



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 06:19 AM BST

PDB ID : 2MSD
Title : NMR data-driven model of GTPase KRas-GNP 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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

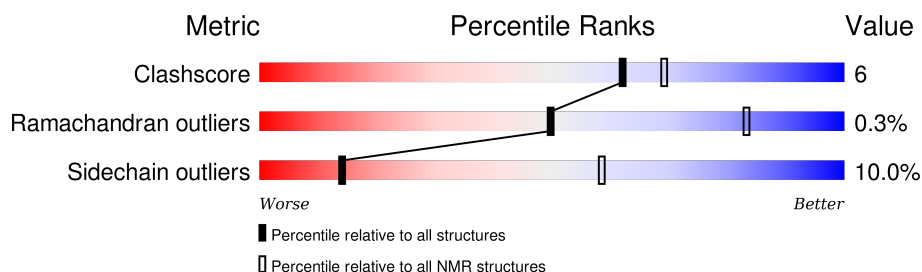
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	200	 81% 17% ...
1	C	200	 80% 18% ...
2	B	187	 76% 14% 8% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:201-A:396, C:401-C:595 (391)	0.26	1
2	B:3-B:172 (170)	0.46	3

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9138 atoms, of which 62 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

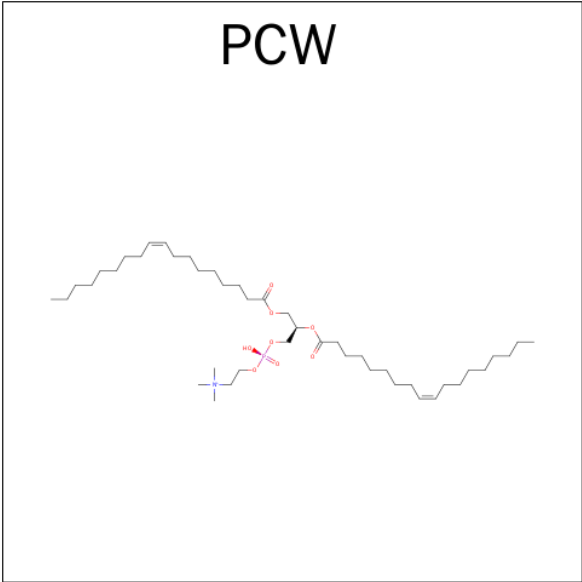
- Molecule 2 is a protein called V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b.

Mol	Chain	Residues	Atoms						Trace
2	B	185	Total	C	H	N	O	S	0
			1494	923	18	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 A0A024RAV5
B	0	SER	-	EXPRESSION TAG	UNP A0A024RAV5

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



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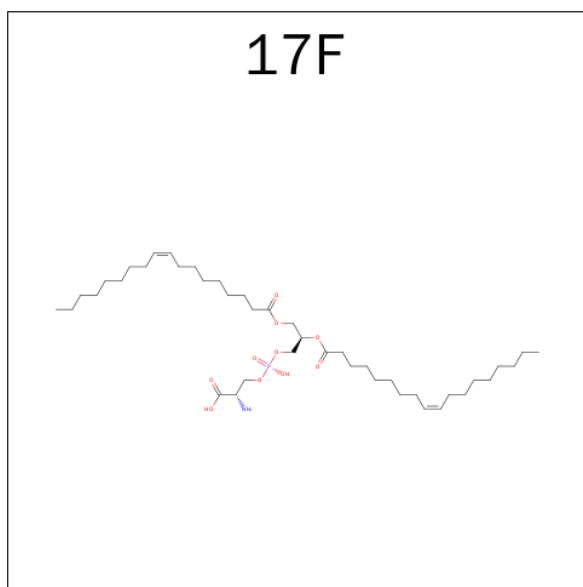
Mol	Chain	Residues	Atoms				
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44	1	8	1
3	A	1	Total	C	N	O	P
			54	44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

- 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).



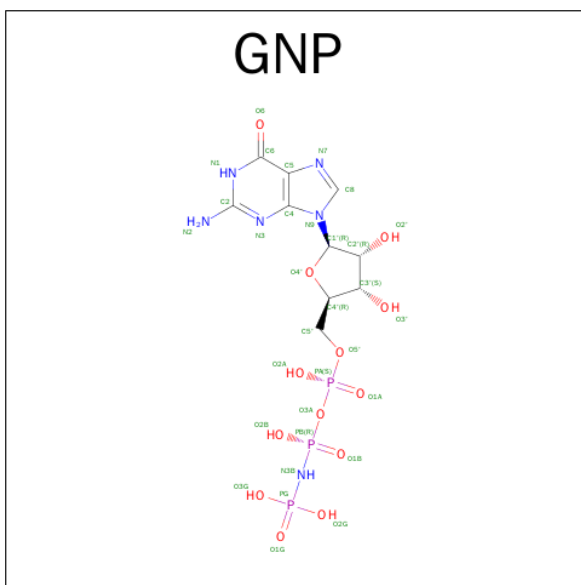
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1
4	A	1	Total	C	N	O	P
			54	42	1	10	1

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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

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



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

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

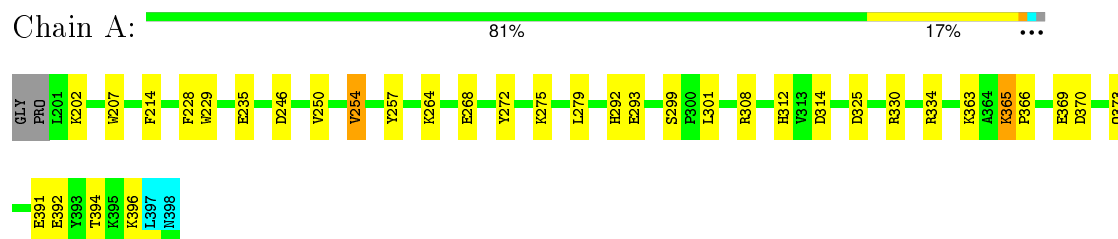
Mol	Chain	Residues	Atoms	
6	B	1	Total	Mg
			1	1

4 Residue-property plots [i](#)

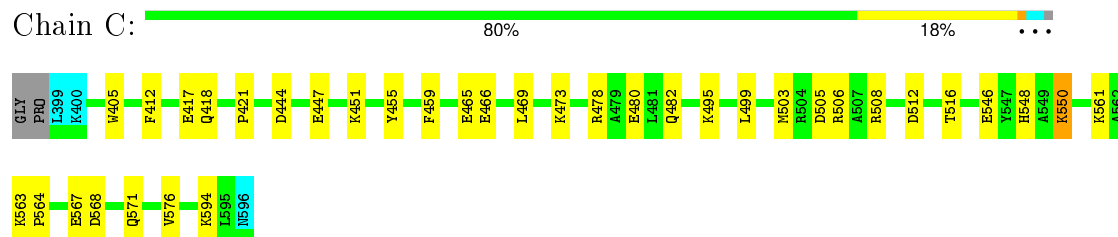
4.1 Average score per residue in the NMR ensemble

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

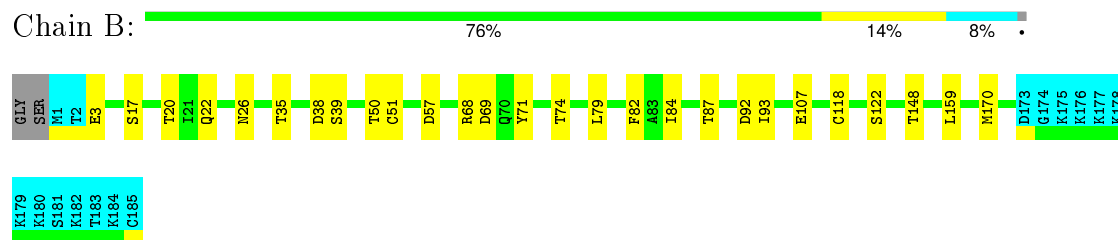
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b

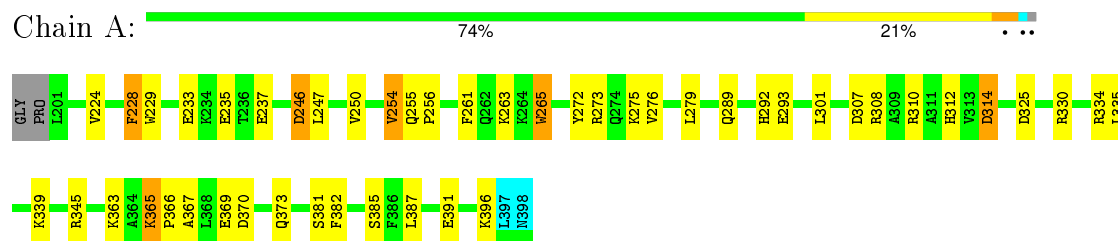


4.2 Scores per residue for each member of the ensemble

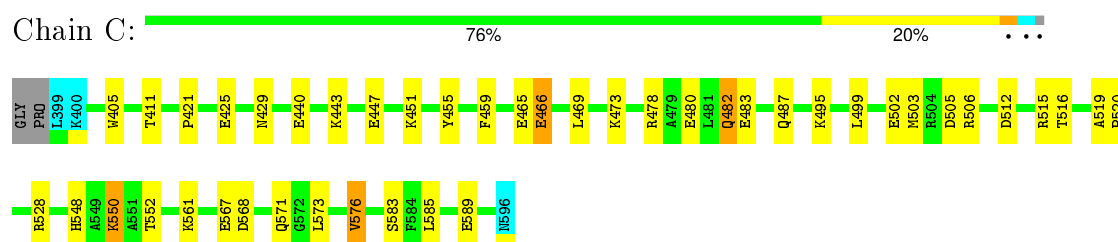
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

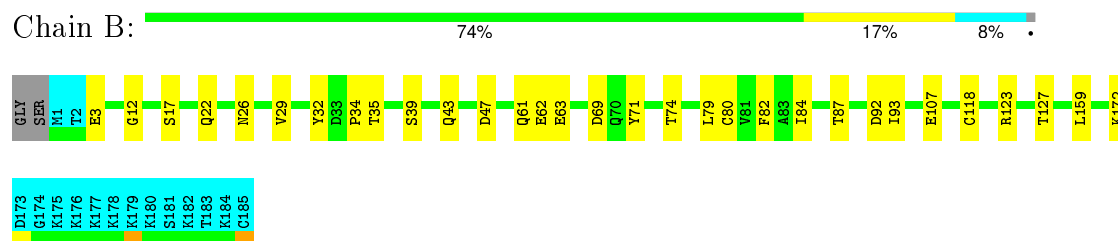
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

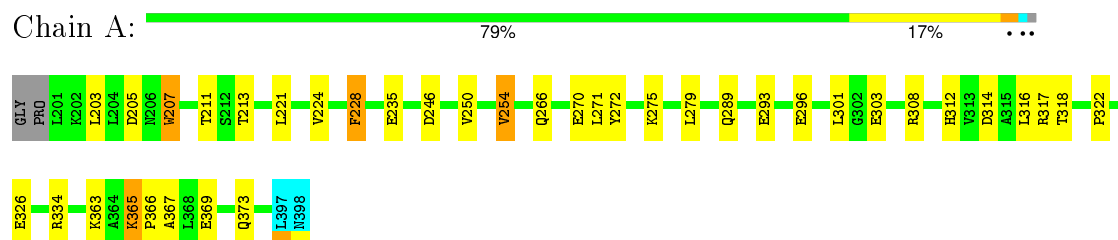


- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b



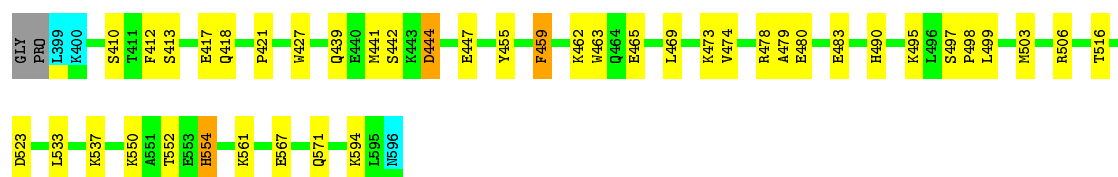
4.2.2 Score per residue for model 2

- Molecule 1: Apolipoprotein A-I



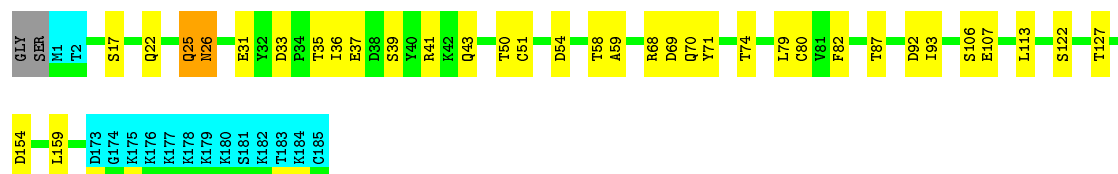
- Molecule 1: Apolipoprotein A-I





- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b

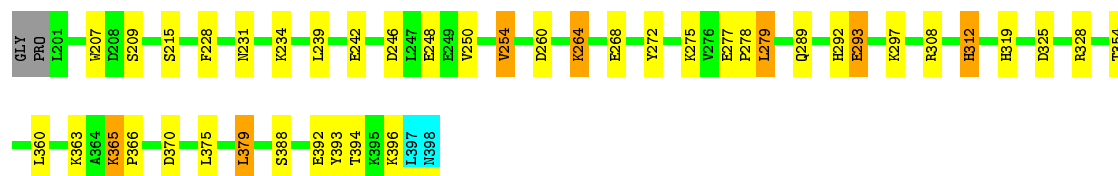
Chain B: 72% 18% 8%



4.2.3 Score per residue for model 3

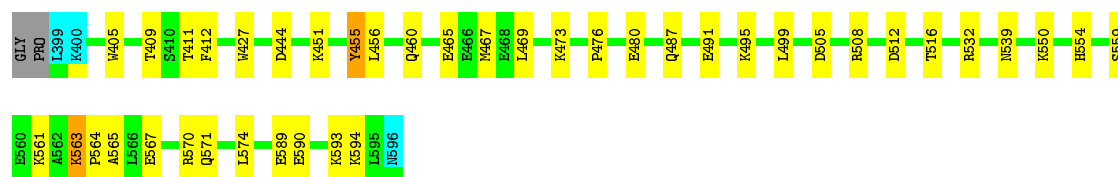
- Molecule 1: Apolipoprotein A-I

Chain A: 77% 18%



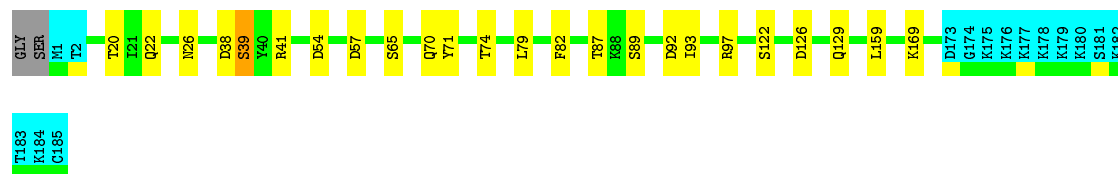
- Molecule 1: Apolipoprotein A-I

Chain C: 77% 20%



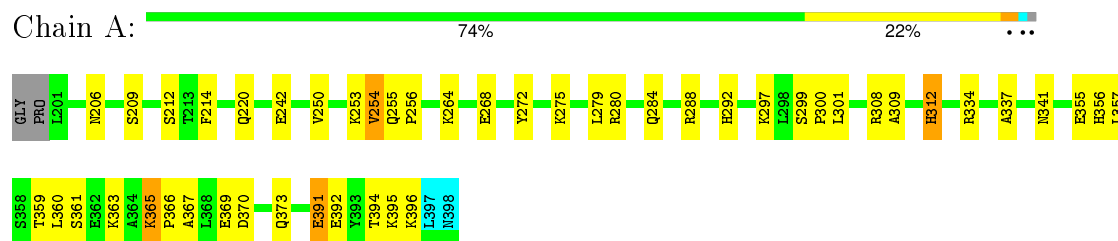
- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b

Chain B: 78% 12% 8%

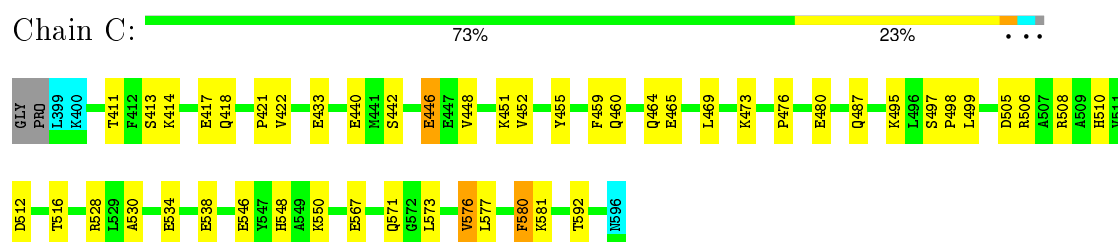


4.2.4 Score per residue for model 4

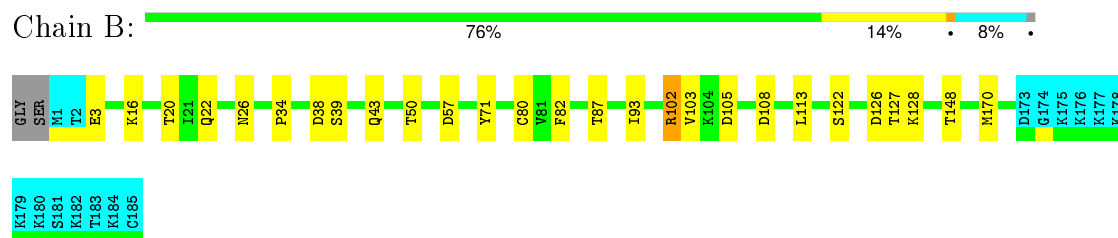
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

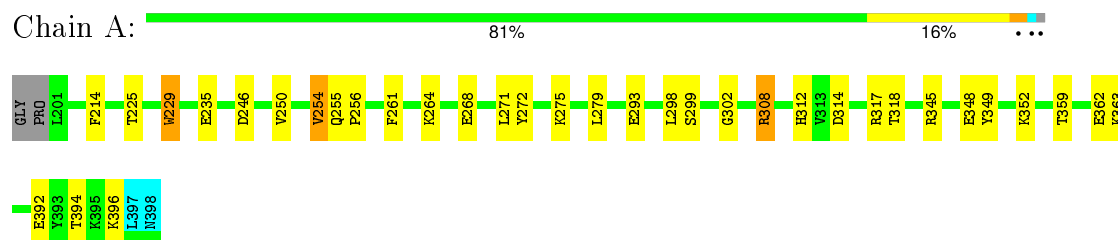


- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b

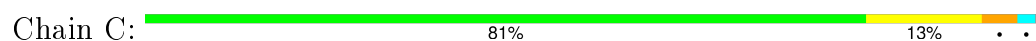


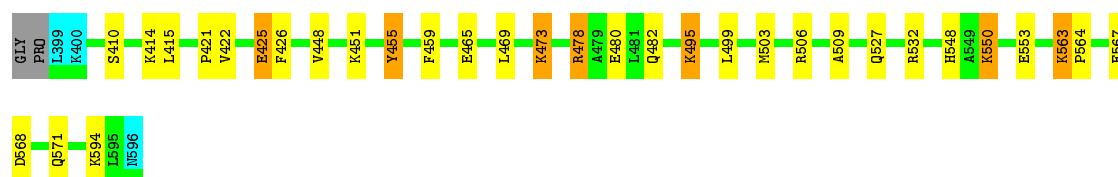
4.2.5 Score per residue for model 5

- Molecule 1: Apolipoprotein A-I



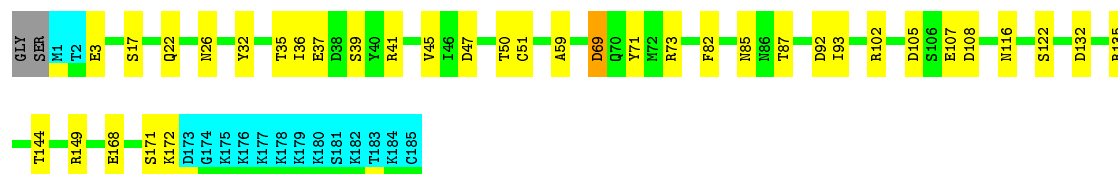
- Molecule 1: Apolipoprotein A-I





- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b

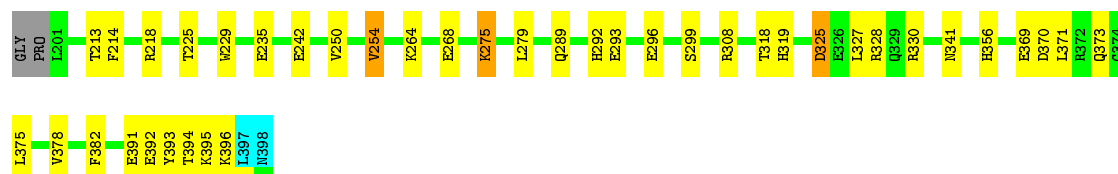
Chain B:



4.2.6 Score per residue for model 6

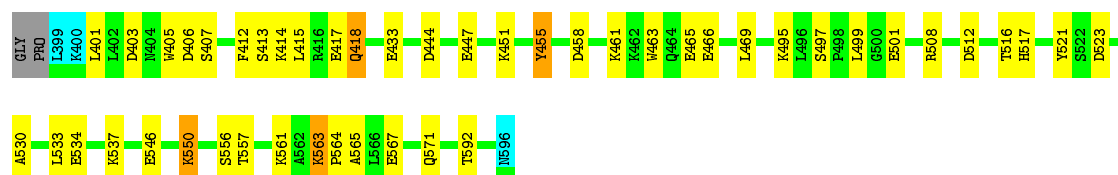
- Molecule 1: Apolipoprotein A-I

Chain A:



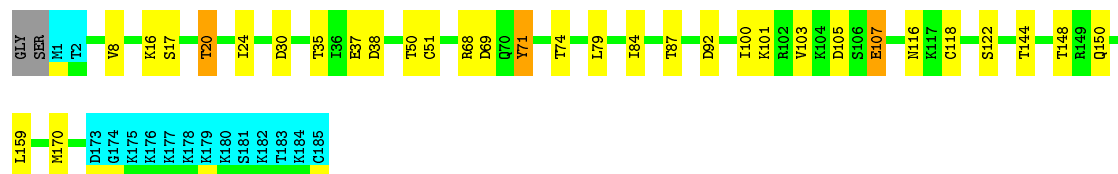
- Molecule 1: Apolipoprotein A-I

Chain C:



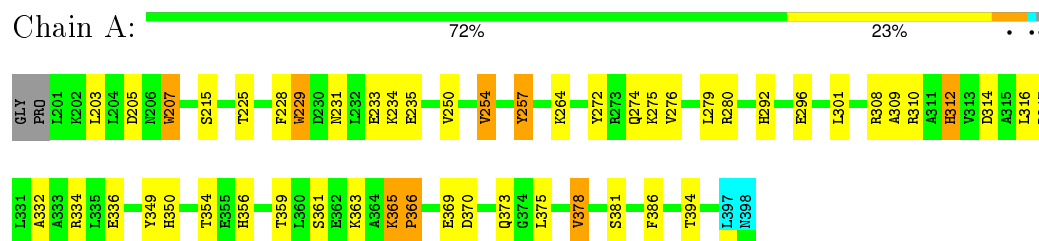
- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b

Chain B:

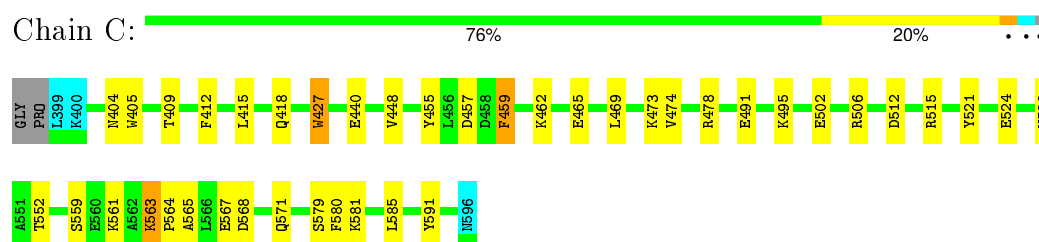


4.2.7 Score per residue for model 7

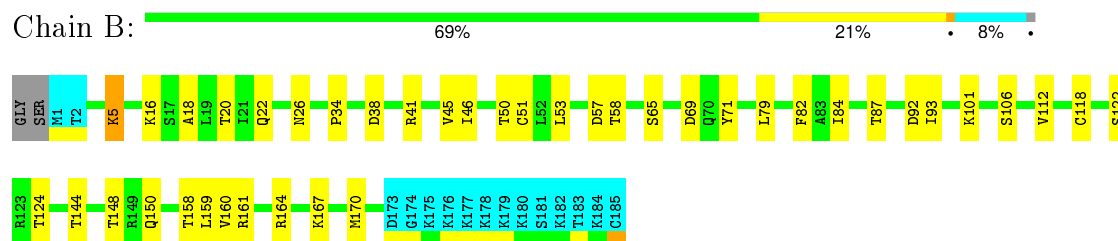
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

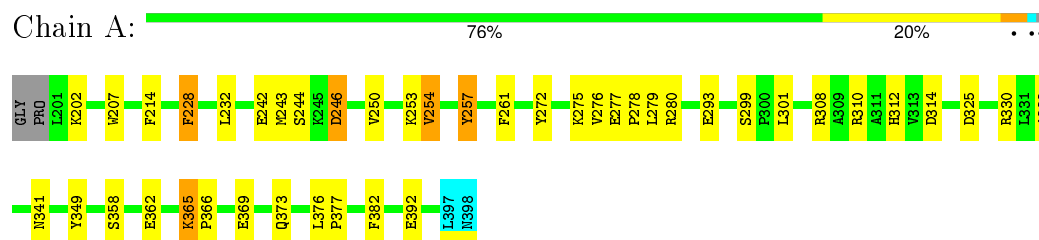


- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b



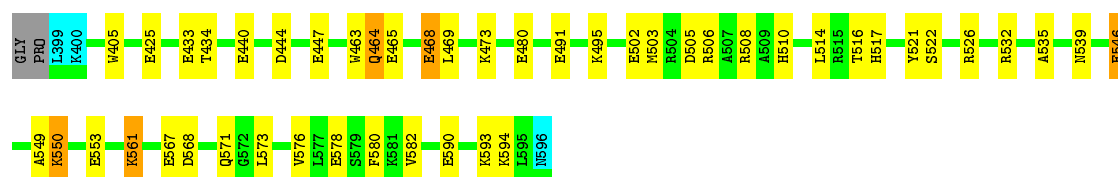
4.2.8 Score per residue for model 8

- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I





- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b

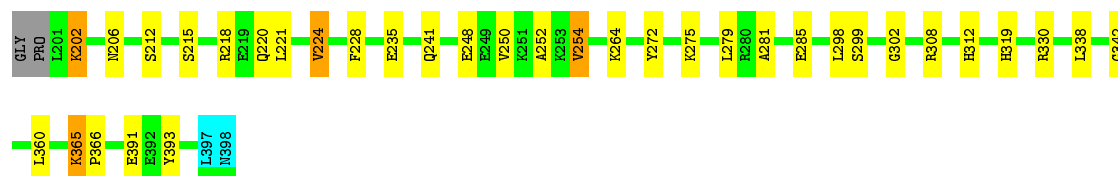
Chain B: 72% 19% 8%



4.2.9 Score per residue for model 9

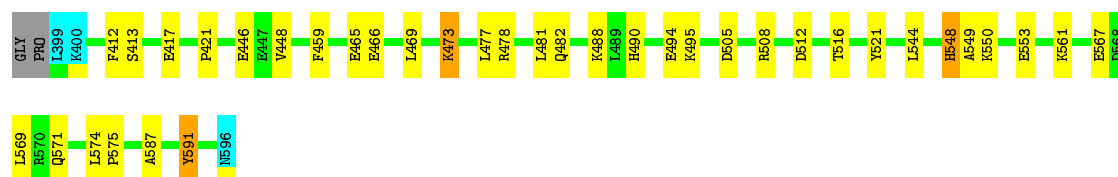
- Molecule 1: Apolipoprotein A-I

Chain A: 81% 16%



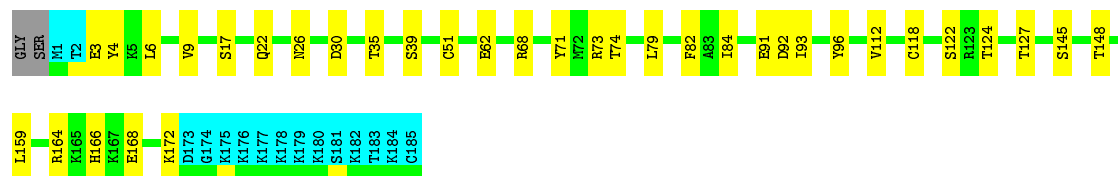
- Molecule 1: Apolipoprotein A-I

Chain C: 79% 17%



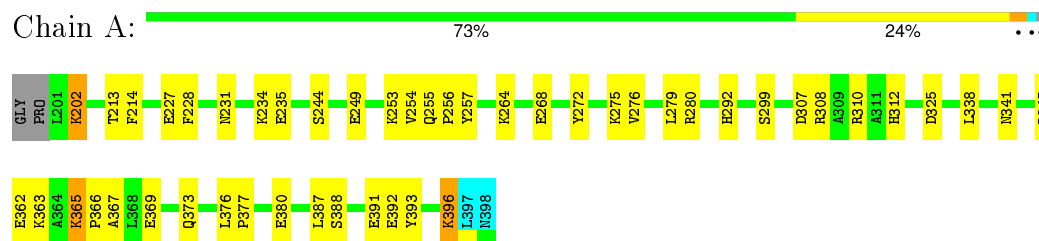
- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b

Chain B: 72% 19% 8%

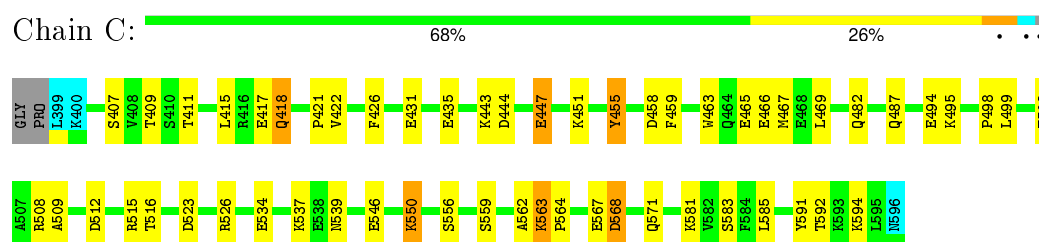


4.2.10 Score per residue for model 10

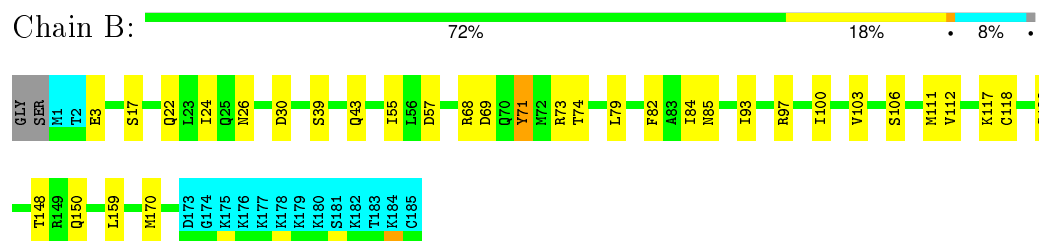
• Molecule 1: Apolipoprotein A-I



• Molecule 1: Apolipoprotein A-I



• Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b



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	
HADDOCK	structure solution	
CHARMM-GUI	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)	2msd_cs.str
Number of chemical shift lists	1
Total number of shifts	44
Number of shifts mapped to atoms	44
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	1607	22	1609	26±6
1	C	1598	22	1597	28±6
2	B	1358	18	1342	13±4
3	A	3456	0	5376	52±4
4	A	864	0	1216	20±5
5	B	32	0	13	1±1
All	All	89160	620	111525	1103

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 5.

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:CG	1:C:469:LEU:HD11	1.44	1.42	5	2
1:C:465:GLU:O	1:C:469:LEU:CG	1.27	1.82	1	8
1:A:308:ARG:HG2	1:C:469:LEU:CD1	1.27	1.59	5	1
1:C:465:GLU:O	1:C:469:LEU:HG	1.21	1.30	7	10
1:A:391:GLU:O	1:A:395:LYS:HG3	1.10	1.46	6	1
1:C:567:GLU:O	1:C:571:GLN:HG3	1.05	1.50	9	10
1:A:308:ARG:CD	1:C:469:LEU:HD21	1.00	1.86	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:HG3	1:C:469:LEU:HD21	0.98	1.32	10	7
1:A:392:GLU:OE1	1:A:395:LYS:HD2	0.94	1.62	6	1
1:C:567:GLU:O	1:C:571:GLN:CG	0.93	2.17	9	4
1:A:369:GLU:OE1	1:A:373:GLN:NE2	0.92	2.02	2	1
1:A:369:GLU:O	1:A:373:GLN:HG3	0.88	1.67	10	7
1:A:308:ARG:HD2	1:C:469:LEU:HD21	0.88	1.43	7	1
4:A:35:17F:HN1A	2:B:73:ARG:HH12	0.88	1.11	5	1
1:A:308:ARG:HG3	1:C:469:LEU:CD2	0.84	2.01	10	4
1:A:392:GLU:OE1	1:A:395:LYS:CD	0.84	2.25	6	1
2:B:38:ASP:HB2	2:B:57:ASP:HB3	0.83	1.46	7	4
1:A:392:GLU:CD	1:A:395:LYS:HD2	0.82	1.93	6	1
1:A:279:LEU:HD22	1:C:495:LYS:HG2	0.82	1.51	7	2
1:A:365:LYS:HB2	1:A:366:PRO:HD3	0.81	1.52	2	8
1:C:465:GLU:O	1:C:469:LEU:CB	0.81	2.27	7	2
3:A:68:PCW:H122	3:A:69:PCW:H331	0.80	1.53	1	2
1:A:308:ARG:CB	1:C:469:LEU:HD11	0.80	2.06	5	2
1:A:314:ASP:HA	1:A:317:ARG:HD2	0.79	1.52	2	3
4:A:36:17F:HN1A	2:B:73:ARG:HH11	0.79	1.19	10	1
1:A:308:ARG:CG	1:C:469:LEU:CD1	0.79	2.39	5	1
1:C:563:LYS:HB2	1:C:564:PRO:HD3	0.78	1.55	5	4
1:A:297:LYS:HE2	1:C:476:PRO:HB2	0.78	1.56	4	2
1:A:392:GLU:O	1:A:396:LYS:HG3	0.77	1.80	6	1
1:C:465:GLU:O	1:C:469:LEU:CD1	0.77	2.32	7	3
1:A:393:TYR:HD1	1:A:396:LYS:HE3	0.77	1.40	6	1
1:A:391:GLU:O	1:A:395:LYS:CG	0.76	2.31	6	1
3:A:13:PCW:H73	4:A:34:17F:HN1	0.76	1.38	9	2
1:A:308:ARG:HD3	1:C:469:LEU:HD21	0.75	1.57	7	1
3:A:11:PCW:H62	3:A:25:PCW:H31	0.74	1.58	10	1
4:A:40:17F:HN1	4:A:40:17F:H4	0.74	1.41	3	2
1:A:393:TYR:HD1	1:A:396:LYS:CE	0.74	1.95	6	1
3:A:45:PCW:H40	3:A:57:PCW:H61	0.73	1.57	10	2
3:A:6:PCW:H39	3:A:7:PCW:H62	0.73	1.59	1	1
1:A:393:TYR:CD1	1:A:396:LYS:HE3	0.73	2.18	6	1
3:A:54:PCW:H321	3:A:72:PCW:H132	0.73	1.61	10	1
4:A:34:17F:HN1A	2:B:167:LYS:HD3	0.72	1.44	7	1
3:A:5:PCW:H2	3:A:5:PCW:H52	0.72	1.61	9	2
1:C:590:GLU:HA	1:C:593:LYS:HE3	0.71	1.62	8	2
2:B:79:LEU:HG	2:B:159:LEU:HD22	0.71	1.61	6	8
1:A:218:ARG:HE	3:A:15:PCW:H19	0.70	1.45	6	2
3:A:4:PCW:H31	3:A:4:PCW:H41	0.70	1.64	1	1
3:A:16:PCW:H351	4:A:39:17F:H8A	0.69	1.63	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:45:PCW:H39	3:A:57:PCW:H71	0.69	1.65	9	1
3:A:26:PCW:H332	4:A:40:17F:H20A	0.69	1.63	4	1
1:A:276:VAL:O	1:A:280:ARG:HB2	0.69	1.88	8	3
1:C:458:ASP:HA	1:C:461:LYS:HE2	0.69	1.63	6	1
1:A:279:LEU:HB3	1:C:495:LYS:HE3	0.69	1.65	10	4
3:A:58:PCW:H332	3:A:61:PCW:H351	0.69	1.64	8	1
1:A:308:ARG:CG	1:C:469:LEU:HD21	0.68	2.14	10	2
3:A:18:PCW:H131	3:A:18:PCW:H341	0.68	1.66	9	1
4:A:34:17F:H20	4:A:34:17F:H8A	0.68	1.66	9	1
1:A:255:GLN:HB2	1:A:256:PRO:HD3	0.67	1.65	4	2
3:A:32:PCW:H62	4:A:38:17F:HN1	0.67	1.49	2	1
1:A:308:ARG:HD3	1:C:469:LEU:HD11	0.67	1.65	7	2
1:A:393:TYR:CD1	1:A:396:LYS:NZ	0.67	2.62	6	1
1:A:388:SER:HB2	1:C:594:LYS:HE2	0.67	1.66	3	1
3:A:53:PCW:H41	3:A:68:PCW:H321	0.66	1.66	7	1
3:A:66:PCW:H212	3:A:67:PCW:H82	0.66	1.66	8	1
1:A:308:ARG:HG2	1:C:469:LEU:HD11	0.66	0.70	5	1
3:A:25:PCW:H452	3:A:25:PCW:H182	0.66	1.66	1	1
3:A:42:PCW:H52	4:A:75:17F:H2	0.66	1.68	8	1
1:A:275:LYS:O	1:A:279:LEU:HG	0.66	1.90	6	9
3:A:7:PCW:H11	3:A:16:PCW:H12	0.66	1.67	9	1
3:A:1:PCW:H52	4:A:35:17F:HN1A	0.65	1.50	3	1
3:A:46:PCW:H42	4:A:73:17F:HN1A	0.65	1.50	8	1
3:A:12:PCW:H52	4:A:37:17F:HN1	0.65	1.51	10	1
1:C:503:MET:HA	1:C:506:ARG:HD2	0.65	1.67	2	4
3:A:16:PCW:H121	4:A:39:17F:H9	0.65	1.68	6	1
1:A:376:LEU:HB2	1:A:377:PRO:HD3	0.65	1.68	10	1
4:A:39:17F:H18A	4:A:39:17F:H9A	0.65	1.69	9	1
1:A:369:GLU:OE1	1:A:373:GLN:CD	0.65	2.34	2	1
3:A:46:PCW:H31	3:A:71:PCW:H362	0.64	1.68	8	1
1:C:512:ASP:HA	1:C:515:ARG:HD2	0.64	1.67	7	3
3:A:9:PCW:H61	3:A:26:PCW:H61	0.64	1.68	10	1
1:A:301:LEU:HD22	1:C:473:LYS:HG2	0.64	1.69	8	2
3:A:28:PCW:H161	3:A:28:PCW:H39	0.64	1.68	8	1
1:C:497:SER:HB2	1:C:498:PRO:HD3	0.64	1.68	4	2
3:A:26:PCW:H152	3:A:26:PCW:H382	0.64	1.70	9	1
1:A:308:ARG:CD	1:C:469:LEU:HD11	0.64	2.23	8	1
1:A:264:LYS:HE2	1:C:509:ALA:HB1	0.64	1.69	10	1
4:A:35:17F:HN1A	2:B:73:ARG:HH22	0.64	1.35	9	1
3:A:49:PCW:H62	4:A:80:17F:HN1	0.64	1.51	3	1
3:A:32:PCW:H81	4:A:38:17F:HN1A	0.64	1.52	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:392:GLU:OE2	1:A:395:LYS:NZ	0.63	2.24	6	1
3:A:13:PCW:H41	4:A:34:17F:N1	0.63	2.08	9	1
3:A:17:PCW:H172	3:A:21:PCW:H141	0.63	1.69	5	1
3:A:17:PCW:H332	3:A:17:PCW:H132	0.63	1.70	1	1
3:A:68:PCW:H121	3:A:69:PCW:H371	0.63	1.70	9	1
1:C:573:LEU:HA	1:C:576:VAL:HG12	0.62	1.69	8	3
1:C:505:ASP:HA	1:C:508:ARG:HD2	0.62	1.72	8	3
3:A:5:PCW:H83	4:A:38:17F:H4A	0.62	1.70	8	1
1:A:393:TYR:CD1	1:A:396:LYS:CE	0.62	2.80	6	1
3:A:66:PCW:H432	4:A:79:17F:H57	0.62	1.71	9	1
4:A:74:17F:H9	4:A:74:17F:H20A	0.62	1.69	5	1
4:A:36:17F:HN1A	2:B:73:ARG:NH1	0.62	1.93	10	1
3:A:58:PCW:H12	3:A:61:PCW:H381	0.62	1.69	9	1
1:C:418:GLN:O	1:C:422:VAL:HB	0.62	1.95	10	2
3:A:60:PCW:H31	3:A:61:PCW:H382	0.62	1.72	5	1
3:A:9:PCW:H122	3:A:11:PCW:H2	0.62	1.70	7	1
3:A:13:PCW:H122	3:A:18:PCW:H122	0.62	1.71	8	1
3:A:30:PCW:H62	4:A:34:17F:H2	0.61	1.71	8	1
1:A:392:GLU:HA	1:A:395:LYS:HB2	0.61	1.71	6	1
4:A:33:17F:HN1	2:B:73:ARG:HH12	0.61	1.39	8	1
1:A:308:ARG:HG3	1:C:469:LEU:HD11	0.61	1.72	8	2
3:A:14:PCW:H31	4:A:34:17F:H57	0.61	1.72	7	1
3:A:19:PCW:H322	3:A:23:PCW:H352	0.61	1.70	5	1
3:A:14:PCW:H432	4:A:34:17F:H20A	0.61	1.72	10	1
2:B:32:TYR:HD1	5:B:201:GNP:H4'	0.61	1.56	1	1
2:B:30:ASP:HA	5:B:201:GNP:H3'	0.61	1.73	9	1
1:C:561:LYS:HA	1:C:565:ALA:HB3	0.61	1.73	7	2
1:A:334:ARG:HD2	1:C:440:GLU:OE1	0.60	1.96	7	2
1:A:231:ASN:HA	1:A:234:LYS:HE2	0.60	1.73	3	3
3:A:1:PCW:H41	4:A:35:17F:H1A	0.60	1.72	8	1
1:A:330:ARG:HH21	1:C:447:GLU:HB2	0.60	1.56	6	1
1:A:365:LYS:O	1:A:369:GLU:HB2	0.60	1.97	2	2
1:A:308:ARG:CB	1:C:469:LEU:CD1	0.60	2.76	5	1
2:B:12:GLY:HA3	2:B:61:GLN:HG3	0.60	1.73	1	1
2:B:84:ILE:HD12	2:B:123:ARG:HG3	0.60	1.72	1	1
3:A:13:PCW:H41	4:A:34:17F:HN1	0.60	1.57	9	1
2:B:25:GLN:HA	2:B:25:GLN:HE21	0.60	1.57	2	1
3:A:53:PCW:H83	3:A:68:PCW:H322	0.59	1.74	3	1
4:A:77:17F:P1	4:A:77:17F:HN1	0.59	2.20	4	1
3:A:3:PCW:H422	3:A:18:PCW:H132	0.59	1.73	1	1
3:A:63:PCW:H122	3:A:63:PCW:H352	0.59	1.74	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:41:PCW:H61	4:A:77:17F:H1A	0.59	1.73	7	1
4:A:74:17F:H46	4:A:75:17F:H35	0.59	1.74	6	1
1:A:250:VAL:O	1:A:254:VAL:HB	0.59	1.97	2	9
3:A:51:PCW:H41	3:A:71:PCW:H412	0.59	1.74	8	1
3:A:32:PCW:H83	4:A:35:17F:H4A	0.59	1.74	4	1
3:A:49:PCW:H121	3:A:57:PCW:H372	0.59	1.74	8	1
3:A:20:PCW:H322	3:A:31:PCW:H11	0.58	1.72	3	1
1:C:451:LYS:O	1:C:455:TYR:HB2	0.58	1.98	5	6
3:A:59:PCW:H451	4:A:77:17F:H46	0.58	1.74	9	1
1:C:466:GLU:HA	1:C:469:LEU:HD12	0.58	1.73	6	2
3:A:20:PCW:H81	3:A:31:PCW:O2P	0.58	1.98	2	1
3:A:42:PCW:H151	3:A:42:PCW:H352	0.58	1.76	3	1
1:A:345:ARG:HG2	1:C:429:ASN:OD1	0.58	1.97	1	1
3:A:68:PCW:H332	3:A:69:PCW:H322	0.58	1.76	10	1
2:B:22:GLN:O	2:B:26:ASN:HA	0.58	1.99	7	9
3:A:42:PCW:H20	3:A:61:PCW:H71	0.58	1.74	6	1
2:B:84:ILE:HD11	2:B:118:CYS:HA	0.57	1.76	10	3
3:A:30:PCW:H121	4:A:40:17F:H6	0.57	1.76	10	1
3:A:6:PCW:H471	3:A:28:PCW:H19	0.57	1.75	2	1
1:A:369:GLU:O	1:A:373:GLN:CG	0.57	2.50	10	1
3:A:12:PCW:H83	4:A:37:17F:H1A	0.57	1.74	10	1
3:A:9:PCW:H39	3:A:14:PCW:H52	0.57	1.76	9	1
3:A:9:PCW:H73	3:A:30:PCW:O2P	0.57	2.00	3	1
3:A:62:PCW:O2P	3:A:63:PCW:H62	0.57	1.99	5	1
1:C:414:LYS:O	1:C:418:GLN:HG3	0.57	2.00	4	2
3:A:16:PCW:H242	4:A:39:17F:H4	0.57	1.76	5	1
1:C:478:ARG:O	1:C:482:GLN:HB2	0.57	1.99	1	3
2:B:82:PHE:HB3	2:B:93:ILE:HD11	0.57	1.76	4	9
1:A:308:ARG:HG2	1:C:469:LEU:CG	0.57	2.29	5	1
3:A:43:PCW:H411	3:A:71:PCW:H232	0.57	1.77	5	1
3:A:3:PCW:H61	3:A:19:PCW:H2	0.56	1.77	7	1
3:A:3:PCW:H361	3:A:18:PCW:H31	0.56	1.76	10	1
3:A:13:PCW:H73	4:A:34:17F:N1	0.56	2.14	9	2
3:A:30:PCW:H31	3:A:30:PCW:H51	0.56	1.75	3	1
3:A:63:PCW:P	4:A:75:17F:HN1A	0.56	2.22	2	2
3:A:68:PCW:H131	3:A:68:PCW:H371	0.56	1.77	1	1
3:A:16:PCW:H322	4:A:39:17F:H8A	0.56	1.77	8	1
3:A:59:PCW:H121	4:A:77:17F:H19A	0.56	1.77	10	1
3:A:25:PCW:H131	3:A:31:PCW:H12	0.56	1.78	10	1
4:A:35:17F:H43	3:A:55:PCW:H222	0.56	1.76	5	1
3:A:42:PCW:H352	3:A:42:PCW:H19	0.56	1.77	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:68:ARG:HA	2:B:71:TYR:CE2	0.56	2.36	9	2
1:A:242:GLU:HB3	1:C:532:ARG:HH21	0.56	1.61	8	1
1:C:447:GLU:OE1	1:C:451:LYS:HE2	0.56	2.01	10	2
1:A:375:LEU:HA	1:A:378:VAL:HG12	0.56	1.75	6	2
4:A:36:17F:HN1A	2:B:41:ARG:HE	0.56	1.40	5	1
3:A:32:PCW:H72	4:A:38:17F:N1	0.56	2.16	3	1
3:A:19:PCW:H42	3:A:29:PCW:O1P	0.56	2.00	4	1
3:A:9:PCW:H331	3:A:14:PCW:H321	0.56	1.78	3	1
2:B:158:THR:HA	2:B:161:ARG:HD2	0.56	1.78	7	1
3:A:45:PCW:H471	4:A:79:17F:H18	0.56	1.77	7	1
1:A:371:LEU:HD22	4:A:38:17F:H54	0.56	1.77	6	1
2:B:101:LYS:HG2	2:B:107:GLU:HA	0.56	1.76	6	1
3:A:30:PCW:H72	4:A:40:17F:O5	0.56	2.00	5	1
1:C:466:GLU:OE1	1:C:469:LEU:HD12	0.55	2.01	1	1
3:A:53:PCW:H141	3:A:68:PCW:H431	0.55	1.77	4	1
3:A:18:PCW:H252	3:A:49:PCW:H422	0.55	1.78	10	1
1:A:277:GLU:HB2	1:A:278:PRO:HD3	0.55	1.77	3	2
3:A:1:PCW:H42	3:A:26:PCW:H331	0.55	1.78	1	1
3:A:49:PCW:O2P	3:A:57:PCW:H71	0.55	2.01	7	1
3:A:70:PCW:H351	3:A:71:PCW:H121	0.55	1.78	5	1
1:A:327:LEU:HD23	1:A:330:ARG:HD2	0.55	1.77	6	1
3:A:25:PCW:H271	3:A:31:PCW:H451	0.55	1.78	10	1
3:A:1:PCW:O2P	3:A:17:PCW:H83	0.55	2.02	10	1
3:A:42:PCW:H231	3:A:52:PCW:H351	0.55	1.76	10	1
3:A:42:PCW:H82	3:A:42:PCW:O31	0.55	2.02	1	1
3:A:6:PCW:H232	3:A:24:PCW:H232	0.55	1.78	10	1
2:B:45:VAL:HA	2:B:50:THR:HA	0.55	1.78	7	2
3:A:11:PCW:H262	4:A:75:17F:H48	0.55	1.78	8	1
3:A:7:PCW:H32	3:A:16:PCW:H31	0.55	1.77	4	1
1:A:243:MET:HA	1:A:246:ASP:HB2	0.55	1.79	8	1
3:A:13:PCW:H11	3:A:18:PCW:H41	0.55	1.77	9	1
3:A:71:PCW:H19	3:A:71:PCW:H71	0.55	1.79	9	1
3:A:44:PCW:H172	4:A:77:17F:H6	0.55	1.79	2	1
3:A:50:PCW:H31	4:A:78:17F:H4	0.54	1.78	7	1
3:A:32:PCW:H81	4:A:38:17F:N1	0.54	2.16	5	1
3:A:7:PCW:H72	2:B:105:ASP:HB2	0.54	1.78	5	1
3:A:4:PCW:H471	4:A:39:17F:H38	0.54	1.78	6	1
1:A:330:ARG:NH2	1:C:444:ASP:HA	0.54	2.17	6	1
3:A:17:PCW:H152	3:A:17:PCW:H341	0.54	1.79	5	2
3:A:42:PCW:H81	3:A:63:PCW:O1P	0.54	2.01	3	1
1:C:465:GLU:O	1:C:469:LEU:HD12	0.54	2.02	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:67:PCW:H2	4:A:74:17F:H63	0.54	1.79	7	1
4:A:74:17F:H20A	4:A:74:17F:H11	0.54	1.77	2	1
1:C:401:LEU:O	1:C:405:TRP:HB2	0.54	2.03	6	1
1:A:239:LEU:HA	1:A:242:GLU:HB2	0.54	1.79	3	1
3:A:43:PCW:H41	3:A:43:PCW:H31	0.54	1.80	9	1
4:A:35:17F:HN1A	2:B:73:ARG:NH1	0.54	1.92	5	1
1:A:279:LEU:HB3	1:C:495:LYS:HD3	0.54	1.78	8	1
3:A:44:PCW:H221	3:A:59:PCW:H222	0.54	1.80	2	1
1:C:465:GLU:O	1:C:469:LEU:HB2	0.54	2.01	7	1
3:A:11:PCW:H39	3:A:28:PCW:H152	0.54	1.79	6	1
1:C:544:LEU:O	1:C:548:HIS:HB2	0.54	2.03	9	1
1:A:312:HIS:HE1	1:C:465:GLU:HB2	0.54	1.63	3	3
4:A:39:17F:H58	4:A:39:17F:H11A	0.54	1.80	5	1
3:A:59:PCW:H19	4:A:77:17F:H33	0.53	1.79	3	1
3:A:51:PCW:H322	3:A:56:PCW:H32	0.53	1.79	8	1
1:A:301:LEU:HD13	1:C:473:LYS:HG2	0.53	1.79	1	2
3:A:29:PCW:H122	3:A:31:PCW:H342	0.53	1.79	5	1
4:A:40:17F:H51	3:A:68:PCW:H212	0.53	1.79	2	1
2:B:18:ALA:HB2	5:B:201:GNP:O1A	0.53	2.03	7	1
4:A:33:17F:H12A	4:A:35:17F:H9A	0.53	1.79	9	1
3:A:19:PCW:H331	3:A:29:PCW:H361	0.53	1.78	2	1
1:C:589:GLU:HG2	1:C:593:LYS:HE2	0.53	1.80	3	1
3:A:9:PCW:H71	3:A:30:PCW:O1P	0.53	2.04	1	1
1:A:288:ARG:O	1:A:292:HIS:HB2	0.53	2.03	4	1
3:A:66:PCW:H19	4:A:78:17F:H5	0.53	1.79	4	1
1:C:469:LEU:HD22	1:C:473:LYS:NZ	0.53	2.18	3	1
3:A:59:PCW:H321	4:A:77:17F:H9A	0.53	1.79	7	1
2:B:160:VAL:HG12	2:B:164:ARG:HD2	0.53	1.80	7	1
3:A:48:PCW:H63	3:A:61:PCW:H411	0.53	1.81	3	1
3:A:66:PCW:H121	4:A:79:17F:H18A	0.53	1.81	1	1
4:A:35:17F:HN1A	2:B:5:LYS:NZ	0.53	2.01	8	1
4:A:74:17F:H71	4:A:79:17F:H9	0.53	1.80	9	1
3:A:1:PCW:H51	3:A:26:PCW:H362	0.53	1.80	5	1
3:A:25:PCW:H422	3:A:31:PCW:H39	0.53	1.80	6	1
3:A:18:PCW:H20	4:A:37:17F:H12	0.53	1.81	4	1
3:A:23:PCW:H372	4:A:34:17F:H67	0.53	1.80	4	1
1:C:567:GLU:O	1:C:571:GLN:CB	0.53	2.57	9	1
1:C:519:ALA:HB3	1:C:520:PRO:HD3	0.53	1.79	1	1
1:C:510:HIS:O	1:C:514:LEU:HG	0.53	2.04	8	1
3:A:51:PCW:H142	3:A:56:PCW:H211	0.53	1.80	4	1
1:C:491:GLU:O	1:C:495:LYS:HG3	0.53	2.03	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:417:GLU:O	1:C:421:PRO:HD2	0.53	2.04	9	4
3:A:9:PCW:H51	3:A:14:PCW:H322	0.52	1.82	7	1
2:B:68:ARG:HA	2:B:71:TYR:CZ	0.52	2.39	6	2
3:A:12:PCW:H71	4:A:37:17F:HN1A	0.52	1.63	6	1
3:A:27:PCW:H81	4:A:37:17F:H4A	0.52	1.80	7	1
3:A:6:PCW:H361	3:A:28:PCW:H2	0.52	1.79	7	1
3:A:25:PCW:H412	3:A:25:PCW:H162	0.52	1.81	9	1
3:A:20:PCW:H321	3:A:20:PCW:H41	0.52	1.82	9	1
3:A:48:PCW:H141	3:A:54:PCW:H141	0.52	1.80	2	1
4:A:35:17F:H47	3:A:55:PCW:H221	0.52	1.82	1	1
3:A:12:PCW:H352	4:A:36:17F:H5	0.52	1.82	2	1
3:A:13:PCW:H42	4:A:34:17F:O1	0.52	2.04	1	1
1:A:307:ASP:HA	1:A:310:ARG:HD2	0.52	1.80	10	2
3:A:30:PCW:H73	4:A:34:17F:O2	0.52	2.04	7	1
3:A:20:PCW:H83	3:A:31:PCW:O2P	0.52	2.04	8	3
3:A:28:PCW:H181	4:A:39:17F:H52	0.52	1.80	6	1
3:A:48:PCW:O31	3:A:48:PCW:H52	0.52	2.03	10	1
3:A:59:PCW:O2P	3:A:61:PCW:H83	0.52	2.05	9	1
3:A:59:PCW:H231	4:A:77:17F:H12	0.52	1.81	5	1
3:A:3:PCW:H71	3:A:19:PCW:H2	0.52	1.81	2	1
1:C:469:LEU:O	1:C:473:LYS:HB2	0.52	2.05	5	3
1:A:338:LEU:HA	1:A:341:ASN:HB3	0.52	1.82	10	1
1:A:363:LYS:HE2	1:C:411:THR:HB	0.52	1.80	3	1
3:A:24:PCW:H73	2:B:37:GLU:HB3	0.52	1.81	2	1
3:A:48:PCW:H322	3:A:54:PCW:H181	0.52	1.80	6	1
3:A:1:PCW:C6	4:A:35:17F:HN1A	0.52	2.18	4	1
3:A:6:PCW:H32	3:A:11:PCW:H322	0.52	1.80	10	1
4:A:40:17F:N1	4:A:40:17F:H4	0.52	2.18	3	1
3:A:65:PCW:H73	3:A:65:PCW:O31	0.52	2.05	3	1
3:A:10:PCW:H131	3:A:22:PCW:H331	0.52	1.81	10	2
1:C:474:VAL:O	1:C:478:ARG:HB2	0.52	2.04	2	2
1:A:301:LEU:HB3	1:C:473:LYS:HE3	0.52	1.81	4	1
1:C:568:ASP:OD1	1:C:571:GLN:OE1	0.52	2.28	10	1
3:A:1:PCW:H2	4:A:35:17F:H18A	0.52	1.80	2	1
3:A:1:PCW:H2	3:A:26:PCW:H372	0.51	1.81	1	1
3:A:42:PCW:H442	3:A:52:PCW:H382	0.51	1.80	1	1
3:A:2:PCW:H62	3:A:5:PCW:O2P	0.51	2.05	1	1
3:A:32:PCW:H71	4:A:38:17F:N1	0.51	2.19	5	1
1:C:427:TRP:HA	1:C:427:TRP:CE3	0.51	2.40	7	1
3:A:2:PCW:H42	3:A:17:PCW:O2P	0.51	2.05	6	1
3:A:13:PCW:H81	4:A:37:17F:H1A	0.51	1.80	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:559:SER:HA	1:C:562:ALA:HB3	0.51	1.82	10	1
4:A:37:17F:O1	2:B:5:LYS:HE2	0.51	2.05	7	1
1:A:275:LYS:O	1:A:279:LEU:HB2	0.51	2.06	3	1
3:A:63:PCW:P	4:A:75:17F:N1	0.51	2.82	2	1
3:A:63:PCW:H152	3:A:63:PCW:H422	0.51	1.82	5	1
3:A:9:PCW:H81	3:A:30:PCW:O2P	0.51	2.06	2	1
3:A:13:PCW:H41	4:A:34:17F:O1	0.51	2.06	4	1
3:A:26:PCW:H42	2:B:3:GLU:OE1	0.51	2.06	10	1
3:A:32:PCW:H61	4:A:38:17F:HN1A	0.51	1.65	5	1
3:A:17:PCW:H73	4:A:38:17F:O1	0.51	2.06	2	1
1:A:330:ARG:HH21	1:C:447:GLU:HB3	0.51	1.67	1	2
3:A:51:PCW:H2	3:A:71:PCW:H382	0.51	1.82	6	1
3:A:49:PCW:C6	4:A:80:17F:HN1	0.50	2.18	3	1
3:A:47:PCW:H172	4:A:76:17F:H4	0.50	1.83	3	1
3:A:44:PCW:H321	3:A:55:PCW:H62	0.50	1.81	10	1
2:B:36:ILE:HA	2:B:59:ALA:HB2	0.50	1.83	5	2
3:A:63:PCW:H412	3:A:72:PCW:H232	0.50	1.82	8	1
3:A:6:PCW:P	3:A:16:PCW:O1P	0.50	2.69	4	1
1:C:421:PRO:O	1:C:425:GLU:HG3	0.50	2.07	5	1
1:A:310:ARG:O	1:A:314:ASP:HB2	0.50	2.07	1	2
3:A:22:PCW:H32	4:A:37:17F:H1A	0.50	1.82	8	1
3:A:6:PCW:H381	3:A:16:PCW:H321	0.50	1.83	4	1
3:A:9:PCW:H71	3:A:30:PCW:O2P	0.50	2.06	10	1
3:A:43:PCW:H451	3:A:69:PCW:H361	0.50	1.83	9	1
2:B:84:ILE:CD1	2:B:118:CYS:HA	0.50	2.37	1	2
3:A:72:PCW:H382	4:A:78:17F:H38	0.50	1.84	7	1
3:A:10:PCW:H281	4:A:37:17F:H61	0.50	1.83	7	1
3:A:4:PCW:H242	3:A:32:PCW:H221	0.50	1.84	7	1
3:A:32:PCW:H83	4:A:38:17F:HN1A	0.50	1.67	8	1
1:C:491:GLU:HB3	1:C:495:LYS:HE2	0.50	1.83	8	1
3:A:41:PCW:H31	3:A:52:PCW:H372	0.50	1.84	6	1
3:A:60:PCW:H182	3:A:62:PCW:H222	0.50	1.81	4	1
3:A:8:PCW:H72	3:A:22:PCW:O1P	0.50	2.07	7	1
3:A:1:PCW:O11	3:A:17:PCW:H83	0.50	2.07	4	1
3:A:5:PCW:H381	3:A:17:PCW:H331	0.50	1.82	10	1
3:A:15:PCW:H81	4:A:39:17F:O2	0.50	2.07	10	1
4:A:74:17F:H5	4:A:74:17F:H20A	0.50	1.84	9	1
3:A:54:PCW:H372	3:A:54:PCW:H31	0.50	1.82	5	1
1:C:455:TYR:O	1:C:459:PHE:HB2	0.50	2.07	10	3
1:A:341:ASN:ND2	1:C:433:GLU:HA	0.50	2.22	8	2
4:A:36:17F:HN1A	2:B:41:ARG:NE	0.50	2.04	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:64:PCW:H442	3:A:68:PCW:H271	0.50	1.82	3	1
3:A:62:PCW:H372	3:A:72:PCW:H152	0.50	1.84	8	1
4:A:33:17F:HN1	2:B:73:ARG:NH1	0.50	2.05	8	1
1:A:332:ALA:O	1:A:336:GLU:HG2	0.50	2.07	8	1
4:A:33:17F:H1	4:A:33:17F:C4	0.50	2.36	4	1
3:A:60:PCW:H51	3:A:61:PCW:H321	0.50	1.82	10	1
1:A:221:LEU:HA	1:A:224:VAL:HG12	0.50	1.82	9	2
3:A:49:PCW:H82	4:A:80:17F:O2	0.49	2.07	7	1
1:A:325:ASP:HA	1:A:328:ARG:HD2	0.49	1.84	6	2
3:A:53:PCW:H331	3:A:68:PCW:H381	0.49	1.84	4	1
1:C:442:SER:O	1:C:446:GLU:HB2	0.49	2.07	4	1
3:A:15:PCW:H71	4:A:39:17F:N1	0.49	2.22	2	1
3:A:9:PCW:H342	3:A:14:PCW:H61	0.49	1.83	3	1
1:C:443:LYS:O	1:C:447:GLU:HB2	0.49	2.06	10	2
3:A:62:PCW:H351	3:A:72:PCW:H332	0.49	1.83	6	1
3:A:26:PCW:O1P	3:A:30:PCW:H83	0.49	2.08	5	1
1:C:508:ARG:O	1:C:512:ASP:HB2	0.49	2.07	3	3
3:A:24:PCW:H322	3:A:25:PCW:H122	0.49	1.85	10	1
3:A:67:PCW:H232	4:A:75:17F:H11A	0.49	1.84	7	1
4:A:35:17F:HN1A	2:B:5:LYS:HZ3	0.49	1.48	8	1
1:C:523:ASP:HA	1:C:526:ARG:HD2	0.49	1.84	10	1
1:A:224:VAL:O	1:A:228:PHE:HB2	0.49	2.08	2	2
1:A:334:ARG:HD2	1:C:440:GLU:OE2	0.49	2.07	8	1
3:A:47:PCW:H31	4:A:73:17F:O5	0.49	2.07	6	1
1:A:392:GLU:O	1:A:396:LYS:HG2	0.49	2.07	10	2
3:A:72:PCW:H41	3:A:72:PCW:O31	0.49	2.08	1	1
1:A:327:LEU:HA	1:A:330:ARG:HG2	0.49	1.84	6	1
1:A:299:SER:HB2	1:A:300:PRO:HD3	0.49	1.84	4	1
3:A:47:PCW:H242	4:A:76:17F:H33	0.49	1.83	10	1
3:A:41:PCW:H73	3:A:44:PCW:O1P	0.49	2.08	5	1
3:A:14:PCW:H232	4:A:37:17F:H11A	0.49	1.84	2	1
2:B:126:ASP:HB3	2:B:129:GLN:HG3	0.49	1.84	3	1
3:A:48:PCW:H39	3:A:54:PCW:H432	0.49	1.84	9	1
3:A:6:PCW:O1P	3:A:16:PCW:H63	0.49	2.08	5	1
3:A:22:PCW:H132	4:A:37:17F:H6	0.49	1.84	1	1
2:B:116:ASN:HA	2:B:144:THR:O	0.49	2.08	6	2
1:A:298:LEU:O	1:A:302:GLY:HA3	0.49	2.07	9	2
3:A:49:PCW:H142	3:A:57:PCW:H331	0.48	1.85	3	1
1:A:253:LYS:O	1:A:257:TYR:HB2	0.48	2.07	8	1
3:A:57:PCW:H2	3:A:57:PCW:H52	0.48	1.84	6	1
3:A:3:PCW:H122	3:A:19:PCW:H121	0.48	1.84	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:32:TYR:HA	5:B:201:GNP:H5'1	0.48	1.84	8	1
1:C:411:THR:O	1:C:415:LEU:HG	0.48	2.09	10	1
1:A:309:ALA:HA	1:A:312:HIS:HB2	0.48	1.85	7	2
1:A:231:ASN:HA	1:A:234:LYS:CE	0.48	2.38	10	2
3:A:44:PCW:H131	4:A:77:17F:H2	0.48	1.85	4	1
3:A:7:PCW:H11	3:A:16:PCW:O2P	0.48	2.08	1	1
3:A:9:PCW:H73	3:A:26:PCW:O2P	0.48	2.09	1	1
1:A:308:ARG:HD3	1:C:469:LEU:CD1	0.48	2.38	7	1
3:A:18:PCW:H42	2:B:41:ARG:HD3	0.48	1.85	7	1
3:A:47:PCW:H242	4:A:76:17F:H60	0.48	1.84	8	1
1:A:391:GLU:O	1:A:395:LYS:HB2	0.48	2.09	4	1
1:A:388:SER:HB2	1:C:594:LYS:CE	0.48	2.38	10	1
1:C:441:MET:HA	1:C:444:ASP:HB2	0.48	1.84	2	1
1:A:363:LYS:HA	1:A:367:ALA:HB3	0.48	1.84	1	1
3:A:12:PCW:H73	2:B:105:ASP:OD2	0.48	2.07	4	1
1:A:355:GLU:HA	1:A:355:GLU:OE1	0.48	2.08	4	1
4:A:79:17F:H69	4:A:79:17F:H58	0.48	1.85	5	1
3:A:32:PCW:H63	4:A:38:17F:N1	0.48	2.24	3	1
3:A:17:PCW:H32	2:B:172:LYS:HG2	0.48	1.86	1	1
4:A:37:17F:N1	2:B:5:LYS:NZ	0.48	2.61	7	1
3:A:32:PCW:H83	4:A:38:17F:N1	0.48	2.23	8	1
3:A:13:PCW:H81	3:A:30:PCW:H321	0.48	1.86	1	1
1:C:546:GLU:O	1:C:550:LYS:HD2	0.48	2.08	6	3
3:A:42:PCW:H341	3:A:52:PCW:H341	0.48	1.84	10	1
1:A:202:LYS:HZ3	1:A:202:LYS:HB3	0.48	1.69	10	1
3:A:70:PCW:H62	3:A:70:PCW:O31	0.48	2.09	7	1
3:A:52:PCW:H122	3:A:60:PCW:H11	0.48	1.85	7	1
3:A:49:PCW:H332	3:A:57:PCW:H371	0.48	1.86	8	1
3:A:2:PCW:O1P	3:A:21:PCW:H31	0.48	2.08	8	1
3:A:20:PCW:H31	3:A:31:PCW:H31	0.48	1.85	4	1
3:A:49:PCW:H322	3:A:57:PCW:H2	0.48	1.86	9	1
3:A:4:PCW:H61	4:A:33:17F:H2	0.48	1.84	2	1
1:A:322:PRO:O	1:A:326:GLU:HG3	0.48	2.09	2	1
1:C:495:LYS:O	1:C:499:LEU:HB2	0.48	2.09	6	7
3:A:66:PCW:H151	4:A:78:17F:H19A	0.48	1.85	6	1
2:B:102:ARG:HH21	2:B:103:VAL:HG12	0.48	1.69	4	1
1:C:534:GLU:HA	1:C:537:LYS:HE3	0.48	1.85	10	1
3:A:42:PCW:H82	3:A:63:PCW:O1P	0.48	2.09	2	1
3:A:8:PCW:H283	1:C:451:LYS:HB3	0.48	1.86	1	1
2:B:144:THR:HA	2:B:150:GLN:O	0.48	2.09	7	2
1:A:358:SER:O	1:A:362:GLU:HG3	0.48	2.09	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:43:PCW:H351	3:A:43:PCW:H122	0.48	1.86	2	1
3:A:48:PCW:H39	3:A:54:PCW:H452	0.47	1.85	1	1
1:C:502:GLU:HG2	1:C:506:ARG:HE	0.47	1.68	8	2
1:A:392:GLU:CD	1:A:395:LYS:CD	0.47	2.76	6	1
3:A:2:PCW:H81	2:B:105:ASP:OD1	0.47	2.08	6	1
1:A:308:ARG:HD3	1:C:469:LEU:CD2	0.47	2.32	7	1
3:A:1:PCW:H422	4:A:36:17F:H43	0.47	1.86	9	1
3:A:13:PCW:H241	3:A:18:PCW:H372	0.47	1.84	3	1
3:A:46:PCW:O2P	3:A:51:PCW:H83	0.47	2.09	10	1
3:A:49:PCW:H331	4:A:80:17F:H19	0.47	1.85	9	1
3:A:41:PCW:H31	3:A:42:PCW:H211	0.47	1.86	2	1
1:C:421:PRO:O	1:C:425:GLU:HG2	0.47	2.10	1	1
4:A:76:17F:H9	4:A:76:17F:H18	0.47	1.86	1	1
3:A:6:PCW:H342	3:A:28:PCW:H62	0.47	1.86	7	1
3:A:62:PCW:H412	4:A:78:17F:H54	0.47	1.87	8	1
3:A:22:PCW:N	4:A:37:17F:N1	0.47	2.62	4	2
3:A:20:PCW:O2P	3:A:24:PCW:H83	0.47	2.09	10	1
3:A:55:PCW:H411	3:A:64:PCW:H352	0.47	1.85	3	1
3:A:57:PCW:H261	4:A:80:17F:H45	0.47	1.85	1	1
1:A:387:LEU:O	1:A:391:GLU:HG3	0.47	2.09	1	2
3:A:2:PCW:H62	3:A:17:PCW:H2	0.47	1.85	7	1
3:A:42:PCW:C20	3:A:61:PCW:H71	0.47	2.40	6	1
1:A:363:LYS:O	1:A:367:ALA:HB3	0.47	2.10	4	3
3:A:44:PCW:H131	4:A:77:17F:H4A	0.47	1.85	3	1
3:A:18:PCW:H222	4:A:37:17F:H64	0.47	1.85	3	1
3:A:16:PCW:H82	3:A:16:PCW:O11	0.47	2.10	3	1
3:A:6:PCW:H40	3:A:7:PCW:H83	0.47	1.85	1	1
1:A:255:GLN:HB2	1:A:256:PRO:CD	0.47	2.39	1	3
1:A:316:LEU:HG	1:C:462:LYS:HE3	0.47	1.86	7	2
3:A:9:PCW:H82	3:A:30:PCW:O2P	0.47	2.09	7	1
1:A:225:THR:O	1:A:229:TRP:HB2	0.47	2.09	6	3
3:A:3:PCW:H122	3:A:19:PCW:H141	0.47	1.85	6	1
3:A:16:PCW:H322	4:A:39:17F:H11	0.47	1.87	4	1
3:A:25:PCW:O2P	3:A:31:PCW:H51	0.47	2.09	4	1
1:C:479:ALA:O	1:C:483:GLU:HG2	0.47	2.09	2	1
3:A:24:PCW:H361	3:A:25:PCW:H121	0.47	1.87	3	1
1:C:570:ARG:O	1:C:574:LEU:HG	0.47	2.09	3	1
3:A:41:PCW:H141	3:A:61:PCW:H141	0.47	1.87	1	1
3:A:5:PCW:O31	3:A:5:PCW:H83	0.47	2.10	1	1
1:A:293:GLU:O	1:A:297:LYS:HB2	0.47	2.09	3	1
1:A:247:LEU:HA	1:A:250:VAL:HG12	0.47	1.87	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:34:17F:H11A	4:A:40:17F:H59	0.47	1.87	6	1
3:A:53:PCW:O2P	3:A:55:PCW:H61	0.47	2.09	10	1
3:A:62:PCW:O31	3:A:62:PCW:H41	0.47	2.10	4	1
3:A:12:PCW:H82	4:A:37:17F:O4	0.46	2.10	8	1
1:A:392:GLU:OE1	1:A:395:LYS:HD3	0.46	2.08	6	1
3:A:20:PCW:O1P	3:A:31:PCW:H11	0.46	2.10	6	1
4:A:77:17F:N1	4:A:77:17F:P1	0.46	2.88	4	1
3:A:13:PCW:H31	4:A:37:17F:H12	0.46	1.86	2	1
3:A:12:PCW:H321	3:A:30:PCW:H141	0.46	1.87	2	1
3:A:6:PCW:P	3:A:24:PCW:O2P	0.46	2.74	1	1
3:A:19:PCW:H362	3:A:19:PCW:H121	0.46	1.86	7	1
3:A:12:PCW:H63	4:A:37:17F:N1	0.46	2.26	9	1
4:A:39:17F:H33	4:A:39:17F:H8	0.46	1.87	5	1
4:A:38:17F:H20A	4:A:38:17F:H8	0.46	1.87	5	1
3:A:42:PCW:H252	3:A:52:PCW:H212	0.46	1.87	1	1
3:A:12:PCW:H151	3:A:22:PCW:H122	0.46	1.86	1	1
1:A:203:LEU:O	1:A:207:TRP:HB2	0.46	2.10	7	2
3:A:26:PCW:H51	3:A:28:PCW:O1P	0.46	2.11	8	1
1:C:561:LYS:O	1:C:565:ALA:HB3	0.46	2.10	6	1
2:B:16:LYS:HB3	2:B:57:ASP:OD1	0.46	2.10	4	1
1:A:299:SER:HB2	1:A:300:PRO:CD	0.46	2.39	4	1
3:A:43:PCW:H471	3:A:70:PCW:H351	0.46	1.87	3	1
2:B:58:THR:HG22	2:B:71:TYR:CE1	0.46	2.46	7	1
2:B:62:GLU:OE1	2:B:68:ARG:HD2	0.46	2.10	8	1
3:A:26:PCW:H372	3:A:26:PCW:H131	0.46	1.86	6	1
3:A:54:PCW:H131	3:A:54:PCW:H331	0.46	1.87	4	1
3:A:30:PCW:H81	2:B:39:SER:OG	0.46	2.10	10	1
3:A:50:PCW:H62	4:A:78:17F:HN1	0.46	1.70	5	1
3:A:30:PCW:H83	4:A:34:17F:O2	0.46	2.10	2	1
1:C:456:LEU:O	1:C:460:GLN:HB2	0.46	2.10	3	1
1:A:310:ARG:O	1:A:314:ASP:HB3	0.46	2.11	7	1
4:A:40:17F:H43	3:A:43:PCW:H252	0.46	1.87	6	1
3:A:28:PCW:H261	3:A:42:PCW:H452	0.46	1.86	10	1
3:A:6:PCW:H341	3:A:28:PCW:H121	0.46	1.87	5	1
4:A:36:17F:H46	3:A:68:PCW:H271	0.46	1.86	2	1
3:A:6:PCW:O1P	3:A:7:PCW:H71	0.46	2.09	2	1
3:A:23:PCW:H212	3:A:49:PCW:H461	0.46	1.87	2	1
3:A:53:PCW:H341	3:A:68:PCW:H372	0.46	1.87	8	1
1:C:534:GLU:O	1:C:538:GLU:HG2	0.46	2.10	4	1
3:A:16:PCW:H212	3:A:24:PCW:H441	0.46	1.88	9	1
3:A:51:PCW:H362	3:A:56:PCW:H11	0.46	1.85	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:41:ARG:HD3	2:B:54:ASP:OD1	0.46	2.11	2	1
3:A:51:PCW:O1P	3:A:56:PCW:H32	0.46	2.11	3	1
3:A:53:PCW:H142	3:A:56:PCW:H382	0.46	1.87	3	1
1:C:563:LYS:HB2	1:C:564:PRO:CD	0.46	2.41	6	2
3:A:68:PCW:H421	3:A:70:PCW:H231	0.46	1.87	5	1
3:A:53:PCW:O2P	3:A:55:PCW:H71	0.46	2.10	1	1
3:A:28:PCW:O4P	3:A:28:PCW:H2	0.46	2.10	1	1
3:A:53:PCW:H31	3:A:64:PCW:H32	0.46	1.88	7	1
3:A:59:PCW:H2	4:A:77:17F:H9	0.46	1.87	4	1
3:A:22:PCW:H341	3:A:22:PCW:H132	0.46	1.87	4	1
1:C:460:GLN:O	1:C:464:GLN:HG3	0.46	2.11	4	1
3:A:41:PCW:O31	3:A:61:PCW:H81	0.46	2.10	1	1
2:B:79:LEU:HD23	2:B:112:VAL:HB	0.46	1.87	8	4
1:C:563:LYS:CB	1:C:564:PRO:HD3	0.46	2.38	3	2
1:A:234:LYS:HE3	1:C:539:ASN:OD1	0.46	2.11	10	3
3:A:60:PCW:O2P	3:A:63:PCW:H81	0.46	2.10	3	1
3:A:53:PCW:H132	3:A:64:PCW:H162	0.46	1.87	4	1
4:A:33:17F:P1	4:A:33:17F:HN1	0.46	2.34	5	2
3:A:24:PCW:N	4:A:39:17F:N1	0.45	2.64	1	1
3:A:44:PCW:H42	3:A:53:PCW:H42	0.45	1.88	6	1
3:A:10:PCW:H51	3:A:21:PCW:O2P	0.45	2.11	4	1
3:A:23:PCW:H451	3:A:29:PCW:H371	0.45	1.88	5	1
4:A:34:17F:HN1A	2:B:167:LYS:CD	0.45	2.20	7	1
3:A:5:PCW:H12	3:A:17:PCW:H342	0.45	1.87	7	1
3:A:30:PCW:H41	3:A:30:PCW:H31	0.45	1.88	8	1
3:A:1:PCW:H472	4:A:36:17F:H45	0.45	1.88	8	1
3:A:25:PCW:H381	3:A:29:PCW:H431	0.45	1.87	6	1
1:C:466:GLU:HA	1:C:469:LEU:HB2	0.45	1.87	10	1
3:A:14:PCW:H42	3:A:25:PCW:H62	0.45	1.86	5	1
1:C:585:LEU:O	1:C:589:GLU:HB2	0.45	2.12	1	1
3:A:22:PCW:O2P	3:A:27:PCW:H62	0.45	2.10	7	1
3:A:48:PCW:H81	3:A:60:PCW:O11	0.45	2.12	7	1
2:B:84:ILE:HG12	2:B:118:CYS:HA	0.45	1.88	6	1
1:A:345:ARG:O	1:A:349:TYR:HB2	0.45	2.12	5	1
3:A:32:PCW:H52	4:A:35:17F:H6	0.45	1.87	2	1
3:A:4:PCW:H251	3:A:32:PCW:H182	0.45	1.87	7	1
1:C:530:ALA:O	1:C:534:GLU:HG3	0.45	2.11	4	2
3:A:11:PCW:H71	2:B:3:GLU:OE1	0.45	2.10	4	1
1:C:422:VAL:HA	1:C:425:GLU:OE2	0.45	2.11	5	1
3:A:12:PCW:H72	3:A:22:PCW:O2P	0.45	2.10	2	1
3:A:4:PCW:H222	3:A:32:PCW:H262	0.45	1.87	10	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:H48	0.45	1.88	10	1
3:A:9:PCW:H62	3:A:9:PCW:O11	0.45	2.12	3	1
3:A:68:PCW:H19	3:A:70:PCW:H262	0.45	1.89	7	1
3:A:3:PCW:O2P	3:A:23:PCW:H62	0.45	2.11	7	1
2:B:100:ILE:HA	2:B:103:VAL:HG22	0.45	1.88	10	2
3:A:26:PCW:H39	4:A:33:17F:H46	0.45	1.88	9	1
4:A:35:17F:HN1A	2:B:73:ARG:NH2	0.45	2.07	9	1
3:A:12:PCW:H63	4:A:37:17F:HN1	0.45	1.72	9	1
3:A:22:PCW:H442	3:A:30:PCW:H261	0.45	1.88	5	1
1:A:264:LYS:CE	1:C:509:ALA:HB1	0.45	2.42	5	1
3:A:9:PCW:H412	3:A:29:PCW:H412	0.45	1.89	3	1
2:B:45:VAL:HG22	2:B:50:THR:HB	0.45	1.88	7	1
3:A:57:PCW:H141	4:A:76:17F:H45	0.45	1.89	6	1
1:A:268:GLU:OE1	1:C:506:ARG:HD3	0.45	2.12	4	3
1:A:376:LEU:O	1:A:380:GLU:HG3	0.45	2.11	10	1
4:A:76:17F:H8A	4:A:76:17F:H20	0.45	1.88	10	1
4:A:79:17F:H64	4:A:80:17F:H67	0.45	1.89	9	1
3:A:6:PCW:H342	3:A:16:PCW:H321	0.45	1.89	9	1
3:A:48:PCW:H41	3:A:48:PCW:O31	0.45	2.12	2	1
3:A:43:PCW:O11	3:A:43:PCW:H83	0.45	2.12	2	1
2:B:46:ILE:HD11	2:B:53:LEU:HD11	0.45	1.88	7	1
1:A:337:ALA:O	1:A:341:ASN:HB2	0.45	2.12	4	1
3:A:43:PCW:H332	3:A:43:PCW:H132	0.45	1.87	5	1
1:C:550:LYS:O	1:C:554:HIS:HB2	0.45	2.12	2	1
1:A:363:LYS:HG2	1:C:411:THR:HG22	0.45	1.88	4	2
3:A:31:PCW:H52	3:A:31:PCW:O31	0.45	2.12	1	1
1:C:415:LEU:HA	1:C:418:GLN:NE2	0.45	2.27	7	1
1:C:448:VAL:O	1:C:452:VAL:HB	0.45	2.12	4	1
1:C:499:LEU:O	1:C:503:MET:HB2	0.45	2.11	10	1
3:A:12:PCW:H342	3:A:30:PCW:H121	0.45	1.89	2	1
3:A:68:PCW:O2P	3:A:69:PCW:H41	0.45	2.12	6	1
3:A:54:PCW:H82	3:A:62:PCW:O2P	0.45	2.12	4	1
3:A:17:PCW:H182	3:A:21:PCW:H122	0.45	1.88	2	1
3:A:54:PCW:O3P	3:A:60:PCW:H82	0.44	2.12	3	1
3:A:27:PCW:H161	3:A:27:PCW:H372	0.44	1.88	7	1
2:B:58:THR:HG22	2:B:71:TYR:HE1	0.44	1.72	7	1
1:A:242:GLU:OE1	1:C:528:ARG:HB3	0.44	2.12	4	1
1:A:365:LYS:CB	1:A:366:PRO:HD3	0.44	2.37	3	5
1:A:308:ARG:CD	1:C:469:LEU:CD2	0.44	2.79	7	1
2:B:6:LEU:HD22	2:B:159:LEU:HD23	0.44	1.88	8	2
1:A:202:LYS:HE3	1:C:576:VAL:HG21	0.44	1.89	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:80:CYS:HB2	2:B:113:LEU:HD12	0.44	1.88	4	1
1:A:308:ARG:HG3	1:C:465:GLU:HB3	0.44	1.88	5	1
3:A:12:PCW:H51	2:B:39:SER:HB2	0.44	1.88	3	1
1:A:330:ARG:O	1:A:334:ARG:HG2	0.44	2.11	7	2
1:A:359:THR:O	1:A:363:LYS:HG3	0.44	2.12	7	2
1:C:464:GLN:O	1:C:468:GLU:HB2	0.44	2.13	8	1
2:B:73:ARG:HH21	2:B:103:VAL:HA	0.44	1.71	10	1
3:A:13:PCW:H152	3:A:18:PCW:H322	0.44	1.89	2	1
3:A:53:PCW:H181	3:A:64:PCW:H182	0.44	1.88	8	1
1:C:549:ALA:O	1:C:553:GLU:HG3	0.44	2.12	8	2
3:A:13:PCW:H161	3:A:18:PCW:H332	0.44	1.88	6	1
1:A:249:GLU:O	1:A:253:LYS:HB2	0.44	2.12	10	1
3:A:24:PCW:H271	3:A:25:PCW:H221	0.44	1.90	2	1
1:A:266:GLN:O	1:A:270:GLU:HG3	0.44	2.13	2	1
3:A:14:PCW:O2P	3:A:23:PCW:H41	0.44	2.12	3	1
3:A:11:PCW:H72	3:A:24:PCW:O2P	0.44	2.12	3	1
3:A:66:PCW:H471	4:A:79:17F:H59	0.44	1.88	1	1
3:A:5:PCW:H142	4:A:38:17F:H8A	0.44	1.88	7	1
1:A:214:PHE:HE1	3:A:15:PCW:H272	0.44	1.72	6	1
3:A:45:PCW:H241	3:A:57:PCW:H371	0.44	1.89	6	1
3:A:44:PCW:H452	3:A:64:PCW:H461	0.44	1.90	2	1
3:A:1:PCW:H232	4:A:38:17F:H58	0.44	1.89	3	1
3:A:43:PCW:O1P	3:A:68:PCW:H73	0.44	2.12	3	1
3:A:18:PCW:H371	3:A:19:PCW:H20	0.44	1.90	3	1
3:A:11:PCW:H52	3:A:24:PCW:O2P	0.44	2.12	3	1
3:A:20:PCW:H151	3:A:31:PCW:H422	0.44	1.89	7	1
1:A:229:TRP:O	1:A:233:GLU:HG3	0.44	2.13	7	1
1:A:292:HIS:O	1:A:296:GLU:HG2	0.44	2.13	7	1
3:A:26:PCW:H32	3:A:28:PCW:H331	0.44	1.88	8	1
1:C:517:HIS:O	1:C:521:TYR:HB2	0.44	2.13	6	2
3:A:32:PCW:O31	4:A:33:17F:H20A	0.44	2.12	9	1
4:A:36:17F:HN1A	2:B:41:ARG:HH21	0.44	1.54	5	1
3:A:10:PCW:H341	3:A:21:PCW:H342	0.44	1.89	2	1
1:C:491:GLU:HB3	1:C:495:LYS:HZ2	0.44	1.73	3	1
1:A:268:GLU:O	1:A:272:TYR:HB2	0.44	2.13	3	1
3:A:44:PCW:H141	4:A:77:17F:H4A	0.44	1.90	4	1
3:A:10:PCW:H332	3:A:21:PCW:H322	0.44	1.89	4	1
1:C:550:LYS:HA	1:C:553:GLU:OE1	0.44	2.13	5	1
3:A:43:PCW:O2P	3:A:45:PCW:H83	0.44	2.13	2	1
3:A:62:PCW:H142	3:A:72:PCW:H172	0.44	1.88	10	1
1:C:473:LYS:O	1:C:477:LEU:HB2	0.44	2.12	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:6:PCW:H372	3:A:7:PCW:H331	0.44	1.88	9	1
1:A:202:LYS:O	1:A:206:ASN:HB2	0.44	2.13	9	1
3:A:70:PCW:H19	3:A:70:PCW:H73	0.44	1.90	9	1
3:A:21:PCW:H441	3:A:51:PCW:H262	0.44	1.90	5	1
1:A:335:LEU:O	1:A:339:LYS:HB2	0.44	2.12	1	1
3:A:47:PCW:H283	4:A:76:17F:H12	0.44	1.90	8	1
1:C:533:LEU:O	1:C:537:LYS:HG3	0.44	2.13	6	2
3:A:12:PCW:H62	2:B:37:GLU:OE1	0.43	2.13	6	1
3:A:6:PCW:H283	3:A:24:PCW:H182	0.43	1.89	10	1
3:A:23:PCW:H31	3:A:23:PCW:H41	0.43	1.90	10	1
1:A:271:LEU:O	1:A:275:LYS:HG2	0.43	2.13	2	2
3:A:44:PCW:H341	3:A:68:PCW:H332	0.43	1.90	3	1
2:B:5:LYS:N	2:B:5:LYS:HD3	0.43	2.28	7	1
3:A:9:PCW:H39	3:A:14:PCW:H82	0.43	1.89	9	1
3:A:15:PCW:H372	3:A:15:PCW:H211	0.43	1.89	5	1
1:A:224:VAL:HG22	1:C:550:LYS:HD3	0.43	1.90	1	1
1:A:273:ARG:HA	1:A:276:VAL:HG12	0.43	1.91	1	1
3:A:58:PCW:H381	3:A:60:PCW:H151	0.43	1.90	8	1
3:A:62:PCW:O1P	3:A:72:PCW:H63	0.43	2.13	6	1
1:C:576:VAL:O	1:C:580:PHE:HB2	0.43	2.14	4	1
3:A:26:PCW:H41	4:A:40:17F:O1	0.43	2.13	10	1
3:A:1:PCW:H212	4:A:35:17F:H32	0.43	1.91	1	1
1:A:312:HIS:HA	1:C:462:LYS:HD3	0.43	1.91	7	1
3:A:20:PCW:O2P	3:A:24:PCW:H81	0.43	2.13	4	1
3:A:21:PCW:H361	3:A:21:PCW:H172	0.43	1.89	4	1
1:C:577:LEU:O	1:C:581:LYS:HB2	0.43	2.14	4	1
3:A:28:PCW:H452	3:A:63:PCW:H222	0.43	1.89	4	1
3:A:42:PCW:H412	3:A:69:PCW:H141	0.43	1.89	9	1
3:A:3:PCW:H40	3:A:19:PCW:H242	0.43	1.89	3	1
3:A:48:PCW:H352	3:A:54:PCW:H152	0.43	1.90	1	1
2:B:126:ASP:OD2	2:B:128:LYS:HB3	0.43	2.13	4	1
1:C:469:LEU:HD22	1:C:473:LYS:HZ2	0.43	1.73	3	1
3:A:27:PCW:H61	4:A:37:17F:O2	0.43	2.14	7	1
3:A:47:PCW:H331	3:A:71:PCW:H241	0.43	1.90	8	1
3:A:20:PCW:H451	3:A:31:PCW:H242	0.43	1.91	6	1
3:A:1:PCW:H372	3:A:5:PCW:H431	0.43	1.91	6	1
1:C:508:ARG:O	1:C:512:ASP:HB3	0.43	2.14	4	1
3:A:46:PCW:O2P	3:A:71:PCW:H352	0.43	2.13	9	1
1:A:362:GLU:HB3	1:C:414:LYS:HD3	0.43	1.90	5	1
3:A:6:PCW:H31	3:A:16:PCW:H332	0.43	1.89	2	1
1:A:357:LEU:HA	1:A:360:LEU:HB2	0.43	1.91	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:9:PCW:H73	2:B:3:GLU:OE1	0.43	2.13	9	1
1:C:422:VAL:O	1:C:426:PHE:HB2	0.43	2.14	5	1
4:A:37:17F:H55	3:A:57:PCW:H452	0.43	1.91	1	1
3:A:62:PCW:H341	4:A:78:17F:H36	0.43	1.91	1	1
3:A:62:PCW:O1P	3:A:72:PCW:H51	0.43	2.14	1	1
1:A:301:LEU:HD13	1:C:473:LYS:HG3	0.43	1.91	4	1
3:A:41:PCW:H182	3:A:58:PCW:H371	0.43	1.90	4	1
3:A:23:PCW:H141	4:A:34:17F:H61	0.43	1.90	6	1
1:A:280:ARG:O	1:A:284:GLN:HB2	0.43	2.13	4	1
3:A:12:PCW:H71	4:A:37:17F:O3	0.43	2.14	5	1
3:A:30:PCW:H142	4:A:40:17F:HN1A	0.43	1.74	3	1
3:A:41:PCW:H62	3:A:44:PCW:O11	0.43	2.14	3	1
1:C:522:SER:O	1:C:526:ARG:HG3	0.43	2.13	8	1
3:A:4:PCW:H82	3:A:7:PCW:O1P	0.42	2.14	1	1
3:A:43:PCW:O31	3:A:45:PCW:H82	0.42	2.14	7	1
3:A:30:PCW:H461	4:A:34:17F:H53	0.42	1.90	8	1
3:A:32:PCW:H421	4:A:35:17F:H49	0.42	1.91	10	1
3:A:42:PCW:H442	3:A:52:PCW:H361	0.42	1.90	9	1
2:B:69:ASP:O	2:B:73:ARG:HG3	0.42	2.14	5	1
3:A:56:PCW:H83	3:A:56:PCW:O11	0.42	2.14	3	1
3:A:49:PCW:H362	3:A:57:PCW:H171	0.42	1.92	7	1
2:B:30:ASP:O	5:B:201:GNP:H3'	0.42	2.14	10	1
1:A:248:GLU:O	1:A:252:ALA:HB3	0.42	2.14	9	1
3:A:48:PCW:H332	3:A:54:PCW:H142	0.42	1.91	5	1
3:A:14:PCW:H372	4:A:34:17F:H34	0.42	1.91	5	1
3:A:72:PCW:O31	3:A:72:PCW:H42	0.42	2.14	7	1
1:C:581:LYS:O	1:C:585:LEU:HG	0.42	2.14	10	2
1:C:578:GLU:O	1:C:582:VAL:HG23	0.42	2.14	8	1
3:A:68:PCW:H31	3:A:70:PCW:H232	0.42	1.90	4	1
3:A:62:PCW:H31	3:A:72:PCW:O11	0.42	2.14	4	1
3:A:10:PCW:H73	3:A:21:PCW:O31	0.42	2.13	10	1
3:A:41:PCW:O2P	3:A:61:PCW:H72	0.42	2.14	10	1
3:A:41:PCW:H451	3:A:58:PCW:H451	0.42	1.90	5	1
3:A:13:PCW:H342	3:A:18:PCW:H121	0.42	1.90	2	1
3:A:42:PCW:H51	4:A:75:17F:O1	0.42	2.14	2	1
3:A:62:PCW:H352	3:A:72:PCW:H122	0.42	1.92	3	1
3:A:12:PCW:H151	3:A:12:PCW:H331	0.42	1.91	8	1
1:C:561:LYS:HE3	1:C:561:LYS:HA	0.42	1.90	8	1
3:A:48:PCW:H341	3:A:54:PCW:H351	0.42	1.92	6	1
1:C:413:SER:O	1:C:417:GLU:HG3	0.42	2.15	6	1
2:B:97:ARG:HD2	2:B:111:MET:SD	0.42	2.54	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:62:PCW:H362	3:A:72:PCW:H331	0.42	1.90	3	1
2:B:41:ARG:HD3	2:B:54:ASP:OD2	0.42	2.14	3	1
3:A:1:PCW:H431	3:A:26:PCW:H221	0.42	1.90	1	1
3:A:14:PCW:H142	4:A:34:17F:H34	0.42	1.90	1	1
1:A:308:ARG:HG3	1:C:469:LEU:CD1	0.42	2.42	8	1
3:A:63:PCW:O2P	3:A:63:PCW:N	0.42	2.52	4	1
3:A:14:PCW:O2P	3:A:19:PCW:H81	0.42	2.15	5	1
1:C:431:GLU:O	1:C:435:GLU:HG3	0.42	2.14	10	1
1:C:587:ALA:O	1:C:591:TYR:HB2	0.42	2.14	9	1
2:B:9:VAL:HB	2:B:96:TYR:CE2	0.42	2.49	9	1
3:A:10:PCW:H172	3:A:10:PCW:H462	0.42	1.91	9	1
3:A:43:PCW:H162	3:A:43:PCW:H442	0.42	1.91	5	1
1:A:348:GLU:O	1:A:352:LYS:HG3	0.42	2.13	5	1
3:A:9:PCW:H321	3:A:14:PCW:H342	0.42	1.90	3	1
3:A:54:PCW:H332	3:A:72:PCW:H121	0.42	1.91	3	1
1:C:412:PHE:HA	1:C:415:LEU:HD12	0.42	1.90	6	1
2:B:20:THR:O	2:B:24:ILE:HG12	0.42	2.14	6	1
2:B:34:PRO:HA	5:B:201:GNP:O3G	0.42	2.15	4	3
3:A:57:PCW:H63	4:A:80:17F:HN1A	0.42	1.74	1	1
3:A:53:PCW:H212	3:A:64:PCW:H212	0.42	1.92	8	1
3:A:68:PCW:H32	3:A:70:PCW:H142	0.42	1.90	6	1
3:A:15:PCW:H61	4:A:39:17F:O2	0.42	2.15	10	1
3:A:4:PCW:H161	3:A:7:PCW:H221	0.42	1.91	10	1
1:A:338:LEU:O	1:A:342:GLY:HA3	0.42	2.15	9	1
4:A:36:17F:HN1A	2:B:41:ARG:NH2	0.42	2.13	5	1
3:A:56:PCW:O2P	3:A:70:PCW:H41	0.42	2.15	7	1
3:A:1:PCW:H20	3:A:32:PCW:H351	0.42	1.91	6	1
3:A:5:PCW:H31	3:A:17:PCW:H321	0.42	1.91	6	1
3:A:11:PCW:H62	3:A:24:PCW:O2P	0.42	2.14	4	1
3:A:58:PCW:H362	3:A:61:PCW:H451	0.42	1.91	4	1
3:A:6:PCW:P	3:A:11:PCW:O2P	0.42	2.78	10	1
1:C:498:PRO:O	1:C:502:GLU:HB2	0.42	2.14	10	1
3:A:3:PCW:H362	3:A:18:PCW:H12	0.42	1.92	9	1
3:A:43:PCW:H32	3:A:69:PCW:O3P	0.42	2.15	9	1
4:A:75:17F:H4	4:A:75:17F:H2	0.42	1.92	1	1
3:A:65:PCW:O4P	3:A:65:PCW:H2	0.42	2.15	1	1
3:A:57:PCW:H41	3:A:57:PCW:O31	0.42	2.15	8	1
1:A:268:GLU:OE2	1:C:510:HIS:NE2	0.42	2.53	4	1
3:A:25:PCW:H42	3:A:31:PCW:O1P	0.42	2.14	9	1
3:A:11:PCW:H171	3:A:28:PCW:H411	0.42	1.92	5	1
3:A:23:PCW:H40	3:A:29:PCW:H351	0.41	1.91	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:49:PCW:O2P	3:A:57:PCW:H61	0.41	2.14	7	1
1:A:264:LYS:O	1:A:268:GLU:HG3	0.41	2.14	6	1
3:A:1:PCW:N	4:A:35:17F:N1	0.41	2.64	4	1
3:A:21:PCW:H142	4:A:36:17F:H57	0.41	1.91	5	1
3:A:13:PCW:H73	4:A:37:17F:O4	0.41	2.15	5	1
4:A:75:17F:H52	4:A:75:17F:H75	0.41	1.91	5	1
1:A:348:GLU:HB3	1:A:352:LYS:HE2	0.41	1.91	5	1
3:A:1:PCW:H40	4:A:33:17F:H51	0.41	1.91	2	1
4:A:77:17F:H18A	4:A:77:17F:H9A	0.41	1.92	2	1
3:A:46:PCW:H39	3:A:47:PCW:H412	0.41	1.91	2	1
3:A:4:PCW:H461	4:A:39:17F:H70	0.41	1.91	3	1
1:C:502:GLU:O	1:C:506:ARG:HG3	0.41	2.15	1	1
3:A:54:PCW:H132	3:A:54:PCW:H362	0.41	1.91	7	1
3:A:16:PCW:H2	3:A:16:PCW:O1P	0.41	2.15	6	1
3:A:55:PCW:H411	3:A:64:PCW:H39	0.41	1.90	9	1
4:A:33:17F:H10	4:A:35:17F:H6A	0.41	1.92	5	1
3:A:49:PCW:H82	4:A:80:17F:HN1	0.41	1.74	2	1
3:A:7:PCW:H231	3:A:61:PCW:H271	0.41	1.93	1	1
1:A:233:GLU:O	1:A:237:GLU:HB2	0.41	2.15	1	1
3:A:59:PCW:H181	4:A:77:17F:H8A	0.41	1.92	7	1
2:B:8:VAL:HG12	2:B:16:LYS:HD2	0.41	1.92	6	1
3:A:19:PCW:H63	3:A:29:PCW:O1P	0.41	2.15	4	1
3:A:69:PCW:H142	3:A:69:PCW:H372	0.41	1.92	10	1
3:A:1:PCW:H422	3:A:68:PCW:H261	0.41	1.92	2	1
3:A:41:PCW:H231	3:A:58:PCW:H431	0.41	1.92	2	1
2:B:80:CYS:HB3	2:B:93:ILE:HD12	0.41	1.91	2	1
2:B:58:THR:HG21	2:B:71:TYR:CE1	0.41	2.50	2	1
1:A:307:ASP:O	1:A:310:ARG:HB2	0.41	2.14	1	1
3:A:12:PCW:H432	3:A:30:PCW:H242	0.41	1.92	8	1
3:A:43:PCW:H11	3:A:70:PCW:H151	0.41	1.92	8	1
3:A:15:PCW:H431	3:A:20:PCW:H212	0.41	1.92	2	1
3:A:42:PCW:H441	3:A:42:PCW:H221	0.41	1.92	10	1
1:A:330:ARG:HH22	1:C:448:VAL:HG23	0.41	1.76	9	1
3:A:1:PCW:H431	3:A:26:PCW:H241	0.41	1.91	5	1
3:A:28:PCW:H262	3:A:69:PCW:H211	0.41	1.93	5	1
3:A:4:PCW:O2P	3:A:16:PCW:H82	0.41	2.16	2	1
1:A:375:LEU:O	1:A:379:LEU:HB2	0.41	2.16	3	1
3:A:15:PCW:H382	3:A:24:PCW:H462	0.41	1.93	1	1
3:A:19:PCW:H62	3:A:23:PCW:O2P	0.41	2.14	7	1
3:A:15:PCW:H412	3:A:24:PCW:H461	0.41	1.93	10	1
1:A:253:LYS:HE2	1:A:257:TYR:OH	0.41	2.15	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:2:PCW:H42	3:A:21:PCW:H11	0.41	1.92	2	1
1:C:427:TRP:HA	1:C:427:TRP:HE3	0.41	1.74	7	1
1:C:521:TYR:HA	1:C:524:GLU:OE1	0.41	2.16	7	1
3:A:44:PCW:H82	4:A:77:17F:O4	0.41	2.16	8	1
1:A:253:LYS:C	1:A:256:PRO:HD2	0.41	2.36	4	1
3:A:21:PCW:H432	3:A:51:PCW:H272	0.41	1.92	10	1
1:A:281:ALA:O	1:A:285:GLU:HG2	0.41	2.16	9	1
3:A:2:PCW:H61	4:A:36:17F:O1	0.41	2.16	2	1
3:A:67:PCW:H241	3:A:69:PCW:H222	0.41	1.93	2	1
3:A:25:PCW:H122	3:A:25:PCW:H351	0.41	1.93	1	1
3:A:3:PCW:O2P	3:A:23:PCW:N	0.41	2.54	1	1
3:A:45:PCW:H73	3:A:71:PCW:H19	0.41	1.91	1	1
3:A:70:PCW:O4P	3:A:70:PCW:H2	0.41	2.16	1	1
3:A:3:PCW:H252	3:A:19:PCW:H241	0.41	1.93	7	1
3:A:3:PCW:H121	3:A:3:PCW:H361	0.41	1.93	7	1
1:A:254:VAL:HA	1:A:257:TYR:HB2	0.41	1.92	7	1
1:A:228:PHE:O	1:A:232:LEU:HG	0.41	2.16	8	1
1:A:330:ARG:NH2	1:C:447:GLU:HB2	0.41	2.27	6	1
3:A:57:PCW:H231	4:A:80:17F:H52	0.41	1.92	6	1
3:A:9:PCW:H341	3:A:14:PCW:H372	0.41	1.92	6	1
3:A:43:PCW:H63	4:A:75:17F:H6	0.41	1.93	4	1
3:A:8:PCW:H40	3:A:27:PCW:H261	0.41	1.92	4	1
3:A:5:PCW:H482	4:A:36:17F:H10A	0.41	1.92	10	1
3:A:16:PCW:H251	3:A:24:PCW:H361	0.41	1.91	10	1
3:A:32:PCW:H483	3:A:59:PCW:H271	0.41	1.91	10	1
2:B:24:ILE:HD11	2:B:55:ILE:HD12	0.41	1.92	10	1
3:A:5:PCW:H39	3:A:17:PCW:H63	0.41	1.93	9	1
3:A:4:PCW:H432	3:A:7:PCW:H212	0.41	1.93	9	1
3:A:42:PCW:H283	3:A:52:PCW:H231	0.41	1.92	9	1
3:A:48:PCW:H452	3:A:54:PCW:H241	0.41	1.93	9	1
1:C:574:LEU:HB2	1:C:575:PRO:CD	0.41	2.46	9	1
3:A:26:PCW:H11	3:A:28:PCW:O1P	0.41	2.16	5	1
3:A:64:PCW:H241	3:A:64:PCW:H351	0.41	1.92	2	1
1:A:376:LEU:HB2	1:A:377:PRO:CD	0.41	2.46	8	1
3:A:20:PCW:H73	3:A:31:PCW:O2P	0.41	2.16	10	1
2:B:3:GLU:HG2	2:B:4:TYR:N	0.41	2.30	9	1
2:B:82:PHE:HE1	2:B:113:LEU:HG	0.41	1.76	2	1
2:B:31:GLU:O	5:B:201:GNP:H5'1	0.41	2.15	2	1
3:A:41:PCW:H152	3:A:58:PCW:H361	0.40	1.92	1	1
3:A:58:PCW:O31	3:A:58:PCW:H12	0.40	2.16	7	1
2:B:111:MET:HB2	2:B:139:ILE:HG21	0.40	1.93	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:12:PCW:H61	4:A:37:17F:O2	0.40	2.15	5	1
1:A:388:SER:O	1:A:392:GLU:HG2	0.40	2.16	3	1
3:A:7:PCW:H52	3:A:16:PCW:O2P	0.40	2.15	3	1
1:A:260:ASP:O	1:A:264:LYS:HD3	0.40	2.16	3	1
1:A:334:ARG:HD3	1:C:440:GLU:OE1	0.40	2.15	1	1
1:C:561:LYS:HA	1:C:565:ALA:CB	0.40	2.45	7	1
1:A:332:ALA:O	1:A:336:GLU:HG3	0.40	2.17	7	1
3:A:60:PCW:H82	3:A:61:PCW:H342	0.40	1.92	8	1
3:A:28:PCW:H462	3:A:63:PCW:H241	0.40	1.94	8	1
3:A:30:PCW:H52	4:A:34:17F:O3	0.40	2.16	8	1
1:C:535:ALA:O	1:C:539:ASN:HB2	0.40	2.16	8	1
2:B:32:TYR:HD1	5:B:201:GNP:H5'1	0.40	1.75	5	1
3:A:2:PCW:H71	4:A:36:17F:O1	0.40	2.16	2	1
1:A:261:PHE:O	1:A:265:TRP:HB2	0.40	2.17	1	1
3:A:20:PCW:H271	4:A:78:17F:H44	0.40	1.92	7	1
1:A:246:ASP:O	1:A:250:VAL:HB	0.40	2.17	8	1
1:A:253:LYS:O	1:A:256:PRO:HD2	0.40	2.17	4	1
3:A:3:PCW:H81	3:A:19:PCW:O11	0.40	2.15	4	1
3:A:22:PCW:C7	4:A:37:17F:HN1	0.40	2.29	4	1
3:A:16:PCW:H472	3:A:16:PCW:H272	0.40	1.93	10	1
3:A:4:PCW:O2P	3:A:16:PCW:H83	0.40	2.16	10	1
4:A:76:17F:H77	1:C:481:LEU:HD12	0.40	1.92	9	1
3:A:9:PCW:O2P	2:B:171:SER:HA	0.40	2.16	5	1
3:A:3:PCW:H361	3:A:18:PCW:H342	0.40	1.93	2	1
3:A:42:PCW:H231	3:A:42:PCW:H451	0.40	1.92	3	1
3:A:42:PCW:O2P	3:A:69:PCW:H11	0.40	2.17	6	1
3:A:52:PCW:H131	3:A:60:PCW:O1P	0.40	2.17	6	1
1:C:469:LEU:O	1:C:473:LYS:HE2	0.40	2.16	9	1
3:A:45:PCW:H382	4:A:74:17F:H8	0.40	1.92	9	1
3:A:48:PCW:H61	3:A:61:PCW:C40	0.40	2.47	5	1
1:A:264:LYS:HE3	1:C:509:ALA:HB1	0.40	1.92	5	1
1:A:279:LEU:HD22	1:C:495:LYS:HE3	0.40	1.93	1	1
3:A:9:PCW:H42	3:A:26:PCW:O2P	0.40	2.17	1	1
1:A:246:ASP:HA	1:C:528:ARG:NH1	0.40	2.32	1	1
3:A:17:PCW:H41	3:A:17:PCW:O11	0.40	2.17	6	1
3:A:1:PCW:H181	3:A:5:PCW:H362	0.40	1.93	4	1
3:A:14:PCW:O1P	3:A:19:PCW:H73	0.40	2.17	9	1
2:B:168:GLU:HG2	2:B:172:LYS:HE2	0.40	1.93	9	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/200 (98%)	191±2 (98±1%)	4±1 (2±1%)	1±1 (0±0%)	38	79
1	C	195/200 (98%)	191±2 (98±1%)	4±2 (2±1%)	1±1 (0±0%)	50	83
2	B	170/187 (91%)	160±2 (94±1%)	10±2 (6±1%)	0±0 (0±0%)	56	85
All	All	5600/5870 (95%)	5416 (97%)	167 (3%)	17 (0%)	50	83

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	365	LYS	8
1	C	563	LYS	5
1	A	366	PRO	1
2	B	34	PRO	1
2	B	117	LYS	1
2	B	47	ASP	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/175 (98%)	155±2 (90±1%)	17±2 (10±1%)	14	58
1	C	171/175 (98%)	155±2 (91±1%)	16±2 (9±1%)	15	60
2	B	150/165 (91%)	134±3 (90±2%)	16±3 (10±2%)	13	57
All	All	4930/5150 (96%)	4438 (90%)	492 (10%)	14	58

All 189 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	254	VAL	10
1	C	550	LYS	9
2	B	122	SER	9
1	A	312	HIS	8
1	C	516	THR	8
2	B	92	ASP	8
2	B	87	THR	8
1	A	272	TYR	8
1	A	235	GLU	7
2	B	39	SER	7
2	B	17	SER	7
1	A	228	PHE	7
2	B	74	THR	7
2	B	69	ASP	7
1	C	459	PHE	6
1	C	480	GLU	6
2	B	71	TYR	6
2	B	51	CYS	6
1	A	293	GLU	6
2	B	170	MET	5
2	B	35	THR	5
1	A	299	SER	5
2	B	148	THR	5
1	C	548	HIS	5
1	A	370	ASP	5
1	C	568	ASP	5
1	A	246	ASP	5
1	A	325	ASP	5
1	A	394	THR	5
2	B	20	THR	5
1	C	561	LYS	4
1	A	292	HIS	4
2	B	107	GLU	4
1	C	412	PHE	4
1	A	289	GLN	4
2	B	127	THR	4
1	C	455	TYR	4
1	C	505	ASP	4
1	A	396	LYS	4
1	A	207	TRP	4
1	A	214	PHE	4
1	C	444	ASP	4
1	A	264	LYS	4

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Mol	Chain	Res	Type	Models (Total)
2	B	43	GLN	4
1	C	487	GLN	4
1	C	405	TRP	4
1	C	463	TRP	4
2	B	50	THR	3
1	C	552	THR	3
2	B	106	SER	3
1	A	382	PHE	3
2	B	124	THR	3
2	B	3	GLU	3
1	A	215	SER	3
1	C	592	THR	3
1	A	319	HIS	3
1	C	413	SER	3
1	A	213	THR	3
1	C	418	GLN	3
1	C	591	TYR	3
1	C	409	THR	3
1	C	427	TRP	3
1	A	318	THR	3
1	A	229	TRP	3
1	A	356	HIS	3
1	A	361	SER	3
1	C	580	PHE	3
1	C	594	LYS	3
1	C	466	GLU	2
1	A	381	SER	2
1	A	360	LEU	2
2	B	70	GLN	2
1	A	209	SER	2
2	B	108	ASP	2
1	A	296	GLU	2
1	A	202	LYS	2
1	C	425	GLU	2
1	A	354	THR	2
1	C	473	LYS	2
1	C	523	ASP	2
1	A	220	GLN	2
1	A	244	SER	2
1	A	205	ASP	2
2	B	102	ARG	2
1	C	482	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	C	494	GLU	2
2	B	65	SER	2
1	C	576	VAL	2
1	C	467	MET	2
1	C	532	ARG	2
1	A	393	TYR	2
1	C	448	VAL	2
1	C	583	SER	2
1	C	546	GLU	2
1	A	261	PHE	2
1	A	392	GLU	2
1	A	391	GLU	2
1	C	407	SER	2
1	C	559	SER	2
2	B	62	GLU	2
1	C	490	HIS	2
2	B	132	ASP	2
1	A	257	TYR	2
1	C	410	SER	2
1	C	446	GLU	2
1	A	212	SER	2
1	A	349	TYR	2
1	C	556	SER	2
2	B	16	LYS	2
2	B	168	GLU	2
2	B	85	ASN	2
1	C	554	HIS	2
1	C	447	GLU	2
1	C	464	GLN	1
2	B	57	ASP	1
2	B	5	LYS	1
1	C	426	PHE	1
1	C	501	GLU	1
1	C	483	GLU	1
1	A	359	THR	1
1	A	303	GLU	1
1	A	206	ASN	1
1	C	579	SER	1
2	B	101	LYS	1
1	C	478	ARG	1
1	C	569	LEU	1
1	A	386	PHE	1

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Mol	Chain	Res	Type	Models (Total)
2	B	76	GLU	1
2	B	47	ASP	1
1	A	345	ARG	1
1	A	242	GLU	1
1	C	527	GLN	1
2	B	169	LYS	1
1	A	265	TRP	1
1	A	314	ASP	1
1	C	439	GLN	1
1	A	350	HIS	1
2	B	126	ASP	1
2	B	58	THR	1
1	C	403	ASP	1
2	B	63	GLU	1
1	A	263	LYS	1
1	C	557	THR	1
2	B	38	ASP	1
1	A	279	LEU	1
1	C	442	SER	1
1	C	434	THR	1
1	A	385	SER	1
2	B	166	HIS	1
1	C	488	LYS	1
2	B	30	ASP	1
2	B	97	ARG	1
2	B	172	LYS	1
2	B	91	GLU	1
1	A	308	ARG	1
1	C	458	ASP	1
2	B	80	CYS	1
1	C	457	ASP	1
1	C	497	SER	1
1	A	334	ARG	1
2	B	25	GLN	1
2	B	33	ASP	1
1	A	274	GLN	1
1	C	495	LYS	1
2	B	29	VAL	1
1	C	468	GLU	1
1	A	224	VAL	1
1	A	241	GLN	1
2	B	135	ARG	1

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Mol	Chain	Res	Type	Models (Total)
2	B	149	ARG	1
2	B	89	SER	1
1	C	433	GLU	1
1	C	406	ASP	1
2	B	164	ARG	1
2	B	145	SER	1
2	B	26	ASN	1
2	B	154	ASP	1
1	A	275	LYS	1
1	C	521	TYR	1
1	A	379	LEU	1
1	A	211	THR	1
1	A	227	GLU	1
2	B	105	ASP	1
1	C	415	LEU	1
2	B	150	GLN	1
1	A	378	VAL	1
1	C	404	ASN	1
1	A	248	GLU	1
2	B	37	GLU	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.

6.6 Ligand geometry ⓘ

Of 82 ligands modelled in this entry, 1 is monoatomic - leaving 81 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard

deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	A	1	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	10	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	11	-	53,53,53	1.04±0.00	0±0 (0±0%)
3	PCW	A	12	-	53,53,53	1.05±0.01	0±0 (0±0%)
3	PCW	A	13	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	14	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	15	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	16	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	17	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	18	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	19	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	2	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	20	-	53,53,53	1.05±0.01	0±0 (0±0%)
3	PCW	A	21	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	22	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	23	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	24	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	25	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	26	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	27	-	53,53,53	1.06±0.01	0±0 (0±0%)
3	PCW	A	28	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	29	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	3	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	30	-	53,53,53	1.04±0.00	0±0 (0±0%)
3	PCW	A	31	-	53,53,53	1.03±0.00	0±0 (0±0%)
3	PCW	A	32	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	17F	A	33	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	34	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	35	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	36	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	37	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	38	-	50,53,53	0.91±0.00	0±0 (0±0%)
4	17F	A	39	-	50,53,53	0.92±0.00	0±0 (0±0%)
3	PCW	A	4	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	17F	A	40	-	50,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	A	41	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	42	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	43	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	44	-	53,53,53	1.04±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PCW	A	45	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	46	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	47	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	48	-	53,53,53	1.03±0.00	0±0 (0±0%)
3	PCW	A	49	-	53,53,53	1.04±0.00	0±0 (0±0%)
3	PCW	A	5	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	50	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	51	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	52	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	53	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	54	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	55	-	53,53,53	1.06±0.00	0±0 (0±0%)
3	PCW	A	56	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	57	-	53,53,53	1.03±0.00	0±0 (0±0%)
3	PCW	A	58	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	59	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	6	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	60	-	53,53,53	1.04±0.00	0±0 (0±0%)
3	PCW	A	61	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	62	-	53,53,53	1.03±0.00	0±0 (0±0%)
3	PCW	A	63	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	64	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	65	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	66	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	67	-	53,53,53	1.04±0.00	0±0 (0±0%)
3	PCW	A	68	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	69	-	53,53,53	1.03±0.01	0±0 (0±0%)
3	PCW	A	7	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	70	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	71	-	53,53,53	1.04±0.01	0±0 (0±0%)
3	PCW	A	72	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	17F	A	73	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	74	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	75	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	76	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	77	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	78	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	17F	A	79	-	50,53,53	0.91±0.01	0±0 (0±0%)
3	PCW	A	8	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	17F	A	80	-	50,53,53	0.92±0.01	0±0 (0±0%)
3	PCW	A	9	-	53,53,53	1.04±0.01	0±0 (0±0%)
5	GNP	B	201	-	29,34,34	1.66±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
3	PCW	A	1	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	10	-	57,61,61	2.37±0.01	3±0 (5±0%)
3	PCW	A	11	-	57,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	12	-	57,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	13	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	14	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	15	-	57,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	16	-	57,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	17	-	57,61,61	2.37±0.01	3±0 (5±0%)
3	PCW	A	18	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	19	-	57,61,61	0.83±0.00	0±0 (0±0%)
3	PCW	A	2	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	20	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	21	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	22	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	23	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	24	-	57,61,61	2.37±0.01	3±0 (5±0%)
3	PCW	A	25	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	26	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	27	-	57,61,61	0.82±0.01	0±0 (0±0%)
3	PCW	A	28	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	29	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	3	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	30	-	57,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	31	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	32	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	17F	A	33	-	50,60,60	1.73±0.03	2±0 (4±0%)
4	17F	A	34	-	50,60,60	1.00±0.03	0±0 (0±0%)
4	17F	A	35	-	50,60,60	0.99±0.02	0±0 (0±0%)
4	17F	A	36	-	50,60,60	0.99±0.02	0±0 (0±0%)
4	17F	A	37	-	50,60,60	1.00±0.03	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
4	17F	A	38	-	50,60,60	1.00±0.03	0±0 (0±0%)
4	17F	A	39	-	50,60,60	1.01±0.02	0±0 (0±0%)
3	PCW	A	4	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	17F	A	40	-	50,60,60	0.99±0.03	0±0 (0±0%)
3	PCW	A	41	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	42	-	57,61,61	2.37±0.01	3±0 (5±0%)
3	PCW	A	43	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	44	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	45	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	46	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	47	-	57,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	48	-	57,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	49	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	5	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	50	-	57,61,61	0.83±0.00	0±0 (0±0%)
3	PCW	A	51	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	52	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	53	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	54	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	55	-	57,61,61	0.82±0.01	0±0 (0±0%)
3	PCW	A	56	-	57,61,61	2.37±0.01	3±0 (5±0%)
3	PCW	A	57	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	58	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	59	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	6	-	57,61,61	2.78±0.01	6±0 (10±0%)
3	PCW	A	60	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	61	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	62	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	63	-	57,61,61	2.78±0.00	6±0 (10±0%)
3	PCW	A	64	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	65	-	57,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	66	-	57,61,61	0.83±0.01	0±0 (0±0%)
3	PCW	A	67	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	68	-	57,61,61	2.37±0.01	3±0 (5±0%)
3	PCW	A	69	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	7	-	57,61,61	0.83±0.00	0±0 (0±0%)
3	PCW	A	70	-	57,61,61	2.37±0.00	3±0 (5±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PCW	A	71	-	57,61,61	2.37±0.00	3±0 (5±0%)
3	PCW	A	72	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	17F	A	73	-	50,60,60	0.99±0.02	0±0 (0±0%)
4	17F	A	74	-	50,60,60	0.99±0.04	0±0 (0±0%)
4	17F	A	75	-	50,60,60	0.98±0.02	0±0 (0±0%)
4	17F	A	76	-	50,60,60	0.99±0.03	0±0 (0±0%)
4	17F	A	77	-	50,60,60	1.73±0.02	2±0 (4±0%)
4	17F	A	78	-	50,60,60	0.97±0.02	0±0 (0±0%)
4	17F	A	79	-	50,60,60	0.99±0.02	0±0 (0±0%)
3	PCW	A	8	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	17F	A	80	-	50,60,60	0.96±0.02	0±0 (0±0%)
3	PCW	A	9	-	57,61,61	0.83±0.01	0±0 (0±0%)
5	GNP	B	201	-	29,54,54	2.46±0.02	2±0 (6±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	1	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	10	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	11	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	12	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	13	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	14	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	15	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	16	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	17	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	18	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	19	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	2	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	20	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	21	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	22	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	23	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	24	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	25	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	26	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	27	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	28	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	29	-	-	0±0,57,57,57	0±0,0,0,0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	3	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	30	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	31	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	32	-	-	0±0,57,57,57	0±0,0,0,0
4	17F	A	33	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	34	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	35	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	36	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	37	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	38	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	39	-	-	0±0,55,59,59	0±0,0,0,0
3	PCW	A	4	-	-	0±0,57,57,57	0±0,0,0,0
4	17F	A	40	-	-	0±0,55,59,59	0±0,0,0,0
3	PCW	A	41	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	42	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	43	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	44	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	45	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	46	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	47	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	48	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	49	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	5	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	50	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	51	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	52	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	53	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	54	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	55	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	56	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	57	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	58	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	59	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	6	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	60	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	61	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	62	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	63	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	64	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	65	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	66	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	67	-	-	0±0,57,57,57	0±0,0,0,0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	68	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	69	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	7	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	70	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	71	-	-	0±0,57,57,57	0±0,0,0,0
3	PCW	A	72	-	-	0±0,57,57,57	0±0,0,0,0
4	17F	A	73	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	74	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	75	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	76	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	77	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	78	-	-	0±0,55,59,59	0±0,0,0,0
4	17F	A	79	-	-	0±0,55,59,59	0±0,0,0,0
3	PCW	A	8	-	-	0±0,57,57,57	0±0,0,0,0
4	17F	A	80	-	-	0±0,55,59,59	0±0,0,0,0
3	PCW	A	9	-	-	0±0,57,57,57	0±0,0,0,0
5	GNP	B	201	-	-	0±0,13,38,38	0±0,3,3,3

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	13	PCW	C8-N-C7	12.21	77.38	108.96	1	10
3	A	42	PCW	C8-N-C7	12.18	77.44	108.96	1	10
3	A	68	PCW	C8-N-C7	12.17	77.48	108.96	3	10
3	A	10	PCW	C8-N-C7	12.16	77.51	108.96	10	10
3	A	46	PCW	C8-N-C7	12.15	77.53	108.96	2	10
3	A	51	PCW	C8-N-C7	12.14	77.55	108.96	8	10
3	A	56	PCW	C8-N-C7	12.13	77.58	108.96	6	10
3	A	4	PCW	C8-N-C7	12.12	77.60	108.96	1	10
3	A	67	PCW	C8-N-C7	12.11	77.63	108.96	7	10
3	A	49	PCW	C8-N-C7	12.11	77.63	108.96	7	10
3	A	44	PCW	C8-N-C7	12.11	77.64	108.96	9	10
3	A	29	PCW	C8-N-C7	12.10	77.64	108.96	2	10
3	A	69	PCW	C8-N-C7	12.10	77.66	108.96	3	10
3	A	22	PCW	C8-N-C7	12.09	77.67	108.96	9	10
3	A	6	PCW	C8-N-C7	12.09	77.68	108.96	10	10
3	A	3	PCW	C8-N-C7	12.08	77.70	108.96	9	10
3	A	21	PCW	C8-N-C7	12.08	77.70	108.96	8	10
3	A	25	PCW	C8-N-C7	12.08	77.70	108.96	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	18	PCW	C8-N-C7	12.08	77.72	108.96	8	10
3	A	59	PCW	C8-N-C7	12.07	77.73	108.96	1	10
3	A	41	PCW	C8-N-C7	12.07	77.73	108.96	9	10
3	A	14	PCW	C8-N-C7	12.07	77.74	108.96	7	10
3	A	54	PCW	C8-N-C7	12.07	77.73	108.96	2	10
3	A	64	PCW	C8-N-C7	12.07	77.74	108.96	8	10
3	A	62	PCW	C8-N-C7	12.07	77.74	108.96	10	10
3	A	24	PCW	C8-N-C7	12.07	77.74	108.96	1	10
3	A	52	PCW	C8-N-C7	12.07	77.74	108.96	5	10
3	A	17	PCW	C8-N-C7	12.07	77.74	108.96	3	10
3	A	45	PCW	C8-N-C7	12.06	77.75	108.96	7	10
3	A	20	PCW	C8-N-C7	12.06	77.76	108.96	10	10
3	A	31	PCW	C8-N-C7	12.06	77.76	108.96	9	10
3	A	5	PCW	C8-N-C7	12.06	77.77	108.96	7	10
3	A	1	PCW	C8-N-C7	12.06	77.77	108.96	7	10
3	A	2	PCW	C8-N-C7	12.06	77.77	108.96	2	10
3	A	61	PCW	C8-N-C7	12.05	77.79	108.96	2	10
3	A	23	PCW	C8-N-C7	12.05	77.79	108.96	7	10
3	A	43	PCW	C8-N-C7	12.05	77.80	108.96	3	10
3	A	28	PCW	C8-N-C7	12.05	77.80	108.96	10	10
3	A	70	PCW	C8-N-C7	12.04	77.80	108.96	5	10
3	A	57	PCW	C8-N-C7	12.04	77.81	108.96	10	10
3	A	26	PCW	C8-N-C7	12.04	77.81	108.96	7	10
3	A	53	PCW	C8-N-C7	12.02	77.86	108.96	10	10
3	A	71	PCW	C8-N-C7	12.02	77.86	108.96	7	10
3	A	60	PCW	C8-N-C7	12.02	77.87	108.96	3	10
3	A	58	PCW	C8-N-C7	12.02	77.87	108.96	8	10
3	A	63	PCW	C8-N-C7	12.01	77.89	108.96	8	10
3	A	43	PCW	C8-N-C6	10.26	82.41	108.96	2	10
3	A	17	PCW	C8-N-C6	10.25	82.44	108.96	7	10
3	A	61	PCW	C8-N-C6	10.24	82.48	108.96	9	10
3	A	23	PCW	C8-N-C6	10.22	82.52	108.96	2	10
3	A	20	PCW	C8-N-C6	10.21	82.54	108.96	5	10
3	A	25	PCW	C8-N-C6	10.20	82.56	108.96	2	10
3	A	21	PCW	C8-N-C6	10.20	82.58	108.96	9	10
3	A	69	PCW	C8-N-C6	10.19	82.58	108.96	9	10
3	A	63	PCW	C8-N-C6	10.20	82.58	108.96	1	10
3	A	10	PCW	C8-N-C6	10.19	82.59	108.96	3	10
3	A	13	PCW	C8-N-C6	10.19	82.61	108.96	9	10
3	A	14	PCW	C8-N-C6	10.18	82.61	108.96	6	10
3	A	24	PCW	C8-N-C6	10.18	82.62	108.96	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	45	PCW	C8-N-C6	10.18	82.62	108.96	4	10
3	A	57	PCW	C8-N-C6	10.18	82.63	108.96	6	10
3	A	1	PCW	C8-N-C6	10.17	82.64	108.96	4	10
3	A	5	PCW	C8-N-C6	10.17	82.65	108.96	3	10
3	A	67	PCW	C8-N-C6	10.17	82.66	108.96	5	10
3	A	18	PCW	C8-N-C6	10.17	82.66	108.96	7	10
3	A	62	PCW	C8-N-C6	10.17	82.66	108.96	5	10
3	A	58	PCW	C8-N-C6	10.17	82.66	108.96	2	10
3	A	28	PCW	C8-N-C6	10.17	82.66	108.96	1	10
3	A	29	PCW	C8-N-C6	10.16	82.67	108.96	8	10
3	A	3	PCW	C8-N-C6	10.16	82.67	108.96	8	10
3	A	64	PCW	C8-N-C6	10.16	82.68	108.96	2	10
3	A	56	PCW	C8-N-C6	10.16	82.69	108.96	10	10
3	A	6	PCW	C8-N-C6	10.15	82.69	108.96	1	10
3	A	46	PCW	C8-N-C6	10.15	82.69	108.96	7	10
3	A	71	PCW	C8-N-C6	10.15	82.69	108.96	9	10
3	A	31	PCW	C8-N-C6	10.15	82.70	108.96	2	10
3	A	44	PCW	C8-N-C6	10.15	82.70	108.96	8	10
3	A	52	PCW	C8-N-C6	10.15	82.71	108.96	8	10
3	A	22	PCW	C8-N-C6	10.15	82.71	108.96	4	10
3	A	41	PCW	C8-N-C6	10.14	82.71	108.96	6	10
3	A	2	PCW	C8-N-C6	10.14	82.71	108.96	10	10
3	A	4	PCW	C8-N-C6	10.14	82.72	108.96	5	10
3	A	70	PCW	C8-N-C6	10.14	82.73	108.96	4	10
3	A	60	PCW	C8-N-C6	10.13	82.74	108.96	7	10
3	A	51	PCW	C8-N-C6	10.13	82.75	108.96	5	10
3	A	59	PCW	C8-N-C6	10.13	82.76	108.96	7	10
3	A	42	PCW	C8-N-C6	10.12	82.77	108.96	6	10
3	A	49	PCW	C8-N-C6	10.12	82.77	108.96	9	10
3	A	54	PCW	C8-N-C6	10.12	82.78	108.96	5	10
3	A	53	PCW	C8-N-C6	10.11	82.79	108.96	7	10
3	A	26	PCW	C8-N-C6	10.11	82.79	108.96	1	10
3	A	68	PCW	C8-N-C6	10.09	82.86	108.96	8	10
5	B	201	GNP	C5-C6-N1	8.16	112.85	123.52	9	10
5	B	201	GNP	C6-N1-C2	7.84	125.07	115.88	9	10
3	A	6	PCW	O4P-P-O2P	7.47	78.62	109.21	10	10
3	A	63	PCW	O4P-P-O2P	7.40	78.93	109.21	9	10
4	A	77	17F	O2-P1-O6	6.18	78.79	108.24	3	10
4	A	33	17F	O2-P1-O6	6.16	78.86	108.24	3	10
4	A	33	17F	O2-P1-O3	5.98	79.74	108.24	4	10
4	A	77	17F	O2-P1-O3	5.94	79.94	108.24	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	63	PCW	O3P-P-O2P	5.70	85.86	109.21	1	10
3	A	6	PCW	O3P-P-O2P	5.67	86.00	109.21	8	10
3	A	23	PCW	C8-N-C5	5.31	88.35	109.92	5	10
3	A	1	PCW	C8-N-C5	5.30	88.41	109.92	1	10
3	A	57	PCW	C8-N-C5	5.30	88.42	109.92	1	10
3	A	60	PCW	C8-N-C5	5.29	88.45	109.92	8	10
3	A	18	PCW	C8-N-C5	5.29	88.47	109.92	1	10
3	A	42	PCW	C8-N-C5	5.28	88.47	109.92	5	10
3	A	59	PCW	C8-N-C5	5.28	88.47	109.92	10	10
3	A	56	PCW	C8-N-C5	5.28	88.48	109.92	5	10
3	A	58	PCW	C8-N-C5	5.28	88.49	109.92	3	10
3	A	45	PCW	C8-N-C5	5.28	88.50	109.92	10	10
3	A	53	PCW	C8-N-C5	5.28	88.50	109.92	1	10
3	A	24	PCW	C8-N-C5	5.27	88.52	109.92	2	10
3	A	68	PCW	C8-N-C5	5.27	88.52	109.92	2	10
3	A	46	PCW	C8-N-C5	5.27	88.53	109.92	8	10
3	A	20	PCW	C8-N-C5	5.27	88.54	109.92	3	10
3	A	5	PCW	C8-N-C5	5.27	88.55	109.92	3	10
3	A	10	PCW	C8-N-C5	5.26	88.55	109.92	1	10
3	A	13	PCW	C8-N-C5	5.26	88.55	109.92	3	10
3	A	28	PCW	C8-N-C5	5.27	88.55	109.92	6	10
3	A	62	PCW	C8-N-C5	5.26	88.57	109.92	7	10
3	A	69	PCW	C8-N-C5	5.26	88.58	109.92	7	10
3	A	31	PCW	C8-N-C5	5.26	88.58	109.92	8	10
3	A	70	PCW	C8-N-C5	5.26	88.59	109.92	7	10
3	A	29	PCW	C8-N-C5	5.26	88.58	109.92	3	10
3	A	22	PCW	C8-N-C5	5.26	88.58	109.92	10	10
3	A	25	PCW	C8-N-C5	5.25	88.60	109.92	6	10
3	A	51	PCW	C8-N-C5	5.25	88.60	109.92	2	10
3	A	6	PCW	C8-N-C5	5.25	88.60	109.92	7	10
3	A	54	PCW	C8-N-C5	5.25	88.59	109.92	1	10
3	A	61	PCW	C8-N-C5	5.25	88.60	109.92	5	10
3	A	63	PCW	C8-N-C5	5.25	88.60	109.92	8	10
3	A	41	PCW	C8-N-C5	5.25	88.60	109.92	3	10
3	A	17	PCW	C8-N-C5	5.25	88.60	109.92	5	10
3	A	4	PCW	C8-N-C5	5.25	88.61	109.92	7	10
3	A	71	PCW	C8-N-C5	5.25	88.61	109.92	2	10
3	A	2	PCW	C8-N-C5	5.25	88.60	109.92	6	10
3	A	44	PCW	C8-N-C5	5.25	88.62	109.92	4	10
3	A	67	PCW	C8-N-C5	5.25	88.61	109.92	3	10
3	A	43	PCW	C8-N-C5	5.25	88.62	109.92	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	3	PCW	C8-N-C5	5.25	88.62	109.92	4	10
3	A	6	PCW	O1P-P-O2P	5.25	85.27	112.56	8	10
3	A	64	PCW	C8-N-C5	5.24	88.64	109.92	1	10
3	A	26	PCW	C8-N-C5	5.24	88.65	109.92	1	10
3	A	21	PCW	C8-N-C5	5.24	88.66	109.92	3	10
3	A	14	PCW	C8-N-C5	5.24	88.67	109.92	4	10
3	A	52	PCW	C8-N-C5	5.23	88.68	109.92	10	10
3	A	49	PCW	C8-N-C5	5.23	88.71	109.92	3	10
3	A	63	PCW	O1P-P-O2P	5.18	85.59	112.56	9	8

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
5	B	201	GNP	O1G-PG-N3B-PB	1

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

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: 2msd_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	44
Number of shifts mapped to atoms	44
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. 22 atoms were assigned a chemical shift out of a possible 7198. 0 out of 106 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/2769 (0%)	0/1104 (0%)	0/1122 (0%)	0/543 (0%)
Sidechain	22/3991 (1%)	11/2340 (0%)	11/1446 (1%)	0/205 (0%)
Aromatic	0/438 (0%)	0/244 (0%)	0/194 (0%)	0/0 (—%)
Overall	22/7198 (0%)	11/3688 (0%)	11/2762 (0%)	0/748 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 22 atoms were assigned a chemical shift out of a possible 7473. 0 out of 108 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/2869 (0%)	0/1144 (0%)	0/1162 (0%)	0/563 (0%)
Sidechain	22/4166 (1%)	11/2445 (0%)	11/1505 (1%)	0/216 (0%)
Aromatic	0/438 (0%)	0/244 (0%)	0/194 (0%)	0/0 (—%)
Overall	22/7473 (0%)	11/3833 (0%)	11/2861 (0%)	0/779 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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.