8-N-C5	5.30	88.45	109.91	6	10
3	B	202	PCW	C8-N-C5	5.29	88.46	109.91	2	10
3	B	220	PCW	C8-N-C5	5.29	88.46	109.91	8	10
3	C	604	PCW	C8-N-C5	5.29	88.46	109.91	7	10
3	C	617	PCW	C8-N-C5	5.29	88.48	109.91	2	10
3	C	620	PCW	C8-N-C5	5.29	88.47	109.91	6	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	B	212	PCW	C8-N-C5	5.29	88.48	109.91	10	10
3	A	408	PCW	C8-N-C5	5.29	88.50	109.91	7	9
3	B	209	PCW	C8-N-C5	5.28	88.52	109.91	4	10
3	B	215	PCW	C8-N-C5	5.28	88.52	109.91	6	10
3	C	627	PCW	C8-N-C5	5.28	88.52	109.91	3	9
3	C	603	PCW	C8-N-C5	5.28	88.53	109.91	10	10
3	A	402	PCW	C8-N-C5	5.28	88.53	109.91	1	10
3	B	213	PCW	C8-N-C5	5.27	88.55	109.91	3	10
3	C	628	PCW	C8-N-C5	5.27	88.56	109.91	6	10
3	C	613	PCW	C8-N-C5	5.27	88.56	109.91	9	10
3	B	233	PCW	C8-N-C5	5.27	88.56	109.91	6	10
3	A	410	PCW	C8-N-C5	5.27	88.57	109.91	6	10
3	A	406	PCW	C8-N-C5	5.27	88.57	109.91	4	10
3	B	206	PCW	C8-N-C5	5.27	88.57	109.91	9	10
3	C	611	PCW	C8-N-C5	5.27	88.58	109.91	10	10
3	C	622	PCW	C8-N-C5	5.26	88.59	109.91	7	10
3	B	232	PCW	C8-N-C5	5.26	88.59	109.91	4	10
3	C	616	PCW	C8-N-C5	5.26	88.60	109.91	8	10
3	B	218	PCW	C8-N-C5	5.26	88.60	109.91	7	10
3	A	409	PCW	C8-N-C5	5.26	88.62	109.91	8	10
3	B	217	PCW	C8-N-C5	5.24	88.69	109.91	5	10
3	B	222	PCW	C8-N-C5	5.20	88.83	109.91	6	9

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)
5	B	235	GNP	O1B-PB-N3B-PG	2
3	B	203	PCW	P-O4P-C4-C5	1

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: 6ccx_cs.cif

Chemical shift list name: *resonance_list_nmrstar_50_51.txt*

7.1.1 Bookkeeping [i](#)

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	268
Number of shifts mapped to atoms	268
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	84	-0.47 ± 0.54	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 204 atoms were assigned a chemical shift out of a possible 7233. 3 out of 107 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	154/2779 (6%)	77/1108 (7%)	0/1126 (0%)	77/545 (14%)
Sidechain	50/4008 (1%)	25/2349 (1%)	25/1453 (2%)	0/206 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/446 (0%)	0/244 (0%)	0/194 (0%)	0/8 (0%)
Overall	204/7233 (3%)	102/3701 (3%)	25/2773 (1%)	77/759 (10%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 217 atoms were assigned a chemical shift out of a possible 7487. 3 out of 109 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	167/2869 (6%)	83/1144 (7%)	0/1162 (0%)	84/563 (15%)
Sidechain	50/4172 (1%)	25/2448 (1%)	25/1508 (2%)	0/216 (0%)
Aromatic	0/446 (0%)	0/244 (0%)	0/194 (0%)	0/8 (0%)
Overall	217/7487 (3%)	108/3836 (3%)	25/2864 (1%)	84/787 (11%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain B:

