WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 05:11 AM BST

PDB ID	:	2RQA
Title	:	Solution structure of LGP2 CTD
Authors	:	Takahasi, K.; Kumeta, H.; Tsuduki, N.; Narita, R.; Shigemoto, T.; Hirai, R.; Yoneyama, M.; Horiuchi, M.; Ogura, K.; Fujita, T.; Fuyuhiko, I.
Deposited on	:	2009-03-17

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	:	unknown
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	Percentile Ranks	Value
Clashscore		57
Ramachandran outliers		4.2%
Sidechain outliers		19.5%

Worse   *Better*

█ Percentile relative to all structures
▯ Percentile relative to all NMR structures
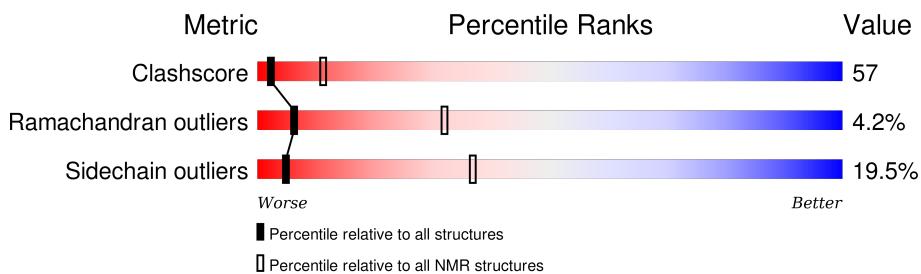
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	137	23% 45% 9% 23%
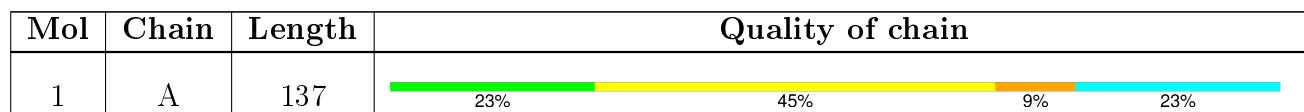
2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy.*

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:546-A:591, A:604-A:662 (105)	0.24	2

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2171 atoms, of which 1080 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ATP-dependent RNA helicase DHX58.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	137	2170	696	1080	194	191	9	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	GLY	-	EXPRESSION TAG	UNP Q96C10
A	543	PRO	-	EXPRESSION TAG	UNP Q96C10
A	544	HIS	-	EXPRESSION TAG	UNP Q96C10
A	545	MET	-	EXPRESSION TAG	UNP Q96C10

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

4   Residue-property plots ⓘ

4.1   Average score per residue in the NMR ensemble

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

• Molecule 1: ATP-dependent RNA helicase DHX58

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: ATP-dependent RNA helicase DHX58

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: ATP-dependent RNA helicase DHX58

Chain A:
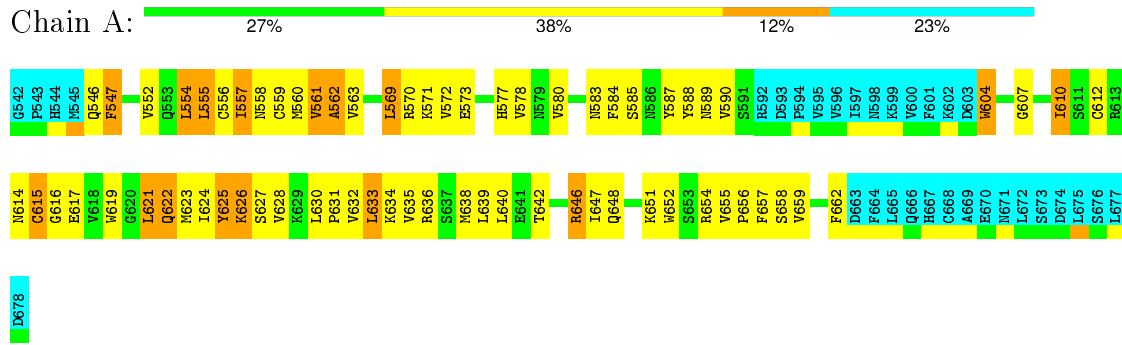
4.2.3 Score per residue for model 3

• Molecule 1: ATP-dependent RNA helicase DHX58

Chain A:
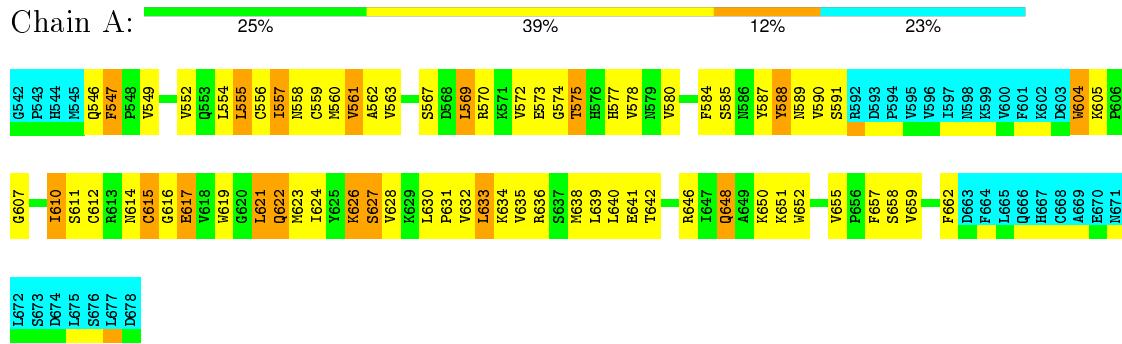
4.2.4 Score per residue for model 4

• Molecule 1: ATP-dependent RNA helicase DHX58

Chain A:
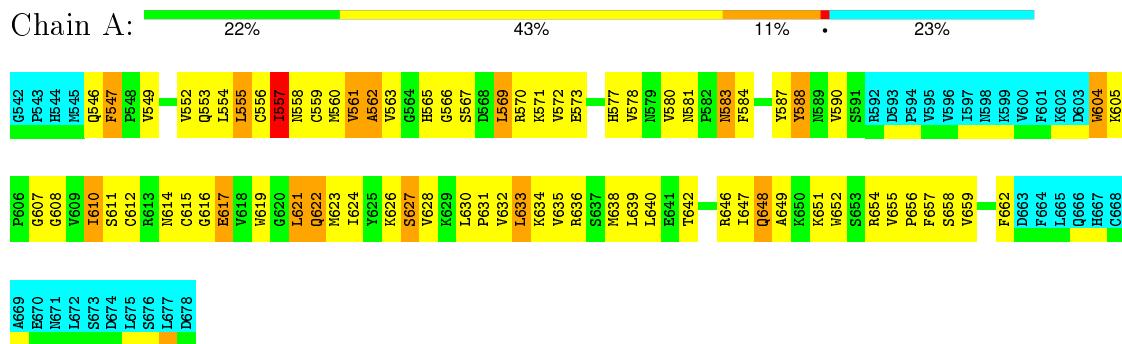
4.2.5　Score per residue for model 5

• Molecule 1: ATP-dependent RNA helicase DHX58
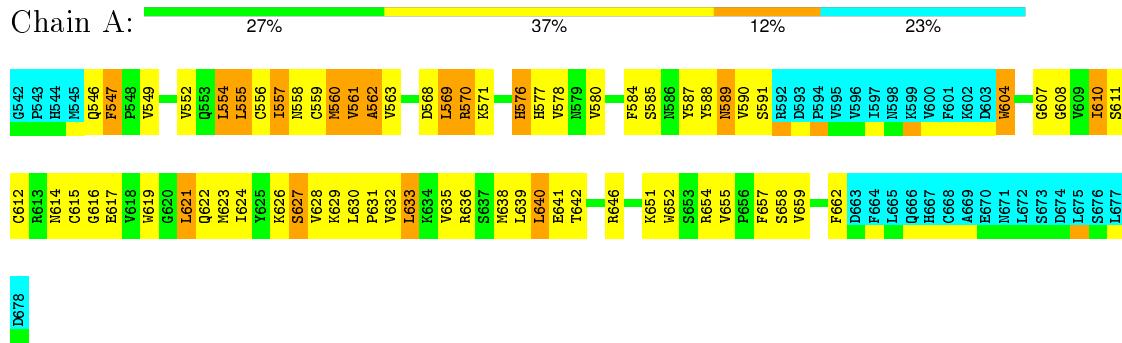
4.2.6　Score per residue for model 6

• Molecule 1: ATP-dependent RNA helicase DHX58
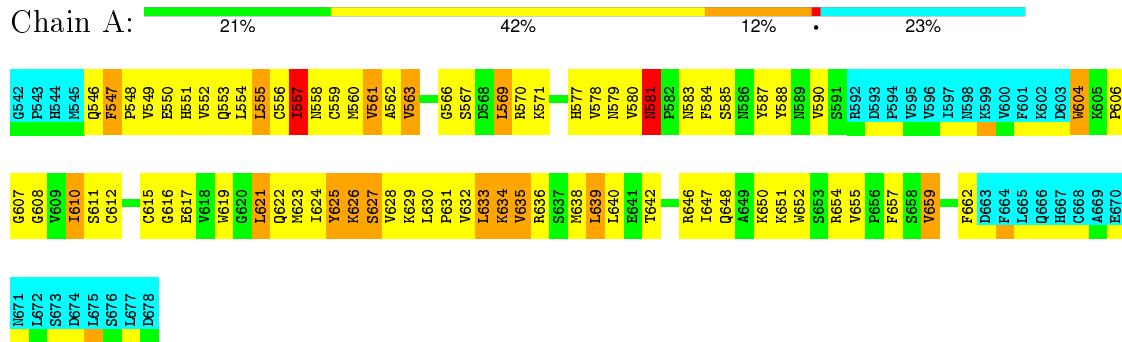
4.2.7　Score per residue for model 7

• Molecule 1: ATP-dependent RNA helicase DHX58
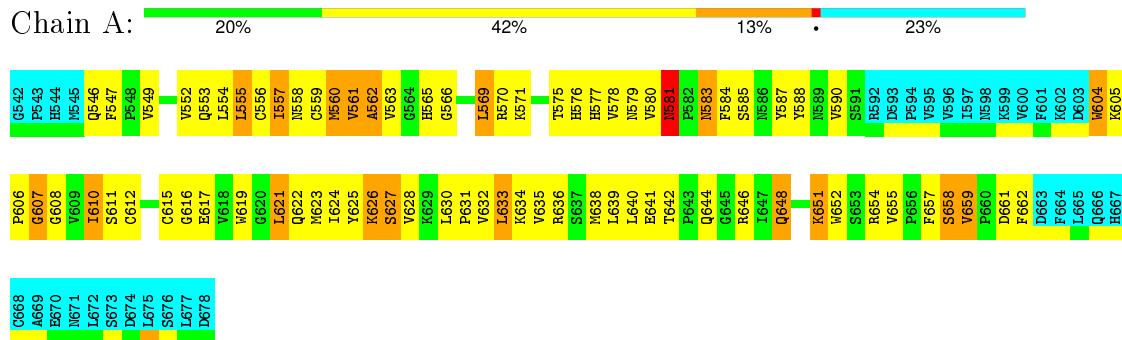
4.2.8 Score per residue for model 8

• Molecule 1: ATP-dependent RNA helicase DHX58

Chain A:

25%   37%   14%   •   23%
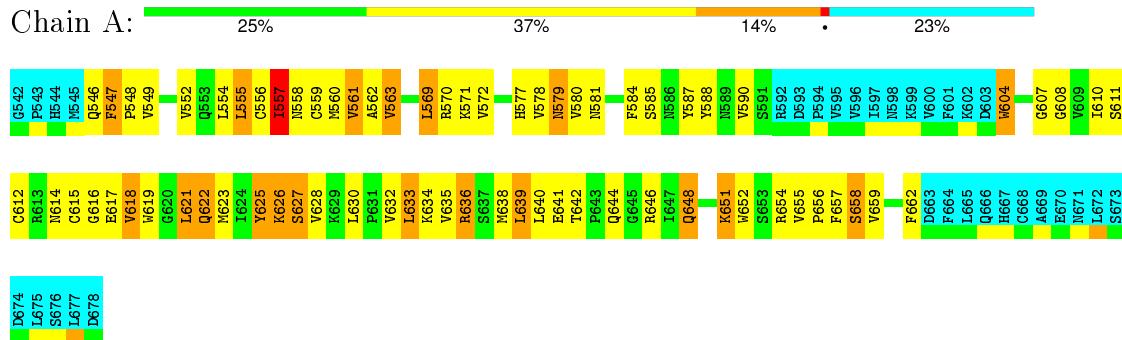
4.2.9 Score per residue for model 9

• Molecule 1: ATP-dependent RNA helicase DHX58

Chain A:

27%   39%   11%   23%
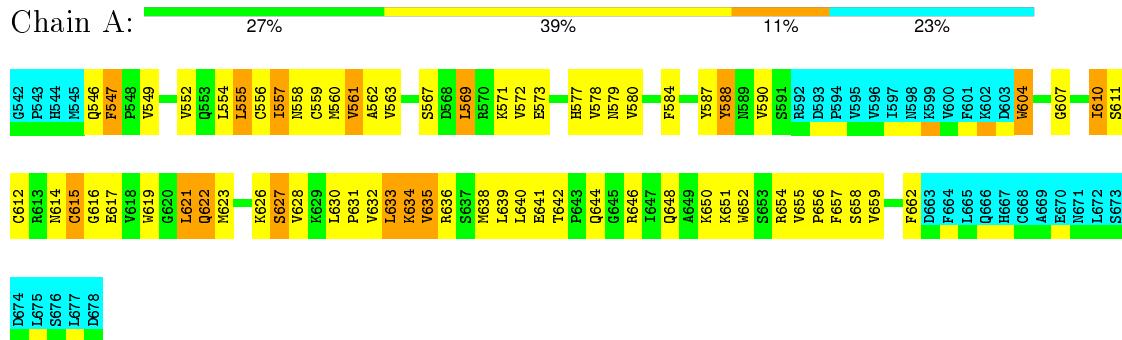
4.2.10 Score per residue for model 10

• Molecule 1: ATP-dependent RNA helicase DHX58

Chain A:

26%   39%   12%   23%
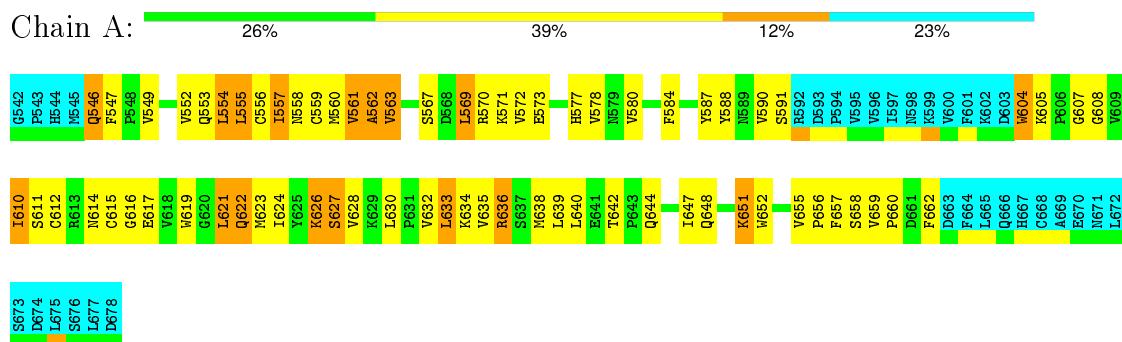
4.2.11 Score per residue for model 11

• Molecule 1: ATP-dependent RNA helicase DHX58
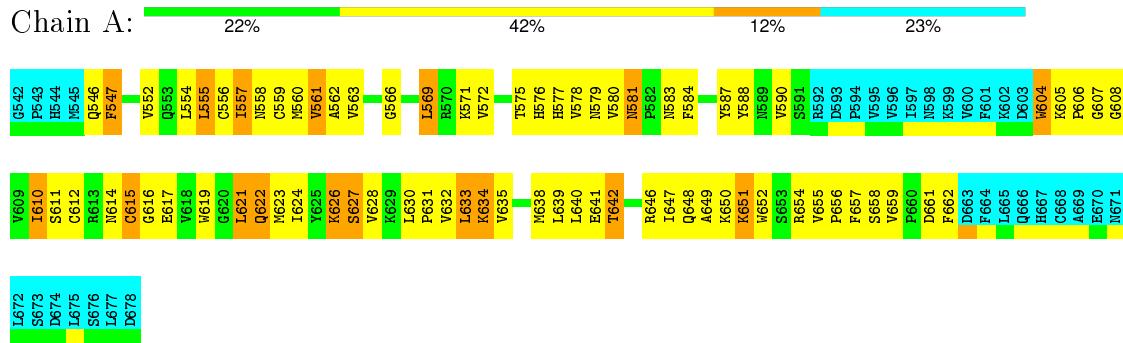
4.2.12 Score per residue for model 12

• Molecule 1: ATP-dependent RNA helicase DHX58
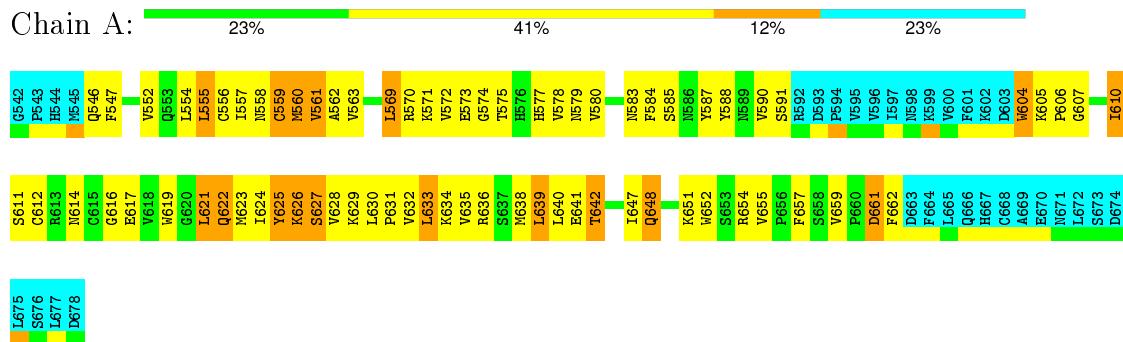
4.2.13 Score per residue for model 13

• Molecule 1: ATP-dependent RNA helicase DHX58
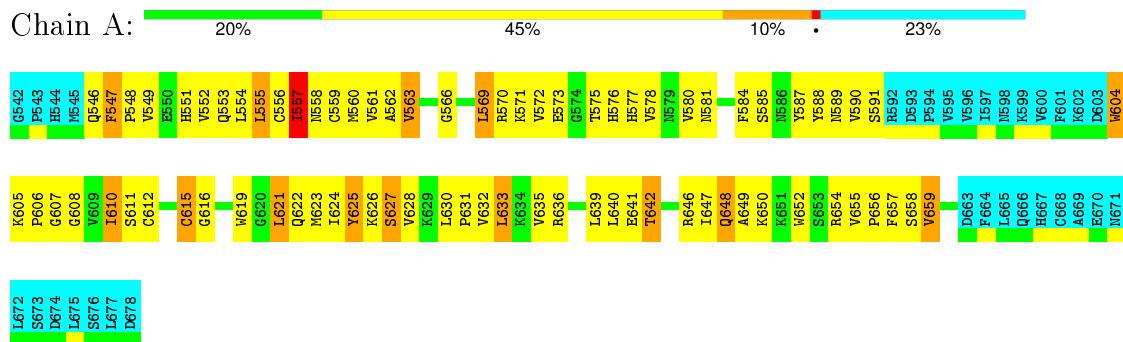
4.2.14　Score per residue for model 14

• Molecule 1: ATP-dependent RNA helicase DHX58

Chain A:
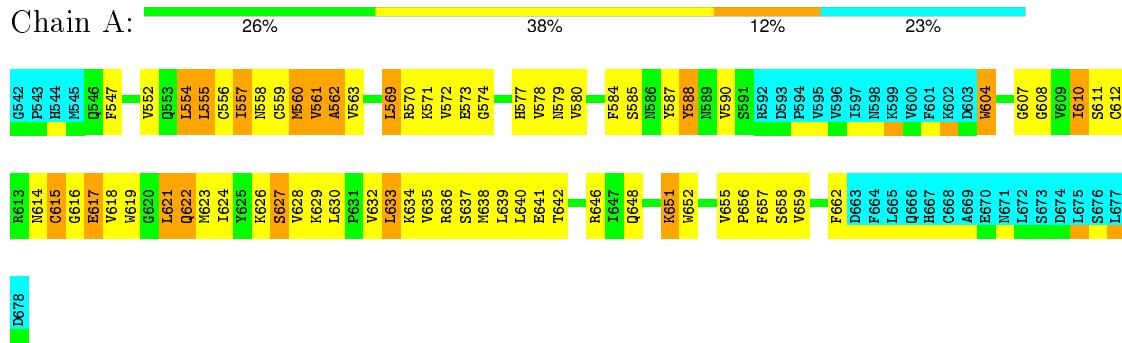
4.2.15　Score per residue for model 15

• Molecule 1: ATP-dependent RNA helicase DHX58

Chain A:
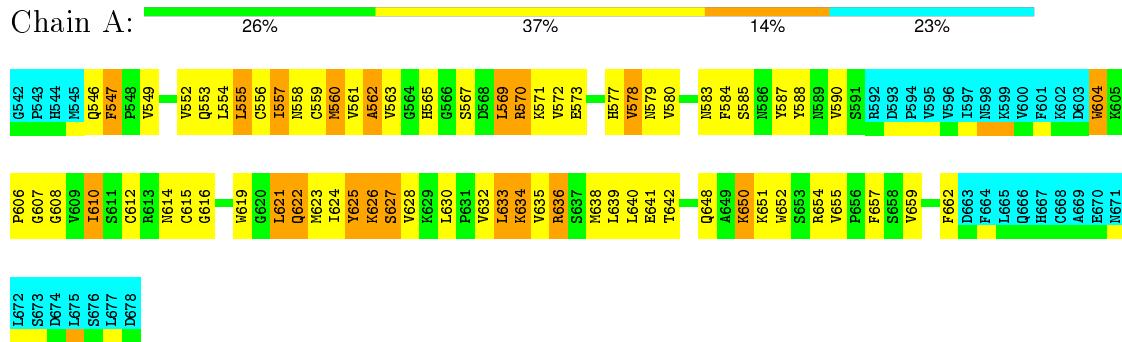
4.2.16　Score per residue for model 16

• Molecule 1: ATP-dependent RNA helicase DHX58

Chain A:
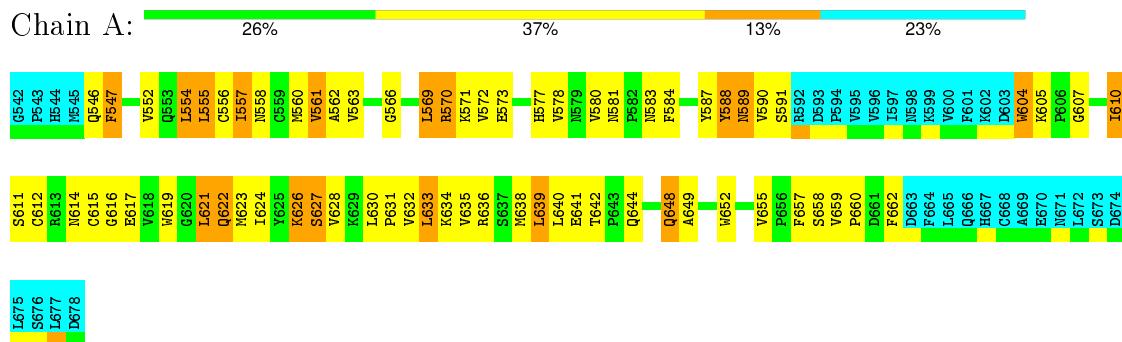
4.2.17 Score per residue for model 17

• Molecule 1: ATP-dependent RNA helicase DHX58
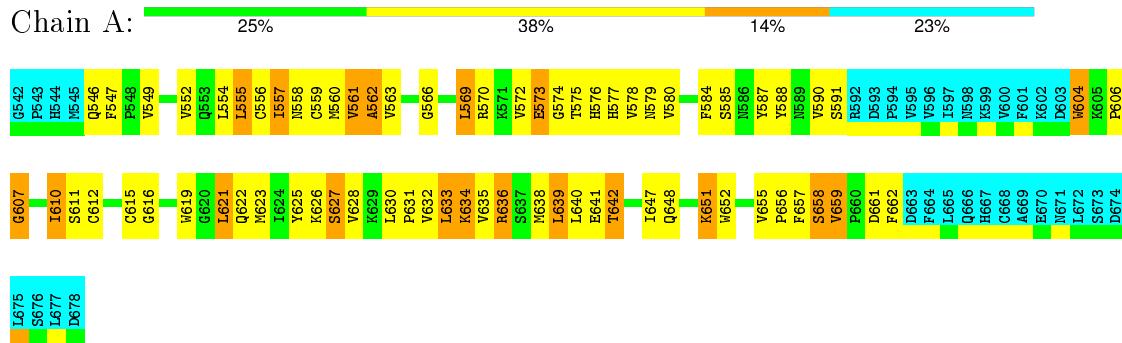
4.2.18 Score per residue for model 18

• Molecule 1: ATP-dependent RNA helicase DHX58
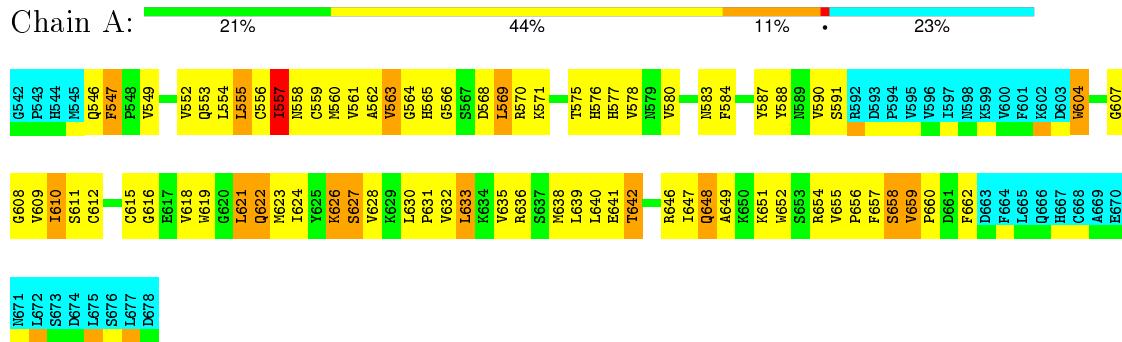
4.2.19 Score per residue for model 19

• Molecule 1: ATP-dependent RNA helicase DHX58
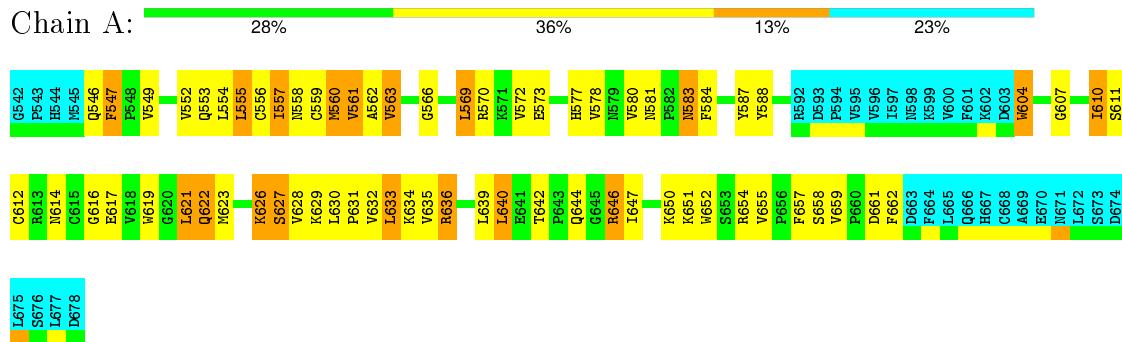
4.2.20　Score per residue for model 20

• Molecule 1: ATP-dependent RNA helicase DHX58

Chain A:

26%　　　　　　　　　　　39%　　　　　　　　12%　　　　　　23%
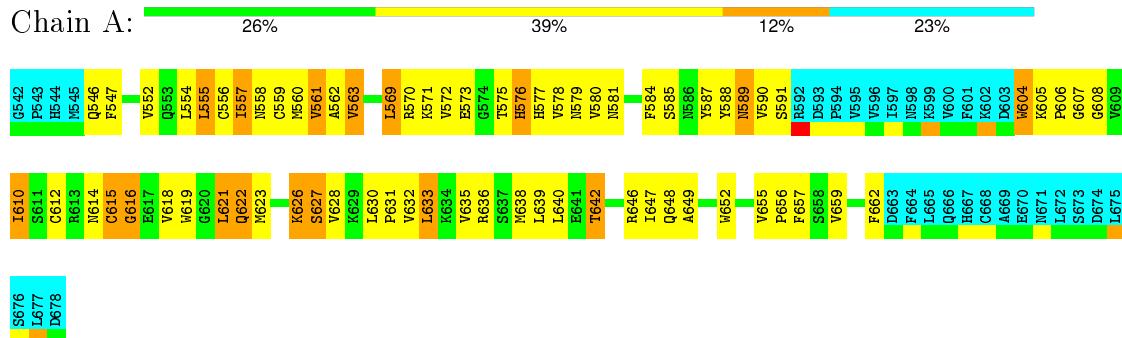
5 Refinement protocol and experimental data overview (i)

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *target function.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

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 (i)

6.1 Standard geometry (i)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	835	832	838	96±9
All	All	16720	16640	16760	1912

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:554:LEU:HD11	1:A:569:LEU:HD23	1.04	1.23	10	19
1:A:572:VAL:HG23	1:A:578:VAL:HG21	1.02	1.27	19	7
1:A:657:PHE:CE1	1:A:659:VAL:HG22	1.01	1.89	11	9
1:A:578:VAL:HG12	1:A:632:VAL:HG22	0.97	1.34	14	15
1:A:578:VAL:CG1	1:A:632:VAL:HG22	0.95	1.91	14	16
1:A:657:PHE:CE2	1:A:659:VAL:HG22	0.94	1.98	12	6
1:A:577:HIS:CD2	1:A:659:VAL:HG11	0.93	1.98	11	6
1:A:572:VAL:HG11	1:A:604:TRP:CE3	0.92	2.00	19	4
1:A:557:ILE:HD13	1:A:636:ARG:O	0.90	1.67	1	19
1:A:605:LYS:NZ	1:A:624:ILE:HD13	0.89	1.81	10	2
1:A:632:VAL:C	1:A:633:LEU:HD13	0.88	1.88	14	19
1:A:555:LEU:HD12	1:A:639:LEU:O	0.88	1.67	11	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:635:VAL:HG11	1:A:651:LYS:C	0.88	1.89	5	12
1:A:563:VAL:HG12	1:A:587:TYR:CD1	0.86	2.05	18	18
1:A:588:TYR:CD1	1:A:610:ILE:HG23	0.85	2.05	19	19
1:A:632:VAL:C	1:A:633:LEU:HD23	0.82	1.95	11	1
1:A:580:VAL:HG22	1:A:630:LEU:HD22	0.81	1.52	1	17
1:A:621:LEU:HD21	1:A:623:MET:SD	0.81	2.15	15	1
1:A:572:VAL:CG2	1:A:578:VAL:HG21	0.81	2.06	10	6
1:A:572:VAL:HG23	1:A:578:VAL:CG2	0.81	2.06	19	12
1:A:555:LEU:N	1:A:555:LEU:HD12	0.80	1.91	13	2
1:A:640:LEU:HD11	1:A:655:VAL:HG22	0.80	1.50	13	3
1:A:584:PHE:CZ	1:A:619:TRP:CZ3	0.80	2.69	11	6
1:A:577:HIS:CD2	1:A:652:TRP:CE3	0.80	2.70	6	8
1:A:555:LEU:HD12	1:A:555:LEU:N	0.79	1.93	8	3
1:A:628:VAL:HG11	1:A:662:PHE:CZ	0.77	2.13	11	4
1:A:569:LEU:HD21	1:A:657:PHE:CZ	0.77	2.14	13	3
1:A:619:TRP:CE2	1:A:638:MET:HE3	0.77	2.15	3	16
1:A:633:LEU:HD13	1:A:633:LEU:N	0.77	1.93	15	10
1:A:633:LEU:N	1:A:633:LEU:HD13	0.76	1.93	6	9
1:A:621:LEU:C	1:A:621:LEU:HD23	0.76	2.01	18	2
1:A:633:LEU:N	1:A:633:LEU:HD23	0.76	1.94	11	1
1:A:557:ILE:HA	1:A:639:LEU:HD23	0.75	1.55	12	1
1:A:554:LEU:HD11	1:A:569:LEU:CD2	0.74	2.11	10	8
1:A:577:HIS:CD2	1:A:652:TRP:CG	0.74	2.75	20	10
1:A:577:HIS:CD2	1:A:652:TRP:CD2	0.74	2.75	14	9
1:A:621:LEU:HD23	1:A:621:LEU:C	0.74	2.02	16	4
1:A:576:HIS:O	1:A:578:VAL:HG13	0.73	1.82	17	3
1:A:639:LEU:HD21	1:A:646:ARG:HD2	0.73	1.61	7	10
1:A:577:HIS:CG	1:A:652:TRP:CE3	0.73	2.76	7	17
1:A:642:THR:HG21	1:A:647:ILE:HD12	0.73	1.59	2	11
1:A:635:VAL:HG21	1:A:655:VAL:HG23	0.72	1.62	11	8
1:A:624:ILE:N	1:A:624:ILE:HD12	0.72	1.98	18	6
1:A:639:LEU:HD12	1:A:640:LEU:N	0.71	2.00	5	7
1:A:639:LEU:HD12	1:A:640:LEU:H	0.71	1.45	10	6
1:A:621:LEU:C	1:A:621:LEU:HD22	0.71	2.06	13	6
1:A:578:VAL:HG12	1:A:632:VAL:HA	0.71	1.63	9	1
1:A:555:LEU:HD23	1:A:562:ALA:CA	0.71	2.16	12	11
1:A:569:LEU:HD13	1:A:659:VAL:HG13	0.71	1.62	15	12
1:A:580:VAL:HG13	1:A:630:LEU:CD2	0.71	2.16	18	10
1:A:628:VAL:HG12	1:A:630:LEU:HG	0.70	1.62	8	20
1:A:655:VAL:HG13	1:A:657:PHE:CD1	0.70	2.20	18	10
1:A:624:ILE:HD12	1:A:624:ILE:N	0.70	2.01	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:552:VAL:HG11	1:A:657:PHE:CD2	0.70	2.22	19	9
1:A:570:ARG:CZ	1:A:662:PHE:CD1	0.70	2.74	14	1
1:A:621:LEU:HD22	1:A:621:LEU:C	0.69	2.06	5	6
1:A:576:HIS:CE1	1:A:604:TRP:CZ2	0.69	2.80	5	1
1:A:628:VAL:CG1	1:A:630:LEU:HD21	0.69	2.17	6	12
1:A:655:VAL:HG13	1:A:657:PHE:CD2	0.69	2.22	19	10
1:A:635:VAL:HG13	1:A:652:TRP:CD2	0.68	2.23	9	2
1:A:588:TYR:CD1	1:A:610:ILE:CG2	0.68	2.77	16	10
1:A:621:LEU:HD23	1:A:621:LEU:O	0.67	1.89	18	5
1:A:555:LEU:HD11	1:A:641:GLU:HB2	0.67	1.67	3	11
1:A:580:VAL:HG13	1:A:630:LEU:HD23	0.67	1.67	18	5
1:A:655:VAL:HG13	1:A:657:PHE:CE1	0.67	2.25	12	10
1:A:554:LEU:C	1:A:555:LEU:HD12	0.66	2.11	6	5
1:A:635:VAL:HG13	1:A:652:TRP:CE2	0.66	2.24	9	2
1:A:552:VAL:HG21	1:A:657:PHE:HB3	0.66	1.66	11	16
1:A:570:ARG:NH2	1:A:630:LEU:HD13	0.65	2.07	14	1
1:A:628:VAL:HG12	1:A:630:LEU:CD2	0.65	2.22	16	13
1:A:561:VAL:O	1:A:562:ALA:HB3	0.65	1.91	17	14
1:A:547:PHE:N	1:A:547:PHE:CD1	0.65	2.65	6	7
1:A:635:VAL:HG11	1:A:651:LYS:CA	0.65	2.22	12	12
1:A:580:VAL:CG2	1:A:630:LEU:HD22	0.64	2.23	7	13
1:A:639:LEU:HD13	1:A:640:LEU:N	0.64	2.07	16	1
1:A:570:ARG:HH21	1:A:580:VAL:CG2	0.64	2.05	14	1
1:A:621:LEU:HD22	1:A:622:GLN:N	0.64	2.08	15	11
1:A:547:PHE:CD1	1:A:547:PHE:N	0.64	2.64	13	8
1:A:576:HIS:NE2	1:A:604:TRP:CZ2	0.64	2.66	5	1
1:A:630:LEU:HD21	1:A:662:PHE:CE2	0.64	2.28	11	3
1:A:639:LEU:HD21	1:A:646:ARG:HB3	0.63	1.68	6	2
1:A:621:LEU:HD12	1:A:621:LEU:C	0.63	2.13	12	1
1:A:635:VAL:HG11	1:A:651:LYS:N	0.63	2.08	1	1
1:A:655:VAL:HG13	1:A:657:PHE:CE2	0.63	2.28	8	10
1:A:623:MET:C	1:A:624:ILE:HD12	0.63	2.14	15	7
1:A:578:VAL:HG12	1:A:631:PRO:O	0.63	1.93	3	6
1:A:588:TYR:CG	1:A:610:ILE:CG2	0.63	2.82	19	10
1:A:555:LEU:HD23	1:A:562:ALA:HB2	0.62	1.70	3	10
1:A:628:VAL:HG12	1:A:630:LEU:CG	0.62	2.24	6	18
1:A:557:ILE:HD12	1:A:648:GLN:OE1	0.62	1.94	12	3
1:A:623:MET:HG3	1:A:632:VAL:HG21	0.62	1.71	4	5
1:A:635:VAL:HG11	1:A:652:TRP:N	0.62	2.10	2	7
1:A:652:TRP:HA	1:A:655:VAL:HG23	0.62	1.70	12	8
1:A:556:CYS:O	1:A:560:MET:N	0.62	2.33	13	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:547:PHE:CE1	1:A:647:ILE:HD11	0.61	2.31	17	1
1:A:555:LEU:CD1	1:A:555:LEU:N	0.61	2.62	13	4
1:A:570:ARG:HH21	1:A:580:VAL:HG21	0.61	1.54	14	1
1:A:566:GLY:O	1:A:569:LEU:HD11	0.61	1.96	6	9
1:A:621:LEU:C	1:A:621:LEU:HD12	0.61	2.16	17	1
1:A:604:TRP:CZ2	1:A:623:MET:SD	0.61	2.94	19	5
1:A:559:CYS:O	1:A:561:VAL:HG13	0.61	1.96	19	2
1:A:570:ARG:HH22	1:A:630:LEU:HD13	0.61	1.54	14	2
1:A:546:GLN:C	1:A:547:PHE:CD1	0.60	2.75	8	16
1:A:555:LEU:HD23	1:A:562:ALA:CB	0.60	2.26	9	4
1:A:640:LEU:HD11	1:A:657:PHE:CE1	0.60	2.32	6	1
1:A:560:MET:SD	1:A:639:LEU:HD23	0.60	2.36	13	2
1:A:628:VAL:HG11	1:A:662:PHE:CE2	0.60	2.31	11	1
1:A:604:TRP:CH2	1:A:623:MET:SD	0.60	2.95	6	4
1:A:581:ASN:HD21	1:A:583:ASN:ND2	0.60	1.94	4	1
1:A:588:TYR:CD1	1:A:588:TYR:C	0.60	2.75	4	13
1:A:619:TRP:CE2	1:A:638:MET:CE	0.60	2.84	9	16
1:A:578:VAL:HG12	1:A:632:VAL:CG2	0.60	2.18	14	4
1:A:579:ASN:OD1	1:A:584:PHE:CE1	0.60	2.55	14	9
1:A:625:TYR:CD1	1:A:625:TYR:C	0.60	2.74	8	3
1:A:569:LEU:O	1:A:569:LEU:HD12	0.60	1.97	6	10
1:A:639:LEU:HD21	1:A:646:ARG:CD	0.60	2.27	20	6
1:A:557:ILE:HA	1:A:639:LEU:HD12	0.60	1.73	15	3
1:A:553:GLN:HB3	1:A:555:LEU:HD11	0.60	1.73	13	4
1:A:576:HIS:CD2	1:A:604:TRP:CZ2	0.60	2.89	5	1
1:A:584:PHE:O	1:A:588:TYR:CD2	0.60	2.54	11	20
1:A:604:TRP:CZ3	1:A:623:MET:SD	0.60	2.95	3	3
1:A:657:PHE:CE2	1:A:659:VAL:CG2	0.60	2.80	12	6
1:A:577:HIS:HD2	1:A:659:VAL:HG11	0.60	1.52	12	1
1:A:590:VAL:HG13	1:A:608:GLY:HA3	0.59	1.74	8	11
1:A:588:TYR:C	1:A:588:TYR:CD1	0.59	2.75	9	7
1:A:633:LEU:CD1	1:A:633:LEU:N	0.59	2.65	6	9
1:A:583:ASN:O	1:A:587:TYR:CD1	0.59	2.55	19	1
1:A:547:PHE:CE2	1:A:644:GLN:NE2	0.59	2.70	8	3
1:A:577:HIS:CD2	1:A:652:TRP:CZ3	0.58	2.90	6	6
1:A:555:LEU:N	1:A:555:LEU:CD1	0.58	2.65	18	1
1:A:569:LEU:HD12	1:A:569:LEU:O	0.58	1.98	13	7
1:A:572:VAL:HG11	1:A:604:TRP:CZ3	0.58	2.33	10	2
1:A:554:LEU:CD1	1:A:579:ASN:ND2	0.58	2.67	8	1
1:A:553:GLN:OE1	1:A:565:HIS:CE1	0.58	2.57	18	3
1:A:634:LYS:CE	1:A:636:ARG:CG	0.58	2.82	16	2

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Full wwPDB NMR Structure Validation Report

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:584:PHE:CE2	1:A:633:LEU:HD11	0.58	2.33	11	1
1:A:572:VAL:HG12	1:A:573:GLU:HG2	0.58	1.73	20	4
1:A:633:LEU:CD2	1:A:633:LEU:N	0.58	2.67	11	1
1:A:584:PHE:CE2	1:A:619:TRP:CZ3	0.58	2.91	13	6
1:A:605:LYS:HZ3	1:A:624:ILE:HD13	0.58	1.55	10	1
1:A:561:VAL:HG22	1:A:614:ASN:ND2	0.57	2.13	2	12
1:A:577:HIS:NE2	1:A:659:VAL:HG21	0.57	2.13	3	1
1:A:552:VAL:HG11	1:A:657:PHE:CD1	0.57	2.34	7	7
1:A:604:TRP:O	1:A:604:TRP:CD1	0.57	2.57	6	2
1:A:639:LEU:HD13	1:A:640:LEU:H	0.57	1.57	16	1
1:A:657:PHE:CE1	1:A:659:VAL:CG2	0.57	2.80	11	7
1:A:553:GLN:O	1:A:555:LEU:HD12	0.57	1.99	10	2
1:A:635:VAL:HG13	1:A:649:ALA:O	0.57	1.99	1	1
1:A:657:PHE:HE1	1:A:659:VAL:HG22	0.57	1.57	2	9
1:A:576:HIS:CD2	1:A:604:TRP:CH2	0.57	2.93	5	1
1:A:625:TYR:C	1:A:625:TYR:CD1	0.57	2.75	6	3
1:A:570:ARG:HA	1:A:659:VAL:HG23	0.56	1.77	17	5
1:A:630:LEU:HD21	1:A:662:PHE:CE1	0.56	2.35	19	1
1:A:570:ARG:NH1	1:A:572:VAL:CG2	0.56	2.68	15	1
1:A:619:TRP:CE2	1:A:638:MET:HE1	0.56	2.35	16	1
1:A:619:TRP:NE1	1:A:638:MET:CE	0.56	2.69	11	17
1:A:633:LEU:N	1:A:633:LEU:CD1	0.56	2.69	18	10
1:A:631:PRO:HB2	1:A:633:LEU:HD11	0.55	1.77	1	14
1:A:564:GLY:O	1:A:565:HIS:CD2	0.55	2.59	18	1
1:A:604:TRP:CD2	1:A:623:MET:SD	0.55	3.00	3	5
1:A:569:LEU:HD21	1:A:657:PHE:CE1	0.55	2.36	13	2
1:A:546:GLN:C	1:A:547:PHE:CG	0.55	2.80	18	10
1:A:557:ILE:HG21	1:A:636:ARG:O	0.55	2.02	18	2
1:A:635:VAL:CG2	1:A:655:VAL:HG23	0.55	2.30	11	3
1:A:604:TRP:CE2	1:A:623:MET:SD	0.55	2.99	3	7
1:A:552:VAL:CG1	1:A:640:LEU:HD12	0.55	2.31	6	3
1:A:588:TYR:CE1	1:A:590:VAL:HG23	0.54	2.37	9	4
1:A:621:LEU:HD21	1:A:623:MET:HG2	0.54	1.78	11	3
1:A:580:VAL:CG1	1:A:630:LEU:CD2	0.54	2.85	18	5
1:A:588:TYR:HE1	1:A:590:VAL:HG23	0.54	1.61	3	13
1:A:640:LEU:CD1	1:A:657:PHE:CE1	0.54	2.90	6	1
1:A:577:HIS:NE2	1:A:652:TRP:CB	0.54	2.70	10	6
1:A:549:VAL:HG11	1:A:658:SER:O	0.54	2.02	7	4
1:A:604:TRP:CE3	1:A:623:MET:SD	0.54	3.01	3	1
1:A:557:ILE:HD12	1:A:648:GLN:CD	0.54	2.23	12	3
1:A:579:ASN:ND2	1:A:633:LEU:HD23	0.54	2.18	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:639:LEU:HD22	1:A:648:GLN:HG3	0.54	1.78	12	1
1:A:546:GLN:O	1:A:547:PHE:CG	0.54	2.60	17	3
1:A:635:VAL:CG1	1:A:651:LYS:N	0.54	2.71	1	2
1:A:604:TRP:CG	1:A:623:MET:SD	0.54	3.00	13	2
1:A:577:HIS:CG	1:A:652:TRP:CD2	0.54	2.96	16	7
1:A:575:THR:O	1:A:576:HIS:CG	0.54	2.60	18	5
1:A:577:HIS:ND1	1:A:652:TRP:CE3	0.54	2.76	19	2
1:A:621:LEU:CD1	1:A:621:LEU:C	0.54	2.76	12	1
1:A:640:LEU:HD13	1:A:656:PRO:HD2	0.54	1.79	11	5
1:A:631:PRO:HB2	1:A:633:LEU:HD21	0.54	1.79	11	1
1:A:575:THR:HG21	1:A:604:TRP:CZ2	0.53	2.38	3	1
1:A:628:VAL:HG12	1:A:630:LEU:HD21	0.53	1.79	16	2
1:A:561:VAL:CG2	1:A:614:ASN:ND2	0.53	2.72	10	4
1:A:634:LYS:HZ1	1:A:636:ARG:HD2	0.53	1.62	9	1
1:A:621:LEU:HD13	1:A:632:VAL:HB	0.53	1.79	11	1
1:A:549:VAL:HG23	1:A:567:SER:OG	0.53	2.04	6	1
1:A:624:ILE:N	1:A:624:ILE:CD1	0.53	2.72	16	5
1:A:639:LEU:HD12	1:A:647:ILE:O	0.53	2.03	4	3
1:A:563:VAL:O	1:A:587:TYR:CD2	0.53	2.61	18	4
1:A:606:PRO:O	1:A:624:ILE:HD13	0.53	2.04	7	1
1:A:556:CYS:O	1:A:558:ASN:N	0.53	2.42	8	20
1:A:621:LEU:C	1:A:621:LEU:CD2	0.53	2.74	18	7
1:A:580:VAL:HG22	1:A:630:LEU:CD2	0.53	2.34	19	3
1:A:588:TYR:HB2	1:A:610:ILE:HG22	0.53	1.81	18	5
1:A:624:ILE:CD1	1:A:624:ILE:N	0.52	2.70	18	3
1:A:572:VAL:CG2	1:A:630:LEU:HD13	0.52	2.34	9	1
1:A:626:LYS:O	1:A:627:SER:CB	0.52	2.58	10	20
1:A:578:VAL:HG11	1:A:632:VAL:HG22	0.52	1.80	14	1
1:A:655:VAL:CG1	1:A:657:PHE:CE1	0.52	2.93	6	3
1:A:552:VAL:HG13	1:A:640:LEU:HB3	0.52	1.81	4	3
1:A:561:VAL:O	1:A:562:ALA:CB	0.52	2.57	17	13
1:A:621:LEU:C	1:A:621:LEU:CD1	0.52	2.78	17	1
1:A:571:LYS:HE2	1:A:577:HIS:CE1	0.52	2.39	11	5
1:A:559:CYS:O	1:A:561:VAL:N	0.52	2.42	19	2
1:A:580:VAL:HG13	1:A:630:LEU:HD22	0.52	1.81	13	1
1:A:569:LEU:CD1	1:A:569:LEU:C	0.51	2.78	19	12
1:A:655:VAL:CG1	1:A:657:PHE:CE2	0.51	2.93	9	9
1:A:556:CYS:O	1:A:557:ILE:C	0.51	2.48	5	20
1:A:569:LEU:C	1:A:569:LEU:CD1	0.51	2.78	8	6
1:A:571:LYS:CE	1:A:577:HIS:CE1	0.51	2.94	11	1
1:A:577:HIS:HB2	1:A:652:TRP:CH2	0.51	2.41	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:621:LEU:CD2	1:A:622:GLN:O	0.51	2.59	19	11
1:A:655:VAL:HG12	1:A:657:PHE:O	0.51	2.06	14	7
1:A:610:ILE:HD11	1:A:622:GLN:HA	0.51	1.83	1	6
1:A:621:LEU:CD2	1:A:621:LEU:C	0.50	2.76	9	6
1:A:621:LEU:HD12	1:A:621:LEU:O	0.50	2.06	12	1
1:A:577:HIS:O	1:A:578:VAL:HG13	0.50	2.06	15	3
1:A:635:VAL:CG1	1:A:650:LYS:C	0.50	2.80	19	5
1:A:563:VAL:HA	1:A:587:TYR:CE2	0.50	2.41	14	1
1:A:622:GLN:OE1	1:A:629:LYS:CE	0.50	2.60	5	5
1:A:566:GLY:O	1:A:569:LEU:CD1	0.50	2.60	19	6
1:A:635:VAL:CG1	1:A:650:LYS:O	0.50	2.60	15	2
1:A:546:GLN:C	1:A:547:PHE:CD2	0.50	2.85	17	1
1:A:578:VAL:CG1	1:A:631:PRO:O	0.49	2.60	11	5
1:A:547:PHE:CE1	1:A:647:ILE:CD1	0.49	2.95	17	1
1:A:549:VAL:CG1	1:A:658:SER:O	0.49	2.60	7	3
1:A:635:VAL:HG23	1:A:650:LYS:C	0.49	2.27	6	2
1:A:556:CYS:O	1:A:559:CYS:N	0.49	2.45	19	6
1:A:549:VAL:HG12	1:A:657:PHE:HB2	0.49	1.85	13	6
1:A:548:PRO:O	1:A:552:VAL:HG23	0.49	2.07	6	2
1:A:607:GLY:N	1:A:622:GLN:O	0.49	2.45	19	20
1:A:584:PHE:CE2	1:A:633:LEU:HD21	0.49	2.42	8	1
1:A:619:TRP:O	1:A:634:LYS:CD	0.49	2.60	12	8
1:A:634:LYS:NZ	1:A:636:ARG:NE	0.49	2.60	9	1
1:A:570:ARG:NE	1:A:578:VAL:HG23	0.49	2.22	15	1
1:A:572:VAL:O	1:A:573:GLU:CG	0.49	2.61	10	9
1:A:577:HIS:CD2	1:A:659:VAL:HG21	0.49	2.43	3	2
1:A:635:VAL:HG21	1:A:655:VAL:CG2	0.49	2.38	4	1
1:A:604:TRP:CE3	1:A:623:MET:HB3	0.48	2.43	9	7
1:A:606:PRO:O	1:A:624:ILE:CD1	0.48	2.61	6	2
1:A:578:VAL:HG23	1:A:578:VAL:O	0.48	2.09	17	3
1:A:570:ARG:C	1:A:659:VAL:CG2	0.48	2.81	7	2
1:A:589:ASN:N	1:A:589:ASN:ND2	0.48	2.61	16	1
1:A:621:LEU:O	1:A:621:LEU:HD23	0.48	2.09	3	1
1:A:577:HIS:HB3	1:A:652:TRP:CH2	0.48	2.43	6	1
1:A:560:MET:HG2	1:A:639:LEU:HD23	0.48	1.85	19	1
1:A:568:ASP:O	1:A:570:ARG:CZ	0.48	2.62	5	1
1:A:625:TYR:CE2	1:A:626:LYS:HG3	0.48	2.42	7	1
1:A:581:ASN:OD1	1:A:584:PHE:N	0.48	2.47	11	4
1:A:578:VAL:CB	1:A:631:PRO:O	0.48	2.61	3	5
1:A:621:LEU:O	1:A:621:LEU:HD12	0.48	2.09	17	1
1:A:610:ILE:HD11	1:A:622:GLN:CA	0.48	2.38	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:569:LEU:CD1	1:A:569:LEU:O	0.48	2.61	13	6
1:A:569:LEU:HD21	1:A:657:PHE:CE2	0.48	2.44	17	3
1:A:584:PHE:CZ	1:A:633:LEU:HD11	0.48	2.44	11	1
1:A:569:LEU:CD2	1:A:657:PHE:CZ	0.48	2.93	13	1
1:A:639:LEU:HD21	1:A:646:ARG:NE	0.48	2.24	9	1
1:A:621:LEU:HD22	1:A:622:GLN:C	0.47	2.29	15	9
1:A:559:CYS:O	1:A:560:MET:CB	0.47	2.62	14	13
1:A:549:VAL:HG23	1:A:567:SER:CB	0.47	2.39	6	5
1:A:578:VAL:O	1:A:578:VAL:HG23	0.47	2.09	7	3
1:A:625:TYR:CD2	1:A:625:TYR:O	0.47	2.68	17	2
1:A:634:LYS:C	1:A:652:TRP:CZ2	0.47	2.88	11	5
1:A:556:CYS:C	1:A:558:ASN:N	0.47	2.67	18	20
1:A:571:LYS:O	1:A:662:PHE:N	0.47	2.48	6	10
1:A:572:VAL:O	1:A:575:THR:N	0.47	2.47	3	3
1:A:571:LYS:HD3	1:A:577:HIS:CE1	0.47	2.45	9	4
1:A:553:GLN:O	1:A:555:LEU:CD1	0.47	2.62	10	1
1:A:559:CYS:O	1:A:560:MET:HB2	0.47	2.10	5	17
1:A:575:THR:HG22	1:A:576:HIS:N	0.47	2.25	20	1
1:A:612:CYS:O	1:A:616:GLY:N	0.47	2.48	12	20
1:A:577:HIS:HB2	1:A:652:TRP:CZ2	0.47	2.45	14	3
1:A:589:ASN:ND2	1:A:589:ASN:N	0.47	2.62	5	1
1:A:605:LYS:HE2	1:A:624:ILE:HD13	0.47	1.85	3	1
1:A:549:VAL:CG2	1:A:567:SER:CB	0.47	2.93	3	1
1:A:577:HIS:NE2	1:A:659:VAL:CG1	0.47	2.78	6	2
1:A:571:LYS:CD	1:A:659:VAL:O	0.46	2.63	13	1
1:A:577:HIS:CB	1:A:652:TRP:CZ3	0.46	2.98	19	7
1:A:569:LEU:O	1:A:569:LEU:CD1	0.46	2.62	6	1
1:A:640:LEU:N	1:A:640:LEU:HD22	0.46	2.25	6	1
1:A:570:ARG:O	1:A:578:VAL:CG2	0.46	2.64	20	1
1:A:619:TRP:NE1	1:A:638:MET:HE3	0.46	2.24	7	11
1:A:628:VAL:CG1	1:A:630:LEU:CD2	0.46	2.89	12	4
1:A:651:LYS:CB	1:A:654:ARG:NH1	0.46	2.79	9	1
1:A:572:VAL:O	1:A:573:GLU:C	0.46	2.54	14	3
1:A:559:CYS:N	1:A:615:CYS:SG	0.46	2.89	7	8
1:A:626:LYS:CE	1:A:626:LYS:HA	0.46	2.40	11	2
1:A:635:VAL:CG2	1:A:650:LYS:C	0.46	2.85	9	2
1:A:577:HIS:CD2	1:A:659:VAL:CG1	0.45	2.87	11	3
1:A:604:TRP:CH2	1:A:623:MET:HG3	0.45	2.46	14	2
1:A:546:GLN:O	1:A:547:PHE:CD2	0.45	2.70	17	1
1:A:550:GLU:OE2	1:A:551:HIS:NE2	0.45	2.50	6	1
1:A:618:VAL:O	1:A:634:LYS:NZ	0.45	2.50	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:568:ASP:O	1:A:570:ARG:NH1	0.45	2.50	1	3
1:A:578:VAL:HG11	1:A:604:TRP:HZ3	0.45	1.72	13	1
1:A:584:PHE:CZ	1:A:633:LEU:HD21	0.45	2.47	8	1
1:A:570:ARG:HE	1:A:580:VAL:HG21	0.45	1.70	14	1
1:A:580:VAL:O	1:A:581:ASN:ND2	0.45	2.50	6	2
1:A:563:VAL:HA	1:A:587:TYR:CD2	0.45	2.46	19	2
1:A:570:ARG:CB	1:A:660:PRO:O	0.45	2.65	16	1
1:A:570:ARG:NH1	1:A:662:PHE:CD1	0.45	2.85	14	1
1:A:572:VAL:O	1:A:574:GLY:N	0.45	2.50	17	1
1:A:579:ASN:CG	1:A:633:LEU:CD2	0.45	2.86	8	1
1:A:555:LEU:HD23	1:A:562:ALA:HA	0.45	1.88	12	2
1:A:555:LEU:HD21	1:A:641:GLU:CD	0.45	2.33	8	3
1:A:635:VAL:CG2	1:A:655:VAL:CG2	0.44	2.95	10	2
1:A:579:ASN:ND2	1:A:579:ASN:C	0.44	2.70	11	2
1:A:635:VAL:HG22	1:A:649:ALA:O	0.44	2.11	20	1
1:A:635:VAL:HB	1:A:652:TRP:CD1	0.44	2.47	2	2
1:A:662:PHE:CD1	1:A:662:PHE:C	0.44	2.91	9	2
1:A:546:GLN:O	1:A:644:GLN:NE2	0.44	2.50	1	5
1:A:604:TRP:CH2	1:A:632:VAL:CG2	0.44	3.00	16	2
1:A:559:CYS:SG	1:A:615:CYS:N	0.44	2.91	2	9
1:A:657:PHE:CD2	1:A:659:VAL:HG22	0.44	2.45	12	2
1:A:569:LEU:C	1:A:570:ARG:CG	0.44	2.85	20	2
1:A:556:CYS:O	1:A:560:MET:CG	0.44	2.65	7	9
1:A:585:SER:HA	1:A:588:TYR:CE2	0.44	2.47	13	11
1:A:577:HIS:NE2	1:A:659:VAL:CG2	0.44	2.81	3	1
1:A:547:PHE:CG	1:A:656:PRO:HB2	0.44	2.48	13	4
1:A:634:LYS:O	1:A:652:TRP:CZ2	0.44	2.71	12	1
1:A:661:ASP:N	1:A:661:ASP:OD2	0.44	2.51	12	1
1:A:570:ARG:NH2	1:A:580:VAL:HG21	0.44	2.26	14	1
1:A:634:LYS:HE2	1:A:636:ARG:CG	0.44	2.43	16	1
1:A:635:VAL:HG13	1:A:650:LYS:C	0.44	2.33	13	2
1:A:604:TRP:CE3	1:A:623:MET:CB	0.44	3.01	15	2
1:A:555:LEU:CD2	1:A:562:ALA:HB2	0.44	2.41	3	2
1:A:558:ASN:ND2	1:A:617:GLU:OE1	0.44	2.51	3	2
1:A:560:MET:SD	1:A:639:LEU:CD2	0.44	3.06	19	1
1:A:634:LYS:CE	1:A:636:ARG:HG3	0.43	2.43	15	1
1:A:626:LYS:CA	1:A:626:LYS:HE2	0.43	2.43	8	3
1:A:555:LEU:HD23	1:A:562:ALA:N	0.43	2.29	12	4
1:A:612:CYS:SG	1:A:619:TRP:CZ2	0.43	3.12	6	1
1:A:570:ARG:NH2	1:A:580:VAL:CG2	0.43	2.78	14	1
1:A:588:TYR:C	1:A:589:ASN:ND2	0.43	2.72	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:549:VAL:CG2	1:A:567:SER:OG	0.43	2.66	6	1
1:A:579:ASN:N	1:A:579:ASN:OD1	0.43	2.52	8	1
1:A:570:ARG:CA	1:A:660:PRO:O	0.43	2.66	16	2
1:A:549:VAL:CG2	1:A:567:SER:HB2	0.43	2.44	3	1
1:A:547:PHE:CD1	1:A:656:PRO:HB2	0.43	2.48	14	1
1:A:574:GLY:O	1:A:575:THR:C	0.43	2.57	3	1
1:A:648:GLN:OE1	1:A:649:ALA:N	0.43	2.51	18	3
1:A:553:GLN:OE1	1:A:565:HIS:NE2	0.43	2.52	4	1
1:A:571:LYS:CE	1:A:659:VAL:O	0.43	2.66	7	2
1:A:580:VAL:CG1	1:A:630:LEU:HD22	0.43	2.44	13	1
1:A:577:HIS:HB2	1:A:652:TRP:CE2	0.43	2.48	6	3
1:A:558:ASN:ND2	1:A:617:GLU:OE2	0.43	2.51	4	1
1:A:580:VAL:O	1:A:581:ASN:CB	0.43	2.67	6	2
1:A:636:ARG:O	1:A:648:GLN:NE2	0.43	2.52	8	1
1:A:604:TRP:CD1	1:A:623:MET:SD	0.43	3.12	13	1
1:A:635:VAL:HG23	1:A:650:LYS:O	0.43	2.13	6	1
1:A:639:LEU:HD11	1:A:646:ARG:HB3	0.43	1.91	19	1
1:A:634:LYS:HZ1	1:A:636:ARG:CD	0.43	2.27	9	1
1:A:634:LYS:NZ	1:A:636:ARG:CZ	0.43	2.82	9	1
1:A:564:GLY:C	1:A:565:HIS:CD2	0.43	2.91	18	1
1:A:571:LYS:N	1:A:660:PRO:O	0.43	2.52	10	2
1:A:657:PHE:CD1	1:A:657:PHE:C	0.43	2.91	13	1
1:A:635:VAL:HG13	1:A:649:ALA:C	0.43	2.35	1	1
1:A:573:GLU:O	1:A:574:GLY:C	0.43	2.56	14	1
1:A:635:VAL:HG11	1:A:651:LYS:O	0.42	2.14	18	1
1:A:579:ASN:CG	1:A:633:LEU:HD23	0.42	2.35	8	1
1:A:634:LYS:HE3	1:A:636:ARG:CG	0.42	2.44	15	1
1:A:605:LYS:HZ2	1:A:624:ILE:HB	0.42	1.74	10	1
1:A:569:LEU:O	1:A:570:ARG:CG	0.42	2.67	12	3
1:A:640:LEU:N	1:A:640:LEU:CD2	0.42	2.83	6	1
1:A:561:VAL:O	1:A:561:VAL:HG23	0.42	2.13	2	1
1:A:577:HIS:O	1:A:578:VAL:CG1	0.42	2.67	5	1
1:A:655:VAL:CG1	1:A:657:PHE:CD2	0.42	3.03	9	2
1:A:556:CYS:O	1:A:560:MET:HG3	0.42	2.15	4	4
1:A:635:VAL:HB	1:A:652:TRP:CE2	0.42	2.50	7	5
1:A:621:LEU:HD13	1:A:621:LEU:O	0.42	2.15	15	1
1:A:546:GLN:O	1:A:547:PHE:CD1	0.42	2.73	20	1
1:A:555:LEU:CD2	1:A:641:GLU:CD	0.42	2.88	18	1
1:A:584:PHE:CD2	1:A:631:PRO:CG	0.42	3.03	5	1
1:A:619:TRP:NE1	1:A:638:MET:HE1	0.42	2.29	16	1
1:A:588:TYR:OH	1:A:622:GLN:NE2	0.41	2.53	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:557:ILE:O	1:A:560:MET:CE	0.41	2.68	12	1
1:A:635:VAL:CG1	1:A:651:LYS:CA	0.41	2.97	5	1
1:A:634:LYS:CE	1:A:636:ARG:CD	0.41	2.98	9	1
1:A:550:GLU:OE2	1:A:551:HIS:CD2	0.41	2.73	6	1
1:A:577:HIS:NE2	1:A:652:TRP:CG	0.41	2.88	20	1
1:A:635:VAL:HG11	1:A:651:LYS:HA	0.41	1.93	12	1
1:A:626:LYS:HE3	1:A:626:LYS:CA	0.41	2.46	13	1
1:A:626:LYS:O	1:A:627:SER:OG	0.41	2.38	7	2
1:A:634:LYS:NZ	1:A:637:SER:OG	0.41	2.49	14	1
1:A:609:VAL:CG1	1:A:618:VAL:CG1	0.41	2.98	18	1
1:A:612:CYS:HB2	1:A:619:TRP:CE2	0.41	2.51	14	1
1:A:654:ARG:O	1:A:655:VAL:C	0.41	2.59	13	14
1:A:577:HIS:NE2	1:A:659:VAL:HG13	0.41	2.31	6	1
1:A:635:VAL:HG21	1:A:652:TRP:HA	0.41	1.92	19	1
1:A:608:GLY:O	1:A:622:GLN:N	0.41	2.53	4	2
1:A:572:VAL:C	1:A:574:GLY:N	0.41	2.71	17	3
1:A:585:SER:O	1:A:588:TYR:O	0.41	2.39	6	6
1:A:639:LEU:HD22	1:A:646:ARG:HG2	0.41	1.92	6	1
1:A:570:ARG:C	1:A:659:VAL:HG12	0.41	2.35	14	1
1:A:560:MET:CG	1:A:639:LEU:HD23	0.41	2.45	19	1
1:A:570:ARG:O	1:A:578:VAL:HG23	0.41	2.16	20	1
1:A:561:VAL:CG2	1:A:614:ASN:OD1	0.41	2.68	20	1
1:A:577:HIS:CG	1:A:652:TRP:CZ3	0.41	3.09	3	1
1:A:635:VAL:O	1:A:638:MET:O	0.41	2.39	18	1
1:A:578:VAL:HG12	1:A:632:VAL:CA	0.41	2.40	9	1
1:A:570:ARG:CZ	1:A:578:VAL:CG2	0.41	2.99	15	1
1:A:583:ASN:N	1:A:583:ASN:OD1	0.41	2.54	7	1
1:A:580:VAL:O	1:A:581:ASN:CG	0.41	2.59	8	3
1:A:584:PHE:O	1:A:587:TYR:N	0.41	2.53	3	1
1:A:563:VAL:CG1	1:A:614:ASN:ND2	0.40	2.84	3	1
1:A:635:VAL:HG12	1:A:652:TRP:CD1	0.40	2.51	16	1
1:A:640:LEU:CD2	1:A:657:PHE:CE2	0.40	3.05	11	1
1:A:635:VAL:HB	1:A:652:TRP:CG	0.40	2.51	2	1
1:A:604:TRP:CZ2	1:A:623:MET:HG3	0.40	2.51	16	1
1:A:605:LYS:O	1:A:623:MET:SD	0.40	2.80	16	1
1:A:570:ARG:NH1	1:A:572:VAL:HG23	0.40	2.31	15	1
1:A:635:VAL:HB	1:A:652:TRP:CD2	0.40	2.51	11	2
1:A:635:VAL:O	1:A:649:ALA:O	0.40	2.39	4	2
1:A:569:LEU:HD13	1:A:659:VAL:HB	0.40	1.92	18	1
1:A:634:LYS:CE	1:A:636:ARG:HG2	0.40	2.46	16	1
1:A:648:GLN:C	1:A:648:GLN:OE1	0.40	2.60	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:640:LEU:HD22	1:A:657:PHE:CE2	0.40	2.51	4	1
1:A:623:MET:O	1:A:630:LEU:O	0.40	2.40	19	1
1:A:648:GLN:OE1	1:A:648:GLN:C	0.40	2.59	13	1
1:A:548:PRO:HG2	1:A:551:HIS:CG	0.40	2.51	13	1
1:A:648:GLN:OE1	1:A:649:ALA:O	0.40	2.40	16	1
1:A:561:VAL:HG23	1:A:561:VAL:O	0.40	2.16	6	1
1:A:555:LEU:CD2	1:A:641:GLU:OE2	0.40	2.70	18	1
1:A:563:VAL:HG11	1:A:619:TRP:CH2	0.40	2.51	15	1
1:A:571:LYS:CG	1:A:574:GLY:HA2	0.40	2.46	14	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	105/137 (77%)	86±2 (82±2%)	15±2 (14±2%)	4±1 (4±1%)	6	32
All	All	2100/2740 (77%)	1717 (82%)	294 (14%)	89 (4%)	6	32

All 16 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	627	SER	19
1	A	557	ILE	19
1	A	617	GLU	15
1	A	562	ALA	11
1	A	560	MET	6
1	A	646	ARG	3
1	A	656	PRO	3
1	A	581	ASN	3
1	A	607	GLY	2
1	A	618	VAL	2
1	A	616	GLY	1
1	A	591	SER	1
1	A	573	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	662	PHE	1
1	A	575	THR	1
1	A	661	ASP	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/125 (76%)	77±2 (81±2%)	19±2 (19±2%)	5	37
All	All	1900/2500 (76%)	1530 (81%)	370 (19%)	5	37

All 43 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	621	LEU	20
1	A	610	ILE	20
1	A	569	LEU	20
1	A	555	LEU	20
1	A	604	TRP	20
1	A	633	LEU	20
1	A	561	VAL	18
1	A	648	GLN	18
1	A	611	SER	17
1	A	642	THR	15
1	A	622	GLN	14
1	A	626	LYS	14
1	A	547	PHE	14
1	A	658	SER	13
1	A	615	CYS	12
1	A	583	ASN	10
1	A	640	LEU	9
1	A	651	LYS	8
1	A	563	VAL	7
1	A	634	LYS	7
1	A	625	TYR	6
1	A	589	ASN	6

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Mol	Chain	Res	Type	Models (Total)
1	A	554	LEU	6
1	A	636	ARG	6
1	A	659	VAL	5
1	A	639	LEU	5
1	A	588	TYR	5
1	A	605	LYS	5
1	A	570	ARG	5
1	A	557	ILE	5
1	A	661	ASP	4
1	A	576	HIS	2
1	A	635	VAL	2
1	A	546	GLN	2
1	A	581	ASN	2
1	A	650	LYS	1
1	A	579	ASN	1
1	A	637	SER	1
1	A	646	ARG	1
1	A	559	CYS	1
1	A	629	LYS	1
1	A	578	VAL	1
1	A	567	SER	1

6.3.3   RNA (i)

There are no RNA molecules in this entry.

6.4   Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5   Carbohydrates (i)

There are no carbohydrates in this entry.

6.6   Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided