Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2020 – 11:25 am BST

PDB ID	:	2MSE
Title	:	NMR data-driven model of GTPase KRas-GNP:ARafRBD complex tethered to a lipid-bilayer nanodisc
Authors	:	Mazhab-Jafari, M.; Stathopoulos, P.; Marshall, C.; Ikura, M.
Deposited on	:	2014-07-29

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

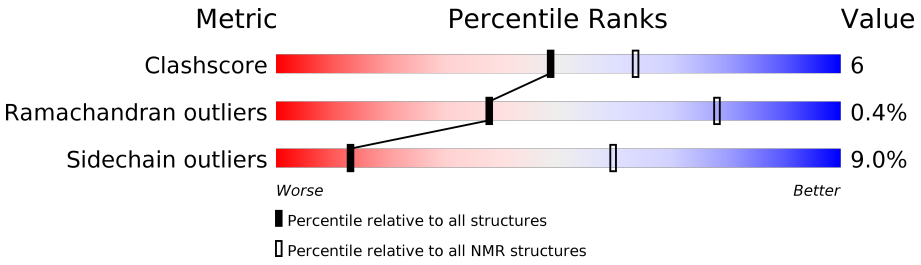
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 0%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	200	64% 14% 21%
1	C	200	80% 18%
2	B	187	75% 16% 8%
3	D	73	75% 25%

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, 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:239-A:395, C:401-C:596 (353)	0.25	3
2	B:2-B:171, D:808-D:880 (243)	0.55	5

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9709 atoms, of which 64 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
			1492	923	16	257	287	9	

There are 2 discrepancies between the modelled and reference sequences:

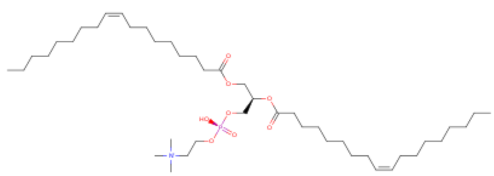
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P01116
B	0	SER	-	expression tag	UNP P01116

- Molecule 3 is a protein called Serine/threonine-protein kinase A-Raf.

Mol	Chain	Residues	Atoms						Trace
3	D	73	Total	C	H	N	O	S	0
			573	360	4	99	107	3	

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).

PCW



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

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

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

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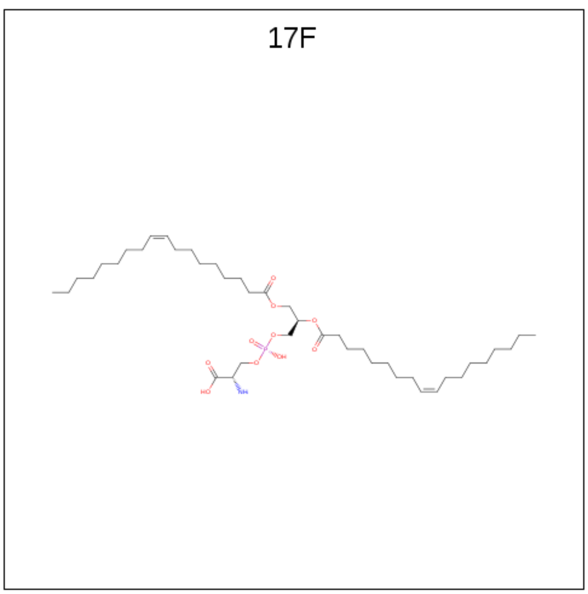
Mol	Chain	Residues	Atoms
4	A	1	Total C N O P 54 44 1 8 1
4	A	1	Total C N O P 54 44 1 8 1
4	A	1	Total C N O P 54 44 1 8 1
4	A	1	Total C N O P 54 44 1 8 1
4	A	1	Total C N O P 54 44 1 8 1
4	A	1	Total C N O P 54 44 1 8 1
4	A	1	Total C N O P 54 44 1 8 1
4	A	1	Total C N O P 54 44 1 8 1

- Molecule 5 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: $C_{42}H_{78}NO_{10}P$).



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

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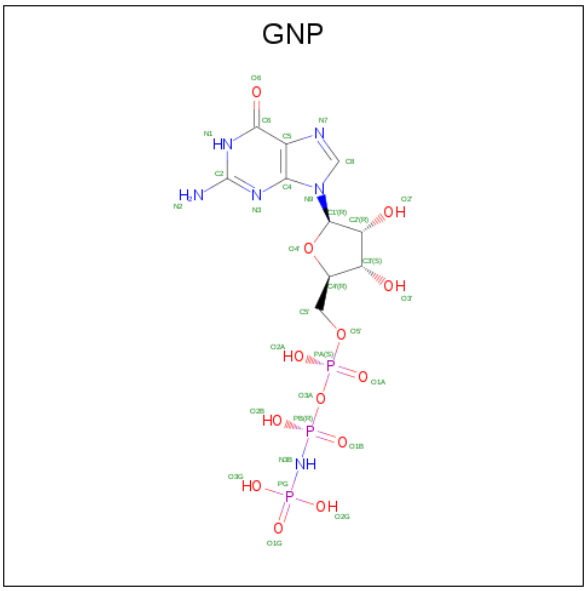
Mol	Chain	Residues	Atoms				
5	A	1	Total 54	C 42	N 1	O 10	P 1
5	A	1	Total 54	C 42	N 1	O 10	P 1
5	A	1	Total 54	C 42	N 1	O 10	P 1
5	A	1	Total 54	C 42	N 1	O 10	P 1
5	A	1	Total 54	C 42	N 1	O 10	P 1
5	A	1	Total 54	C 42	N 1	O 10	P 1
5	A	1	Total 54	C 42	N 1	O 10	P 1
5	A	1	Total 54	C 42	N 1	O 10	P 1
5	A	1	Total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

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
			Total	Mg
7	B	1	1	1

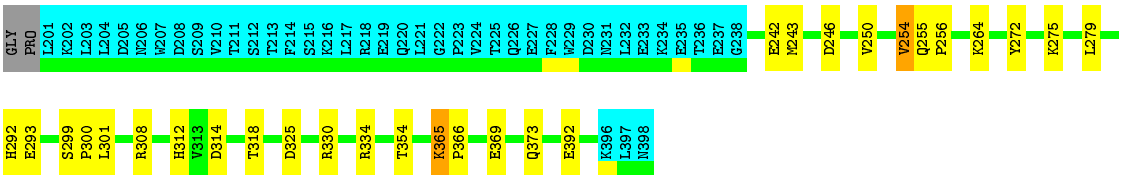
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

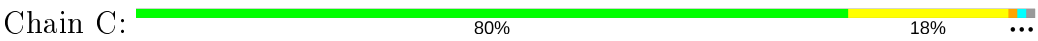
• Molecule 1: Apolipoprotein A-I

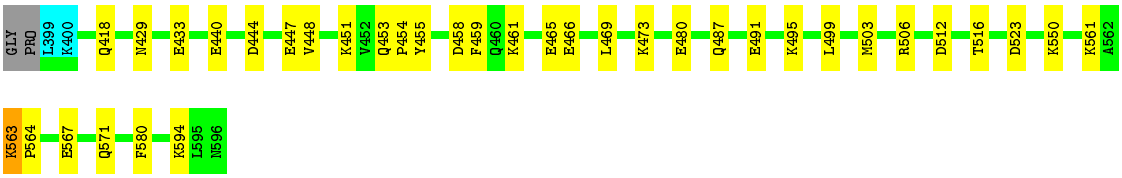
Chain A:



• Molecule 1: Apolipoprotein A-I

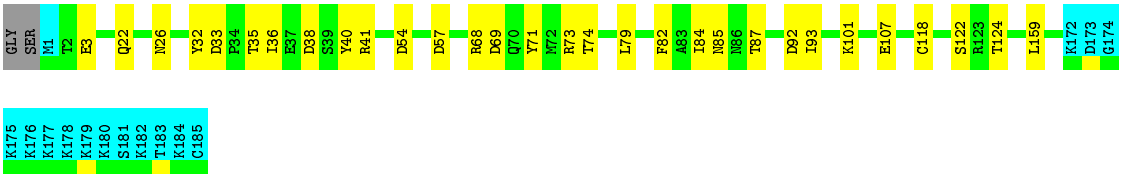
Chain C:





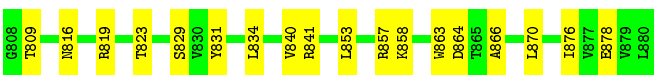
• Molecule 2: GTPase KRas

Chain B:



• Molecule 3: Serine/threonine-protein kinase A-Raf

Chain D:



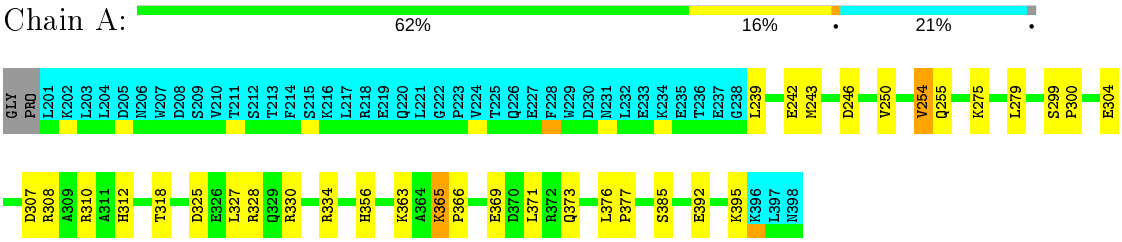
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

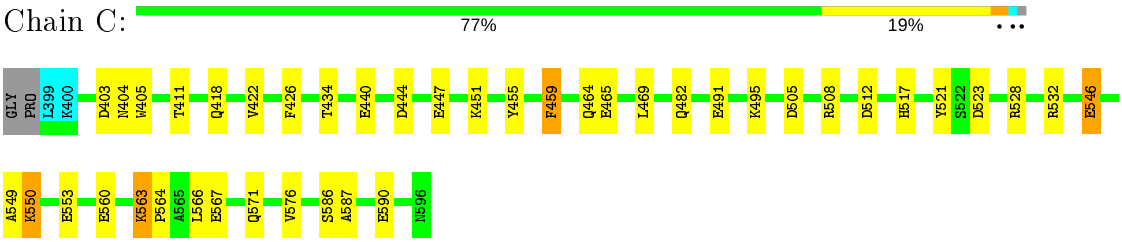
• Molecule 1: Apolipoprotein A-I

Chain A:



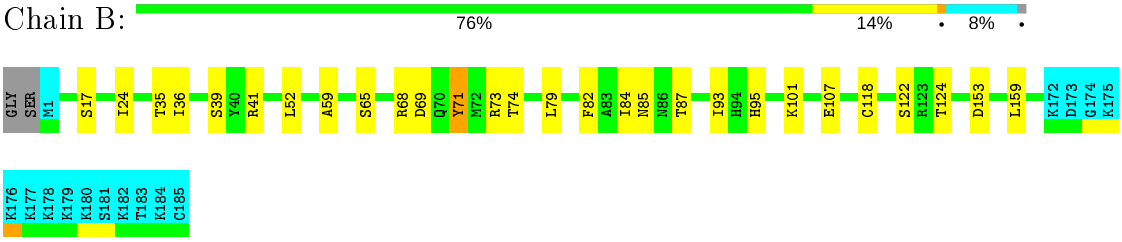
• Molecule 1: Apolipoprotein A-I

Chain C:



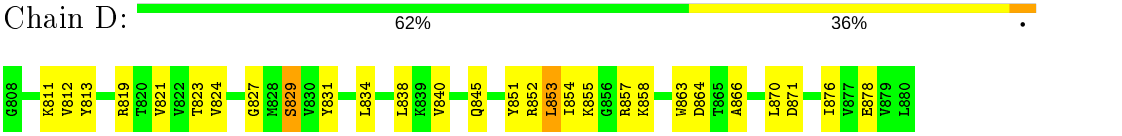
• Molecule 2: GTPase KRas

Chain B:



• Molecule 3: Serine/threonine-protein kinase A-Raf

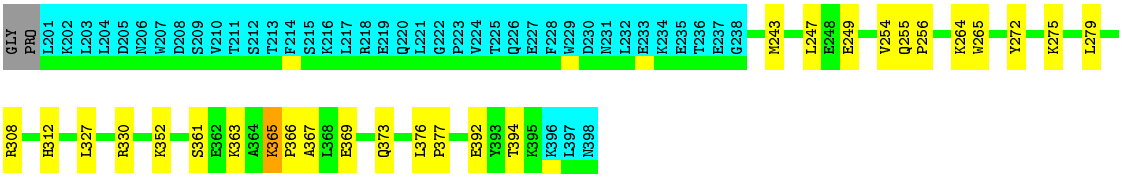
Chain D:



4.2.2 Score per residue for model 2

• Molecule 1: Apolipoprotein A-I

Chain A:

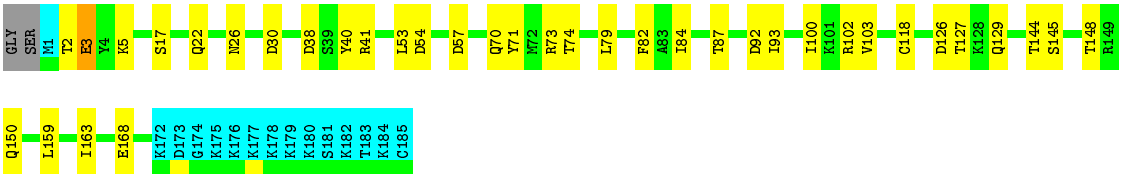


• Molecule 1: Apolipoprotein A-I

Chain C:

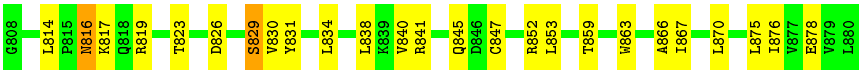
• Molecule 2: GTPase KRas

Chain B:



• Molecule 3: Serine/threonine-protein kinase A-Raf

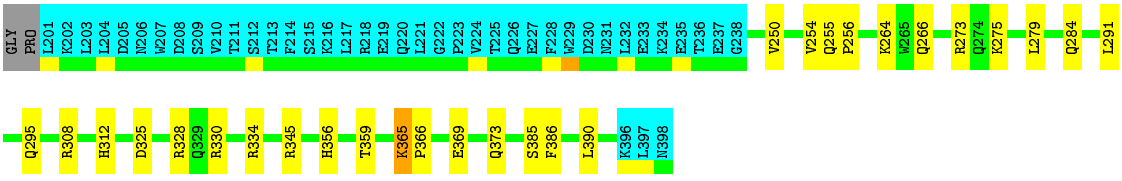
Chain D:



4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: Apolipoprotein A-I

Chain A:

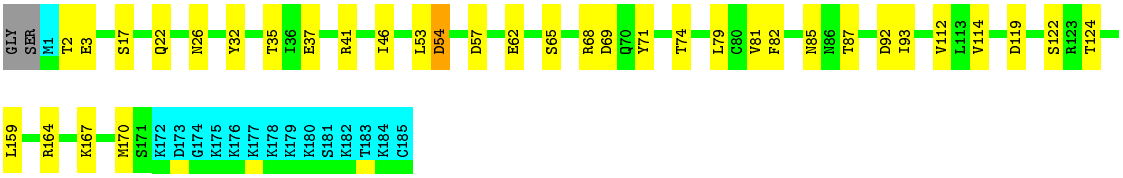


• Molecule 1: Apolipoprotein A-I

Chain C:

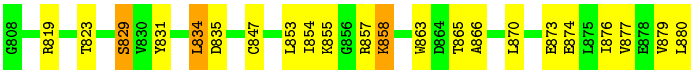
- Molecule 2: GTPase KRas

Chain B:



- Molecule 3: Serine/threonine-protein kinase A-Raf

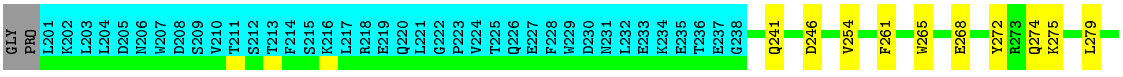
Chain D:

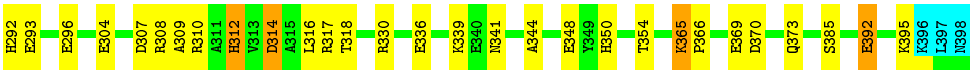


4.2.4 Score per residue for model 4

- Molecule 1: Apolipoprotein A-I

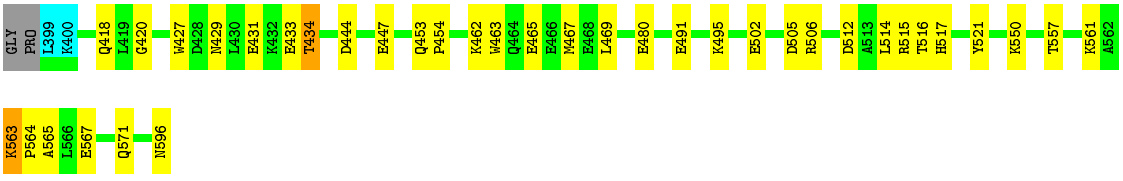
Chain A:





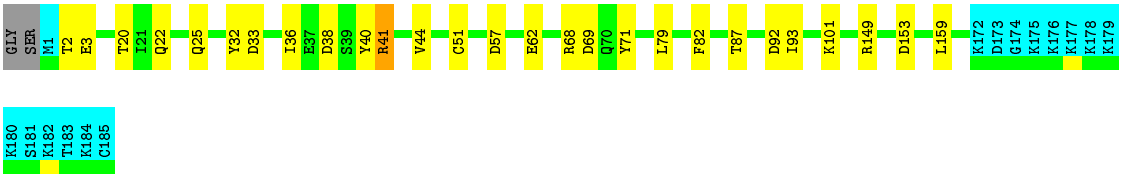
- Molecule 1: Apolipoprotein A-I

Chain C:



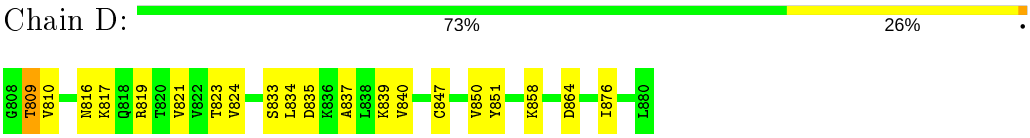
- Molecule 2: GTPase KRas

Chain B:



- Molecule 3: Serine/threonine-protein kinase A-Raf

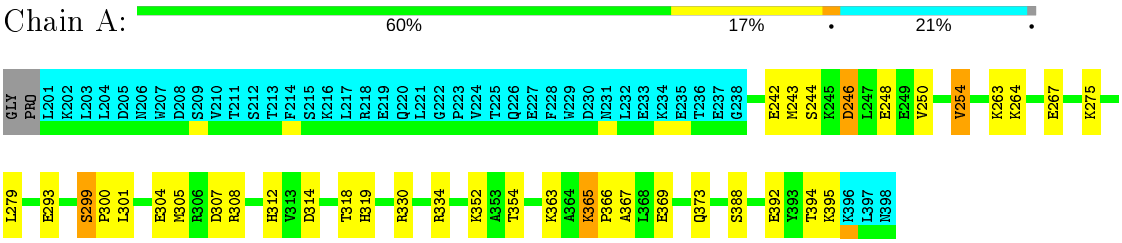
Chain D:



4.2.5 Score per residue for model 5

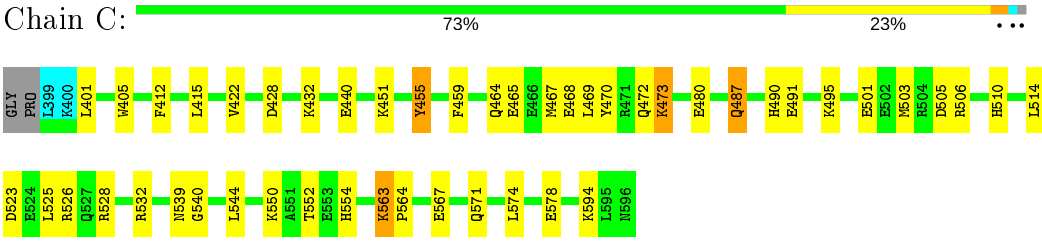
- Molecule 1: Apolipoprotein A-I

Chain A:



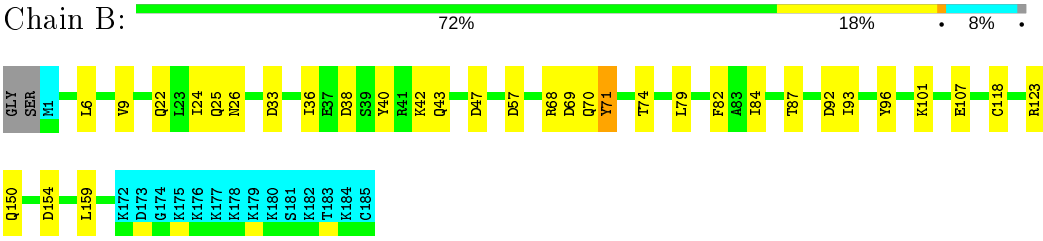
- Molecule 1: Apolipoprotein A-I

Chain C:



- Molecule 2: GTPase KRas

Chain B:



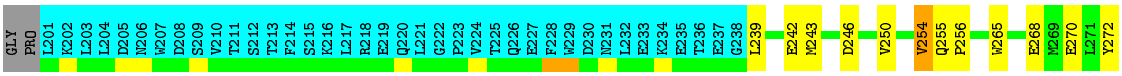
- Molecule 3: Serine/threonine-protein kinase A-Raf

Chain D:

4.2.6 Score per residue for model 6

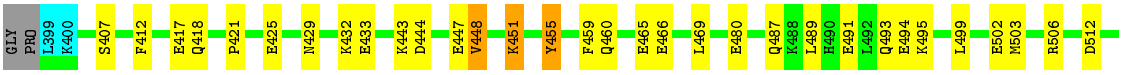
- Molecule 1: Apolipoprotein A-I

Chain A:



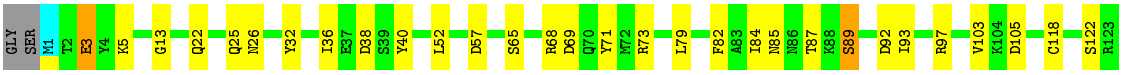
- Molecule 1: Apolipoprotein A-I

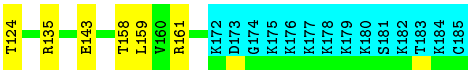
Chain C:



- Molecule 2: GTPase KRas

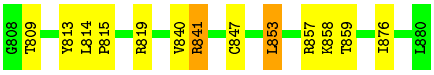
Chain B:





- Molecule 3: Serine/threonine-protein kinase A-Raf

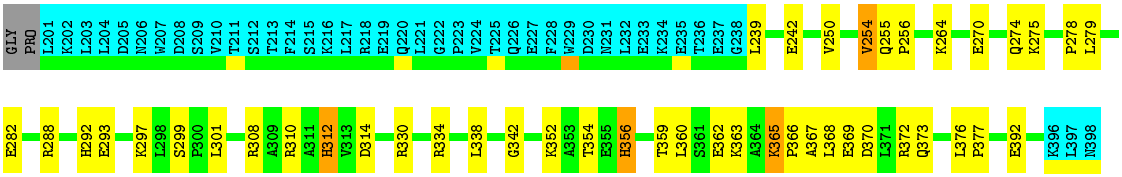
Chain D:



4.2.7 Score per residue for model 7

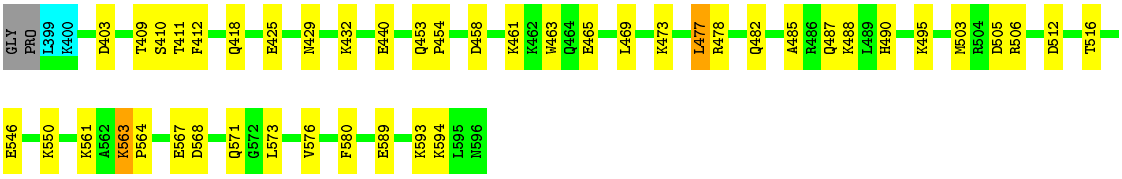
- Molecule 1: Apolipoprotein A-I

Chain A:



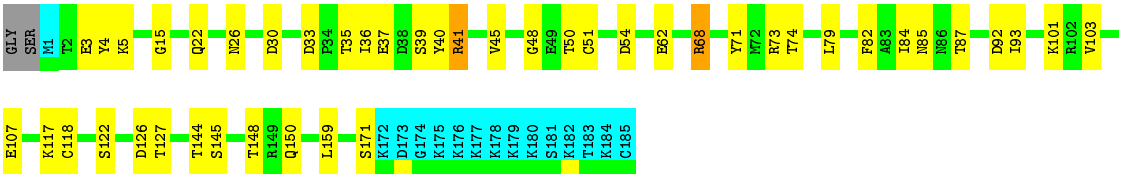
• Molecule 1: Apolipoprotein A-I

Chain C:



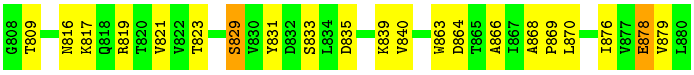
• Molecule 2: GTPase KRas

Chain B:



• Molecule 3: Serine/threonine-protein kinase A-Raf

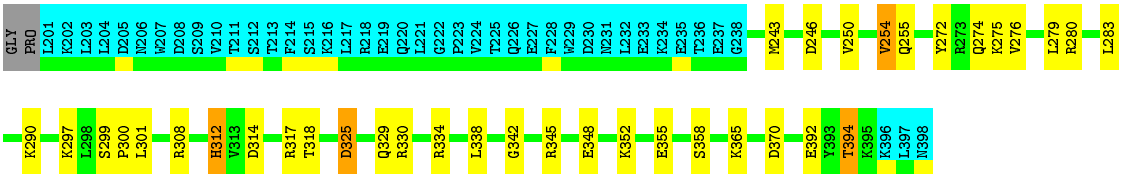
Chain D:



4.2.8 Score per residue for model 8

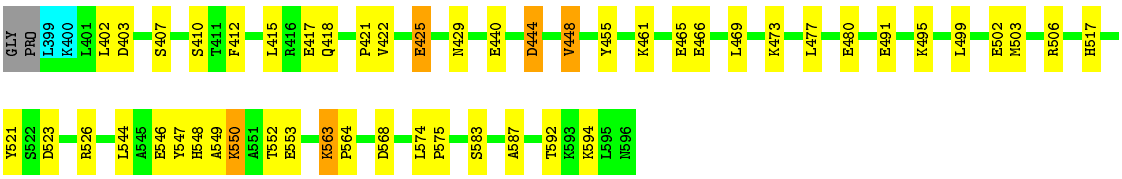
• Molecule 1: Apolipoprotein A-I

Chain A:



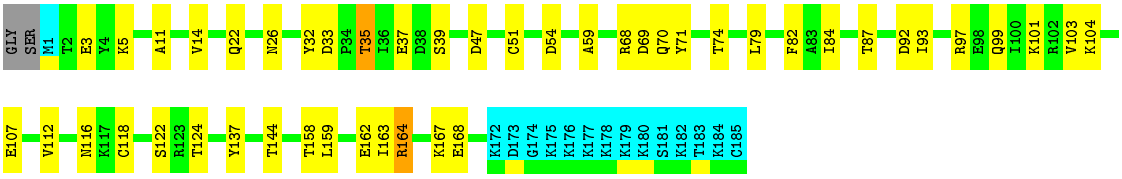
• Molecule 1: Apolipoprotein A-I

Chain C:



- Molecule 2: GTPase KRas

Chain B:



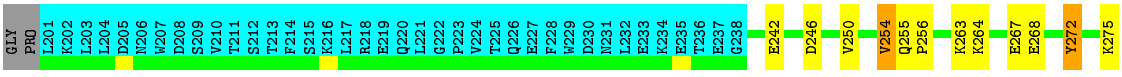
- Molecule 3: Serine/threonine-protein kinase A-Raf

Chain D:

4.2.9 Score per residue for model 9

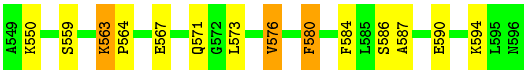
- Molecule 1: Apolipoprotein A-I

Chain A:



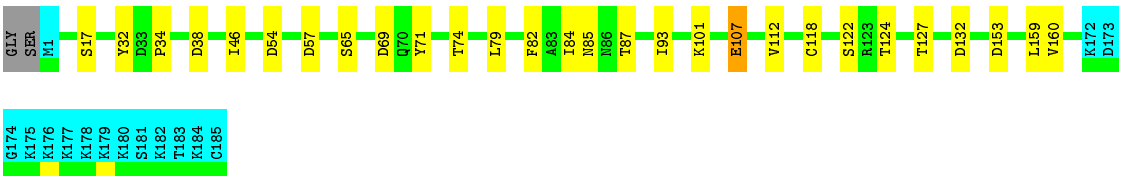
- Molecule 1: Apolipoprotein A-I

Chain C:



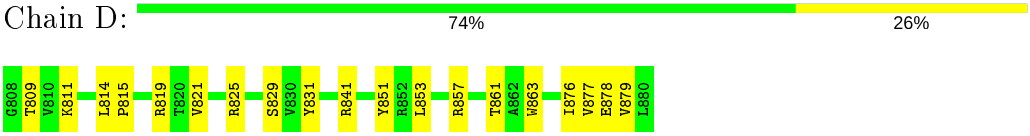
- Molecule 2: GTPase KRas

Chain B:



- Molecule 3: Serine/threonine-protein kinase A-Raf

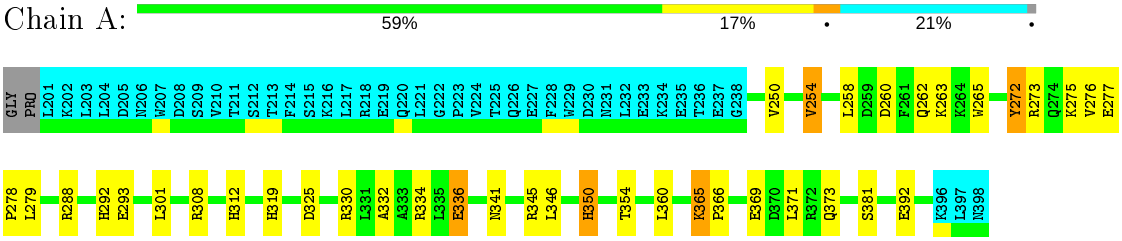
Chain D:



4.2.10 Score per residue for model 10

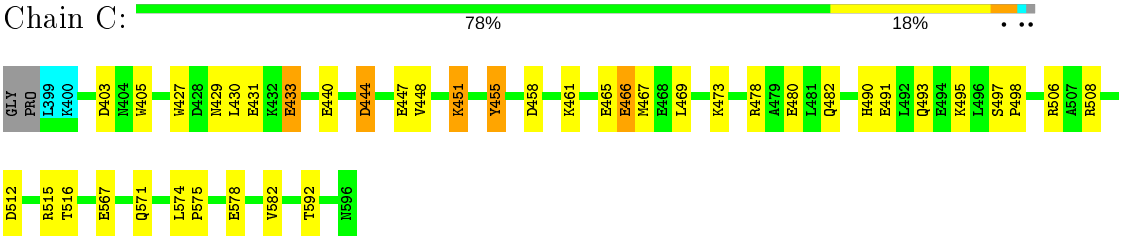
- Molecule 1: Apolipoprotein A-I

Chain A:



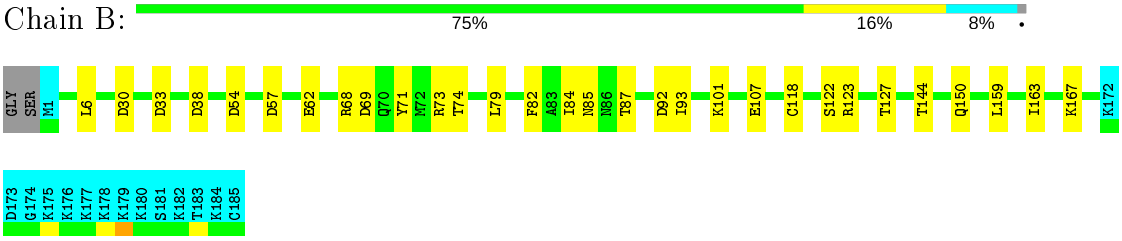
- Molecule 1: Apolipoprotein A-I

Chain C:



- Molecule 2: GTPase KRas

Chain B:



- Molecule 3: Serine/threonine-protein kinase A-Raf

Chain D:


G808
V812
R819
T823
V824
S829
L834
L853
R857
K858
T859
D864
T865
A866
D871
I876
W877
E878
V879
L880

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: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	
CHARMM-GUI	structure solution	
HADDOCK	structure solution	
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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	52
Number of shifts mapped to atoms	52
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 17F, MG, GNP, PCW

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1284	18	1297	24±6
1	C	1607	22	1603	30±6
2	B	1356	16	1336	16±5
3	D	569	4	598	15±5
4	A	3456	0	5376	60±9
5	A	864	0	1216	23±4
6	B	32	0	13	0±0
All	All	91690	600	114390	1282

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:CD	1:C:469:LEU:HD11	1.48	1.34	1	1
1:C:465:GLU:O	1:C:469:LEU:HG	1.32	1.19	2	9
1:C:465:GLU:O	1:C:469:LEU:CG	1.26	1.82	7	6
1:A:308:ARG:CG	1:C:469:LEU:HD11	1.21	1.63	1	3
1:A:308:ARG:CD	1:C:469:LEU:CD1	1.17	2.21	1	1
1:A:308:ARG:HG3	1:C:469:LEU:CD1	1.15	1.72	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:HD3	1:C:469:LEU:CD1	1.10	1.75	1	2
1:C:567:GLU:O	1:C:571:GLN:HG3	1.07	1.48	2	7
1:A:308:ARG:CG	1:C:469:LEU:CD1	1.05	2.34	1	2
1:A:308:ARG:CD	1:C:469:LEU:HD21	1.03	1.82	4	2
1:A:308:ARG:HG3	1:C:469:LEU:HD11	1.01	1.26	9	3
1:A:308:ARG:HG3	1:C:469:LEU:HD21	1.01	1.27	10	6
1:A:308:ARG:HD2	1:C:469:LEU:HD21	0.99	1.33	1	2
1:A:369:GLU:O	1:A:373:GLN:HG3	0.99	1.58	10	8
1:A:308:ARG:HD3	1:C:469:LEU:HD11	0.96	0.97	1	2
1:C:465:GLU:O	1:C:469:LEU:CB	0.94	2.16	7	2
5:A:38:17F:H1	5:A:38:17F:H4	0.90	1.43	1	1
1:A:297:LYS:HE2	1:C:477:LEU:HG	0.90	1.39	7	1
2:B:38:ASP:HB2	2:B:57:ASP:HB3	0.89	1.39	9	6
1:C:465:GLU:O	1:C:469:LEU:CD1	0.85	2.25	7	2
1:A:308:ARG:HD2	1:C:469:LEU:CD2	0.84	2.00	1	2
5:A:37:17F:HN1	3:D:857:ARG:HH21	0.83	1.16	1	1
5:A:74:17F:HN1	5:A:74:17F:H4	0.82	1.30	4	1
4:A:30:PCW:H73	5:A:40:17F:HN1	0.81	1.35	3	1
1:A:279:LEU:HD22	1:C:495:LYS:HG2	0.80	1.53	1	7
1:C:563:LYS:HB2	1:C:564:PRO:HD3	0.80	1.52	2	9
1:A:308:ARG:HD3	1:C:469:LEU:HD21	0.78	1.55	4	1
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.78	1.56	3	8
1:C:466:GLU:OE1	1:C:469:LEU:HD12	0.77	1.79	10	1
4:A:24:PCW:H41	3:D:853:LEU:HG	0.76	1.58	9	1
5:A:74:17F:H4A	5:A:79:17F:HN1A	0.75	1.41	8	1
1:C:567:GLU:O	1:C:571:GLN:CG	0.75	2.34	2	3
2:B:36:ILE:HD11	3:D:809:THR:HG21	0.75	1.59	4	4
4:A:7:PCW:H20	3:D:857:ARG:HH12	0.75	1.42	5	1
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.74	1.59	8	7
1:A:308:ARG:CD	1:C:469:LEU:CG	0.74	2.65	1	1
4:A:6:PCW:H341	4:A:28:PCW:H152	0.73	1.58	7	1
2:B:79:LEU:HG	2:B:159:LEU:HD22	0.73	1.60	9	10
4:A:7:PCW:H72	3:D:879:VAL:HB	0.72	1.60	9	1
4:A:9:PCW:H322	4:A:14:PCW:H351	0.71	1.62	8	1
4:A:7:PCW:H2	4:A:16:PCW:H11	0.71	1.62	8	1
1:A:260:ASP:HA	1:A:263:LYS:HE2	0.71	1.60	10	1
4:A:12:PCW:H362	4:A:30:PCW:H152	0.71	1.62	4	1
4:A:43:PCW:H82	5:A:74:17F:HN1A	0.71	1.45	9	1
1:C:453:GLN:HB2	1:C:454:PRO:HD3	0.71	1.61	4	5
3:D:829:SER:HA	3:D:866:ALA:HA	0.70	1.60	3	7
4:A:45:PCW:H331	4:A:45:PCW:H132	0.70	1.62	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:45:PCW:H40	4:A:57:PCW:H61	0.70	1.61	8	1
4:A:57:PCW:H42	5:A:80:17F:HN1A	0.70	1.46	3	1
4:A:9:PCW:H31	4:A:9:PCW:H41	0.70	1.64	2	2
1:A:341:ASN:HD21	1:C:433:GLU:HA	0.70	1.47	6	4
4:A:6:PCW:H122	4:A:16:PCW:H352	0.69	1.64	10	1
1:A:316:LEU:HG	1:C:462:LYS:HE3	0.69	1.63	4	2
4:A:56:PCW:H132	4:A:56:PCW:H331	0.69	1.63	2	1
1:C:465:GLU:O	1:C:469:LEU:HB2	0.69	1.86	7	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.69	1.87	10	9
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.69	1.63	1	2
1:A:308:ARG:CG	1:C:469:LEU:HD21	0.68	2.15	8	2
4:A:23:PCW:H32	5:A:34:17F:H63	0.68	1.65	5	1
4:A:15:PCW:H321	4:A:16:PCW:H19	0.68	1.64	10	1
4:A:10:PCW:H131	4:A:22:PCW:H351	0.68	1.65	4	1
1:A:308:ARG:CB	1:C:469:LEU:HD11	0.67	2.20	1	3
4:A:12:PCW:H73	5:A:37:17F:HN1A	0.67	1.48	4	1
1:A:308:ARG:HD2	1:C:469:LEU:CG	0.67	2.17	1	1
1:A:352:LYS:HG2	1:C:422:VAL:HG13	0.67	1.66	2	1
4:A:12:PCW:H72	5:A:40:17F:HN1	0.66	1.49	8	1
2:B:101:LYS:HD2	2:B:107:GLU:HG3	0.66	1.66	8	2
1:C:418:GLN:O	1:C:422:VAL:HB	0.66	1.89	2	3
4:A:67:PCW:H81	5:A:78:17F:H37	0.66	1.67	10	1
4:A:54:PCW:H131	4:A:54:PCW:H331	0.66	1.66	2	1
4:A:15:PCW:H71	5:A:39:17F:H2	0.66	1.67	9	1
2:B:101:LYS:HG2	2:B:107:GLU:HA	0.66	1.67	9	2
2:B:101:LYS:HE3	2:B:107:GLU:HB3	0.66	1.67	9	1
1:A:308:ARG:CD	1:C:469:LEU:CD2	0.66	2.73	1	2
4:A:31:PCW:H52	4:A:31:PCW:H2	0.65	1.68	3	1
3:D:851:TYR:HB3	3:D:858:LYS:HB3	0.65	1.67	1	1
1:C:547:TYR:HA	1:C:550:LYS:HB2	0.65	1.69	8	1
2:B:36:ILE:CD1	3:D:809:THR:HG21	0.65	2.21	7	4
1:A:369:GLU:O	1:A:373:GLN:CG	0.65	2.43	10	2
4:A:1:PCW:H41	5:A:35:17F:H1	0.65	1.67	4	1
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.65	1.69	6	3
4:A:1:PCW:H152	5:A:38:17F:H33	0.65	1.69	9	1
4:A:13:PCW:H122	5:A:37:17F:H37	0.65	1.69	2	1
1:A:308:ARG:HD3	1:C:469:LEU:CD2	0.64	2.21	4	1
5:A:38:17F:H1	5:A:38:17F:C4	0.64	2.22	1	1
4:A:12:PCW:H72	5:A:40:17F:N1	0.64	2.07	8	1
4:A:23:PCW:H73	5:A:34:17F:HN1A	0.64	1.52	1	1
4:A:31:PCW:H71	3:D:853:LEU:HG	0.64	1.67	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.64	1.69	3	2
2:B:82:PHE:HB2	2:B:89:SER:HB2	0.64	1.69	6	1
4:A:3:PCW:H322	4:A:3:PCW:H51	0.64	1.69	7	1
4:A:6:PCW:H152	4:A:24:PCW:H132	0.64	1.69	3	1
1:A:308:ARG:HG3	1:C:469:LEU:CD2	0.64	2.16	8	6
3:D:812:VAL:HG11	3:D:834:LEU:HD11	0.63	1.71	8	3
4:A:17:PCW:H81	5:A:38:17F:O1	0.63	1.93	3	2
4:A:43:PCW:H62	4:A:69:PCW:H11	0.63	1.71	1	1
1:C:465:GLU:O	1:C:469:LEU:HD12	0.63	1.92	7	2
4:A:60:PCW:H151	4:A:61:PCW:H442	0.63	1.70	9	1
4:A:42:PCW:H71	5:A:75:17F:HN1	0.63	1.53	2	1
2:B:25:GLN:NE2	3:D:840:VAL:HA	0.63	2.09	4	3
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.63	1.69	1	1
4:A:3:PCW:H11	4:A:18:PCW:H11	0.62	1.71	4	1
5:A:34:17F:H9	5:A:40:17F:H63	0.62	1.71	9	1
4:A:32:PCW:H61	5:A:38:17F:N1	0.62	2.09	3	1
4:A:62:PCW:H431	5:A:78:17F:H47	0.62	1.70	5	1
4:A:30:PCW:H352	4:A:30:PCW:H122	0.62	1.72	2	1
1:C:574:LEU:HB2	1:C:575:PRO:HD3	0.62	1.72	8	2
4:A:5:PCW:H73	3:D:853:LEU:HD22	0.62	1.71	6	1
4:A:71:PCW:H71	4:A:71:PCW:H19	0.62	1.72	1	1
4:A:54:PCW:H352	4:A:72:PCW:H11	0.61	1.71	10	1
4:A:9:PCW:H81	3:D:876:ILE:HG23	0.61	1.73	3	1
4:A:17:PCW:H12	2:B:70:GLN:HB2	0.61	1.72	8	1
2:B:103:VAL:HG23	2:B:104:LYS:HE2	0.61	1.72	8	1
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.61	1.72	7	2
5:A:34:17F:HN1A	3:D:858:LYS:H	0.61	1.35	3	1
4:A:27:PCW:H41	5:A:37:17F:O2	0.61	1.96	4	2
3:D:840:VAL:HG13	3:D:841:ARG:HG3	0.61	1.73	2	2
4:A:13:PCW:H31	4:A:14:PCW:H151	0.60	1.72	6	1
4:A:67:PCW:H83	5:A:78:17F:H37	0.60	1.71	4	1
4:A:30:PCW:H31	4:A:30:PCW:H52	0.60	1.73	2	1
4:A:20:PCW:H62	3:D:879:VAL:HB	0.60	1.73	10	1
1:A:301:LEU:HD22	1:C:473:LYS:HE2	0.60	1.72	5	1
4:A:21:PCW:H72	5:A:36:17F:H1	0.60	1.73	6	1
3:D:852:ARG:HD3	3:D:870:LEU:HD11	0.60	1.73	2	2
1:A:250:VAL:O	1:A:254:VAL:HB	0.60	1.97	6	8
2:B:40:TYR:CE2	3:D:840:VAL:HG22	0.60	2.31	7	5
2:B:35:THR:HG22	2:B:59:ALA:HA	0.60	1.73	8	1
4:A:14:PCW:H451	5:A:34:17F:H19A	0.60	1.74	10	1
3:D:813:TYR:HB2	3:D:876:ILE:HG12	0.60	1.72	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.60	1.73	3	10
4:A:50:PCW:H31	5:A:78:17F:H4	0.60	1.73	9	2
4:A:43:PCW:O1P	4:A:68:PCW:H83	0.60	1.97	3	1
1:A:352:LYS:HZ2	1:C:425:GLU:HB3	0.60	1.55	7	1
5:A:73:17F:H57	5:A:73:17F:H30	0.60	1.73	6	1
4:A:1:PCW:H181	5:A:35:17F:H18	0.59	1.73	10	1
2:B:32:TYR:HA	6:B:201:GNP:H5'1	0.59	1.73	8	3
5:A:40:17F:HN1	2:B:5:LYS:NZ	0.59	1.94	6	1
4:A:49:PCW:H32	4:A:57:PCW:H62	0.59	1.72	9	1
4:A:12:PCW:H42	5:A:37:17F:N1	0.59	2.12	2	1
4:A:49:PCW:H122	4:A:57:PCW:H361	0.59	1.71	5	1
4:A:30:PCW:H73	5:A:40:17F:N1	0.59	2.10	3	1
4:A:46:PCW:H182	4:A:46:PCW:H252	0.59	1.74	10	1
4:A:17:PCW:H41	4:A:17:PCW:H322	0.59	1.75	6	1
4:A:9:PCW:H132	4:A:26:PCW:H12	0.59	1.73	3	1
3:D:811:LYS:HB3	3:D:821:VAL:HG22	0.59	1.73	1	1
1:C:503:MET:HA	1:C:506:ARG:HD2	0.59	1.74	5	5
2:B:73:ARG:HD3	2:B:103:VAL:HB	0.59	1.75	6	1
4:A:67:PCW:H61	5:A:78:17F:H8	0.59	1.74	3	1
4:A:59:PCW:H342	5:A:77:17F:H9A	0.59	1.74	3	1
4:A:57:PCW:O31	4:A:57:PCW:H41	0.59	1.98	9	1
4:A:46:PCW:H11	4:A:71:PCW:H381	0.59	1.73	2	1
1:C:561:LYS:HA	1:C:565:ALA:HB3	0.58	1.74	2	1
1:A:242:GLU:HB3	1:C:532:ARG:HH21	0.58	1.58	6	2
4:A:12:PCW:H11	4:A:30:PCW:H121	0.58	1.74	3	1
4:A:3:PCW:H332	4:A:23:PCW:H31	0.58	1.76	8	1
5:A:75:17F:H4	5:A:75:17F:HN1	0.58	1.57	1	1
4:A:12:PCW:H152	4:A:22:PCW:H352	0.58	1.75	10	1
4:A:60:PCW:H381	4:A:62:PCW:H152	0.58	1.74	5	1
4:A:10:PCW:H83	5:A:36:17F:HN1A	0.58	1.58	6	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.58	1.75	9	3
4:A:67:PCW:H141	5:A:75:17F:H60	0.58	1.74	10	1
4:A:11:PCW:H322	4:A:28:PCW:H62	0.58	1.74	9	1
1:C:491:GLU:HB3	1:C:495:LYS:HE2	0.58	1.76	4	5
4:A:10:PCW:H62	3:D:876:ILE:HG23	0.58	1.76	7	1
4:A:3:PCW:H61	4:A:19:PCW:H2	0.58	1.76	6	1
1:A:264:LYS:HE3	1:C:509:ALA:HB1	0.58	1.73	2	2
4:A:1:PCW:H122	5:A:35:17F:H20	0.57	1.76	8	1
1:A:334:ARG:HD2	1:C:440:GLU:OE1	0.57	1.99	8	6
1:A:330:ARG:O	1:A:334:ARG:HG2	0.57	1.98	7	5
4:A:2:PCW:H341	4:A:5:PCW:H152	0.57	1.76	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:451:LYS:O	1:C:455:TYR:HB2	0.57	1.99	3	6
1:A:288:ARG:O	1:A:292:HIS:HB2	0.57	1.98	6	3
4:A:42:PCW:H39	4:A:69:PCW:H451	0.57	1.76	5	1
3:D:815:PRO:HD3	3:D:877:VAL:HB	0.57	1.76	5	2
3:D:814:LEU:HD13	3:D:841:ARG:HD2	0.57	1.74	6	3
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.57	1.77	6	2
4:A:26:PCW:H321	5:A:40:17F:H19	0.57	1.76	4	1
1:C:491:GLU:HG2	1:C:495:LYS:HE3	0.57	1.75	8	1
4:A:18:PCW:H232	4:A:49:PCW:H442	0.57	1.75	8	1
4:A:59:PCW:H40	4:A:61:PCW:H161	0.57	1.77	8	1
2:B:68:ARG:HA	2:B:71:TYR:CE2	0.57	2.34	6	8
1:A:308:ARG:HD3	1:C:469:LEU:CG	0.57	2.30	4	1
4:A:71:PCW:H181	4:A:71:PCW:H132	0.57	1.75	4	1
4:A:24:PCW:H39	3:D:857:ARG:HH12	0.56	1.60	9	1
4:A:4:PCW:H332	4:A:7:PCW:H31	0.56	1.75	4	1
5:A:36:17F:H18A	5:A:40:17F:H36	0.56	1.77	1	1
4:A:53:PCW:H361	4:A:64:PCW:H122	0.56	1.77	8	1
2:B:47:ASP:HB2	2:B:164:ARG:HH22	0.56	1.59	8	1
4:A:59:PCW:H121	5:A:77:17F:H11	0.56	1.76	7	1
1:A:352:LYS:NZ	1:C:425:GLU:HB2	0.56	2.15	8	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.56	2.00	7	6
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.56	1.77	9	1
4:A:6:PCW:H2	4:A:11:PCW:H322	0.56	1.76	3	1
4:A:44:PCW:H371	4:A:69:PCW:H431	0.56	1.77	8	1
5:A:74:17F:N1	5:A:74:17F:H4	0.56	2.11	4	1
5:A:38:17F:H1A	2:B:43:GLN:NE2	0.56	2.15	5	1
4:A:7:PCW:H122	4:A:16:PCW:H32	0.56	1.76	7	1
4:A:5:PCW:H122	5:A:38:17F:H18A	0.56	1.78	4	1
4:A:19:PCW:H241	4:A:19:PCW:H161	0.56	1.76	8	1
3:D:809:THR:HG22	3:D:823:THR:HA	0.56	1.77	7	1
4:A:43:PCW:O2P	4:A:45:PCW:H61	0.56	2.01	3	1
1:A:345:ARG:HA	1:C:429:ASN:HD21	0.56	1.61	8	2
4:A:3:PCW:H321	4:A:18:PCW:H322	0.56	1.78	5	1
4:A:20:PCW:H32	4:A:24:PCW:H331	0.55	1.76	10	1
4:A:10:PCW:H142	4:A:10:PCW:H381	0.55	1.76	8	1
2:B:46:ILE:HD11	2:B:53:LEU:HD11	0.55	1.78	3	1
3:D:852:ARG:HD2	3:D:873:GLU:OE1	0.55	2.01	8	1
4:A:9:PCW:H81	4:A:30:PCW:O2P	0.55	2.01	5	1
1:C:444:ASP:O	1:C:448:VAL:HB	0.55	2.02	8	2
1:C:508:ARG:O	1:C:512:ASP:HB2	0.55	2.01	2	3
1:C:528:ARG:HB3	1:C:532:ARG:NH2	0.55	2.16	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:101:LYS:HE2	2:B:107:GLU:HG3	0.55	1.79	10	1
2:B:41:ARG:NH1	3:D:817:LYS:HB2	0.55	2.16	7	3
4:A:19:PCW:H2	4:A:23:PCW:H11	0.55	1.77	3	1
3:D:851:TYR:HE1	3:D:878:GLU:HB3	0.55	1.62	5	1
3:D:838:LEU:HD12	3:D:845:GLN:HG3	0.55	1.78	1	2
4:A:66:PCW:H452	5:A:79:17F:H59	0.55	1.78	10	1
4:A:44:PCW:H41	4:A:44:PCW:H2	0.55	1.78	6	1
4:A:8:PCW:H321	4:A:22:PCW:H331	0.54	1.79	10	1
2:B:144:THR:HA	2:B:150:GLN:O	0.54	2.02	7	3
4:A:1:PCW:H82	5:A:35:17F:HN1A	0.54	1.61	6	1
1:C:544:LEU:O	1:C:548:HIS:HB2	0.54	2.03	8	1
4:A:48:PCW:H321	4:A:54:PCW:H131	0.54	1.78	5	1
2:B:158:THR:HA	2:B:161:ARG:HD2	0.54	1.78	6	1
1:A:308:ARG:CB	1:C:469:LEU:CD1	0.54	2.84	1	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.54	1.63	8	2
1:C:473:LYS:O	1:C:477:LEU:HB2	0.54	2.03	7	2
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.54	2.37	7	2
1:C:458:ASP:HA	1:C:461:LYS:HE3	0.54	1.78	7	1
4:A:67:PCW:H41	5:A:78:17F:H30	0.54	1.78	2	1
4:A:20:PCW:H332	4:A:20:PCW:H131	0.54	1.80	6	1
4:A:20:PCW:H361	4:A:20:PCW:H122	0.54	1.78	7	1
4:A:55:PCW:H63	4:A:64:PCW:H11	0.54	1.78	4	1
4:A:53:PCW:H212	4:A:64:PCW:H151	0.54	1.80	2	1
4:A:9:PCW:H71	3:D:876:ILE:CG2	0.54	2.33	3	1
4:A:42:PCW:H162	4:A:52:PCW:H141	0.54	1.80	8	1
4:A:30:PCW:H71	5:A:37:17F:O4	0.54	2.03	7	1
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.54	1.79	3	2
4:A:32:PCW:H371	5:A:38:17F:H32	0.54	1.78	6	1
4:A:67:PCW:H371	4:A:67:PCW:H142	0.54	1.80	9	1
5:A:40:17F:HN1A	2:B:5:LYS:NZ	0.54	2.00	7	1
1:A:352:LYS:NZ	1:C:425:GLU:HB3	0.54	2.17	7	1
5:A:40:17F:H46	4:A:51:PCW:H432	0.54	1.80	4	1
1:C:478:ARG:O	1:C:482:GLN:HB2	0.54	2.02	7	2
2:B:41:ARG:HB3	3:D:816:ASN:ND2	0.54	2.18	4	1
1:C:469:LEU:O	1:C:473:LYS:HB2	0.53	2.03	5	1
4:A:13:PCW:H422	4:A:27:PCW:H371	0.53	1.80	6	1
2:B:73:ARG:HG2	2:B:103:VAL:HB	0.53	1.78	7	1
4:A:5:PCW:H431	4:A:17:PCW:H352	0.53	1.80	3	1
3:D:870:LEU:HD12	3:D:873:GLU:HG2	0.53	1.80	3	1
4:A:12:PCW:H41	3:D:855:LYS:HB2	0.53	1.79	1	1
4:A:30:PCW:H83	5:A:34:17F:O2	0.53	2.03	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:495:LYS:O	1:C:499:LEU:HB2	0.53	2.04	9	5
4:A:48:PCW:H81	4:A:58:PCW:O2P	0.53	2.03	5	1
4:A:67:PCW:H341	4:A:72:PCW:H20	0.53	1.80	9	1
4:A:16:PCW:H451	5:A:39:17F:H60	0.53	1.78	2	1
1:C:546:GLU:O	1:C:550:LYS:HD2	0.53	2.03	1	2
1:A:244:SER:O	1:A:248:GLU:HB2	0.53	2.03	5	1
4:A:42:PCW:H19	4:A:52:PCW:H121	0.53	1.80	2	1
4:A:19:PCW:H63	4:A:23:PCW:H2	0.53	1.79	3	1
1:A:308:ARG:HG3	1:C:469:LEU:HD13	0.53	1.76	1	1
4:A:51:PCW:H361	4:A:70:PCW:H341	0.53	1.79	10	1
4:A:16:PCW:H152	5:A:39:17F:H19	0.53	1.80	9	1
4:A:12:PCW:H342	4:A:30:PCW:H121	0.53	1.81	4	1
1:A:332:ALA:O	1:A:336:GLU:HB2	0.53	2.03	10	1
5:A:33:17F:O2	3:D:817:LYS:HA	0.53	2.03	5	1
4:A:8:PCW:H51	3:D:879:VAL:O	0.53	2.04	7	1
4:A:29:PCW:H62	3:D:880:LEU:HB2	0.53	1.78	3	1
3:D:811:LYS:HE3	3:D:819:ARG:HG3	0.53	1.79	5	1
4:A:53:PCW:H61	4:A:68:PCW:O2P	0.53	2.04	9	1
4:A:62:PCW:H31	4:A:72:PCW:H2	0.53	1.80	9	1
4:A:30:PCW:H73	2:B:3:GLU:HB2	0.53	1.80	7	1
4:A:12:PCW:H352	5:A:36:17F:H5	0.53	1.81	4	1
5:A:79:17F:H4	5:A:79:17F:H1	0.53	1.81	1	1
4:A:42:PCW:O1P	4:A:42:PCW:H2	0.53	2.04	7	1
4:A:12:PCW:H142	4:A:22:PCW:H361	0.53	1.80	4	1
4:A:17:PCW:H39	5:A:38:17F:H18	0.53	1.81	2	1
4:A:14:PCW:H131	4:A:23:PCW:H151	0.53	1.80	3	1
4:A:12:PCW:H62	3:D:854:ILE:HB	0.53	1.79	1	1
5:A:34:17F:H29	5:A:40:17F:H66	0.53	1.79	10	1
4:A:6:PCW:O1P	4:A:7:PCW:H83	0.53	2.04	5	1
4:A:13:PCW:H72	3:D:854:ILE:HB	0.53	1.80	3	1
4:A:42:PCW:H40	4:A:52:PCW:H482	0.52	1.81	10	1
4:A:44:PCW:H121	5:A:77:17F:H6	0.52	1.80	5	1
3:D:852:ARG:HD2	3:D:870:LEU:HD11	0.52	1.82	5	1
2:B:46:ILE:HD13	2:B:160:VAL:HG11	0.52	1.81	9	1
4:A:5:PCW:H63	5:A:38:17F:H4A	0.52	1.81	4	1
4:A:1:PCW:C6	5:A:35:17F:HN1A	0.52	2.17	3	1
4:A:26:PCW:H441	5:A:33:17F:H44	0.52	1.80	6	1
1:C:514:LEU:HA	1:C:517:HIS:HB2	0.52	1.81	4	1
4:A:44:PCW:H12	4:A:69:PCW:H83	0.52	1.80	6	1
3:D:851:TYR:HB2	3:D:876:ILE:HG13	0.52	1.81	9	1
4:A:11:PCW:O31	4:A:26:PCW:H71	0.52	2.05	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:465:GLU:HB3	1:C:469:LEU:HD11	0.52	1.80	7	2
4:A:12:PCW:H63	5:A:37:17F:N1	0.52	2.18	2	1
4:A:16:PCW:H352	5:A:39:17F:H8A	0.52	1.82	3	1
4:A:15:PCW:H63	5:A:39:17F:O1	0.52	2.04	3	1
1:C:417:GLU:O	1:C:421:PRO:HD2	0.52	2.05	9	3
5:A:37:17F:O1	3:D:855:LYS:HD2	0.52	2.05	3	1
4:A:42:PCW:H19	4:A:52:PCW:H322	0.52	1.81	10	1
3:D:858:LYS:HE2	3:D:876:ILE:HD13	0.52	1.80	5	3
4:A:13:PCW:H181	4:A:18:PCW:H162	0.52	1.81	9	1
4:A:9:PCW:H2	4:A:11:PCW:H32	0.52	1.81	7	1
4:A:13:PCW:H71	5:A:34:17F:O1	0.52	2.05	4	2
4:A:64:PCW:H352	4:A:64:PCW:H162	0.52	1.80	2	1
4:A:13:PCW:O1P	4:A:18:PCW:H82	0.52	2.05	3	1
4:A:70:PCW:H63	4:A:70:PCW:H19	0.52	1.82	5	1
4:A:3:PCW:H321	4:A:18:PCW:O1P	0.52	2.05	7	1
5:A:33:17F:HN1	5:A:33:17F:P1	0.52	2.28	1	1
4:A:49:PCW:H122	4:A:57:PCW:H352	0.52	1.82	1	1
4:A:6:PCW:P	4:A:11:PCW:O2P	0.52	2.68	6	1
4:A:10:PCW:H331	4:A:21:PCW:H322	0.52	1.82	6	1
2:B:3:GLU:HG2	2:B:52:LEU:HB2	0.52	1.82	6	1
1:A:310:ARG:O	1:A:314:ASP:HB2	0.52	2.05	4	2
4:A:54:PCW:H352	4:A:72:PCW:H122	0.52	1.81	4	1
4:A:7:PCW:O11	4:A:16:PCW:H73	0.52	2.05	1	1
4:A:10:PCW:H61	5:A:36:17F:H2	0.51	1.82	10	1
4:A:62:PCW:H361	4:A:72:PCW:H322	0.51	1.81	5	1
4:A:46:PCW:H61	5:A:73:17F:O1	0.51	2.05	9	1
4:A:27:PCW:H73	2:B:70:GLN:HB2	0.51	1.82	2	1
1:C:489:LEU:O	1:C:493:GLN:HB2	0.51	2.06	2	1
1:C:525:LEU:HD23	1:C:528:ARG:HD2	0.51	1.83	5	1
4:A:42:PCW:H81	4:A:63:PCW:O2P	0.51	2.06	8	1
1:A:388:SER:HB3	1:C:594:LYS:HE2	0.51	1.81	5	1
4:A:25:PCW:H421	4:A:29:PCW:H141	0.51	1.81	1	1
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.51	1.66	2	4
4:A:66:PCW:H451	5:A:79:17F:H37	0.51	1.81	10	1
3:D:831:TYR:HB2	3:D:863:TRP:HB3	0.51	1.81	9	5
4:A:6:PCW:O2P	4:A:28:PCW:H81	0.51	2.06	7	1
4:A:56:PCW:H131	4:A:56:PCW:H331	0.51	1.81	8	2
4:A:62:PCW:H122	4:A:72:PCW:H152	0.51	1.82	8	1
4:A:70:PCW:O31	4:A:70:PCW:H41	0.51	2.04	6	1
4:A:22:PCW:H52	4:A:22:PCW:H2	0.51	1.83	3	1
5:A:40:17F:N1	3:D:855:LYS:HA	0.51	2.20	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:352:LYS:HZ1	1:C:425:GLU:HB2	0.51	1.63	8	1
1:A:341:ASN:ND2	1:C:433:GLU:HA	0.51	2.17	6	1
4:A:41:PCW:H351	4:A:52:PCW:H39	0.51	1.82	7	1
3:D:809:THR:HB	3:D:821:VAL:HG12	0.51	1.83	7	1
4:A:1:PCW:H342	4:A:26:PCW:H351	0.51	1.81	1	1
4:A:70:PCW:H2	4:A:70:PCW:H51	0.51	1.83	1	1
1:A:314:ASP:HA	1:A:317:ARG:HD2	0.51	1.82	9	3
4:A:65:PCW:H142	5:A:80:17F:H18A	0.51	1.83	5	1
4:A:62:PCW:H351	4:A:72:PCW:H332	0.51	1.83	8	1
4:A:17:PCW:O2P	3:D:876:ILE:HD11	0.51	2.06	6	1
4:A:43:PCW:H221	4:A:51:PCW:H462	0.51	1.83	3	1
4:A:4:PCW:H71	2:B:167:LYS:HB3	0.51	1.82	3	1
4:A:67:PCW:H352	4:A:72:PCW:H241	0.51	1.82	3	1
4:A:13:PCW:H73	5:A:34:17F:N1	0.51	2.21	8	1
2:B:79:LEU:HD23	2:B:112:VAL:HB	0.51	1.82	9	3
1:C:447:GLU:O	1:C:451:LYS:HB2	0.51	2.06	6	2
3:D:853:LEU:HD21	3:D:858:LYS:HE3	0.50	1.84	6	1
4:A:24:PCW:H41	4:A:24:PCW:H322	0.50	1.83	10	1
4:A:3:PCW:H212	4:A:19:PCW:H181	0.50	1.82	8	1
4:A:17:PCW:H132	4:A:17:PCW:H62	0.50	1.82	5	1
1:A:279:LEU:HB3	1:C:495:LYS:HE3	0.50	1.83	9	1
2:B:45:VAL:HG22	2:B:50:THR:HB	0.50	1.84	7	1
4:A:30:PCW:H361	5:A:40:17F:H61	0.50	1.83	2	1
1:C:414:LYS:HA	1:C:417:GLU:HG3	0.50	1.82	2	1
4:A:51:PCW:H442	4:A:70:PCW:H442	0.50	1.82	1	1
4:A:13:PCW:H31	5:A:37:17F:H10	0.50	1.82	9	1
5:A:75:17F:H4	5:A:75:17F:N1	0.50	2.20	1	1
1:C:491:GLU:O	1:C:495:LYS:HG3	0.50	2.06	6	5
4:A:5:PCW:H12	4:A:17:PCW:H321	0.50	1.82	6	3
1:A:239:LEU:O	1:A:243:MET:HB2	0.50	2.06	6	1
4:A:16:PCW:H63	2:B:3:GLU:HB2	0.50	1.83	4	1
4:A:44:PCW:H82	4:A:44:PCW:H11	0.50	1.84	8	1
2:B:32:TYR:O	2:B:34:PRO:HD3	0.50	2.07	9	1
1:A:276:VAL:O	1:A:280:ARG:HB2	0.50	2.07	9	2
3:D:835:ASP:O	3:D:839:LYS:HG2	0.50	2.05	7	2
4:A:25:PCW:H122	4:A:31:PCW:H12	0.50	1.84	2	1
4:A:4:PCW:H332	4:A:7:PCW:H132	0.50	1.84	9	1
5:A:37:17F:HN1	3:D:817:LYS:HZ2	0.50	1.49	7	1
2:B:41:ARG:HH11	2:B:52:LEU:HD21	0.50	1.65	1	1
1:A:279:LEU:HD22	1:C:495:LYS:HE2	0.50	1.83	8	1
4:A:14:PCW:H141	5:A:34:17F:H19	0.50	1.83	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:42:PCW:H82	4:A:42:PCW:O11	0.50	2.06	10	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.50	2.06	6	1
4:A:5:PCW:H39	4:A:17:PCW:H83	0.50	1.82	9	1
1:A:365:LYS:O	1:A:369:GLU:HB2	0.50	2.07	3	1
1:A:301:LEU:HB3	1:C:473:LYS:HE2	0.49	1.84	10	1
4:A:5:PCW:H382	5:A:38:17F:H18	0.49	1.83	10	1
4:A:12:PCW:H11	4:A:30:PCW:H132	0.49	1.83	4	1
3:D:851:TYR:CD2	3:D:858:LYS:HB3	0.49	2.42	4	1
4:A:43:PCW:O1P	4:A:68:PCW:H42	0.49	2.07	1	1
4:A:47:PCW:H122	4:A:49:PCW:H181	0.49	1.82	7	1
1:A:363:LYS:HD3	1:C:411:THR:HG23	0.49	1.84	2	2
4:A:16:PCW:H362	5:A:39:17F:H10A	0.49	1.83	1	1
4:A:18:PCW:H171	5:A:37:17F:H12	0.49	1.84	1	1
3:D:824:VAL:HG11	3:D:871:ASP:HB2	0.49	1.84	10	2
2:B:45:VAL:HA	2:B:50:THR:HA	0.49	1.83	7	1
4:A:10:PCW:H83	5:A:36:17F:HN1	0.49	1.66	4	1
1:A:275:LYS:O	1:A:279:LEU:HB2	0.49	2.07	2	1
2:B:41:ARG:HB3	3:D:816:ASN:OD1	0.49	2.08	2	1
4:A:43:PCW:H31	4:A:69:PCW:H12	0.49	1.85	8	1
4:A:9:PCW:H332	4:A:14:PCW:H341	0.49	1.83	10	1
1:A:308:ARG:HD2	1:C:465:GLU:OE1	0.49	2.08	5	1
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.49	2.38	9	3
4:A:61:PCW:O31	4:A:61:PCW:H41	0.49	2.06	6	1
4:A:58:PCW:H12	4:A:61:PCW:H431	0.49	1.85	9	1
4:A:44:PCW:H62	5:A:77:17F:N1	0.49	2.22	4	1
4:A:24:PCW:H42	4:A:25:PCW:H131	0.49	1.84	10	1
4:A:2:PCW:H331	4:A:17:PCW:H421	0.49	1.83	5	1
4:A:42:PCW:O2P	4:A:43:PCW:H81	0.49	2.08	2	1
4:A:41:PCW:H322	4:A:52:PCW:H372	0.49	1.85	6	1
1:A:268:GLU:O	1:A:272:TYR:HB2	0.49	2.08	9	3
1:A:297:LYS:O	1:A:301:LEU:HB2	0.49	2.08	8	2
3:D:838:LEU:HD21	3:D:877:VAL:HG11	0.49	1.85	8	2
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.49	1.85	10	1
1:C:479:ALA:O	1:C:483:GLU:HG2	0.49	2.08	9	1
4:A:13:PCW:H82	3:D:857:ARG:HB2	0.49	1.83	3	1
4:A:26:PCW:H11	4:A:28:PCW:O2P	0.49	2.08	10	1
4:A:68:PCW:H39	4:A:68:PCW:H141	0.49	1.85	9	1
4:A:1:PCW:H352	5:A:35:17F:H32	0.49	1.85	2	1
4:A:43:PCW:H372	4:A:43:PCW:H122	0.49	1.83	8	1
4:A:15:PCW:H71	5:A:39:17F:O2	0.49	2.08	7	1
4:A:8:PCW:H63	3:D:880:LEU:OXT	0.48	2.08	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:489:LEU:O	1:C:493:GLN:HG3	0.48	2.07	6	1
4:A:20:PCW:O2P	3:D:857:ARG:HG2	0.48	2.08	9	1
4:A:3:PCW:H82	4:A:3:PCW:H331	0.48	1.85	7	1
4:A:48:PCW:H332	4:A:54:PCW:H181	0.48	1.84	8	1
4:A:16:PCW:H341	4:A:28:PCW:H19	0.48	1.84	9	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.48	2.08	8	2
1:C:517:HIS:O	1:C:521:TYR:HB2	0.48	2.07	4	3
4:A:49:PCW:H322	4:A:57:PCW:H352	0.48	1.85	5	1
1:C:574:LEU:O	1:C:578:GLU:HG3	0.48	2.07	5	1
4:A:19:PCW:H321	4:A:23:PCW:H361	0.48	1.85	6	1
4:A:16:PCW:H61	5:A:39:17F:HN1	0.48	1.68	9	1
1:A:291:LEU:O	1:A:295:GLN:HG3	0.48	2.07	3	1
4:A:62:PCW:H472	4:A:72:PCW:H151	0.48	1.83	3	1
4:A:46:PCW:H321	4:A:71:PCW:H372	0.48	1.85	6	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.48	2.39	9	5
4:A:26:PCW:H472	4:A:68:PCW:H261	0.48	1.84	9	1
4:A:46:PCW:H71	5:A:73:17F:O1	0.48	2.08	9	1
4:A:49:PCW:O1P	4:A:57:PCW:H61	0.48	2.08	2	1
4:A:5:PCW:H73	5:A:38:17F:H4A	0.48	1.84	3	1
4:A:58:PCW:H121	4:A:61:PCW:H382	0.48	1.86	3	1
4:A:6:PCW:H121	4:A:16:PCW:H371	0.48	1.85	1	1
4:A:44:PCW:O31	4:A:55:PCW:H62	0.48	2.08	1	1
3:D:852:ARG:O	3:D:858:LYS:HA	0.48	2.08	1	1
2:B:22:GLN:HG3	2:B:149:ARG:HG3	0.48	1.85	5	2
4:A:11:PCW:H321	4:A:28:PCW:H2	0.48	1.83	9	1
4:A:2:PCW:H321	4:A:17:PCW:H351	0.48	1.85	7	1
4:A:52:PCW:H152	4:A:60:PCW:H331	0.48	1.86	1	1
4:A:13:PCW:H332	4:A:18:PCW:H142	0.48	1.86	8	1
4:A:59:PCW:H39	4:A:61:PCW:H132	0.48	1.85	8	1
4:A:64:PCW:H162	4:A:64:PCW:H352	0.48	1.86	10	1
5:A:38:17F:H1A	2:B:43:GLN:HE22	0.48	1.67	5	1
4:A:11:PCW:H351	4:A:28:PCW:H40	0.48	1.84	6	1
4:A:13:PCW:H73	5:A:37:17F:N1	0.48	2.23	4	1
4:A:1:PCW:H61	4:A:28:PCW:O2P	0.48	2.09	4	1
4:A:45:PCW:H152	5:A:74:17F:H19	0.48	1.84	3	1
4:A:25:PCW:H42	3:D:879:VAL:O	0.48	2.07	3	1
4:A:71:PCW:H321	4:A:71:PCW:H19	0.48	1.86	8	1
4:A:59:PCW:H231	5:A:77:17F:H44	0.48	1.86	5	1
4:A:26:PCW:H19	5:A:40:17F:H72	0.48	1.85	2	1
4:A:11:PCW:H442	4:A:63:PCW:H241	0.48	1.84	5	1
4:A:49:PCW:O11	4:A:57:PCW:H73	0.48	2.08	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:9:PCW:H73	4:A:14:PCW:O31	0.48	2.09	1	1
4:A:7:PCW:H52	4:A:16:PCW:O2P	0.48	2.09	1	1
5:A:40:17F:HN1	3:D:855:LYS:HA	0.48	1.68	1	1
4:A:45:PCW:H371	4:A:49:PCW:H32	0.48	1.85	5	1
4:A:13:PCW:H382	4:A:18:PCW:H141	0.48	1.86	9	1
4:A:60:PCW:H483	4:A:63:PCW:H462	0.48	1.86	9	1
4:A:60:PCW:H461	4:A:63:PCW:H40	0.48	1.85	7	1
4:A:49:PCW:O1P	4:A:57:PCW:H71	0.48	2.09	2	1
4:A:44:PCW:H481	4:A:55:PCW:H212	0.48	1.85	1	1
2:B:40:TYR:CE2	3:D:840:VAL:CG2	0.48	2.97	6	4
1:C:429:ASN:HA	1:C:432:LYS:HD2	0.48	1.86	6	2
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.48	1.86	7	2
5:A:79:17F:C4	5:A:79:17F:H1	0.48	2.38	1	1
3:D:850:VAL:HG12	3:D:877:VAL:HG22	0.47	1.86	8	1
4:A:41:PCW:H71	4:A:59:PCW:O1P	0.47	2.09	10	1
4:A:30:PCW:H41	5:A:34:17F:O2	0.47	2.09	5	1
5:A:33:17F:H11A	5:A:35:17F:H11A	0.47	1.86	9	1
4:A:66:PCW:H451	5:A:79:17F:H29	0.47	1.86	9	1
1:A:336:GLU:HA	1:A:339:LYS:HE3	0.47	1.85	4	1
4:A:12:PCW:H131	4:A:22:PCW:H122	0.47	1.85	1	1
4:A:12:PCW:H471	4:A:70:PCW:H471	0.47	1.85	1	1
5:A:74:17F:H12	5:A:79:17F:H44	0.47	1.86	10	1
4:A:56:PCW:O1P	4:A:70:PCW:H41	0.47	2.09	3	2
1:C:559:SER:HB2	1:C:563:LYS:HE2	0.47	1.85	6	1
4:A:50:PCW:H61	4:A:67:PCW:O2P	0.47	2.09	9	1
1:A:359:THR:HA	1:A:362:GLU:OE1	0.47	2.08	7	1
3:D:837:ALA:O	3:D:840:VAL:HG12	0.47	2.10	4	1
1:C:466:GLU:OE1	1:C:469:LEU:CD1	0.47	2.58	10	1
1:A:363:LYS:O	1:A:367:ALA:HB3	0.47	2.10	7	3
3:D:810:VAL:HG23	3:D:824:VAL:HG22	0.47	1.86	4	2
4:A:45:PCW:H261	5:A:79:17F:H49	0.47	1.85	6	1
1:A:242:GLU:HB3	1:C:532:ARG:NH2	0.47	2.24	1	1
4:A:41:PCW:H412	4:A:59:PCW:H421	0.47	1.85	1	1
4:A:23:PCW:H441	4:A:29:PCW:H371	0.47	1.87	8	1
1:C:440:GLU:O	1:C:444:ASP:HB2	0.47	2.10	10	1
4:A:3:PCW:H32	3:D:876:ILE:HG21	0.47	1.86	2	1
1:C:430:LEU:HA	1:C:433:GLU:HB2	0.47	1.86	10	1
4:A:63:PCW:H212	4:A:63:PCW:H481	0.47	1.85	5	1
3:D:841:ARG:HH11	3:D:841:ARG:HB3	0.47	1.68	6	1
4:A:11:PCW:H431	4:A:28:PCW:H231	0.47	1.86	7	1
4:A:13:PCW:H42	5:A:34:17F:H2	0.47	1.87	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:23:PCW:H172	4:A:23:PCW:H341	0.47	1.84	8	1
5:A:74:17F:H65	5:A:75:17F:H63	0.47	1.85	10	1
3:D:851:TYR:HD2	3:D:858:LYS:HB3	0.47	1.67	4	1
4:A:30:PCW:H461	4:A:30:PCW:H251	0.47	1.85	2	1
4:A:54:PCW:H321	4:A:72:PCW:H32	0.47	1.87	10	1
4:A:58:PCW:H151	4:A:61:PCW:H472	0.47	1.87	5	1
4:A:21:PCW:H152	4:A:51:PCW:H272	0.47	1.87	9	1
3:D:834:LEU:HG	3:D:850:VAL:HG21	0.47	1.85	4	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.47	1.86	4	1
4:A:66:PCW:H20	4:A:67:PCW:H62	0.47	1.86	4	1
1:A:308:ARG:CG	1:C:469:LEU:CD2	0.47	2.91	1	1
4:A:13:PCW:H141	4:A:18:PCW:H171	0.47	1.86	8	1
1:C:563:LYS:HB2	1:C:564:PRO:CD	0.47	2.39	1	4
4:A:71:PCW:H19	4:A:71:PCW:H81	0.47	1.85	9	1
4:A:6:PCW:H381	4:A:16:PCW:H11	0.47	1.87	7	1
1:C:561:LYS:O	1:C:565:ALA:HB3	0.47	2.10	3	2
4:A:8:PCW:H152	4:A:10:PCW:H141	0.47	1.86	8	1
1:C:549:ALA:O	1:C:553:GLU:HG3	0.47	2.09	8	2
2:B:22:GLN:CG	2:B:149:ARG:HG3	0.47	2.40	5	1
4:A:14:PCW:H382	5:A:34:17F:H8	0.47	1.87	3	1
4:A:66:PCW:H20	4:A:67:PCW:H321	0.47	1.86	8	1
4:A:3:PCW:H362	4:A:18:PCW:H321	0.47	1.86	10	1
1:A:272:TYR:HD2	1:C:506:ARG:HH22	0.47	1.53	10	1
2:B:101:LYS:HE3	2:B:107:GLU:HG2	0.47	1.86	7	1
1:A:376:LEU:HB2	1:A:377:PRO:CD	0.47	2.40	2	3
4:A:42:PCW:H81	4:A:63:PCW:O3P	0.47	2.10	3	1
1:A:392:GLU:HA	1:A:395:LYS:HG2	0.47	1.87	1	1
1:A:352:LYS:HZ2	1:C:425:GLU:CB	0.46	2.23	7	1
4:A:23:PCW:O2P	2:B:73:ARG:HD2	0.46	2.10	10	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.46	2.38	5	5
4:A:67:PCW:H39	5:A:74:17F:H66	0.46	1.87	6	1
2:B:32:TYR:CD2	6:B:201:GNP:H5'1	0.46	2.45	6	1
4:A:28:PCW:H461	4:A:63:PCW:H482	0.46	1.88	2	1
4:A:25:PCW:H61	4:A:29:PCW:O2P	0.46	2.10	3	1
4:A:53:PCW:H421	4:A:64:PCW:H481	0.46	1.88	5	1
5:A:34:17F:HN1A	5:A:37:17F:H2	0.46	1.70	4	1
4:A:13:PCW:H73	5:A:34:17F:HN1	0.46	1.69	8	1
2:B:97:ARG:NH1	2:B:137:TYR:HB3	0.46	2.26	8	1
4:A:64:PCW:H431	4:A:64:PCW:H141	0.46	1.85	4	1
4:A:44:PCW:H62	5:A:77:17F:HN1A	0.46	1.70	2	1
2:B:126:ASP:HB3	2:B:129:GLN:HG3	0.46	1.87	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:45:PCW:H39	4:A:57:PCW:H71	0.46	1.87	8	1
1:A:315:ALA:O	1:A:319:HIS:HB2	0.46	2.11	6	1
4:A:13:PCW:H283	4:A:18:PCW:H352	0.46	1.86	4	1
4:A:22:PCW:H73	4:A:22:PCW:O31	0.46	2.11	3	1
4:A:48:PCW:H442	4:A:54:PCW:H172	0.46	1.87	1	1
4:A:43:PCW:H452	4:A:43:PCW:H121	0.46	1.88	8	1
4:A:12:PCW:H61	5:A:37:17F:HN1A	0.46	1.69	10	1
2:B:84:ILE:HD12	2:B:123:ARG:HG3	0.46	1.88	10	2
1:A:351:ALA:O	1:A:355:GLU:HG2	0.46	2.10	6	1
4:A:31:PCW:H352	4:A:31:PCW:H172	0.46	1.87	9	1
1:C:586:SER:O	1:C:590:GLU:HG3	0.46	2.10	1	2
4:A:10:PCW:H41	3:D:876:ILE:CD1	0.46	2.41	7	1
1:A:372:ARG:O	1:A:376:LEU:HG	0.46	2.10	7	1
2:B:41:ARG:HH12	3:D:817:LYS:HB2	0.46	1.71	7	1
4:A:22:PCW:H52	4:A:22:PCW:O31	0.46	2.11	4	1
4:A:13:PCW:H83	3:D:854:ILE:HB	0.46	1.87	3	1
4:A:6:PCW:H331	4:A:28:PCW:H81	0.46	1.86	1	1
1:C:466:GLU:HA	1:C:469:LEU:HD12	0.46	1.87	6	1
4:A:72:PCW:H221	5:A:78:17F:H50	0.46	1.87	4	1
4:A:3:PCW:O2P	4:A:23:PCW:H63	0.46	2.11	3	1
4:A:30:PCW:H72	2:B:3:GLU:OE2	0.46	2.10	8	1
4:A:22:PCW:H2	4:A:22:PCW:O4P	0.46	2.11	10	1
1:A:346:LEU:O	1:A:350:HIS:HB2	0.46	2.11	10	1
4:A:21:PCW:H221	4:A:51:PCW:H271	0.46	1.87	5	1
4:A:28:PCW:H412	4:A:28:PCW:H172	0.46	1.88	6	1
4:A:13:PCW:H12	5:A:37:17F:H8A	0.46	1.87	9	1
4:A:60:PCW:H131	4:A:61:PCW:H421	0.46	1.88	9	1
4:A:6:PCW:H332	4:A:16:PCW:H12	0.46	1.88	7	1
4:A:30:PCW:H42	5:A:34:17F:O2	0.46	2.10	7	1
4:A:6:PCW:O1P	4:A:28:PCW:H321	0.46	2.11	3	1
5:A:33:17F:P1	5:A:33:17F:N1	0.46	2.89	1	1
4:A:11:PCW:H372	4:A:63:PCW:H281	0.46	1.86	1	1
1:A:355:GLU:HA	1:A:355:GLU:OE1	0.46	2.11	8	1
1:A:307:ASP:HA	1:A:310:ARG:CD	0.46	2.41	6	1
3:D:858:LYS:HG2	3:D:876:ILE:HD12	0.46	1.88	6	1
4:A:18:PCW:H20	5:A:37:17F:H12A	0.46	1.88	9	1
4:A:12:PCW:H182	4:A:22:PCW:H262	0.46	1.87	1	1
4:A:47:PCW:H31	5:A:73:17F:H4A	0.45	1.86	10	1
4:A:1:PCW:H2	5:A:35:17F:H18A	0.45	1.87	5	1
1:A:352:LYS:HG2	1:C:422:VAL:HG22	0.45	1.88	5	1
4:A:69:PCW:H331	4:A:69:PCW:H131	0.45	1.88	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:47:PCW:H241	5:A:76:17F:H11A	0.45	1.86	4	1
4:A:20:PCW:H131	4:A:20:PCW:H332	0.45	1.88	8	1
1:C:461:LYS:O	1:C:465:GLU:HG3	0.45	2.11	10	2
4:A:7:PCW:H42	5:A:35:17F:O5	0.45	2.12	6	1
4:A:4:PCW:H51	4:A:7:PCW:O2P	0.45	2.11	9	1
4:A:13:PCW:C7	5:A:34:17F:HN1	0.45	2.24	7	1
4:A:8:PCW:H62	3:D:878:GLU:OE2	0.45	2.11	7	1
4:A:10:PCW:H81	4:A:12:PCW:H322	0.45	1.88	4	1
4:A:9:PCW:H73	4:A:30:PCW:O2P	0.45	2.12	4	1
4:A:67:PCW:H73	5:A:78:17F:H37	0.45	1.87	2	1
4:A:6:PCW:H39	4:A:16:PCW:H11	0.45	1.88	1	1
4:A:32:PCW:H321	5:A:33:17F:H20A	0.45	1.86	1	1
4:A:25:PCW:H40	4:A:29:PCW:H231	0.45	1.88	7	1
1:C:465:GLU:C	1:C:469:LEU:HD12	0.45	2.30	7	1
4:A:14:PCW:H421	5:A:34:17F:H12	0.45	1.89	2	1
1:A:327:LEU:HD23	1:A:330:ARG:HD3	0.45	1.88	2	1
4:A:23:PCW:H42	2:B:3:GLU:OE2	0.45	2.11	2	1
4:A:44:PCW:O2P	4:A:53:PCW:H62	0.45	2.10	10	1
2:B:6:LEU:HD22	2:B:159:LEU:HD23	0.45	1.88	10	2
2:B:62:GLU:OE1	2:B:68:ARG:HD2	0.45	2.12	10	1
1:A:291:LEU:HD23	1:A:294:LEU:HD12	0.45	1.88	6	1
4:A:30:PCW:H32	5:A:40:17F:HN1	0.45	1.71	9	1
4:A:13:PCW:N	5:A:34:17F:N1	0.45	2.63	7	1
4:A:42:PCW:H61	4:A:63:PCW:O2P	0.45	2.12	3	1
4:A:20:PCW:H42	4:A:24:PCW:H61	0.45	1.88	10	1
4:A:32:PCW:H331	5:A:35:17F:H11	0.45	1.88	10	1
1:C:563:LYS:CB	1:C:564:PRO:HD3	0.45	2.36	9	3
4:A:13:PCW:H42	5:A:34:17F:H1A	0.45	1.88	6	1
4:A:50:PCW:H451	5:A:78:17F:H65	0.45	1.89	9	1
4:A:12:PCW:H63	5:A:37:17F:HN1	0.45	1.71	2	1
4:A:71:PCW:H52	4:A:71:PCW:H332	0.45	1.89	10	1
4:A:8:PCW:C32	4:A:22:PCW:H331	0.45	2.42	10	1
4:A:9:PCW:H452	4:A:25:PCW:H221	0.45	1.89	7	1
4:A:28:PCW:H81	2:B:3:GLU:OE2	0.45	2.11	3	1
4:A:43:PCW:H62	4:A:43:PCW:O11	0.45	2.11	3	1
2:B:85:ASN:HB3	2:B:122:SER:O	0.45	2.11	3	1
4:A:22:PCW:C7	5:A:37:17F:HN1	0.45	2.25	10	1
1:A:278:PRO:O	1:A:282:GLU:HG3	0.45	2.12	6	2
4:A:48:PCW:H61	4:A:61:PCW:H422	0.45	1.88	9	1
1:A:392:GLU:HA	1:A:395:LYS:HD2	0.45	1.89	4	1
4:A:8:PCW:H72	4:A:27:PCW:O2P	0.45	2.11	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:42:PCW:H71	5:A:75:17F:N1	0.45	2.26	2	1
4:A:15:PCW:H42	5:A:39:17F:O1	0.45	2.10	3	1
4:A:17:PCW:H261	5:A:36:17F:H61	0.45	1.88	1	1
4:A:50:PCW:C4	5:A:78:17F:HN1	0.45	2.25	8	1
1:A:242:GLU:OE1	1:C:528:ARG:HA	0.45	2.11	5	1
4:A:44:PCW:O11	4:A:44:PCW:H82	0.45	2.12	9	1
3:D:868:ALA:HB3	3:D:869:PRO:HD3	0.45	1.88	7	1
4:A:62:PCW:H142	4:A:72:PCW:H152	0.45	1.88	3	1
3:D:834:LEU:HD11	3:D:877:VAL:HG21	0.45	1.87	3	1
4:A:41:PCW:H361	4:A:42:PCW:H272	0.45	1.89	1	1
4:A:54:PCW:H73	4:A:72:PCW:O11	0.45	2.12	1	1
4:A:47:PCW:H472	5:A:73:17F:H12A	0.45	1.88	1	1
2:B:116:ASN:HA	2:B:144:THR:O	0.45	2.12	8	1
4:A:21:PCW:H442	4:A:51:PCW:H251	0.45	1.88	5	1
5:A:34:17F:H37	5:A:40:17F:H71	0.45	1.87	5	1
5:A:39:17F:H33	5:A:39:17F:H8	0.45	1.89	7	1
4:A:32:PCW:H71	5:A:38:17F:HN1A	0.45	1.72	3	1
5:A:33:17F:H54	4:A:52:PCW:H461	0.45	1.88	1	1
4:A:41:PCW:H81	4:A:59:PCW:O1P	0.45	2.12	8	1
4:A:32:PCW:H482	4:A:55:PCW:H221	0.45	1.89	6	1
4:A:48:PCW:H332	4:A:54:PCW:H152	0.45	1.88	6	1
5:A:37:17F:H1	3:D:858:LYS:HD3	0.45	1.89	1	1
4:A:8:PCW:H82	4:A:22:PCW:H362	0.44	1.88	10	1
4:A:10:PCW:H81	4:A:22:PCW:O3P	0.44	2.12	7	1
4:A:53:PCW:H341	4:A:68:PCW:H151	0.44	1.89	2	1
4:A:24:PCW:H61	4:A:31:PCW:O1P	0.44	2.12	3	1
3:D:831:TYR:O	3:D:835:ASP:HB2	0.44	2.12	3	1
4:A:1:PCW:H121	5:A:35:17F:H32	0.44	1.87	7	1
4:A:42:PCW:H262	4:A:52:PCW:H241	0.44	1.89	7	1
4:A:55:PCW:H382	4:A:64:PCW:H362	0.44	1.88	8	1
4:A:43:PCW:H371	5:A:75:17F:H10	0.44	1.89	6	1
1:A:363:LYS:HG2	1:C:411:THR:HG22	0.44	1.87	7	1
2:B:41:ARG:HA	2:B:53:LEU:O	0.44	2.12	2	1
4:A:29:PCW:H71	3:D:847:CYS:HA	0.44	1.90	3	1
4:A:10:PCW:H71	5:A:36:17F:O2	0.44	2.11	1	1
1:C:455:TYR:O	1:C:459:PHE:HB2	0.44	2.12	1	1
4:A:5:PCW:H152	4:A:5:PCW:H211	0.44	1.90	5	1
4:A:42:PCW:H12	4:A:69:PCW:H121	0.44	1.88	5	1
4:A:16:PCW:H73	4:A:16:PCW:O31	0.44	2.12	7	1
4:A:71:PCW:H41	5:A:73:17F:O4	0.44	2.12	8	1
4:A:45:PCW:H362	4:A:49:PCW:H152	0.44	1.88	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:49:PCW:H421	5:A:80:17F:H58	0.44	1.89	4	1
4:A:22:PCW:O2P	4:A:27:PCW:H83	0.44	2.13	3	1
4:A:48:PCW:H341	4:A:54:PCW:H121	0.44	1.89	3	1
1:C:465:GLU:C	1:C:469:LEU:HG	0.44	2.23	7	1
4:A:52:PCW:O2P	4:A:60:PCW:H71	0.44	2.13	4	1
2:B:73:ARG:HH21	2:B:103:VAL:HA	0.44	1.72	2	1
4:A:27:PCW:H82	5:A:37:17F:O2	0.44	2.13	5	2
4:A:10:PCW:H452	4:A:12:PCW:H232	0.44	1.89	6	1
1:C:431:GLU:HA	1:C:434:THR:OG1	0.44	2.12	4	1
1:C:458:ASP:HA	1:C:461:LYS:HD2	0.44	1.90	2	1
4:A:10:PCW:H262	5:A:73:17F:H53	0.44	1.88	8	1
4:A:17:PCW:H31	4:A:17:PCW:O1P	0.44	2.12	8	1
4:A:25:PCW:H132	4:A:31:PCW:H31	0.44	1.88	10	1
1:C:464:GLN:O	1:C:468:GLU:HG3	0.44	2.12	5	1
1:C:487:GLN:O	1:C:491:GLU:HG3	0.44	2.12	5	1
1:C:530:ALA:O	1:C:534:GLU:HG2	0.44	2.12	9	1
4:A:22:PCW:H11	5:A:37:17F:O2	0.44	2.12	3	1
4:A:32:PCW:H11	5:A:33:17F:H4	0.44	1.90	3	1
1:A:356:HIS:HA	1:C:418:GLN:OE1	0.44	2.13	1	1
4:A:57:PCW:H351	4:A:57:PCW:H122	0.44	1.90	8	1
4:A:62:PCW:H71	4:A:67:PCW:O2P	0.44	2.13	8	1
2:B:11:ALA:O	2:B:14:VAL:HG22	0.44	2.13	8	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.44	2.42	1	2
4:A:2:PCW:H19	3:D:857:ARG:HE	0.44	1.73	6	1
3:D:853:LEU:HD12	3:D:874:GLU:HB2	0.44	1.88	3	1
4:A:14:PCW:H32	5:A:34:17F:H1	0.43	1.90	8	1
4:A:1:PCW:H432	4:A:26:PCW:H182	0.43	1.89	6	1
4:A:42:PCW:H211	4:A:52:PCW:H342	0.43	1.88	6	1
1:A:335:LEU:O	1:A:339:LYS:HG3	0.43	2.13	9	1
4:A:3:PCW:H39	4:A:3:PCW:H161	0.43	1.90	1	1
4:A:27:PCW:H73	5:A:37:17F:O2	0.43	2.13	5	1
4:A:5:PCW:H39	4:A:17:PCW:H63	0.43	1.89	5	1
4:A:66:PCW:H20	4:A:67:PCW:H82	0.43	1.88	5	1
1:C:428:ASP:O	1:C:432:LYS:HG3	0.43	2.12	5	1
4:A:26:PCW:O3P	5:A:40:17F:H19	0.43	2.13	6	1
4:A:62:PCW:H422	4:A:72:PCW:H172	0.43	1.89	6	1
1:C:458:ASP:O	1:C:462:LYS:HG3	0.43	2.13	9	1
1:C:465:GLU:C	1:C:469:LEU:CD1	0.43	2.86	7	1
4:A:44:PCW:O1P	4:A:55:PCW:H82	0.43	2.13	2	1
4:A:1:PCW:H212	5:A:38:17F:H19	0.43	1.90	1	1
4:A:42:PCW:H332	4:A:69:PCW:H132	0.43	1.89	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:44:PCW:H262	4:A:55:PCW:H19	0.43	1.89	10	1
4:A:60:PCW:H461	4:A:63:PCW:H432	0.43	1.90	10	1
4:A:31:PCW:C7	3:D:876:ILE:HD11	0.43	2.43	10	1
4:A:8:PCW:H411	4:A:27:PCW:H251	0.43	1.89	5	1
1:A:330:ARG:HD3	1:C:444:ASP:OD2	0.43	2.14	4	1
4:A:44:PCW:C5	5:A:77:17F:HN1A	0.43	2.26	4	1
5:A:34:17F:HN1A	3:D:857:ARG:HA	0.43	1.73	3	1
4:A:17:PCW:H271	5:A:36:17F:H71	0.43	1.91	3	1
4:A:4:PCW:O2P	4:A:16:PCW:H82	0.43	2.13	10	1
4:A:46:PCW:H361	4:A:71:PCW:H212	0.43	1.90	10	1
4:A:14:PCW:H12	4:A:23:PCW:O31	0.43	2.13	9	1
4:A:23:PCW:H241	4:A:49:PCW:H40	0.43	1.90	1	1
5:A:76:17F:H70	1:C:470:TYR:HB3	0.43	1.90	5	1
4:A:32:PCW:H483	5:A:38:17F:H55	0.43	1.90	6	1
4:A:59:PCW:H162	5:A:77:17F:H34	0.43	1.90	6	1
1:A:279:LEU:HB3	1:C:495:LYS:HD3	0.43	1.90	4	1
1:C:567:GLU:HG2	1:C:571:GLN:NE2	0.43	2.27	2	1
4:A:14:PCW:H471	4:A:30:PCW:H442	0.43	1.89	8	1
1:C:510:HIS:O	1:C:514:LEU:HG	0.43	2.14	3	2
1:A:365:LYS:HB2	1:A:366:PRO:CD	0.43	2.43	2	3
4:A:41:PCW:H212	4:A:61:PCW:H152	0.43	1.91	7	1
1:A:386:PHE:O	1:A:390:LEU:HG	0.43	2.14	3	1
4:A:53:PCW:H31	4:A:64:PCW:C3	0.43	2.44	3	1
1:A:345:ARG:HD3	1:C:433:GLU:OE2	0.43	2.13	3	1
1:A:239:LEU:HD22	4:A:20:PCW:H462	0.43	1.91	1	1
4:A:55:PCW:H62	5:A:77:17F:HN1A	0.43	1.72	8	1
1:A:277:GLU:HB3	1:A:278:PRO:CD	0.43	2.43	10	1
1:C:458:ASP:HA	1:C:461:LYS:HE2	0.43	1.91	10	1
1:C:485:ALA:HA	1:C:488:LYS:HG2	0.43	1.90	7	1
4:A:43:PCW:O2P	4:A:45:PCW:H71	0.43	2.14	3	1
4:A:17:PCW:C1	2:B:70:GLN:HB2	0.43	2.41	8	1
1:C:512:ASP:O	1:C:515:ARG:HB2	0.43	2.13	10	2
2:B:9:VAL:HB	2:B:96:TYR:CE1	0.43	2.49	5	1
4:A:48:PCW:H372	4:A:54:PCW:H252	0.43	1.90	6	1
4:A:3:PCW:H221	4:A:19:PCW:H182	0.43	1.90	9	1
3:D:811:LYS:HG2	3:D:821:VAL:HG22	0.43	1.90	9	1
4:A:52:PCW:H31	4:A:52:PCW:H41	0.43	1.90	8	1
4:A:20:PCW:H462	4:A:31:PCW:H411	0.43	1.90	9	1
1:A:344:ALA:O	1:A:348:GLU:HG2	0.43	2.14	4	1
3:D:858:LYS:HE3	3:D:876:ILE:HB	0.43	1.89	1	1
4:A:56:PCW:H131	4:A:56:PCW:H332	0.43	1.90	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
5:A:40:17F:H37	5:A:40:17F:H69	0.43	1.91	2	1
4:A:31:PCW:H73	4:A:31:PCW:H331	0.43	1.90	1	1
4:A:30:PCW:H361	5:A:34:17F:H18	0.42	1.90	8	1
4:A:47:PCW:H20	5:A:76:17F:H20	0.42	1.91	8	1
2:B:163:ILE:O	2:B:167:LYS:HG2	0.42	2.14	8	2
1:A:263:LYS:O	1:A:267:GLU:HG3	0.42	2.14	9	2
4:A:53:PCW:H362	4:A:53:PCW:H151	0.42	1.90	6	1
4:A:7:PCW:H321	5:A:33:17F:H9	0.42	1.89	4	1
1:A:243:MET:HA	1:A:246:ASP:HB2	0.42	1.90	5	1
5:A:37:17F:N1	3:D:817:LYS:NZ	0.42	2.67	7	1
1:C:589:GLU:O	1:C:593:LYS:HG3	0.42	2.14	7	1
4:A:53:PCW:H152	4:A:64:PCW:H171	0.42	1.90	10	1
2:B:24:ILE:HA	2:B:42:LYS:HD2	0.42	1.90	5	1
4:A:68:PCW:O31	4:A:69:PCW:H73	0.42	2.15	6	1
4:A:7:PCW:H42	3:D:879:VAL:O	0.42	2.14	9	1
5:A:40:17F:N1	2:B:5:LYS:NZ	0.42	2.65	7	1
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.42	1.91	2	2
4:A:10:PCW:H352	4:A:21:PCW:H341	0.42	1.91	4	1
4:A:23:PCW:H71	2:B:54:ASP:OD2	0.42	2.13	2	1
4:A:8:PCW:O31	4:A:22:PCW:H71	0.42	2.14	8	1
4:A:44:PCW:O31	4:A:55:PCW:H83	0.42	2.13	5	1
4:A:9:PCW:H142	4:A:11:PCW:H132	0.42	1.90	5	1
3:D:830:VAL:O	3:D:834:LEU:HB2	0.42	2.14	2	2
2:B:118:CYS:HB3	2:B:143:GLU:HG2	0.42	1.91	6	1
4:A:20:PCW:H432	4:A:31:PCW:H122	0.42	1.90	7	1
5:A:38:17F:H2	5:A:38:17F:O2	0.42	2.13	1	1
2:B:69:ASP:O	2:B:73:ARG:HG3	0.42	2.14	1	1
4:A:9:PCW:H261	4:A:63:PCW:H241	0.42	1.91	3	1
4:A:12:PCW:O1P	3:D:855:LYS:HD3	0.42	2.14	3	1
4:A:5:PCW:H12	4:A:17:PCW:H361	0.42	1.91	8	1
4:A:42:PCW:O11	4:A:42:PCW:H82	0.42	2.14	5	1
4:A:17:PCW:H121	5:A:36:17F:H6	0.42	1.90	6	1
4:A:20:PCW:P	3:D:876:ILE:HG12	0.42	2.55	4	1
4:A:10:PCW:C7	5:A:37:17F:HN1A	0.42	2.27	3	1
5:A:33:17F:H8A	5:A:35:17F:H11A	0.42	1.92	1	1
4:A:16:PCW:C8	5:A:39:17F:H6	0.42	2.44	8	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.42	2.15	2	4
1:A:258:LEU:O	1:A:262:GLN:HB2	0.42	2.14	10	1
1:A:270:GLU:O	1:A:274:GLN:HB2	0.42	2.14	6	1
4:A:14:PCW:H432	5:A:34:17F:H12	0.42	1.92	6	1
4:A:70:PCW:H351	4:A:71:PCW:H141	0.42	1.91	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:576:VAL:O	1:C:580:PHE:HB2	0.42	2.15	9	1
5:A:33:17F:H1	5:A:33:17F:C4	0.42	2.44	7	1
4:A:16:PCW:H2	4:A:16:PCW:O1P	0.42	2.15	8	1
4:A:15:PCW:H42	5:A:39:17F:H1	0.42	1.91	8	1
4:A:60:PCW:H322	4:A:63:PCW:H62	0.42	1.91	8	1
4:A:58:PCW:H351	4:A:61:PCW:H441	0.42	1.91	9	1
4:A:53:PCW:H371	4:A:68:PCW:H411	0.42	1.91	9	1
4:A:32:PCW:H342	5:A:35:17F:H12A	0.42	1.91	4	1
4:A:23:PCW:H62	2:B:5:LYS:HG2	0.42	1.92	2	1
4:A:1:PCW:H471	4:A:26:PCW:H461	0.42	1.92	8	1
1:A:243:MET:HA	1:A:246:ASP:HB3	0.42	1.92	8	1
4:A:9:PCW:H81	4:A:26:PCW:O2P	0.42	2.14	8	1
1:C:427:TRP:O	1:C:431:GLU:HG2	0.42	2.15	10	1
1:A:304:GLU:O	1:A:308:ARG:HG2	0.42	2.14	5	1
4:A:5:PCW:H461	4:A:17:PCW:H171	0.42	1.92	6	1
1:A:345:ARG:O	1:A:349:TYR:HB2	0.42	2.15	9	1
4:A:42:PCW:H31	4:A:69:PCW:H151	0.42	1.92	9	1
4:A:59:PCW:O11	4:A:59:PCW:H83	0.42	2.14	2	1
2:B:159:LEU:O	2:B:163:ILE:HG13	0.42	2.15	2	1
4:A:8:PCW:H73	4:A:22:PCW:O1P	0.42	2.14	3	1
4:A:12:PCW:H71	3:D:874:GLU:OE1	0.42	2.15	3	1
4:A:68:PCW:H31	4:A:70:PCW:H171	0.42	1.91	8	1
4:A:26:PCW:H62	4:A:28:PCW:O1P	0.42	2.15	10	1
4:A:7:PCW:H382	5:A:33:17F:H9A	0.42	1.91	5	1
1:A:356:HIS:O	1:A:360:LEU:HB2	0.42	2.14	7	1
4:A:48:PCW:H62	4:A:61:PCW:H39	0.42	1.91	7	1
4:A:6:PCW:H331	4:A:7:PCW:H81	0.42	1.91	7	1
4:A:11:PCW:H83	2:B:171:SER:HB3	0.42	1.92	7	1
4:A:2:PCW:N	4:A:5:PCW:O2P	0.42	2.53	4	1
4:A:12:PCW:O1P	3:D:857:ARG:HD3	0.42	2.14	1	1
4:A:31:PCW:O2P	3:D:876:ILE:HG21	0.41	2.15	10	1
4:A:44:PCW:H32	5:A:77:17F:HN1A	0.41	1.76	10	1
1:C:491:GLU:HB3	1:C:495:LYS:CE	0.41	2.44	5	3
4:A:30:PCW:H73	4:A:30:PCW:O11	0.41	2.15	6	1
5:A:74:17F:H56	5:A:79:17F:H4	0.41	1.92	9	1
4:A:48:PCW:H371	4:A:54:PCW:H431	0.41	1.91	7	1
4:A:59:PCW:H221	5:A:77:17F:H11A	0.41	1.91	7	1
2:B:15:GLY:HA2	6:B:201:GNP:O1A	0.41	2.16	7	1
4:A:59:PCW:H51	5:A:77:17F:H8A	0.41	1.90	2	1
2:B:158:THR:O	2:B:162:GLU:HG2	0.41	2.15	8	1
4:A:26:PCW:H471	4:A:26:PCW:H152	0.41	1.92	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:13:PCW:H61	5:A:34:17F:O1	0.41	2.15	10	1
4:A:44:PCW:H82	5:A:77:17F:C3	0.41	2.46	5	1
4:A:44:PCW:H42	4:A:53:PCW:O1P	0.41	2.14	6	1
4:A:8:PCW:H41	4:A:22:PCW:O1P	0.41	2.15	3	1
1:C:458:ASP:HA	1:C:461:LYS:NZ	0.41	2.30	3	1
5:A:34:17F:H42	5:A:75:17F:H52	0.41	1.91	8	1
4:A:48:PCW:H82	4:A:61:PCW:H411	0.41	1.91	10	1
4:A:14:PCW:H352	5:A:34:17F:H59	0.41	1.92	7	1
1:A:330:ARG:NH2	1:C:447:GLU:HB3	0.41	2.31	1	1
4:A:13:PCW:H442	5:A:37:17F:H73	0.41	1.92	7	1
1:A:304:GLU:O	1:A:308:ARG:HG3	0.41	2.14	4	1
4:A:30:PCW:H82	5:A:34:17F:O3	0.41	2.16	4	1
4:A:1:PCW:H181	5:A:35:17F:H56	0.41	1.92	2	1
5:A:34:17F:HN1A	3:D:858:LYS:N	0.41	2.10	3	1
4:A:42:PCW:H231	4:A:42:PCW:H432	0.41	1.91	3	1
4:A:13:PCW:H411	4:A:27:PCW:H351	0.41	1.91	6	1
4:A:5:PCW:H42	3:D:853:LEU:HD13	0.41	1.92	6	1
5:A:40:17F:HN1A	2:B:5:LYS:HZ2	0.41	1.50	7	1
2:B:41:ARG:HD3	2:B:54:ASP:OD2	0.41	2.16	3	1
4:A:17:PCW:H181	5:A:36:17F:H19	0.41	1.92	8	1
4:A:62:PCW:H332	4:A:72:PCW:H19	0.41	1.90	8	1
4:A:43:PCW:H211	4:A:51:PCW:H431	0.41	1.92	10	1
4:A:51:PCW:H82	4:A:71:PCW:O31	0.41	2.16	10	1
1:A:330:ARG:HH12	1:C:448:VAL:HG23	0.41	1.76	10	1
4:A:6:PCW:P	5:A:39:17F:O1	0.41	2.79	7	1
2:B:37:GLU:O	3:D:821:VAL:HG23	0.41	2.16	7	1
4:A:14:PCW:H131	4:A:23:PCW:H2	0.41	1.92	2	1
4:A:4:PCW:H63	5:A:33:17F:P1	0.41	2.56	3	1
4:A:5:PCW:H442	5:A:36:17F:H36	0.41	1.92	10	1
1:A:285:GLU:HA	1:A:288:ARG:HD2	0.41	1.92	9	1
4:A:30:PCW:H39	5:A:40:17F:H74	0.41	1.93	9	1
4:A:6:PCW:P	3:D:878:GLU:OE2	0.41	2.79	9	1
5:A:37:17F:HN1	3:D:817:LYS:NZ	0.41	2.13	7	1
4:A:50:PCW:H441	5:A:78:17F:H59	0.41	1.93	4	1
4:A:8:PCW:H63	4:A:27:PCW:O2P	0.41	2.15	4	1
4:A:67:PCW:H141	5:A:74:17F:H70	0.41	1.93	2	1
4:A:14:PCW:H151	4:A:23:PCW:H172	0.41	1.91	3	1
4:A:1:PCW:N	5:A:35:17F:N1	0.41	2.68	3	1
4:A:56:PCW:H51	4:A:56:PCW:H31	0.41	1.92	1	1
4:A:42:PCW:H341	4:A:42:PCW:H19	0.41	1.93	8	1
4:A:42:PCW:H382	4:A:69:PCW:H152	0.41	1.92	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:53:PCW:H40	4:A:68:PCW:H462	0.41	1.93	10	1
1:C:508:ARG:O	1:C:512:ASP:HB3	0.41	2.16	10	1
1:A:277:GLU:HB2	1:A:278:PRO:CD	0.41	2.45	6	1
4:A:11:PCW:H62	4:A:24:PCW:O11	0.41	2.15	9	1
4:A:6:PCW:H272	4:A:24:PCW:H481	0.41	1.93	9	1
4:A:41:PCW:H231	4:A:61:PCW:H232	0.41	1.93	4	1
4:A:9:PCW:H52	4:A:14:PCW:O31	0.41	2.16	2	1
5:A:79:17F:C1	5:A:79:17F:H4	0.41	2.45	1	1
1:A:325:ASP:O	1:A:329:GLN:HG3	0.41	2.15	8	1
5:A:40:17F:O4	2:B:5:LYS:HE2	0.41	2.16	8	1
4:A:28:PCW:H242	4:A:42:PCW:H481	0.41	1.92	10	1
1:C:578:GLU:O	1:C:582:VAL:HG23	0.41	2.16	10	1
1:C:412:PHE:O	1:C:415:LEU:HB2	0.41	2.16	5	1
1:C:540:GLY:O	1:C:544:LEU:HG	0.41	2.16	5	1
4:A:46:PCW:O3P	4:A:71:PCW:H372	0.41	2.16	5	1
4:A:48:PCW:H63	4:A:58:PCW:O11	0.41	2.16	6	1
4:A:14:PCW:H72	4:A:25:PCW:H31	0.41	1.92	6	1
4:A:14:PCW:H42	4:A:23:PCW:H371	0.41	1.92	9	1
1:A:264:LYS:O	1:A:268:GLU:HG3	0.41	2.15	9	1
4:A:25:PCW:O31	4:A:31:PCW:H62	0.41	2.16	7	1
4:A:5:PCW:H161	5:A:38:17F:H10A	0.41	1.91	4	1
4:A:44:PCW:H432	4:A:64:PCW:H40	0.41	1.93	4	1
4:A:8:PCW:H83	4:A:22:PCW:O1P	0.41	2.15	2	1
1:A:243:MET:O	1:A:247:LEU:HB2	0.41	2.16	2	1
4:A:43:PCW:H12	4:A:68:PCW:O1P	0.41	2.16	2	1
4:A:62:PCW:H41	4:A:67:PCW:O2P	0.41	2.16	2	1
2:B:100:ILE:HA	2:B:103:VAL:HG22	0.41	1.92	2	1
2:B:81:VAL:HA	2:B:114:VAL:HB	0.41	1.92	3	1
4:A:30:PCW:H61	3:D:853:LEU:HD11	0.41	1.93	1	1
4:A:41:PCW:O31	4:A:61:PCW:H81	0.41	2.16	8	1
1:C:490:HIS:HA	1:C:493:GLN:OE1	0.41	2.15	10	1
4:A:6:PCW:H82	5:A:39:17F:H2	0.41	1.91	5	1
4:A:9:PCW:O11	4:A:9:PCW:H51	0.41	2.15	5	1
4:A:52:PCW:H42	4:A:60:PCW:O1P	0.41	2.16	6	1
4:A:9:PCW:H121	4:A:11:PCW:H122	0.41	1.91	6	1
4:A:13:PCW:H141	5:A:37:17F:H37	0.41	1.93	7	1
4:A:60:PCW:H411	4:A:72:PCW:H162	0.41	1.93	4	1
4:A:25:PCW:H40	4:A:29:PCW:H321	0.41	1.92	1	1
4:A:30:PCW:H71	3:D:853:LEU:HD21	0.41	1.93	1	1
4:A:13:PCW:O1P	4:A:18:PCW:H62	0.40	2.16	8	1
4:A:12:PCW:H362	4:A:30:PCW:H181	0.40	1.93	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:48:PCW:H61	4:A:60:PCW:O11	0.40	2.15	10	1
1:C:574:LEU:HB2	1:C:575:PRO:CD	0.40	2.45	10	1
4:A:42:PCW:H73	4:A:42:PCW:O31	0.40	2.16	6	1
4:A:28:PCW:H451	4:A:63:PCW:H272	0.40	1.91	6	1
4:A:8:PCW:H83	4:A:27:PCW:O2P	0.40	2.16	6	1
1:A:290:LYS:HE3	1:C:487:GLN:OE1	0.40	2.16	6	1
4:A:12:PCW:H411	5:A:36:17F:H12A	0.40	1.92	9	1
3:D:867:ILE:HD11	3:D:875:LEU:HD11	0.40	1.93	2	1
4:A:5:PCW:H2	4:A:5:PCW:O4P	0.40	2.16	1	1
4:A:18:PCW:H261	4:A:49:PCW:H442	0.40	1.91	10	1
1:A:260:ASP:HA	1:A:263:LYS:CE	0.40	2.38	10	1
5:A:33:17F:N1	3:D:858:LYS:NZ	0.40	2.70	5	1
4:A:13:PCW:H42	5:A:34:17F:O5	0.40	2.16	6	1
4:A:2:PCW:H61	3:D:815:PRO:HA	0.40	1.93	6	1
1:A:272:TYR:O	1:A:276:VAL:HG23	0.40	2.17	9	1
4:A:54:PCW:O31	4:A:62:PCW:H131	0.40	2.17	7	1
4:A:12:PCW:H372	5:A:36:17F:H18A	0.40	1.93	4	1
4:A:43:PCW:O2P	4:A:45:PCW:H51	0.40	2.16	4	1
4:A:16:PCW:H122	5:A:39:17F:H69	0.40	1.93	2	1
4:A:9:PCW:H172	4:A:26:PCW:H131	0.40	1.92	2	1
4:A:41:PCW:H351	4:A:59:PCW:H362	0.40	1.93	1	1
4:A:41:PCW:H261	4:A:58:PCW:H452	0.40	1.92	8	1
4:A:70:PCW:H62	4:A:70:PCW:O31	0.40	2.15	8	1
4:A:8:PCW:H341	4:A:10:PCW:H172	0.40	1.91	8	1
4:A:17:PCW:H72	5:A:38:17F:O1	0.40	2.16	10	1
4:A:45:PCW:H141	5:A:74:17F:HN1	0.40	1.76	10	1
4:A:16:PCW:H62	2:B:105:ASP:OD1	0.40	2.16	6	1
4:A:26:PCW:O31	5:A:40:17F:H19A	0.40	2.17	9	1
5:A:34:17F:H40	5:A:40:17F:H73	0.40	1.93	9	1
4:A:53:PCW:O2P	4:A:64:PCW:H81	0.40	2.17	9	1
2:B:85:ASN:OD1	2:B:117:LYS:HD2	0.40	2.17	7	1
4:A:48:PCW:H61	4:A:58:PCW:O11	0.40	2.16	2	1
1:C:561:LYS:HA	1:C:565:ALA:CB	0.40	2.46	2	1
4:A:41:PCW:H32	4:A:52:PCW:H122	0.40	1.92	3	1
4:A:5:PCW:H151	4:A:17:PCW:H382	0.40	1.93	1	1
4:A:26:PCW:H432	4:A:26:PCW:H121	0.40	1.93	10	1
4:A:58:PCW:H132	4:A:61:PCW:H451	0.40	1.91	5	1
1:A:341:ASN:O	1:A:345:ARG:HG3	0.40	2.16	9	1
1:A:239:LEU:HA	1:A:242:GLU:HB2	0.40	1.91	7	1
2:B:36:ILE:HB	3:D:821:VAL:HB	0.40	1.92	4	1
4:A:58:PCW:O2P	4:A:60:PCW:H81	0.40	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:12:PCW:H131	5:A:37:17F:H6	0.40	1.93	3	1
4:A:65:PCW:O11	4:A:65:PCW:H82	0.40	2.17	3	1
4:A:14:PCW:H442	4:A:14:PCW:H252	0.40	1.94	1	1
4:A:23:PCW:H73	5:A:34:17F:N1	0.40	2.29	1	1
4:A:8:PCW:H82	4:A:22:PCW:O1P	0.40	2.16	5	1
4:A:46:PCW:O2P	4:A:71:PCW:H332	0.40	2.15	9	1
4:A:62:PCW:H11	4:A:72:PCW:O3P	0.40	2.16	9	1
4:A:1:PCW:H162	5:A:35:17F:H33	0.40	1.91	7	1
4:A:55:PCW:O2P	4:A:64:PCW:H12	0.40	2.16	2	1
5:A:34:17F:O4	3:D:857:ARG:HD3	0.40	2.17	3	1
5:A:38:17F:H18A	5:A:38:17F:H9	0.40	1.92	1	1
4:A:46:PCW:H83	5:A:73:17F:O2	0.40	2.17	1	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	157/200 (78%)	153±1 (98±1%)	3±1 (2±1%)	1±0 (1±0%)	29	74
1	C	195/200 (98%)	190±1 (98±1%)	4±2 (2±1%)	1±0 (1±0%)	32	76
2	B	170/187 (91%)	161±3 (95±2%)	9±3 (5±1%)	0±0 (0±0%)	50	82
3	D	71/73 (97%)	66±2 (93±2%)	5±2 (7±2%)	0±0 (0±0%)	54	85
All	All	5930/6600 (90%)	5702 (96%)	204 (3%)	24 (0%)	38	78

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	10
1	C	563	LYS	9
1	C	420	GLY	1
2	B	24	ILE	1
2	B	48	GLY	1
3	D	827	GLY	1

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Mol	Chain	Res	Type	Models (Total)
2	B	13	GLY	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	135/175 (77%)	123±3 (91±2%)	12±3 (9±2%)	14	60
1	C	172/175 (98%)	157±3 (91±2%)	15±3 (9±2%)	14	60
2	B	150/165 (91%)	137±2 (91±2%)	13±2 (9±2%)	13	60
3	D	64/64 (100%)	57±2 (89±3%)	7±2 (11±3%)	10	55
All	All	5210/5790 (90%)	4743 (91%)	467 (9%)	13	60

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)
3	D	819	ARG	10
2	B	87	THR	10
1	A	254	VAL	9
1	A	392	GLU	8
2	B	74	THR	8
1	C	550	LYS	8
1	A	312	HIS	8
1	C	516	THR	8
2	B	92	ASP	8
1	C	480	GLU	7
3	D	829	SER	7
2	B	69	ASP	7
1	C	455	TYR	6
3	D	823	THR	6
2	B	122	SER	6
1	A	354	THR	6
1	A	318	THR	5
2	B	33	ASP	5
3	D	864	ASP	5
1	A	246	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	293	GLU	5
3	D	853	LEU	5
2	B	124	THR	5
1	C	594	LYS	5
2	B	54	ASP	5
1	C	459	PHE	5
2	B	65	SER	4
2	B	17	SER	4
1	C	405	TRP	4
1	C	580	PHE	4
1	A	370	ASP	4
1	C	403	ASP	4
2	B	35	THR	4
1	C	568	ASP	4
2	B	127	THR	4
3	D	878	GLU	4
1	A	265	TRP	4
2	B	85	ASN	4
1	C	444	ASP	4
1	C	505	ASP	4
2	B	71	TYR	4
1	A	272	TYR	4
1	A	292	HIS	3
2	B	51	CYS	3
1	C	412	PHE	3
1	A	350	HIS	3
2	B	39	SER	3
1	A	385	SER	3
3	D	859	THR	3
1	C	451	LYS	3
3	D	809	THR	3
1	C	447	GLU	3
1	C	512	ASP	3
3	D	816	ASN	3
1	A	314	ASP	3
1	C	467	MET	3
2	B	30	ASP	3
1	C	407	SER	3
1	C	552	THR	3
1	C	418	GLN	3
1	C	487	GLN	3
1	A	394	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	274	GLN	3
3	D	847	CYS	3
2	B	153	ASP	3
2	B	62	GLU	3
1	C	466	GLU	3
2	B	2	THR	3
1	A	319	HIS	3
3	D	833	SER	3
1	C	592	THR	2
1	C	490	HIS	2
1	C	434	THR	2
1	A	255	GLN	2
2	B	145	SER	2
2	B	41	ARG	2
3	D	834	LEU	2
2	B	3	GLU	2
2	B	132	ASP	2
1	A	325	ASP	2
1	C	410	SER	2
1	C	404	ASN	2
1	A	371	LEU	2
1	A	264	LYS	2
1	C	463	TRP	2
1	A	296	GLU	2
3	D	841	ARG	2
1	A	299	SER	2
3	D	865	THR	2
1	C	546	GLU	2
1	C	583	SER	2
2	B	168	GLU	2
1	C	523	ASP	2
2	B	148	THR	2
2	B	164	ARG	2
1	A	356	HIS	2
1	C	448	VAL	2
1	C	561	LYS	2
1	A	327	LEU	2
2	B	37	GLU	2
2	B	135	ARG	1
1	C	464	GLN	1
3	D	857	ARG	1
1	A	249	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	C	457	ASP	1
1	A	261	PHE	1
2	B	20	THR	1
1	A	284	GLN	1
1	C	401	LEU	1
2	B	57	ASP	1
1	C	584	PHE	1
1	C	559	SER	1
1	C	558	LEU	1
2	B	126	ASP	1
1	C	402	LEU	1
1	C	433	GLU	1
1	C	522	SER	1
1	C	429	ASN	1
3	D	844	ASN	1
1	C	557	THR	1
2	B	89	SER	1
3	D	861	THR	1
1	A	378	VAL	1
3	D	813	TYR	1
1	A	358	SER	1
2	B	70	GLN	1
1	A	241	GLN	1
1	A	283	LEU	1
1	A	336	GLU	1
1	C	415	LEU	1
1	C	427	TRP	1
2	B	119	ASP	1
1	A	368	LEU	1
2	B	99	GLN	1
3	D	870	LEU	1
1	A	359	THR	1
3	D	825	ARG	1
1	C	460	GLN	1
1	C	554	HIS	1
1	C	494	GLU	1
1	C	501	GLU	1
1	A	360	LEU	1
1	C	576	VAL	1
3	D	858	LYS	1
1	C	521	TYR	1
2	B	97	ARG	1

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Mol	Chain	Res	Type	Models (Total)
3	D	811	LYS	1
1	A	273	ARG	1
1	C	461	LYS	1
3	D	840	VAL	1
2	B	170	MET	1
1	C	566	LEU	1
1	A	381	SER	1
1	A	290	LYS	1
1	A	304	GLU	1
1	A	270	GLU	1
1	C	596	ASN	1
1	A	307	ASP	1
1	C	482	GLN	1
1	A	348	GLU	1
1	C	443	LYS	1
2	B	4	TYR	1
1	C	409	THR	1
1	C	548	HIS	1
2	B	47	ASP	1
2	B	95	HIS	1
2	B	44	VAL	1
1	A	305	MET	1
1	A	243	MET	1
1	C	556	SER	1
1	A	266	GLN	1
1	C	495	LYS	1
1	A	361	SER	1
2	B	32	TYR	1
3	D	826	ASP	1
2	B	101	LYS	1
2	B	150	GLN	1
2	B	102	ARG	1
1	C	560	GLU	1
1	C	477	LEU	1
2	B	107	GLU	1
2	B	154	ASP	1
1	C	473	LYS	1
1	C	426	PHE	1
1	C	472	GLN	1
1	C	425	GLU	1
2	B	68	ARG	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

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6.6 Other polymers

There are no such molecules in this entry.

6.7 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	52
Number of shifts mapped to atoms	52
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

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 26 atoms were assigned a chemical shift out of a possible 7601. 0 out of 118 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/2942 (0%)	0/1173 (0%)	0/1192 (0%)	0/577 (0%)
Sidechain	26/4226 (1%)	13/2472 (1%)	13/1535 (1%)	0/219 (0%)
Aromatic	0/433 (0%)	0/240 (0%)	0/193 (0%)	0/0 (—%)
Overall	26/7601 (0%)	13/3885 (0%)	13/2920 (0%)	0/796 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 26 atoms were assigned a chemical shift out of a possible 8369. 0 out of 128 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/3230 (0%)	0/1288 (0%)	0/1308 (0%)	0/634 (0%)
Sidechain	26/4666 (1%)	13/2732 (0%)	13/1693 (1%)	0/241 (0%)
Aromatic	0/473 (0%)	0/262 (0%)	0/211 (0%)	0/0 (—%)
Overall	26/8369 (0%)	13/4282 (0%)	13/3212 (0%)	0/875 (0%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.