



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 01:20 AM UTC

PDB ID : 1K2M / pdb_00001k2m
Title : Solution Structure of the FHA2 Domain of Rad53 Complexed with a Phosphotyrosyl 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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

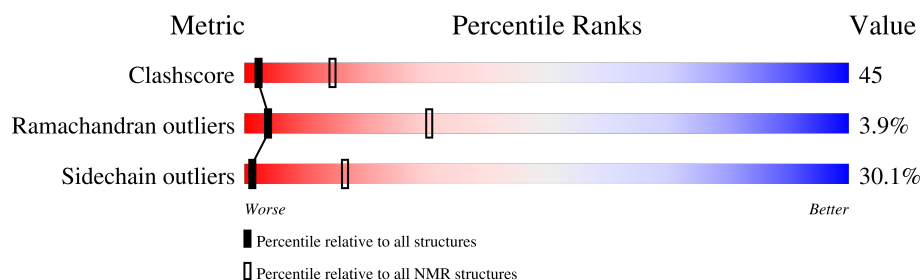
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

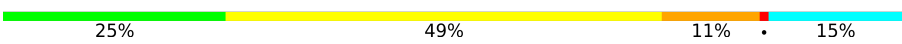
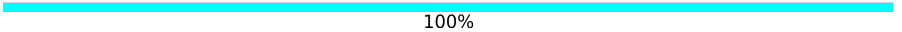
The overall completeness of chemical shifts assignment was not calculated.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	158	
2	P	7	

2 Ensemble composition and analysis

This entry contains 22 models. Model 11 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:575-A:630, A:643-A:705, A:715-A:730 (135)	0.44	11

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 5 clusters and 2 single-model clusters were found.

Cluster number	Models
1	4, 5, 8, 11, 13, 18, 21
2	1, 3, 6, 14, 17
3	9, 15, 16
4	10, 20, 22
5	2, 19
Single-model clusters	7; 12

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2676 atoms, of which 1332 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein Kinase SPK1.

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

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

Mol	Chain	Residues	Atoms						Trace
2	P	7	Total	C	H	N	O	P	0
			125	43	55	7	19	1	

There is a discrepancy between the modelled and reference sequences:

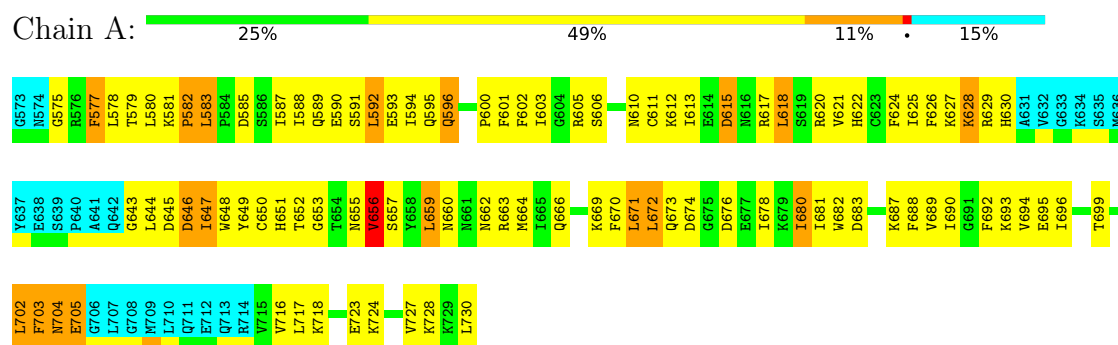
Chain	Residue	Modelled	Actual	Comment	Reference
P	829	PTR	TYR	modified residue	UNP P14737

4 Residue-property plots

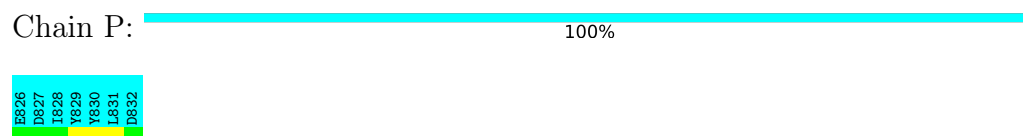
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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: Protein Kinase SPK1



• Molecule 2: DNA repair protein Rad9

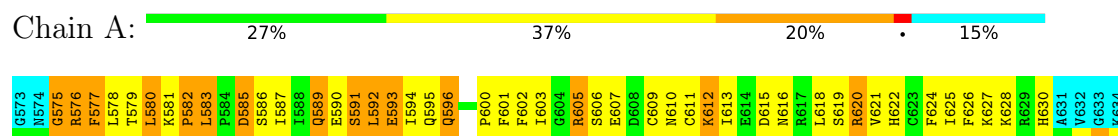


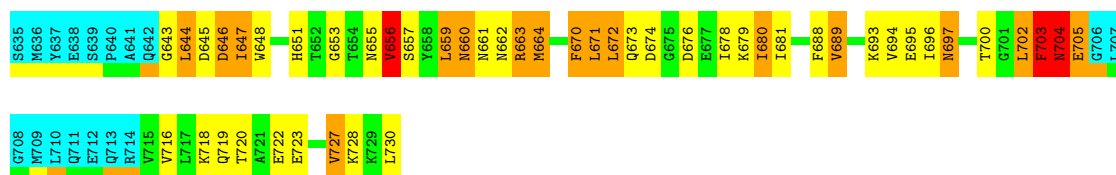
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

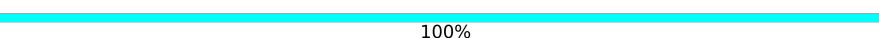
4.2.1 Score per residue for model 1

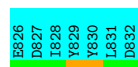
• Molecule 1: Protein Kinase SPK1





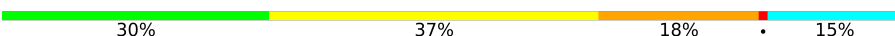
- Molecule 2: DNA repair protein Rad9

Chain P:  100%



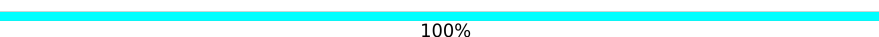
4.2.2 Score per residue for model 2

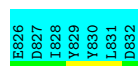
- Molecule 1: Protein Kinase SPK1

Chain A:  30% 37% 18% 15%



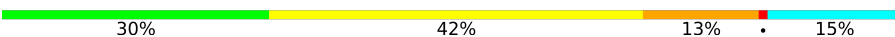
- Molecule 2: DNA repair protein Rad9

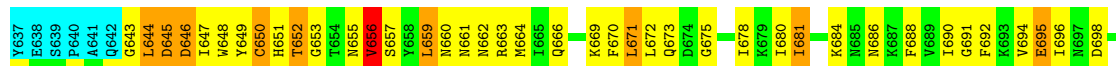
Chain P:  100%

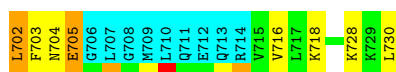


4.2.3 Score per residue for model 3

- Molecule 1: Protein Kinase SPK1

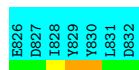
Chain A:  30% 42% 13% 15%





- Molecule 2: DNA repair protein Rad9

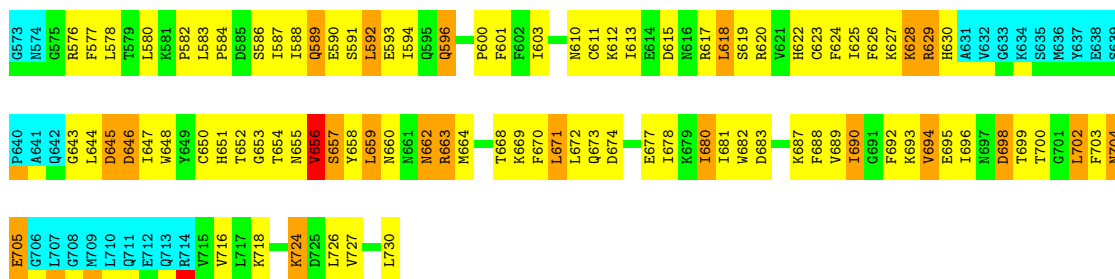
Chain P: 100%



4.2.4 Score per residue for model 4

- Molecule 1: Protein Kinase SPK1

Chain A: 27% 45% 13% 15%



- Molecule 2: DNA repair protein Rad9

Chain P: 100%



4.2.5 Score per residue for model 5

- Molecule 1: Protein Kinase SPK1

Chain A: 30% 40% 15% 15%



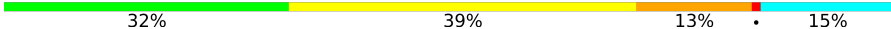
- Molecule 2: DNA repair protein Rad9

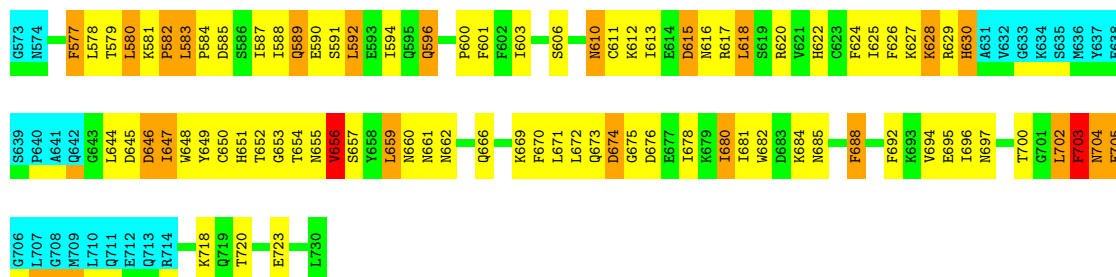
Chain P:  100%



4.2.6 Score per residue for model 6

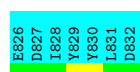
- Molecule 1: Protein Kinase SPK1

Chain A:  32% 39% 13% 15%



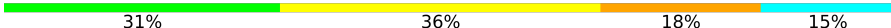
- Molecule 2: DNA repair protein Rad9

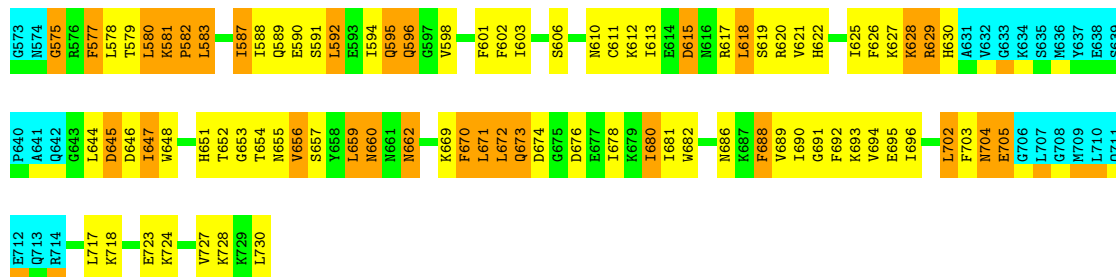
Chain P:  100%



4.2.7 Score per residue for model 7

- Molecule 1: Protein Kinase SPK1

Chain A:  31% 36% 18% 15%



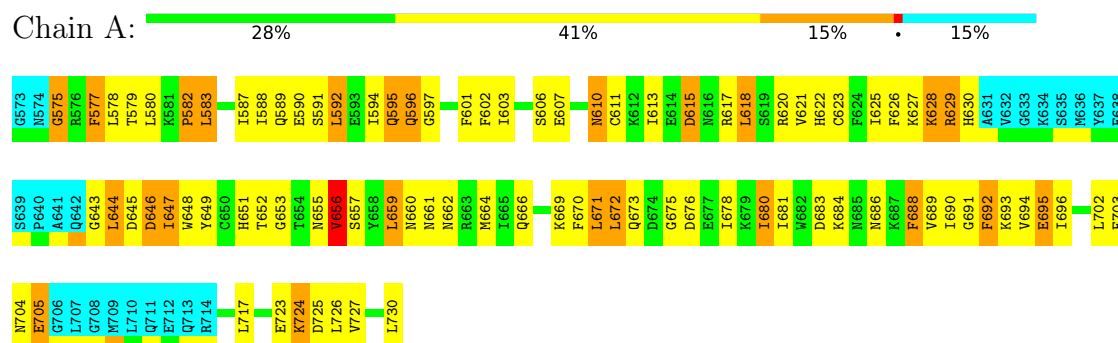
- Molecule 2: DNA repair protein Rad9

Chain P:  100%

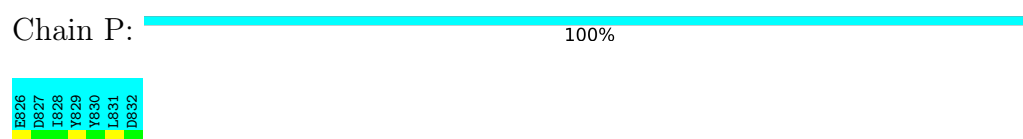


4.2.8 Score per residue for model 8

- Molecule 1: Protein Kinase SPK1

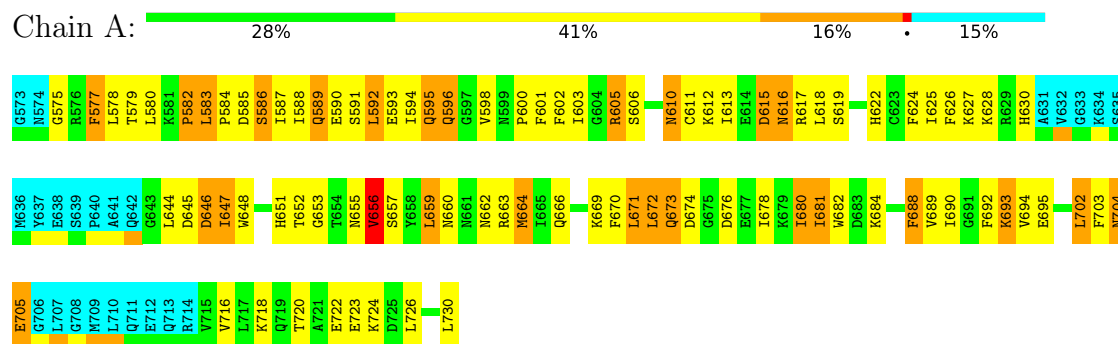


- Molecule 2: DNA repair protein Rad9

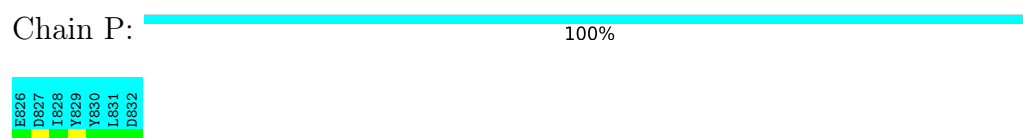


4.2.9 Score per residue for model 9

- Molecule 1: Protein Kinase SPK1

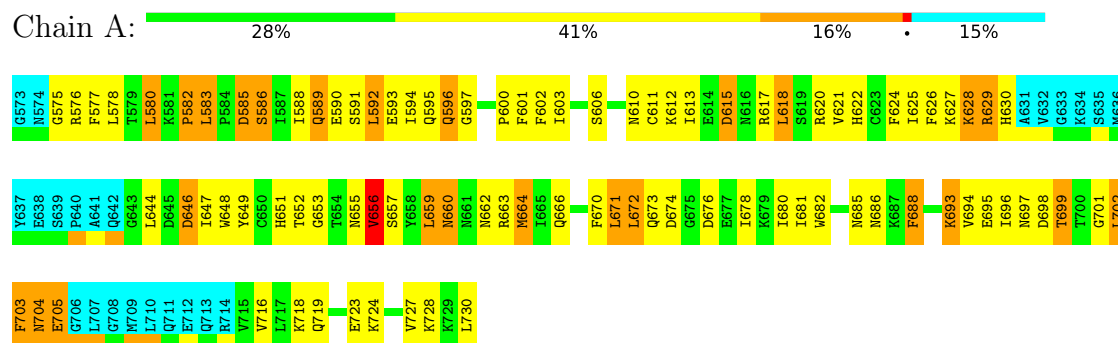


- Molecule 2: DNA repair protein Rad9

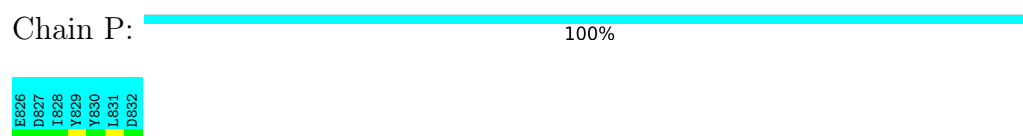


4.2.10 Score per residue for model 10

- Molecule 1: Protein Kinase SPK1

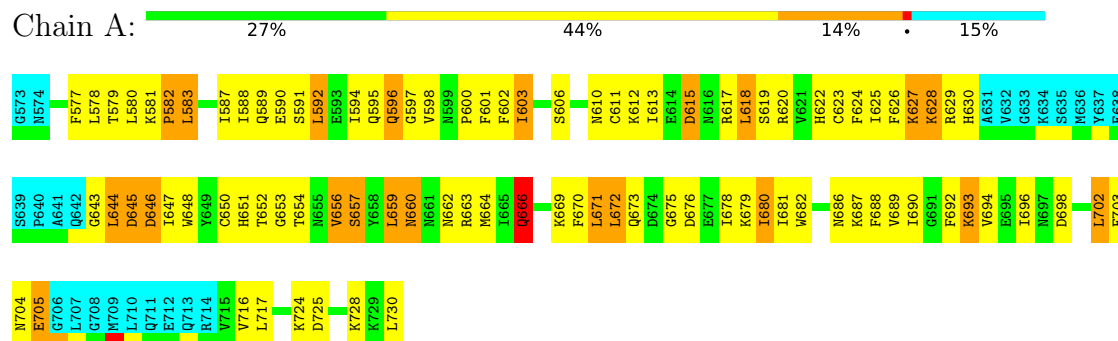


- Molecule 2: DNA repair protein Rad9

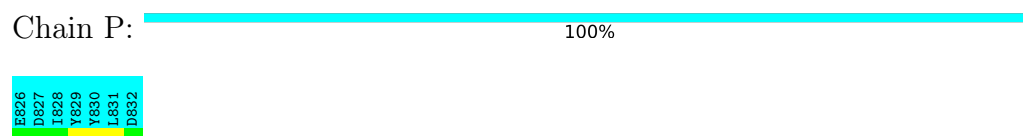


4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Protein Kinase SPK1

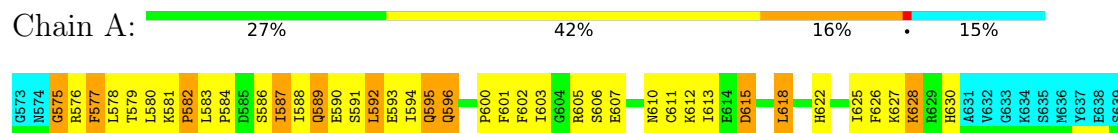


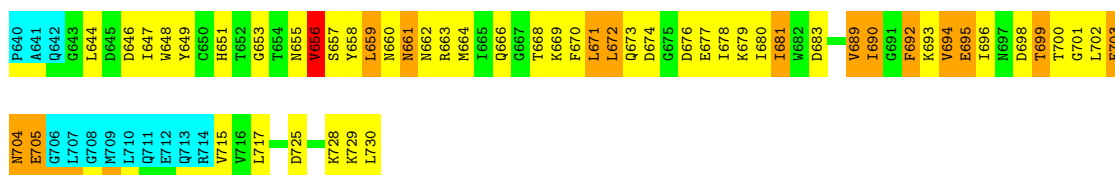
- Molecule 2: DNA repair protein Rad9



4.2.12 Score per residue for model 12

- Molecule 1: Protein Kinase SPK1





- Molecule 2: DNA repair protein Rad9

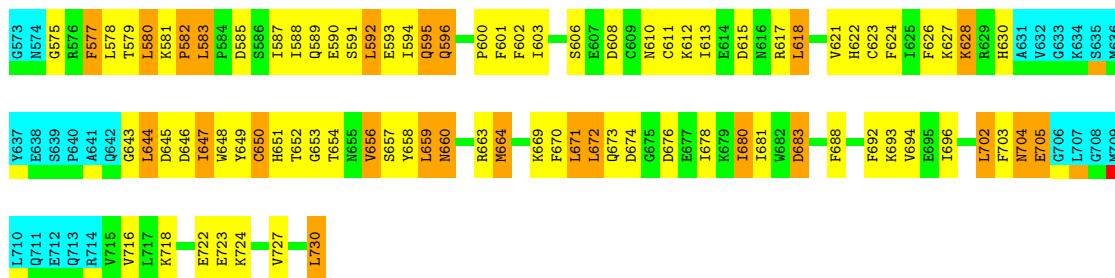
Chain P: 100%



4.2.13 Score per residue for model 13

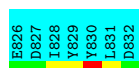
- Molecule 1: Protein Kinase SPK1

Chain A: 31% 39% 15% 15%



- Molecule 2: DNA repair protein Rad9

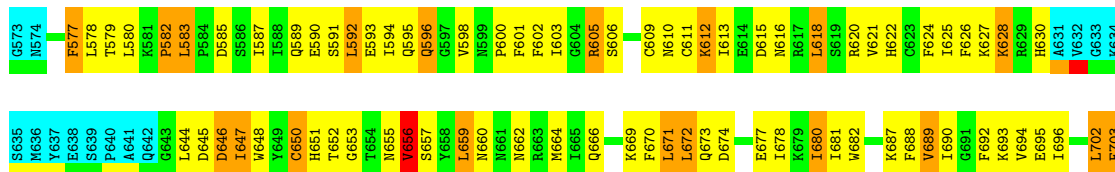
Chain P: 100%



4.2.14 Score per residue for model 14

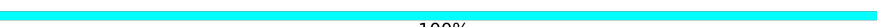
- Molecule 1: Protein Kinase SPK1

Chain A: 29% 42% 13% 15%





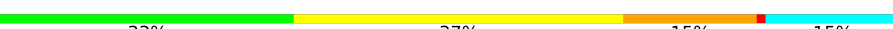
- Molecule 2: DNA repair protein Rad9

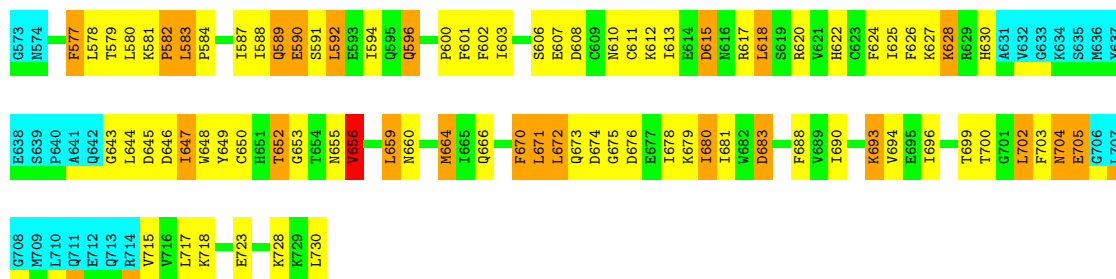
Chain P:  100%



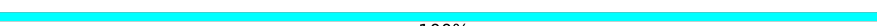
4.2.15 Score per residue for model 15

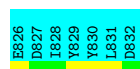
- Molecule 1: Protein Kinase SPK1

Chain A:  33% 37% 15% • 15%



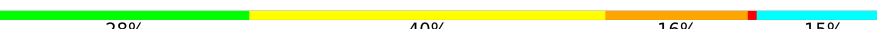
- Molecule 2: DNA repair protein Rad9

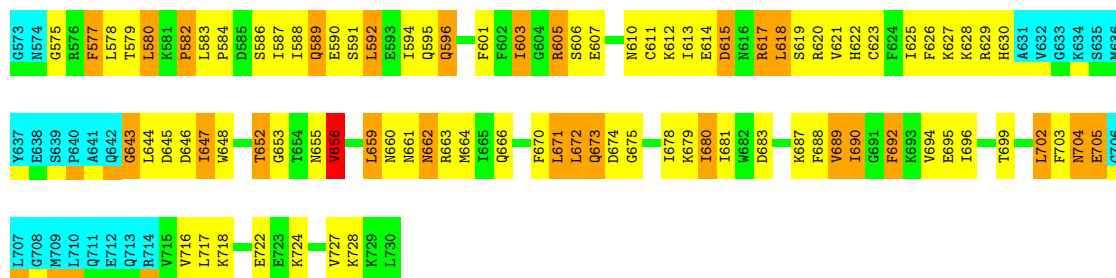
Chain P:  100%



4.2.16 Score per residue for model 16

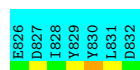
- Molecule 1: Protein Kinase SPK1

Chain A:  28% 40% 16% • 15%



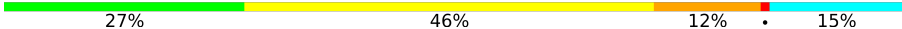
- Molecule 2: DNA repair protein Rad9

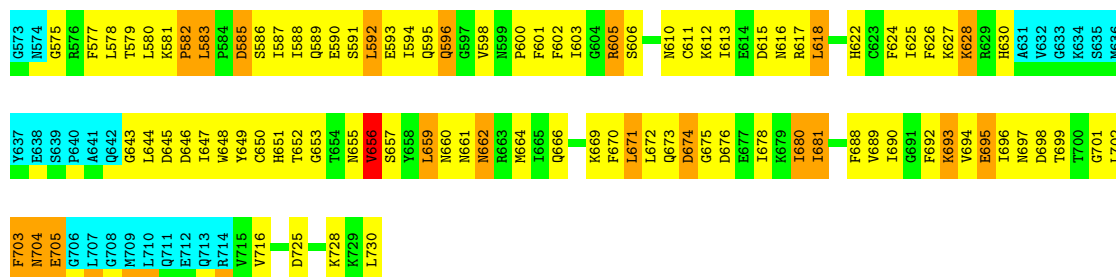
Chain P:  100%



4.2.17 Score per residue for model 17

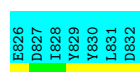
- Molecule 1: Protein Kinase SPK1

Chain A:  27% 46% 12% 15%



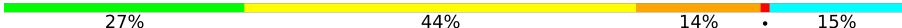
- Molecule 2: DNA repair protein Rad9

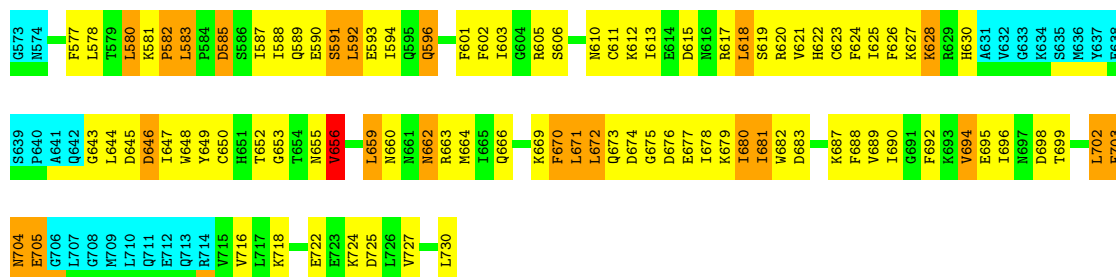
Chain P:  100%



4.2.18 Score per residue for model 18

- Molecule 1: Protein Kinase SPK1

Chain A:  27% 44% 14% 15%



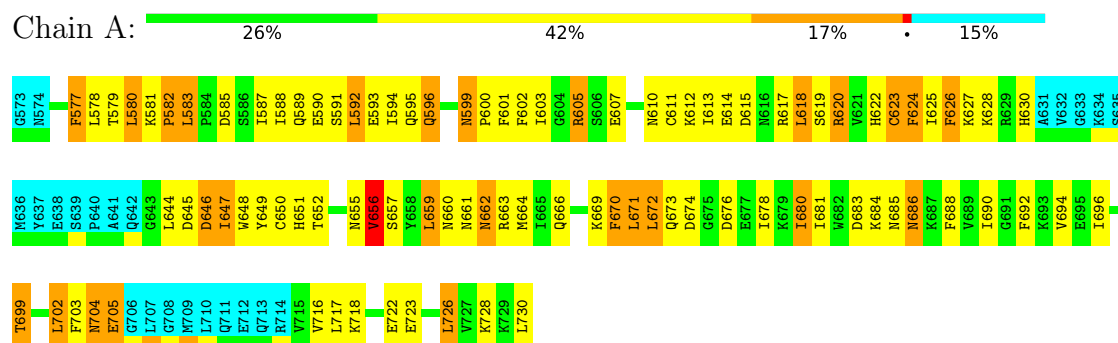
- Molecule 2: DNA repair protein Rad9

Chain P:  100%

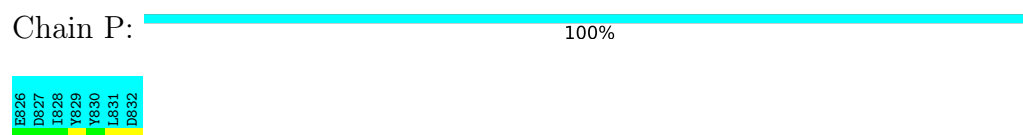


4.2.19 Score per residue for model 19

- Molecule 1: Protein Kinase SPK1

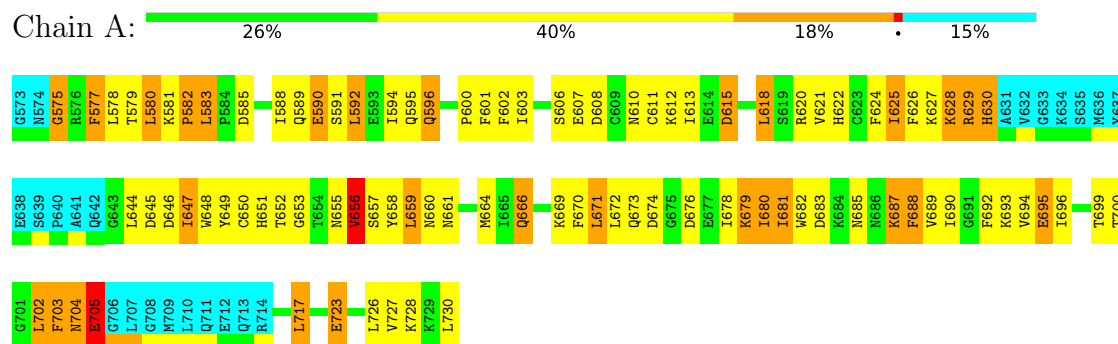


- Molecule 2: DNA repair protein Rad9

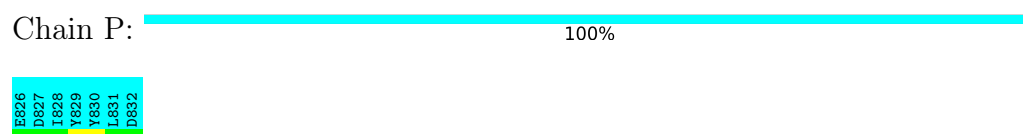


4.2.20 Score per residue for model 20

- Molecule 1: Protein Kinase SPK1

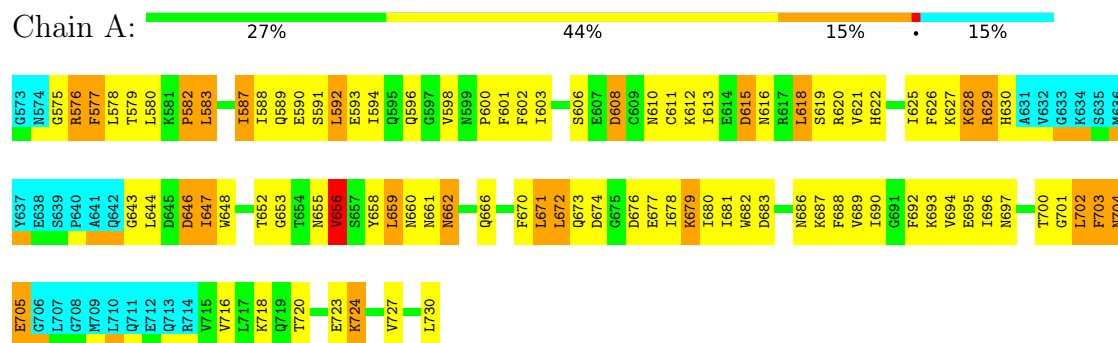


- Molecule 2: DNA repair protein Rad9

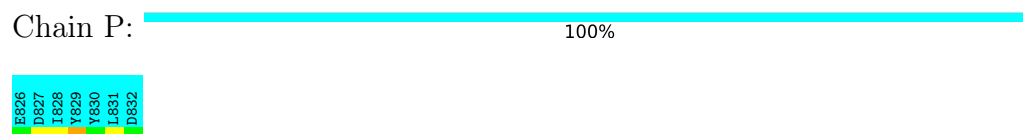


4.2.21 Score per residue for model 21

- Molecule 1: Protein Kinase SPK1

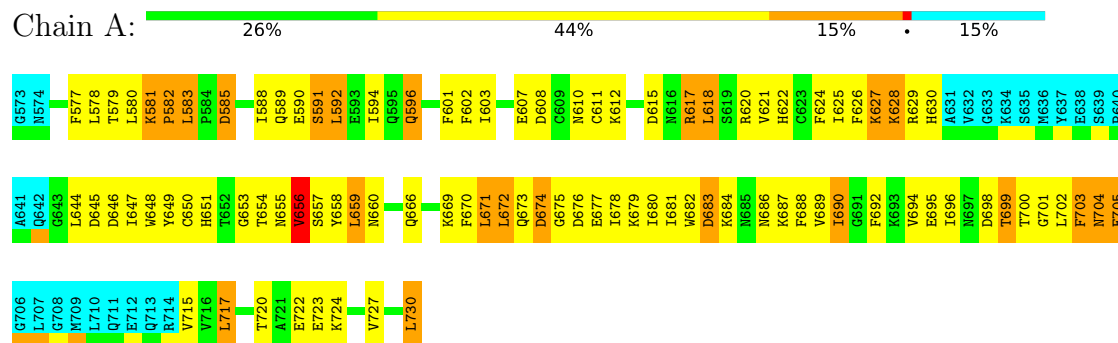


- Molecule 2: DNA repair protein Rad9

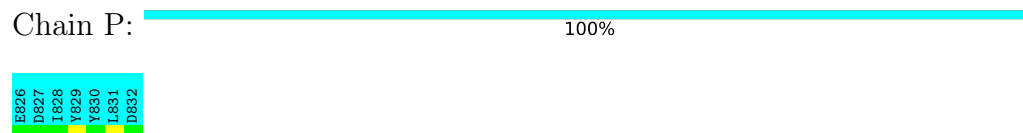


4.2.22 Score per residue for model 22

- Molecule 1: Protein Kinase SPK1



- Molecule 2: DNA repair protein Rad9



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 22 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.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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	1105	1112	1109	99±8
2	P	0	0	0	0±0
All	All	24310	24464	24398	2188

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 45.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:580:LEU:HD22	1:A:694:VAL:HG22	1.04	1.25	20	1
1:A:618:LEU:HD12	1:A:681:ILE:HD12	1.02	1.30	5	9
1:A:592:LEU:HD21	1:A:613:ILE:HD11	1.01	1.32	19	7
1:A:578:LEU:HD12	1:A:647:ILE:HD13	1.00	1.32	9	12
1:A:588:ILE:HD12	1:A:690:ILE:HD11	1.00	1.31	4	1
1:A:578:LEU:HD22	1:A:594:ILE:HD12	0.99	1.33	21	8
1:A:578:LEU:HD11	1:A:694:VAL:HG13	0.98	1.33	4	9
1:A:580:LEU:HD11	1:A:594:ILE:HD11	0.95	1.34	20	2
1:A:659:LEU:HD13	1:A:678:ILE:HG22	0.93	1.40	19	10
1:A:594:ILE:HD11	1:A:625:ILE:HD12	0.93	1.40	22	10
1:A:672:LEU:HD13	1:A:694:VAL:HG21	0.89	1.43	4	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:648:TRP:CH2	1:A:671:LEU:HD22	0.88	2.03	17	17
1:A:580:LEU:HD12	1:A:594:ILE:HD11	0.84	1.44	6	3
1:A:580:LEU:CD2	1:A:694:VAL:HG23	0.83	2.04	4	6
1:A:618:LEU:HD11	1:A:680:ILE:CG2	0.82	2.05	8	5
1:A:663:ARG:O	1:A:716:VAL:HG21	0.80	1.76	18	11
1:A:615:ASP:HB2	1:A:618:LEU:HD22	0.80	1.54	3	2
1:A:578:LEU:HD23	1:A:579:THR:N	0.80	1.92	2	10
1:A:594:ILE:CD1	1:A:625:ILE:HD12	0.80	2.05	22	8
1:A:662:ASN:OD1	1:A:716:VAL:HG23	0.79	1.78	18	4
1:A:598:VAL:HG11	1:A:610:ASN:OD1	0.79	1.77	17	3
1:A:577:PHE:CE2	1:A:702:LEU:HD13	0.78	2.14	17	1
1:A:648:TRP:CZ3	1:A:671:LEU:HD22	0.78	2.13	10	15
1:A:577:PHE:CZ	1:A:647:ILE:HG21	0.78	2.14	12	9
1:A:618:LEU:HD12	1:A:681:ILE:CD1	0.78	2.07	8	6
1:A:644:LEU:HD12	1:A:702:LEU:C	0.77	2.04	11	6
1:A:702:LEU:HD11	1:A:705:GLU:O	0.77	1.79	6	3
1:A:618:LEU:HD11	1:A:680:ILE:HG21	0.77	1.57	8	1
1:A:617:ARG:HB3	1:A:681:ILE:HD13	0.77	1.56	16	7
1:A:703:PHE:O	1:A:705:GLU:N	0.77	2.17	10	6
1:A:696:ILE:HG21	1:A:705:GLU:HB2	0.77	1.56	20	3
1:A:592:LEU:HD13	1:A:611:CYS:SG	0.76	2.20	15	18
1:A:580:LEU:CD2	1:A:694:VAL:HG22	0.76	2.10	20	1
1:A:602:PHE:CG	1:A:730:LEU:HD12	0.76	2.15	13	12
1:A:578:LEU:HD11	1:A:647:ILE:CD1	0.76	2.11	18	1
1:A:588:ILE:CD1	1:A:613:ILE:HG23	0.75	2.11	15	13
1:A:645:ASP:O	1:A:702:LEU:HD12	0.75	1.81	22	2
1:A:680:ILE:HD11	1:A:692:PHE:CE2	0.75	2.16	4	3
1:A:587:ILE:CD1	1:A:690:ILE:HD11	0.75	2.12	15	1
1:A:615:ASP:CB	1:A:618:LEU:HD22	0.74	2.13	12	2
1:A:615:ASP:OD2	1:A:690:ILE:HD13	0.74	1.81	22	2
1:A:580:LEU:HD21	1:A:694:VAL:HG23	0.74	1.58	14	6
1:A:645:ASP:O	1:A:702:LEU:HD13	0.74	1.82	3	10
1:A:578:LEU:HD11	1:A:694:VAL:CG1	0.74	2.13	17	9
1:A:659:LEU:CD2	1:A:678:ILE:HG22	0.74	2.13	4	2
1:A:659:LEU:HD21	1:A:678:ILE:HG22	0.74	1.59	4	2
1:A:649:TYR:CE2	1:A:678:ILE:HG21	0.73	2.18	13	4
1:A:580:LEU:HD22	1:A:694:VAL:CG2	0.73	2.12	20	1
1:A:577:PHE:CE1	1:A:647:ILE:HG21	0.73	2.17	10	8
1:A:588:ILE:HD13	1:A:613:ILE:HG12	0.73	1.61	3	1
1:A:587:ILE:HD11	1:A:615:ASP:OD1	0.73	1.82	19	4
1:A:578:LEU:HD12	1:A:647:ILE:CD1	0.72	2.13	6	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:578:LEU:HD13	1:A:647:ILE:HD13	0.72	1.61	5	7
1:A:578:LEU:HD22	1:A:647:ILE:HD13	0.72	1.59	20	3
1:A:696:ILE:HD12	1:A:705:GLU:O	0.72	1.85	13	5
1:A:618:LEU:HD23	1:A:681:ILE:HD12	0.72	1.59	6	1
1:A:603:ILE:HG23	1:A:611:CYS:SG	0.72	2.24	16	22
1:A:680:ILE:HD12	1:A:692:PHE:CZ	0.72	2.20	19	2
1:A:615:ASP:HB2	1:A:618:LEU:HD13	0.71	1.62	22	12
1:A:615:ASP:CB	1:A:618:LEU:HD13	0.71	2.15	2	14
1:A:647:ILE:HD12	1:A:672:LEU:CB	0.71	2.15	2	16
1:A:622:HIS:CD2	1:A:680:ILE:HG23	0.71	2.20	3	8
1:A:594:ILE:HD13	1:A:625:ILE:HG21	0.71	1.61	20	1
1:A:580:LEU:HD11	1:A:625:ILE:HD11	0.70	1.61	15	5
1:A:580:LEU:HD21	1:A:625:ILE:HD11	0.70	1.62	17	2
1:A:577:PHE:CZ	1:A:702:LEU:HD11	0.70	2.21	14	1
1:A:578:LEU:HD13	1:A:647:ILE:CD1	0.69	2.17	14	7
1:A:578:LEU:HD21	1:A:694:VAL:HG22	0.69	1.63	12	12
1:A:680:ILE:HD12	1:A:692:PHE:CE2	0.69	2.22	8	5
1:A:646:ASP:HB3	1:A:671:LEU:HD21	0.69	1.62	6	2
1:A:659:LEU:HD23	1:A:670:PHE:CD2	0.69	2.23	19	1
1:A:580:LEU:HD11	1:A:625:ILE:CD1	0.69	2.18	3	6
1:A:620:ARG:HG2	1:A:621:VAL:HG23	0.69	1.63	3	2
1:A:582:PRO:HD2	1:A:590:GLU:O	0.69	1.86	12	22
1:A:657:SER:OG	1:A:680:ILE:HG22	0.69	1.88	11	1
1:A:681:ILE:HG22	1:A:690:ILE:HG22	0.68	1.65	12	2
1:A:664:MET:HE1	1:A:670:PHE:HB2	0.68	1.64	14	12
1:A:644:LEU:HD13	1:A:703:PHE:HA	0.68	1.63	10	10
1:A:649:TYR:CD2	1:A:664:MET:HE2	0.67	2.24	8	3
1:A:618:LEU:HD21	1:A:680:ILE:CD1	0.67	2.19	22	1
1:A:603:ILE:CD1	1:A:625:ILE:HD12	0.67	2.19	19	9
1:A:618:LEU:HD23	1:A:618:LEU:O	0.67	1.90	3	2
1:A:645:ASP:O	1:A:702:LEU:HD23	0.66	1.90	14	3
1:A:592:LEU:HD22	1:A:611:CYS:SG	0.66	2.31	22	16
1:A:647:ILE:O	1:A:671:LEU:HD23	0.66	1.91	20	2
1:A:603:ILE:HD11	1:A:625:ILE:HD12	0.66	1.67	2	6
1:A:647:ILE:HD12	1:A:672:LEU:HB2	0.66	1.66	6	19
1:A:592:LEU:N	1:A:592:LEU:HD13	0.65	2.06	12	1
1:A:583:LEU:HD12	1:A:693:LYS:HB2	0.65	1.66	8	1
1:A:587:ILE:CG2	1:A:690:ILE:HD13	0.65	2.22	14	2
1:A:578:LEU:CD2	1:A:694:VAL:HG13	0.65	2.22	18	2
1:A:621:VAL:HG11	1:A:727:VAL:CG2	0.65	2.21	18	10
1:A:657:SER:HG	1:A:680:ILE:HG22	0.65	1.52	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:583:LEU:HD12	1:A:585:ASP:HB2	0.64	1.69	17	12
1:A:696:ILE:HD12	1:A:705:GLU:HG3	0.64	1.67	21	1
1:A:659:LEU:HD11	1:A:672:LEU:CD2	0.64	2.23	4	2
1:A:580:LEU:HG	1:A:694:VAL:HG22	0.64	1.69	22	12
1:A:602:PHE:CE2	1:A:624:PHE:CZ	0.64	2.85	2	2
1:A:659:LEU:HD21	1:A:672:LEU:CD2	0.64	2.23	22	10
1:A:594:ILE:CD1	1:A:625:ILE:HG21	0.64	2.23	20	1
1:A:702:LEU:HD21	1:A:705:GLU:HA	0.64	1.69	22	1
1:A:647:ILE:HD12	1:A:672:LEU:HB3	0.64	1.68	9	6
1:A:703:PHE:O	1:A:704:ASN:C	0.64	2.39	20	1
1:A:623:CYS:SG	1:A:680:ILE:HD11	0.63	2.33	19	5
1:A:577:PHE:CD1	1:A:577:PHE:C	0.63	2.77	19	20
1:A:644:LEU:N	1:A:644:LEU:HD23	0.63	2.08	13	7
1:A:594:ILE:HG23	1:A:601:PHE:CD2	0.63	2.29	22	4
1:A:592:LEU:HD21	1:A:613:ILE:CD1	0.63	2.24	8	2
1:A:594:ILE:HD11	1:A:625:ILE:HD13	0.63	1.70	8	1
1:A:621:VAL:HG11	1:A:727:VAL:HG23	0.63	1.70	5	5
1:A:621:VAL:HG11	1:A:727:VAL:HG21	0.63	1.70	18	2
1:A:649:TYR:CD2	1:A:664:MET:HE1	0.62	2.29	5	2
1:A:587:ILE:HD11	1:A:690:ILE:HD11	0.62	1.68	9	1
1:A:592:LEU:CD2	1:A:613:ILE:HD11	0.62	2.20	19	2
1:A:580:LEU:HD11	1:A:594:ILE:CD1	0.62	2.17	20	4
1:A:618:LEU:CD1	1:A:681:ILE:HD12	0.62	2.19	5	6
1:A:702:LEU:HD11	1:A:705:GLU:C	0.62	2.20	6	1
1:A:575:GLY:O	1:A:595:GLN:NE2	0.62	2.33	8	5
1:A:603:ILE:N	1:A:603:ILE:HD12	0.61	2.10	11	3
1:A:672:LEU:CD1	1:A:694:VAL:HG21	0.61	2.22	4	2
1:A:643:GLY:C	1:A:644:LEU:HD23	0.61	2.21	13	6
1:A:602:PHE:CD2	1:A:730:LEU:HD12	0.61	2.31	2	4
1:A:615:ASP:OD2	1:A:681:ILE:HG21	0.61	1.96	17	1
1:A:588:ILE:CD1	1:A:690:ILE:HD11	0.60	2.18	4	1
1:A:696:ILE:HD13	1:A:705:GLU:O	0.60	1.96	3	6
1:A:723:GLU:HA	1:A:726:LEU:HD12	0.60	1.74	19	7
1:A:587:ILE:HD13	1:A:688:PHE:CE1	0.60	2.32	11	3
1:A:594:ILE:HG23	1:A:601:PHE:CD1	0.60	2.31	19	14
1:A:674:ASP:HB2	1:A:696:ILE:HD12	0.60	1.73	10	6
1:A:578:LEU:HD22	1:A:647:ILE:CD1	0.60	2.27	22	4
1:A:587:ILE:HD13	1:A:690:ILE:HD11	0.60	1.73	15	2
1:A:618:LEU:HG	1:A:622:HIS:CD2	0.60	2.32	4	2
1:A:659:LEU:C	1:A:659:LEU:HD12	0.60	2.21	12	17
1:A:662:ASN:CG	1:A:716:VAL:HG23	0.60	2.21	21	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:615:ASP:CG	1:A:690:ILE:HD13	0.60	2.22	16	2
1:A:644:LEU:HD23	1:A:701:GLY:O	0.60	1.97	17	1
1:A:578:LEU:HD11	1:A:647:ILE:HD13	0.60	1.74	18	1
1:A:615:ASP:HB3	1:A:618:LEU:HD22	0.60	1.73	18	1
1:A:681:ILE:HG22	1:A:690:ILE:CG2	0.59	2.27	4	1
1:A:674:ASP:N	1:A:696:ILE:HD12	0.59	2.12	22	2
1:A:644:LEU:HD13	1:A:703:PHE:CA	0.59	2.27	10	3
1:A:730:LEU:O	1:A:730:LEU:HD23	0.59	1.97	19	1
1:A:578:LEU:HD11	1:A:647:ILE:HD12	0.59	1.74	18	1
1:A:612:LYS:O	1:A:613:ILE:HD13	0.59	1.98	1	2
1:A:696:ILE:HD13	1:A:705:GLU:HB2	0.59	1.75	22	5
1:A:578:LEU:CD1	1:A:647:ILE:HD13	0.59	2.24	2	8
1:A:702:LEU:HD22	1:A:705:GLU:C	0.59	2.23	17	1
1:A:578:LEU:HD23	1:A:578:LEU:C	0.59	2.22	16	9
1:A:578:LEU:HD22	1:A:580:LEU:CD1	0.59	2.28	8	1
1:A:591:SER:C	1:A:592:LEU:HD13	0.59	2.22	12	3
1:A:703:PHE:O	1:A:703:PHE:CG	0.59	2.56	6	4
1:A:583:LEU:HD22	1:A:693:LYS:HB2	0.59	1.74	14	13
1:A:578:LEU:HD22	1:A:594:ILE:CD1	0.58	2.21	21	2
1:A:603:ILE:HD12	1:A:624:PHE:HA	0.58	1.75	18	6
1:A:674:ASP:CB	1:A:696:ILE:HD12	0.58	2.28	20	2
1:A:577:PHE:CE1	1:A:702:LEU:HD11	0.58	2.33	14	1
1:A:674:ASP:CA	1:A:696:ILE:HD12	0.58	2.27	20	1
1:A:671:LEU:HD12	1:A:672:LEU:N	0.58	2.13	16	2
1:A:588:ILE:HD13	1:A:613:ILE:HD12	0.58	1.74	9	2
1:A:578:LEU:CD1	1:A:694:VAL:HG13	0.58	2.28	17	8
1:A:644:LEU:HD12	1:A:701:GLY:O	0.58	1.97	21	1
1:A:588:ILE:HD13	1:A:613:ILE:HG23	0.58	1.75	7	6
1:A:681:ILE:HG22	1:A:690:ILE:CG1	0.58	2.29	2	4
1:A:649:TYR:CE2	1:A:664:MET:HE2	0.58	2.34	18	3
1:A:578:LEU:C	1:A:578:LEU:HD23	0.57	2.25	1	3
1:A:624:PHE:O	1:A:650:CYS:N	0.57	2.35	2	12
1:A:623:CYS:SG	1:A:680:ILE:HG21	0.57	2.39	11	3
1:A:580:LEU:CD1	1:A:594:ILE:HD11	0.57	2.30	16	7
1:A:644:LEU:HD12	1:A:703:PHE:N	0.57	2.14	1	7
1:A:655:ASN:O	1:A:656:VAL:O	0.57	2.22	6	18
1:A:644:LEU:HD12	1:A:703:PHE:HA	0.57	1.76	6	2
1:A:644:LEU:HD13	1:A:703:PHE:CB	0.57	2.29	17	1
1:A:587:ILE:HG22	1:A:690:ILE:CD1	0.57	2.30	21	1
1:A:680:ILE:HD11	1:A:692:PHE:CZ	0.57	2.34	16	1
1:A:615:ASP:CB	1:A:618:LEU:HD21	0.57	2.30	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:649:TYR:CE1	1:A:678:ILE:HD12	0.57	2.34	12	1
1:A:655:ASN:C	1:A:656:VAL:HG13	0.57	2.25	4	4
1:A:577:PHE:CD2	1:A:698:ASP:O	0.57	2.58	18	7
1:A:648:TRP:CZ3	1:A:671:LEU:HG	0.56	2.35	20	5
1:A:659:LEU:HG	1:A:678:ILE:HG23	0.56	1.76	18	3
1:A:688:PHE:CG	1:A:688:PHE:O	0.56	2.58	9	4
1:A:584:PRO:HA	1:A:589:GLN:CD	0.56	2.25	12	2
1:A:588:ILE:HD12	1:A:613:ILE:HG23	0.56	1.76	6	1
1:A:681:ILE:CG2	1:A:690:ILE:HG22	0.56	2.30	12	1
1:A:586:SER:O	1:A:589:GLN:NE2	0.56	2.38	12	7
1:A:703:PHE:C	1:A:703:PHE:CD1	0.56	2.83	6	1
1:A:594:ILE:HG23	1:A:601:PHE:CG	0.56	2.36	6	10
1:A:615:ASP:HB2	1:A:618:LEU:HD21	0.56	1.78	6	2
1:A:578:LEU:HD12	1:A:696:ILE:HG12	0.56	1.75	14	2
1:A:644:LEU:HD12	1:A:703:PHE:CA	0.55	2.31	6	2
1:A:613:ILE:HD13	1:A:692:PHE:CZ	0.55	2.36	3	1
1:A:622:HIS:CE1	1:A:681:ILE:HD11	0.55	2.36	13	5
1:A:648:TRP:CZ2	1:A:671:LEU:HD22	0.55	2.35	7	2
1:A:659:LEU:HD13	1:A:678:ILE:HG12	0.55	1.78	21	6
1:A:659:LEU:HD13	1:A:678:ILE:CG2	0.55	2.23	19	5
1:A:681:ILE:HG21	1:A:688:PHE:CE1	0.55	2.36	20	1
1:A:648:TRP:CH2	1:A:671:LEU:HD12	0.55	2.37	20	1
1:A:624:PHE:CE1	1:A:727:VAL:HG22	0.55	2.36	1	1
1:A:625:ILE:HG23	1:A:648:TRP:O	0.55	2.01	5	2
1:A:622:HIS:O	1:A:653:GLY:N	0.55	2.39	12	21
1:A:648:TRP:CH2	1:A:671:LEU:CD2	0.55	2.89	7	14
1:A:644:LEU:HD13	1:A:703:PHE:HB2	0.55	1.78	17	1
1:A:580:LEU:N	1:A:592:LEU:O	0.55	2.39	19	15
1:A:670:PHE:CE1	1:A:716:VAL:HG22	0.54	2.37	16	2
1:A:618:LEU:HD12	1:A:680:ILE:HG21	0.54	1.78	3	2
1:A:577:PHE:HE2	1:A:702:LEU:HD13	0.54	1.61	17	1
1:A:580:LEU:O	1:A:592:LEU:N	0.54	2.40	11	14
1:A:580:LEU:HB3	1:A:592:LEU:HD12	0.54	1.78	14	3
1:A:587:ILE:CG1	1:A:690:ILE:HD11	0.54	2.32	7	1
1:A:577:PHE:CE2	1:A:647:ILE:HG21	0.54	2.38	12	11
1:A:655:ASN:O	1:A:656:VAL:HG13	0.54	2.02	12	19
1:A:730:LEU:C	1:A:730:LEU:HD23	0.54	2.28	4	10
1:A:613:ILE:HD13	1:A:692:PHE:CE2	0.54	2.38	3	1
1:A:577:PHE:HE1	1:A:647:ILE:HG21	0.54	1.63	4	5
1:A:703:PHE:CD2	1:A:704:ASN:OD1	0.54	2.60	21	4
1:A:582:PRO:CB	1:A:588:ILE:HG23	0.54	2.33	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:582:PRO:CD	1:A:590:GLU:O	0.54	2.55	12	22
1:A:618:LEU:CB	1:A:622:HIS:CG	0.54	2.91	17	2
1:A:648:TRP:CZ3	1:A:717:LEU:HD13	0.54	2.38	22	1
1:A:682:TRP:CD1	1:A:689:VAL:HG23	0.53	2.38	7	1
1:A:601:PHE:CZ	1:A:610:ASN:HB3	0.53	2.39	18	20
1:A:630:HIS:CD2	1:A:630:HIS:C	0.53	2.86	20	8
1:A:702:LEU:O	1:A:702:LEU:HD12	0.53	2.04	20	2
1:A:587:ILE:HD13	1:A:688:PHE:CZ	0.53	2.39	16	2
1:A:580:LEU:HD21	1:A:625:ILE:CD1	0.53	2.33	22	2
1:A:702:LEU:HD22	1:A:705:GLU:HA	0.53	1.81	21	1
1:A:603:ILE:CG1	1:A:611:CYS:HB3	0.53	2.34	8	10
1:A:644:LEU:HD22	1:A:702:LEU:C	0.53	2.28	14	5
1:A:664:MET:HE3	1:A:716:VAL:HG13	0.53	1.81	10	2
1:A:630:HIS:N	1:A:644:LEU:O	0.53	2.41	22	19
1:A:630:HIS:CE1	1:A:703:PHE:CD2	0.53	2.97	5	1
1:A:704:ASN:O	1:A:705:GLU:CB	0.52	2.56	2	13
1:A:584:PRO:O	1:A:589:GLN:NE2	0.52	2.42	4	4
1:A:622:HIS:CD2	1:A:680:ILE:CG2	0.52	2.92	21	5
1:A:703:PHE:O	1:A:703:PHE:CD1	0.52	2.61	10	2
1:A:586:SER:OG	1:A:690:ILE:HD13	0.52	2.05	3	2
1:A:615:ASP:OD2	1:A:690:ILE:HD12	0.52	2.05	18	1
1:A:618:LEU:HD21	1:A:680:ILE:HD11	0.52	1.81	22	1
1:A:644:LEU:HD22	1:A:702:LEU:O	0.52	2.04	16	5
1:A:644:LEU:HD12	1:A:703:PHE:H	0.52	1.63	20	1
1:A:656:VAL:HG23	1:A:664:MET:O	0.52	2.04	3	3
1:A:724:LYS:O	1:A:727:VAL:HG12	0.52	2.04	22	7
1:A:592:LEU:HD11	1:A:692:PHE:CE2	0.52	2.40	7	8
1:A:648:TRP:CH2	1:A:671:LEU:HG	0.52	2.40	20	5
1:A:618:LEU:HD23	1:A:622:HIS:CB	0.52	2.34	19	1
1:A:598:VAL:HG11	1:A:610:ASN:ND2	0.52	2.19	7	3
1:A:648:TRP:CH2	1:A:671:LEU:CD1	0.52	2.93	20	1
1:A:696:ILE:HG21	1:A:705:GLU:CB	0.52	2.31	20	2
1:A:652:THR:O	1:A:666:GLN:NE2	0.51	2.43	17	15
1:A:583:LEU:HD11	1:A:677:GLU:OE2	0.51	2.05	22	1
1:A:575:GLY:O	1:A:595:GLN:HG3	0.51	2.06	16	5
1:A:592:LEU:HD11	1:A:613:ILE:HD11	0.51	1.82	15	1
1:A:618:LEU:HD21	1:A:680:ILE:HD12	0.51	1.81	22	1
1:A:730:LEU:HD23	1:A:730:LEU:C	0.51	2.31	19	1
1:A:617:ARG:HB2	1:A:681:ILE:HD13	0.51	1.83	10	3
1:A:669:LYS:HE2	1:A:717:LEU:HD13	0.51	1.82	20	1
1:A:618:LEU:HD23	1:A:680:ILE:CG2	0.51	2.35	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:578:LEU:HD12	1:A:696:ILE:CG1	0.51	2.35	14	3
1:A:594:ILE:HD13	1:A:625:ILE:HD13	0.51	1.81	20	1
1:A:689:VAL:O	1:A:690:ILE:HD13	0.51	2.06	8	1
1:A:580:LEU:HD11	1:A:625:ILE:HD13	0.51	1.82	16	4
1:A:644:LEU:N	1:A:644:LEU:CD2	0.51	2.74	13	7
1:A:659:LEU:HD23	1:A:670:PHE:CD1	0.51	2.41	13	1
1:A:587:ILE:HG22	1:A:689:VAL:O	0.50	2.06	14	2
1:A:680:ILE:CG2	1:A:690:ILE:HG21	0.50	2.36	17	1
1:A:577:PHE:HZ	1:A:647:ILE:HG21	0.50	1.62	12	1
1:A:618:LEU:HD12	1:A:680:ILE:CG2	0.50	2.36	3	1
1:A:664:MET:HE3	1:A:670:PHE:HB2	0.50	1.82	15	2
1:A:675:GLY:N	1:A:694:VAL:O	0.50	2.44	17	10
1:A:582:PRO:HB2	1:A:588:ILE:HG22	0.50	1.82	9	1
1:A:702:LEU:HD12	1:A:705:GLU:CA	0.50	2.35	18	1
1:A:586:SER:OG	1:A:690:ILE:HA	0.50	2.07	16	2
1:A:651:HIS:CG	1:A:657:SER:OG	0.50	2.65	13	1
1:A:578:LEU:HD13	1:A:647:ILE:HD11	0.50	1.83	14	1
1:A:702:LEU:HD12	1:A:705:GLU:C	0.50	2.32	18	1
1:A:662:ASN:HB2	1:A:670:PHE:CZ	0.50	2.42	16	2
1:A:682:TRP:HB2	1:A:689:VAL:HG23	0.50	1.83	9	1
1:A:608:ASP:CG	1:A:730:LEU:HD21	0.50	2.32	15	1
1:A:618:LEU:HB2	1:A:622:HIS:CG	0.50	2.42	17	1
1:A:618:LEU:HD12	1:A:622:HIS:CB	0.50	2.36	18	1
1:A:578:LEU:HD21	1:A:694:VAL:HG13	0.50	1.83	18	2
1:A:600:PRO:HD3	1:A:726:LEU:HD22	0.50	1.82	4	1
1:A:578:LEU:HD13	1:A:696:ILE:HG12	0.49	1.84	4	1
1:A:603:ILE:HG13	1:A:611:CYS:HB3	0.49	1.83	20	10
1:A:659:LEU:CD1	1:A:678:ILE:HG22	0.49	2.27	19	4
1:A:655:ASN:C	1:A:656:VAL:CG1	0.49	2.85	12	19
1:A:592:LEU:HD22	1:A:592:LEU:N	0.49	2.22	10	1
1:A:617:ARG:O	1:A:655:ASN:ND2	0.49	2.45	18	6
1:A:659:LEU:HG	1:A:670:PHE:CD2	0.49	2.43	16	6
1:A:681:ILE:HB	1:A:690:ILE:HD12	0.49	1.85	19	1
1:A:583:LEU:H	1:A:583:LEU:HD13	0.49	1.67	8	1
1:A:608:ASP:OD1	1:A:730:LEU:HD21	0.49	2.07	15	1
1:A:680:ILE:CD1	1:A:692:PHE:CE2	0.49	2.95	20	1
1:A:618:LEU:HD21	1:A:680:ILE:HD13	0.49	1.85	2	2
1:A:580:LEU:HD12	1:A:594:ILE:CD1	0.49	2.38	16	3
1:A:606:SER:CB	1:A:620:ARG:HB2	0.49	2.38	3	1
1:A:703:PHE:CG	1:A:704:ASN:N	0.49	2.80	20	3
1:A:615:ASP:OD2	1:A:690:ILE:HD11	0.49	2.07	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:654:THR:O	1:A:654:THR:HG22	0.49	2.07	5	4
1:A:594:ILE:HD11	1:A:625:ILE:CD1	0.49	2.35	15	5
1:A:587:ILE:HG22	1:A:690:ILE:HD13	0.49	1.84	11	2
1:A:680:ILE:HG13	1:A:690:ILE:HG21	0.49	1.83	11	1
1:A:645:ASP:O	1:A:702:LEU:HG	0.48	2.07	17	1
1:A:602:PHE:CB	1:A:730:LEU:HD12	0.48	2.39	13	1
1:A:649:TYR:CD2	1:A:664:MET:HE3	0.48	2.43	17	1
1:A:589:GLN:OE1	1:A:589:GLN:CA	0.48	2.61	16	2
1:A:618:LEU:HD12	1:A:622:HIS:CG	0.48	2.42	18	1
1:A:659:LEU:HD12	1:A:670:PHE:HB3	0.48	1.85	4	1
1:A:580:LEU:CD2	1:A:625:ILE:HD11	0.48	2.37	17	2
1:A:595:GLN:O	1:A:596:GLN:C	0.48	2.55	19	1
1:A:577:PHE:CB	1:A:596:GLN:HB3	0.48	2.38	8	16
1:A:662:ASN:CB	1:A:670:PHE:CE1	0.48	2.97	9	1
1:A:587:ILE:HD11	1:A:688:PHE:CE1	0.48	2.44	4	1
1:A:662:ASN:CB	1:A:670:PHE:CZ	0.48	2.97	16	2
1:A:577:PHE:CG	1:A:578:LEU:N	0.48	2.82	1	8
1:A:630:HIS:ND1	1:A:646:ASP:OD2	0.48	2.46	9	3
1:A:703:PHE:N	1:A:703:PHE:CD1	0.48	2.82	1	1
1:A:649:TYR:HB2	1:A:672:LEU:HD11	0.48	1.86	19	2
1:A:580:LEU:HD23	1:A:580:LEU:N	0.48	2.23	20	1
1:A:659:LEU:CD1	1:A:670:PHE:CD2	0.47	2.97	5	3
1:A:659:LEU:CG	1:A:678:ILE:HG22	0.47	2.39	4	2
1:A:617:ARG:CB	1:A:681:ILE:HD13	0.47	2.39	8	4
1:A:646:ASP:CB	1:A:671:LEU:HD21	0.47	2.38	20	1
1:A:602:PHE:CD2	1:A:624:PHE:CE1	0.47	3.02	19	2
1:A:649:TYR:CD1	1:A:664:MET:HE2	0.47	2.44	3	1
1:A:662:ASN:CB	1:A:670:PHE:CE2	0.47	2.98	7	2
1:A:582:PRO:CG	1:A:613:ILE:HD11	0.47	2.39	12	1
1:A:659:LEU:HD22	1:A:678:ILE:HG12	0.47	1.86	15	1
1:A:577:PHE:HB2	1:A:596:GLN:HB3	0.47	1.85	18	9
1:A:646:ASP:CG	1:A:703:PHE:CE1	0.47	2.93	9	9
1:A:704:ASN:O	1:A:705:GLU:HB3	0.47	2.09	13	6
1:A:618:LEU:CB	1:A:622:HIS:ND1	0.47	2.77	1	4
1:A:577:PHE:CE1	1:A:647:ILE:CG2	0.47	2.97	3	5
1:A:627:LYS:HD3	1:A:647:ILE:HG23	0.47	1.86	11	1
1:A:651:HIS:ND1	1:A:657:SER:CB	0.47	2.77	22	7
1:A:615:ASP:CB	1:A:618:LEU:CD2	0.47	2.92	6	2
1:A:651:HIS:CE1	1:A:657:SER:N	0.47	2.83	12	5
1:A:704:ASN:ND2	1:A:705:GLU:CG	0.47	2.78	8	6
1:A:704:ASN:O	1:A:704:ASN:CG	0.47	2.58	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:692:PHE:N	1:A:692:PHE:CD1	0.47	2.81	12	5
1:A:615:ASP:OD1	1:A:690:ILE:HD11	0.47	2.10	9	1
1:A:602:PHE:HA	1:A:624:PHE:CB	0.47	2.40	1	5
1:A:577:PHE:CD1	1:A:578:LEU:HB2	0.47	2.45	10	3
1:A:656:VAL:CG2	1:A:658:TYR:CZ	0.47	2.98	4	1
1:A:624:PHE:CE1	1:A:727:VAL:CG2	0.47	2.98	1	1
1:A:587:ILE:CD1	1:A:688:PHE:CE1	0.47	2.97	18	3
1:A:649:TYR:HD2	1:A:664:MET:HE1	0.47	1.70	5	1
1:A:575:GLY:O	1:A:595:GLN:CG	0.47	2.63	7	2
1:A:674:ASP:HB3	1:A:696:ILE:HD12	0.47	1.87	12	1
1:A:648:TRP:CZ3	1:A:671:LEU:CG	0.47	2.97	20	1
1:A:649:TYR:HB3	1:A:672:LEU:HD21	0.46	1.86	2	2
1:A:681:ILE:HG22	1:A:690:ILE:HB	0.46	1.86	2	1
1:A:627:LYS:CE	1:A:647:ILE:HG23	0.46	2.39	22	2
1:A:587:ILE:HD13	1:A:689:VAL:O	0.46	2.10	12	1
1:A:704:ASN:ND2	1:A:705:GLU:N	0.46	2.62	4	5
1:A:659:LEU:HD23	1:A:670:PHE:HB3	0.46	1.87	20	7
1:A:702:LEU:HD22	1:A:705:GLU:CA	0.46	2.40	21	1
1:A:575:GLY:CA	1:A:596:GLN:OE1	0.46	2.64	1	6
1:A:578:LEU:CD1	1:A:696:ILE:CG1	0.46	2.93	20	4
1:A:587:ILE:HG12	1:A:690:ILE:HD11	0.46	1.86	7	2
1:A:618:LEU:CD1	1:A:680:ILE:HG21	0.46	2.40	3	2
1:A:716:VAL:HG13	1:A:716:VAL:O	0.46	2.09	3	1
1:A:658:TYR:N	1:A:658:TYR:CD1	0.46	2.83	4	2
1:A:602:PHE:CD1	1:A:730:LEU:HD12	0.46	2.46	1	1
1:A:649:TYR:CB	1:A:672:LEU:HD21	0.46	2.41	2	6
1:A:671:LEU:HD12	1:A:671:LEU:C	0.46	2.35	7	1
1:A:577:PHE:CE1	1:A:702:LEU:CD1	0.46	2.98	14	1
1:A:703:PHE:CE2	1:A:704:ASN:OD1	0.46	2.68	18	2
1:A:696:ILE:CD1	1:A:705:GLU:O	0.46	2.63	2	5
1:A:681:ILE:HG22	1:A:690:ILE:HG13	0.46	1.87	17	1
1:A:618:LEU:HD11	1:A:680:ILE:HD11	0.46	1.87	22	1
1:A:659:LEU:HB3	1:A:670:PHE:CD2	0.46	2.45	15	1
1:A:702:LEU:HD22	1:A:705:GLU:O	0.46	2.10	17	1
1:A:578:LEU:CD1	1:A:647:ILE:CD1	0.46	2.93	12	3
1:A:618:LEU:HB3	1:A:622:HIS:CG	0.46	2.46	6	2
1:A:577:PHE:CE2	1:A:627:LYS:CE	0.46	2.99	19	2
1:A:577:PHE:CE2	1:A:647:ILE:CG2	0.46	2.99	19	2
1:A:599:ASN:ND2	1:A:626:PHE:CD2	0.46	2.84	19	1
1:A:582:PRO:CB	1:A:588:ILE:HG22	0.46	2.41	9	1
1:A:703:PHE:CD1	1:A:703:PHE:N	0.46	2.84	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:649:TYR:O	1:A:669:LYS:HA	0.46	2.11	6	3
1:A:651:HIS:CE1	1:A:657:SER:OG	0.46	2.69	6	3
1:A:578:LEU:HD22	1:A:694:VAL:HG13	0.46	1.86	18	1
1:A:609:CYS:SG	1:A:621:VAL:HG22	0.46	2.51	14	2
1:A:579:THR:O	1:A:695:GLU:N	0.46	2.49	8	12
1:A:578:LEU:CG	1:A:694:VAL:HG13	0.46	2.40	14	3
1:A:702:LEU:O	1:A:702:LEU:CG	0.46	2.63	6	2
1:A:682:TRP:CB	1:A:689:VAL:HG23	0.46	2.41	9	2
1:A:622:HIS:CD2	1:A:680:ILE:HB	0.46	2.45	11	2
1:A:651:HIS:NE2	1:A:653:GLY:O	0.46	2.49	12	1
1:A:588:ILE:HD11	1:A:613:ILE:HG23	0.46	1.84	21	1
1:A:615:ASP:O	1:A:618:LEU:HB2	0.45	2.10	16	1
1:A:658:TYR:O	1:A:679:LYS:N	0.45	2.42	21	2
1:A:681:ILE:CG2	1:A:688:PHE:CE1	0.45	2.99	20	1
1:A:626:PHE:CZ	1:A:628:LYS:CG	0.45	3.00	4	15
1:A:582:PRO:CB	1:A:588:ILE:CG2	0.45	2.95	12	2
1:A:580:LEU:CD2	1:A:678:ILE:HD11	0.45	2.42	16	2
1:A:644:LEU:HD12	1:A:703:PHE:CB	0.45	2.41	6	1
1:A:577:PHE:CE1	1:A:696:ILE:HG23	0.45	2.47	7	3
1:A:664:MET:HE1	1:A:716:VAL:HG13	0.45	1.88	16	2
1:A:580:LEU:HD22	1:A:692:PHE:HB2	0.45	1.87	14	1
1:A:646:ASP:OD2	1:A:703:PHE:CE1	0.45	2.70	21	7
1:A:680:ILE:HG22	1:A:690:ILE:CG2	0.45	2.41	18	1
1:A:587:ILE:CD1	1:A:688:PHE:CZ	0.45	3.00	13	3
1:A:578:LEU:O	1:A:594:ILE:N	0.45	2.49	21	6
1:A:592:LEU:HD11	1:A:692:PHE:CD2	0.45	2.46	19	1
1:A:601:PHE:HB3	1:A:625:ILE:CG2	0.45	2.42	20	1
1:A:704:ASN:O	1:A:705:GLU:HG2	0.45	2.11	9	2
1:A:605:ARG:CD	1:A:615:ASP:O	0.45	2.65	16	1
1:A:594:ILE:CD1	1:A:625:ILE:CD1	0.45	2.94	5	4
1:A:659:LEU:CD2	1:A:670:PHE:CD2	0.45	2.99	19	1
1:A:651:HIS:ND1	1:A:657:SER:OG	0.45	2.50	19	5
1:A:580:LEU:CD1	1:A:625:ILE:CD1	0.45	2.94	5	1
1:A:601:PHE:CE2	1:A:610:ASN:HB3	0.45	2.46	8	4
1:A:580:LEU:CD2	1:A:694:VAL:CG2	0.45	2.95	21	3
1:A:600:PRO:HG2	1:A:602:PHE:CZ	0.45	2.47	10	11
1:A:626:PHE:N	1:A:648:TRP:O	0.45	2.48	4	4
1:A:598:VAL:HG11	1:A:610:ASN:CG	0.45	2.37	9	2
1:A:618:LEU:HG	1:A:622:HIS:CG	0.45	2.47	2	6
1:A:670:PHE:CD1	1:A:671:LEU:N	0.45	2.85	22	1
1:A:594:ILE:HG12	1:A:601:PHE:CD2	0.44	2.48	2	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:594:ILE:HG23	1:A:601:PHE:CB	0.44	2.42	6	1
1:A:651:HIS:ND1	1:A:657:SER:HB3	0.44	2.27	8	2
1:A:613:ILE:HG13	1:A:692:PHE:CZ	0.44	2.46	12	2
1:A:681:ILE:CB	1:A:690:ILE:HG22	0.44	2.42	12	1
1:A:646:ASP:OD2	1:A:703:PHE:CZ	0.44	2.71	18	3
1:A:624:PHE:CE1	1:A:650:CYS:CB	0.44	3.00	3	1
1:A:646:ASP:OD1	1:A:703:PHE:CD1	0.44	2.71	10	4
1:A:617:ARG:CG	1:A:688:PHE:CD2	0.44	3.01	6	1
1:A:700:THR:HG23	1:A:700:THR:O	0.44	2.12	12	4
1:A:657:SER:HG	1:A:680:ILE:CG2	0.44	2.24	11	1
1:A:618:LEU:HB2	1:A:622:HIS:ND1	0.44	2.27	9	2
1:A:608:ASP:HB3	1:A:730:LEU:HD21	0.44	1.90	21	2
1:A:577:PHE:CZ	1:A:647:ILE:CG2	0.44	3.01	19	2
1:A:605:ARG:HG2	1:A:618:LEU:CD1	0.44	2.43	1	3
1:A:659:LEU:C	1:A:659:LEU:CD1	0.44	2.90	9	7
1:A:600:PRO:CG	1:A:624:PHE:CZ	0.44	3.01	2	1
1:A:577:PHE:HE1	1:A:647:ILE:HD13	0.44	1.72	5	1
1:A:603:ILE:N	1:A:603:ILE:CD1	0.44	2.80	11	2
1:A:619:SER:O	1:A:620:ARG:C	0.44	2.61	19	2
1:A:662:ASN:ND2	1:A:716:VAL:HG23	0.44	2.27	16	1
1:A:702:LEU:O	1:A:703:PHE:C	0.44	2.61	18	2
1:A:629:ARG:O	1:A:629:ARG:HG3	0.44	2.12	7	3
1:A:594:ILE:HG23	1:A:601:PHE:HB2	0.44	1.88	6	1
1:A:582:PRO:HB2	1:A:588:ILE:HG23	0.44	1.89	19	2
1:A:588:ILE:O	1:A:588:ILE:CG2	0.44	2.66	16	1
1:A:704:ASN:ND2	1:A:705:GLU:HG2	0.44	2.27	17	1
1:A:646:ASP:OD2	1:A:671:LEU:HD11	0.44	2.13	20	1
1:A:644:LEU:HD22	1:A:644:LEU:H	0.44	1.72	21	1
1:A:582:PRO:CD	1:A:592:LEU:CD2	0.44	2.95	18	3
1:A:600:PRO:HB2	1:A:624:PHE:CE1	0.44	2.47	19	2
1:A:615:ASP:CB	1:A:618:LEU:CD1	0.44	2.94	2	3
1:A:699:THR:O	1:A:699:THR:OG1	0.44	2.35	12	4
1:A:615:ASP:CG	1:A:688:PHE:CZ	0.44	2.96	4	1
1:A:702:LEU:HD12	1:A:705:GLU:O	0.44	2.12	11	2
1:A:578:LEU:HD22	1:A:580:LEU:HD12	0.44	1.88	8	1
1:A:696:ILE:HD13	1:A:705:GLU:C	0.44	2.38	10	1
1:A:699:THR:O	1:A:701:GLY:N	0.44	2.50	10	3
1:A:644:LEU:CD2	1:A:644:LEU:N	0.44	2.81	20	1
1:A:673:GLN:O	1:A:674:ASP:C	0.44	2.61	1	5
1:A:580:LEU:HD22	1:A:692:PHE:CB	0.44	2.42	14	2
1:A:603:ILE:CD1	1:A:625:ILE:CD1	0.44	2.96	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:594:ILE:HG12	1:A:601:PHE:CD1	0.44	2.47	22	3
1:A:600:PRO:HB3	1:A:626:PHE:HB2	0.44	1.90	15	11
1:A:575:GLY:O	1:A:596:GLN:N	0.44	2.51	10	1
1:A:618:LEU:HB3	1:A:681:ILE:HD11	0.44	1.89	14	1
1:A:588:ILE:HG23	1:A:588:ILE:O	0.44	2.13	16	1
1:A:702:LEU:HD13	1:A:703:PHE:CD1	0.44	2.48	18	1
1:A:703:PHE:CZ	1:A:704:ASN:HB3	0.44	2.48	20	1
1:A:645:ASP:O	1:A:702:LEU:CD2	0.43	2.66	1	2
1:A:662:ASN:CG	1:A:670:PHE:CE2	0.43	2.96	6	7
1:A:644:LEU:HB2	1:A:703:PHE:CA	0.43	2.43	9	2
1:A:581:LYS:HA	1:A:591:SER:HA	0.43	1.88	12	2
1:A:588:ILE:HG21	1:A:613:ILE:HD12	0.43	1.90	16	1
1:A:646:ASP:OD1	1:A:703:PHE:CZ	0.43	2.71	21	4
1:A:644:LEU:HD22	1:A:703:PHE:HA	0.43	1.90	9	3
1:A:646:ASP:OD2	1:A:703:PHE:CD1	0.43	2.71	19	2
1:A:670:PHE:CE1	1:A:715:VAL:C	0.43	2.96	15	1
1:A:577:PHE:CE2	1:A:702:LEU:HD23	0.43	2.49	18	1
1:A:582:PRO:CD	1:A:592:LEU:HD22	0.43	2.43	1	2
1:A:646:ASP:OD1	1:A:703:PHE:CE1	0.43	2.71	14	6
1:A:577:PHE:CE2	1:A:578:LEU:HB2	0.43	2.48	12	1
1:A:647:ILE:CD1	1:A:672:LEU:HB2	0.43	2.44	22	2
1:A:699:THR:HB	1:A:702:LEU:CD2	0.43	2.44	22	1
1:A:626:PHE:CZ	1:A:628:LYS:HG3	0.43	2.49	4	10
1:A:621:VAL:CG2	1:A:730:LEU:HD13	0.43	2.42	5	1
1:A:645:ASP:O	1:A:702:LEU:O	0.43	2.35	6	1
1:A:658:TYR:CD1	1:A:658:TYR:N	0.43	2.86	22	2
1:A:699:THR:CB	1:A:702:LEU:CD2	0.43	2.97	22	1
1:A:659:LEU:HD13	1:A:670:PHE:CD2	0.43	2.48	5	1
1:A:702:LEU:HD11	1:A:705:GLU:HA	0.43	1.90	10	1
1:A:626:PHE:CE1	1:A:627:LYS:O	0.43	2.72	1	18
1:A:689:VAL:O	1:A:689:VAL:CG1	0.43	2.66	18	8
1:A:659:LEU:HB3	1:A:670:PHE:CE2	0.43	2.48	7	2
1:A:690:ILE:O	1:A:690:ILE:HG23	0.43	2.13	12	1
1:A:580:LEU:CD1	1:A:594:ILE:CD1	0.43	2.96	8	4
1:A:615:ASP:H	1:A:618:LEU:HD11	0.43	1.74	17	3
1:A:596:GLN:HG2	1:A:597:GLY:N	0.43	2.28	5	4
1:A:587:ILE:CG2	1:A:690:ILE:CD1	0.43	2.97	11	2
1:A:703:PHE:CE2	1:A:704:ASN:ND2	0.43	2.86	21	1
1:A:659:LEU:O	1:A:661:ASN:N	0.43	2.52	16	10
1:A:659:LEU:CD2	1:A:672:LEU:CD2	0.43	2.96	6	3
1:A:601:PHE:CE1	1:A:610:ASN:OD1	0.43	2.72	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:587:ILE:HG21	1:A:688:PHE:HD1	0.43	1.74	7	1
1:A:664:MET:CE	1:A:716:VAL:HG13	0.43	2.44	10	1
1:A:577:PHE:CZ	1:A:702:LEU:HD13	0.43	2.47	17	1
1:A:578:LEU:HD23	1:A:594:ILE:HD12	0.43	1.90	11	1
1:A:644:LEU:CB	1:A:703:PHE:HB3	0.43	2.44	20	1
1:A:662:ASN:HB3	1:A:716:VAL:HG23	0.43	1.90	5	1
1:A:648:TRP:CH2	1:A:671:LEU:CG	0.43	3.02	20	1
1:A:580:LEU:CD1	1:A:625:ILE:HD13	0.42	2.44	9	1
1:A:674:ASP:HB2	1:A:705:GLU:O	0.42	2.13	13	1
1:A:626:PHE:CE2	1:A:627:LYS:O	0.42	2.72	19	1
1:A:688:PHE:O	1:A:688:PHE:CD1	0.42	2.72	5	1
1:A:624:PHE:O	1:A:650:CYS:CB	0.42	2.67	20	1
1:A:703:PHE:CD1	1:A:703:PHE:C	0.42	2.95	22	1
1:A:682:TRP:CD1	1:A:682:TRP:C	0.42	2.97	6	8
1:A:577:PHE:CZ	1:A:578:LEU:HB2	0.42	2.49	12	1
1:A:646:ASP:OD2	1:A:671:LEU:HD21	0.42	2.14	17	1
1:A:577:PHE:CE2	1:A:702:LEU:CD2	0.42	3.02	18	1
1:A:644:LEU:CB	1:A:703:PHE:N	0.42	2.82	12	4
1:A:618:LEU:N	1:A:681:ILE:CD1	0.42	2.82	12	1
1:A:662:ASN:HB2	1:A:670:PHE:CE2	0.42	2.49	12	1
1:A:656:VAL:HG13	1:A:664:MET:O	0.42	2.15	13	1
1:A:659:LEU:CB	1:A:670:PHE:CD2	0.42	3.02	15	1
1:A:587:ILE:CG1	1:A:690:ILE:CD1	0.42	2.98	7	1
1:A:655:ASN:C	1:A:656:VAL:HG23	0.42	2.39	7	1
1:A:655:ASN:O	1:A:656:VAL:CG1	0.42	2.68	16	3
1:A:727:VAL:HG23	1:A:730:LEU:HD13	0.42	1.90	2	1
1:A:613:ILE:O	1:A:613:ILE:HG22	0.42	2.14	3	1
1:A:656:VAL:HG22	1:A:658:TYR:CZ	0.42	2.50	4	1
1:A:578:LEU:HG	1:A:694:VAL:HG13	0.42	1.91	7	1
1:A:575:GLY:C	1:A:596:GLN:NE2	0.42	2.78	10	1
1:A:659:LEU:HD11	1:A:676:ASP:OD1	0.42	2.14	1	1
1:A:681:ILE:HG22	1:A:690:ILE:CB	0.42	2.45	2	1
1:A:644:LEU:HD12	1:A:703:PHE:HB2	0.42	1.92	6	1
1:A:662:ASN:CG	1:A:670:PHE:CZ	0.42	2.98	11	3
1:A:577:PHE:CD1	1:A:696:ILE:HG23	0.42	2.50	2	1
1:A:582:PRO:HA	1:A:692:PHE:CD1	0.42	2.50	18	1
1:A:618:LEU:HD23	1:A:680:ILE:HG23	0.42	1.92	1	1
1:A:624:PHE:CZ	1:A:723:GLU:OE2	0.42	2.73	10	2
1:A:582:PRO:HG3	1:A:692:PHE:CE1	0.42	2.50	11	7
1:A:613:ILE:CD1	1:A:692:PHE:CZ	0.42	3.02	3	1
1:A:577:PHE:CD1	1:A:578:LEU:N	0.42	2.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:578:LEU:C	1:A:578:LEU:CD2	0.42	2.91	16	2
1:A:629:ARG:CZ	1:A:643:GLY:CA	0.42	2.98	16	1
1:A:645:ASP:O	1:A:702:LEU:CG	0.42	2.68	17	1
1:A:690:ILE:CG2	1:A:690:ILE:O	0.41	2.66	4	1
1:A:681:ILE:O	1:A:690:ILE:N	0.41	2.52	8	2
1:A:644:LEU:HD22	1:A:703:PHE:CA	0.41	2.45	9	1
1:A:685:ASN:ND2	1:A:686:ASN:N	0.41	2.68	19	2
1:A:580:LEU:HD21	1:A:694:VAL:CG2	0.41	2.44	11	1
1:A:605:ARG:HD3	1:A:615:ASP:O	0.41	2.15	16	1
1:A:605:ARG:HD3	1:A:618:LEU:O	0.41	2.15	19	1
1:A:644:LEU:CB	1:A:703:PHE:CB	0.41	2.97	20	1
1:A:681:ILE:CG2	1:A:690:ILE:CG1	0.41	2.99	2	1
1:A:629:ARG:CD	1:A:629:ARG:C	0.41	2.94	4	3
1:A:615:ASP:OD1	1:A:688:PHE:CE1	0.41	2.74	7	1
1:A:702:LEU:O	1:A:702:LEU:CD1	0.41	2.68	6	1
1:A:592:LEU:CD1	1:A:692:PHE:CE2	0.41	3.03	7	1
1:A:582:PRO:HB3	1:A:588:ILE:CG2	0.41	2.46	8	1
1:A:588:ILE:CG2	1:A:588:ILE:O	0.41	2.69	12	1
1:A:692:PHE:CD1	1:A:692:PHE:N	0.41	2.88	18	2
1:A:618:LEU:CD2	1:A:680:ILE:CG2	0.41	2.99	1	1
1:A:664:MET:HE1	1:A:670:PHE:CB	0.41	2.45	8	1
1:A:630:HIS:CB	1:A:646:ASP:OD1	0.41	2.69	10	1
1:A:659:LEU:HD21	1:A:672:LEU:HD22	0.41	1.92	15	1
1:A:618:LEU:HD12	1:A:622:HIS:CD2	0.41	2.51	18	1
1:A:659:LEU:HD12	1:A:660:ASN:N	0.41	2.31	1	1
1:A:592:LEU:CD1	1:A:692:PHE:CD2	0.41	3.04	5	2
1:A:629:ARG:CD	1:A:644:LEU:O	0.41	2.69	6	2
1:A:575:GLY:N	1:A:596:GLN:OE1	0.41	2.53	12	1
1:A:670:PHE:CE1	1:A:715:VAL:O	0.41	2.74	12	1
1:A:578:LEU:CD1	1:A:696:ILE:HG12	0.41	2.46	3	2
1:A:649:TYR:HD2	1:A:664:MET:HE2	0.41	1.75	12	1
1:A:674:ASP:HA	1:A:696:ILE:HD12	0.41	1.92	20	1
1:A:602:PHE:HB2	1:A:609:CYS:HA	0.41	1.93	2	1
1:A:587:ILE:HG21	1:A:688:PHE:CD1	0.41	2.50	7	1
1:A:582:PRO:HB3	1:A:588:ILE:HG23	0.41	1.91	8	1
1:A:618:LEU:HB3	1:A:681:ILE:HD12	0.41	1.91	9	1
1:A:576:ARG:NH1	1:A:697:ASN:CB	0.41	2.83	21	2
1:A:600:PRO:HG2	1:A:624:PHE:CZ	0.41	2.51	2	1
1:A:615:ASP:OD1	1:A:688:PHE:CE2	0.41	2.74	3	1
1:A:690:ILE:CG2	1:A:691:GLY:N	0.41	2.83	3	2
1:A:654:THR:HG22	1:A:654:THR:O	0.41	2.16	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:626:PHE:CE2	1:A:628:LYS:HG3	0.41	2.51	5	2
1:A:579:THR:HG22	1:A:581:LYS:HG3	0.41	1.92	7	1
1:A:583:LEU:HD22	1:A:583:LEU:N	0.41	2.31	8	1
1:A:678:ILE:O	1:A:691:GLY:HA2	0.41	2.16	8	1
1:A:662:ASN:CG	1:A:670:PHE:CE1	0.41	2.99	9	1
1:A:689:VAL:O	1:A:689:VAL:HG13	0.41	2.15	18	1
1:A:577:PHE:CB	1:A:596:GLN:HG2	0.41	2.45	19	1
1:A:578:LEU:CD2	1:A:647:ILE:CD1	0.41	2.99	22	2
1:A:646:ASP:OD1	1:A:703:PHE:CD2	0.41	2.74	22	1
1:A:615:ASP:OD1	1:A:688:PHE:CZ	0.41	2.74	17	4
1:A:615:ASP:OD2	1:A:688:PHE:CE2	0.41	2.73	6	1
1:A:674:ASP:CB	1:A:705:GLU:CD	0.41	2.94	6	1
1:A:576:ARG:CG	1:A:593:GLU:HB3	0.41	2.46	12	1
1:A:576:ARG:CG	1:A:593:GLU:CB	0.40	2.98	1	1
1:A:577:PHE:CE2	1:A:627:LYS:HE3	0.40	2.51	7	1
1:A:617:ARG:CB	1:A:681:ILE:CD1	0.40	3.00	10	1
1:A:649:TYR:CD1	1:A:649:TYR:C	0.40	2.99	19	3
1:A:615:ASP:HB2	1:A:618:LEU:CD2	0.40	2.46	6	1
1:A:657:SER:O	1:A:664:MET:N	0.40	2.52	8	1
1:A:615:ASP:O	1:A:616:ASN:C	0.40	2.64	21	2
1:A:657:SER:C	1:A:658:TYR:CD1	0.40	2.99	13	1
1:A:704:ASN:CG	1:A:705:GLU:N	0.40	2.80	13	1
1:A:580:LEU:HD21	1:A:594:ILE:HD12	0.40	1.94	20	1
1:A:675:GLY:CA	1:A:694:VAL:O	0.40	2.70	3	1
1:A:664:MET:HB2	1:A:668:THR:OG1	0.40	2.16	4	1
1:A:704:ASN:CG	1:A:705:GLU:HG2	0.40	2.41	6	1
1:A:605:ARG:NE	1:A:618:LEU:O	0.40	2.54	9	1
1:A:627:LYS:CE	1:A:647:ILE:CG2	0.40	2.99	11	1
1:A:648:TRP:HB3	1:A:669:LYS:CG	0.40	2.46	14	1
1:A:615:ASP:CB	1:A:618:LEU:HB2	0.40	2.46	20	1
1:A:605:ARG:HD3	1:A:615:ASP:C	0.40	2.42	1	1
1:A:669:LYS:O	1:A:717:LEU:HD12	0.40	2.16	2	1
1:A:662:ASN:HB3	1:A:670:PHE:CE2	0.40	2.51	7	1
1:A:615:ASP:HB3	1:A:618:LEU:HG	0.40	1.93	9	1
1:A:576:ARG:O	1:A:698:ASP:CB	0.40	2.69	10	1
1:A:579:THR:HG22	1:A:581:LYS:CG	0.40	2.46	11	1
1:A:655:ASN:ND2	1:A:681:ILE:HD11	0.40	2.32	18	1
1:A:646:ASP:OD1	1:A:703:PHE:CE2	0.40	2.75	22	1
1:A:682:TRP:CD1	1:A:683:ASP:N	0.40	2.89	22	1
1:A:615:ASP:O	1:A:618:LEU:N	0.40	2.55	4	1
1:A:651:HIS:ND1	1:A:657:SER:HB2	0.40	2.30	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:671:LEU:C	1:A:671:LEU:CD1	0.40	2.95	7	1
1:A:581:LYS:O	1:A:583:LEU:N	0.40	2.55	11	1
1:A:659:LEU:HD23	1:A:670:PHE:CG	0.40	2.52	13	1
1:A:615:ASP:CG	1:A:688:PHE:CE1	0.40	2.99	14	1
1:A:683:ASP:O	1:A:687:LYS:N	0.40	2.55	20	1
1:A:688:PHE:CD1	1:A:688:PHE:C	0.40	2.99	22	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	134/158 (85%)	117±1 (87±1%)	12±2 (9±1%)	5±1 (4±1%)	4	30
2	P	0	-	-	-	-	-
All	All	2948/3630 (81%)	2564 (87%)	268 (9%)	116 (4%)	4	30

All 12 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	656	VAL	22
1	A	660	ASN	22
1	A	582	PRO	21
1	A	705	GLU	18
1	A	704	ASN	8
1	A	643	GLY	7
1	A	575	GLY	6
1	A	616	ASN	4
1	A	674	ASP	3
1	A	703	PHE	2
1	A	666	GLN	2
1	A	700	THR	1

6.3.2 Protein sidechains ⓘ

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	125/142 (88%)	87±4 (70±4%)	38±4 (30±4%)	1 16
2	P	0	-	-	-
All	All	2750/3256 (84%)	1923 (70%)	827 (30%)	1 16

All 99 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	583	LEU	22
1	A	589	GLN	22
1	A	592	LEU	22
1	A	596	GLN	22
1	A	628	LYS	22
1	A	659	LEU	22
1	A	591	SER	21
1	A	612	LYS	21
1	A	671	LEU	21
1	A	656	VAL	20
1	A	618	LEU	20
1	A	702	LEU	19
1	A	606	SER	18
1	A	672	LEU	17
1	A	680	ILE	17
1	A	676	ASP	17
1	A	646	ASP	16
1	A	620	ARG	15
1	A	718	LYS	15
1	A	577	PHE	14
1	A	728	LYS	14
1	A	647	ILE	13
1	A	581	LYS	12
1	A	695	GLU	12
1	A	704	ASN	12
1	A	669	LYS	12
1	A	615	ASP	12
1	A	580	LEU	11

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Mol	Chain	Res	Type	Models (Total)
1	A	593	GLU	11
1	A	703	PHE	11
1	A	687	LYS	10
1	A	699	THR	10
1	A	717	LEU	10
1	A	688	PHE	10
1	A	605	ARG	9
1	A	679	LYS	9
1	A	683	ASP	9
1	A	595	GLN	9
1	A	607	GLU	8
1	A	670	PHE	8
1	A	629	ARG	8
1	A	652	THR	8
1	A	662	ASN	8
1	A	686	ASN	8
1	A	693	LYS	8
1	A	723	GLU	8
1	A	724	LYS	8
1	A	619	SER	7
1	A	644	LEU	7
1	A	681	ILE	7
1	A	722	GLU	7
1	A	645	ASP	7
1	A	684	LYS	7
1	A	585	ASP	6
1	A	720	THR	6
1	A	725	ASP	6
1	A	664	MET	5
1	A	689	VAL	5
1	A	705	GLU	5
1	A	608	ASP	5
1	A	677	GLU	5
1	A	663	ARG	4
1	A	697	ASN	4
1	A	587	ILE	4
1	A	650	CYS	4
1	A	690	ILE	4
1	A	673	GLN	4
1	A	660	ASN	4
1	A	576	ARG	3
1	A	617	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	730	LEU	3
1	A	614	GLU	3
1	A	694	VAL	3
1	A	700	THR	3
1	A	590	GLU	3
1	A	610	ASN	3
1	A	692	PHE	3
1	A	666	GLN	3
1	A	719	GLN	2
1	A	623	CYS	2
1	A	624	PHE	2
1	A	726	LEU	2
1	A	657	SER	2
1	A	698	ASP	2
1	A	630	HIS	2
1	A	654	THR	2
1	A	685	ASN	2
1	A	586	SER	2
1	A	603	ILE	2
1	A	627	LYS	2
1	A	727	VAL	1
1	A	613	ILE	1
1	A	616	ASN	1
1	A	661	ASN	1
1	A	668	THR	1
1	A	729	LYS	1
1	A	599	ASN	1
1	A	626	PHE	1
1	A	625	ILE	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	PTR	P	829	2	15,16,17	0.76±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	PTR	P	829	2	17,22,24	0.88±0.01	1±0 (5±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	PTR	P	829	2	-	0±0,10,11,13	0±0,1,1,1

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	P	829	PTR	O3P-P-OH	2.50	112.70	105.32	11	22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

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