



Full wwPDB NMR Structure Validation Report ⓘ

Jun 7, 2020 – 04:13 am BST

PDB ID : 6CCH
Title : NMR data-driven model of GTPase KRas-GMPPNP tethered to a nanodisc (E3 state)
Authors : Fang, Z.; Marshall, C.B.; Nishikawa, T.; Gossert, A.D.; Jansen, J.M.; Jahnke, W.; Ikura, M.
Deposited on : 2018-02-07

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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	:	1.8.5 (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

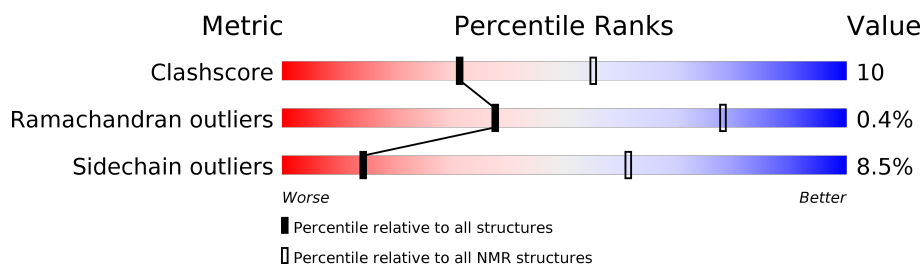
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	200	
1	C	200	
2	B	187	

2 Ensemble composition and analysis

This entry contains 7 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:231-A:395, C:401-C:596 (361)	0.25	3
2	B:1-B:172 (172)	0.42	1

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 and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4
2	3, 5, 7
Single-model clusters	6

3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9487 atoms, of which 407 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

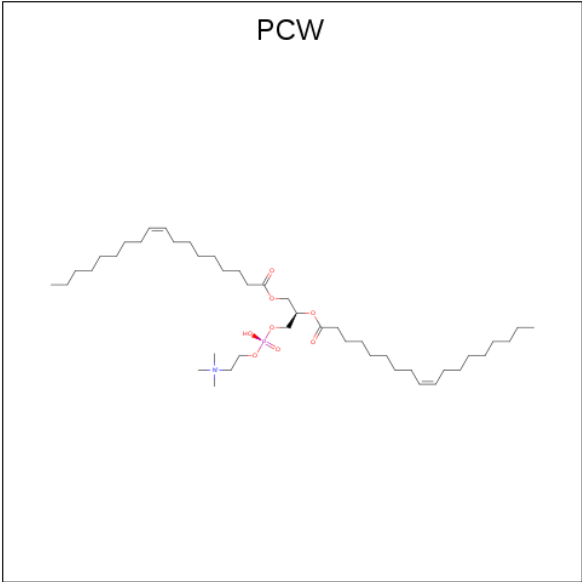
- Molecule 2 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
2	B	185	Total	C	H	N	O	S	0
			1843	926	363	257	288	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: $C_{44}H_{85}NO_8P$).



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	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

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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	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	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

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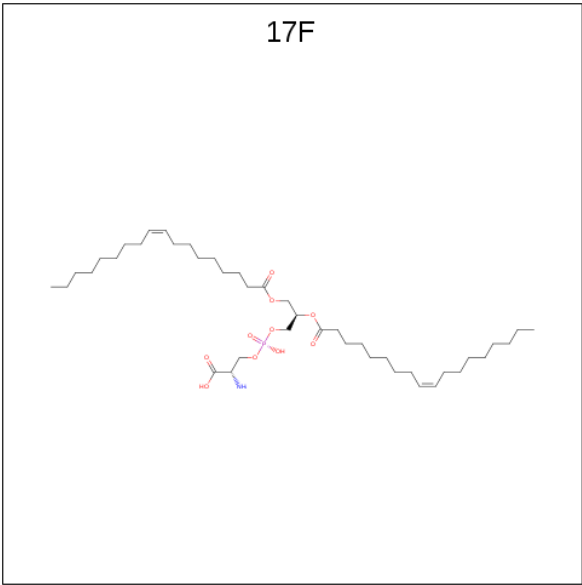
Mol	Chain	Residues	Atoms				
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44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

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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

- 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).



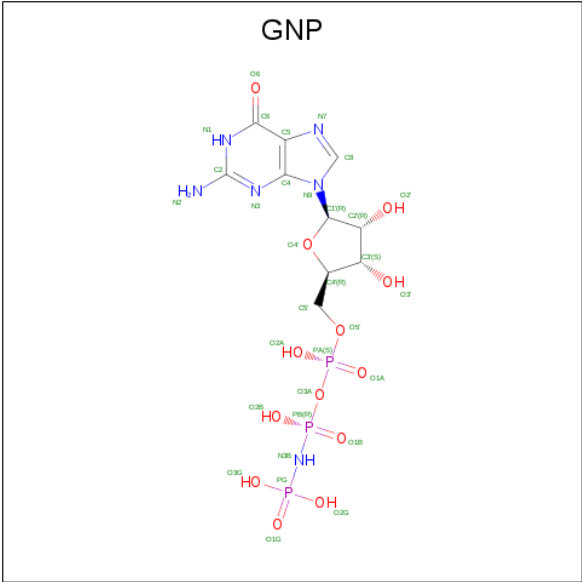
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1

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Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	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				
			Total	C	N	O	P
5	B	1	32	10	6	13	3

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

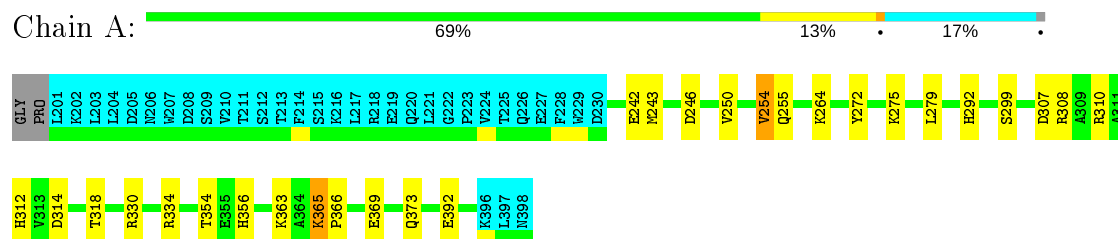
Mol	Chain	Residues	Atoms	
			Total	Mg
6	B	1	1	1

4 Residue-property plots

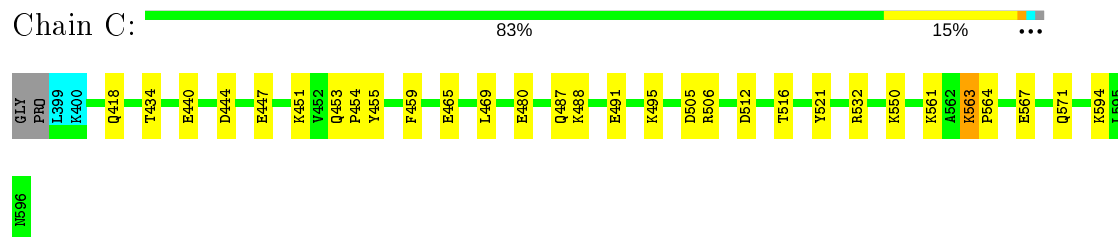
4.1 Average score per residue in the NMR ensemble

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.

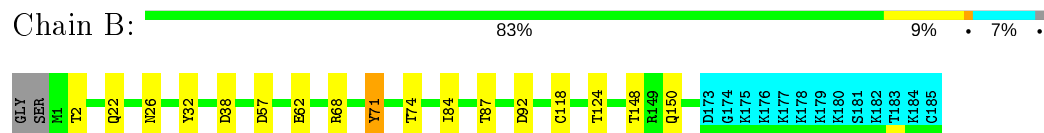
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas

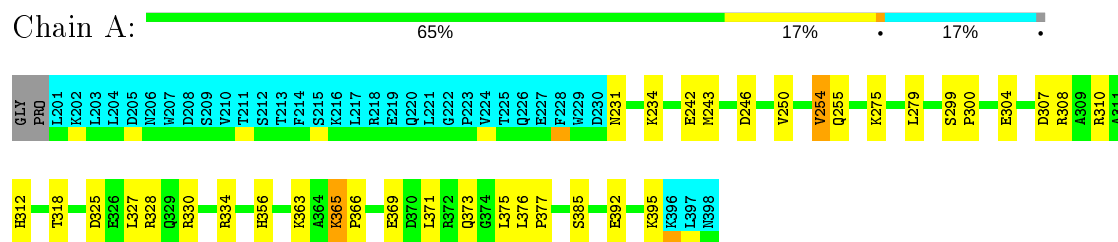


4.2 Scores per residue for each member of the ensemble

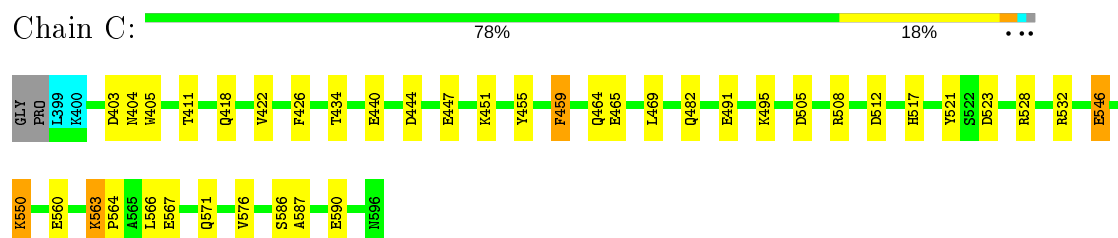
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

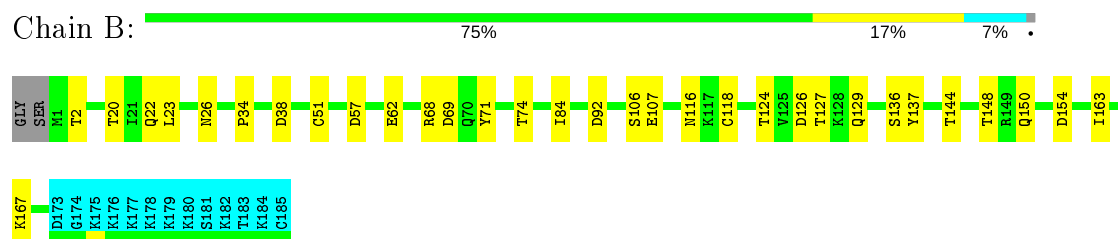
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

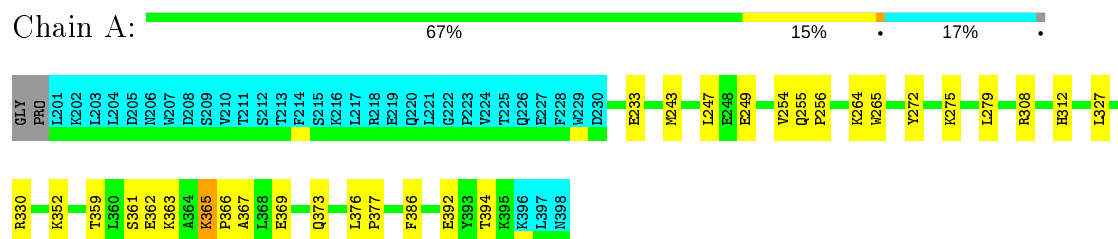


- Molecule 2: GTPase KRas

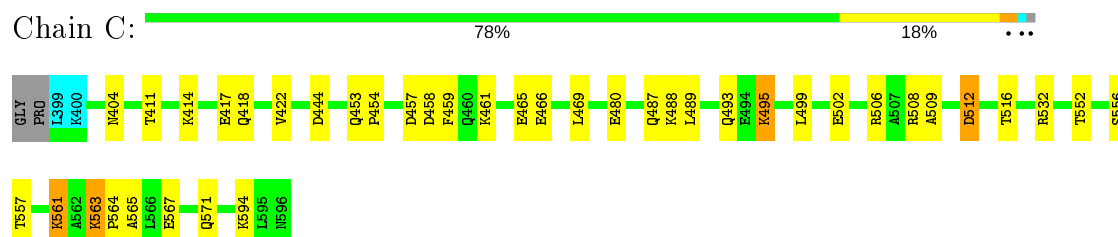


4.2.2 Score per residue for model 2

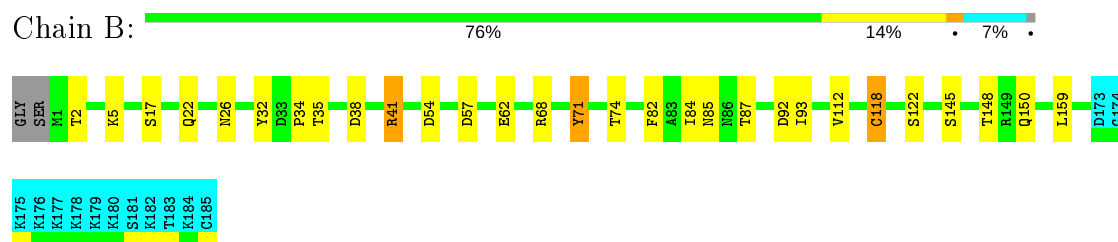
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

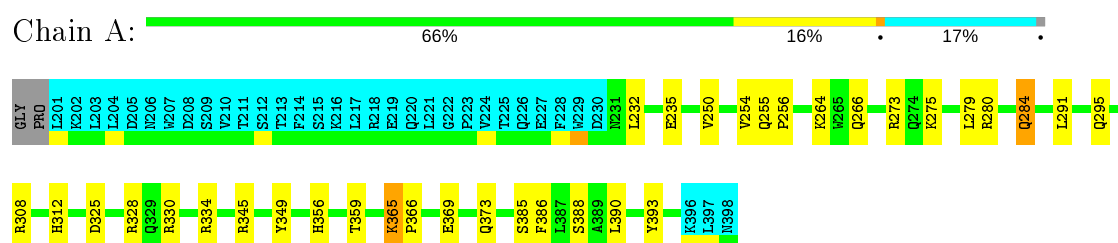


- Molecule 2: GTPase KRas

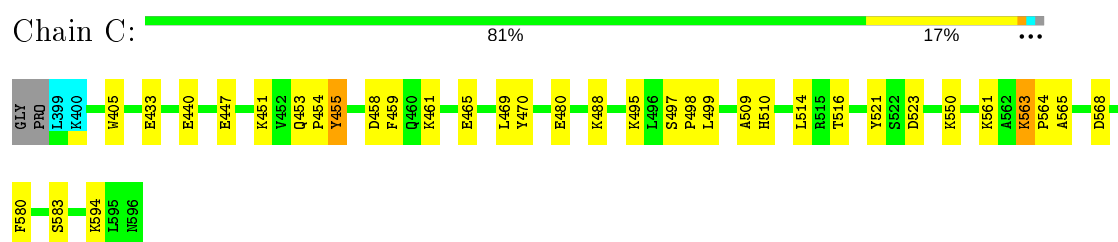


4.2.3 Score per residue for model 3 (medoid)

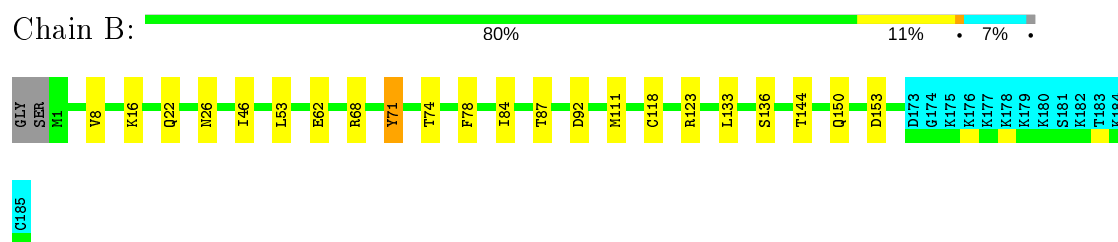
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



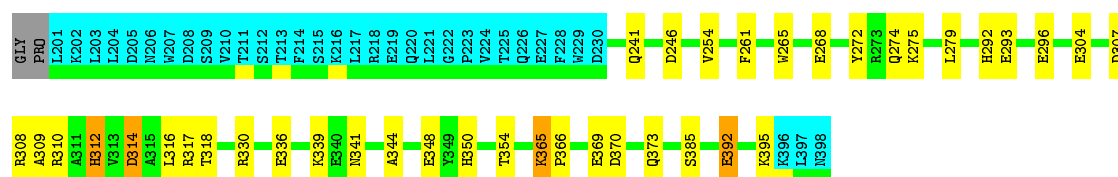
- Molecule 2: GTPase KRas



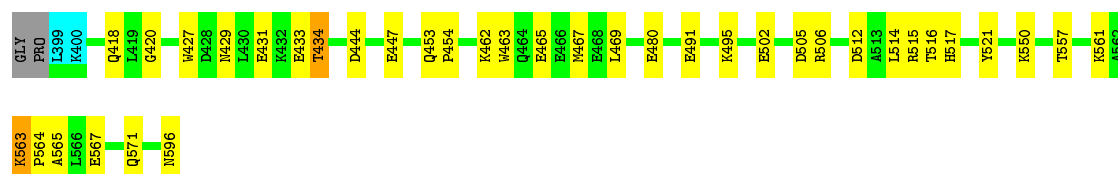
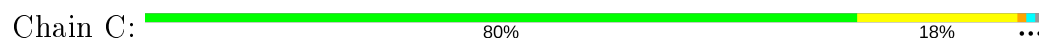
4.2.4 Score per residue for model 4

- Molecule 1: Apolipoprotein A-I

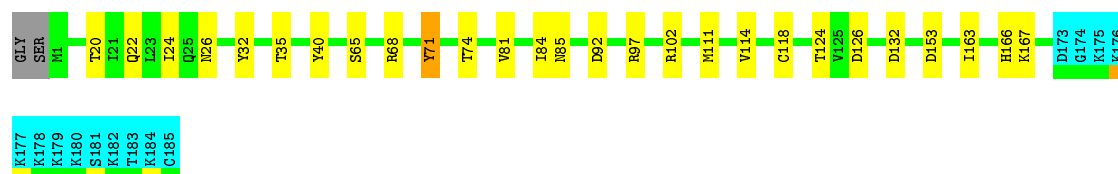




- Molecule 1: Apolipoprotein A-I

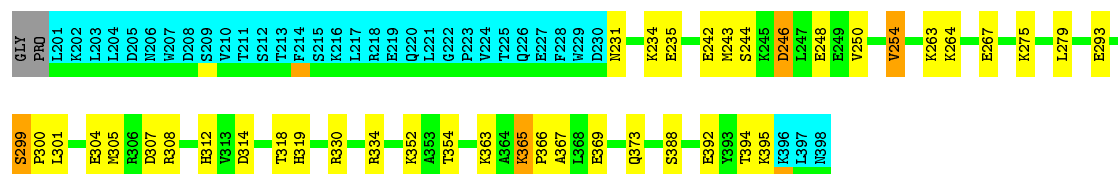


- Molecule 2: GTPase KRas

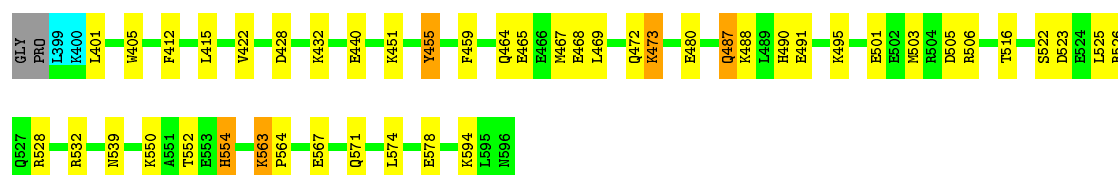


4.2.5 Score per residue for model 5

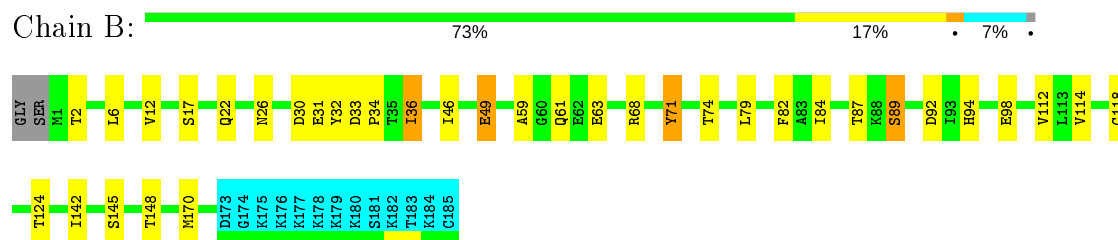
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

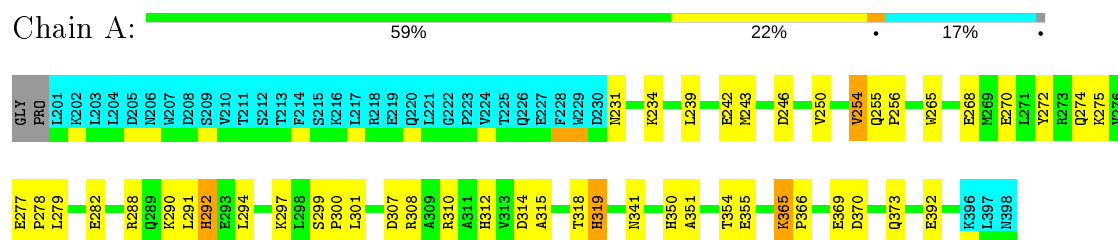


- Molecule 2: GTPase KRas

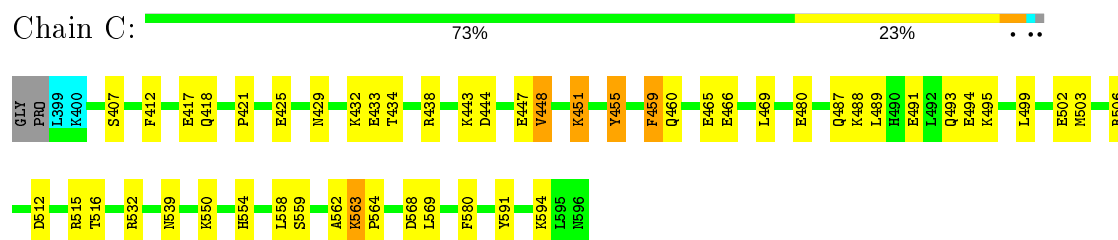


4.2.6 Score per residue for model 6

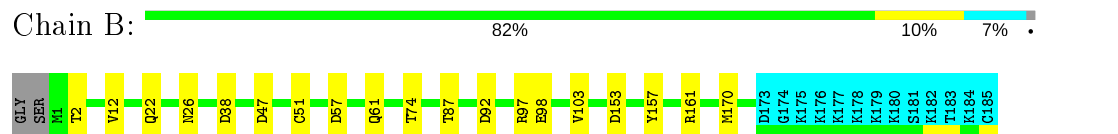
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

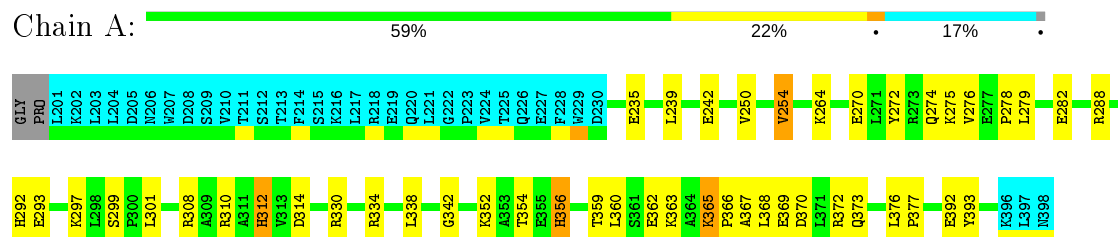


- Molecule 2: GTPase KRas

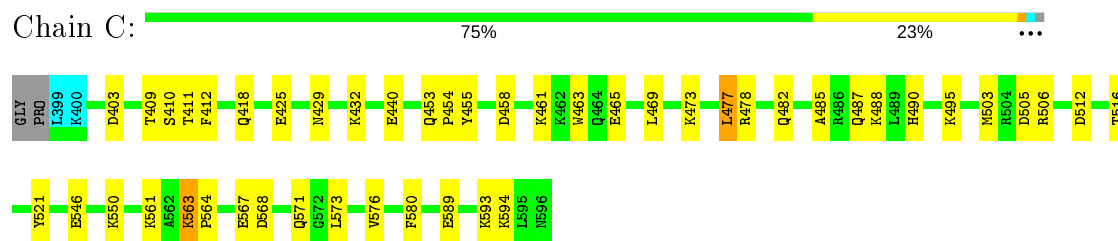


4.2.7 Score per residue for model 7

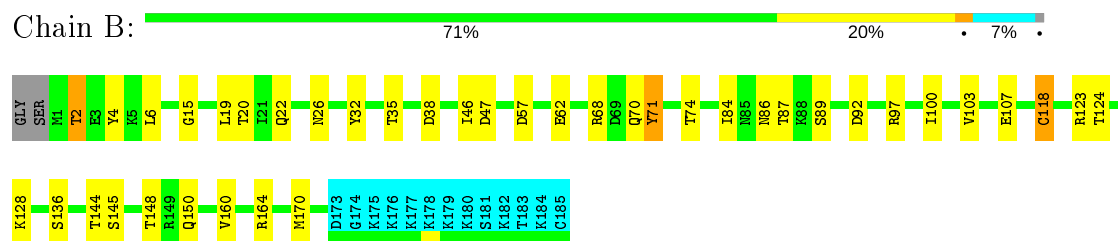
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



5 Refinement protocol and experimental data overview

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

Of the 3000 calculated structures, 7 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
HADDOCK	structure calculation	
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	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: 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 [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	1347	18	1355	30±7
1	C	1607	22	1601	41±15
2	B	1376	323	1366	12±4
3	A	3456	0	5374	126±20
4	A	864	0	1216	47±4
5	B	32	0	13	1±1
All	All	60781	2541	76490	1312

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:8:PCW:H272	1:C:459:PHE:CZ	1.65	1.18	6	1
3:A:15:PCW:H281	1:C:554:HIS:CE1	1.64	1.26	6	1
3:A:15:PCW:C28	1:C:554:HIS:CE1	1.55	1.85	6	1
3:A:65:PCW:H281	1:C:488:LYS:CE	1.54	1.23	6	2
1:A:308:ARG:CD	1:C:469:LEU:HD11	1.51	1.34	1	1
3:A:29:PCW:C26	1:C:521:TYR:OH	1.44	1.65	1	1
3:A:65:PCW:H281	1:C:488:LYS:CD	1.41	1.43	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:65:PCW:C28	1:C:488:LYS:HD3	1.39	1.44	5	1
3:A:8:PCW:C27	1:C:459:PHE:CZ	1.37	2.08	6	1
3:A:65:PCW:C28	1:C:488:LYS:CE	1.36	1.87	6	2
3:A:8:PCW:H271	1:C:455:TYR:CE2	1.36	1.53	7	1
1:C:465:GLU:O	1:C:469:LEU:HG	1.32	1.19	2	6
3:A:15:PCW:C28	1:C:554:HIS:NE2	1.25	1.97	6	1
1:C:465:GLU:O	1:C:469:LEU:CG	1.25	1.82	7	4
3:A:15:PCW:H281	1:C:554:HIS:NE2	1.25	1.42	6	1
1:A:308:ARG:CG	1:C:469:LEU:HD11	1.24	1.63	1	2
3:A:65:PCW:C27	1:C:488:LYS:NZ	1.23	2.01	6	1
1:A:308:ARG:CD	1:C:469:LEU:CD1	1.19	2.21	1	1
3:A:29:PCW:C27	1:C:521:TYR:OH	1.19	1.90	1	1
1:A:308:ARG:HG3	1:C:469:LEU:CD1	1.13	1.72	5	3
3:A:15:PCW:H283	1:C:554:HIS:CE1	1.12	1.77	6	1
1:A:308:ARG:HD3	1:C:469:LEU:CD1	1.12	1.75	1	2
3:A:29:PCW:C28	1:C:521:TYR:OH	1.10	1.97	1	2
1:C:567:GLU:O	1:C:571:GLN:HG3	1.07	1.48	2	5
3:A:8:PCW:C27	1:C:455:TYR:CZ	1.06	2.38	7	1
3:A:29:PCW:H283	1:C:521:TYR:CZ	1.05	1.86	1	1
3:A:8:PCW:C27	1:C:455:TYR:CE2	1.05	2.39	7	1
1:A:308:ARG:CG	1:C:469:LEU:CD1	1.04	2.34	1	2
1:A:308:ARG:CD	1:C:469:LEU:HD21	1.03	1.82	4	2
3:A:65:PCW:C28	1:C:488:LYS:CD	1.02	2.19	5	1
3:A:8:PCW:H272	1:C:459:PHE:CE1	1.00	1.91	6	1
3:A:65:PCW:H281	1:C:488:LYS:HE3	0.99	1.30	6	1
1:A:393:TYR:CE1	3:A:32:PCW:H283	0.98	1.93	3	1
3:A:29:PCW:H283	1:C:521:TYR:OH	0.98	1.52	1	1
3:A:65:PCW:C28	1:C:488:LYS:HD2	0.98	1.88	3	1
3:A:65:PCW:C27	1:C:488:LYS:CE	0.97	2.41	6	1
3:A:8:PCW:H271	1:C:455:TYR:CZ	0.97	1.93	7	1
3:A:15:PCW:C27	1:C:554:HIS:NE2	0.96	2.29	6	1
1:A:308:ARG:HD3	1:C:469:LEU:HD11	0.96	0.97	1	2
1:A:308:ARG:HD2	1:C:469:LEU:HD21	0.96	1.33	1	2
3:A:65:PCW:H281	1:C:488:LYS:HD2	0.96	1.00	3	1
1:A:308:ARG:HG3	1:C:469:LEU:HD11	0.95	1.01	5	2
3:A:59:PCW:H332	4:A:77:17F:H29	0.94	1.35	6	1
1:A:393:TYR:CE1	3:A:32:PCW:C28	0.94	2.50	3	1
1:A:349:TYR:CD1	3:A:2:PCW:H281	0.93	1.99	3	1
1:A:349:TYR:CE1	3:A:2:PCW:C28	0.93	2.52	3	1
1:C:465:GLU:O	1:C:469:LEU:CB	0.93	2.16	7	2
3:A:8:PCW:H262	1:C:455:TYR:OH	0.93	1.63	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:29:PCW:H261	1:C:521:TYR:OH	0.93	1.63	1	1
1:A:297:LYS:HE2	1:C:477:LEU:HG	0.92	1.39	7	1
3:A:8:PCW:H272	1:C:459:PHE:HZ	0.92	1.22	6	1
3:A:65:PCW:H282	1:C:488:LYS:HZ1	0.91	0.75	6	1
1:A:349:TYR:CD1	3:A:2:PCW:C28	0.91	2.53	3	1
3:A:8:PCW:H272	1:C:459:PHE:CE2	0.90	2.02	6	1
2:B:38:ASP:HB2	2:B:57:ASP:HB3	0.90	1.44	6	4
3:A:15:PCW:H281	1:C:554:HIS:ND1	0.88	1.83	6	1
1:A:393:TYR:CE1	3:A:32:PCW:H261	0.87	2.04	3	1
1:A:308:ARG:HD2	1:C:469:LEU:CD2	0.85	2.00	1	2
3:A:15:PCW:H281	1:C:554:HIS:CD2	0.85	2.06	6	1
3:A:41:PCW:H332	3:A:59:PCW:H341	0.85	1.47	3	2
3:A:29:PCW:H281	1:C:521:TYR:OH	0.84	1.73	7	1
1:C:465:GLU:O	1:C:469:LEU:CD1	0.84	2.25	7	2
3:A:16:PCW:H52	3:A:16:PCW:H32	0.83	1.48	3	1
3:A:59:PCW:H382	4:A:77:17F:H36	0.83	1.50	5	3
3:A:65:PCW:C27	1:C:488:LYS:HD3	0.82	2.03	5	1
3:A:8:PCW:C26	1:C:455:TYR:CZ	0.82	2.63	7	1
1:A:393:TYR:HE1	3:A:32:PCW:H283	0.82	1.34	3	1
1:C:563:LYS:HB2	1:C:564:PRO:HD3	0.82	1.51	2	7
3:A:65:PCW:C28	1:C:488:LYS:HZ1	0.81	0.35	6	1
3:A:62:PCW:H381	3:A:72:PCW:H171	0.81	1.49	7	2
3:A:62:PCW:H122	3:A:72:PCW:H182	0.81	1.52	5	1
3:A:20:PCW:H42	3:A:31:PCW:H11	0.81	1.50	7	1
3:A:29:PCW:C28	1:C:521:TYR:CZ	0.80	2.61	1	1
3:A:65:PCW:H281	1:C:488:LYS:HE2	0.80	1.54	5	1
3:A:26:PCW:H12	3:A:28:PCW:H12	0.80	1.51	4	2
3:A:7:PCW:H322	4:A:33:17F:H8A	0.79	1.53	2	1
4:A:77:17F:H4A	4:A:77:17F:H2	0.79	1.53	5	2
3:A:65:PCW:C28	1:C:488:LYS:NZ	0.79	0.74	6	1
4:A:74:17F:H38	4:A:75:17F:H10	0.79	1.53	3	1
1:A:279:LEU:HD22	1:C:495:LYS:HG2	0.79	1.53	1	5
3:A:65:PCW:C27	1:C:488:LYS:HZ1	0.79	1.73	6	1
1:A:393:TYR:HE1	3:A:32:PCW:C28	0.79	1.89	3	1
1:A:308:ARG:HD3	1:C:469:LEU:HD21	0.78	1.54	4	1
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.78	1.55	3	6
3:A:20:PCW:C48	1:C:532:ARG:HH11	0.78	1.92	2	1
3:A:20:PCW:H82	3:A:31:PCW:H132	0.77	1.56	4	1
3:A:20:PCW:H471	1:C:532:ARG:NH1	0.77	1.94	2	1
3:A:8:PCW:C27	1:C:459:PHE:HZ	0.77	1.79	6	1
3:A:13:PCW:H122	3:A:18:PCW:H142	0.76	1.57	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:15:PCW:H271	1:C:554:HIS:NE2	0.76	1.94	6	1
3:A:8:PCW:H262	1:C:455:TYR:CZ	0.76	2.16	7	1
1:A:349:TYR:CE1	3:A:2:PCW:H281	0.76	2.12	3	1
3:A:59:PCW:H331	4:A:77:17F:H29	0.75	1.58	2	2
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.75	1.58	7	4
3:A:53:PCW:H162	3:A:64:PCW:H161	0.75	1.57	6	1
3:A:12:PCW:H12	3:A:22:PCW:H31	0.74	1.58	2	1
3:A:32:PCW:H331	4:A:33:17F:H32	0.74	1.59	3	4
1:A:369:GLU:O	1:A:373:GLN:HG3	0.74	1.81	1	7
3:A:48:PCW:H372	3:A:54:PCW:H182	0.74	1.59	2	3
1:A:308:ARG:CD	1:C:469:LEU:CG	0.74	2.65	1	1
3:A:65:PCW:C28	1:C:488:LYS:HZ2	0.73	1.46	6	1
3:A:62:PCW:H352	3:A:72:PCW:H152	0.73	1.58	3	1
3:A:14:PCW:H381	4:A:34:17F:H32	0.73	1.60	7	2
3:A:32:PCW:H342	4:A:35:17F:H11	0.73	1.59	6	2
3:A:49:PCW:H442	4:A:80:17F:H43	0.73	1.61	6	2
3:A:15:PCW:H283	1:C:554:HIS:HE1	0.73	1.40	6	1
3:A:20:PCW:H481	1:C:532:ARG:HH11	0.72	1.43	2	1
3:A:3:PCW:H212	3:A:19:PCW:H242	0.72	1.62	4	1
3:A:65:PCW:H271	1:C:488:LYS:HE2	0.72	1.61	6	1
3:A:49:PCW:H152	3:A:57:PCW:H321	0.72	1.62	1	3
1:C:465:GLU:O	1:C:469:LEU:HB2	0.71	1.85	7	1
3:A:14:PCW:H151	4:A:37:17F:H11	0.71	1.62	7	1
1:A:308:ARG:HG3	1:C:469:LEU:HD21	0.71	1.62	2	3
3:A:15:PCW:H272	1:C:554:HIS:HE1	0.71	1.45	5	1
3:A:62:PCW:H352	3:A:72:PCW:H162	0.71	1.62	1	1
3:A:8:PCW:C26	1:C:459:PHE:CZ	0.71	2.73	6	1
1:A:393:TYR:CZ	3:A:32:PCW:H283	0.71	2.20	3	1
1:A:393:TYR:HE1	3:A:32:PCW:H261	0.70	1.42	3	1
3:A:4:PCW:H152	3:A:4:PCW:H351	0.70	1.63	7	2
1:A:316:LEU:HG	1:C:462:LYS:HE3	0.70	1.63	4	1
4:A:39:17F:H52	3:A:52:PCW:H481	0.70	1.61	5	1
3:A:30:PCW:H342	4:A:40:17F:H11A	0.70	1.63	2	1
3:A:15:PCW:H71	4:A:39:17F:N1	0.70	2.01	2	1
1:C:567:GLU:O	1:C:571:GLN:CG	0.70	2.34	2	2
3:A:8:PCW:H271	1:C:455:TYR:CD2	0.70	2.18	7	1
3:A:57:PCW:H20	4:A:80:17F:H40	0.70	1.61	2	1
3:A:30:PCW:H472	4:A:37:17F:H52	0.70	1.60	3	1
3:A:20:PCW:H471	1:C:532:ARG:HH12	0.70	1.46	2	1
1:C:453:GLN:HB2	1:C:454:PRO:HD3	0.70	1.61	4	4
3:A:65:PCW:H271	1:C:488:LYS:CE	0.69	2.17	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:29:PCW:C27	1:C:521:TYR:CZ	0.69	2.74	1	1
3:A:30:PCW:H2	4:A:40:17F:H4A	0.69	1.64	5	1
3:A:48:PCW:H431	3:A:54:PCW:H162	0.69	1.63	5	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.69	1.63	1	2
3:A:29:PCW:H283	1:C:521:TYR:CE1	0.69	2.22	1	1
1:A:308:ARG:HD2	1:C:469:LEU:CG	0.69	2.17	1	1
3:A:41:PCW:H371	3:A:59:PCW:H362	0.69	1.64	2	1
3:A:8:PCW:H261	1:C:459:PHE:CE2	0.69	2.22	6	1
1:A:308:ARG:CD	1:C:469:LEU:CD2	0.68	2.69	4	2
3:A:17:PCW:H121	4:A:36:17F:H6	0.68	1.64	6	1
3:A:57:PCW:H182	4:A:76:17F:H42	0.68	1.62	7	2
3:A:45:PCW:H332	3:A:49:PCW:H132	0.68	1.63	4	1
3:A:57:PCW:H231	4:A:76:17F:H41	0.68	1.63	5	1
1:A:341:ASN:HD21	1:C:433:GLU:HA	0.68	1.47	6	2
3:A:11:PCW:H412	3:A:16:PCW:H39	0.68	1.65	4	1
3:A:6:PCW:H151	3:A:16:PCW:H39	0.68	1.65	1	1
3:A:65:PCW:H283	1:C:488:LYS:HD3	0.68	1.60	5	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.67	1.88	1	6
3:A:63:PCW:H341	3:A:63:PCW:H131	0.67	1.66	7	1
3:A:15:PCW:H411	3:A:24:PCW:H421	0.67	1.67	6	2
3:A:8:PCW:C27	1:C:459:PHE:CE2	0.67	2.74	6	1
3:A:45:PCW:H61	3:A:71:PCW:H232	0.67	1.66	5	1
3:A:20:PCW:C48	1:C:532:ARG:NH1	0.67	2.58	2	1
1:A:352:LYS:HG2	1:C:422:VAL:HG13	0.67	1.66	2	1
3:A:6:PCW:H332	3:A:16:PCW:H321	0.67	1.66	5	1
3:A:41:PCW:H461	3:A:61:PCW:H271	0.67	1.67	5	1
3:A:10:PCW:H372	3:A:21:PCW:H341	0.67	1.67	3	1
3:A:15:PCW:H272	1:C:554:HIS:CE1	0.67	2.25	5	1
3:A:16:PCW:H411	4:A:39:17F:H36	0.67	1.65	4	1
1:A:308:ARG:CB	1:C:469:LEU:HD11	0.67	2.20	1	1
1:A:349:TYR:CG	3:A:2:PCW:H281	0.67	2.24	3	1
3:A:14:PCW:H331	4:A:34:17F:H20A	0.66	1.66	3	1
3:A:8:PCW:H242	1:C:459:PHE:CZ	0.66	2.24	1	1
1:C:418:GLN:O	1:C:422:VAL:HB	0.66	1.89	2	2
3:A:66:PCW:H141	4:A:79:17F:H6	0.66	1.67	4	1
3:A:20:PCW:C47	1:C:532:ARG:NH1	0.66	2.59	2	1
3:A:59:PCW:H382	4:A:77:17F:H12A	0.66	1.68	3	3
3:A:1:PCW:H241	3:A:5:PCW:H251	0.66	1.68	3	1
4:A:40:17F:H49	3:A:70:PCW:H283	0.66	1.68	6	1
3:A:48:PCW:H361	3:A:54:PCW:H151	0.66	1.66	7	1
2:B:145:SER:HB3	2:B:150:GLN:HB3	0.65	1.67	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:60:PCW:H422	3:A:62:PCW:H471	0.65	1.68	1	1
3:A:13:PCW:H161	3:A:18:PCW:H361	0.65	1.67	2	1
3:A:32:PCW:H342	4:A:35:17F:H9	0.65	1.68	7	1
1:A:393:TYR:CD1	3:A:32:PCW:H271	0.65	2.25	7	1
1:A:393:TYR:OH	3:A:32:PCW:C28	0.65	2.45	3	1
3:A:47:PCW:H221	4:A:76:17F:H47	0.65	1.67	3	1
3:A:21:PCW:H172	4:A:36:17F:H58	0.65	1.67	7	1
3:A:20:PCW:H32	3:A:24:PCW:H371	0.65	1.68	3	1
3:A:44:PCW:H482	3:A:64:PCW:H422	0.65	1.67	7	1
3:A:45:PCW:H242	4:A:79:17F:H54	0.65	1.67	7	1
3:A:32:PCW:H331	4:A:33:17F:C1Y	0.65	2.22	2	1
3:A:14:PCW:H121	4:A:34:17F:H34	0.65	1.69	3	1
3:A:65:PCW:H282	1:C:488:LYS:NZ	0.65	1.53	6	1
3:A:9:PCW:H212	3:A:26:PCW:H122	0.65	1.69	4	2
3:A:15:PCW:H281	1:C:554:HIS:CG	0.64	2.26	6	1
3:A:5:PCW:H19	4:A:38:17F:H12	0.64	1.67	6	1
3:A:13:PCW:H382	3:A:18:PCW:H152	0.64	1.68	7	2
1:A:308:ARG:HD3	1:C:469:LEU:CD2	0.64	2.21	4	1
1:A:393:TYR:CZ	3:A:32:PCW:C28	0.64	2.80	3	1
1:A:393:TYR:OH	3:A:32:PCW:H283	0.64	1.92	3	1
3:A:6:PCW:H431	3:A:7:PCW:H39	0.64	1.68	3	1
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.64	1.69	3	1
3:A:12:PCW:H141	3:A:22:PCW:H362	0.64	1.68	1	1
1:A:231:ASN:HA	1:A:234:LYS:HE2	0.64	1.68	5	2
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.64	1.69	6	2
4:A:38:17F:H11A	4:A:38:17F:H31	0.64	1.69	7	1
4:A:74:17F:H68	4:A:75:17F:H73	0.64	1.69	7	2
4:A:35:17F:H63	4:A:35:17F:H12A	0.64	1.68	4	2
3:A:19:PCW:H51	3:A:23:PCW:H322	0.64	1.68	2	1
3:A:30:PCW:H372	4:A:40:17F:H61	0.64	1.69	1	1
3:A:68:PCW:H121	3:A:69:PCW:H342	0.64	1.70	7	2
3:A:32:PCW:H331	4:A:33:17F:H31	0.64	1.70	2	1
4:A:74:17F:H72	4:A:75:17F:H73	0.64	1.69	2	1
4:A:40:17F:H55	3:A:70:PCW:H272	0.64	1.68	1	1
3:A:2:PCW:H342	3:A:17:PCW:H351	0.63	1.68	3	1
3:A:21:PCW:H182	3:A:51:PCW:H252	0.63	1.68	1	1
3:A:57:PCW:H232	4:A:76:17F:H41	0.63	1.69	6	1
4:A:35:17F:H12A	4:A:35:17F:H63	0.63	1.71	2	1
3:A:16:PCW:H232	3:A:24:PCW:H432	0.63	1.70	6	1
1:A:393:TYR:HD1	3:A:32:PCW:C28	0.63	2.06	7	1
3:A:12:PCW:H141	3:A:30:PCW:H212	0.63	1.69	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:114:VAL:HG22	2:B:142:ILE:HB	0.63	1.70	5	1
4:A:77:17F:C4	4:A:77:17F:H1	0.63	2.24	6	3
3:A:49:PCW:H32	3:A:57:PCW:H62	0.63	1.70	7	1
3:A:67:PCW:H141	4:A:75:17F:H57	0.63	1.70	3	1
2:B:12:VAL:HG11	2:B:61:GLN:HG3	0.62	1.71	6	1
1:C:465:GLU:O	1:C:469:LEU:HD12	0.62	1.92	7	2
3:A:26:PCW:H472	4:A:33:17F:H41	0.62	1.68	1	1
1:A:352:LYS:HZ2	1:C:425:GLU:HB3	0.62	1.54	7	1
3:A:5:PCW:H421	4:A:36:17F:H11	0.62	1.69	1	2
4:A:39:17F:H47	3:A:62:PCW:H262	0.62	1.71	1	1
3:A:49:PCW:H462	4:A:80:17F:H42	0.62	1.71	1	1
3:A:64:PCW:H381	3:A:64:PCW:H151	0.62	1.71	6	3
3:A:57:PCW:H422	4:A:79:17F:H47	0.62	1.72	6	1
3:A:70:PCW:H39	3:A:71:PCW:H421	0.62	1.70	4	1
3:A:5:PCW:H411	3:A:17:PCW:H181	0.62	1.70	3	1
3:A:4:PCW:H182	3:A:7:PCW:H182	0.62	1.70	7	1
3:A:17:PCW:H142	4:A:36:17F:H19A	0.62	1.71	4	1
3:A:44:PCW:H461	3:A:55:PCW:H172	0.62	1.71	4	1
3:A:53:PCW:H132	3:A:64:PCW:H121	0.62	1.69	3	1
3:A:1:PCW:H361	4:A:35:17F:H19A	0.62	1.70	4	1
1:A:301:LEU:HD22	1:C:473:LYS:HE2	0.61	1.72	5	1
3:A:20:PCW:H161	3:A:24:PCW:H171	0.61	1.72	5	1
3:A:10:PCW:H62	3:A:22:PCW:H352	0.61	1.70	6	1
3:A:7:PCW:H483	3:A:52:PCW:H442	0.61	1.73	6	1
3:A:5:PCW:H342	3:A:5:PCW:H131	0.61	1.73	1	1
4:A:77:17F:H2	4:A:77:17F:H4A	0.61	1.71	1	1
3:A:14:PCW:H483	3:A:30:PCW:H411	0.61	1.72	5	1
3:A:66:PCW:H152	4:A:79:17F:H6	0.61	1.72	3	3
3:A:3:PCW:H462	3:A:13:PCW:H251	0.61	1.71	7	1
3:A:11:PCW:H411	3:A:28:PCW:H152	0.61	1.71	4	1
3:A:49:PCW:H211	3:A:57:PCW:H372	0.61	1.73	6	1
3:A:62:PCW:H31	3:A:72:PCW:H132	0.61	1.72	1	1
3:A:65:PCW:H283	1:C:488:LYS:HZ2	0.61	1.11	6	1
3:A:62:PCW:H361	3:A:72:PCW:H212	0.61	1.71	7	3
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.61	1.72	7	1
3:A:32:PCW:H152	4:A:33:17F:H20	0.61	1.73	1	2
4:A:35:17F:H8	4:A:35:17F:H33	0.61	1.72	4	1
3:A:13:PCW:H152	3:A:23:PCW:H181	0.61	1.73	3	1
3:A:13:PCW:H41	4:A:34:17F:HN1A	0.60	1.56	1	1
3:A:59:PCW:H121	4:A:77:17F:H30	0.60	1.72	6	3
3:A:1:PCW:H41	4:A:35:17F:O1	0.60	1.96	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:32:PCW:H471	3:A:55:PCW:H221	0.60	1.73	7	1
3:A:45:PCW:H252	4:A:74:17F:H39	0.60	1.72	7	1
3:A:65:PCW:C27	1:C:488:LYS:HZ3	0.60	1.87	6	1
1:A:393:TYR:HD1	3:A:32:PCW:C27	0.60	2.09	7	1
3:A:19:PCW:H371	3:A:23:PCW:H431	0.60	1.73	4	1
3:A:20:PCW:H251	4:A:78:17F:H54	0.60	1.73	1	1
3:A:67:PCW:H331	3:A:67:PCW:H73	0.60	1.74	2	2
3:A:20:PCW:H251	3:A:72:PCW:H451	0.60	1.73	6	1
3:A:9:PCW:H371	4:A:34:17F:H31	0.60	1.72	6	1
3:A:1:PCW:H362	4:A:36:17F:H37	0.60	1.73	1	1
3:A:1:PCW:H40	3:A:68:PCW:H252	0.60	1.73	7	1
2:B:84:ILE:HD12	2:B:123:ARG:HG3	0.60	1.74	3	2
3:A:13:PCW:H382	3:A:18:PCW:H161	0.60	1.71	4	1
3:A:9:PCW:H221	3:A:69:PCW:H272	0.60	1.72	7	1
3:A:44:PCW:H472	3:A:55:PCW:H222	0.60	1.74	4	1
4:A:77:17F:C4	4:A:77:17F:H2	0.59	2.27	5	2
3:A:26:PCW:H212	3:A:67:PCW:H241	0.59	1.72	7	1
2:B:32:TYR:HD1	5:B:201:GNP:H5'2	0.59	1.56	2	1
3:A:26:PCW:H441	4:A:33:17F:H41	0.59	1.74	7	1
3:A:8:PCW:H212	3:A:27:PCW:H251	0.59	1.72	3	1
3:A:12:PCW:H121	3:A:30:PCW:H171	0.59	1.74	1	1
3:A:24:PCW:H82	2:B:128:LYS:HD3	0.59	1.75	7	1
3:A:10:PCW:H11	3:A:21:PCW:H52	0.59	1.73	5	1
3:A:21:PCW:H361	3:A:21:PCW:H122	0.59	1.75	6	2
3:A:8:PCW:C26	1:C:459:PHE:CE2	0.59	2.85	6	1
3:A:8:PCW:C27	1:C:455:TYR:CE1	0.59	2.84	7	1
4:A:37:17F:H50	3:A:49:PCW:H251	0.59	1.73	3	1
3:A:57:PCW:H452	4:A:79:17F:H48	0.59	1.73	5	1
3:A:7:PCW:H11	3:A:16:PCW:O2P	0.59	1.97	5	1
3:A:6:PCW:H371	3:A:7:PCW:H142	0.59	1.73	6	1
3:A:63:PCW:H121	3:A:67:PCW:H171	0.59	1.75	5	1
4:A:75:17F:H40	4:A:75:17F:H69	0.59	1.73	2	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.59	1.97	6	5
1:A:288:ARG:O	1:A:292:HIS:HB2	0.59	1.98	6	2
1:A:264:LYS:HE3	1:C:509:ALA:HB1	0.59	1.74	2	2
3:A:57:PCW:H211	4:A:76:17F:H42	0.59	1.73	3	1
1:A:242:GLU:HB3	1:C:532:ARG:HH21	0.58	1.58	6	1
3:A:47:PCW:H212	4:A:73:17F:H37	0.58	1.75	2	1
1:C:561:LYS:HA	1:C:565:ALA:HB3	0.58	1.73	2	1
1:A:330:ARG:O	1:A:334:ARG:HG2	0.58	1.98	7	3
3:A:59:PCW:H381	4:A:77:17F:H36	0.58	1.74	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:24:PCW:H42	4:A:39:17F:H1	0.58	1.73	5	1
1:C:491:GLU:HB3	1:C:495:LYS:HE2	0.58	1.76	4	4
4:A:37:17F:HN1	4:A:37:17F:H4	0.58	1.57	6	1
3:A:16:PCW:H331	4:A:39:17F:H8A	0.58	1.74	6	1
3:A:59:PCW:H11	3:A:59:PCW:H51	0.58	1.75	7	1
1:C:503:MET:HA	1:C:506:ARG:HD2	0.58	1.74	5	3
3:A:1:PCW:H462	4:A:36:17F:H46	0.58	1.74	2	1
3:A:15:PCW:H71	4:A:39:17F:HN1A	0.58	1.58	2	1
3:A:6:PCW:H71	3:A:24:PCW:O2P	0.58	1.98	5	1
3:A:7:PCW:H471	3:A:41:PCW:H411	0.58	1.74	2	1
3:A:45:PCW:H412	3:A:49:PCW:H31	0.58	1.74	4	2
4:A:76:17F:H78	1:C:470:TYR:CE1	0.58	2.33	3	1
1:A:393:TYR:HD1	3:A:32:PCW:H271	0.58	1.59	7	1
3:A:17:PCW:H141	4:A:36:17F:H32	0.58	1.76	3	1
3:A:58:PCW:H331	3:A:61:PCW:H382	0.58	1.75	6	1
3:A:41:PCW:H331	3:A:41:PCW:H131	0.58	1.75	1	1
3:A:66:PCW:H451	4:A:79:17F:H70	0.58	1.76	1	1
3:A:17:PCW:H262	3:A:21:PCW:H172	0.57	1.76	6	1
3:A:45:PCW:H271	4:A:74:17F:H45	0.57	1.76	2	1
3:A:42:PCW:H472	3:A:69:PCW:H161	0.57	1.75	1	1
3:A:21:PCW:H332	3:A:22:PCW:H39	0.57	1.75	3	1
4:A:73:17F:H11	4:A:76:17F:H31	0.57	1.73	5	1
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.57	1.77	6	2
3:A:54:PCW:H331	3:A:54:PCW:H132	0.57	1.75	4	1
3:A:57:PCW:H421	4:A:79:17F:H52	0.57	1.76	5	1
3:A:53:PCW:H352	3:A:68:PCW:H411	0.57	1.77	5	1
3:A:8:PCW:H272	1:C:455:TYR:CE1	0.57	2.35	7	1
3:A:23:PCW:H42	2:B:136:SER:HB2	0.57	1.76	1	1
3:A:70:PCW:H372	3:A:71:PCW:H162	0.57	1.76	6	1
3:A:3:PCW:H412	3:A:13:PCW:H271	0.57	1.77	2	1
3:A:4:PCW:H382	3:A:4:PCW:H151	0.57	1.76	3	1
3:A:48:PCW:H361	3:A:54:PCW:H152	0.57	1.76	2	2
1:C:451:LYS:O	1:C:455:TYR:HB2	0.57	1.99	3	4
3:A:32:PCW:H352	4:A:33:17F:H56	0.57	1.76	2	2
4:A:35:17F:H40	3:A:55:PCW:H241	0.57	1.77	2	1
4:A:37:17F:H9A	4:A:37:17F:H18	0.56	1.76	5	1
3:A:2:PCW:H462	3:A:53:PCW:H271	0.56	1.77	7	2
2:B:68:ARG:HA	2:B:71:TYR:CE2	0.56	2.35	4	2
3:A:16:PCW:C8	2:B:133:LEU:HA	0.56	2.30	3	1
4:A:34:17F:H40	4:A:75:17F:H43	0.56	1.77	4	2
1:A:308:ARG:HD3	1:C:469:LEU:CG	0.56	2.30	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:40:17F:HN1	4:A:40:17F:H4	0.56	1.60	2	1
4:A:34:17F:H43	4:A:75:17F:H47	0.56	1.74	1	1
3:A:8:PCW:H181	3:A:8:PCW:H461	0.56	1.77	6	1
3:A:32:PCW:H342	4:A:33:17F:H57	0.56	1.77	3	1
3:A:57:PCW:H182	4:A:76:17F:H38	0.56	1.77	4	1
3:A:12:PCW:H222	3:A:22:PCW:H451	0.56	1.77	2	1
3:A:27:PCW:H341	4:A:37:17F:H19	0.56	1.76	1	1
3:A:9:PCW:H483	4:A:34:17F:H75	0.56	1.76	4	1
1:C:508:ARG:O	1:C:512:ASP:HB2	0.56	2.01	2	2
3:A:16:PCW:H41	2:B:98:GLU:HB3	0.56	1.77	5	1
3:A:8:PCW:H182	3:A:27:PCW:H211	0.56	1.76	6	1
3:A:10:PCW:H262	3:A:22:PCW:H20	0.56	1.76	7	1
3:A:32:PCW:H332	4:A:35:17F:H11A	0.56	1.77	3	1
1:A:308:ARG:HG3	1:C:469:LEU:HD13	0.56	1.76	1	1
3:A:5:PCW:H481	3:A:12:PCW:H411	0.56	1.78	7	1
3:A:9:PCW:H51	3:A:9:PCW:H31	0.56	1.76	4	1
1:A:386:PHE:HZ	4:A:33:17F:H78	0.56	1.61	2	1
3:A:9:PCW:H211	3:A:28:PCW:H412	0.56	1.77	5	1
3:A:44:PCW:H41	4:A:77:17F:H2	0.56	1.78	4	1
4:A:36:17F:H53	4:A:40:17F:H48	0.56	1.78	1	1
2:B:34:PRO:HA	5:B:201:GNP:O3G	0.55	1.99	1	3
3:A:17:PCW:H472	3:A:53:PCW:H451	0.55	1.77	7	1
1:C:458:ASP:HA	1:C:461:LYS:HE3	0.55	1.78	7	1
3:A:65:PCW:C28	1:C:488:LYS:HE2	0.55	2.23	5	1
3:A:14:PCW:H381	4:A:34:17F:H18A	0.55	1.78	2	1
4:A:39:17F:H20A	4:A:39:17F:H8	0.55	1.77	2	1
3:A:45:PCW:H481	3:A:49:PCW:H371	0.55	1.78	1	1
3:A:56:PCW:H381	3:A:56:PCW:H171	0.55	1.76	6	1
1:A:349:TYR:CD1	3:A:2:PCW:H282	0.55	2.35	3	1
3:A:25:PCW:H483	3:A:66:PCW:H251	0.55	1.78	4	1
1:A:308:ARG:CB	1:C:469:LEU:CD1	0.55	2.84	1	1
3:A:48:PCW:H352	3:A:54:PCW:H212	0.55	1.79	1	1
2:B:82:PHE:HB2	2:B:89:SER:HB2	0.55	1.77	5	1
1:A:341:ASN:ND2	1:C:433:GLU:HA	0.55	2.17	6	1
3:A:45:PCW:H283	4:A:75:17F:H77	0.55	1.77	7	1
3:A:47:PCW:H252	4:A:76:17F:H48	0.55	1.78	2	1
1:A:334:ARG:HD2	1:C:440:GLU:OE1	0.55	2.02	7	4
3:A:53:PCW:H182	3:A:64:PCW:H181	0.55	1.79	1	4
3:A:3:PCW:H71	3:A:19:PCW:H32	0.55	1.78	2	2
4:A:35:17F:H73	4:A:38:17F:H69	0.55	1.77	3	1
2:B:78:PHE:HB2	2:B:111:MET:HG2	0.55	1.79	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:16:PCW:H63	2:B:98:GLU:HB2	0.55	1.78	5	1
3:A:60:PCW:H362	3:A:62:PCW:H121	0.55	1.75	5	1
3:A:48:PCW:H362	3:A:54:PCW:H351	0.55	1.77	4	2
4:A:35:17F:H44	3:A:55:PCW:H241	0.55	1.79	6	1
3:A:47:PCW:H221	4:A:76:17F:H52	0.55	1.78	7	1
1:C:528:ARG:HB3	1:C:532:ARG:NH2	0.55	2.16	1	2
3:A:43:PCW:H122	3:A:43:PCW:H351	0.55	1.77	6	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.55	2.02	1	7
3:A:43:PCW:H351	3:A:43:PCW:H122	0.55	1.79	2	2
3:A:30:PCW:H40	4:A:34:17F:H49	0.55	1.78	4	1
3:A:25:PCW:H142	3:A:25:PCW:H382	0.54	1.78	6	1
3:A:16:PCW:H371	4:A:39:17F:H57	0.54	1.78	2	1
3:A:57:PCW:H231	4:A:76:17F:H45	0.54	1.78	2	1
1:A:352:LYS:NZ	1:C:425:GLU:HB3	0.54	2.17	7	1
3:A:8:PCW:C27	1:C:455:TYR:CD2	0.54	2.85	7	1
3:A:6:PCW:H121	3:A:11:PCW:H352	0.54	1.78	1	1
3:A:30:PCW:H431	4:A:34:17F:H54	0.54	1.78	4	1
1:A:393:TYR:CE1	3:A:32:PCW:H282	0.54	2.35	3	1
3:A:22:PCW:H61	4:A:37:17F:O2	0.54	2.03	1	1
3:A:47:PCW:H283	4:A:76:17F:H49	0.54	1.79	5	1
3:A:59:PCW:C33	4:A:77:17F:H29	0.54	2.32	2	3
1:C:478:ARG:O	1:C:482:GLN:HB2	0.54	2.02	7	1
3:A:63:PCW:H182	3:A:63:PCW:H442	0.54	1.78	2	1
3:A:55:PCW:H31	3:A:64:PCW:H342	0.54	1.79	3	1
3:A:42:PCW:H212	3:A:63:PCW:H83	0.54	1.80	7	1
3:A:62:PCW:H372	3:A:72:PCW:H141	0.54	1.77	2	1
4:A:33:17F:H30	4:A:35:17F:H34	0.54	1.78	1	1
1:A:244:SER:O	1:A:248:GLU:HB2	0.54	2.03	5	1
3:A:18:PCW:H483	4:A:79:17F:H63	0.54	1.79	5	1
3:A:32:PCW:C34	4:A:35:17F:H11	0.54	2.33	6	1
3:A:15:PCW:H82	4:A:39:17F:HN1	0.54	1.63	7	1
2:B:46:ILE:HD13	2:B:160:VAL:HG21	0.54	1.78	7	1
3:A:11:PCW:H472	3:A:63:PCW:H171	0.54	1.80	7	1
3:A:23:PCW:H19	4:A:34:17F:H61	0.54	1.79	2	1
4:A:39:17F:H8	4:A:39:17F:H57	0.53	1.79	6	1
3:A:63:PCW:H452	3:A:63:PCW:H242	0.53	1.80	6	1
1:A:369:GLU:O	1:A:373:GLN:CG	0.53	2.55	1	1
3:A:28:PCW:H40	3:A:63:PCW:H232	0.53	1.79	5	1
3:A:57:PCW:H182	4:A:80:17F:H12	0.53	1.78	6	1
1:A:231:ASN:HA	1:A:234:LYS:CE	0.53	2.34	5	1
1:C:473:LYS:O	1:C:477:LEU:HB2	0.53	2.03	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:GLY:O	2:B:19:LEU:HG	0.53	2.03	7	1
2:B:2:THR:HB	2:B:4:TYR:CE2	0.53	2.39	7	1
3:A:49:PCW:H372	3:A:57:PCW:H412	0.53	1.80	4	3
3:A:25:PCW:O2P	3:A:31:PCW:H41	0.53	2.03	3	1
3:A:45:PCW:H241	4:A:79:17F:H53	0.53	1.79	1	1
1:C:469:LEU:O	1:C:473:LYS:HB2	0.53	2.03	5	1
3:A:5:PCW:H231	4:A:38:17F:H63	0.53	1.79	7	1
1:C:514:LEU:HA	1:C:517:HIS:HB2	0.53	1.81	4	1
3:A:6:PCW:H351	3:A:16:PCW:H321	0.53	1.79	3	1
3:A:5:PCW:H361	3:A:17:PCW:H61	0.53	1.80	1	1
4:A:74:17F:H41	4:A:75:17F:H8	0.53	1.80	7	1
2:B:2:THR:HB	2:B:4:TYR:HE2	0.53	1.63	7	1
3:A:32:PCW:C33	4:A:33:17F:H32	0.53	2.34	4	1
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.53	1.79	3	2
3:A:48:PCW:H162	3:A:54:PCW:H161	0.53	1.80	5	1
3:A:45:PCW:H71	3:A:71:PCW:H222	0.53	1.80	4	1
3:A:1:PCW:H242	4:A:38:17F:H66	0.53	1.81	5	1
3:A:6:PCW:H231	3:A:24:PCW:H151	0.53	1.80	5	1
3:A:30:PCW:H39	4:A:40:17F:H63	0.53	1.80	5	1
3:A:59:PCW:H351	4:A:77:17F:H12A	0.53	1.82	4	1
3:A:45:PCW:H421	3:A:49:PCW:H11	0.53	1.80	2	1
3:A:41:PCW:H341	3:A:52:PCW:H39	0.53	1.81	1	1
3:A:28:PCW:H441	3:A:63:PCW:H482	0.52	1.81	5	1
1:A:393:TYR:CD1	3:A:32:PCW:H261	0.52	2.38	3	1
3:A:20:PCW:H19	3:A:31:PCW:H241	0.52	1.82	1	1
4:A:74:17F:H62	4:A:75:17F:H67	0.52	1.81	1	1
3:A:44:PCW:H131	4:A:77:17F:H9	0.52	1.79	1	1
1:C:546:GLU:O	1:C:550:LYS:HD2	0.52	2.03	1	1
3:A:13:PCW:H142	3:A:18:PCW:H151	0.52	1.81	7	2
3:A:49:PCW:H82	4:A:80:17F:N1	0.52	2.19	7	1
3:A:13:PCW:H151	3:A:18:PCW:H172	0.52	1.79	1	1
3:A:10:PCW:O2P	3:A:21:PCW:H83	0.52	2.05	5	1
3:A:9:PCW:H412	3:A:29:PCW:H40	0.52	1.81	5	1
3:A:21:PCW:H162	3:A:51:PCW:H252	0.52	1.80	2	1
3:A:21:PCW:H171	4:A:36:17F:H58	0.52	1.82	2	1
3:A:57:PCW:H40	4:A:79:17F:H52	0.52	1.81	3	1
3:A:63:PCW:H151	3:A:67:PCW:H162	0.52	1.80	3	1
3:A:5:PCW:H271	4:A:38:17F:H70	0.52	1.81	1	1
3:A:23:PCW:H421	3:A:29:PCW:H382	0.52	1.81	4	1
3:A:16:PCW:H242	3:A:24:PCW:H431	0.52	1.81	1	1
3:A:5:PCW:H481	3:A:17:PCW:H20	0.52	1.81	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:388:SER:HB3	1:C:594:LYS:HE2	0.52	1.81	5	1
1:A:310:ARG:O	1:A:314:ASP:HB2	0.52	2.05	4	2
3:A:21:PCW:H172	4:A:36:17F:H66	0.52	1.82	2	1
3:A:57:PCW:H212	4:A:76:17F:H46	0.52	1.80	2	1
3:A:62:PCW:H381	3:A:72:PCW:H161	0.52	1.80	2	1
4:A:75:17F:H75	4:A:75:17F:H44	0.52	1.81	3	1
3:A:3:PCW:H212	3:A:19:PCW:H272	0.52	1.82	1	1
4:A:36:17F:H51	4:A:40:17F:H38	0.52	1.82	5	1
3:A:63:PCW:P	3:A:67:PCW:O1P	0.52	2.67	7	1
3:A:32:PCW:H152	4:A:33:17F:H33	0.52	1.82	4	1
3:A:27:PCW:H462	3:A:47:PCW:H261	0.52	1.81	2	1
3:A:18:PCW:H42	3:A:23:PCW:H62	0.52	1.82	1	1
1:A:393:TYR:CD1	3:A:32:PCW:C27	0.52	2.92	7	1
3:A:16:PCW:H332	4:A:39:17F:H11	0.52	1.80	4	1
3:A:16:PCW:H282	3:A:16:PCW:H472	0.52	1.81	1	1
3:A:21:PCW:H332	3:A:22:PCW:H40	0.51	1.81	6	1
3:A:65:PCW:H283	1:C:488:LYS:NZ	0.51	0.70	6	1
3:A:59:PCW:H51	3:A:59:PCW:H11	0.51	1.82	4	1
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.51	2.35	3	3
3:A:48:PCW:H361	3:A:54:PCW:H132	0.51	1.81	1	1
4:A:79:17F:H32	4:A:79:17F:H8A	0.51	1.81	1	1
3:A:5:PCW:H83	4:A:38:17F:H9A	0.51	1.81	5	1
3:A:20:PCW:H72	3:A:31:PCW:O2P	0.51	2.06	1	2
3:A:53:PCW:H431	3:A:64:PCW:H452	0.51	1.83	4	1
3:A:9:PCW:H482	3:A:11:PCW:H242	0.51	1.82	4	1
3:A:30:PCW:H11	4:A:40:17F:H20A	0.51	1.83	2	1
3:A:6:PCW:H462	3:A:28:PCW:H232	0.51	1.82	5	1
3:A:49:PCW:H341	3:A:57:PCW:H341	0.51	1.81	4	1
3:A:9:PCW:H282	3:A:63:PCW:H211	0.51	1.82	4	1
1:C:465:GLU:HB3	1:C:469:LEU:HD11	0.51	1.80	7	2
1:A:308:ARG:HG3	1:C:469:LEU:CD2	0.51	2.35	1	4
3:A:19:PCW:H141	3:A:23:PCW:H121	0.51	1.83	2	1
4:A:39:17F:H53	3:A:52:PCW:H172	0.51	1.81	1	1
3:A:1:PCW:H52	4:A:35:17F:HN1	0.51	1.66	5	1
2:B:79:LEU:HD23	2:B:112:VAL:HB	0.51	1.82	5	1
3:A:21:PCW:H141	3:A:21:PCW:H382	0.51	1.81	6	1
4:A:35:17F:H71	3:A:55:PCW:H222	0.51	1.80	7	1
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.51	2.41	3	4
3:A:20:PCW:H322	3:A:20:PCW:H52	0.51	1.82	4	1
3:A:13:PCW:H122	3:A:18:PCW:H131	0.51	1.81	3	1
3:A:27:PCW:H231	4:A:73:17F:H47	0.51	1.82	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:44:PCW:H39	3:A:53:PCW:H361	0.51	1.83	1	1
1:A:239:LEU:O	1:A:243:MET:HB2	0.51	2.06	6	1
3:A:19:PCW:H331	3:A:23:PCW:H421	0.51	1.82	7	1
3:A:57:PCW:H232	4:A:76:17F:H45	0.51	1.83	7	1
3:A:14:PCW:H382	4:A:34:17F:H8	0.51	1.81	2	2
3:A:47:PCW:H221	4:A:73:17F:H37	0.51	1.82	6	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.51	2.06	6	1
3:A:10:PCW:H142	3:A:22:PCW:H421	0.51	1.82	4	1
3:A:32:PCW:H322	4:A:35:17F:H9	0.51	1.82	3	1
1:A:393:TYR:HE1	3:A:32:PCW:C26	0.51	2.17	3	1
3:A:65:PCW:H142	4:A:80:17F:H59	0.51	1.82	3	1
3:A:13:PCW:H61	3:A:14:PCW:H172	0.51	1.82	7	1
1:A:365:LYS:O	1:A:369:GLU:HB2	0.51	2.07	3	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.50	1.82	5	1
3:A:70:PCW:H331	3:A:71:PCW:H152	0.50	1.82	2	1
1:C:525:LEU:HD23	1:C:528:ARG:HD2	0.50	1.83	5	1
3:A:6:PCW:H121	3:A:11:PCW:H342	0.50	1.82	5	1
3:A:66:PCW:H481	4:A:74:17F:H71	0.50	1.83	5	1
3:A:6:PCW:H32	3:A:11:PCW:O3P	0.50	2.06	6	1
1:C:417:GLU:O	1:C:421:PRO:HD2	0.50	2.07	6	1
1:A:275:LYS:O	1:A:279:LEU:HB2	0.50	2.07	2	1
3:A:72:PCW:H40	4:A:78:17F:H44	0.50	1.82	2	1
3:A:45:PCW:O1P	3:A:47:PCW:H82	0.50	2.06	3	1
3:A:49:PCW:H252	3:A:57:PCW:H431	0.50	1.82	6	1
3:A:44:PCW:H2	3:A:44:PCW:O1P	0.50	2.07	7	1
2:B:62:GLU:OE1	2:B:68:ARG:HD2	0.50	2.06	7	3
2:B:24:ILE:HG13	2:B:40:TYR:CD2	0.50	2.42	4	1
3:A:16:PCW:H121	4:A:39:17F:H9A	0.50	1.84	2	1
1:C:489:LEU:O	1:C:493:GLN:HB2	0.50	2.05	2	1
3:A:17:PCW:H432	3:A:17:PCW:H20	0.50	1.81	3	1
3:A:53:PCW:H151	3:A:68:PCW:H431	0.50	1.82	1	1
3:A:46:PCW:H82	4:A:73:17F:H2	0.50	1.83	6	1
3:A:32:PCW:H422	4:A:35:17F:H70	0.50	1.84	7	1
3:A:2:PCW:H42	3:A:17:PCW:O3P	0.50	2.06	3	1
3:A:44:PCW:H222	3:A:55:PCW:H172	0.50	1.83	1	1
3:A:20:PCW:H221	4:A:78:17F:H55	0.50	1.82	5	1
1:C:447:GLU:O	1:C:451:LYS:HB2	0.50	2.06	6	1
3:A:9:PCW:H141	3:A:28:PCW:H361	0.50	1.83	7	1
3:A:16:PCW:H63	3:A:16:PCW:O11	0.50	2.07	3	1
3:A:50:PCW:H82	4:A:78:17F:O1	0.50	2.07	1	1
1:C:491:GLU:O	1:C:495:LYS:HG3	0.50	2.07	4	4

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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	0.50	2.07	6	1
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.50	1.66	2	2
3:A:22:PCW:H63	3:A:22:PCW:O31	0.50	2.07	4	1
1:C:414:LYS:HA	1:C:417:GLU:HG3	0.50	1.82	2	1
3:A:21:PCW:H472	3:A:51:PCW:H242	0.50	1.84	3	1
1:A:308:ARG:CG	1:C:469:LEU:HD21	0.50	2.37	1	1
3:A:45:PCW:H481	3:A:49:PCW:H372	0.49	1.83	6	1
3:A:63:PCW:H122	3:A:67:PCW:H161	0.49	1.83	6	1
1:C:517:HIS:O	1:C:521:TYR:HB2	0.49	2.07	4	2
3:A:6:PCW:H321	3:A:16:PCW:O31	0.49	2.06	2	1
3:A:49:PCW:H341	3:A:57:PCW:H361	0.49	1.84	2	1
3:A:5:PCW:H352	3:A:17:PCW:H71	0.49	1.83	2	1
3:A:21:PCW:H432	3:A:51:PCW:H251	0.49	1.84	1	1
3:A:12:PCW:H141	3:A:22:PCW:H372	0.49	1.84	5	1
3:A:26:PCW:C1	3:A:28:PCW:H12	0.49	2.35	6	1
3:A:4:PCW:H11	3:A:7:PCW:H12	0.49	1.84	6	1
1:C:495:LYS:O	1:C:499:LEU:HB2	0.49	2.07	3	3
1:A:291:LEU:O	1:A:295:GLN:HG3	0.49	2.07	3	1
3:A:4:PCW:H122	3:A:4:PCW:H372	0.49	1.83	5	1
3:A:65:PCW:H281	1:C:488:LYS:CG	0.49	2.28	5	1
3:A:46:PCW:H51	4:A:73:17F:HN1A	0.49	1.67	4	2
3:A:44:PCW:H482	3:A:55:PCW:H182	0.49	1.84	2	1
3:A:18:PCW:H412	3:A:23:PCW:H252	0.49	1.83	1	1
1:A:308:ARG:HD2	1:C:465:GLU:OE1	0.49	2.08	5	1
3:A:55:PCW:H132	3:A:64:PCW:H382	0.49	1.84	5	1
3:A:51:PCW:H412	3:A:70:PCW:H212	0.49	1.85	2	1
3:A:49:PCW:O3P	3:A:57:PCW:H62	0.49	2.08	5	1
3:A:48:PCW:H352	3:A:54:PCW:H211	0.49	1.83	4	2
4:A:34:17F:H12A	4:A:40:17F:H65	0.49	1.83	2	1
3:A:48:PCW:H432	3:A:60:PCW:H212	0.49	1.84	3	1
3:A:17:PCW:H152	3:A:17:PCW:H341	0.49	1.84	6	1
3:A:26:PCW:H483	3:A:69:PCW:H232	0.49	1.85	3	1
3:A:4:PCW:H352	3:A:4:PCW:C31	0.49	2.38	3	1
3:A:53:PCW:O1P	3:A:55:PCW:H62	0.49	2.07	1	1
1:A:352:LYS:HZ2	1:C:425:GLU:CB	0.49	2.21	7	1
3:A:49:PCW:H361	3:A:57:PCW:H381	0.49	1.85	7	1
3:A:13:PCW:H31	4:A:37:17F:H10	0.49	1.83	1	1
4:A:38:17F:H19	4:A:38:17F:H8A	0.49	1.85	5	1
3:A:9:PCW:H232	3:A:28:PCW:H142	0.49	1.84	1	1
1:C:574:LEU:O	1:C:578:GLU:HG3	0.49	2.07	5	1
3:A:43:PCW:H11	3:A:45:PCW:H83	0.49	1.83	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:44:PCW:H82	4:A:77:17F:N1	0.49	2.23	6	1
3:A:12:PCW:H151	3:A:22:PCW:H381	0.49	1.84	4	1
3:A:26:PCW:H441	4:A:33:17F:H45	0.49	1.84	4	1
3:A:13:PCW:H351	3:A:18:PCW:H141	0.49	1.83	7	1
3:A:49:PCW:H82	4:A:80:17F:HN1A	0.49	1.68	7	1
1:A:336:GLU:HA	1:A:339:LYS:HE3	0.49	1.85	4	1
3:A:48:PCW:H141	3:A:54:PCW:H162	0.49	1.85	4	1
3:A:21:PCW:H421	3:A:51:PCW:H221	0.49	1.85	1	1
3:A:6:PCW:H141	3:A:11:PCW:H362	0.48	1.85	5	1
3:A:44:PCW:H232	3:A:55:PCW:H172	0.48	1.84	5	1
3:A:5:PCW:H252	3:A:64:PCW:H271	0.48	1.84	6	1
3:A:47:PCW:H282	4:A:76:17F:H48	0.48	1.83	6	1
3:A:6:PCW:H321	3:A:16:PCW:H341	0.48	1.85	1	2
3:A:24:PCW:H73	3:A:24:PCW:H331	0.48	1.85	2	1
3:A:41:PCW:H362	3:A:41:PCW:H172	0.48	1.84	2	1
4:A:39:17F:H43	3:A:62:PCW:H283	0.48	1.84	3	1
2:B:144:THR:HA	2:B:150:GLN:O	0.48	2.08	1	2
3:A:15:PCW:H382	3:A:24:PCW:H421	0.48	1.85	5	1
3:A:4:PCW:H362	3:A:7:PCW:H212	0.48	1.84	5	1
3:A:51:PCW:H372	3:A:70:PCW:H212	0.48	1.86	5	1
3:A:6:PCW:H39	3:A:28:PCW:H172	0.48	1.84	7	1
3:A:2:PCW:H83	4:A:36:17F:H1A	0.48	1.86	7	1
2:B:68:ARG:HA	2:B:71:TYR:CE1	0.48	2.44	5	1
3:A:26:PCW:H161	4:A:40:17F:H73	0.48	1.85	6	1
1:C:563:LYS:HB2	1:C:564:PRO:CD	0.48	2.39	1	2
3:A:59:PCW:H322	4:A:77:17F:H29	0.48	1.84	5	3
3:A:44:PCW:H171	3:A:55:PCW:H122	0.48	1.85	4	1
3:A:45:PCW:H362	3:A:45:PCW:H121	0.48	1.86	2	1
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.48	1.84	2	1
3:A:8:PCW:H242	3:A:27:PCW:H262	0.48	1.86	3	1
3:A:8:PCW:C24	1:C:459:PHE:HZ	0.48	2.22	1	1
1:A:308:ARG:CG	1:C:469:LEU:CD2	0.48	2.91	1	1
3:A:14:PCW:H462	3:A:30:PCW:H381	0.48	1.84	5	1
3:A:32:PCW:H221	3:A:61:PCW:H262	0.48	1.83	5	1
3:A:52:PCW:H442	3:A:69:PCW:H472	0.48	1.85	5	1
3:A:10:PCW:O2P	3:A:21:PCW:H52	0.48	2.08	7	1
1:A:359:THR:HA	1:A:362:GLU:OE1	0.48	2.08	7	2
3:A:49:PCW:H151	3:A:57:PCW:H321	0.48	1.84	2	1
4:A:35:17F:H53	3:A:44:PCW:H441	0.48	1.85	4	1
3:A:1:PCW:H52	4:A:35:17F:N1	0.48	2.23	3	2
3:A:66:PCW:H132	4:A:79:17F:H4A	0.48	1.85	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.48	1.86	7	1
3:A:62:PCW:H122	3:A:72:PCW:H172	0.48	1.86	2	1
1:A:242:GLU:HB3	1:C:532:ARG:NH2	0.48	2.24	1	1
3:A:13:PCW:H332	3:A:27:PCW:H82	0.47	1.84	5	1
1:C:429:ASN:HA	1:C:432:LYS:HD2	0.47	1.86	6	2
3:A:13:PCW:C4	4:A:34:17F:HN1A	0.47	2.21	1	2
3:A:18:PCW:H332	3:A:18:PCW:C13	0.47	2.39	2	1
1:A:363:LYS:HD3	1:C:411:THR:HG23	0.47	1.85	2	2
3:A:19:PCW:O1P	3:A:29:PCW:H41	0.47	2.08	3	1
3:A:25:PCW:H281	3:A:67:PCW:H40	0.47	1.85	7	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.47	1.86	4	1
3:A:49:PCW:H212	3:A:57:PCW:H352	0.47	1.87	4	1
3:A:4:PCW:H321	3:A:7:PCW:H31	0.47	1.85	4	1
3:A:12:PCW:H39	3:A:21:PCW:H362	0.47	1.84	5	1
3:A:9:PCW:H82	3:A:14:PCW:O2P	0.47	2.09	6	1
3:A:41:PCW:H72	3:A:59:PCW:O1P	0.47	2.09	6	1
2:B:97:ARG:HD3	2:B:98:GLU:OE1	0.47	2.09	6	1
2:B:35:THR:HB	5:B:201:GNP:O3G	0.47	2.10	7	1
3:A:9:PCW:H482	3:A:11:PCW:H122	0.47	1.86	3	1
1:A:231:ASN:HA	1:A:234:LYS:HE3	0.47	1.86	1	1
3:A:55:PCW:H381	3:A:64:PCW:H371	0.47	1.86	6	2
3:A:8:PCW:H81	3:A:22:PCW:O1P	0.47	2.08	6	1
3:A:48:PCW:H361	3:A:54:PCW:H161	0.47	1.86	4	1
1:A:392:GLU:HA	1:A:395:LYS:HG2	0.47	1.87	1	1
2:B:94:HIS:O	2:B:98:GLU:HG2	0.47	2.09	5	1
3:A:68:PCW:H421	3:A:70:PCW:H20	0.47	1.86	4	1
3:A:3:PCW:H351	3:A:19:PCW:H151	0.47	1.84	2	1
3:A:13:PCW:H32	3:A:14:PCW:H141	0.47	1.87	1	1
3:A:10:PCW:H331	3:A:21:PCW:H31	0.47	1.87	7	1
3:A:13:PCW:H20	3:A:18:PCW:H432	0.47	1.86	2	1
1:A:234:LYS:HE3	1:C:539:ASN:OD1	0.47	2.10	5	2
3:A:43:PCW:H171	3:A:68:PCW:H132	0.47	1.87	7	2
2:B:32:TYR:HD1	5:B:201:GNP:H5'1	0.47	1.69	7	2
3:A:49:PCW:H272	3:A:57:PCW:H451	0.47	1.85	6	1
3:A:53:PCW:H332	3:A:68:PCW:H382	0.47	1.85	6	1
3:A:56:PCW:H172	3:A:56:PCW:H412	0.47	1.86	7	1
3:A:26:PCW:H472	3:A:69:PCW:H242	0.47	1.86	4	1
3:A:16:PCW:H20	3:A:24:PCW:H382	0.47	1.87	2	1
3:A:5:PCW:H462	3:A:12:PCW:H432	0.47	1.85	2	1
3:A:9:PCW:H63	3:A:30:PCW:O2P	0.47	2.09	6	1
4:A:40:17F:H49	3:A:51:PCW:H471	0.47	1.85	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:13:PCW:N	4:A:34:17F:N1	0.47	2.63	6	1
3:A:44:PCW:H181	3:A:55:PCW:H122	0.47	1.86	6	1
3:A:45:PCW:H272	4:A:74:17F:H45	0.47	1.85	7	1
3:A:25:PCW:H131	3:A:31:PCW:H322	0.47	1.86	2	1
3:A:26:PCW:H371	3:A:28:PCW:H31	0.47	1.87	3	1
3:A:4:PCW:H122	3:A:4:PCW:H371	0.47	1.85	3	1
3:A:1:PCW:H431	3:A:26:PCW:H431	0.47	1.86	6	1
3:A:24:PCW:O2P	3:A:25:PCW:H32	0.47	2.10	7	1
3:A:16:PCW:H283	4:A:39:17F:H61	0.47	1.85	7	1
2:B:163:ILE:HG22	2:B:167:LYS:HE2	0.47	1.87	4	2
3:A:32:PCW:H481	3:A:44:PCW:H242	0.47	1.87	2	1
4:A:33:17F:H18A	4:A:33:17F:C7	0.47	2.39	3	1
3:A:57:PCW:H221	4:A:80:17F:H44	0.47	1.85	3	1
3:A:5:PCW:H481	4:A:36:17F:H34	0.47	1.87	3	1
3:A:41:PCW:H172	3:A:41:PCW:H362	0.46	1.86	7	1
3:A:70:PCW:H371	3:A:71:PCW:H412	0.46	1.87	7	1
4:A:39:17F:H66	4:A:39:17F:H12	0.46	1.87	2	1
1:C:586:SER:O	1:C:590:GLU:HG3	0.46	2.10	1	1
3:A:10:PCW:H371	3:A:21:PCW:H352	0.46	1.87	5	1
3:A:15:PCW:H351	3:A:16:PCW:H271	0.46	1.87	6	1
3:A:9:PCW:H483	4:A:75:17F:H55	0.46	1.87	6	1
1:C:559:SER:HB2	1:C:563:LYS:HE2	0.46	1.85	6	1
1:A:376:LEU:HB2	1:A:377:PRO:CD	0.46	2.40	2	3
3:A:57:PCW:H142	4:A:80:17F:H8	0.46	1.86	4	1
4:A:35:17F:H75	3:A:55:PCW:H231	0.46	1.87	3	1
2:B:118:CYS:SG	2:B:145:SER:HB2	0.46	2.50	5	1
1:A:363:LYS:O	1:A:367:ALA:HB3	0.46	2.09	7	3
3:A:17:PCW:H131	3:A:17:PCW:H332	0.46	1.87	6	1
3:A:6:PCW:H142	3:A:11:PCW:H351	0.46	1.88	7	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.46	2.38	5	3
2:B:79:LEU:CD2	2:B:112:VAL:HB	0.46	2.41	5	1
3:A:53:PCW:H31	3:A:64:PCW:C3	0.46	2.40	7	1
2:B:97:ARG:HG3	2:B:111:MET:SD	0.46	2.51	4	1
3:A:9:PCW:O31	3:A:25:PCW:H81	0.46	2.10	1	1
1:A:307:ASP:HA	1:A:310:ARG:CD	0.46	2.41	6	1
3:A:59:PCW:C38	4:A:77:17F:H12A	0.46	2.39	7	2
3:A:10:PCW:H40	3:A:21:PCW:H431	0.46	1.87	2	1
3:A:32:PCW:H121	4:A:33:17F:C1Z	0.46	2.40	2	1
3:A:62:PCW:H381	3:A:72:PCW:H182	0.46	1.88	2	1
3:A:62:PCW:H411	4:A:78:17F:H53	0.46	1.88	3	1
3:A:9:PCW:H232	3:A:28:PCW:H371	0.46	1.86	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:49:PCW:H262	3:A:57:PCW:H441	0.46	1.87	5	1
3:A:14:PCW:H332	4:A:34:17F:O10	0.46	2.10	6	1
1:A:315:ALA:O	1:A:319:HIS:HB2	0.46	2.11	6	1
2:B:32:TYR:CD1	5:B:201:GNP:H5'1	0.46	2.46	4	1
1:A:351:ALA:O	1:A:355:GLU:HG2	0.46	2.10	6	1
3:A:16:PCW:H63	4:A:39:17F:O1	0.46	2.09	6	1
2:B:157:TYR:O	2:B:161:ARG:HG3	0.46	2.11	6	1
3:A:12:PCW:H62	3:A:22:PCW:O2P	0.46	2.10	7	1
1:C:465:GLU:C	1:C:469:LEU:HD12	0.46	2.30	7	1
3:A:41:PCW:H31	3:A:52:PCW:H351	0.46	1.87	4	1
3:A:14:PCW:H331	4:A:34:17F:H5	0.46	1.86	2	1
4:A:36:17F:H35	4:A:40:17F:H8	0.46	1.88	5	1
3:A:29:PCW:H462	3:A:67:PCW:H472	0.46	1.88	6	1
3:A:67:PCW:H321	3:A:67:PCW:H41	0.46	1.87	6	1
3:A:68:PCW:H131	3:A:70:PCW:H182	0.46	1.86	1	1
4:A:36:17F:H73	3:A:71:PCW:H483	0.46	1.87	6	1
2:B:81:VAL:HA	2:B:114:VAL:O	0.46	2.11	4	1
1:C:561:LYS:O	1:C:565:ALA:HB3	0.46	2.10	3	2
3:A:42:PCW:H63	3:A:42:PCW:O11	0.46	2.11	2	1
3:A:14:PCW:H351	4:A:34:17F:H78	0.46	1.87	3	1
2:B:46:ILE:HD11	2:B:53:LEU:HD11	0.46	1.87	3	1
3:A:12:PCW:H11	3:A:30:PCW:H121	0.46	1.88	6	1
3:A:12:PCW:H131	3:A:22:PCW:H122	0.46	1.88	6	1
3:A:14:PCW:H271	3:A:30:PCW:H411	0.46	1.88	7	1
3:A:67:PCW:H121	4:A:75:17F:H56	0.46	1.88	7	1
2:B:47:ASP:HB2	2:B:164:ARG:HH22	0.45	1.71	7	1
3:A:10:PCW:H381	3:A:10:PCW:H141	0.45	1.87	4	1
1:A:349:TYR:CZ	3:A:2:PCW:H281	0.45	2.45	3	1
3:A:24:PCW:H31	3:A:25:PCW:H32	0.45	1.87	1	1
3:A:16:PCW:H182	4:A:39:17F:H57	0.45	1.87	1	1
3:A:45:PCW:H332	3:A:49:PCW:H122	0.45	1.88	1	1
3:A:53:PCW:H231	3:A:64:PCW:H242	0.45	1.88	5	1
3:A:21:PCW:H461	3:A:51:PCW:H20	0.45	1.88	2	1
3:A:18:PCW:H261	3:A:49:PCW:H412	0.45	1.89	3	1
3:A:18:PCW:H283	4:A:37:17F:H51	0.45	1.87	5	1
4:A:36:17F:H54	3:A:68:PCW:H242	0.45	1.86	6	1
1:C:466:GLU:HA	1:C:469:LEU:HD12	0.45	1.87	6	1
1:A:372:ARG:O	1:A:376:LEU:HG	0.45	2.10	7	1
1:A:363:LYS:HG2	1:C:411:THR:HG22	0.45	1.87	7	1
3:A:1:PCW:C7	4:A:35:17F:HN1A	0.45	2.25	4	1
3:A:65:PCW:H281	1:C:488:LYS:HD3	0.45	1.86	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:37:17F:H35	3:A:57:PCW:H483	0.45	1.88	3	1
3:A:21:PCW:H422	4:A:36:17F:H70	0.45	1.88	1	1
3:A:47:PCW:H32	4:A:76:17F:O1	0.45	2.12	5	2
4:A:34:17F:H52	4:A:74:17F:H54	0.45	1.87	5	1
3:A:5:PCW:H171	4:A:38:17F:H10	0.45	1.87	6	1
3:A:53:PCW:C33	3:A:68:PCW:H382	0.45	2.42	6	1
3:A:32:PCW:H121	4:A:33:17F:H33	0.45	1.87	2	2
3:A:16:PCW:C5	3:A:16:PCW:H32	0.45	2.33	3	1
3:A:6:PCW:H142	3:A:11:PCW:H381	0.45	1.88	1	1
3:A:59:PCW:H461	3:A:61:PCW:H182	0.45	1.88	5	1
3:A:3:PCW:H182	3:A:19:PCW:H251	0.45	1.87	6	1
3:A:24:PCW:H252	3:A:25:PCW:H282	0.45	1.87	7	1
3:A:63:PCW:H382	3:A:63:PCW:H152	0.45	1.89	7	1
3:A:19:PCW:O1P	3:A:29:PCW:H42	0.45	2.12	2	1
1:C:563:LYS:CB	1:C:564:PRO:HD3	0.45	2.41	5	3
1:A:278:PRO:O	1:A:282:GLU:HG3	0.45	2.12	6	2
4:A:37:17F:N1	4:A:37:17F:H4	0.45	2.24	6	1
3:A:10:PCW:H432	3:A:21:PCW:H451	0.45	1.88	2	1
4:A:36:17F:H72	3:A:70:PCW:H482	0.45	1.89	2	1
2:B:41:ARG:HD2	2:B:54:ASP:OD1	0.45	2.12	2	1
3:A:13:PCW:H172	3:A:18:PCW:H171	0.45	1.89	7	1
3:A:29:PCW:H462	3:A:67:PCW:H441	0.45	1.89	2	1
3:A:13:PCW:H211	3:A:18:PCW:H372	0.45	1.89	5	1
3:A:32:PCW:H121	4:A:33:17F:H20	0.45	1.89	4	1
3:A:3:PCW:H52	3:A:3:PCW:H322	0.45	1.88	4	1
3:A:32:PCW:H352	4:A:35:17F:H11	0.45	1.90	5	1
1:C:464:GLN:O	1:C:468:GLU:HG3	0.45	2.12	5	1
3:A:65:PCW:H281	1:C:488:LYS:NZ	0.45	0.92	6	1
3:A:11:PCW:H211	3:A:11:PCW:H171	0.45	1.88	4	1
3:A:12:PCW:H242	3:A:22:PCW:H262	0.45	1.88	4	1
3:A:67:PCW:H241	3:A:69:PCW:H211	0.45	1.87	2	1
2:B:84:ILE:HD13	2:B:118:CYS:HA	0.45	1.87	3	1
3:A:6:PCW:H131	4:A:39:17F:H18	0.44	1.89	5	1
3:A:44:PCW:H62	4:A:77:17F:N1	0.44	2.27	5	1
3:A:3:PCW:H40	3:A:13:PCW:H39	0.44	1.88	7	1
3:A:5:PCW:H161	4:A:38:17F:H34	0.44	1.89	2	1
3:A:1:PCW:H271	3:A:17:PCW:H422	0.44	1.87	3	1
1:C:455:TYR:O	1:C:459:PHE:HB2	0.44	2.12	1	1
3:A:48:PCW:H351	3:A:54:PCW:H382	0.44	1.88	7	5
3:A:10:PCW:H62	3:A:22:PCW:H332	0.44	1.88	7	1
3:A:2:PCW:H342	3:A:17:PCW:H20	0.44	1.87	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:291:LEU:HD23	1:A:294:LEU:HD12	0.44	1.88	6	1
3:A:20:PCW:H332	3:A:31:PCW:H122	0.44	1.88	6	1
3:A:62:PCW:H361	3:A:72:PCW:H182	0.44	1.88	6	1
3:A:3:PCW:H211	3:A:19:PCW:H442	0.44	1.88	7	1
3:A:4:PCW:H483	3:A:62:PCW:H262	0.44	1.89	7	1
3:A:66:PCW:H431	4:A:79:17F:H58	0.44	1.89	7	1
3:A:57:PCW:H162	4:A:80:17F:H10	0.44	1.90	2	1
3:A:14:PCW:O1P	2:B:137:TYR:HA	0.44	2.12	1	1
3:A:14:PCW:H221	4:A:37:17F:H41	0.44	1.89	5	1
3:A:14:PCW:O1P	3:A:23:PCW:H72	0.44	2.13	6	1
3:A:55:PCW:O31	3:A:55:PCW:H31	0.44	2.12	2	2
1:A:299:SER:HB2	1:A:300:PRO:CD	0.44	2.42	1	1
3:A:17:PCW:H83	4:A:38:17F:O2	0.44	2.13	1	1
3:A:55:PCW:H361	3:A:55:PCW:H122	0.44	1.89	1	1
3:A:45:PCW:H381	3:A:49:PCW:H31	0.44	1.90	5	1
3:A:32:PCW:H331	4:A:33:17F:H19	0.44	1.89	6	1
4:A:33:17F:H18A	4:A:33:17F:H6	0.44	1.88	6	1
3:A:3:PCW:H142	3:A:19:PCW:H162	0.44	1.90	7	1
3:A:15:PCW:H81	4:A:39:17F:N1	0.44	2.28	2	1
1:C:567:GLU:HG2	1:C:571:GLN:NE2	0.44	2.27	2	1
3:A:14:PCW:H161	4:A:37:17F:H8A	0.44	1.87	1	1
3:A:26:PCW:H41	3:A:28:PCW:O1P	0.44	2.12	1	1
3:A:8:PCW:H431	3:A:27:PCW:H182	0.44	1.89	5	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.44	1.72	6	1
3:A:13:PCW:H331	3:A:18:PCW:H141	0.44	1.88	7	2
3:A:21:PCW:H182	3:A:51:PCW:H232	0.44	1.89	7	1
3:A:21:PCW:H162	3:A:51:PCW:H261	0.44	1.90	7	1
3:A:52:PCW:H32	3:A:61:PCW:H341	0.44	1.88	7	1
3:A:63:PCW:H481	4:A:74:17F:H76	0.44	1.90	1	1
1:A:242:GLU:OE1	1:C:528:ARG:HA	0.44	2.12	5	1
3:A:6:PCW:H122	3:A:16:PCW:H371	0.44	1.90	5	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.44	2.43	6	3
3:A:47:PCW:H20	4:A:73:17F:H58	0.44	1.88	6	1
3:A:48:PCW:H381	3:A:54:PCW:H152	0.44	1.89	6	1
3:A:44:PCW:H222	3:A:55:PCW:H171	0.44	1.88	2	1
3:A:47:PCW:H162	4:A:76:17F:H18	0.44	1.88	2	1
3:A:62:PCW:H331	3:A:72:PCW:H182	0.44	1.89	3	1
2:B:126:ASP:HB3	2:B:129:GLN:HG3	0.44	1.89	1	1
3:A:19:PCW:H372	3:A:23:PCW:H431	0.44	1.89	5	1
1:A:243:MET:HA	1:A:246:ASP:HB2	0.44	1.90	5	1
3:A:6:PCW:H352	3:A:28:PCW:H132	0.44	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:12:PCW:C1	3:A:22:PCW:H31	0.44	2.36	2	1
1:A:327:LEU:HD23	1:A:330:ARG:HD3	0.44	1.88	2	1
2:B:116:ASN:HA	2:B:144:THR:O	0.44	2.13	1	1
3:A:9:PCW:H261	3:A:28:PCW:H181	0.44	1.90	7	1
1:A:392:GLU:HA	1:A:395:LYS:HD2	0.44	1.89	4	1
4:A:75:17F:H69	4:A:75:17F:H40	0.44	1.88	4	2
3:A:15:PCW:H39	3:A:24:PCW:H432	0.44	1.89	1	1
3:A:27:PCW:H82	4:A:37:17F:O2	0.44	2.13	1	1
3:A:13:PCW:H121	3:A:18:PCW:H341	0.43	1.90	5	1
1:C:487:GLN:O	1:C:491:GLU:HG3	0.43	2.12	5	1
3:A:56:PCW:H472	3:A:56:PCW:H221	0.43	1.89	6	1
3:A:9:PCW:H122	3:A:11:PCW:H131	0.43	1.90	4	1
3:A:15:PCW:H52	3:A:16:PCW:H142	0.43	1.89	2	1
3:A:3:PCW:H281	3:A:65:PCW:H471	0.43	1.90	3	1
1:A:345:ARG:HD3	1:C:433:GLU:OE2	0.43	2.13	3	1
3:A:45:PCW:H283	4:A:75:17F:H78	0.43	1.90	6	1
1:A:393:TYR:HD1	3:A:32:PCW:H283	0.43	1.72	7	1
3:A:51:PCW:O31	3:A:70:PCW:H362	0.43	2.12	7	1
3:A:17:PCW:H261	3:A:21:PCW:H172	0.43	1.90	3	1
3:A:6:PCW:H372	3:A:28:PCW:H151	0.43	1.90	3	1
3:A:6:PCW:P	4:A:39:17F:O1	0.43	2.76	3	1
3:A:26:PCW:H161	4:A:40:17F:H60	0.43	1.88	5	1
1:C:428:ASP:O	1:C:432:LYS:HG3	0.43	2.12	5	1
3:A:43:PCW:H371	3:A:43:PCW:H141	0.43	1.91	6	1
1:A:268:GLU:O	1:A:272:TYR:HB2	0.43	2.13	4	2
3:A:11:PCW:H161	3:A:28:PCW:H411	0.43	1.90	7	1
3:A:6:PCW:H321	3:A:16:PCW:H322	0.43	1.90	4	1
3:A:65:PCW:H142	4:A:80:17F:H29	0.43	1.89	2	1
1:C:458:ASP:HA	1:C:461:LYS:HD2	0.43	1.90	2	1
3:A:41:PCW:H131	3:A:41:PCW:H331	0.43	1.89	3	1
3:A:41:PCW:H39	3:A:59:PCW:H411	0.43	1.89	3	1
3:A:60:PCW:H472	3:A:63:PCW:H40	0.43	1.89	7	1
3:A:13:PCW:H142	3:A:18:PCW:H142	0.43	1.88	4	1
1:A:365:LYS:HB2	1:A:366:PRO:CD	0.43	2.43	2	1
1:C:510:HIS:O	1:C:514:LEU:HG	0.43	2.14	3	1
4:A:36:17F:H49	3:A:53:PCW:H462	0.43	1.90	1	1
3:A:16:PCW:H41	2:B:98:GLU:CB	0.43	2.42	5	1
3:A:49:PCW:H181	3:A:57:PCW:H352	0.43	1.89	5	1
3:A:10:PCW:H421	3:A:12:PCW:H221	0.43	1.90	6	1
3:A:66:PCW:H281	4:A:78:17F:H38	0.43	1.88	6	1
3:A:49:PCW:H232	3:A:57:PCW:H432	0.43	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:77:17F:H2	4:A:77:17F:C4	0.43	2.42	1	1
3:A:15:PCW:H483	3:A:20:PCW:H122	0.43	1.90	5	1
3:A:53:PCW:H31	3:A:64:PCW:H31	0.43	1.91	7	1
1:C:465:GLU:C	1:C:469:LEU:CD1	0.43	2.86	7	1
4:A:74:17F:H78	4:A:75:17F:H45	0.43	1.91	4	1
1:A:279:LEU:HB3	1:C:495:LYS:HD3	0.43	1.90	4	1
3:A:21:PCW:H212	3:A:51:PCW:H222	0.43	1.91	2	1
1:A:356:HIS:HA	1:C:418:GLN:OE1	0.43	2.13	1	1
1:A:263:LYS:O	1:A:267:GLU:HG3	0.43	2.14	5	1
3:A:53:PCW:H161	3:A:53:PCW:H351	0.43	1.90	6	1
3:A:21:PCW:H40	4:A:36:17F:H69	0.43	1.91	1	1
3:A:6:PCW:H231	3:A:24:PCW:C15	0.43	2.44	5	1
4:A:33:17F:H77	3:A:44:PCW:H272	0.43	1.90	7	1
3:A:17:PCW:H252	3:A:53:PCW:H461	0.43	1.90	4	1
3:A:6:PCW:H141	3:A:11:PCW:H371	0.43	1.91	2	1
1:C:485:ALA:HA	1:C:488:LYS:HG2	0.43	1.90	7	1
3:A:13:PCW:H232	3:A:49:PCW:H482	0.43	1.91	4	1
4:A:73:17F:H68	4:A:76:17F:H55	0.43	1.91	4	1
3:A:19:PCW:H322	3:A:23:PCW:H381	0.43	1.90	2	1
3:A:62:PCW:H371	3:A:72:PCW:H412	0.43	1.90	2	1
3:A:27:PCW:H20	3:A:27:PCW:H252	0.43	1.90	3	1
2:B:8:VAL:HG12	2:B:16:LYS:HD2	0.43	1.90	3	1
1:A:352:LYS:HG2	1:C:422:VAL:HG22	0.43	1.89	5	1
1:A:356:HIS:O	1:A:360:LEU:HB2	0.43	2.14	7	1
3:A:27:PCW:H462	4:A:37:17F:H70	0.43	1.91	7	1
3:A:1:PCW:H281	3:A:5:PCW:H282	0.43	1.90	2	1
3:A:66:PCW:H412	4:A:79:17F:H34	0.43	1.91	3	1
3:A:12:PCW:H73	4:A:37:17F:HN1	0.42	1.74	5	1
3:A:6:PCW:H20	3:A:60:PCW:H462	0.42	1.90	7	1
3:A:1:PCW:H451	3:A:68:PCW:H231	0.42	1.91	4	1
3:A:18:PCW:H332	3:A:18:PCW:H132	0.42	1.89	2	1
3:A:48:PCW:H141	3:A:54:PCW:H141	0.42	1.89	2	1
4:A:36:17F:H10	4:A:40:17F:H9A	0.42	1.90	3	1
3:A:2:PCW:H39	3:A:5:PCW:H211	0.42	1.90	3	1
3:A:20:PCW:H172	3:A:31:PCW:H39	0.42	1.89	5	1
3:A:49:PCW:H482	4:A:80:17F:H39	0.42	1.91	7	1
3:A:70:PCW:H372	3:A:71:PCW:H161	0.42	1.90	7	1
3:A:16:PCW:H351	4:A:39:17F:H11	0.42	1.90	4	1
3:A:41:PCW:H83	3:A:59:PCW:O1P	0.42	2.14	4	1
3:A:65:PCW:C8	4:A:80:17F:H4A	0.42	2.44	4	1
3:A:3:PCW:H432	3:A:13:PCW:H222	0.42	1.91	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:14:PCW:H181	4:A:34:17F:H34	0.42	1.90	5	1
3:A:3:PCW:H382	3:A:18:PCW:H321	0.42	1.91	4	1
3:A:12:PCW:H221	3:A:22:PCW:H262	0.42	1.91	4	1
1:A:330:ARG:HD3	1:C:444:ASP:OD2	0.42	2.14	4	1
1:A:344:ALA:O	1:A:348:GLU:HG2	0.42	2.14	4	1
3:A:57:PCW:H421	4:A:79:17F:H50	0.42	1.92	4	1
1:C:431:GLU:HA	1:C:434:THR:OG1	0.42	2.12	4	1
3:A:2:PCW:H381	3:A:17:PCW:H441	0.42	1.91	2	1
3:A:13:PCW:H182	3:A:18:PCW:H422	0.42	1.90	1	1
3:A:55:PCW:H131	3:A:64:PCW:H382	0.42	1.89	1	1
1:A:304:GLU:O	1:A:308:ARG:HG2	0.42	2.14	5	1
1:A:270:GLU:O	1:A:274:GLN:HB2	0.42	2.14	6	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.42	2.15	7	1
3:A:14:PCW:H161	4:A:34:17F:H31	0.42	1.91	7	1
3:A:18:PCW:H452	3:A:49:PCW:H472	0.42	1.90	4	1
3:A:1:PCW:O31	3:A:1:PCW:H341	0.42	2.14	2	1
3:A:16:PCW:H20	3:A:24:PCW:H362	0.42	1.91	5	1
1:A:297:LYS:O	1:A:301:LEU:HB2	0.42	2.14	6	1
3:A:30:PCW:H39	4:A:40:17F:H71	0.42	1.92	6	1
3:A:32:PCW:H122	4:A:33:17F:H20	0.42	1.90	7	1
3:A:47:PCW:H20	4:A:76:17F:H47	0.42	1.91	7	1
1:C:589:GLU:O	1:C:593:LYS:HG3	0.42	2.14	7	1
4:A:36:17F:H71	3:A:51:PCW:H19	0.42	1.92	4	1
1:A:386:PHE:O	1:A:390:LEU:HG	0.42	2.14	3	1
3:A:55:PCW:H31	3:A:55:PCW:O31	0.42	2.15	1	1
4:A:77:17F:H4	4:A:77:17F:H1	0.42	1.89	6	1
3:A:13:PCW:H132	3:A:23:PCW:H141	0.42	1.90	7	1
3:A:8:PCW:H272	1:C:455:TYR:CD1	0.42	2.49	7	1
3:A:57:PCW:H211	4:A:76:17F:C24	0.42	2.45	3	1
3:A:29:PCW:H271	1:C:521:TYR:CZ	0.42	2.49	1	1
3:A:14:PCW:H412	4:A:34:17F:H8	0.42	1.91	5	1
3:A:10:PCW:H441	3:A:12:PCW:H252	0.42	1.92	6	1
3:A:68:PCW:H331	3:A:69:PCW:H332	0.42	1.92	6	1
3:A:27:PCW:H12	3:A:27:PCW:O31	0.42	2.14	7	1
3:A:24:PCW:O2P	2:B:102:ARG:HD2	0.42	2.15	4	1
2:B:112:VAL:HG23	2:B:159:LEU:HD13	0.42	1.90	2	1
2:B:5:LYS:HA	2:B:54:ASP:HB3	0.42	1.91	2	1
1:A:349:TYR:CE1	3:A:2:PCW:H283	0.42	2.44	3	1
3:A:16:PCW:H461	3:A:24:PCW:H442	0.42	1.91	1	1
3:A:2:PCW:H452	3:A:56:PCW:H252	0.42	1.92	7	1
3:A:45:PCW:H471	3:A:49:PCW:H352	0.42	1.91	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:57:PCW:H212	4:A:80:17F:C2X	0.42	2.44	3	1
1:C:458:ASP:HA	1:C:461:LYS:NZ	0.42	2.30	3	1
3:A:18:PCW:H242	4:A:80:17F:H47	0.42	1.90	1	1
3:A:17:PCW:H121	4:A:36:17F:O9	0.42	2.15	5	1
3:A:22:PCW:H482	4:A:36:17F:H78	0.42	1.92	6	1
3:A:22:PCW:H282	3:A:46:PCW:H431	0.42	1.92	7	1
3:A:46:PCW:H82	4:A:73:17F:HN1A	0.42	1.75	4	1
3:A:45:PCW:H451	3:A:49:PCW:H321	0.42	1.92	2	1
3:A:18:PCW:H262	3:A:57:PCW:H20	0.42	1.92	3	1
3:A:14:PCW:H232	3:A:14:PCW:H262	0.42	1.73	5	1
3:A:62:PCW:H362	3:A:72:PCW:H412	0.42	1.91	5	1
3:A:14:PCW:H161	4:A:34:17F:H19	0.42	1.92	7	1
1:A:239:LEU:HA	1:A:242:GLU:HB2	0.42	1.91	7	1
4:A:74:17F:H6A	4:A:79:17F:HN1	0.42	1.75	2	1
3:A:21:PCW:H432	3:A:51:PCW:H231	0.42	1.91	3	1
3:A:42:PCW:H411	3:A:69:PCW:H71	0.41	1.91	5	1
1:C:491:GLU:HB3	1:C:495:LYS:CE	0.41	2.44	5	2
1:C:502:GLU:O	1:C:506:ARG:HG3	0.41	2.15	4	3
3:A:13:PCW:H121	3:A:23:PCW:H122	0.41	1.92	7	1
3:A:42:PCW:H11	3:A:69:PCW:O2P	0.41	2.15	7	1
3:A:48:PCW:H141	3:A:54:PCW:H152	0.41	1.91	7	1
3:A:32:PCW:H361	4:A:35:17F:H8A	0.41	1.92	5	1
3:A:13:PCW:C33	3:A:18:PCW:H141	0.41	2.44	6	1
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.41	1.92	7	2
3:A:62:PCW:H351	3:A:72:PCW:H382	0.41	1.91	7	1
4:A:77:17F:H1A	4:A:77:17F:C4	0.41	2.45	4	1
3:A:16:PCW:H231	4:A:39:17F:H59	0.41	1.92	2	1
3:A:5:PCW:H321	3:A:17:PCW:H81	0.41	1.92	2	1
2:B:35:THR:HB	5:B:201:GNP:O1G	0.41	2.15	2	1
3:A:5:PCW:H421	4:A:36:17F:C11	0.41	2.44	1	1
3:A:11:PCW:H282	3:A:24:PCW:H283	0.41	1.92	5	1
3:A:49:PCW:H341	3:A:57:PCW:H362	0.41	1.92	6	2
1:A:277:GLU:HB2	1:A:278:PRO:CD	0.41	2.45	6	1
3:A:3:PCW:H232	3:A:19:PCW:H451	0.41	1.91	7	1
3:A:19:PCW:H82	3:A:23:PCW:H322	0.41	1.93	7	1
3:A:52:PCW:H481	3:A:52:PCW:H241	0.41	1.91	3	1
3:A:27:PCW:H452	4:A:73:17F:H44	0.41	1.93	5	1
3:A:20:PCW:H42	3:A:31:PCW:O11	0.41	2.16	6	1
3:A:44:PCW:H82	4:A:77:17F:HN1A	0.41	1.76	6	1
1:C:444:ASP:O	1:C:448:VAL:HB	0.41	2.15	6	1
3:A:41:PCW:H341	3:A:52:PCW:C39	0.41	2.46	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:4:PCW:H442	3:A:58:PCW:H481	0.41	1.90	7	1
3:A:48:PCW:H432	3:A:60:PCW:H19	0.41	1.92	2	1
3:A:48:PCW:H382	3:A:54:PCW:H371	0.41	1.90	5	1
3:A:50:PCW:H31	4:A:78:17F:H4A	0.41	1.92	4	1
3:A:13:PCW:H321	3:A:18:PCW:H122	0.41	1.92	3	1
3:A:53:PCW:H322	3:A:64:PCW:H122	0.41	1.90	3	1
3:A:14:PCW:H11	3:A:23:PCW:H73	0.41	1.93	6	1
3:A:2:PCW:H432	3:A:17:PCW:H483	0.41	1.91	7	1
3:A:4:PCW:H332	3:A:4:PCW:H131	0.41	1.91	4	1
4:A:33:17F:H53	3:A:69:PCW:H39	0.41	1.92	3	1
4:A:39:17F:H56	4:A:39:17F:H8	0.41	1.90	1	1
3:A:19:PCW:H32	3:A:29:PCW:O1P	0.41	2.15	6	1
3:A:22:PCW:H42	4:A:37:17F:O3	0.41	2.16	6	1
3:A:63:PCW:H441	3:A:63:PCW:H211	0.41	1.93	6	1
3:A:8:PCW:H381	3:A:27:PCW:H182	0.41	1.91	7	1
2:B:100:ILE:HA	2:B:103:VAL:HG22	0.41	1.93	7	1
3:A:30:PCW:H151	4:A:40:17F:H9A	0.41	1.91	4	1
1:A:330:ARG:NH2	1:C:447:GLU:HB3	0.41	2.31	1	1
3:A:32:PCW:H342	4:A:33:17F:H56	0.41	1.93	5	1
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.41	1.93	5	1
3:A:23:PCW:H172	4:A:34:17F:H59	0.41	1.91	6	1
3:A:1:PCW:H262	3:A:64:PCW:H472	0.41	1.92	7	1
3:A:21:PCW:H472	3:A:51:PCW:H222	0.41	1.92	7	1
3:A:41:PCW:O31	3:A:61:PCW:H63	0.41	2.15	4	1
3:A:49:PCW:H232	3:A:57:PCW:H411	0.41	1.92	2	1
4:A:39:17F:H47	3:A:62:PCW:H241	0.41	1.92	2	1
3:A:18:PCW:H282	3:A:49:PCW:H381	0.41	1.93	3	1
1:A:375:LEU:HD11	4:A:38:17F:C29	0.41	2.46	1	1
3:A:6:PCW:H483	3:A:28:PCW:H262	0.41	1.93	5	1
3:A:1:PCW:O11	4:A:35:17F:H6	0.41	2.16	6	1
3:A:8:PCW:H261	1:C:459:PHE:HE2	0.41	1.69	6	1
3:A:44:PCW:H141	3:A:44:PCW:H172	0.41	1.51	7	1
3:A:13:PCW:H52	4:A:34:17F:HN1	0.41	1.76	7	1
3:A:24:PCW:H222	3:A:31:PCW:H411	0.41	1.93	4	1
3:A:17:PCW:H20	3:A:17:PCW:H461	0.41	1.93	4	1
3:A:57:PCW:H222	4:A:80:17F:H40	0.41	1.92	4	1
3:A:10:PCW:H371	3:A:21:PCW:H131	0.41	1.92	2	1
1:A:243:MET:O	1:A:247:LEU:HB2	0.41	2.16	2	1
3:A:13:PCW:H121	3:A:18:PCW:H332	0.41	1.92	3	1
3:A:47:PCW:H221	4:A:76:17F:C27	0.41	2.43	3	1
3:A:4:PCW:H31	3:A:4:PCW:O1P	0.41	2.16	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:13:PCW:H231	3:A:49:PCW:H482	0.41	1.93	1	1
3:A:13:PCW:H441	4:A:37:17F:H71	0.41	1.93	1	1
1:C:412:PHE:O	1:C:415:LEU:HB2	0.41	2.16	5	1
3:A:27:PCW:O31	3:A:27:PCW:H31	0.41	2.16	6	1
3:A:32:PCW:H351	3:A:32:PCW:H322	0.41	1.71	6	1
4:A:74:17F:H59	4:A:75:17F:H61	0.41	1.92	6	1
3:A:59:PCW:H361	4:A:77:17F:H12A	0.41	1.92	6	1
1:C:559:SER:HA	1:C:562:ALA:HB3	0.41	1.93	6	1
1:A:304:GLU:O	1:A:308:ARG:HG3	0.41	2.14	4	1
4:A:74:17F:H1A	4:A:74:17F:H4	0.41	1.92	4	1
4:A:74:17F:H68	4:A:75:17F:C40	0.41	2.46	4	1
3:A:18:PCW:H482	3:A:49:PCW:H471	0.41	1.93	2	1
1:C:461:LYS:O	1:C:465:GLU:HG3	0.41	2.16	2	1
3:A:24:PCW:H131	3:A:25:PCW:H152	0.40	1.92	6	1
1:A:393:TYR:CD1	3:A:32:PCW:H283	0.40	2.51	7	1
3:A:8:PCW:H242	1:C:459:PHE:CE1	0.40	2.51	1	1
3:A:12:PCW:H361	4:A:36:17F:H18A	0.40	1.93	5	1
3:A:30:PCW:H321	4:A:34:17F:H8A	0.40	1.92	5	1
1:A:314:ASP:HA	1:A:317:ARG:HD2	0.40	1.92	4	1
1:A:280:ARG:O	1:A:284:GLN:HB2	0.40	2.16	3	1
3:A:54:PCW:H252	3:A:54:PCW:H471	0.40	1.93	3	1
1:A:388:SER:HB2	1:C:594:LYS:HD3	0.40	1.93	3	1
3:A:1:PCW:H362	4:A:36:17F:C21	0.40	2.45	1	1
3:A:48:PCW:H142	3:A:54:PCW:H171	0.40	1.93	5	1
2:B:46:ILE:O	2:B:49:GLU:HG3	0.40	2.16	5	1
1:C:434:THR:HB	1:C:438:ARG:CZ	0.40	2.47	6	1
1:A:290:LYS:HE3	1:C:487:GLN:OE1	0.40	2.16	6	1
3:A:21:PCW:H441	3:A:51:PCW:H20	0.40	1.94	7	1
3:A:32:PCW:H451	4:A:35:17F:H38	0.40	1.94	2	1
3:A:45:PCW:H431	4:A:74:17F:H9A	0.40	1.93	3	1
3:A:59:PCW:H71	4:A:77:17F:H19	0.40	1.92	1	1
3:A:51:PCW:H371	3:A:70:PCW:H341	0.40	1.92	1	1
3:A:59:PCW:H11	3:A:59:PCW:C5	0.40	2.46	7	1
3:A:65:PCW:H31	3:A:66:PCW:H331	0.40	1.93	3	1
3:A:21:PCW:H12	4:A:36:17F:O1	0.40	2.16	1	1
3:A:8:PCW:H341	3:A:22:PCW:H61	0.40	1.94	5	1
3:A:13:PCW:H362	3:A:18:PCW:H161	0.40	1.93	7	1
1:A:272:TYR:O	1:A:276:VAL:HG23	0.40	2.16	7	1
3:A:20:PCW:H252	4:A:78:17F:H55	0.40	1.94	3	1
3:A:24:PCW:H71	3:A:31:PCW:O1P	0.40	2.16	3	1
4:A:36:17F:H48	3:A:53:PCW:H483	0.40	1.93	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:41:PCW:H161	3:A:61:PCW:H152	0.40	1.94	1	1
3:A:49:PCW:H221	3:A:57:PCW:H411	0.40	1.94	1	1
3:A:5:PCW:H321	4:A:38:17F:H6	0.40	1.93	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	165/200 (82%)	161±1 (98±1%)	3±1 (2±1%)	1±0 (1±0%)	29	74
1	C	195/200 (98%)	190±1 (97±1%)	4±1 (2±1%)	1±0 (1±0%)	29	74
2	B	171/187 (91%)	164±3 (96±2%)	7±3 (4±2%)	0±0 (0±0%)	54	85
All	All	3717/4109 (90%)	3605 (97%)	96 (3%)	16 (0%)	38	78

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	7
1	C	563	LYS	7
1	C	420	GLY	1
2	B	36	ILE	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	142/175 (81%)	130±3 (92±2%)	12±3 (8±2%)	15	62
1	C	172/175 (98%)	157±2 (91±1%)	15±2 (9±1%)	13	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	153/166 (92%)	140±4 (92±3%)	13±4 (8±3%)	14 61
All	All	3269/3612 (91%)	2991 (91%)	278 (9%)	14 61

All 142 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)
2	B	92	ASP	7
2	B	74	THR	7
1	A	254	VAL	6
1	C	516	THR	6
1	C	550	LYS	6
1	A	312	HIS	6
2	B	2	THR	5
2	B	71	TYR	5
1	C	459	PHE	5
2	B	87	THR	5
1	C	480	GLU	5
1	A	392	GLU	5
1	A	246	ASP	4
2	B	124	THR	4
1	A	318	THR	4
1	C	505	ASP	4
2	B	148	THR	4
1	A	354	THR	4
2	B	170	MET	3
1	C	405	TRP	3
1	C	580	PHE	3
1	A	314	ASP	3
1	C	418	GLN	3
1	A	235	GLU	3
1	C	568	ASP	3
1	C	594	LYS	3
2	B	153	ASP	3
2	B	20	THR	3
1	A	370	ASP	3
1	C	487	GLN	3
1	A	385	SER	3
1	C	455	TYR	3
1	A	293	GLU	3
1	A	265	TRP	3
1	C	552	THR	2

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Mol	Chain	Res	Type	Models (Total)
2	B	17	SER	2
1	A	274	GLN	2
1	A	292	HIS	2
1	C	561	LYS	2
1	C	546	GLU	2
1	C	463	TRP	2
1	C	490	HIS	2
1	C	467	MET	2
2	B	6	LEU	2
2	B	85	ASN	2
2	B	89	SER	2
2	B	107	GLU	2
1	A	299	SER	2
1	A	264	LYS	2
1	C	512	ASP	2
2	B	51	CYS	2
1	A	319	HIS	2
1	A	394	THR	2
1	C	404	ASN	2
1	C	523	ASP	2
2	B	136	SER	2
1	C	434	THR	2
1	C	412	PHE	2
1	C	447	GLU	2
1	C	403	ASP	2
1	C	444	ASP	2
1	A	356	HIS	2
2	B	118	CYS	2
1	A	350	HIS	2
1	C	466	GLU	1
1	A	255	GLN	1
1	C	472	GLN	1
2	B	61	GLN	1
2	B	132	ASP	1
1	C	596	ASN	1
2	B	127	THR	1
1	C	583	SER	1
2	B	33	ASP	1
1	A	371	LEU	1
1	A	261	PHE	1
2	B	63	GLU	1
1	A	270	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	C	566	LEU	1
1	C	410	SER	1
1	A	241	GLN	1
2	B	122	SER	1
1	C	560	GLU	1
2	B	65	SER	1
1	C	451	LYS	1
1	C	457	ASP	1
2	B	106	SER	1
1	C	556	SER	1
1	C	494	GLU	1
1	A	307	ASP	1
1	A	359	THR	1
2	B	86	ASN	1
1	A	296	GLU	1
2	B	35	THR	1
1	A	368	LEU	1
1	A	327	LEU	1
1	C	557	THR	1
1	C	554	HIS	1
1	A	273	ARG	1
1	C	429	ASN	1
2	B	145	SER	1
2	B	166	HIS	1
1	C	427	TRP	1
2	B	144	THR	1
1	C	521	TYR	1
1	C	443	LYS	1
1	A	284	GLN	1
2	B	62	GLU	1
2	B	70	GLN	1
1	C	401	LEU	1
2	B	97	ARG	1
1	C	482	GLN	1
1	C	464	GLN	1
2	B	154	ASP	1
1	C	558	LEU	1
1	C	448	VAL	1
1	C	473	LYS	1
1	A	243	MET	1
1	A	305	MET	1
1	C	522	SER	1

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Mol	Chain	Res	Type	Models (Total)
2	B	126	ASP	1
1	A	361	SER	1
1	C	407	SER	1
2	B	30	ASP	1
1	C	495	LYS	1
2	B	31	GLU	1
1	C	501	GLU	1
2	B	103	VAL	1
2	B	12	VAL	1
1	C	426	PHE	1
1	A	272	TYR	1
1	A	266	GLN	1
1	C	477	LEU	1
2	B	47	ASP	1
2	B	23	LEU	1
2	B	41	ARG	1
1	C	460	GLN	1
1	C	409	THR	1
1	A	304	GLU	1
2	B	49	GLU	1
1	A	249	GLU	1
2	B	150	GLN	1
2	B	69	ASP	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.

LIGAND-GEOMETRY INFOmissingINFO

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 [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: input_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	-0.46 ± 0.64	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. 205 atoms were assigned a chemical shift out of a possible 6844. 3 out of 100 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	155/2631 (6%)	77/1049 (7%)	0/1066 (0%)	78/516 (15%)
Sidechain	50/3807 (1%)	25/2232 (1%)	25/1378 (2%)	0/197 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/406 (0%)	0/222 (0%)	0/176 (0%)	0/8 (0%)
Overall	205/6844 (3%)	102/3503 (3%)	25/2620 (1%)	78/721 (11%)

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:

