Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 03:31 PM BST

PDB ID	:	1K2N
Title	:	Solution Structure of the FHA2 domain of Rad53 Complexed with a Phosphothreonyl Peptide Derived from Rad9
Authors	:	Byeon, I.-J.L.; Yongkiettrakul, S.; Tsai, M.-D.
Deposited on	:	2001-09-28

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 (i) symbol.

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

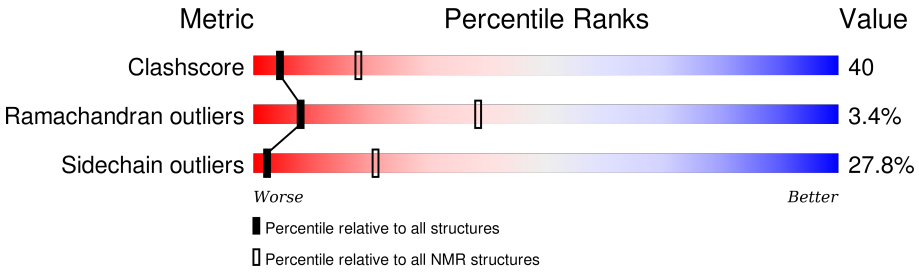
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 (i)

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	158	23% 47% 8% • 21%
2	P	9	100%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:576-A:630, A:644-A:699, A:716-A:729 (125)	0.20	13

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 8, 9, 10, 11, 12, 13, 14, 15, 18, 20
2	16, 17
Single-model clusters	4; 7; 19

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2701 atoms, of which 1349 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein Kinase SPK1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	158	2551	806	1277	222	239	7	0

- Molecule 2 is a protein called DNA repair protein Rad9.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	P	9	150	46	72	10	21	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	603	TPO	THR	MODIFIED RESIDUE	UNP P14737

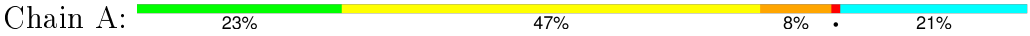
4 Residue-property plots

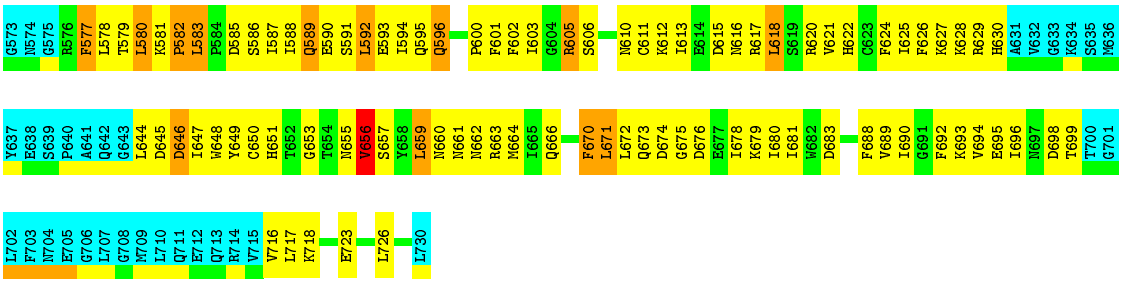
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Protein Kinase SPK1

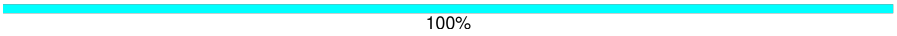
Chain A:

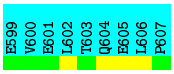




• Molecule 2: DNA repair protein Rad9

Chain P:





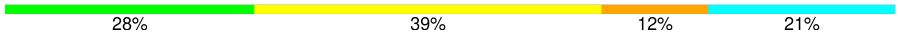
4.2 Scores per residue for each member of the ensemble

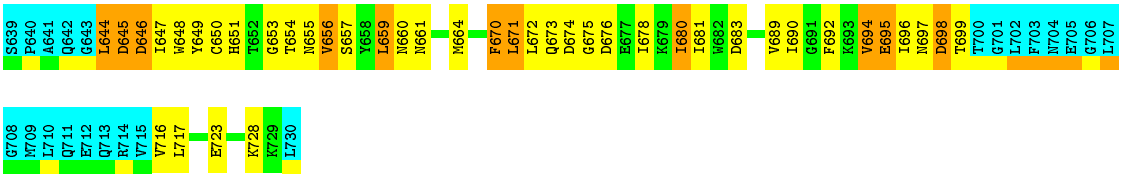
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Protein Kinase SPK1

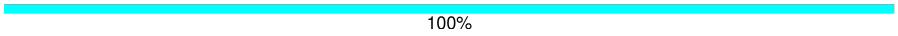
Chain A:

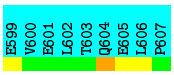




• Molecule 2: DNA repair protein Rad9

Chain P:

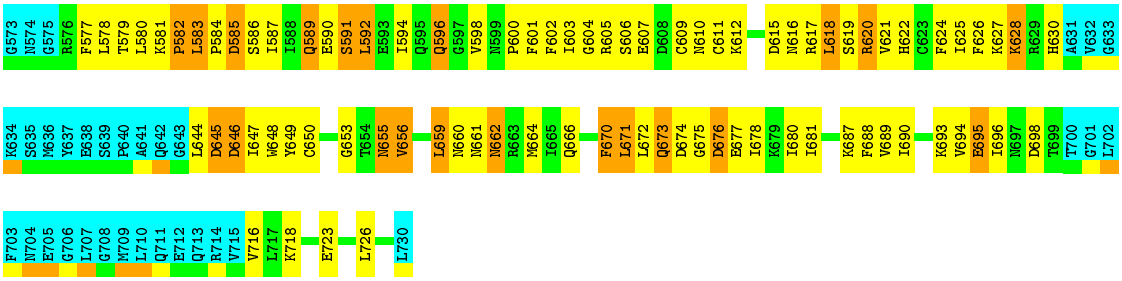




4.2.2 Score per residue for model 2

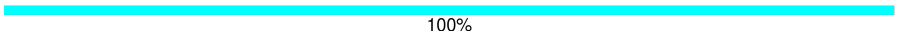
• Molecule 1: Protein Kinase SPK1

Chain A:



• Molecule 2: DNA repair protein Rad9

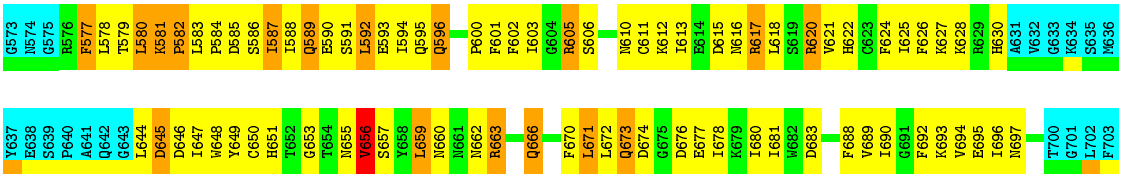
Chain P:

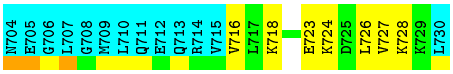


4.2.3 Score per residue for model 3

• Molecule 1: Protein Kinase SPK1

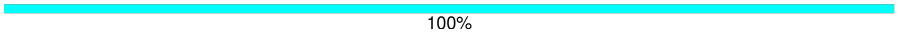
Chain A:

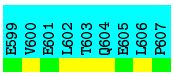




• Molecule 2: DNA repair protein Rad9

Chain P:

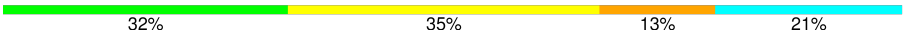


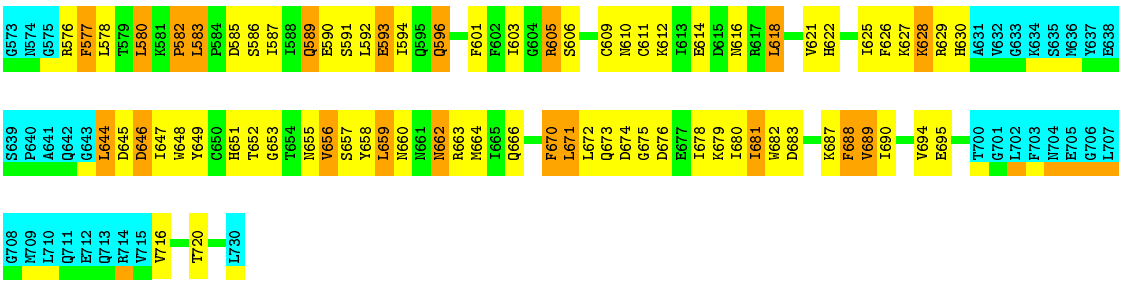


4.2.4 Score per residue for model 4

• Molecule 1: Protein Kinase SPK1

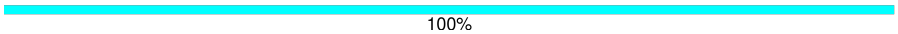
Chain A:

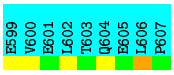




• Molecule 2: DNA repair protein Rad9

Chain P:

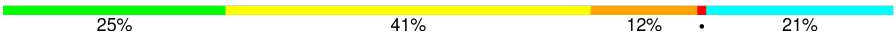


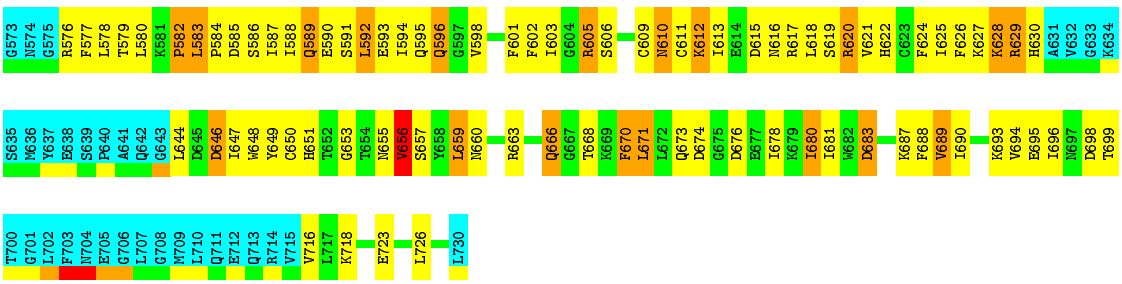


4.2.5 Score per residue for model 5

• Molecule 1: Protein Kinase SPK1

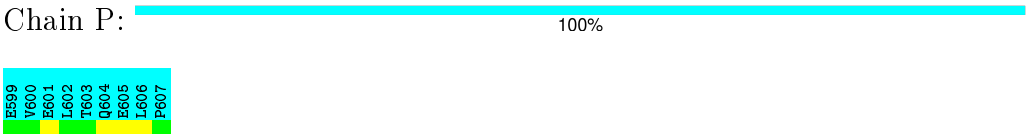
Chain A:





• Molecule 2: DNA repair protein Rad9

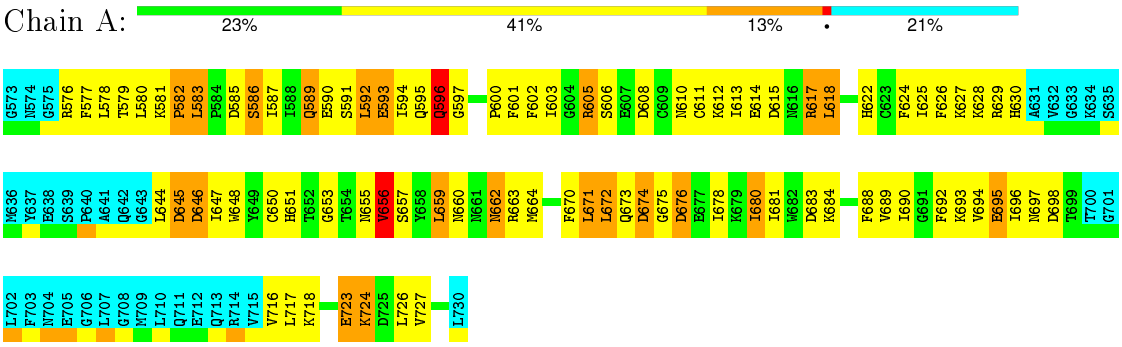
Chain P:



4.2.6 Score per residue for model 6

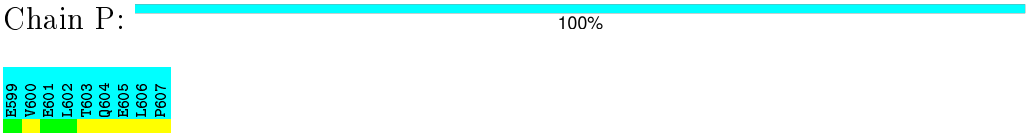
- Molecule 1: Protein Kinase SPK1

Chain A:



- Molecule 2: DNA repair protein Rad9

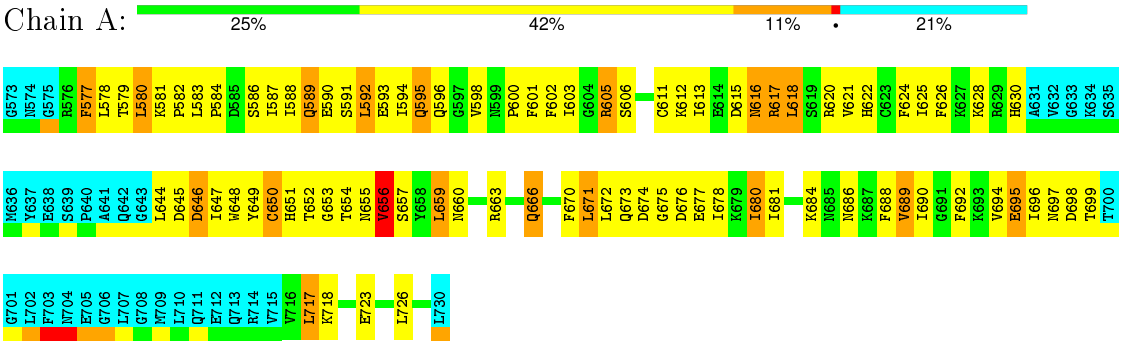
Chain P:



4.2.7 Score per residue for model 7

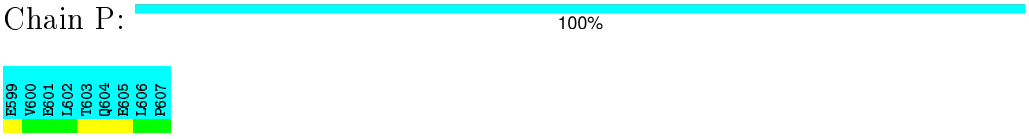
- Molecule 1: Protein Kinase SPK1

Chain A:



- Molecule 2: DNA repair protein Rad9

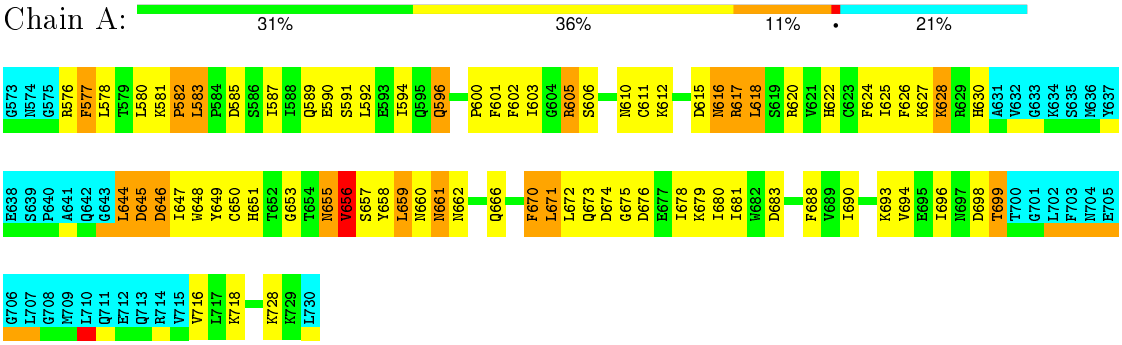
Chain P:



4.2.8 Score per residue for model 8

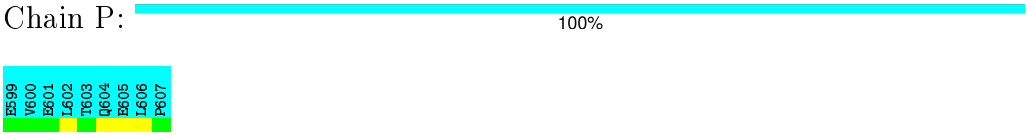
- Molecule 1: Protein Kinase SPK1

Chain A:



- Molecule 2: DNA repair protein Rad9

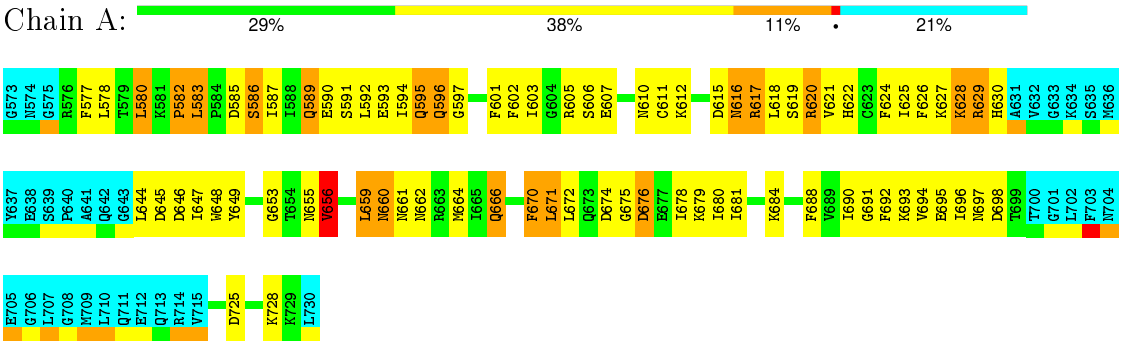
Chain P:



4.2.9 Score per residue for model 9

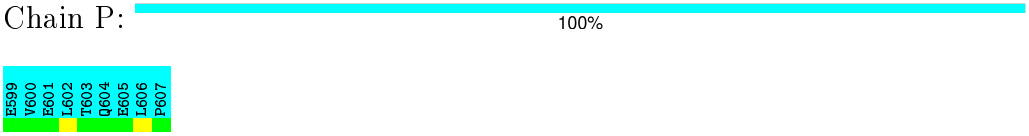
- Molecule 1: Protein Kinase SPK1

Chain A:



- Molecule 2: DNA repair protein Rad9

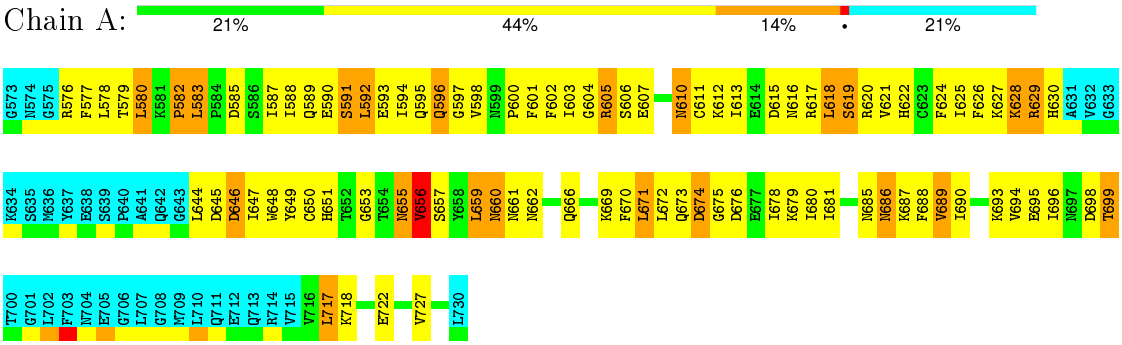
Chain P:



4.2.10 Score per residue for model 10

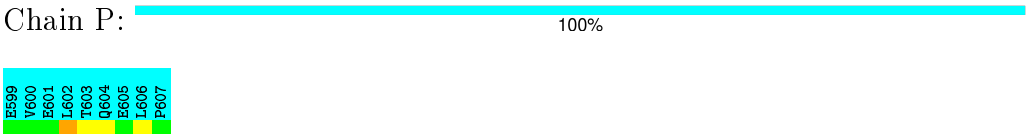
- Molecule 1: Protein Kinase SPK1

Chain A:



- Molecule 2: DNA repair protein Rad9

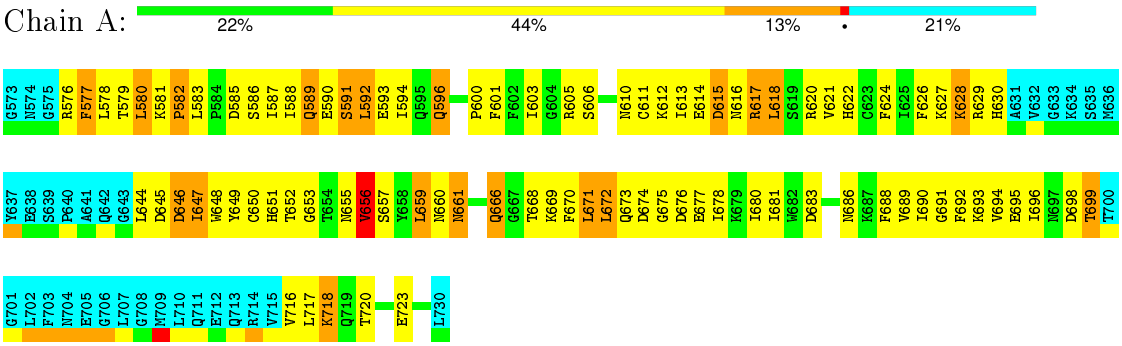
Chain P:



4.2.11 Score per residue for model 11

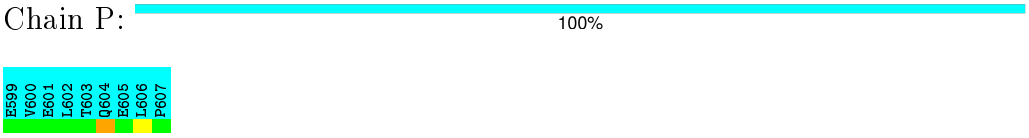
- Molecule 1: Protein Kinase SPK1

Chain A:



- Molecule 2: DNA repair protein Rad9

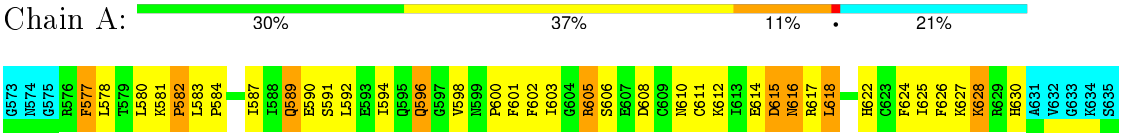
Chain P:

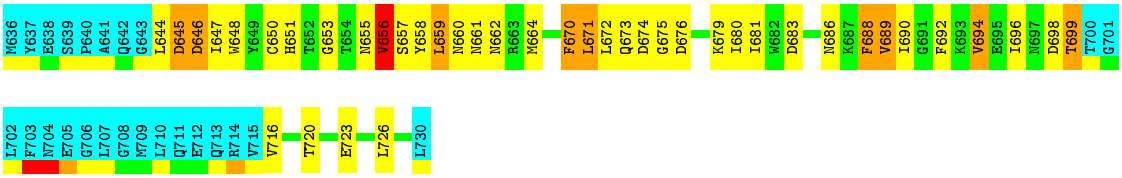


4.2.12 Score per residue for model 12

- Molecule 1: Protein Kinase SPK1

Chain A:





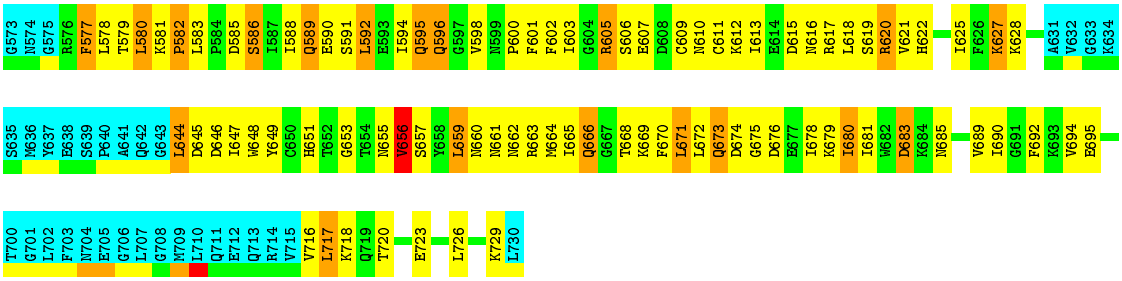
• Molecule 2: DNA repair protein Rad9

Chain P: 100%

4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Protein Kinase SPK1

Chain A: 24% 42% 12% 21%



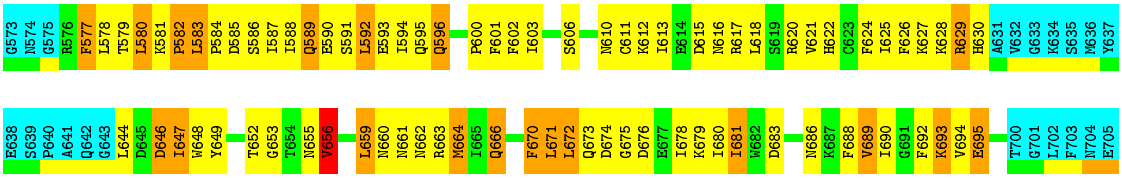
• Molecule 2: DNA repair protein Rad9

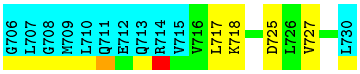
Chain P: 100%

4.2.14 Score per residue for model 14

• Molecule 1: Protein Kinase SPK1

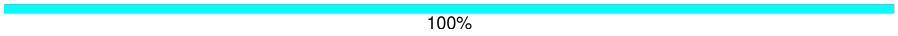
Chain A: 27% 39% 13% 21%

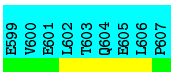




• Molecule 2: DNA repair protein Rad9

Chain P:

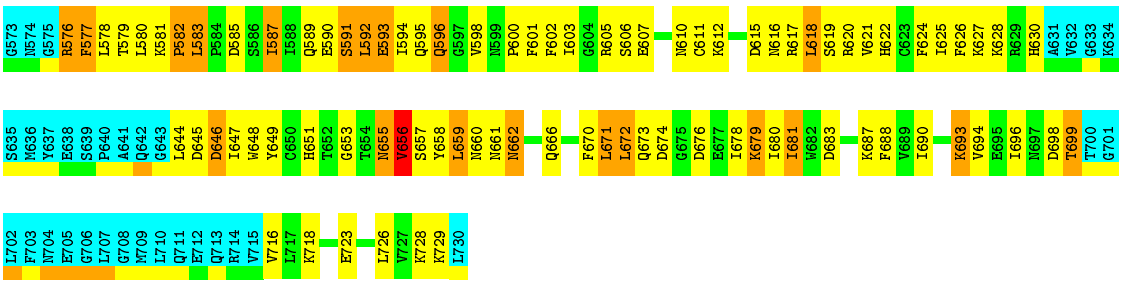




4.2.15 Score per residue for model 15

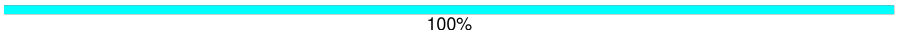
• Molecule 1: Protein Kinase SPK1

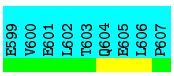
Chain A:



• Molecule 2: DNA repair protein Rad9

Chain P:

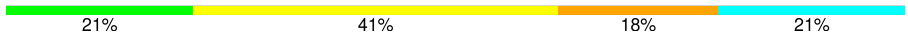


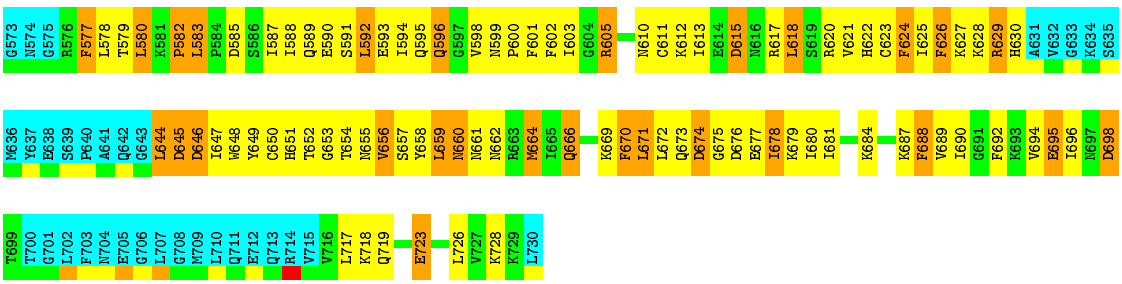


4.2.16 Score per residue for model 16

• Molecule 1: Protein Kinase SPK1

Chain A:





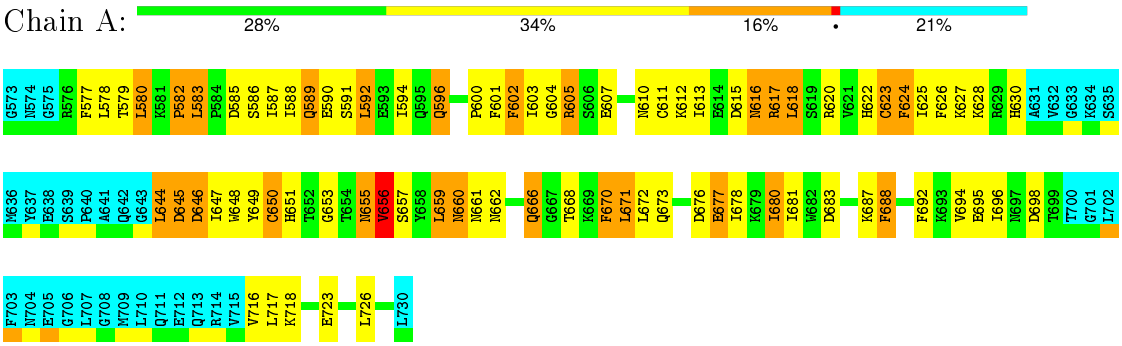
• Molecule 2: DNA repair protein Rad9

Chain P:

4.2.17 Score per residue for model 17

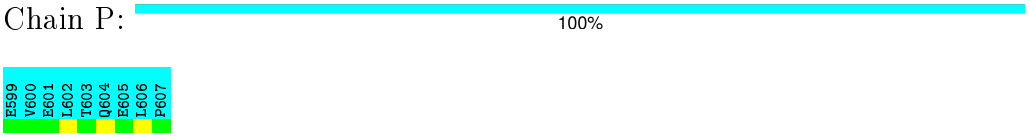
- Molecule 1: Protein Kinase SPK1

Chain A:



- Molecule 2: DNA repair protein Rad9

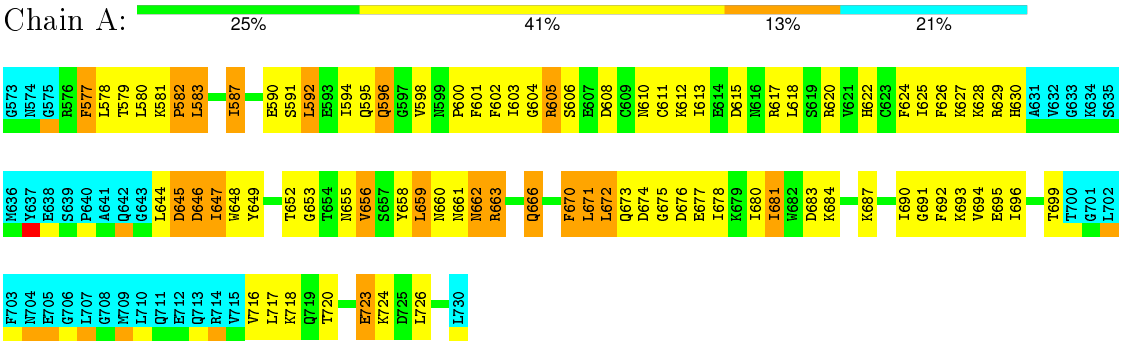
Chain P:



4.2.18 Score per residue for model 18

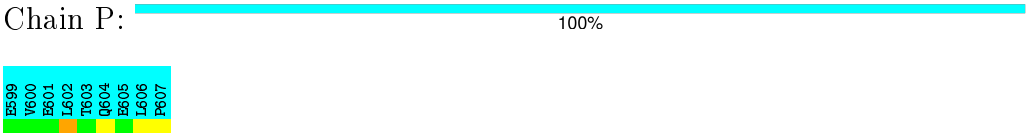
- Molecule 1: Protein Kinase SPK1

Chain A:



- Molecule 2: DNA repair protein Rad9

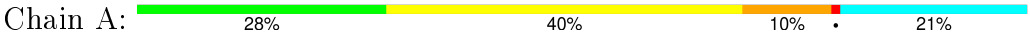
Chain P:

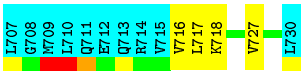


4.2.19 Score per residue for model 19

- Molecule 1: Protein Kinase SPK1

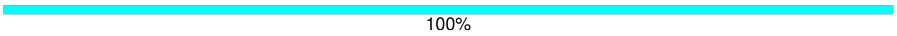
Chain A:

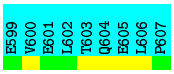




- Molecule 2: DNA repair protein Rad9

Chain P:

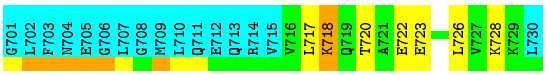




4.2.20 Score per residue for model 20

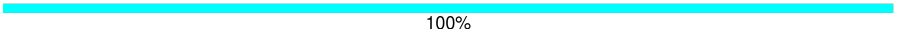
- Molecule 1: Protein Kinase SPK1

Chain A:



- Molecule 2: DNA repair protein Rad9

Chain P:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *The complex structures are generated using a total of 3369 restraints, 3181 distance restraints, and 188 TALOS-derived dihedral angle restraints.*.

Of the 100 calculated structures, 20 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
X-PLOR	structure solution	3.851
X-PLOR	refinement	3.851

No chemical shift data was provided. 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: TPO

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	1034	1044	1041	83±8
2	P	0	0	0	0±0
All	All	20680	20880	20820	1652

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:578:LEU:HD11	1:A:694:VAL:HG13	1.04	1.26	12	10
1:A:578:LEU:HD21	1:A:694:VAL:HG13	1.03	1.29	16	2
1:A:580:LEU:HD22	1:A:694:VAL:HG22	0.95	1.34	7	2
1:A:578:LEU:HD12	1:A:647:ILE:HD13	0.95	1.35	14	10
1:A:594:ILE:HD11	1:A:625:ILE:HD12	0.93	1.41	6	10
1:A:577:PHE:CZ	1:A:647:ILE:HG21	0.87	2.05	19	9
1:A:592:LEU:HD21	1:A:613:ILE:HD11	0.86	1.46	7	10
1:A:578:LEU:CD1	1:A:694:VAL:HG13	0.86	1.99	17	9
1:A:648:TRP:CH2	1:A:671:LEU:HD22	0.86	2.05	2	15
1:A:659:LEU:HD13	1:A:678:ILE:HG22	0.84	1.49	15	4
1:A:672:LEU:HD13	1:A:694:VAL:HG21	0.84	1.47	10	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:580:LEU:CD2	1:A:694:VAL:HG23	0.84	2.03	1	4
1:A:681:ILE:HG22	1:A:690:ILE:HG22	0.83	1.48	19	1
1:A:578:LEU:HD23	1:A:594:ILE:HD12	0.83	1.51	7	3
1:A:659:LEU:HD22	1:A:678:ILE:HG22	0.81	1.52	11	1
1:A:648:TRP:CZ3	1:A:671:LEU:HD22	0.80	2.12	19	14
1:A:662:ASN:OD1	1:A:716:VAL:HG23	0.77	1.78	15	3
1:A:621:VAL:HG11	1:A:727:VAL:HG23	0.77	1.55	14	3
1:A:580:LEU:HD11	1:A:594:ILE:HD11	0.77	1.55	10	1
1:A:681:ILE:HG22	1:A:690:ILE:HB	0.77	1.56	12	12
1:A:598:VAL:HG11	1:A:610:ASN:OD1	0.76	1.80	12	6
1:A:578:LEU:HD13	1:A:647:ILE:HD13	0.76	1.55	9	6
1:A:580:LEU:HD12	1:A:594:ILE:HD11	0.76	1.57	15	5
1:A:580:LEU:CD2	1:A:694:VAL:HG22	0.76	2.09	10	2
1:A:580:LEU:HD21	1:A:694:VAL:HG23	0.76	1.58	12	4
1:A:622:HIS:CD2	1:A:680:ILE:HG23	0.76	2.15	18	13
1:A:578:LEU:HD22	1:A:594:ILE:HD12	0.75	1.55	18	7
1:A:580:LEU:HD22	1:A:694:VAL:CG2	0.74	2.12	7	2
1:A:578:LEU:HD12	1:A:647:ILE:CD1	0.73	2.12	18	9
1:A:620:ARG:HG2	1:A:621:VAL:HG23	0.73	1.59	5	5
1:A:578:LEU:HD23	1:A:579:THR:N	0.73	1.98	14	8
1:A:592:LEU:HD13	1:A:611:CYS:SG	0.72	2.25	7	13
1:A:659:LEU:HD22	1:A:678:ILE:CG2	0.72	2.13	11	1
1:A:579:THR:HG23	1:A:593:GLU:HG3	0.72	1.58	7	1
1:A:587:ILE:HD13	1:A:688:PHE:CE1	0.72	2.20	15	5
1:A:603:ILE:HG23	1:A:611:CYS:SG	0.72	2.25	9	20
1:A:578:LEU:HD11	1:A:694:VAL:CG1	0.71	2.14	8	13
1:A:647:ILE:HD12	1:A:672:LEU:CB	0.71	2.15	11	10
1:A:577:PHE:CE1	1:A:647:ILE:HG21	0.71	2.20	16	10
1:A:587:ILE:HD11	1:A:690:ILE:HD11	0.70	1.62	7	5
1:A:580:LEU:CD1	1:A:594:ILE:HD11	0.70	2.16	15	8
1:A:680:ILE:HD12	1:A:692:PHE:CE2	0.70	2.22	3	5
1:A:646:ASP:OD2	1:A:671:LEU:HD11	0.70	1.86	9	3
1:A:578:LEU:HD22	1:A:647:ILE:CD1	0.70	2.16	17	7
1:A:681:ILE:HG22	1:A:690:ILE:CG2	0.70	2.16	19	1
1:A:578:LEU:HD22	1:A:647:ILE:HD13	0.69	1.64	7	8
1:A:579:THR:HG23	1:A:593:GLU:CG	0.69	2.18	7	1
1:A:594:ILE:HD11	1:A:625:ILE:CD1	0.69	2.15	6	8
1:A:578:LEU:HD21	1:A:694:VAL:CG1	0.68	2.16	16	1
1:A:577:PHE:CB	1:A:596:GLN:HA	0.67	2.19	7	1
1:A:659:LEU:HD21	1:A:672:LEU:CD2	0.67	2.20	19	16
1:A:586:SER:O	1:A:589:GLN:NE2	0.67	2.28	2	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:592:LEU:HD22	1:A:611:CYS:SG	0.67	2.28	19	13
1:A:623:CYS:SG	1:A:680:ILE:HD11	0.67	2.29	17	1
1:A:618:LEU:HD23	1:A:618:LEU:O	0.67	1.90	2	2
1:A:588:ILE:HD13	1:A:613:ILE:HG23	0.67	1.67	7	5
1:A:672:LEU:CD1	1:A:694:VAL:HG21	0.66	2.19	10	3
1:A:664:MET:CE	1:A:716:VAL:HG13	0.66	2.20	6	1
1:A:578:LEU:HD21	1:A:694:VAL:HG22	0.66	1.65	4	9
1:A:587:ILE:CD1	1:A:690:ILE:HD11	0.65	2.22	7	2
1:A:594:ILE:CD1	1:A:625:ILE:HD12	0.65	2.22	2	6
1:A:674:ASP:HB2	1:A:696:ILE:HD12	0.65	1.68	6	7
1:A:580:LEU:HG	1:A:694:VAL:HG22	0.65	1.66	5	10
1:A:580:LEU:HD23	1:A:678:ILE:HD11	0.65	1.68	16	1
1:A:615:ASP:CB	1:A:618:LEU:HD22	0.65	2.21	10	2
1:A:583:LEU:HD12	1:A:693:LYS:HB2	0.64	1.67	18	3
1:A:578:LEU:HD13	1:A:647:ILE:CD1	0.64	2.23	9	6
1:A:603:ILE:CD1	1:A:625:ILE:HD12	0.64	2.22	14	7
1:A:594:ILE:HG23	1:A:601:PHE:CD1	0.64	2.28	7	14
1:A:587:ILE:HG22	1:A:690:ILE:HG12	0.63	1.70	2	1
1:A:622:HIS:O	1:A:653:GLY:N	0.63	2.32	4	20
1:A:644:LEU:N	1:A:644:LEU:HD23	0.63	2.09	1	4
1:A:649:TYR:CE1	1:A:678:ILE:HD12	0.63	2.29	15	2
1:A:659:LEU:HG	1:A:678:ILE:HG22	0.63	1.71	4	1
1:A:580:LEU:HD11	1:A:625:ILE:HD11	0.63	1.68	8	4
1:A:647:ILE:HD12	1:A:672:LEU:HB2	0.62	1.70	1	13
1:A:644:LEU:HD23	1:A:644:LEU:N	0.62	2.08	17	2
1:A:615:ASP:HB3	1:A:618:LEU:HD22	0.62	1.71	10	2
1:A:615:ASP:CB	1:A:618:LEU:HD13	0.62	2.24	19	2
1:A:680:ILE:HD12	1:A:692:PHE:CZ	0.62	2.30	19	3
1:A:682:TRP:CD1	1:A:689:VAL:CG1	0.62	2.82	4	1
1:A:583:LEU:HD12	1:A:585:ASP:HB2	0.62	1.69	8	10
1:A:664:MET:HE1	1:A:716:VAL:HG13	0.61	1.72	6	1
1:A:609:CYS:SG	1:A:621:VAL:HG22	0.61	2.35	5	6
1:A:577:PHE:CE2	1:A:647:ILE:HG21	0.61	2.30	13	8
1:A:580:LEU:HD11	1:A:625:ILE:CD1	0.61	2.25	8	5
1:A:649:TYR:CD2	1:A:678:ILE:HD13	0.61	2.30	5	6
1:A:602:PHE:CE2	1:A:624:PHE:CZ	0.61	2.88	16	2
1:A:624:PHE:O	1:A:650:CYS:N	0.60	2.32	17	12
1:A:603:ILE:HD12	1:A:624:PHE:HA	0.60	1.74	6	10
1:A:582:PRO:HD2	1:A:590:GLU:O	0.60	1.97	11	20
1:A:621:VAL:HG11	1:A:727:VAL:CG2	0.59	2.28	14	1
1:A:580:LEU:HD21	1:A:625:ILE:HD11	0.59	1.75	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:594:ILE:HG23	1:A:601:PHE:CG	0.59	2.33	3	10
1:A:655:ASN:O	1:A:656:VAL:O	0.59	2.21	12	16
1:A:622:HIS:HD2	1:A:680:ILE:HG23	0.59	1.57	18	3
1:A:587:ILE:HD13	1:A:688:PHE:CZ	0.58	2.33	10	8
1:A:663:ARG:O	1:A:716:VAL:HG21	0.58	1.97	3	6
1:A:598:VAL:HG11	1:A:610:ASN:ND2	0.58	2.14	15	1
1:A:592:LEU:CD2	1:A:613:ILE:HD11	0.58	2.24	7	1
1:A:615:ASP:HB3	1:A:618:LEU:HD13	0.58	1.76	14	2
1:A:723:GLU:HA	1:A:726:LEU:HD12	0.58	1.74	17	12
1:A:681:ILE:HG22	1:A:690:ILE:CG1	0.58	2.29	10	4
1:A:591:SER:C	1:A:592:LEU:HD13	0.58	2.19	10	3
1:A:618:LEU:HB2	1:A:622:HIS:CG	0.57	2.33	17	13
1:A:668:THR:HG22	1:A:718:LYS:HA	0.57	1.75	20	2
1:A:580:LEU:HD12	1:A:594:ILE:CD1	0.57	2.29	20	7
1:A:659:LEU:HD12	1:A:659:LEU:C	0.57	2.20	17	6
1:A:601:PHE:CZ	1:A:610:ASN:HB3	0.57	2.34	2	18
1:A:647:ILE:HD12	1:A:672:LEU:HB3	0.57	1.76	3	6
1:A:659:LEU:HA	1:A:678:ILE:HG23	0.57	1.76	10	1
1:A:603:ILE:HD11	1:A:625:ILE:HD12	0.57	1.76	14	4
1:A:617:ARG:HB3	1:A:681:ILE:HD11	0.56	1.75	10	6
1:A:580:LEU:N	1:A:592:LEU:O	0.56	2.37	7	19
1:A:594:ILE:HG23	1:A:601:PHE:CD2	0.56	2.34	1	3
1:A:580:LEU:HD11	1:A:625:ILE:HD13	0.56	1.77	15	1
1:A:603:ILE:CG1	1:A:611:CYS:HB3	0.56	2.31	14	10
1:A:665:ILE:HG13	1:A:668:THR:HG23	0.56	1.77	13	1
1:A:577:PHE:HE1	1:A:647:ILE:HG21	0.56	1.61	16	5
1:A:577:PHE:HZ	1:A:647:ILE:HG21	0.56	1.58	19	2
1:A:594:ILE:HD11	1:A:625:ILE:HD13	0.56	1.78	18	2
1:A:649:TYR:CB	1:A:672:LEU:HD21	0.55	2.31	17	10
1:A:659:LEU:C	1:A:659:LEU:HD12	0.55	2.22	14	10
1:A:579:THR:HG22	1:A:581:LYS:HG3	0.55	1.77	3	1
1:A:578:LEU:CD1	1:A:647:ILE:HD13	0.55	2.26	3	5
1:A:648:TRP:CH2	1:A:671:LEU:CD2	0.55	2.89	18	14
1:A:649:TYR:HH	1:A:657:SER:CB	0.55	2.14	17	2
1:A:649:TYR:CE2	1:A:678:ILE:HD12	0.55	2.36	9	1
1:A:659:LEU:HD11	1:A:672:LEU:CD2	0.55	2.32	4	1
1:A:662:ASN:CG	1:A:716:VAL:HG23	0.55	2.21	18	3
1:A:577:PHE:CD1	1:A:577:PHE:C	0.55	2.81	15	1
1:A:659:LEU:HD13	1:A:678:ILE:HG12	0.54	1.79	2	9
1:A:630:HIS:N	1:A:644:LEU:O	0.54	2.41	5	19
1:A:655:ASN:O	1:A:656:VAL:HG13	0.54	2.01	10	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:602:PHE:CD2	1:A:624:PHE:CE1	0.54	2.96	17	2
1:A:577:PHE:HB3	1:A:596:GLN:HA	0.54	1.77	7	1
1:A:621:VAL:O	1:A:621:VAL:HG13	0.54	2.02	11	1
1:A:578:LEU:C	1:A:578:LEU:HD23	0.54	2.23	18	5
1:A:583:LEU:HD22	1:A:693:LYS:HB2	0.54	1.79	10	6
1:A:578:LEU:HD23	1:A:594:ILE:CD1	0.54	2.30	7	1
1:A:577:PHE:CD2	1:A:698:ASP:O	0.54	2.61	7	11
1:A:615:ASP:HB2	1:A:618:LEU:HD21	0.54	1.78	16	2
1:A:600:PRO:HG2	1:A:602:PHE:CZ	0.53	2.38	7	14
1:A:580:LEU:O	1:A:592:LEU:N	0.53	2.39	18	9
1:A:621:VAL:HG13	1:A:621:VAL:O	0.53	2.03	7	2
1:A:594:ILE:CD1	1:A:625:ILE:HG21	0.53	2.33	17	2
1:A:659:LEU:HG	1:A:678:ILE:HG23	0.53	1.79	18	1
1:A:578:LEU:HD23	1:A:579:THR:H	0.53	1.63	16	1
1:A:618:LEU:HD12	1:A:622:HIS:CG	0.53	2.38	2	1
1:A:618:LEU:O	1:A:618:LEU:HD23	0.53	2.04	10	1
1:A:669:LYS:O	1:A:717:LEU:HD12	0.53	2.04	13	1
1:A:644:LEU:N	1:A:644:LEU:CD2	0.53	2.72	4	2
1:A:578:LEU:HD23	1:A:578:LEU:C	0.53	2.24	20	4
1:A:594:ILE:HG12	1:A:601:PHE:CD2	0.52	2.39	5	10
1:A:659:LEU:HD22	1:A:678:ILE:HG12	0.52	1.80	19	4
1:A:625:ILE:HG23	1:A:648:TRP:O	0.52	2.05	7	3
1:A:618:LEU:HD22	1:A:680:ILE:HG21	0.52	1.81	9	1
1:A:655:ASN:C	1:A:656:VAL:HG13	0.52	2.25	18	5
1:A:662:ASN:CB	1:A:670:PHE:CE2	0.52	2.93	14	5
1:A:579:THR:HG21	1:A:581:LYS:CE	0.52	2.35	13	1
1:A:577:PHE:HB2	1:A:596:GLN:HB3	0.52	1.82	17	10
1:A:656:VAL:HG13	1:A:664:MET:O	0.52	2.04	4	3
1:A:594:ILE:HG23	1:A:601:PHE:HB2	0.52	1.82	12	3
1:A:624:PHE:N	1:A:650:CYS:O	0.52	2.39	17	1
1:A:578:LEU:CD2	1:A:694:VAL:HG13	0.52	2.19	16	2
1:A:618:LEU:CB	1:A:622:HIS:CG	0.52	2.92	11	9
1:A:676:ASP:O	1:A:694:VAL:HB	0.52	2.05	17	1
1:A:618:LEU:CB	1:A:622:HIS:ND1	0.51	2.72	8	14
1:A:578:LEU:CD2	1:A:594:ILE:HD12	0.51	2.32	7	1
1:A:592:LEU:HD22	1:A:592:LEU:N	0.51	2.20	8	1
1:A:577:PHE:CG	1:A:578:LEU:N	0.51	2.79	13	7
1:A:588:ILE:CD1	1:A:613:ILE:HG23	0.51	2.35	10	7
1:A:659:LEU:HD23	1:A:670:PHE:CD2	0.51	2.40	5	1
1:A:618:LEU:HB3	1:A:622:HIS:CE1	0.51	2.40	17	1
1:A:577:PHE:CD1	1:A:578:LEU:HB2	0.51	2.40	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:579:THR:O	1:A:695:GLU:N	0.51	2.42	7	13
1:A:577:PHE:CZ	1:A:578:LEU:HB2	0.51	2.41	19	1
1:A:594:ILE:HG23	1:A:601:PHE:CB	0.51	2.36	12	3
1:A:627:LYS:HB2	1:A:647:ILE:HG22	0.51	1.82	19	1
1:A:582:PRO:CD	1:A:592:LEU:HD22	0.50	2.36	11	3
1:A:583:LEU:H	1:A:583:LEU:HD13	0.50	1.66	18	1
1:A:627:LYS:CE	1:A:647:ILE:HG23	0.50	2.35	5	1
1:A:649:TYR:HB2	1:A:672:LEU:HD11	0.50	1.83	19	4
1:A:615:ASP:HB3	1:A:618:LEU:CD1	0.50	2.36	14	2
1:A:578:LEU:CG	1:A:694:VAL:HG13	0.50	2.36	6	6
1:A:577:PHE:HB3	1:A:596:GLN:CA	0.50	2.37	7	1
1:A:582:PRO:CD	1:A:590:GLU:O	0.50	2.59	10	20
1:A:587:ILE:HG22	1:A:689:VAL:O	0.50	2.07	14	1
1:A:595:GLN:O	1:A:596:GLN:C	0.50	2.49	6	2
1:A:644:LEU:CD2	1:A:644:LEU:N	0.50	2.73	17	3
1:A:577:PHE:CD1	1:A:578:LEU:N	0.50	2.79	16	2
1:A:716:VAL:HG13	1:A:716:VAL:O	0.50	2.07	1	3
1:A:648:TRP:CZ3	1:A:671:LEU:HG	0.50	2.41	1	5
1:A:662:ASN:HB3	1:A:716:VAL:HG23	0.50	1.83	12	1
1:A:580:LEU:HD23	1:A:694:VAL:CG2	0.50	2.37	6	1
1:A:592:LEU:HD11	1:A:692:PHE:CD2	0.49	2.41	17	3
1:A:595:GLN:O	1:A:597:GLY:N	0.49	2.45	6	1
1:A:618:LEU:HD23	1:A:680:ILE:CG2	0.49	2.37	5	6
1:A:656:VAL:HG23	1:A:664:MET:O	0.49	2.07	2	3
1:A:659:LEU:HD12	1:A:660:ASN:N	0.49	2.23	9	2
1:A:659:LEU:CD2	1:A:678:ILE:HG22	0.49	2.33	11	1
1:A:584:PRO:HA	1:A:589:GLN:CD	0.49	2.28	5	3
1:A:648:TRP:CZ3	1:A:717:LEU:HD12	0.49	2.42	10	1
1:A:584:PRO:O	1:A:589:GLN:NE2	0.49	2.45	7	3
1:A:580:LEU:HD21	1:A:625:ILE:CD1	0.49	2.37	6	1
1:A:649:TYR:HB3	1:A:672:LEU:HD21	0.49	1.83	17	1
1:A:587:ILE:CD1	1:A:688:PHE:CZ	0.49	2.95	7	11
1:A:648:TRP:CZ2	1:A:671:LEU:HD22	0.49	2.42	2	1
1:A:651:HIS:CE1	1:A:657:SER:HG	0.49	2.26	16	1
1:A:615:ASP:OD2	1:A:681:ILE:HG21	0.49	2.07	3	5
1:A:578:LEU:CD1	1:A:647:ILE:CD1	0.48	2.91	9	5
1:A:652:THR:O	1:A:666:GLN:NE2	0.48	2.46	16	4
1:A:577:PHE:C	1:A:577:PHE:CD1	0.48	2.85	3	2
1:A:651:HIS:CG	1:A:657:SER:HG	0.48	2.26	4	1
1:A:659:LEU:HD13	1:A:678:ILE:CG2	0.48	2.31	15	2
1:A:627:LYS:HD3	1:A:647:ILE:HG23	0.48	1.85	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:659:LEU:CD1	1:A:670:PHE:CD2	0.48	2.97	18	1
1:A:577:PHE:CB	1:A:596:GLN:HB3	0.48	2.38	3	11
1:A:682:TRP:CD1	1:A:689:VAL:HG13	0.48	2.42	4	1
1:A:622:HIS:CD2	1:A:680:ILE:CG2	0.48	2.96	15	3
1:A:587:ILE:HG12	1:A:690:ILE:HD11	0.48	1.84	9	1
1:A:659:LEU:O	1:A:661:ASN:N	0.48	2.47	9	14
1:A:587:ILE:CD1	1:A:688:PHE:CE1	0.48	2.97	11	3
1:A:579:THR:HG22	1:A:581:LYS:HG2	0.47	1.86	11	1
1:A:675:GLY:N	1:A:694:VAL:O	0.47	2.47	6	16
1:A:578:LEU:HD13	1:A:696:ILE:HG12	0.47	1.86	1	1
1:A:659:LEU:CD1	1:A:678:ILE:HG22	0.47	2.32	15	1
1:A:583:LEU:HD12	1:A:585:ASP:CB	0.47	2.39	15	2
1:A:617:ARG:HB3	1:A:681:ILE:HD13	0.47	1.85	14	1
1:A:662:ASN:CB	1:A:670:PHE:CE1	0.47	2.97	13	2
1:A:658:TYR:O	1:A:679:LYS:N	0.47	2.43	8	3
1:A:692:PHE:N	1:A:692:PHE:CD1	0.47	2.81	19	3
1:A:605:ARG:CG	1:A:618:LEU:HD12	0.47	2.40	16	1
1:A:644:LEU:HD12	1:A:644:LEU:N	0.47	2.25	6	2
1:A:578:LEU:HD12	1:A:579:THR:N	0.47	2.23	17	1
1:A:662:ASN:HB2	1:A:670:PHE:CE2	0.47	2.45	2	4
1:A:582:PRO:CB	1:A:588:ILE:HG23	0.47	2.40	19	2
1:A:577:PHE:HB2	1:A:596:GLN:HA	0.47	1.86	7	1
1:A:580:LEU:HB3	1:A:592:LEU:HD12	0.47	1.87	19	1
1:A:592:LEU:HD11	1:A:692:PHE:CE2	0.47	2.44	18	2
1:A:592:LEU:CD1	1:A:692:PHE:CD2	0.47	2.98	17	4
1:A:649:TYR:O	1:A:669:LYS:HA	0.47	2.10	20	3
1:A:618:LEU:HD12	1:A:622:HIS:CB	0.47	2.40	15	1
1:A:615:ASP:CB	1:A:618:LEU:HD21	0.46	2.40	16	2
1:A:577:PHE:CE2	1:A:578:LEU:HB2	0.46	2.44	13	3
1:A:583:LEU:HD22	1:A:583:LEU:N	0.46	2.25	19	1
1:A:671:LEU:HD12	1:A:672:LEU:N	0.46	2.25	2	1
1:A:587:ILE:CG2	1:A:690:ILE:HD13	0.46	2.41	10	1
1:A:621:VAL:HG12	1:A:621:VAL:O	0.46	2.10	9	1
1:A:578:LEU:O	1:A:594:ILE:N	0.46	2.48	4	7
1:A:583:LEU:HD13	1:A:583:LEU:H	0.46	1.71	6	2
1:A:580:LEU:CD1	1:A:594:ILE:CD1	0.46	2.94	14	3
1:A:594:ILE:HG12	1:A:601:PHE:CD1	0.46	2.46	9	2
1:A:681:ILE:HG22	1:A:690:ILE:CB	0.46	2.35	12	1
1:A:617:ARG:CB	1:A:681:ILE:CD1	0.46	2.94	8	4
1:A:651:HIS:CE1	1:A:657:SER:N	0.46	2.84	15	13
1:A:583:LEU:HD21	1:A:677:GLU:HG3	0.46	1.87	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:681:ILE:HG22	1:A:690:ILE:HG13	0.46	1.88	10	2
1:A:655:ASN:O	1:A:656:VAL:CG1	0.46	2.64	2	2
1:A:577:PHE:CD1	1:A:696:ILE:HG23	0.46	2.46	20	1
1:A:602:PHE:HA	1:A:624:PHE:CB	0.46	2.41	15	10
1:A:615:ASP:OD1	1:A:688:PHE:CZ	0.46	2.68	9	5
1:A:577:PHE:CE1	1:A:647:ILE:CG2	0.45	2.99	9	6
1:A:655:ASN:C	1:A:656:VAL:CG1	0.45	2.85	10	16
1:A:659:LEU:HD21	1:A:672:LEU:HD22	0.45	1.88	19	3
1:A:617:ARG:O	1:A:655:ASN:ND2	0.45	2.48	7	3
1:A:605:ARG:HG2	1:A:618:LEU:CD1	0.45	2.41	6	11
1:A:618:LEU:HB2	1:A:622:HIS:ND1	0.45	2.25	9	2
1:A:681:ILE:CG2	1:A:690:ILE:HD12	0.45	2.41	14	1
1:A:579:THR:HG22	1:A:581:LYS:CG	0.45	2.41	3	3
1:A:648:TRP:CH2	1:A:671:LEU:HG	0.45	2.47	10	5
1:A:579:THR:HG21	1:A:581:LYS:HE2	0.45	1.88	13	1
1:A:600:PRO:HB2	1:A:624:PHE:CE1	0.45	2.47	16	2
1:A:589:GLN:OE1	1:A:589:GLN:CA	0.45	2.64	5	2
1:A:587:ILE:CG2	1:A:690:ILE:CD1	0.45	2.95	10	1
1:A:587:ILE:HG21	1:A:688:PHE:CE1	0.45	2.45	2	1
1:A:587:ILE:HG23	1:A:588:ILE:HG13	0.45	1.89	14	1
1:A:615:ASP:H	1:A:618:LEU:HD11	0.45	1.72	7	8
1:A:627:LYS:HB3	1:A:647:ILE:HG22	0.45	1.89	13	1
1:A:670:PHE:CE1	1:A:716:VAL:HG22	0.45	2.46	6	2
1:A:689:VAL:O	1:A:689:VAL:CG1	0.45	2.64	12	6
1:A:603:ILE:HG13	1:A:611:CYS:HB3	0.45	1.88	18	4
1:A:580:LEU:HD11	1:A:594:ILE:CD1	0.45	2.42	16	1
1:A:618:LEU:HD12	1:A:622:HIS:CD2	0.45	2.47	2	1
1:A:594:ILE:CD1	1:A:625:ILE:HD13	0.45	2.42	18	1
1:A:580:LEU:N	1:A:580:LEU:HD23	0.45	2.26	7	1
1:A:618:LEU:HD23	1:A:618:LEU:C	0.45	2.31	2	1
1:A:699:THR:O	1:A:699:THR:OG1	0.45	2.35	12	2
1:A:582:PRO:HB3	1:A:588:ILE:CG2	0.45	2.42	3	1
1:A:612:LYS:O	1:A:613:ILE:HD13	0.45	2.11	20	2
1:A:648:TRP:HB3	1:A:669:LYS:CG	0.44	2.42	13	2
1:A:662:ASN:HB3	1:A:670:PHE:CE2	0.44	2.47	14	1
1:A:662:ASN:ND2	1:A:716:VAL:HG23	0.44	2.27	6	2
1:A:615:ASP:HB3	1:A:618:LEU:CD2	0.44	2.40	10	4
1:A:716:VAL:O	1:A:716:VAL:HG13	0.44	2.12	11	1
1:A:577:PHE:CE1	1:A:696:ILE:HG23	0.44	2.47	3	1
1:A:583:LEU:HD22	1:A:583:LEU:H	0.44	1.72	19	1
1:A:592:LEU:HD13	1:A:592:LEU:N	0.44	2.26	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:583:LEU:N	1:A:583:LEU:HD22	0.44	2.28	6	2
1:A:651:HIS:ND1	1:A:657:SER:OG	0.44	2.51	17	4
1:A:603:ILE:CD1	1:A:625:ILE:CD1	0.44	2.96	4	3
1:A:578:LEU:HD12	1:A:696:ILE:CG1	0.44	2.42	2	2
1:A:583:LEU:HD12	1:A:585:ASP:HB3	0.44	1.89	15	1
1:A:627:LYS:HA	1:A:646:ASP:O	0.44	2.13	13	1
1:A:678:ILE:CD1	1:A:694:VAL:HG23	0.44	2.42	16	1
1:A:615:ASP:OD2	1:A:688:PHE:CE1	0.44	2.71	11	3
1:A:724:LYS:O	1:A:727:VAL:HG12	0.44	2.12	6	2
1:A:594:ILE:CD1	1:A:625:ILE:CD1	0.44	2.94	8	4
1:A:580:LEU:HD22	1:A:692:PHE:HB2	0.44	1.88	1	2
1:A:654:THR:HG23	1:A:655:ASN:N	0.44	2.27	1	2
1:A:659:LEU:HD11	1:A:676:ASP:OD1	0.44	2.13	9	3
1:A:655:ASN:CB	1:A:681:ILE:HD12	0.44	2.43	4	2
1:A:626:PHE:CE1	1:A:627:LYS:O	0.44	2.71	6	16
1:A:601:PHE:CE2	1:A:610:ASN:HB3	0.44	2.47	5	3
1:A:655:ASN:HB3	1:A:681:ILE:HD12	0.44	1.90	14	2
1:A:699:THR:OG1	1:A:699:THR:O	0.44	2.36	20	3
1:A:600:PRO:CG	1:A:624:PHE:CZ	0.44	3.00	16	1
1:A:648:TRP:CZ3	1:A:717:LEU:CD1	0.44	3.01	7	2
1:A:592:LEU:N	1:A:592:LEU:HD22	0.44	2.28	9	3
1:A:577:PHE:CZ	1:A:647:ILE:CG2	0.44	3.01	11	1
1:A:626:PHE:CZ	1:A:628:LYS:CG	0.44	3.01	2	8
1:A:589:GLN:CA	1:A:589:GLN:OE1	0.44	2.65	14	1
1:A:617:ARG:NH1	1:A:688:PHE:CE1	0.43	2.86	19	1
1:A:669:LYS:O	1:A:717:LEU:N	0.43	2.51	16	1
1:A:615:ASP:OD1	1:A:690:ILE:HD11	0.43	2.13	12	1
1:A:659:LEU:HD12	1:A:670:PHE:HB3	0.43	1.89	4	1
1:A:676:ASP:OD1	1:A:678:ILE:HG23	0.43	2.13	17	1
1:A:659:LEU:CD2	1:A:672:LEU:CD2	0.43	2.97	1	2
1:A:618:LEU:CD2	1:A:680:ILE:CG2	0.43	2.96	5	2
1:A:577:PHE:CE1	1:A:578:LEU:HB2	0.43	2.48	19	1
1:A:651:HIS:ND1	1:A:657:SER:CB	0.43	2.81	10	4
1:A:689:VAL:CG1	1:A:689:VAL:O	0.43	2.65	5	7
1:A:681:ILE:CG2	1:A:690:ILE:HB	0.43	2.43	9	1
1:A:617:ARG:HB3	1:A:681:ILE:CD1	0.43	2.43	19	3
1:A:617:ARG:NH1	1:A:688:PHE:CD2	0.43	2.86	2	1
1:A:576:ARG:O	1:A:698:ASP:CB	0.43	2.66	11	4
1:A:615:ASP:HB3	1:A:618:LEU:HG	0.43	1.90	11	1
1:A:604:GLY:HA3	1:A:620:ARG:O	0.43	2.12	1	5
1:A:578:LEU:HD23	1:A:580:LEU:HD21	0.43	1.90	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:629:ARG:HG3	1:A:629:ARG:O	0.43	2.14	9	2
1:A:583:LEU:HD22	1:A:691:GLY:O	0.43	2.13	18	1
1:A:582:PRO:CD	1:A:592:LEU:CD2	0.43	2.96	9	6
1:A:655:ASN:C	1:A:656:VAL:HG23	0.43	2.33	16	2
1:A:622:HIS:NE2	1:A:680:ILE:HG23	0.43	2.28	19	1
1:A:615:ASP:CB	1:A:618:LEU:CD2	0.43	2.96	11	2
1:A:681:ILE:O	1:A:690:ILE:N	0.43	2.50	15	1
1:A:580:LEU:CD2	1:A:694:VAL:CG2	0.43	2.96	8	3
1:A:600:PRO:HB3	1:A:626:PHE:HB2	0.43	1.91	11	8
1:A:595:GLN:CB	1:A:598:VAL:HG23	0.43	2.43	16	1
1:A:617:ARG:NH1	1:A:688:PHE:CE2	0.43	2.87	2	1
1:A:577:PHE:HB3	1:A:596:GLN:HB3	0.43	1.91	19	1
1:A:690:ILE:CG2	1:A:691:GLY:N	0.43	2.82	11	4
1:A:670:PHE:CD1	1:A:671:LEU:N	0.43	2.87	11	1
1:A:692:PHE:CD1	1:A:692:PHE:N	0.42	2.85	6	4
1:A:577:PHE:HE1	1:A:647:ILE:HD13	0.42	1.74	9	1
1:A:651:HIS:ND1	1:A:657:SER:HB3	0.42	2.29	3	2
1:A:648:TRP:CZ3	1:A:717:LEU:HD11	0.42	2.48	7	1
1:A:617:ARG:NH1	1:A:688:PHE:CZ	0.42	2.87	19	1
1:A:620:ARG:CG	1:A:621:VAL:HG23	0.42	2.44	3	2
1:A:659:LEU:CD1	1:A:659:LEU:C	0.42	2.87	17	1
1:A:618:LEU:CD2	1:A:680:ILE:HG21	0.42	2.44	3	1
1:A:587:ILE:HG21	1:A:688:PHE:CZ	0.42	2.49	3	1
1:A:605:ARG:NE	1:A:618:LEU:O	0.42	2.53	10	5
1:A:615:ASP:OD2	1:A:688:PHE:CZ	0.42	2.72	11	1
1:A:587:ILE:CD1	1:A:690:ILE:CG1	0.42	2.97	18	1
1:A:656:VAL:HG22	1:A:658:TYR:CZ	0.42	2.49	18	1
1:A:656:VAL:CG1	1:A:664:MET:O	0.42	2.67	4	1
1:A:576:ARG:CG	1:A:593:GLU:CB	0.42	2.97	4	1
1:A:586:SER:OG	1:A:690:ILE:HA	0.42	2.14	5	1
1:A:659:LEU:HG	1:A:670:PHE:CD2	0.42	2.49	9	5
1:A:674:ASP:HB3	1:A:696:ILE:HD12	0.42	1.91	2	1
1:A:596:GLN:HG2	1:A:597:GLY:N	0.42	2.29	10	2
1:A:664:MET:HE1	1:A:670:PHE:HB2	0.42	1.91	13	2
1:A:615:ASP:HB2	1:A:618:LEU:HD13	0.42	1.89	19	1
1:A:583:LEU:HD12	1:A:693:LYS:CB	0.42	2.41	18	1
1:A:670:PHE:CD1	1:A:716:VAL:HG22	0.42	2.50	13	1
1:A:582:PRO:HB2	1:A:588:ILE:HG23	0.42	1.92	3	1
1:A:662:ASN:ND2	1:A:670:PHE:CE2	0.42	2.88	8	1
1:A:578:LEU:CD1	1:A:696:ILE:HG12	0.42	2.45	2	2
1:A:651:HIS:CE1	1:A:657:SER:OG	0.42	2.72	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:626:PHE:CZ	1:A:628:LYS:HG3	0.42	2.49	10	4
1:A:598:VAL:HG11	1:A:610:ASN:CG	0.42	2.35	18	3
1:A:592:LEU:HD13	1:A:611:CYS:HG	0.42	1.72	18	1
1:A:659:LEU:CG	1:A:678:ILE:HG22	0.42	2.42	4	1
1:A:577:PHE:CB	1:A:596:GLN:HG2	0.42	2.45	4	2
1:A:578:LEU:CD1	1:A:696:ILE:CG1	0.42	2.97	2	3
1:A:578:LEU:HD21	1:A:694:VAL:CG2	0.41	2.45	8	1
1:A:674:ASP:N	1:A:696:ILE:HD12	0.41	2.29	8	1
1:A:659:LEU:CA	1:A:678:ILE:HG23	0.41	2.44	10	1
1:A:580:LEU:HD11	1:A:625:ILE:HD12	0.41	1.92	10	1
1:A:649:TYR:CD2	1:A:664:MET:CE	0.41	3.04	4	1
1:A:618:LEU:HG	1:A:622:HIS:CG	0.41	2.50	14	1
1:A:618:LEU:HD23	1:A:680:ILE:HG23	0.41	1.91	7	1
1:A:658:TYR:N	1:A:679:LYS:O	0.41	2.46	16	1
1:A:675:GLY:CA	1:A:694:VAL:O	0.41	2.68	10	1
1:A:624:PHE:O	1:A:650:CYS:HB2	0.41	2.15	10	1
1:A:647:ILE:HD11	1:A:672:LEU:O	0.41	2.16	9	1
1:A:651:HIS:CE1	1:A:657:SER:HB3	0.41	2.51	1	2
1:A:659:LEU:C	1:A:659:LEU:CD1	0.41	2.89	11	1
1:A:587:ILE:N	1:A:689:VAL:O	0.41	2.49	3	1
1:A:587:ILE:HD13	1:A:587:ILE:N	0.41	2.30	19	1
1:A:580:LEU:HD12	1:A:594:ILE:HG13	0.41	1.92	16	1
1:A:626:PHE:CE2	1:A:627:LYS:O	0.41	2.73	16	1
1:A:581:LYS:HA	1:A:591:SER:HA	0.41	1.91	2	1
1:A:630:HIS:CD2	1:A:630:HIS:C	0.41	2.93	11	1
1:A:588:ILE:HD12	1:A:690:ILE:HD13	0.41	1.93	5	1
1:A:662:ASN:OD1	1:A:670:PHE:CZ	0.41	2.74	16	2
1:A:582:PRO:HG3	1:A:692:PHE:CE1	0.41	2.51	12	2
1:A:600:PRO:HG2	1:A:602:PHE:CE2	0.41	2.50	7	1
1:A:659:LEU:HD23	1:A:670:PHE:HB3	0.41	1.92	20	1
1:A:657:SER:O	1:A:664:MET:CB	0.41	2.69	16	1
1:A:629:ARG:O	1:A:629:ARG:HG3	0.41	2.15	16	1
1:A:685:ASN:ND2	1:A:686:ASN:N	0.41	2.69	10	1
1:A:626:PHE:O	1:A:648:TRP:N	0.41	2.46	2	1
1:A:578:LEU:HD13	1:A:696:ILE:CG1	0.41	2.46	12	1
1:A:600:PRO:HG2	1:A:602:PHE:CE1	0.41	2.51	13	1
1:A:622:HIS:CD2	1:A:680:ILE:O	0.41	2.74	4	1
1:A:595:GLN:O	1:A:598:VAL:HG23	0.41	2.15	7	1
1:A:676:ASP:HB3	1:A:694:VAL:HB	0.41	1.93	17	1
1:A:580:LEU:CD1	1:A:625:ILE:HD13	0.41	2.44	15	1
1:A:603:ILE:HD11	1:A:625:ILE:CD1	0.41	2.45	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:662:ASN:HB2	1:A:670:PHE:CZ	0.41	2.50	6	1
1:A:621:VAL:O	1:A:652:THR:OG1	0.40	2.38	16	1
1:A:652:THR:O	1:A:666:GLN:CG	0.40	2.69	14	2
1:A:658:TYR:CD1	1:A:658:TYR:N	0.40	2.89	12	1
1:A:578:LEU:CD2	1:A:647:ILE:CD1	0.40	2.97	10	1
1:A:655:ASN:CB	1:A:681:ILE:CD1	0.40	2.99	4	1
1:A:688:PHE:CD1	1:A:688:PHE:O	0.40	2.74	4	1
1:A:649:TYR:CE2	1:A:678:ILE:HG21	0.40	2.51	7	1
1:A:655:ASN:ND2	1:A:681:ILE:HD11	0.40	2.30	17	1
1:A:576:ARG:CG	1:A:593:GLU:HB3	0.40	2.46	15	1
1:A:662:ASN:HB3	1:A:716:VAL:CG2	0.40	2.46	12	1
1:A:615:ASP:HB3	1:A:618:LEU:CG	0.40	2.46	17	1
1:A:578:LEU:HG	1:A:694:VAL:HG13	0.40	1.93	19	1
1:A:657:SER:O	1:A:664:MET:N	0.40	2.53	13	1
1:A:576:ARG:CD	1:A:593:GLU:HB3	0.40	2.46	6	1
1:A:664:MET:CE	1:A:670:PHE:HB2	0.40	2.46	20	1
1:A:654:THR:CG2	1:A:655:ASN:N	0.40	2.85	16	1
1:A:649:TYR:OH	1:A:657:SER:CB	0.40	2.69	11	1
1:A:618:LEU:HB3	1:A:622:HIS:CG	0.40	2.52	7	1
1:A:646:ASP:CG	1:A:671:LEU:HD11	0.40	2.37	3	1
1:A:651:HIS:NE2	1:A:656:VAL:HA	0.40	2.32	20	1

6.3 Torsion angles

6.3.1 Protein backbone

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	125/158 (79%)	112±2 (90±2%)	9±2 (7±1%)	4±1 (3±1%)	8 38
2	P	0	-	-	-	-
All	All	2500/3340 (75%)	2239 (90%)	176 (7%)	85 (3%)	8 38

All 8 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	660	ASN	20
1	A	656	VAL	20
1	A	582	PRO	19
1	A	666	GLN	15
1	A	616	ASN	5
1	A	674	ASP	4
1	A	619	SER	1
1	A	596	GLN	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	118/142 (83%)	85±3 (72±3%)	33±3 (28±3%)	2 21
2	P	0	-	-	-
All	All	2360/3000 (79%)	1704 (72%)	656 (28%)	2 21

All 85 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	612	LYS	20
1	A	671	LEU	20
1	A	628	LYS	20
1	A	591	SER	20
1	A	583	LEU	20
1	A	659	LEU	20
1	A	596	GLN	19
1	A	676	ASP	19
1	A	589	GLN	19
1	A	606	SER	18
1	A	605	ARG	18
1	A	592	LEU	16
1	A	616	ASN	16
1	A	718	LYS	16
1	A	646	ASP	15
1	A	656	VAL	15
1	A	620	ARG	13

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Mol	Chain	Res	Type	Models (Total)
1	A	577	PHE	13
1	A	670	PHE	13
1	A	618	LEU	13
1	A	580	LEU	12
1	A	593	GLU	12
1	A	617	ARG	11
1	A	717	LEU	11
1	A	629	ARG	10
1	A	645	ASP	9
1	A	680	ILE	9
1	A	695	GLU	9
1	A	607	GLU	8
1	A	687	LYS	8
1	A	677	GLU	8
1	A	686	ASN	7
1	A	728	LYS	7
1	A	581	LYS	7
1	A	699	THR	7
1	A	679	LYS	7
1	A	693	LYS	7
1	A	644	LEU	7
1	A	672	LEU	7
1	A	684	LYS	7
1	A	720	THR	6
1	A	585	ASP	6
1	A	673	GLN	6
1	A	689	VAL	6
1	A	595	GLN	6
1	A	619	SER	6
1	A	662	ASN	5
1	A	666	GLN	5
1	A	723	GLU	5
1	A	697	ASN	5
1	A	655	ASN	5
1	A	587	ILE	4
1	A	663	ARG	4
1	A	608	ASP	4
1	A	688	PHE	4
1	A	681	ILE	4
1	A	586	SER	4
1	A	614	GLU	4
1	A	647	ILE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	576	ARG	3
1	A	615	ASP	3
1	A	650	CYS	3
1	A	664	MET	3
1	A	668	THR	3
1	A	683	ASP	3
1	A	624	PHE	2
1	A	724	LYS	2
1	A	626	PHE	2
1	A	729	LYS	2
1	A	722	GLU	2
1	A	661	ASN	2
1	A	725	ASP	2
1	A	610	ASN	2
1	A	623	CYS	2
1	A	698	ASP	2
1	A	694	VAL	2
1	A	660	ASN	2
1	A	692	PHE	1
1	A	678	ILE	1
1	A	669	LYS	1
1	A	685	ASN	1
1	A	602	PHE	1
1	A	627	LYS	1
1	A	599	ASN	1
1	A	719	GLN	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
2	TPO	P	603	2	7,10,11	0.86±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	TPO	P	603	2	10,14,16	1.17±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	P	603	2	-	0±0,8,11,13	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

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