Full wwPDB NMR Structure Validation Report (i)

Sep 30, 2021 – 02:49 PM EDT

PDB ID	:	2KWI
Title	:	RalB-RLIP76 (RalBP1) complex
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Deposited on	:	2010-04-12

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

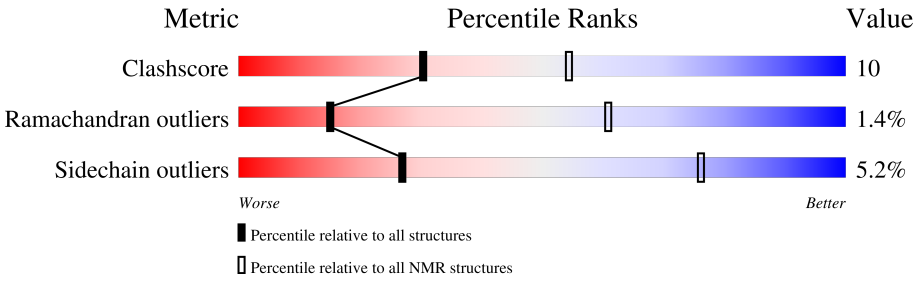
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	178	80% 15%
2	B	56	64% 30% 5%

2 Ensemble composition and analysis

This entry contains 51 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:12-A:181, B:394-B:446 (223)	0.59	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 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 7, 8, 9, 15, 16, 17, 19, 20, 22, 24, 25, 26, 28, 29, 31, 34, 37, 38, 39, 42, 43, 44, 45, 46, 47, 49, 50, 51
2	6, 10, 18, 23, 27, 30, 33, 40, 41, 48
3	21, 32
4	12, 14
Single-model clusters	11; 13; 35; 36

3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3841 atoms, of which 1917 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ras-related protein Ral-B.

Mol	Chain	Residues	Atoms						Trace
1	A	178	Total	C	H	N	O	S	0
			2838	897	1413	240	284	4	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	LEU	GLN	engineered mutation	UNP P11234

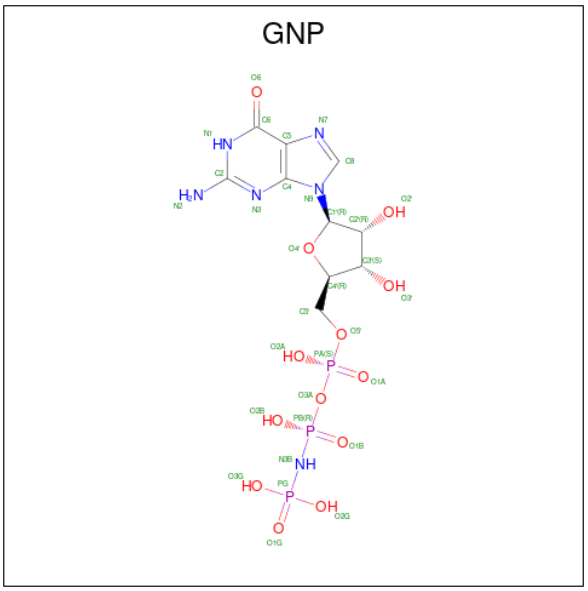
- Molecule 2 is a protein called RalA-binding protein 1.

Mol	Chain	Residues	Atoms					Trace
2	B	56	Total	C	H	N	O	0
			951	287	487	90	87	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	391	GLY	-	expression tag	UNP Q15311
B	392	SER	-	expression tag	UNP Q15311
B	411	SER	CYS	engineered mutation	UNP Q15311

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					
3	A	1	Total	C	H	N	O	P
			45	10	13	6	13	3

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Mg
			1	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		
5	A	2	Total	H	O
			6	4	2

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Ras-related protein Ral-B

Chain A:

• Molecule 2: RalA-binding protein 1

Chain B:

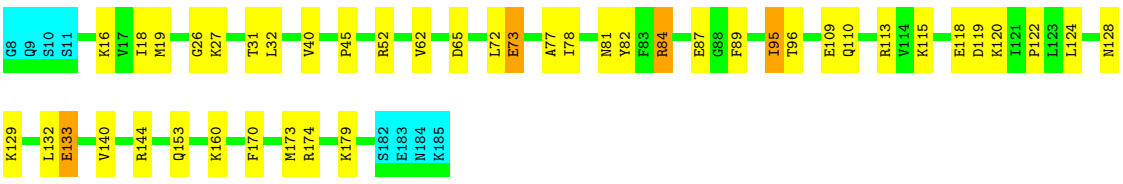
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

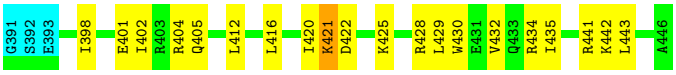
• Molecule 1: Ras-related protein Ral-B

Chain A:



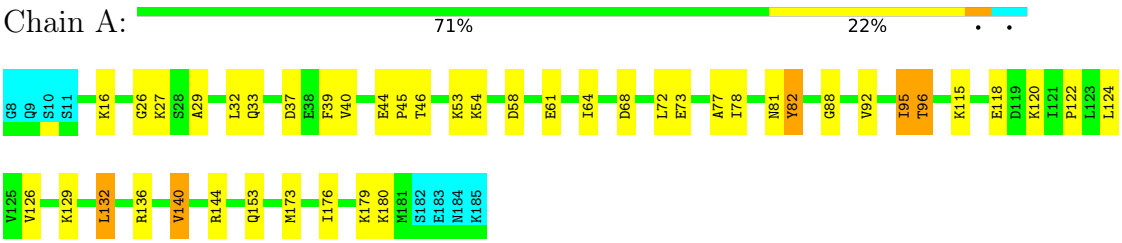
• Molecule 2: RalA-binding protein 1

Chain B:

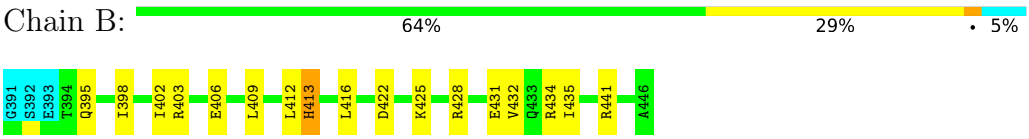


4.2.2 Score per residue for model 2

• Molecule 1: Ras-related protein Ral-B

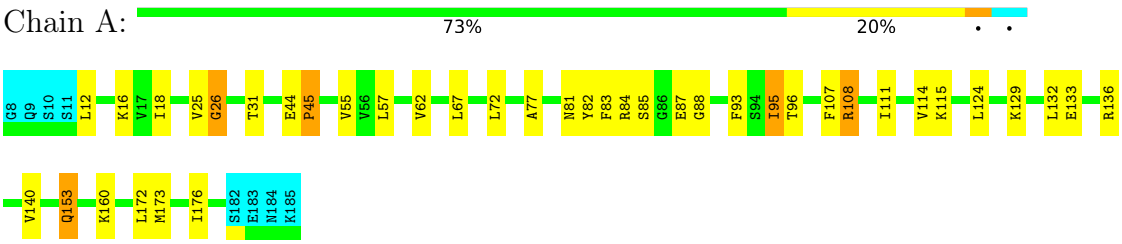


• Molecule 2: RalA-binding protein 1

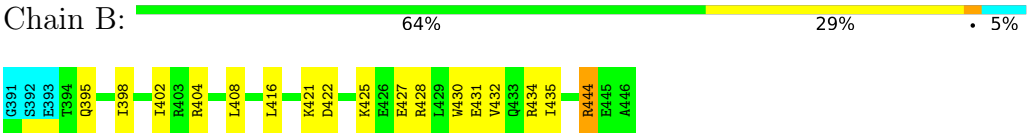


4.2.3 Score per residue for model 3

• Molecule 1: Ras-related protein Ral-B

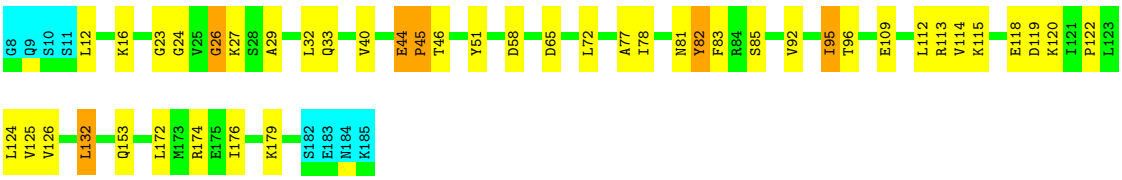


• Molecule 2: RalA-binding protein 1

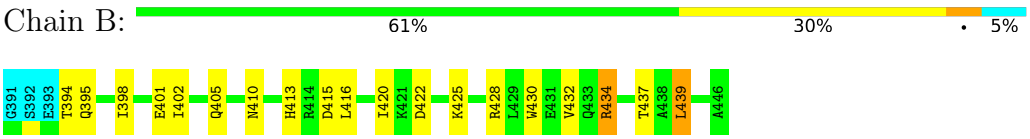


4.2.4 Score per residue for model 4

• Molecule 1: Ras-related protein Ral-B

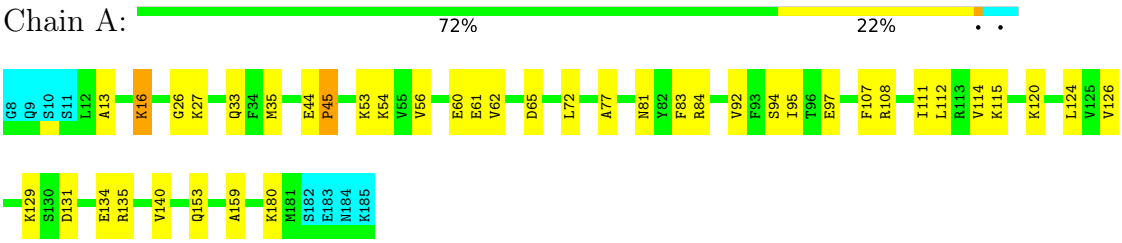


• Molecule 2: RalA-binding protein 1

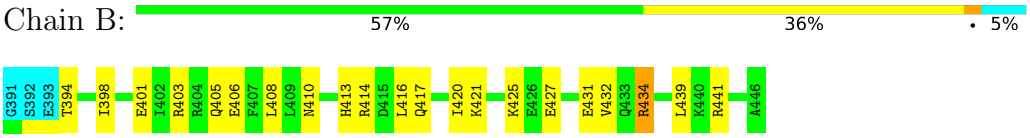


4.2.5 Score per residue for model 5

• Molecule 1: Ras-related protein Ral-B

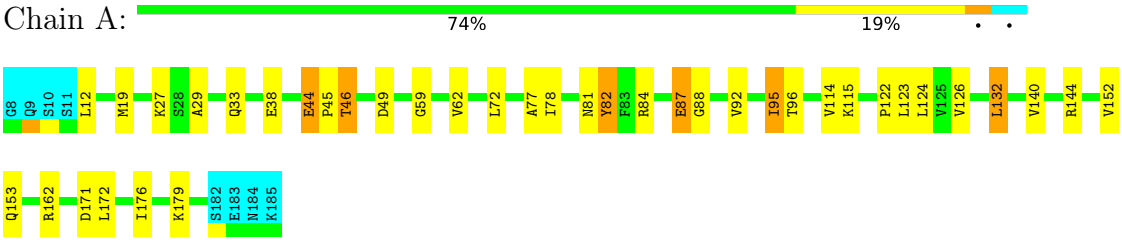


• Molecule 2: RalA-binding protein 1



4.2.6 Score per residue for model 6

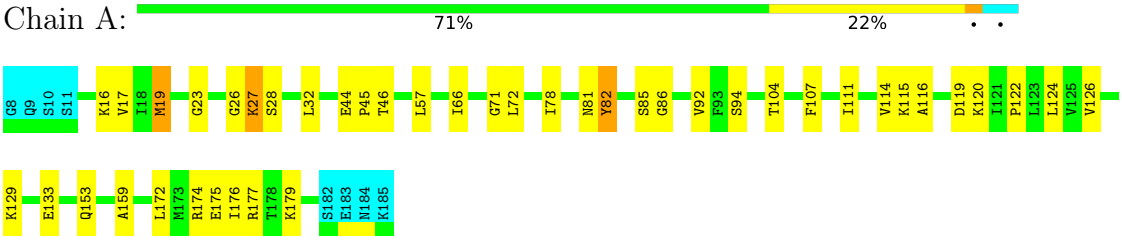
• Molecule 1: Ras-related protein Ral-B



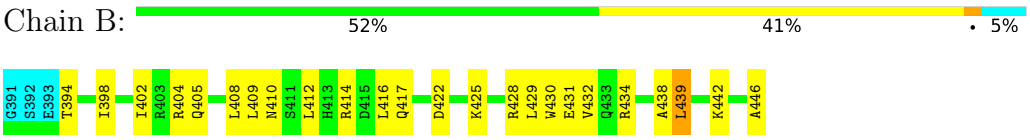
• Molecule 2: RalA-binding protein 1

4.2.7 Score per residue for model 7

• Molecule 1: Ras-related protein Ral-B

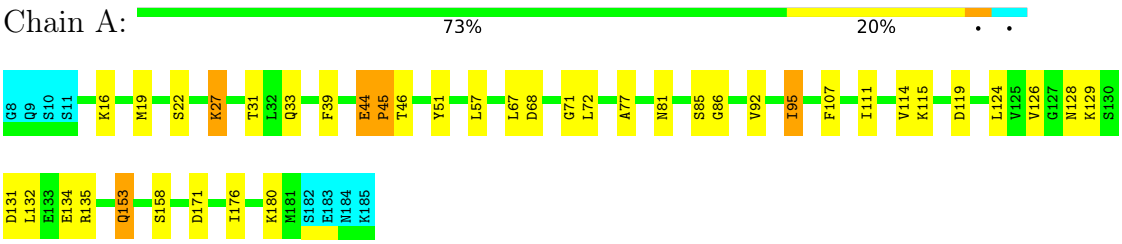


• Molecule 2: RalA-binding protein 1

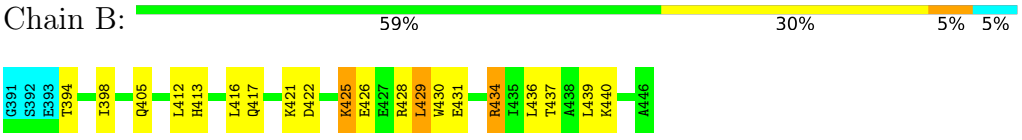


4.2.8 Score per residue for model 8

• Molecule 1: Ras-related protein Ral-B



• Molecule 2: RalA-binding protein 1



4.2.9 Score per residue for model 9

• Molecule 1: Ras-related protein Ral-B

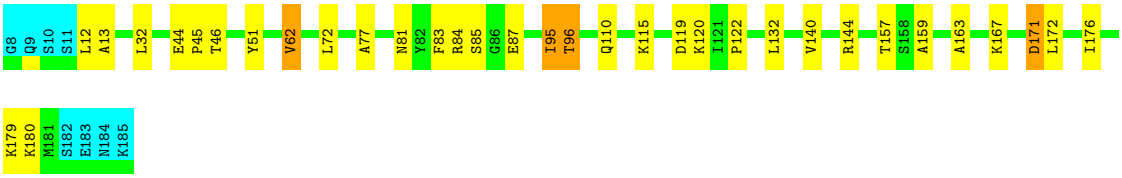
• Molecule 2: RalA-binding protein 1

Chain B:

4.2.10 Score per residue for model 10

• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

Chain B:

4.2.11 Score per residue for model 11

• Molecule 1: Ras-related protein Ral-B

Chain A:

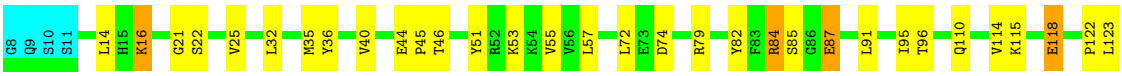
• Molecule 2: RalA-binding protein 1

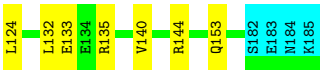
Chain B:

4.2.12 Score per residue for model 12

• Molecule 1: Ras-related protein Ral-B

Chain A:





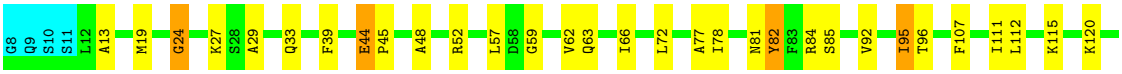
• Molecule 2: RalA-binding protein 1

Chain B:

4.2.13 Score per residue for model 13

• Molecule 1: Ras-related protein Ral-B

Chain A:



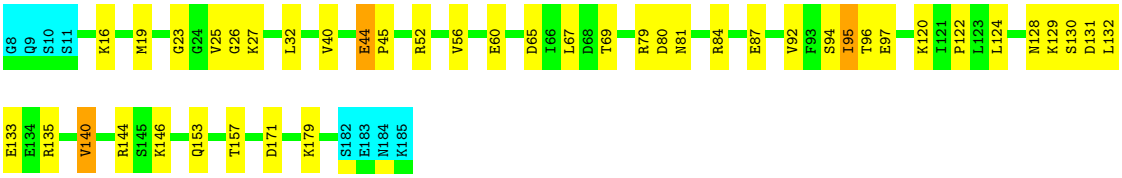
• Molecule 2: RalA-binding protein 1

Chain B:

4.2.14 Score per residue for model 14

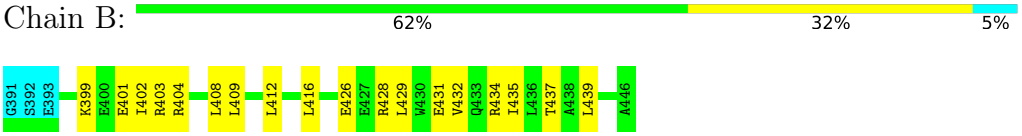
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

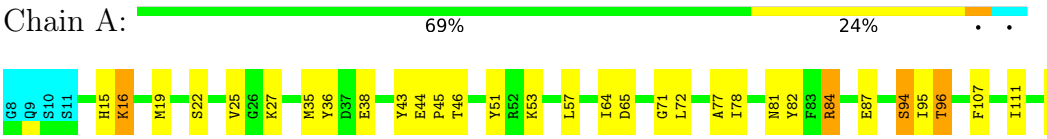
Chain B:



4.2.15 Score per residue for model 15

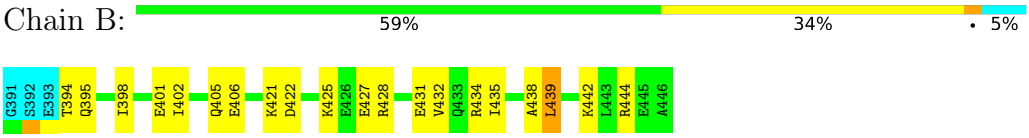
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

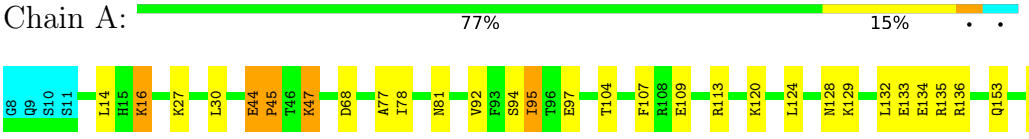
Chain B:



4.2.16 Score per residue for model 16

• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

Chain B:

4.2.17 Score per residue for model 17

• Molecule 1: Ras-related protein Ral-B

Chain A:

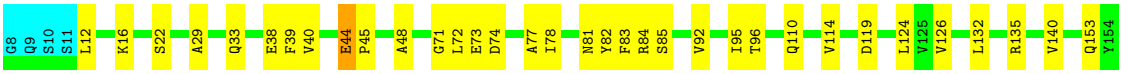
• Molecule 2: RalA-binding protein 1

Chain B:

4.2.18 Score per residue for model 18

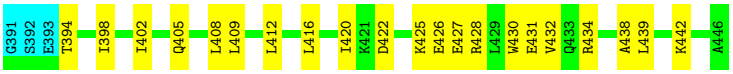
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

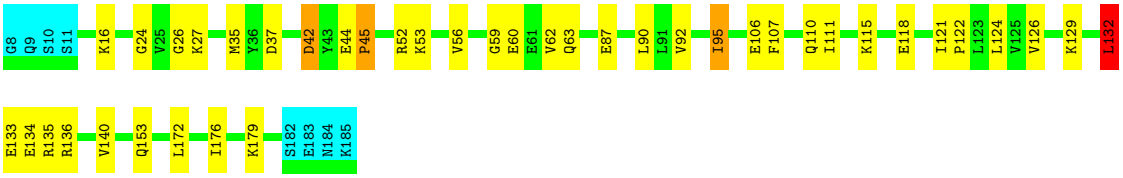
Chain B:



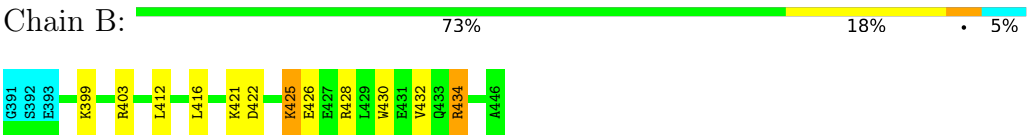
4.2.19 Score per residue for model 19

• Molecule 1: Ras-related protein Ral-B

Chain A:

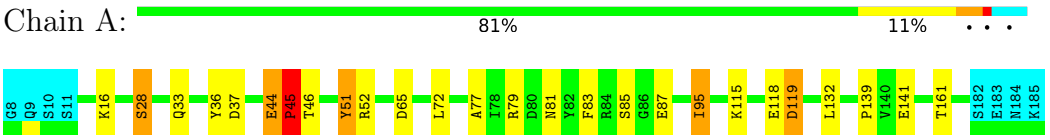


• Molecule 2: RalA-binding protein 1

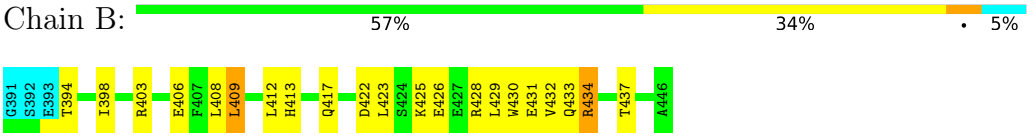


4.2.20 Score per residue for model 20

• Molecule 1: Ras-related protein Ral-B

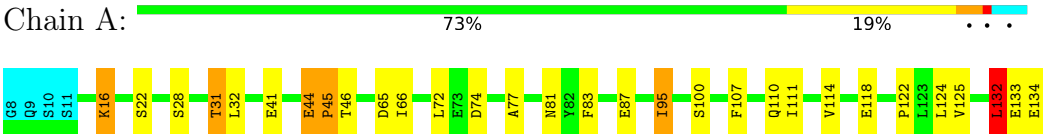


• Molecule 2: RalA-binding protein 1

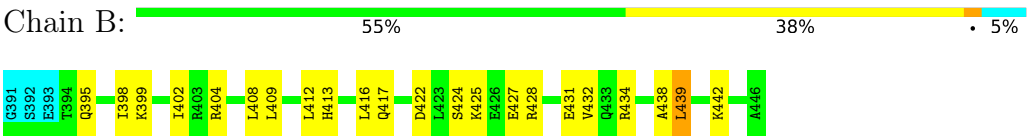


4.2.21 Score per residue for model 21

• Molecule 1: Ras-related protein Ral-B



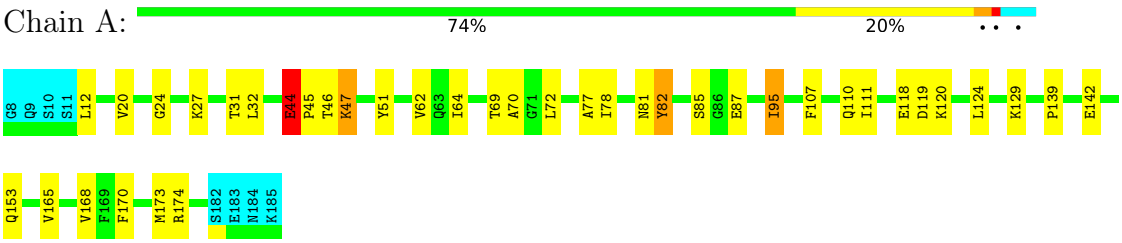
• Molecule 2: RalA-binding protein 1



4.2.22 Score per residue for model 22

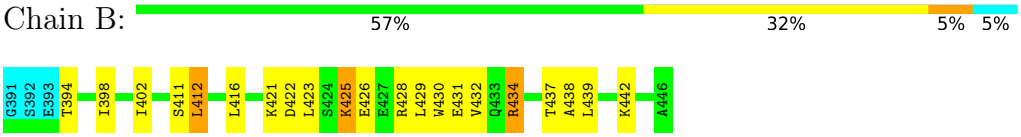
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

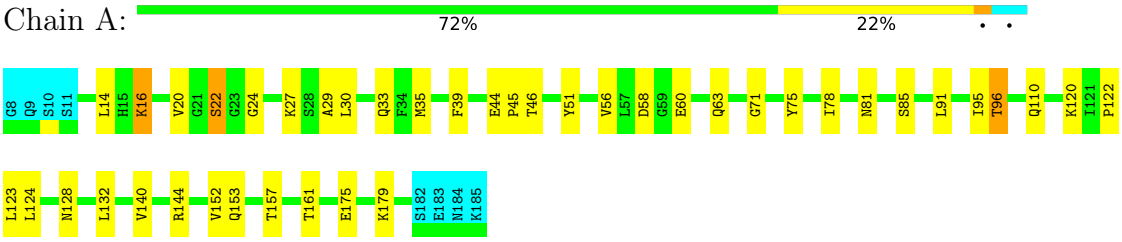
Chain B:



4.2.23 Score per residue for model 23

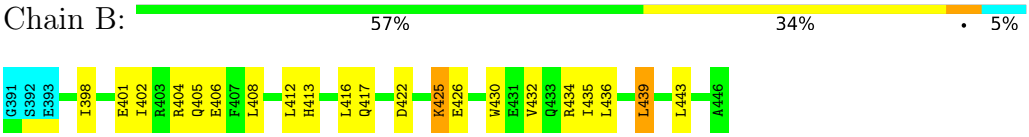
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

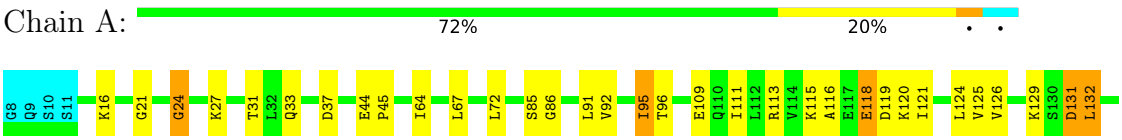
Chain B:



4.2.24 Score per residue for model 24

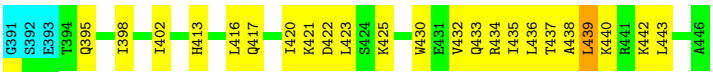
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

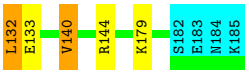
Chain B:



4.2.25 Score per residue for model 25

• Molecule 1: Ras-related protein Ral-B

Chain A:



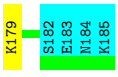
• Molecule 2: RalA-binding protein 1

Chain B:

4.2.26 Score per residue for model 26

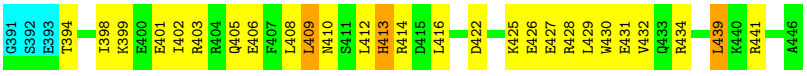
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

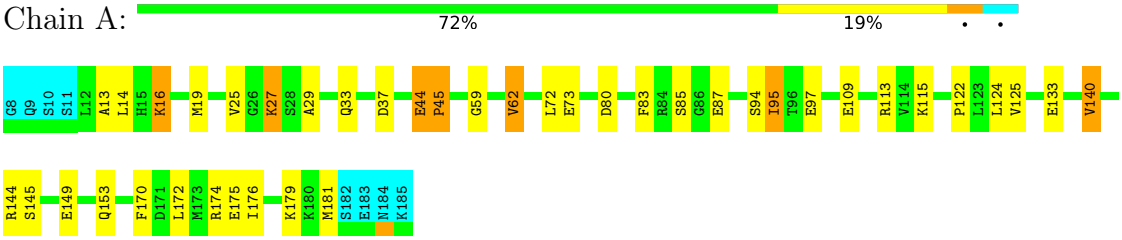
Chain B:



4.2.27 Score per residue for model 27

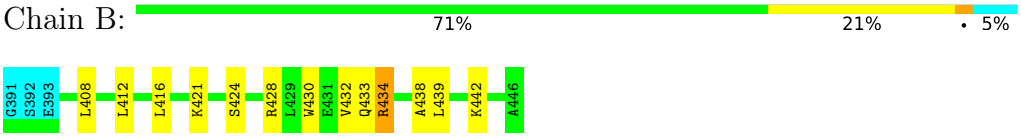
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

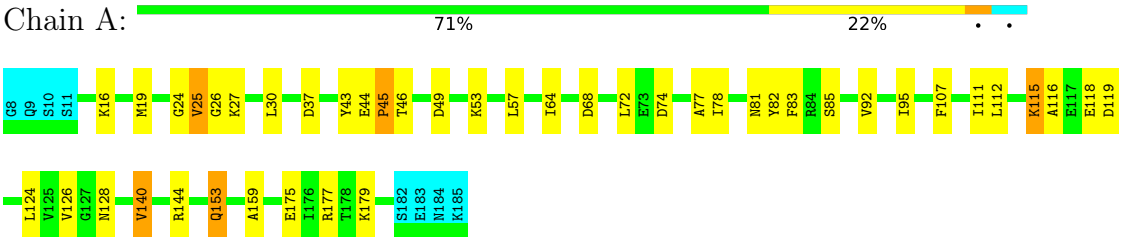
Chain B:



4.2.28 Score per residue for model 28

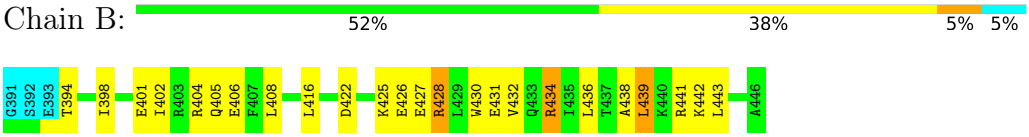
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

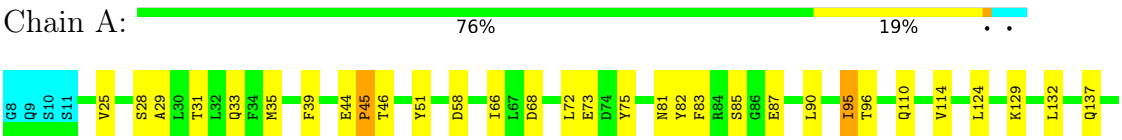
Chain B:



4.2.29 Score per residue for model 29

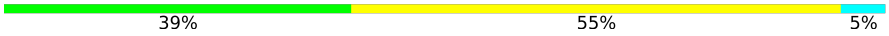
• Molecule 1: Ras-related protein Ral-B

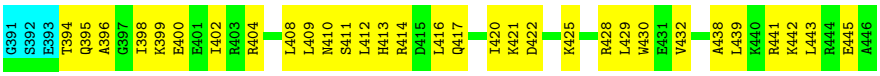
Chain A:



• Molecule 2: RalA-binding protein 1

Chain B:

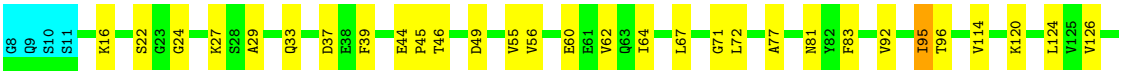




4.2.30 Score per residue for model 30

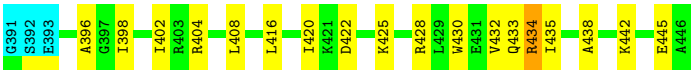
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

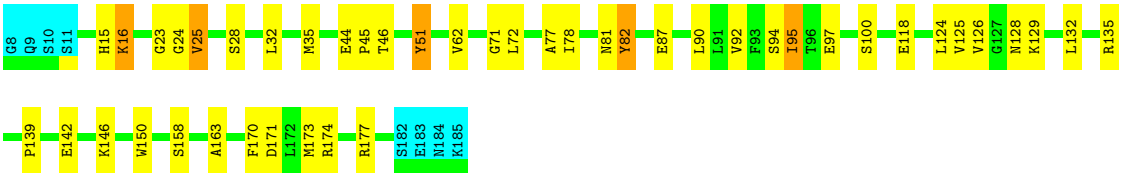
Chain B:



4.2.31 Score per residue for model 31

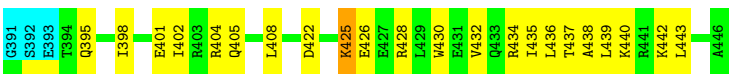
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

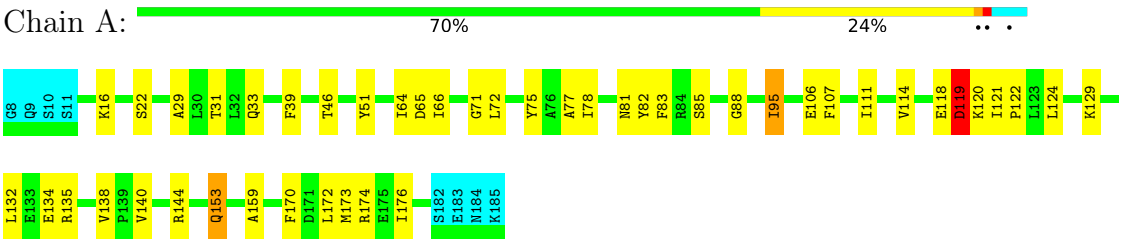
Chain B:



4.2.32 Score per residue for model 32

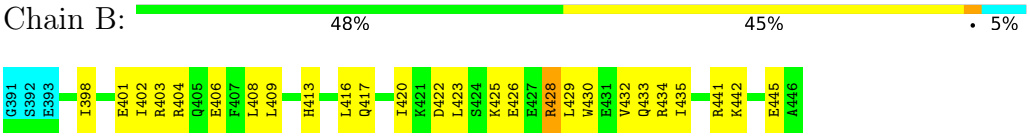
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

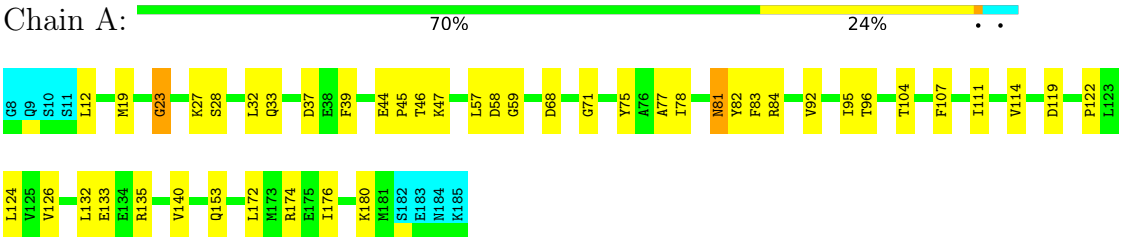
Chain B:



4.2.33 Score per residue for model 33

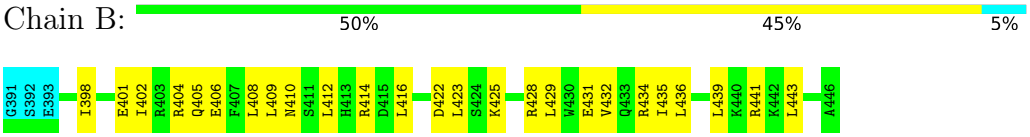
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

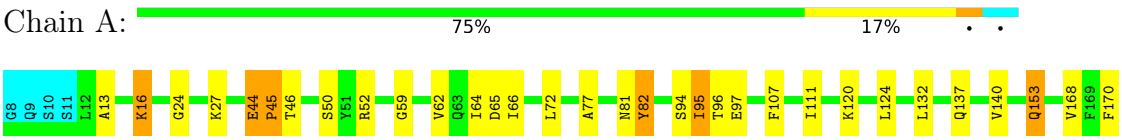
Chain B:

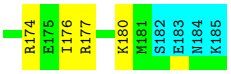


4.2.34 Score per residue for model 34

• Molecule 1: Ras-related protein Ral-B

Chain A:





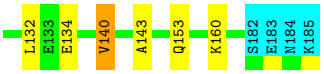
• Molecule 2: RalA-binding protein 1

Chain B: 

4.2.35 Score per residue for model 35

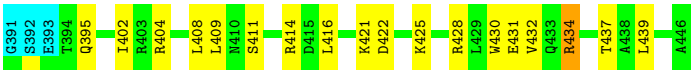
• Molecule 1: Ras-related protein Ral-B

Chain A: 



• Molecule 2: RalA-binding protein 1

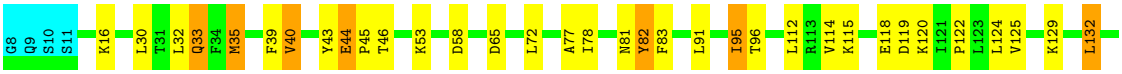
Chain B: 

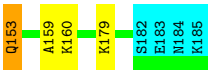


4.2.36 Score per residue for model 36

• Molecule 1: Ras-related protein Ral-B

Chain A: 





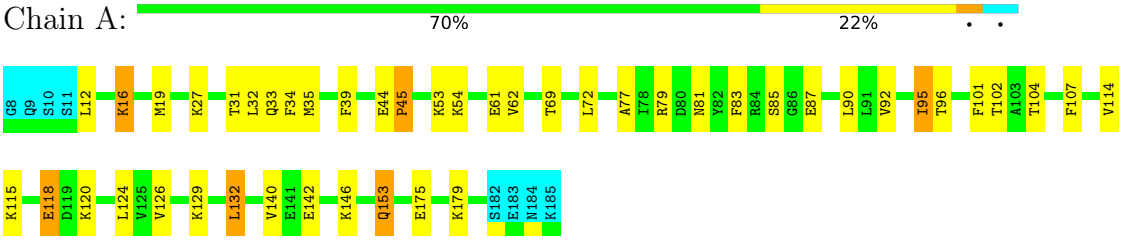
• Molecule 2: RalA-binding protein 1

Chain B: 

4.2.37 Score per residue for model 37

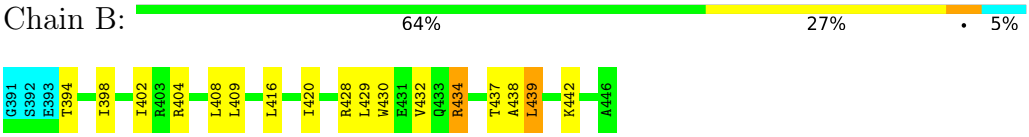
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

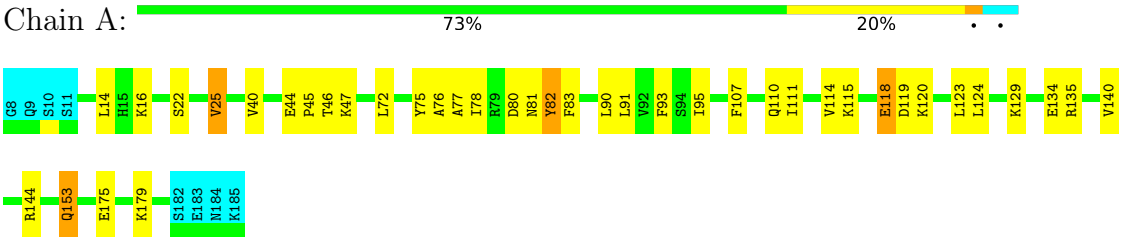
Chain B:



4.2.38 Score per residue for model 38

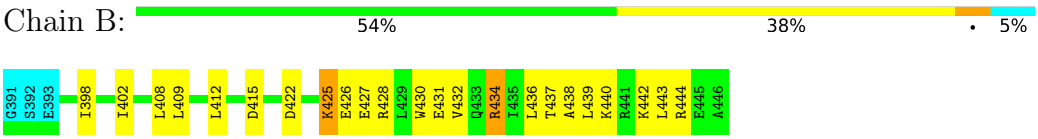
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

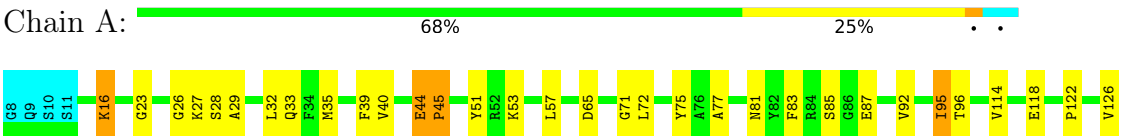
Chain B:



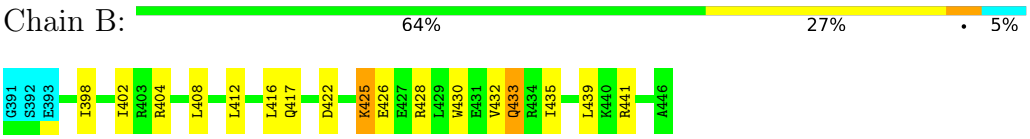
4.2.39 Score per residue for model 39

• Molecule 1: Ras-related protein Ral-B

Chain A:

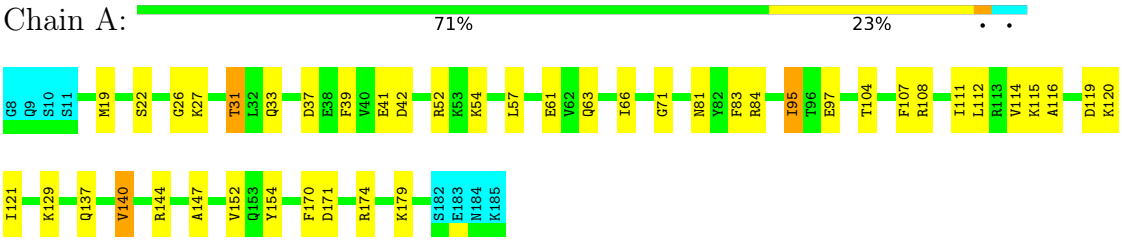


• Molecule 2: RalA-binding protein 1

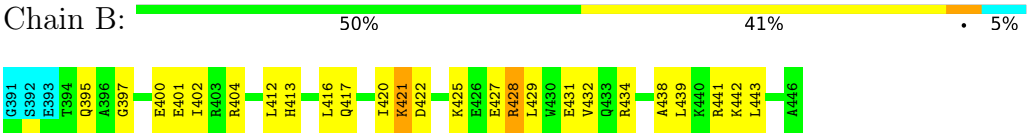


4.2.40 Score per residue for model 40

• Molecule 1: Ras-related protein Ral-B

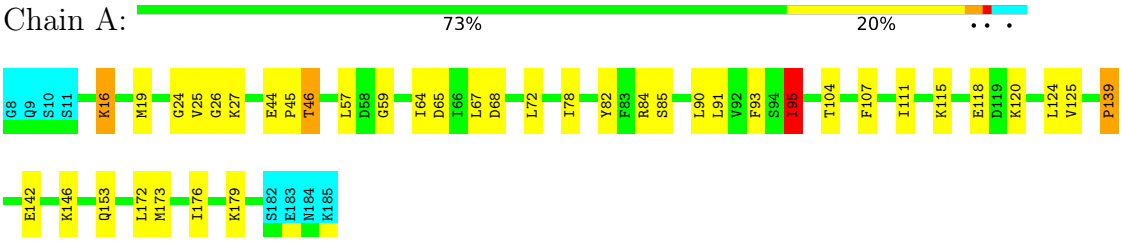


• Molecule 2: RalA-binding protein 1

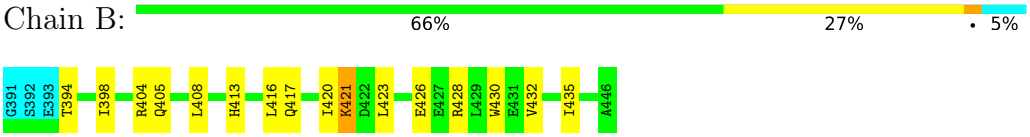


4.2.41 Score per residue for model 41

• Molecule 1: Ras-related protein Ral-B



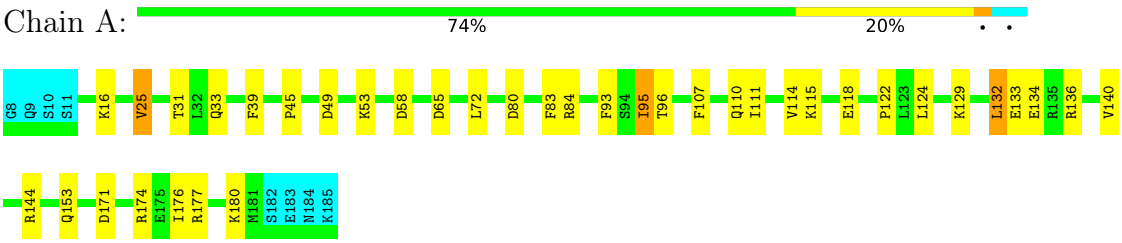
• Molecule 2: RalA-binding protein 1



4.2.42 Score per residue for model 42

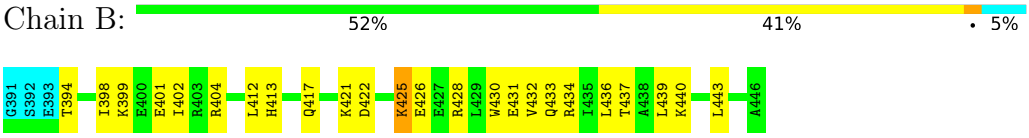
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

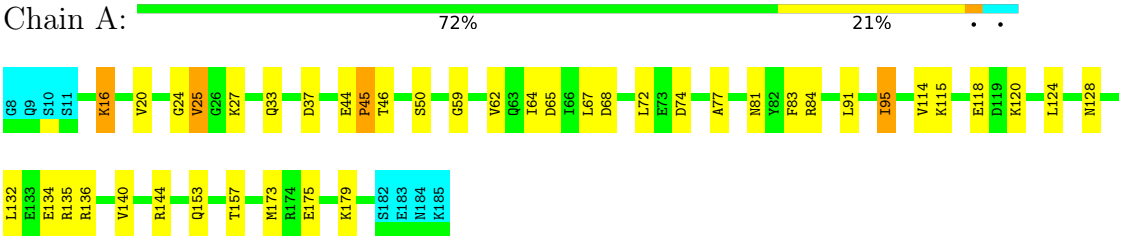
Chain B:



4.2.43 Score per residue for model 43

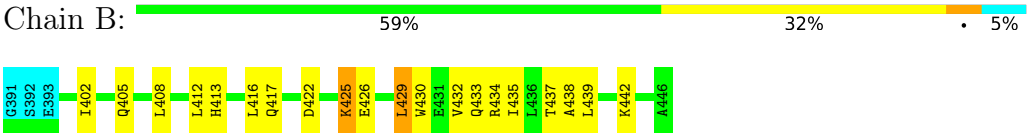
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

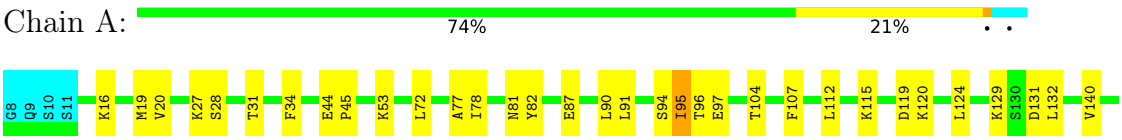
Chain B:

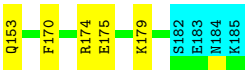


4.2.44 Score per residue for model 44

• Molecule 1: Ras-related protein Ral-B

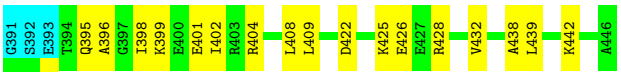
Chain A:





• Molecule 2: RalA-binding protein 1

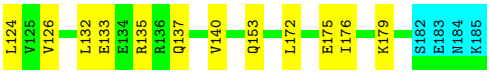
Chain B:



4.2.45 Score per residue for model 45

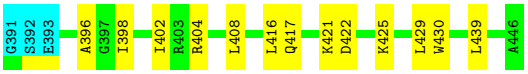
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

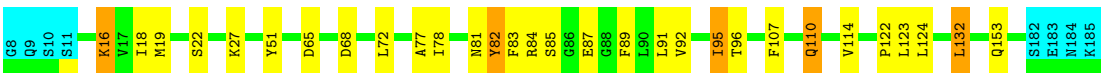
Chain B:



4.2.46 Score per residue for model 46

• Molecule 1: Ras-related protein Ral-B

Chain A:



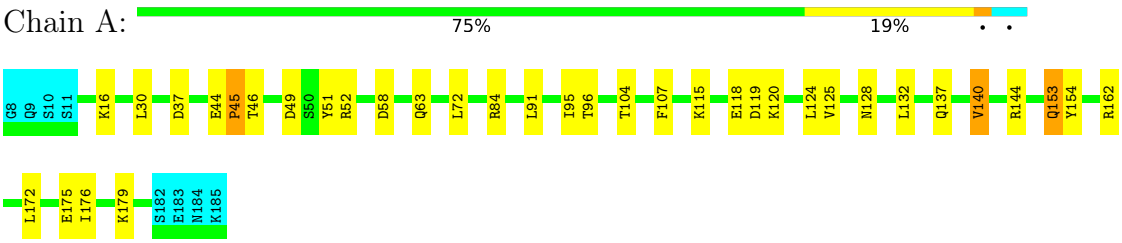
• Molecule 2: RalA-binding protein 1

Chain B:

4.2.47 Score per residue for model 47

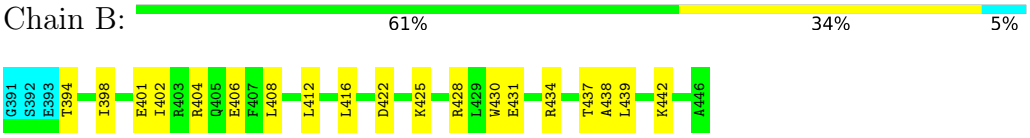
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

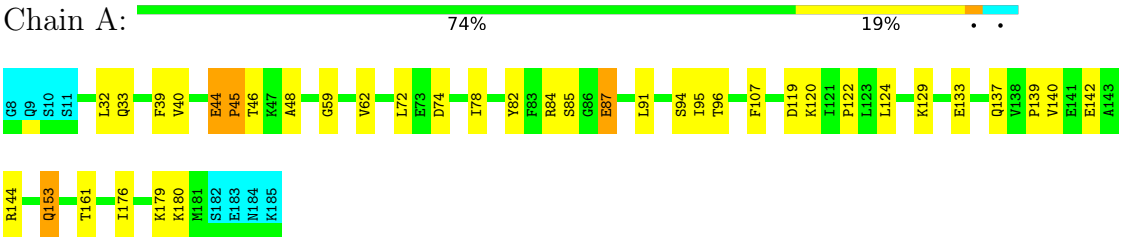
Chain B:



4.2.48 Score per residue for model 48

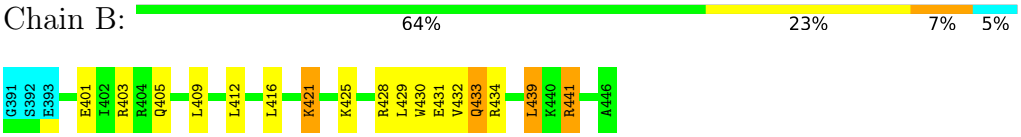
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

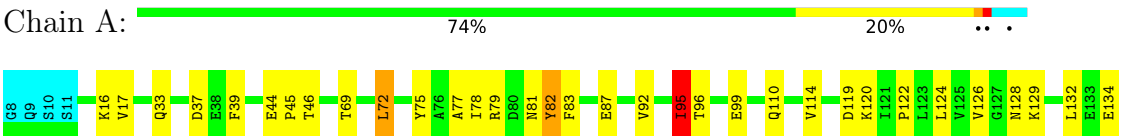
Chain B:



4.2.49 Score per residue for model 49

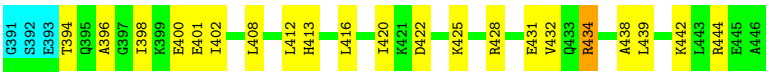
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

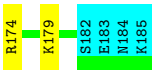
Chain B:



4.2.50 Score per residue for model 50

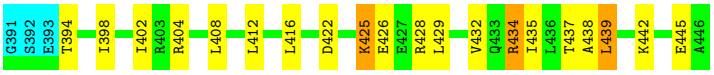
• Molecule 1: Ras-related protein Ral-B

Chain A:



• Molecule 2: RalA-binding protein 1

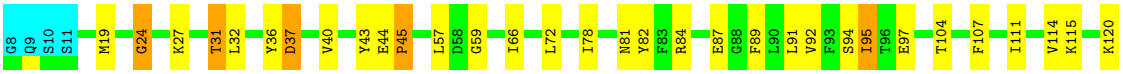
Chain B:

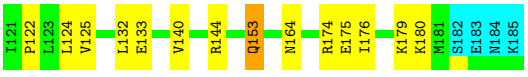


4.2.51 Score per residue for model 51

• Molecule 1: Ras-related protein Ral-B

Chain A:





• Molecule 2: RalA-binding protein 1

Chain B:

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 51 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	
CNS	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.0±0.1
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	36	TYR	Peptide	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1367	1360	1358	24±4
2	B	445	471	470	14±4
3	A	32	13	13	2±1
5	A	2	4	0	0±0
All	All	94197	94248	93891	1867

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
1:A:96:THR:HG21	1:A:132:LEU:HD22	0.97	1.36	26	5
1:A:22:SER:HA	1:A:71:GLY:HA3	0.91	1.41	8	5
1:A:16:LYS:HE2	1:A:65:ASP:HB2	0.90	1.41	39	2
2:B:439:LEU:HD23	2:B:442:LYS:HD3	0.88	1.43	51	2
1:A:77:ALA:HA	1:A:81:ASN:HB3	0.86	1.48	50	1
1:A:92:VAL:HG12	1:A:126:VAL:HB	0.85	1.49	45	22
1:A:27:LYS:HB3	1:A:92:VAL:HG21	0.85	1.47	33	9
1:A:44:GLU:H	1:A:45:PRO:HD2	0.83	1.32	20	14
1:A:27:LYS:HE2	1:A:68:ASP:HA	0.83	1.49	41	1
1:A:77:ALA:HA	1:A:81:ASN:HB2	0.82	1.49	38	16
1:A:120:LYS:HB2	1:A:179:LYS:HG3	0.82	1.52	16	11
1:A:94:SER:HB3	1:A:97:GLU:HG2	0.81	1.50	27	6
1:A:96:THR:HG23	1:A:132:LEU:HD13	0.80	1.54	4	5
1:A:78:ILE:HA	1:A:82:TYR:HD2	0.79	1.36	15	14
1:A:134:GLU:HG3	1:A:135:ARG:HG3	0.79	1.54	21	10
2:B:431:GLU:HA	2:B:434:ARG:HD3	0.78	1.56	42	7
2:B:439:LEU:HD13	2:B:442:LYS:HD3	0.78	1.55	6	7
1:A:32:LEU:HD23	1:A:40:VAL:HB	0.77	1.53	4	2
1:A:124:LEU:HD13	1:A:153:GLN:HG2	0.76	1.57	24	33
1:A:120:LYS:HE3	1:A:180:LYS:HA	0.76	1.55	5	1
1:A:16:LYS:HG3	1:A:65:ASP:HB3	0.76	1.56	43	4
3:A:500:GNP:H2'	3:A:500:GNP:N3	0.76	1.96	36	7
2:B:444:ARG:HA	2:B:444:ARG:NE	0.75	1.97	49	2
1:A:24:GLY:HA2	1:A:27:LYS:HE2	0.75	1.57	23	3
1:A:96:THR:HG23	1:A:132:LEU:HD22	0.74	1.58	1	4
1:A:16:LYS:HG2	1:A:65:ASP:HB2	0.74	1.59	36	1
1:A:120:LYS:HB2	1:A:179:LYS:HB3	0.74	1.59	7	4
1:A:33:GLN:HE22	1:A:39:PHE:HA	0.73	1.44	23	15
1:A:77:ALA:HA	1:A:81:ASN:HD22	0.73	1.43	17	22
1:A:77:ALA:HA	1:A:81:ASN:ND2	0.72	2.00	43	17
1:A:24:GLY:HA2	1:A:27:LYS:HD3	0.71	1.62	17	2
1:A:16:LYS:HE2	1:A:65:ASP:HB3	0.70	1.62	17	2
1:A:84:ARG:HA	1:A:115:LYS:HD3	0.70	1.63	15	2
1:A:115:LYS:HD2	1:A:118:GLU:HG2	0.70	1.64	38	2
1:A:30:LEU:HD11	1:A:128:ASN:HD21	0.70	1.47	23	1
2:B:416:LEU:HA	2:B:420:ILE:O	0.69	1.87	9	17
1:A:46:THR:HA	1:A:49:ASP:HB2	0.69	1.64	17	4
1:A:132:LEU:HD21	1:A:135:ARG:HB2	0.69	1.63	8	1
1:A:77:ALA:H	2:B:417:GLN:HG3	0.69	1.47	45	1
2:B:441:ARG:HH11	2:B:445:GLU:HG3	0.69	1.46	29	1
1:A:19:MET:HG3	1:A:27:LYS:HD2	0.69	1.63	33	1
1:A:55:VAL:HG23	1:A:62:VAL:HG23	0.68	1.66	26	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LYS:HG2	1:A:86:GLY:HA2	0.68	1.64	7	2
1:A:114:VAL:HG23	1:A:115:LYS:HG3	0.68	1.65	8	7
1:A:14:LEU:HG	1:A:16:LYS:HE3	0.68	1.65	16	3
2:B:444:ARG:HA	2:B:444:ARG:HE	0.68	1.46	49	3
2:B:430:TRP:O	2:B:434:ARG:HD3	0.67	1.90	32	10
1:A:115:LYS:HD2	1:A:118:GLU:HG3	0.67	1.65	35	2
1:A:50:SER:HB3	2:B:433:GLN:NE2	0.66	2.05	43	1
1:A:96:THR:CG2	1:A:132:LEU:HD13	0.66	2.21	15	7
1:A:131:ASP:HB3	1:A:158:SER:HB3	0.66	1.68	8	1
1:A:24:GLY:HA2	1:A:27:LYS:HE3	0.65	1.68	22	2
2:B:412:LEU:O	2:B:416:LEU:HG	0.65	1.91	51	10
1:A:44:GLU:N	1:A:45:PRO:HD3	0.65	2.07	18	1
1:A:75:TYR:HB3	1:A:78:ILE:HG12	0.65	1.69	23	1
1:A:32:LEU:HD12	1:A:40:VAL:HB	0.65	1.69	51	1
1:A:78:ILE:HA	1:A:82:TYR:CD2	0.65	2.23	15	15
1:A:81:ASN:HD21	2:B:416:LEU:HD23	0.65	1.52	23	1
2:B:432:VAL:HA	2:B:435:ILE:HD12	0.64	1.68	39	16
2:B:425:LYS:HD2	2:B:426:GLU:N	0.64	2.07	23	13
1:A:159:ALA:HB3	3:A:500:GNP:HN22	0.64	1.50	39	3
2:B:416:LEU:HD22	2:B:420:ILE:HG13	0.64	1.70	32	1
1:A:22:SER:HB2	1:A:100:SER:HB3	0.63	1.69	21	1
1:A:95:ILE:HB	1:A:136:ARG:HG3	0.63	1.71	2	10
1:A:81:ASN:HD22	2:B:416:LEU:HB3	0.63	1.53	14	2
1:A:68:ASP:OD2	5:A:502:HOH:O	0.63	2.15	2	1
1:A:104:THR:HA	1:A:107:PHE:CD2	0.63	2.29	37	13
1:A:92:VAL:HG22	1:A:126:VAL:HB	0.63	1.71	28	1
2:B:428:ARG:O	2:B:432:VAL:HG23	0.63	1.93	3	10
1:A:44:GLU:HB2	1:A:45:PRO:HD3	0.62	1.70	6	11
1:A:132:LEU:HB3	1:A:135:ARG:HB2	0.62	1.70	12	8
1:A:82:TYR:HE2	2:B:413:HIS:HE1	0.62	1.38	36	2
2:B:430:TRP:O	2:B:434:ARG:HG3	0.62	1.95	3	6
1:A:81:ASN:ND2	2:B:416:LEU:HB3	0.62	2.10	3	11
1:A:85:SER:HB2	2:B:430:TRP:CD1	0.62	2.30	48	17
1:A:91:LEU:HD12	1:A:125:VAL:HG22	0.61	1.72	24	4
1:A:139:PRO:O	1:A:142:GLU:HG2	0.61	1.95	41	4
2:B:439:LEU:HA	2:B:442:LYS:HD3	0.61	1.71	28	1
2:B:416:LEU:HD11	2:B:425:LYS:HB3	0.61	1.71	34	5
1:A:174:ARG:O	1:A:177:ARG:HG2	0.61	1.96	42	3
2:B:422:ASP:O	2:B:425:LYS:HG3	0.61	1.96	26	13
1:A:129:LYS:HG3	3:A:500:GNP:C6	0.61	2.25	38	1
1:A:24:GLY:HA3	3:A:500:GNP:O1B	0.61	1.96	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:GLY:HA2	1:A:122:PRO:HD2	0.60	1.72	2	2
1:A:44:GLU:N	1:A:45:PRO:HD2	0.60	2.11	43	23
2:B:413:HIS:O	2:B:417:GLN:HB2	0.60	1.96	24	10
2:B:431:GLU:O	2:B:434:ARG:HG2	0.60	1.95	21	8
1:A:96:THR:CG2	1:A:132:LEU:HD22	0.60	2.26	1	9
1:A:112:LEU:HA	1:A:115:LYS:O	0.60	1.96	5	6
1:A:113:ARG:HE	1:A:113:ARG:HA	0.60	1.55	25	1
1:A:19:MET:HB2	1:A:27:LYS:HE3	0.60	1.73	44	2
1:A:19:MET:SD	1:A:27:LYS:HB2	0.60	2.36	14	6
1:A:115:LYS:HD3	1:A:118:GLU:HG3	0.60	1.72	43	2
1:A:16:LYS:HG3	1:A:65:ASP:HB2	0.60	1.74	45	1
1:A:124:LEU:HD13	1:A:153:GLN:HG3	0.60	1.73	7	8
2:B:416:LEU:HD11	2:B:429:LEU:HD11	0.60	1.71	14	2
1:A:176:ILE:HA	1:A:179:LYS:HG2	0.60	1.74	18	1
1:A:81:ASN:HB3	2:B:416:LEU:HD23	0.60	1.73	29	1
1:A:160:LYS:HB2	3:A:500:GNP:HN22	0.60	1.56	35	1
1:A:88:GLY:HA2	1:A:122:PRO:HG2	0.59	1.71	6	2
1:A:75:TYR:HB3	1:A:78:ILE:CG1	0.59	2.27	23	1
1:A:176:ILE:O	1:A:180:LYS:HG2	0.59	1.97	34	10
2:B:434:ARG:HA	2:B:437:THR:HG22	0.59	1.74	37	14
1:A:77:ALA:HA	1:A:81:ASN:CB	0.59	2.25	50	2
1:A:44:GLU:H	1:A:45:PRO:HD3	0.59	1.57	18	1
1:A:22:SER:O	1:A:71:GLY:HA3	0.59	1.96	23	3
1:A:144:ARG:HG2	1:A:154:TYR:CD2	0.59	2.33	47	2
2:B:428:ARG:O	2:B:432:VAL:HG12	0.59	1.98	11	29
1:A:123:LEU:O	1:A:152:VAL:HB	0.59	1.97	6	2
1:A:47:LYS:HA	1:A:47:LYS:HE3	0.59	1.73	16	1
1:A:55:VAL:HG23	1:A:62:VAL:CG2	0.59	2.26	26	2
2:B:413:HIS:O	2:B:417:GLN:HG3	0.59	1.97	29	1
1:A:96:THR:HG21	1:A:132:LEU:CD2	0.59	2.28	47	2
2:B:422:ASP:HB3	2:B:425:LYS:HG2	0.59	1.75	46	16
1:A:26:GLY:HA2	3:A:500:GNP:O1A	0.59	1.97	14	1
1:A:33:GLN:HE22	1:A:159:ALA:HB1	0.59	1.57	5	1
1:A:27:LYS:HG2	1:A:92:VAL:HG21	0.59	1.73	37	2
2:B:394:THR:O	2:B:398:ILE:HG12	0.59	1.97	37	19
1:A:85:SER:HB3	2:B:430:TRP:CD1	0.59	2.33	13	5
1:A:140:VAL:O	1:A:144:ARG:HG3	0.58	1.97	39	20
2:B:410:ASN:HA	2:B:413:HIS:CD2	0.58	2.33	4	3
2:B:401:GLU:O	2:B:405:GLN:HG2	0.58	1.98	33	8
2:B:438:ALA:O	2:B:442:LYS:HG3	0.58	1.98	50	15
2:B:442:LYS:HA	2:B:445:GLU:HB3	0.58	1.74	30	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:GLU:HG3	1:A:176:ILE:HD13	0.58	1.73	15	1
2:B:411:SER:HA	2:B:414:ARG:HE	0.58	1.58	35	2
1:A:77:ALA:CA	1:A:81:ASN:HB2	0.58	2.27	38	1
2:B:402:ILE:HG12	2:B:439:LEU:HG	0.58	1.74	16	3
1:A:26:GLY:HA2	3:A:500:GNP:O2A	0.58	1.99	11	2
2:B:431:GLU:HA	2:B:434:ARG:NE	0.58	2.14	20	3
1:A:47:LYS:HD2	1:A:75:TYR:CE2	0.58	2.34	33	1
1:A:175:GLU:HB3	1:A:179:LYS:HE2	0.58	1.76	43	5
1:A:96:THR:HG21	1:A:132:LEU:HD13	0.58	1.75	9	4
1:A:16:LYS:HD3	1:A:65:ASP:HB2	0.58	1.75	34	2
1:A:124:LEU:HD13	1:A:153:GLN:CG	0.57	2.29	47	9
1:A:109:GLU:O	1:A:113:ARG:HG3	0.57	1.99	4	3
2:B:431:GLU:HA	2:B:434:ARG:CD	0.57	2.29	13	10
1:A:115:LYS:HB3	1:A:118:GLU:HG3	0.57	1.77	2	3
1:A:16:LYS:HE3	1:A:16:LYS:HA	0.57	1.77	5	1
1:A:175:GLU:O	1:A:179:LYS:HG2	0.57	1.99	47	8
1:A:57:LEU:HD11	1:A:174:ARG:HE	0.57	1.59	51	1
2:B:422:ASP:HB3	2:B:425:LYS:HG3	0.57	1.74	40	3
1:A:115:LYS:HB3	1:A:118:GLU:OE1	0.57	2.00	12	1
2:B:439:LEU:HD12	2:B:442:LYS:HD3	0.57	1.77	18	3
2:B:404:ARG:O	2:B:408:LEU:HG	0.56	2.00	51	24
1:A:95:ILE:HD13	1:A:95:ILE:H	0.56	1.60	24	33
1:A:44:GLU:HA	5:A:503:HOH:O	0.56	1.99	47	4
1:A:81:ASN:OD1	2:B:421:LYS:HD3	0.56	2.01	29	4
2:B:431:GLU:HA	2:B:434:ARG:HD2	0.56	1.76	28	7
2:B:430:TRP:HB3	2:B:434:ARG:NH1	0.56	2.15	27	1
2:B:412:LEU:HB3	2:B:429:LEU:HG	0.56	1.77	46	2
1:A:25:VAL:HG11	1:A:93:PHE:HA	0.56	1.75	38	4
1:A:175:GLU:O	1:A:179:LYS:HD3	0.56	2.01	45	8
2:B:430:TRP:O	2:B:434:ARG:HD2	0.56	2.01	11	9
1:A:32:LEU:HD22	1:A:40:VAL:HG22	0.56	1.76	1	1
1:A:16:LYS:CG	1:A:86:GLY:HA2	0.56	2.31	24	1
1:A:129:LYS:HE2	3:A:500:GNP:N3	0.56	2.16	3	1
1:A:16:LYS:HB2	1:A:87:GLU:HG2	0.56	1.77	37	1
1:A:64:ILE:HD12	1:A:173:MET:SD	0.55	2.41	15	9
1:A:52:ARG:HD3	1:A:63:GLN:HB3	0.55	1.77	13	2
2:B:427:GLU:O	2:B:431:GLU:HG2	0.55	2.01	3	2
1:A:16:LYS:CE	1:A:65:ASP:HB3	0.55	2.30	32	3
2:B:422:ASP:O	2:B:425:LYS:HG2	0.55	2.00	28	1
1:A:115:LYS:CE	1:A:118:GLU:HG3	0.55	2.32	15	1
1:A:22:SER:HB2	1:A:107:PHE:HE1	0.55	1.61	46	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:MET:HB3	1:A:27:LYS:HD2	0.55	1.77	27	2
1:A:87:GLU:O	1:A:122:PRO:HD2	0.55	2.01	17	15
1:A:57:LEU:O	1:A:57:LEU:HG	0.55	2.02	3	2
2:B:442:LYS:HA	2:B:445:GLU:CB	0.55	2.32	10	3
2:B:401:GLU:OE2	2:B:404:ARG:HD3	0.54	2.03	40	4
2:B:405:GLN:HE21	2:B:432:VAL:HG23	0.54	1.62	18	6
1:A:26:GLY:HA2	3:A:500:GNP:C3'	0.54	2.33	1	3
1:A:159:ALA:HB3	3:A:500:GNP:N1	0.54	2.17	17	1
1:A:50:SER:HA	1:A:66:ILE:O	0.54	2.02	34	1
1:A:170:PHE:O	1:A:174:ARG:HG2	0.54	2.02	1	11
1:A:14:LEU:HD21	2:B:434:ARG:HH22	0.54	1.63	9	1
2:B:439:LEU:HD23	2:B:442:LYS:CD	0.54	2.29	29	2
1:A:159:ALA:HB3	3:A:500:GNP:N2	0.54	2.18	18	3
1:A:20:VAL:HG22	1:A:91:LEU:HA	0.54	1.79	44	1
2:B:405:GLN:NE2	2:B:432:VAL:HG23	0.53	2.18	43	5
1:A:94:SER:HB3	1:A:97:GLU:HB2	0.53	1.79	34	3
1:A:109:GLU:O	1:A:113:ARG:HG2	0.53	2.03	27	1
2:B:410:ASN:O	2:B:414:ARG:HG3	0.53	2.03	7	5
1:A:23:GLY:HA2	1:A:71:GLY:HA3	0.53	1.79	39	5
1:A:96:THR:HG21	1:A:132:LEU:CD1	0.53	2.34	12	2
2:B:408:LEU:HB2	2:B:432:VAL:HG21	0.53	1.79	36	11
2:B:409:LEU:HD22	2:B:432:VAL:HG13	0.53	1.81	20	1
2:B:422:ASP:HB2	2:B:425:LYS:HG2	0.53	1.81	32	2
1:A:98:HIS:HB2	1:A:137:GLN:OE1	0.53	2.03	45	1
2:B:412:LEU:HB3	2:B:429:LEU:HD11	0.53	1.79	26	1
2:B:401:GLU:OE2	2:B:404:ARG:HD2	0.53	2.04	47	3
1:A:19:MET:HB3	1:A:27:LYS:HD3	0.53	1.81	7	1
1:A:46:THR:HG21	3:A:500:GNP:O2G	0.53	2.04	50	1
1:A:46:THR:HB	1:A:68:ASP:HB3	0.53	1.80	33	2
1:A:57:LEU:HD21	1:A:174:ARG:HD3	0.53	1.81	13	1
1:A:115:LYS:CB	1:A:118:GLU:HG3	0.53	2.33	2	1
1:A:23:GLY:HA2	3:A:500:GNP:O1B	0.53	2.04	14	1
1:A:96:THR:HA	1:A:137:GLN:HB3	0.53	1.80	34	3
1:A:83:PHE:O	1:A:115:LYS:HD3	0.52	2.03	27	2
1:A:122:PRO:HB2	1:A:172:LEU:HD11	0.52	1.81	4	2
1:A:84:ARG:HA	1:A:115:LYS:HG2	0.52	1.81	47	1
1:A:29:ALA:O	1:A:33:GLN:HG2	0.52	2.04	4	11
1:A:122:PRO:HG3	1:A:179:LYS:NZ	0.52	2.19	6	1
1:A:32:LEU:HG	1:A:40:VAL:HB	0.52	1.81	39	3
1:A:84:ARG:HG2	1:A:114:VAL:HB	0.52	1.79	35	1
2:B:398:ILE:O	2:B:402:ILE:HG13	0.52	2.04	38	27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ILE:HG12	1:A:67:LEU:HD12	0.52	1.81	3	1
2:B:438:ALA:O	2:B:442:LYS:HG2	0.52	2.04	34	14
1:A:54:LYS:HD2	1:A:61:GLU:HB3	0.52	1.79	50	1
1:A:35:MET:HG3	1:A:53:LYS:HB2	0.52	1.81	36	3
1:A:35:MET:SD	1:A:66:ILE:HD12	0.52	2.45	11	1
3:A:500:GNP:N3	3:A:500:GNP:C2'	0.52	2.72	25	5
2:B:416:LEU:HD21	2:B:425:LYS:CB	0.52	2.35	32	2
2:B:436:LEU:O	2:B:440:LYS:HG2	0.52	2.04	38	4
1:A:94:SER:HB3	1:A:129:LYS:HG3	0.52	1.81	48	1
1:A:120:LYS:HG3	1:A:179:LYS:HB3	0.52	1.79	2	1
1:A:19:MET:SD	1:A:27:LYS:HA	0.52	2.44	25	4
1:A:16:LYS:HD2	1:A:87:GLU:HG2	0.52	1.80	31	1
2:B:409:LEU:HD23	2:B:432:VAL:HG13	0.52	1.81	7	5
1:A:31:THR:O	1:A:35:MET:HG3	0.52	2.05	37	1
1:A:51:TYR:HA	2:B:437:THR:OG1	0.52	2.04	4	6
2:B:416:LEU:HD11	2:B:425:LYS:HB2	0.52	1.82	25	3
1:A:72:LEU:HG	1:A:73:GLU:N	0.52	2.20	1	1
2:B:402:ILE:HG12	2:B:439:LEU:HB3	0.52	1.81	47	19
1:A:44:GLU:N	1:A:45:PRO:CD	0.52	2.73	18	5
1:A:83:PHE:HB3	1:A:114:VAL:HG21	0.52	1.82	43	8
2:B:425:LYS:HD2	2:B:426:GLU:HG2	0.52	1.81	39	2
1:A:115:LYS:HB2	1:A:118:GLU:OE2	0.52	2.04	28	1
1:A:157:THR:HB	1:A:165:VAL:HG22	0.52	1.82	39	1
1:A:16:LYS:N	1:A:16:LYS:HD3	0.52	2.20	46	1
1:A:54:LYS:HD3	1:A:61:GLU:HB3	0.51	1.81	5	5
1:A:128:ASN:HA	1:A:157:THR:O	0.51	2.05	43	3
1:A:44:GLU:HB3	1:A:45:PRO:HD3	0.51	1.81	17	3
1:A:28:SER:O	1:A:32:LEU:HG	0.51	2.05	21	2
2:B:416:LEU:HG	2:B:425:LYS:HD2	0.51	1.82	28	1
2:B:425:LYS:HG3	2:B:426:GLU:N	0.51	2.20	28	1
2:B:396:ALA:O	2:B:400:GLU:HG2	0.51	2.04	46	2
2:B:425:LYS:O	2:B:429:LEU:HG	0.51	2.05	51	1
1:A:114:VAL:HG23	1:A:115:LYS:HG2	0.51	1.82	12	1
1:A:56:VAL:HG23	1:A:60:GLU:O	0.51	2.06	14	3
1:A:160:LYS:HB2	3:A:500:GNP:N1	0.51	2.20	1	2
1:A:44:GLU:OE1	3:A:500:GNP:N3B	0.51	2.44	13	14
1:A:75:TYR:HA	2:B:417:GLN:HG2	0.51	1.82	29	1
1:A:84:ARG:HG3	2:B:426:GLU:HB2	0.51	1.82	46	1
2:B:395:GLN:O	2:B:399:LYS:HG3	0.51	2.05	29	2
1:A:84:ARG:HH21	1:A:115:LYS:HA	0.51	1.66	43	1
1:A:139:PRO:HB2	1:A:142:GLU:HG2	0.51	1.83	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:THR:CG2	1:A:66:ILE:HG21	0.51	2.36	40	2
2:B:433:GLN:NE2	2:B:437:THR:HB	0.51	2.19	42	1
1:A:20:VAL:CG2	1:A:91:LEU:HA	0.51	2.36	44	1
1:A:129:LYS:HG3	1:A:132:LEU:HG	0.51	1.82	32	1
1:A:78:ILE:HA	1:A:82:TYR:CD1	0.51	2.41	33	4
1:A:93:PHE:HB2	1:A:100:SER:HB3	0.51	1.82	11	1
1:A:84:ARG:HD3	2:B:426:GLU:OE2	0.51	2.06	43	1
1:A:128:ASN:O	1:A:129:LYS:HB2	0.50	2.06	8	2
1:A:160:LYS:HB2	3:A:500:GNP:C2	0.50	2.36	30	2
2:B:408:LEU:O	2:B:412:LEU:HD23	0.50	2.06	39	19
1:A:83:PHE:O	1:A:115:LYS:HE2	0.50	2.05	20	2
1:A:16:LYS:HD2	2:B:434:ARG:NH2	0.50	2.22	18	1
1:A:107:PHE:O	1:A:111:ILE:HG13	0.50	2.07	19	21
2:B:398:ILE:HD12	2:B:442:LYS:HB3	0.50	1.82	24	4
1:A:120:LYS:HB3	1:A:179:LYS:HG3	0.50	1.82	4	1
1:A:172:LEU:O	1:A:176:ILE:HG13	0.50	2.06	33	10
1:A:82:TYR:CE1	2:B:429:LEU:HB3	0.50	2.42	11	3
1:A:129:LYS:HB3	1:A:132:LEU:HD23	0.50	1.82	1	3
1:A:19:MET:HG2	1:A:90:LEU:HD12	0.50	1.84	37	1
1:A:92:VAL:HA	1:A:126:VAL:O	0.50	2.06	49	1
1:A:16:LYS:HA	1:A:16:LYS:HE2	0.50	1.82	41	2
1:A:119:ASP:OD1	1:A:120:LYS:HG2	0.50	2.07	15	2
2:B:405:GLN:OE1	2:B:432:VAL:HG23	0.50	2.06	41	3
1:A:48:ALA:HB1	2:B:409:LEU:HD21	0.50	1.83	18	1
1:A:137:GLN:HA	1:A:137:GLN:OE1	0.50	2.07	40	2
1:A:39:PHE:O	1:A:40:VAL:HB	0.50	2.07	36	1
1:A:75:TYR:O	1:A:77:ALA:N	0.49	2.43	38	1
2:B:434:ARG:HD3	2:B:435:ILE:HG13	0.49	1.82	50	1
1:A:96:THR:HG23	1:A:132:LEU:CD2	0.49	2.32	1	3
1:A:124:LEU:HD12	1:A:125:VAL:N	0.49	2.22	27	3
1:A:47:LYS:HE2	1:A:70:ALA:HB2	0.49	1.82	22	1
1:A:52:ARG:HA	1:A:64:ILE:O	0.49	2.07	34	1
1:A:83:PHE:HB2	1:A:114:VAL:HG21	0.49	1.84	29	11
1:A:78:ILE:HG12	2:B:413:HIS:CE1	0.49	2.42	41	2
1:A:26:GLY:HA2	3:A:500:GNP:H3'	0.49	1.84	28	2
2:B:436:LEU:HG	2:B:440:LYS:HE3	0.49	1.83	8	1
1:A:82:TYR:OH	2:B:409:LEU:HD11	0.49	2.08	44	6
1:A:129:LYS:HB2	3:A:500:GNP:C6	0.49	2.37	17	1
1:A:30:LEU:HD23	1:A:159:ALA:HB2	0.49	1.83	28	2
1:A:115:LYS:HB3	1:A:118:GLU:CG	0.49	2.37	42	2
2:B:416:LEU:HD22	2:B:429:LEU:HD11	0.49	1.85	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LYS:CB	1:A:179:LYS:HG3	0.49	2.37	11	4
1:A:96:THR:HG22	1:A:135:ARG:O	0.49	2.08	39	6
1:A:77:ALA:HA	1:A:81:ASN:CG	0.49	2.28	33	2
1:A:16:LYS:HD2	2:B:430:TRP:CZ3	0.49	2.43	28	2
2:B:412:LEU:HB3	2:B:429:LEU:CD2	0.49	2.38	12	2
1:A:25:VAL:HA	1:A:94:SER:OG	0.49	2.08	15	1
1:A:16:LYS:HD3	2:B:430:TRP:CZ3	0.49	2.42	17	1
1:A:35:MET:SD	1:A:51:TYR:HB3	0.49	2.48	31	3
1:A:164:ASN:OD1	1:A:167:LYS:HE2	0.49	2.07	30	1
1:A:75:TYR:HA	2:B:417:GLN:HG3	0.49	1.85	32	1
1:A:120:LYS:O	1:A:122:PRO:HD3	0.49	2.06	17	3
2:B:416:LEU:CD1	2:B:429:LEU:HD11	0.49	2.37	14	3
1:A:90:LEU:HD23	1:A:124:LEU:HB3	0.49	1.85	29	5
1:A:33:GLN:HA	1:A:37:ASP:O	0.49	2.07	20	1
2:B:431:GLU:O	2:B:434:ARG:HD3	0.49	2.08	22	1
1:A:44:GLU:HA	3:A:500:GNP:O1G	0.49	2.07	35	1
1:A:122:PRO:HB3	1:A:179:LYS:HE2	0.49	1.83	36	1
1:A:95:ILE:HG12	1:A:132:LEU:HD11	0.49	1.85	2	2
1:A:120:LYS:HB2	1:A:179:LYS:CG	0.49	2.38	51	2
2:B:430:TRP:HB3	2:B:434:ARG:CZ	0.48	2.37	1	1
1:A:26:GLY:HA2	3:A:500:GNP:C2'	0.48	2.39	28	2
1:A:32:LEU:HD13	1:A:40:VAL:HG22	0.48	1.85	45	1
2:B:421:LYS:NZ	2:B:421:LYS:HB2	0.48	2.24	48	1
2:B:421:LYS:HA	2:B:425:LYS:HE2	0.48	1.86	19	2
1:A:129:LYS:HG2	3:A:500:GNP:C4	0.48	2.38	35	1
1:A:140:VAL:HG12	1:A:144:ARG:HG3	0.48	1.84	48	5
2:B:409:LEU:O	2:B:413:HIS:HB2	0.48	2.07	2	1
1:A:32:LEU:HD22	1:A:40:VAL:HB	0.48	1.84	12	1
1:A:129:LYS:O	1:A:132:LEU:HG	0.48	2.08	16	1
2:B:416:LEU:HD21	2:B:425:LYS:HB2	0.48	1.86	23	1
1:A:46:THR:HA	1:A:49:ASP:OD1	0.48	2.09	28	1
2:B:422:ASP:H	2:B:425:LYS:HG3	0.48	1.69	9	1
1:A:122:PRO:HG3	1:A:179:LYS:HG2	0.48	1.85	19	1
1:A:129:LYS:HD3	3:A:500:GNP:C4	0.48	2.38	19	1
1:A:94:SER:CB	1:A:129:LYS:HG3	0.48	2.39	48	1
1:A:46:THR:HB	1:A:68:ASP:OD2	0.48	2.09	8	6
2:B:439:LEU:HD12	2:B:442:LYS:CD	0.48	2.39	15	3
2:B:410:ASN:HA	2:B:413:HIS:NE2	0.48	2.23	4	1
1:A:124:LEU:HG	1:A:153:GLN:HG2	0.48	1.84	29	1
1:A:78:ILE:O	1:A:82:TYR:HB2	0.48	2.08	48	2
1:A:77:ALA:HB2	2:B:416:LEU:HB2	0.48	1.86	49	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LYS:HD3	1:A:65:ASP:HB3	0.47	1.86	1	1
2:B:412:LEU:HD11	2:B:428:ARG:HG3	0.47	1.86	8	2
1:A:33:GLN:HA	1:A:39:PHE:HB3	0.47	1.84	36	1
1:A:67:LEU:HD12	2:B:430:TRP:CH2	0.47	2.44	43	1
1:A:96:THR:HG23	1:A:132:LEU:CD1	0.47	2.39	2	1
1:A:83:PHE:CB	1:A:114:VAL:HG21	0.47	2.40	21	6
1:A:176:ILE:O	1:A:180:LYS:HB2	0.47	2.08	8	1
1:A:28:SER:HB2	5:A:503:HOH:O	0.47	2.09	9	1
1:A:16:LYS:HB2	1:A:87:GLU:HB3	0.47	1.85	20	2
1:A:26:GLY:HA2	3:A:500:GNP:H8	0.47	1.84	5	1
1:A:15:HIS:HA	1:A:87:GLU:OE1	0.47	2.08	15	2
1:A:28:SER:HB2	3:A:500:GNP:O1A	0.47	2.09	29	1
2:B:402:ILE:HD11	2:B:443:LEU:HB2	0.47	1.86	42	11
1:A:84:ARG:HB3	2:B:426:GLU:HG2	0.47	1.87	14	1
1:A:16:LYS:HB2	1:A:87:GLU:HG3	0.47	1.86	25	1
1:A:34:PHE:O	1:A:53:LYS:HE2	0.47	2.10	37	1
1:A:52:ARG:HD2	1:A:63:GLN:HB3	0.47	1.84	40	1
1:A:19:MET:HG2	1:A:90:LEU:HB2	0.47	1.85	44	2
1:A:28:SER:CB	5:A:503:HOH:O	0.47	2.62	9	1
1:A:115:LYS:HZ1	1:A:118:GLU:CD	0.47	2.13	28	1
1:A:17:VAL:O	1:A:66:ILE:HA	0.47	2.09	35	1
2:B:427:GLU:O	2:B:431:GLU:HG3	0.47	2.10	28	7
1:A:115:LYS:HE2	1:A:118:GLU:OE1	0.47	2.09	12	1
1:A:176:ILE:O	1:A:180:LYS:HG3	0.47	2.10	17	1
2:B:431:GLU:O	2:B:434:ARG:HD2	0.47	2.10	17	1
1:A:124:LEU:HG	1:A:153:GLN:CG	0.47	2.40	29	1
1:A:160:LYS:HB2	3:A:500:GNP:N2	0.47	2.25	35	1
1:A:16:LYS:HE3	1:A:16:LYS:CA	0.47	2.39	5	1
2:B:402:ILE:HA	2:B:439:LEU:HD23	0.47	1.87	35	7
1:A:56:VAL:HA	1:A:60:GLU:O	0.47	2.10	30	2
1:A:48:ALA:HB3	2:B:409:LEU:HD21	0.47	1.87	48	1
1:A:57:LEU:O	1:A:58:ASP:HB3	0.47	2.10	11	1
1:A:124:LEU:HD21	1:A:168:VAL:HB	0.47	1.86	22	1
2:B:428:ARG:HD3	2:B:431:GLU:OE1	0.47	2.10	9	5
1:A:128:ASN:OD1	1:A:129:LYS:HD3	0.46	2.09	13	1
2:B:424:SER:HA	2:B:427:GLU:OE2	0.46	2.10	21	1
1:A:15:HIS:HE1	1:A:177:ARG:HG3	0.46	1.70	31	1
1:A:32:LEU:HA	1:A:35:MET:SD	0.46	2.50	36	1
2:B:403:ARG:HD3	2:B:406:GLU:OE1	0.46	2.10	2	1
2:B:426:GLU:HA	2:B:429:LEU:HD12	0.46	1.86	14	1
1:A:115:LYS:HZ2	1:A:118:GLU:CD	0.46	2.13	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LYS:HG3	1:A:86:GLY:HA2	0.46	1.87	24	1
1:A:124:LEU:CD1	1:A:153:GLN:HG3	0.46	2.39	4	2
1:A:132:LEU:O	1:A:134:GLU:HG2	0.46	2.09	21	1
1:A:16:LYS:HD2	1:A:65:ASP:HB3	0.46	1.88	42	1
1:A:16:LYS:HD2	1:A:16:LYS:N	0.46	2.26	9	1
2:B:416:LEU:HD12	2:B:429:LEU:HD11	0.46	1.88	33	3
1:A:48:ALA:HB1	2:B:413:HIS:CE1	0.46	2.46	13	1
1:A:129:LYS:HG3	1:A:132:LEU:HD11	0.46	1.87	15	1
2:B:431:GLU:OE2	2:B:434:ARG:HD3	0.46	2.11	11	2
1:A:67:LEU:HB2	2:B:430:TRP:HH2	0.46	1.70	24	2
1:A:24:GLY:HA2	3:A:500:GNP:O1B	0.46	2.10	31	1
1:A:129:LYS:HG3	3:A:500:GNP:C5	0.46	2.40	44	1
1:A:18:ILE:HD12	1:A:89:PHE:CE2	0.46	2.45	1	2
2:B:397:GLY:HA2	2:B:400:GLU:HG2	0.46	1.87	40	1
2:B:402:ILE:O	2:B:406:GLU:HG3	0.46	2.10	11	5
2:B:422:ASP:HB3	2:B:425:LYS:HE2	0.46	1.87	18	2
1:A:136:ARG:HH11	1:A:140:VAL:HB	0.46	1.71	17	1
2:B:416:LEU:HG	2:B:425:LYS:HD3	0.46	1.87	19	1
2:B:421:LYS:HA	2:B:425:LYS:HD2	0.46	1.87	1	1
1:A:129:LYS:HE2	3:A:500:GNP:C4	0.46	2.41	2	2
1:A:27:LYS:HE3	1:A:68:ASP:OD1	0.46	2.11	46	1
1:A:129:LYS:HG2	3:A:500:GNP:C2	0.46	2.41	35	1
2:B:401:GLU:HB3	2:B:439:LEU:HD21	0.46	1.88	49	1
2:B:416:LEU:HD22	2:B:421:LYS:HA	0.46	1.87	27	2
1:A:122:PRO:HG2	1:A:176:ILE:HG12	0.46	1.87	15	1
1:A:27:LYS:HG3	1:A:68:ASP:OD1	0.46	2.11	16	1
1:A:16:LYS:N	1:A:16:LYS:HE3	0.46	2.26	23	1
1:A:45:PRO:HA	1:A:49:ASP:HB2	0.46	1.88	42	1
1:A:20:VAL:HG21	1:A:91:LEU:HD12	0.45	1.88	35	1
1:A:139:PRO:HD2	1:A:142:GLU:OE2	0.45	2.11	48	1
1:A:132:LEU:HD12	1:A:133:GLU:N	0.45	2.26	19	2
1:A:108:ARG:HA	1:A:111:ILE:HD12	0.45	1.88	3	1
1:A:51:TYR:CE1	1:A:66:ILE:HB	0.45	2.46	25	1
1:A:70:ALA:O	1:A:79:ARG:HB2	0.45	2.12	9	1
1:A:158:SER:HB2	1:A:163:ALA:HB3	0.45	1.87	31	1
1:A:84:ARG:O	1:A:115:LYS:HD3	0.45	2.11	41	1
1:A:89:PHE:CE1	1:A:115:LYS:HE2	0.45	2.47	51	1
2:B:406:GLU:CG	2:B:436:LEU:HD21	0.45	2.41	23	3
2:B:398:ILE:HG21	2:B:443:LEU:HA	0.45	1.89	1	1
1:A:159:ALA:HB3	3:A:500:GNP:C6	0.45	2.42	7	2
1:A:92:VAL:HB	1:A:128:ASN:ND2	0.45	2.27	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:412:LEU:O	2:B:416:LEU:HB2	0.45	2.11	19	2
1:A:129:LYS:HD2	1:A:132:LEU:HG	0.45	1.87	29	1
2:B:416:LEU:HD11	2:B:425:LYS:CB	0.45	2.41	34	1
1:A:91:LEU:O	1:A:125:VAL:HA	0.45	2.10	36	1
1:A:13:ALA:HA	1:A:62:VAL:HG13	0.45	1.86	5	5
1:A:129:LYS:HG3	1:A:132:LEU:HD23	0.45	1.88	11	2
1:A:16:LYS:O	1:A:87:GLU:HG2	0.45	2.11	15	1
1:A:139:PRO:HB2	1:A:141:GLU:HG2	0.45	1.89	20	1
1:A:24:GLY:O	1:A:27:LYS:HG3	0.45	2.11	43	1
1:A:84:ARG:HD3	1:A:84:ARG:C	0.45	2.32	1	1
1:A:35:MET:SD	1:A:53:LYS:HB2	0.45	2.51	19	1
3:A:500:GNP:C2'	3:A:500:GNP:N3	0.45	2.80	19	1
1:A:31:THR:HG21	1:A:66:ILE:HG21	0.45	1.88	21	3
1:A:129:LYS:HE2	3:A:500:GNP:H1'	0.45	1.89	40	1
2:B:412:LEU:HB3	2:B:429:LEU:HD21	0.45	1.89	1	4
1:A:60:GLU:O	1:A:62:VAL:HG23	0.45	2.11	19	1
1:A:146:LYS:HD2	1:A:150:TRP:CZ2	0.45	2.47	31	1
2:B:412:LEU:O	2:B:416:LEU:HD13	0.45	2.12	34	3
2:B:431:GLU:O	2:B:434:ARG:HB3	0.45	2.12	2	1
1:A:21:GLY:O	1:A:22:SER:HB2	0.45	2.12	12	1
1:A:44:GLU:H	1:A:45:PRO:CD	0.45	2.17	20	1
1:A:33:GLN:O	1:A:37:ASP:HA	0.45	2.12	24	2
1:A:31:THR:HB	1:A:66:ILE:HG21	0.45	1.88	29	1
1:A:19:MET:HB3	1:A:27:LYS:HB2	0.45	1.88	51	2
2:B:433:GLN:HE21	2:B:437:THR:HB	0.45	1.71	42	1
2:B:430:TRP:O	2:B:433:GLN:HB3	0.44	2.13	32	6
1:A:36:TYR:HB3	1:A:38:GLU:HG2	0.44	1.88	15	1
1:A:132:LEU:O	1:A:134:GLU:N	0.44	2.50	16	4
1:A:33:GLN:HG2	1:A:39:PHE:HA	0.44	1.89	48	1
1:A:94:SER:HB2	1:A:129:LYS:HB3	0.44	1.89	7	1
2:B:409:LEU:HD13	2:B:432:VAL:HG13	0.44	1.89	16	5
2:B:423:LEU:O	2:B:427:GLU:HG3	0.44	2.12	17	1
2:B:403:ARG:HD2	2:B:406:GLU:OE2	0.44	2.12	32	2
1:A:125:VAL:HG13	1:A:154:TYR:HD1	0.44	1.71	21	1
1:A:35:MET:HG2	1:A:53:LYS:HD3	0.44	1.88	39	1
1:A:115:LYS:HB2	1:A:121:ILE:HD11	0.44	1.90	40	1
1:A:16:LYS:HG2	1:A:87:GLU:OE2	0.44	2.11	44	1
1:A:174:ARG:O	1:A:177:ARG:HB2	0.44	2.11	18	3
1:A:52:ARG:HA	1:A:65:ASP:HA	0.44	1.90	20	1
2:B:406:GLU:HG2	2:B:436:LEU:HD21	0.44	1.88	28	3
1:A:26:GLY:HA3	1:A:128:ASN:ND2	0.44	2.27	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ARG:HB3	1:A:65:ASP:OD1	0.44	2.11	14	1
1:A:52:ARG:NH1	2:B:434:ARG:HB3	0.44	2.27	1	1
2:B:396:ALA:O	2:B:400:GLU:HG3	0.44	2.12	9	2
1:A:157:THR:HA	1:A:163:ALA:O	0.44	2.12	10	1
1:A:53:LYS:HG3	1:A:55:VAL:HG13	0.44	1.89	12	2
1:A:35:MET:HB2	1:A:53:LYS:HD3	0.44	1.90	15	1
2:B:441:ARG:HD3	2:B:441:ARG:C	0.44	2.33	48	2
1:A:81:ASN:HB3	2:B:429:LEU:HD12	0.44	1.89	43	1
1:A:165:VAL:O	1:A:168:VAL:HG22	0.44	2.13	22	1
2:B:401:GLU:HB3	2:B:439:LEU:HD11	0.44	1.90	26	1
1:A:115:LYS:HB3	1:A:118:GLU:OE2	0.44	2.12	45	1
1:A:124:LEU:CD1	1:A:153:GLN:HG2	0.44	2.43	48	1
1:A:128:ASN:OD1	1:A:129:LYS:HG2	0.44	2.13	49	1
1:A:119:ASP:C	1:A:120:LYS:HD2	0.44	2.32	4	2
2:B:394:THR:HG23	2:B:446:ALA:HB1	0.44	1.90	7	1
1:A:24:GLY:O	1:A:25:VAL:HG22	0.44	2.13	28	2
1:A:91:LEU:HD11	1:A:123:LEU:HD23	0.44	1.90	46	1
1:A:12:LEU:HB3	1:A:177:ARG:NH1	0.43	2.28	18	1
1:A:132:LEU:HB2	1:A:135:ARG:HB2	0.43	1.89	24	1
1:A:28:SER:HA	1:A:31:THR:OG1	0.43	2.13	44	1
2:B:399:LYS:O	2:B:403:ARG:HG3	0.43	2.13	6	3
1:A:96:THR:CB	1:A:132:LEU:HD22	0.43	2.42	14	1
1:A:29:ALA:O	1:A:33:GLN:HG3	0.43	2.13	17	3
1:A:24:GLY:O	1:A:27:LYS:HB2	0.43	2.12	13	1
1:A:175:GLU:OE1	1:A:175:GLU:HA	0.43	2.12	13	1
2:B:422:ASP:HB3	2:B:425:LYS:HE3	0.43	1.90	29	2
1:A:129:LYS:HA	1:A:131:ASP:OD2	0.43	2.13	24	1
1:A:72:LEU:O	1:A:79:ARG:HD2	0.43	2.13	26	1
1:A:25:VAL:CG1	1:A:93:PHE:HA	0.43	2.42	35	1
1:A:84:ARG:NH2	2:B:423:LEU:HG	0.43	2.28	33	1
1:A:115:LYS:HD2	1:A:118:GLU:OE1	0.43	2.13	1	1
2:B:413:HIS:CD2	2:B:429:LEU:HD21	0.43	2.48	8	1
1:A:22:SER:CB	1:A:100:SER:HB3	0.43	2.42	21	1
1:A:20:VAL:HG21	1:A:91:LEU:HD23	0.43	1.90	43	1
1:A:170:PHE:O	1:A:173:MET:HG2	0.43	2.14	1	1
1:A:36:TYR:O	1:A:37:ASP:HB2	0.43	2.14	51	3
1:A:109:GLU:HB3	1:A:113:ARG:NH2	0.43	2.28	16	1
1:A:57:LEU:HB3	1:A:174:ARG:HH21	0.43	1.72	33	1
1:A:142:GLU:O	1:A:146:LYS:HG2	0.43	2.13	41	1
1:A:26:GLY:HA2	3:A:500:GNP:O3'	0.43	2.13	3	1
1:A:134:GLU:HG2	1:A:135:ARG:HG3	0.43	1.89	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:THR:HB	1:A:79:ARG:HA	0.43	1.88	14	1
1:A:129:LYS:HE3	1:A:132:LEU:HD21	0.43	1.90	15	1
1:A:91:LEU:HD21	1:A:123:LEU:HD23	0.43	1.91	38	1
1:A:17:VAL:HG12	1:A:172:LEU:HD23	0.43	1.90	49	1
2:B:416:LEU:HD21	2:B:425:LYS:CG	0.43	2.43	35	1
1:A:24:GLY:HA2	1:A:27:LYS:CD	0.43	2.43	51	1
2:B:444:ARG:NE	2:B:444:ARG:CA	0.43	2.80	15	1
1:A:145:SER:O	1:A:149:GLU:HG3	0.43	2.14	27	1
1:A:129:LYS:HB3	1:A:132:LEU:HD21	0.43	1.90	36	1
1:A:20:VAL:HG23	1:A:91:LEU:HD23	0.43	1.91	9	2
1:A:25:VAL:HB	1:A:92:VAL:HG13	0.43	1.88	14	1
1:A:79:ARG:HE	1:A:110:GLN:HG2	0.43	1.73	17	1
1:A:92:VAL:HB	1:A:128:ASN:OD1	0.43	2.14	31	1
1:A:27:LYS:HG3	1:A:28:SER:N	0.43	2.28	39	1
1:A:108:ARG:O	1:A:112:LEU:HD23	0.43	2.14	40	1
1:A:96:THR:HA	1:A:137:GLN:HB2	0.43	1.90	47	1
2:B:436:LEU:O	2:B:440:LYS:HD3	0.42	2.14	9	1
1:A:69:THR:HG22	1:A:79:ARG:HA	0.42	1.91	37	1
1:A:20:VAL:HA	1:A:69:THR:OG1	0.42	2.13	22	1
1:A:81:ASN:ND2	2:B:420:ILE:HD11	0.42	2.29	32	1
1:A:69:THR:CG2	1:A:79:ARG:HA	0.42	2.44	49	1
1:A:14:LEU:O	1:A:180:LYS:HE3	0.42	2.14	11	1
1:A:72:LEU:HG	1:A:74:ASP:H	0.42	1.74	12	1
2:B:405:GLN:HB2	2:B:436:LEU:HD23	0.42	1.89	12	1
2:B:436:LEU:O	2:B:440:LYS:HG3	0.42	2.15	24	1
2:B:442:LYS:HE3	2:B:445:GLU:OE2	0.42	2.13	32	1
1:A:33:GLN:NE2	1:A:39:PHE:HA	0.42	2.29	42	2
1:A:129:LYS:C	1:A:131:ASP:H	0.42	2.18	5	1
1:A:129:LYS:HG3	1:A:132:LEU:CD1	0.42	2.45	15	1
2:B:431:GLU:HG2	2:B:434:ARG:NH1	0.42	2.30	15	1
1:A:16:LYS:HE2	1:A:16:LYS:N	0.42	2.30	37	1
2:B:430:TRP:O	2:B:433:GLN:HG3	0.42	2.14	39	1
2:B:421:LYS:HD2	2:B:421:LYS:C	0.42	2.35	40	2
1:A:129:LYS:HE2	3:A:500:GNP:C2	0.42	2.45	14	1
1:A:106:GLU:O	1:A:110:GLN:HB2	0.42	2.15	19	1
1:A:129:LYS:HD2	3:A:500:GNP:C2	0.42	2.43	22	1
2:B:422:ASP:H	2:B:425:LYS:CG	0.42	2.28	43	3
1:A:35:MET:SD	1:A:51:TYR:HB2	0.42	2.55	23	1
1:A:109:GLU:O	1:A:113:ARG:HB2	0.42	2.15	24	1
2:B:399:LYS:HA	2:B:402:ILE:HD12	0.42	1.92	26	2
1:A:83:PHE:O	1:A:115:LYS:HD2	0.42	2.14	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:VAL:HA	1:A:143:ALA:HB3	0.42	1.92	35	1
1:A:91:LEU:HD11	1:A:107:PHE:CD2	0.42	2.49	48	1
1:A:111:ILE:HG22	1:A:121:ILE:HD13	0.42	1.92	19	3
1:A:25:VAL:O	1:A:25:VAL:HG12	0.42	2.14	43	1
1:A:55:VAL:O	1:A:62:VAL:HB	0.42	2.15	3	1
1:A:42:ASP:OD2	3:A:500:GNP:N3B	0.42	2.51	19	1
1:A:53:LYS:HB3	1:A:64:ILE:HG23	0.42	1.91	28	1
1:A:129:LYS:HA	3:A:500:GNP:C6	0.42	2.44	42	1
1:A:30:LEU:HD21	1:A:128:ASN:ND2	0.42	2.30	47	1
1:A:75:TYR:HA	2:B:417:GLN:NE2	0.42	2.30	39	1
1:A:94:SER:HB3	1:A:97:GLU:CG	0.42	2.39	44	1
1:A:172:LEU:HD11	1:A:176:ILE:HD11	0.42	1.91	45	1
1:A:44:GLU:OE2	3:A:500:GNP:O2G	0.41	2.38	14	1
2:B:434:ARG:HG2	2:B:435:ILE:N	0.41	2.30	15	1
1:A:30:LEU:HD11	1:A:128:ASN:ND2	0.41	2.24	23	1
1:A:96:THR:HA	1:A:137:GLN:CB	0.41	2.44	29	1
1:A:129:LYS:HD2	3:A:500:GNP:N2	0.41	2.30	39	1
1:A:16:LYS:HB2	1:A:87:GLU:OE1	0.41	2.14	49	1
1:A:173:MET:HA	1:A:176:ILE:HD12	0.41	1.92	3	1
1:A:146:LYS:HA	1:A:146:LYS:HE2	0.41	1.92	14	1
1:A:110:GLN:O	1:A:113:ARG:HB3	0.41	2.14	17	1
1:A:95:ILE:O	1:A:138:VAL:HG12	0.41	2.15	32	1
1:A:95:ILE:CG1	1:A:132:LEU:HD11	0.41	2.46	37	1
1:A:67:LEU:HD22	2:B:430:TRP:CZ2	0.41	2.50	41	1
1:A:26:GLY:HA2	3:A:500:GNP:O2'	0.41	2.15	2	1
1:A:167:LYS:O	1:A:171:ASP:HB2	0.41	2.15	10	2
1:A:51:TYR:HA	2:B:437:THR:HG1	0.41	1.76	12	1
1:A:147:ALA:HB1	1:A:152:VAL:HG23	0.41	1.93	13	2
1:A:17:VAL:HB	1:A:66:ILE:CD1	0.41	2.46	7	1
1:A:101:PHE:CE1	1:A:143:ALA:HA	0.41	2.49	9	1
1:A:120:LYS:HB2	1:A:179:LYS:HG2	0.41	1.92	14	1
2:B:423:LEU:O	2:B:426:GLU:HG2	0.41	2.16	20	1
1:A:101:PHE:HZ	1:A:146:LYS:HG3	0.41	1.75	37	1
1:A:111:ILE:HA	1:A:114:VAL:HG22	0.41	1.91	40	1
1:A:110:GLN:NE2	1:A:110:GLN:HA	0.41	2.29	46	1
1:A:52:ARG:HD2	1:A:63:GLN:OE1	0.41	2.15	47	1
1:A:115:LYS:CG	1:A:118:GLU:HG3	0.41	2.45	2	1
2:B:414:ARG:O	2:B:417:GLN:HB2	0.41	2.15	7	1
2:B:436:LEU:HD11	2:B:440:LYS:HE2	0.41	1.91	16	1
1:A:92:VAL:HB	1:A:128:ASN:HD22	0.41	1.75	17	1
1:A:26:GLY:HA3	3:A:500:GNP:H8	0.41	1.92	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:SER:O	1:A:32:LEU:HD23	0.41	2.15	33	2
2:B:432:VAL:HA	2:B:435:ILE:CD1	0.41	2.44	34	1
1:A:50:SER:HB3	1:A:66:ILE:O	0.41	2.14	50	1
1:A:33:GLN:HA	1:A:38:GLU:O	0.41	2.16	6	1
2:B:429:LEU:O	2:B:433:GLN:HB2	0.41	2.16	20	1
1:A:35:MET:HG2	1:A:53:LYS:HB2	0.41	1.92	25	1
1:A:25:VAL:HG13	1:A:94:SER:HB2	0.41	1.92	26	1
1:A:170:PHE:HA	1:A:173:MET:HG2	0.41	1.93	31	1
2:B:416:LEU:HD21	2:B:425:LYS:HB3	0.41	1.92	32	1
1:A:129:LYS:HB3	1:A:132:LEU:CD2	0.41	2.45	13	1
1:A:47:LYS:O	1:A:78:ILE:HG21	0.41	2.15	16	1
1:A:162:ARG:HD2	1:A:162:ARG:O	0.41	2.16	16	1
2:B:403:ARG:HD3	2:B:406:GLU:OE2	0.41	2.15	26	1
1:A:57:LEU:HD12	1:A:177:ARG:HH21	0.41	1.75	28	1
2:B:423:LEU:HA	2:B:426:GLU:OE2	0.41	2.16	32	1
1:A:80:ASP:O	1:A:84:ARG:HG2	0.41	2.15	42	1
1:A:27:LYS:HE2	1:A:68:ASP:OD1	0.41	2.16	43	1
1:A:89:PHE:CZ	1:A:115:LYS:HE2	0.41	2.51	51	1
1:A:84:ARG:HD2	1:A:84:ARG:O	0.41	2.15	3	1
2:B:403:ARG:HD2	2:B:406:GLU:OE1	0.41	2.15	12	2
1:A:33:GLN:NE2	1:A:162:ARG:HG2	0.41	2.30	6	1
1:A:67:LEU:HG	1:A:68:ASP:O	0.41	2.15	8	1
2:B:401:GLU:HG2	2:B:439:LEU:HD21	0.41	1.93	15	1
1:A:30:LEU:HD21	1:A:128:ASN:HD21	0.41	1.75	16	2
1:A:77:ALA:O	1:A:81:ASN:HB2	0.41	2.16	28	1
1:A:95:ILE:H	1:A:95:ILE:HD13	0.41	1.75	31	1
2:B:395:GLN:O	2:B:398:ILE:HB	0.41	2.16	44	1
2:B:400:GLU:HG2	2:B:403:ARG:HH21	0.41	1.76	51	1
1:A:87:GLU:OE2	1:A:176:ILE:HG23	0.41	2.16	3	1
1:A:95:ILE:HD11	1:A:130:SER:HA	0.41	1.92	14	1
2:B:420:ILE:N	2:B:420:ILE:CD1	0.41	2.84	32	1
1:A:120:LYS:N	1:A:120:LYS:HD2	0.41	2.30	34	1
1:A:34:PHE:CE2	1:A:53:LYS:HG2	0.41	2.50	44	1
2:B:401:GLU:HB2	2:B:439:LEU:HD11	0.41	1.93	48	1
1:A:140:VAL:HG12	1:A:144:ARG:HD2	0.41	1.91	23	1
1:A:28:SER:HB3	3:A:500:GNP:O1A	0.40	2.15	7	1
1:A:167:LYS:HG2	1:A:171:ASP:OD2	0.40	2.15	39	1
1:A:44:GLU:CD	3:A:500:GNP:HNB3	0.40	2.20	41	1
1:A:27:LYS:CB	1:A:92:VAL:HG21	0.40	2.44	7	1
1:A:12:LEU:CD2	1:A:180:LYS:HB2	0.40	2.46	10	1
1:A:32:LEU:HG	1:A:36:TYR:CD1	0.40	2.52	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:THR:HG21	1:A:132:LEU:HD12	0.40	1.92	12	1
1:A:79:ARG:HH21	1:A:110:GLN:HG2	0.40	1.76	17	1
1:A:16:LYS:N	1:A:16:LYS:HD2	0.40	2.31	27	1
1:A:120:LYS:HB3	1:A:179:LYS:HE3	0.40	1.93	30	1
1:A:141:GLU:OE1	1:A:144:ARG:HD3	0.40	2.16	39	1
1:A:120:LYS:HD2	1:A:120:LYS:N	0.40	2.31	2	1
1:A:84:ARG:HG3	2:B:426:GLU:OE2	0.40	2.17	10	1
1:A:35:MET:HG2	1:A:51:TYR:CD1	0.40	2.52	11	1
1:A:14:LEU:HA	1:A:63:GLN:O	0.40	2.16	23	1
1:A:128:ASN:HD22	1:A:128:ASN:C	0.40	2.20	25	1
2:B:424:SER:O	2:B:428:ARG:HB2	0.40	2.16	27	1
2:B:423:LEU:HA	2:B:426:GLU:OE1	0.40	2.16	41	1
2:B:401:GLU:OE1	2:B:404:ARG:HD2	0.40	2.16	42	1
1:A:131:ASP:HB3	3:A:500:GNP:O6	0.40	2.17	44	1
1:A:45:PRO:O	1:A:46:THR:HB	0.40	2.16	50	1
2:B:441:ARG:NH1	2:B:445:GLU:HG3	0.40	2.23	29	1
1:A:47:LYS:HE3	1:A:72:LEU:HD21	0.40	1.91	38	1
1:A:120:LYS:HG3	1:A:179:LYS:HD2	0.40	1.93	44	1
2:B:396:ALA:HA	2:B:399:LYS:HG2	0.40	1.93	44	1
1:A:88:GLY:HA3	1:A:172:LEU:HD21	0.40	1.93	3	1
2:B:405:GLN:HB2	2:B:436:LEU:HD13	0.40	1.92	8	1
2:B:434:ARG:HA	2:B:437:THR:CG2	0.40	2.47	35	1
1:A:41:GLU:HG3	1:A:42:ASP:N	0.40	2.32	40	1
1:A:72:LEU:HD13	1:A:75:TYR:H	0.40	1.76	49	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	170/178 (96%)	146±3 (86±2%)	21±3 (12±2%)	3±2 (2±1%)	11	53
2	B	52/56 (93%)	52±0 (100±1%)	0±0 (0±1%)	0±0 (0±0%)	100	100
All	All	11322/11934 (95%)	10097 (89%)	1061 (9%)	164 (1%)	15	61

All 29 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	45	PRO	26
1	A	133	GLU	18
1	A	119	ASP	15
1	A	59	GLY	14
1	A	44	GLU	13
1	A	37	ASP	10
1	A	25	VAL	9
1	A	24	GLY	8
1	A	58	ASP	7
1	A	26	GLY	6
1	A	116	ALA	5
1	A	74	ASP	5
1	A	23	GLY	3
1	A	40	VAL	3
1	A	46	THR	3
1	A	73	GLU	2
1	A	84	ARG	2
1	A	132	LEU	2
1	A	22	SER	2
1	A	95	ILE	2
1	A	164	ASN	1
1	A	43	TYR	1
1	A	42	ASP	1
1	A	28	SER	1
1	A	21	GLY	1
1	A	27	LYS	1
1	A	87	GLU	1
1	A	76	ALA	1
1	A	139	PRO	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	147/154 (95%)	139±3 (95±2%)	8±3 (5±2%)	26 75
2	B	47/49 (96%)	45±1 (95±3%)	2±1 (5±3%)	31 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9894/10353 (96%)	9383 (95%)	511 (5%)	27 76

All 94 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	95	ILE	50
1	A	72	LEU	40
2	B	434	ARG	24
1	A	16	LYS	22
1	A	140	VAL	21
1	A	46	THR	21
1	A	82	TYR	18
2	B	439	LEU	18
1	A	132	LEU	17
1	A	153	GLN	15
1	A	118	GLU	13
1	A	171	ASP	13
2	B	425	LYS	13
1	A	110	GLN	12
1	A	62	VAL	11
2	B	421	LYS	11
1	A	57	LEU	10
1	A	31	THR	9
1	A	84	ARG	9
2	B	441	ARG	9
1	A	51	TYR	9
2	B	429	LEU	7
1	A	96	THR	5
1	A	119	ASP	5
1	A	27	LYS	4
1	A	73	GLU	4
1	A	12	LEU	4
1	A	174	ARG	4
1	A	87	GLU	4
1	A	131	ASP	4
1	A	44	GLU	3
1	A	179	LYS	3
1	A	32	LEU	3
1	A	85	SER	3
1	A	102	THR	3
2	B	423	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	80	ASP	3
2	B	426	GLU	3
1	A	161	THR	3
1	A	43	TYR	3
2	B	428	ARG	3
1	A	53	LYS	2
2	B	413	HIS	2
1	A	108	ARG	2
2	B	444	ARG	2
2	B	415	ASP	2
2	B	417	GLN	2
1	A	79	ARG	2
1	A	66	ILE	2
1	A	67	LEU	2
1	A	47	LYS	2
2	B	403	ARG	2
1	A	74	ASP	2
2	B	409	LEU	2
2	B	412	LEU	2
1	A	120	LYS	2
1	A	128	ASN	2
1	A	37	ASP	2
1	A	129	LYS	2
2	B	433	GLN	2
1	A	19	MET	1
1	A	124	LEU	1
1	A	91	LEU	1
1	A	123	LEU	1
1	A	94	SER	1
1	A	38	GLU	1
1	A	155	VAL	1
1	A	28	SER	1
1	A	45	PRO	1
1	A	41	GLU	1
2	B	411	SER	1
1	A	113	ARG	1
1	A	115	LYS	1
1	A	49	ASP	1
1	A	100	SER	1
1	A	106	GLU	1
1	A	58	ASP	1
1	A	81	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	168	VAL	1
1	A	134	GLU	1
1	A	33	GLN	1
1	A	35	MET	1
1	A	160	LYS	1
1	A	142	GLU	1
1	A	14	LEU	1
1	A	166	ASP	1
1	A	97	GLU	1
2	B	443	LEU	1
1	A	122	PRO	1
2	B	401	GLU	1
1	A	162	ARG	1
1	A	99	GLU	1
1	A	146	LYS	1
1	A	164	ASN	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 monosaccharides in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	GNP	A	500	-	28,34,34	2.28±0.03	7±1 (23±2%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	GNP	A	500	-	30,54,54	2.08±0.03	6±0 (21±1%)

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	GNP	A	500	-	-	0±0,17,38,38	0±0,3,3,3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	500	GNP	C4-N9	7.60	1.37	1.47	49	51
3	A	500	GNP	C5-C6	6.28	1.42	1.52	38	51
3	A	500	GNP	C6-N1	4.14	1.40	1.33	37	51
3	A	500	GNP	PB-O2B	3.02	1.48	1.56	21	51
3	A	500	GNP	PB-N3B	2.71	1.70	1.63	5	16
3	A	500	GNP	C5-C4	2.42	1.38	1.53	18	51
3	A	500	GNP	C8-N9	2.37	1.37	1.45	31	51
3	A	500	GNP	PG-N3B	2.15	1.69	1.63	44	7
3	A	500	GNP	PB-O1B	2.06	1.49	1.46	51	4
3	A	500	GNP	PG-O1G	2.05	1.49	1.46	43	6

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	500	GNP	C4-C5-N7	6.49	111.06	102.46	5	51
3	A	500	GNP	C5-C6-N1	5.23	111.74	118.19	12	51
3	A	500	GNP	O2B-PB-O1B	4.51	119.37	109.92	1	51
3	A	500	GNP	O6-C6-C5	4.31	128.65	119.86	12	51
3	A	500	GNP	PA-O3A-PB	3.70	119.60	132.62	20	51
3	A	500	GNP	O1B-PB-N3B	3.29	106.93	111.77	8	19
3	A	500	GNP	O6-C6-N1	2.54	119.28	122.69	47	51
3	A	500	GNP	O3A-PB-N3B	2.27	100.28	106.59	29	2

There are no chirality outliers.

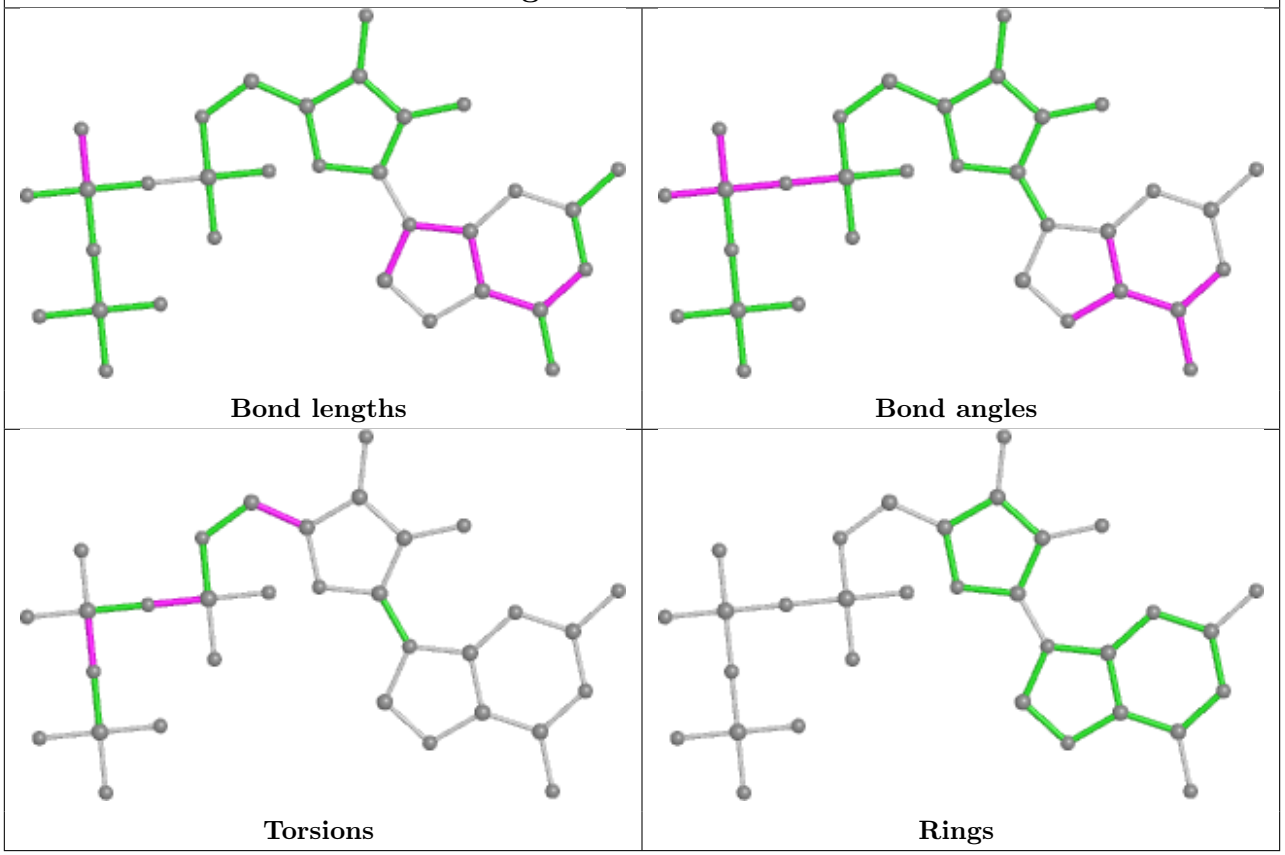
All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
3	A	500	GNP	PG-N3B-PB-O1B	1

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GNP A 500



6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided