



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:44 PM BST

PDB ID : 1Z23  
Title : The serine-rich domain from Crk-associated substrate (p130Cas)  
Authors : Briknarova, K.; Nasertorabi, F.; Havert, M.L.; Eggleston, E.; Hoyt, D.W.; Li, C.; Olson, A.J.; Vuori, K.; Ely, K.R.  
Deposited on : 2005-03-07

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 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

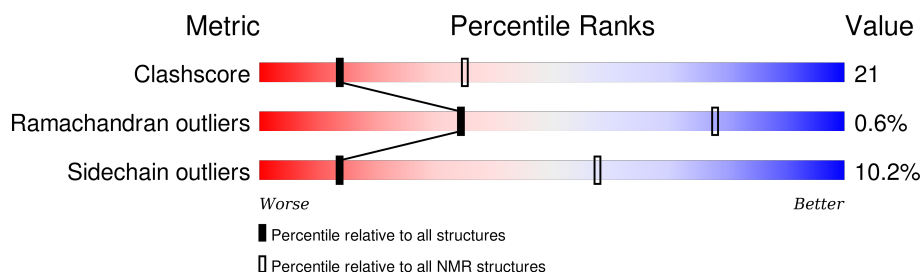
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	163	

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 10 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:553-A:579, A:599-A:625, A:634-A:661, A:670-A:704 (117)	0.39	10

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 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2439 atoms, of which 1219 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CRK-associated substrate.

Mol	Chain	Residues	Atoms						Trace
1	A	163	Total	C	H	N	O	S	0
			2439	754	1219	226	238	2	

There are 2 discrepancies between the modelled and reference sequences:

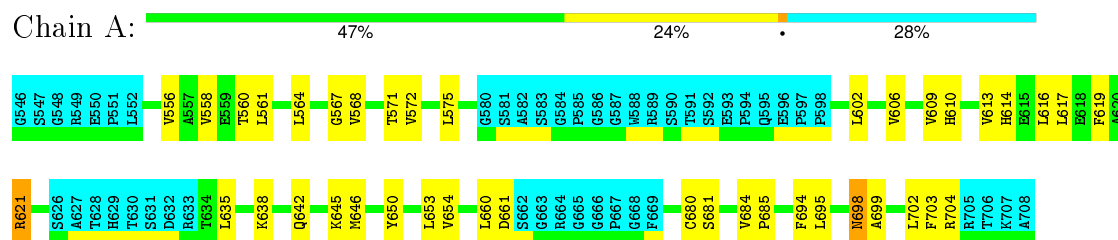
Chain	Residue	Modelled	Actual	Comment	Reference
A	546	GLY	VAL	ENGINEERED	UNP Q63767
A	547	SER	PRO	ENGINEERED	UNP Q63767

## 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: CRK-associated substrate

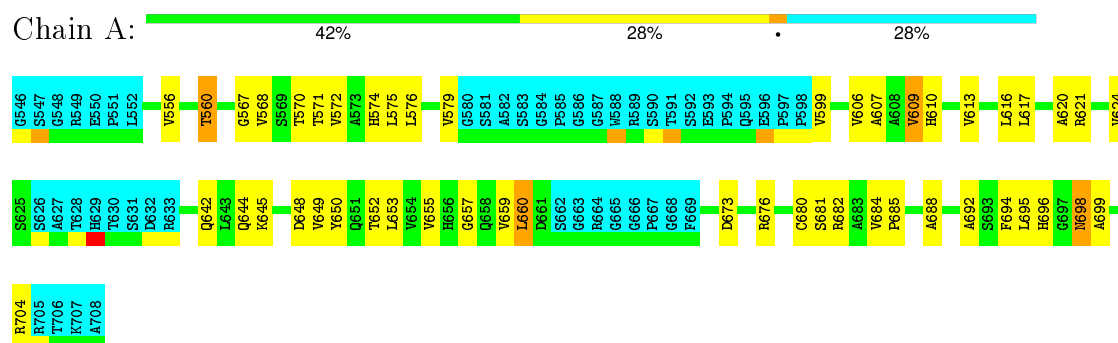


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

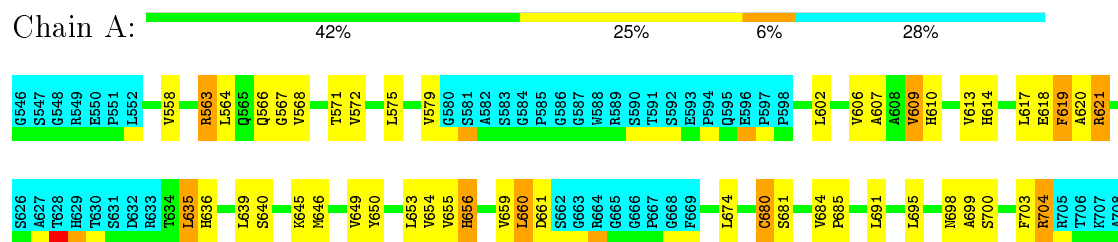
#### 4.2.1 Score per residue for model 1

- Molecule 1: CRK-associated substrate



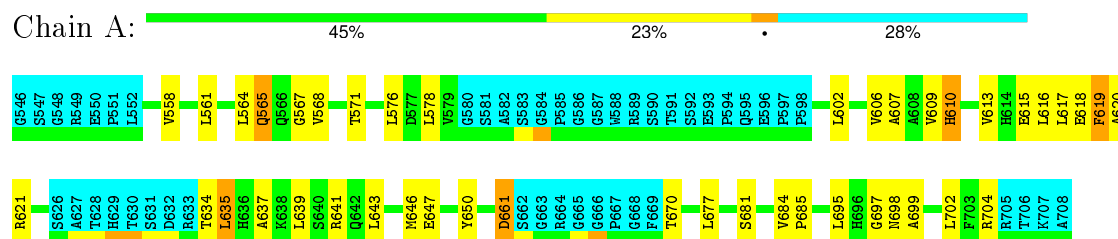
#### 4.2.2 Score per residue for model 2

- Molecule 1: CRK-associated substrate



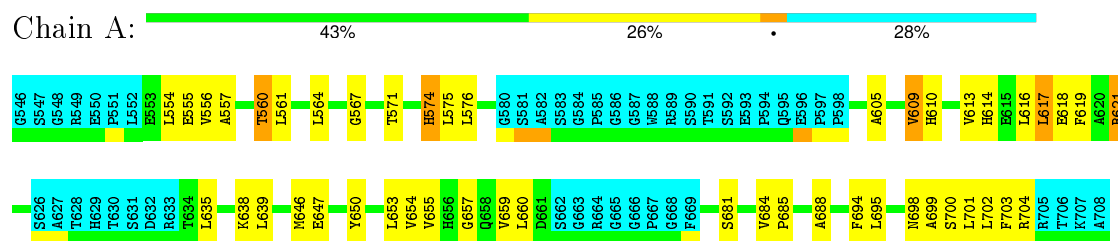
### 4.2.3 Score per residue for model 3

- Molecule 1: CRK-associated substrate



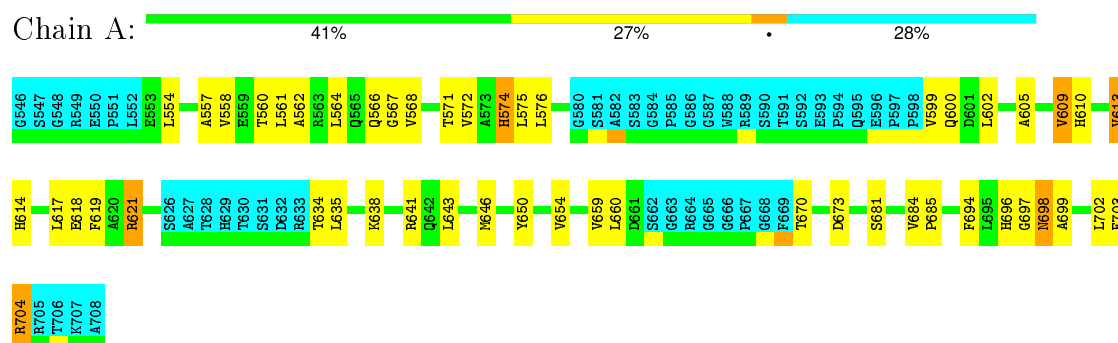
### 4.2.4 Score per residue for model 4

- Molecule 1: CRK-associated substrate



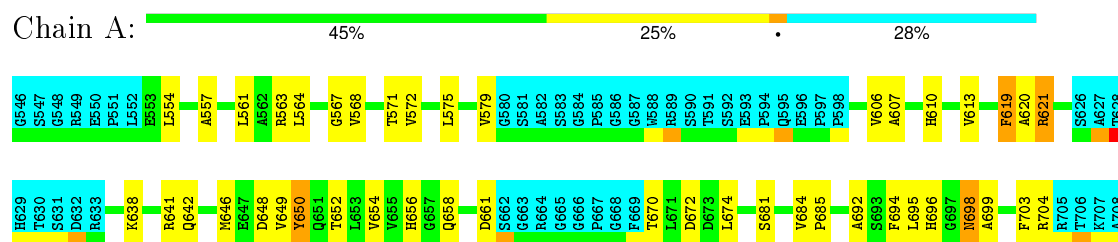
### 4.2.5 Score per residue for model 5

- Molecule 1: CRK-associated substrate



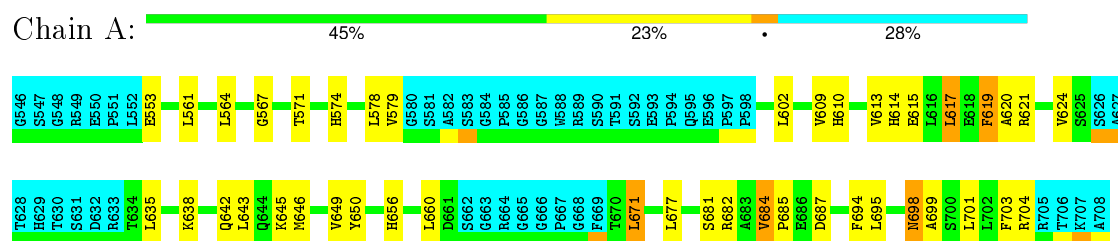
### 4.2.6 Score per residue for model 6

- Molecule 1: CRK-associated substrate



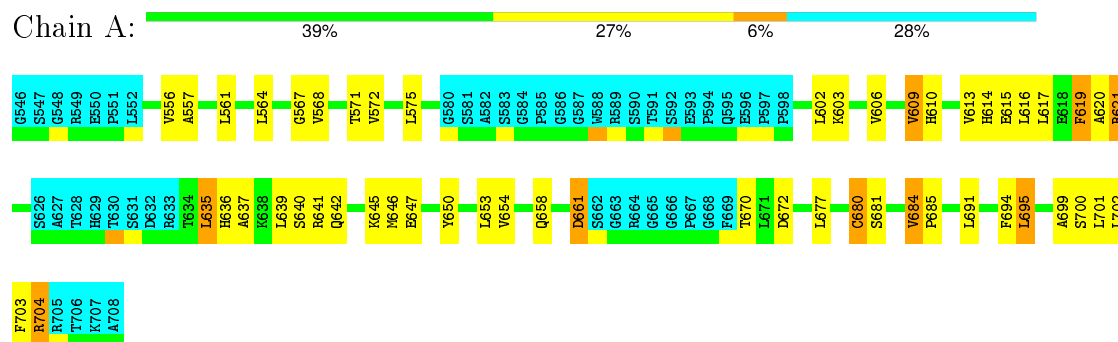
### 4.2.7 Score per residue for model 7

- Molecule 1: CRK-associated substrate



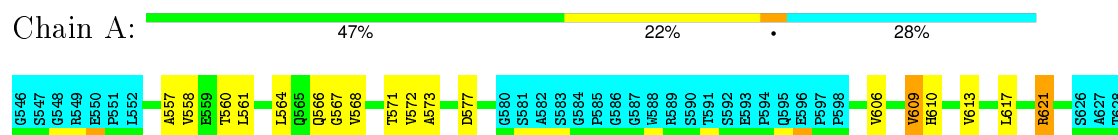
### 4.2.8 Score per residue for model 8

- Molecule 1: CRK-associated substrate



### 4.2.9 Score per residue for model 9

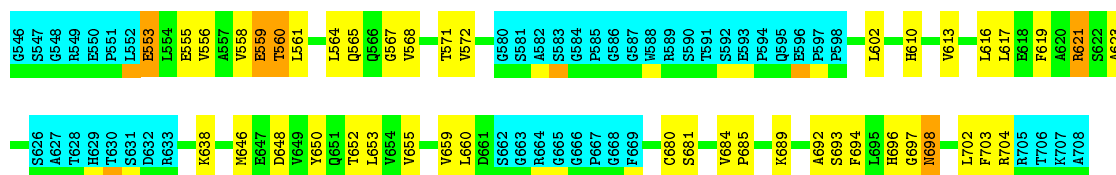
- Molecule 1: CRK-associated substrate





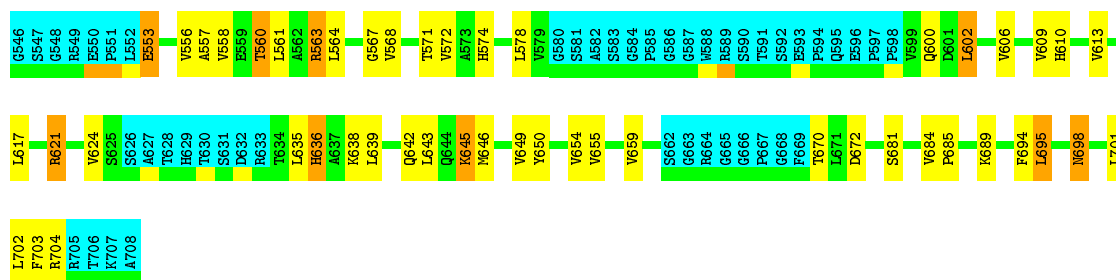
#### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: CRK-associated substrate



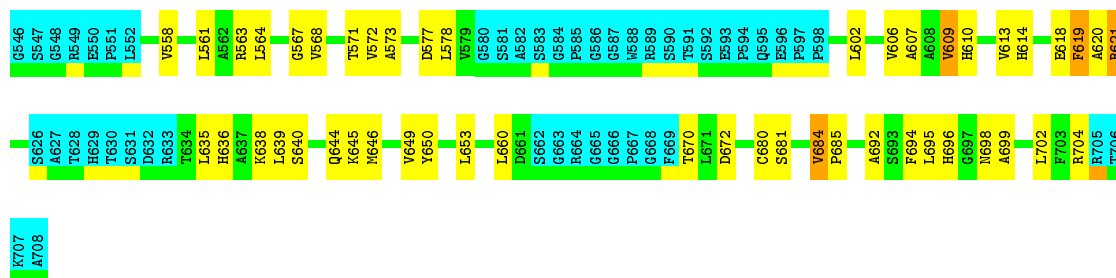
#### 4.2.11 Score per residue for model 11

- Molecule 1: CRK-associated substrate



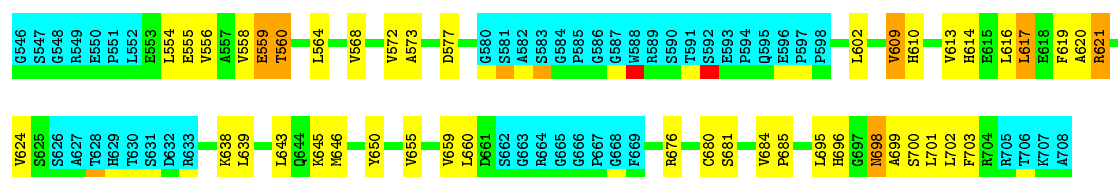
#### 4.2.12 Score per residue for model 12

- Molecule 1: CRK-associated substrate



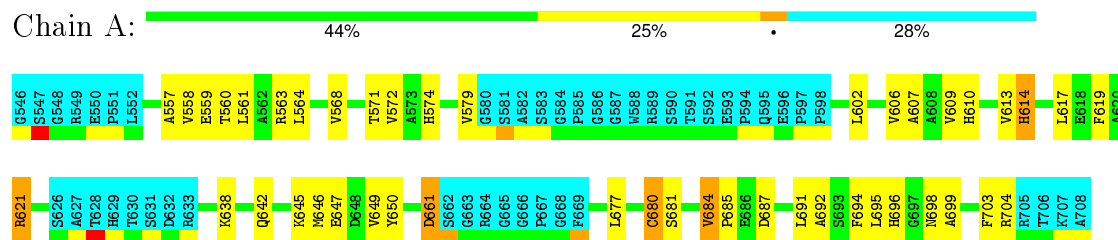






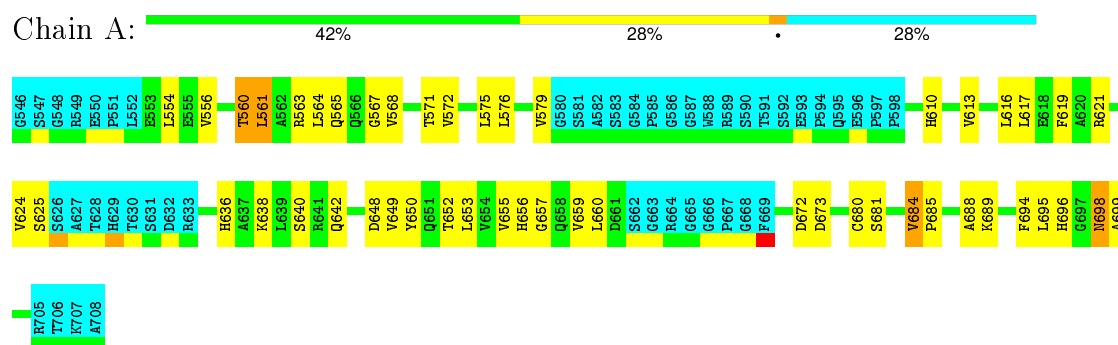
#### 4.2.17 Score per residue for model 17

- Molecule 1: CRK-associated substrate



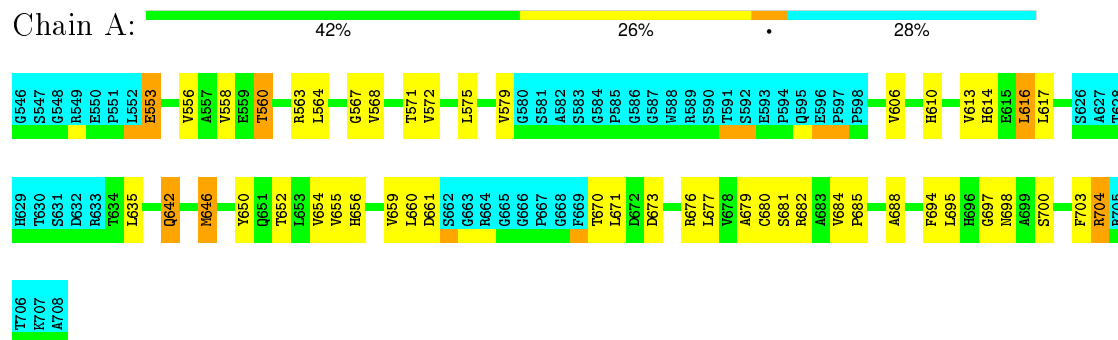
#### 4.2.18 Score per residue for model 18

- Molecule 1: CRK-associated substrate



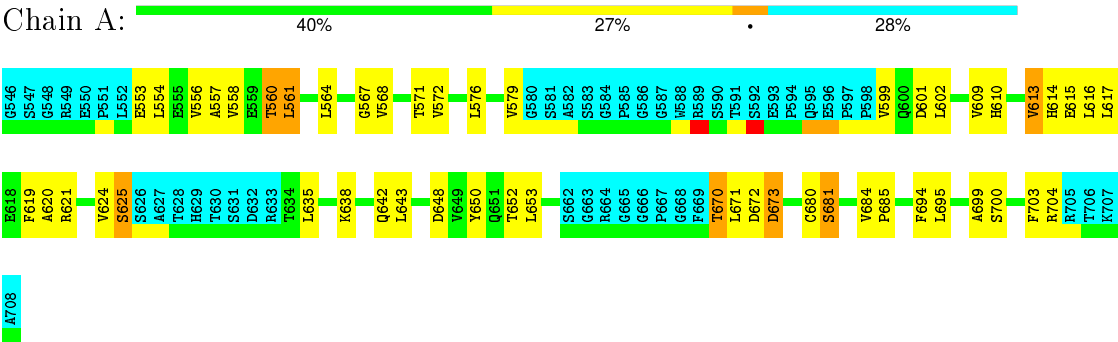
#### 4.2.19 Score per residue for model 19

- Molecule 1: CRK-associated substrate



4.2.20 Score per residue for model 20

● Molecule 1: CRK-associated substrate



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *Torsion angle dynamics*.

Of the 99 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
Xplor-NIH	structure solution	2.9.4a
Xplor-NIH	refinement	2.9.4a

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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	895	917	917	38±4
All	All	17900	18340	18340	755

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:613:VAL:HG11	1:A:650:TYR:CD1	0.84	2.08	19	5
1:A:617:LEU:HD13	1:A:650:TYR:CE2	0.83	2.07	4	6
1:A:617:LEU:HD22	1:A:650:TYR:CD2	0.79	2.12	2	3
1:A:695:LEU:O	1:A:695:LEU:HD12	0.78	1.78	11	1
1:A:653:LEU:HD13	1:A:680:CYS:SG	0.76	2.20	2	2
1:A:619:PHE:CD1	1:A:620:ALA:N	0.76	2.54	3	6
1:A:677:LEU:C	1:A:677:LEU:HD13	0.76	2.00	7	1
1:A:561:LEU:HD13	1:A:561:LEU:C	0.76	2.01	6	1
1:A:609:VAL:O	1:A:613:VAL:HG23	0.75	1.81	2	4
1:A:564:LEU:O	1:A:568:VAL:HG23	0.75	1.81	2	16
1:A:561:LEU:C	1:A:561:LEU:HD13	0.75	2.01	7	1
1:A:655:VAL:O	1:A:659:VAL:HG23	0.75	1.81	9	9
1:A:613:VAL:HG22	1:A:650:TYR:CE2	0.74	2.18	16	5
1:A:648:ASP:O	1:A:652:THR:HG23	0.73	1.82	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:554:LEU:C	1:A:554:LEU:HD13	0.73	2.04	18	1
1:A:574:HIS:NE2	1:A:578:LEU:HD11	0.73	1.98	11	2
1:A:575:LEU:O	1:A:579:VAL:HG23	0.73	1.84	18	4
1:A:620:ALA:O	1:A:624:VAL:HG23	0.72	1.84	16	3
1:A:567:GLY:O	1:A:571:THR:HG23	0.72	1.84	9	17
1:A:610:HIS:O	1:A:650:TYR:OH	0.72	2.06	14	11
1:A:554:LEU:HD13	1:A:699:ALA:HB1	0.72	1.61	6	2
1:A:571:THR:OG1	1:A:609:VAL:HG23	0.71	1.85	3	9
1:A:554:LEU:O	1:A:558:VAL:HG13	0.69	1.87	20	1
1:A:660:LEU:O	1:A:660:LEU:HD12	0.69	1.86	1	2
1:A:572:VAL:HG13	1:A:681:SER:OG	0.69	1.86	17	5
1:A:645:LYS:O	1:A:649:VAL:HG23	0.69	1.88	14	7
1:A:637:ALA:HB1	1:A:641:ARG:HH21	0.67	1.48	8	1
1:A:660:LEU:HD12	1:A:660:LEU:C	0.67	2.09	9	4
1:A:660:LEU:C	1:A:660:LEU:HD12	0.67	2.10	1	2
1:A:613:VAL:HG22	1:A:650:TYR:CZ	0.67	2.24	16	5
1:A:681:SER:O	1:A:685:PRO:CD	0.67	2.43	14	20
1:A:617:LEU:HD13	1:A:650:TYR:CZ	0.67	2.24	20	6
1:A:565:GLN:HE22	1:A:616:LEU:HD13	0.67	1.48	18	1
1:A:646:MET:SD	1:A:691:LEU:HD12	0.67	2.30	8	1
1:A:613:VAL:HG11	1:A:650:TYR:CE1	0.67	2.25	18	10
1:A:617:LEU:HD21	1:A:647:GLU:CD	0.67	2.10	8	1
1:A:671:LEU:HD23	1:A:671:LEU:H	0.66	1.51	7	1
1:A:635:LEU:HD23	1:A:635:LEU:H	0.66	1.50	8	2
1:A:653:LEU:HD21	1:A:680:CYS:CB	0.66	2.21	20	4
1:A:701:LEU:HD12	1:A:701:LEU:N	0.66	2.06	16	4
1:A:571:THR:O	1:A:574:HIS:ND1	0.65	2.29	4	2
1:A:574:HIS:CD2	1:A:575:LEU:N	0.65	2.64	4	2
1:A:556:VAL:O	1:A:560:THR:OG1	0.65	2.14	14	11
1:A:650:TYR:O	1:A:654:VAL:HG23	0.65	1.91	9	6
1:A:660:LEU:HD23	1:A:660:LEU:O	0.64	1.93	5	1
1:A:698:ASN:ND2	1:A:698:ASN:N	0.64	2.44	6	3
1:A:574:HIS:CG	1:A:575:LEU:N	0.64	2.66	5	2
1:A:610:HIS:CD2	1:A:650:TYR:CZ	0.64	2.86	12	2
1:A:635:LEU:CD2	1:A:635:LEU:H	0.64	2.06	8	2
1:A:642:GLN:NE2	1:A:694:PHE:CE2	0.64	2.66	7	1
1:A:701:LEU:N	1:A:701:LEU:HD12	0.63	2.08	4	2
1:A:563:ARG:NH2	1:A:566:GLN:NE2	0.63	2.47	2	1
1:A:610:HIS:ND1	1:A:650:TYR:CZ	0.62	2.67	3	1
1:A:575:LEU:O	1:A:579:VAL:HG22	0.62	1.93	15	1
1:A:561:LEU:HD23	1:A:561:LEU:C	0.62	2.14	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:574:HIS:CE1	1:A:578:LEU:HD11	0.62	2.30	7	1
1:A:606:VAL:HG22	1:A:610:HIS:CD2	0.62	2.30	6	5
1:A:610:HIS:CG	1:A:650:TYR:OH	0.61	2.53	14	2
1:A:613:VAL:HG12	1:A:650:TYR:OH	0.61	1.95	5	2
1:A:574:HIS:CD2	1:A:574:HIS:C	0.61	2.72	4	1
1:A:670:THR:HG23	1:A:672:ASP:H	0.61	1.56	8	4
1:A:610:HIS:CE1	1:A:650:TYR:CE2	0.61	2.89	14	1
1:A:613:VAL:HG12	1:A:650:TYR:CE2	0.61	2.30	2	1
1:A:696:HIS:CD2	1:A:697:GLY:N	0.61	2.68	10	1
1:A:639:LEU:HD22	1:A:698:ASN:HD22	0.60	1.56	15	2
1:A:613:VAL:HG11	1:A:650:TYR:CZ	0.60	2.31	6	1
1:A:574:HIS:C	1:A:574:HIS:CD2	0.60	2.75	5	2
1:A:624:VAL:O	1:A:625:SER:C	0.60	2.39	18	2
1:A:617:LEU:HD21	1:A:647:GLU:OE2	0.60	1.96	8	1
1:A:561:LEU:O	1:A:561:LEU:HD23	0.60	1.96	4	1
1:A:695:LEU:O	1:A:699:ALA:N	0.60	2.35	8	15
1:A:698:ASN:N	1:A:698:ASN:HD22	0.60	1.94	16	2
1:A:619:PHE:CG	1:A:620:ALA:N	0.60	2.70	8	6
1:A:565:GLN:N	1:A:565:GLN:HE21	0.60	1.94	3	1
1:A:564:LEU:HD22	1:A:619:PHE:CD2	0.59	2.32	4	3
1:A:610:HIS:ND1	1:A:650:TYR:CE1	0.59	2.70	10	1
1:A:575:LEU:HD23	1:A:575:LEU:C	0.59	2.18	8	1
1:A:616:LEU:CD1	1:A:688:ALA:HB1	0.59	2.27	1	1
1:A:613:VAL:CG1	1:A:650:TYR:CE1	0.59	2.86	18	8
1:A:694:PHE:O	1:A:698:ASN:ND2	0.58	2.37	15	10
1:A:638:LYS:NZ	1:A:694:PHE:CE2	0.58	2.72	4	1
1:A:693:SER:O	1:A:696:HIS:ND1	0.58	2.36	10	1
1:A:613:VAL:CG1	1:A:614:HIS:N	0.58	2.66	7	5
1:A:696:HIS:CD2	1:A:696:HIS:C	0.58	2.75	10	4
1:A:601:ASP:OD1	1:A:602:LEU:N	0.58	2.37	20	1
1:A:643:LEU:HD23	1:A:643:LEU:O	0.57	2.00	3	2
1:A:616:LEU:HD23	1:A:616:LEU:O	0.56	2.00	10	2
1:A:610:HIS:CE1	1:A:654:VAL:CG2	0.56	2.88	5	2
1:A:653:LEU:HD21	1:A:680:CYS:HB3	0.56	1.75	18	4
1:A:642:GLN:CD	1:A:645:LYS:HZ1	0.56	2.03	17	1
1:A:698:ASN:OD1	1:A:698:ASN:N	0.56	2.38	14	3
1:A:703:PHE:O	1:A:704:ARG:CB	0.56	2.53	19	5
1:A:602:LEU:O	1:A:602:LEU:HD23	0.56	2.01	2	3
1:A:696:HIS:CG	1:A:697:GLY:N	0.56	2.73	10	1
1:A:578:LEU:O	1:A:578:LEU:HD23	0.56	2.01	12	1
1:A:680:CYS:SG	1:A:681:SER:N	0.56	2.79	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:568:VAL:O	1:A:572:VAL:HG23	0.55	2.00	12	7
1:A:672:ASP:OD1	1:A:673:ASP:N	0.55	2.38	18	2
1:A:610:HIS:NE2	1:A:650:TYR:CZ	0.55	2.75	14	2
1:A:691:LEU:O	1:A:691:LEU:HD23	0.55	2.01	8	1
1:A:653:LEU:HD22	1:A:680:CYS:SG	0.55	2.41	15	4
1:A:698:ASN:HD22	1:A:698:ASN:N	0.55	1.99	9	1
1:A:635:LEU:N	1:A:635:LEU:HD12	0.55	2.15	20	2
1:A:660:LEU:HD12	1:A:660:LEU:O	0.55	2.02	18	2
1:A:660:LEU:C	1:A:660:LEU:CD1	0.54	2.75	1	3
1:A:635:LEU:HD23	1:A:635:LEU:N	0.54	2.17	8	2
1:A:639:LEU:HD23	1:A:639:LEU:C	0.54	2.22	4	1
1:A:671:LEU:CD2	1:A:671:LEU:H	0.54	2.13	7	1
1:A:639:LEU:HD23	1:A:639:LEU:O	0.54	2.01	4	1
1:A:560:THR:CG2	1:A:561:LEU:N	0.54	2.71	9	3
1:A:610:HIS:O	1:A:614:HIS:ND1	0.54	2.41	8	2
1:A:617:LEU:HD22	1:A:650:TYR:CE2	0.54	2.37	2	1
1:A:561:LEU:O	1:A:565:GLN:NE2	0.54	2.40	3	1
1:A:642:GLN:OE1	1:A:694:PHE:CZ	0.54	2.61	13	3
1:A:703:PHE:O	1:A:704:ARG:C	0.54	2.45	5	1
1:A:687:ASP:OD1	1:A:691:LEU:HD23	0.54	2.02	17	1
1:A:677:LEU:C	1:A:677:LEU:HD23	0.54	2.23	9	1
1:A:643:LEU:O	1:A:643:LEU:HD23	0.53	2.03	16	3
1:A:642:GLN:OE1	1:A:694:PHE:CE2	0.53	2.61	20	4
1:A:636:HIS:CE1	1:A:640:SER:OG	0.53	2.62	2	3
1:A:610:HIS:CD2	1:A:650:TYR:OH	0.53	2.61	12	2
1:A:564:LEU:HD21	1:A:619:PHE:CG	0.53	2.39	16	3
1:A:617:LEU:HD11	1:A:650:TYR:CD2	0.53	2.38	17	1
1:A:642:GLN:OE1	1:A:694:PHE:CD2	0.53	2.62	7	3
1:A:698:ASN:O	1:A:702:LEU:N	0.52	2.41	5	6
1:A:561:LEU:HD21	1:A:692:ALA:HB1	0.52	1.81	12	1
1:A:554:LEU:C	1:A:554:LEU:CD1	0.52	2.77	18	1
1:A:639:LEU:CD1	1:A:702:LEU:HD11	0.52	2.33	11	2
1:A:602:LEU:HD23	1:A:602:LEU:O	0.52	2.03	20	2
1:A:677:LEU:C	1:A:677:LEU:CD1	0.52	2.74	7	1
1:A:635:LEU:H	1:A:635:LEU:HD23	0.52	1.64	3	1
1:A:563:ARG:O	1:A:563:ARG:NH1	0.52	2.42	11	1
1:A:618:GLU:OE1	1:A:621:ARG:NH1	0.52	2.42	4	1
1:A:652:THR:O	1:A:656:HIS:CD2	0.52	2.63	6	2
1:A:564:LEU:HD13	1:A:619:PHE:CE2	0.52	2.40	17	2
1:A:553:GLU:N	1:A:553:GLU:OE1	0.52	2.43	20	2
1:A:565:GLN:HE22	1:A:616:LEU:CD1	0.52	2.18	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:578:LEU:HD11	1:A:601:ASP:OD2	0.52	2.05	15	1
1:A:572:VAL:HG22	1:A:681:SER:OG	0.52	2.04	17	1
1:A:701:LEU:N	1:A:701:LEU:CD1	0.52	2.73	4	2
1:A:642:GLN:NE2	1:A:694:PHE:CD2	0.52	2.78	20	1
1:A:692:ALA:O	1:A:696:HIS:ND1	0.52	2.43	6	3
1:A:684:VAL:N	1:A:685:PRO:HD2	0.52	2.20	14	13
1:A:639:LEU:CD1	1:A:698:ASN:HD21	0.52	2.18	12	1
1:A:599:VAL:HG13	1:A:600:GLN:N	0.52	2.19	5	1
1:A:559:GLU:OE2	1:A:563:ARG:NH2	0.51	2.43	17	1
1:A:701:LEU:CD1	1:A:701:LEU:N	0.51	2.72	15	3
1:A:554:LEU:O	1:A:554:LEU:HD13	0.51	2.05	18	1
1:A:673:ASP:OD1	1:A:676:ARG:NH2	0.51	2.42	1	1
1:A:646:MET:O	1:A:650:TYR:CD1	0.51	2.63	5	6
1:A:700:SER:O	1:A:704:ARG:O	0.51	2.29	4	5
1:A:610:HIS:ND1	1:A:650:TYR:OH	0.51	2.44	3	1
1:A:599:VAL:CG1	1:A:600:GLN:N	0.51	2.74	5	1
1:A:653:LEU:O	1:A:657:GLY:N	0.51	2.40	18	5
1:A:578:LEU:HD23	1:A:578:LEU:O	0.51	2.05	3	1
1:A:677:LEU:O	1:A:677:LEU:HD23	0.51	2.06	19	3
1:A:635:LEU:CD2	1:A:635:LEU:N	0.51	2.74	11	1
1:A:691:LEU:O	1:A:695:LEU:HD13	0.51	2.05	9	2
1:A:610:HIS:O	1:A:614:HIS:CG	0.51	2.64	20	1
1:A:575:LEU:HD23	1:A:575:LEU:O	0.51	2.06	8	1
1:A:671:LEU:N	1:A:671:LEU:CD2	0.51	2.73	19	1
1:A:673:ASP:OD2	1:A:676:ARG:NH2	0.50	2.45	19	1
1:A:677:LEU:HD23	1:A:677:LEU:O	0.50	2.06	3	2
1:A:613:VAL:HG21	1:A:650:TYR:OH	0.50	2.05	6	1
1:A:695:LEU:C	1:A:695:LEU:HD12	0.50	2.26	11	1
1:A:635:LEU:HD22	1:A:698:ASN:OD1	0.50	2.06	7	1
1:A:639:LEU:O	1:A:639:LEU:HD23	0.50	2.07	8	1
1:A:618:GLU:CG	1:A:619:PHE:N	0.50	2.73	3	1
1:A:609:VAL:CG1	1:A:610:HIS:N	0.50	2.74	2	14
1:A:698:ASN:N	1:A:698:ASN:ND2	0.50	2.60	16	3
1:A:646:MET:SD	1:A:646:MET:O	0.50	2.69	3	1
1:A:671:LEU:N	1:A:671:LEU:HD22	0.50	2.21	19	1
1:A:606:VAL:HG22	1:A:610:HIS:NE2	0.50	2.22	6	2
1:A:561:LEU:O	1:A:561:LEU:HD13	0.50	2.07	15	1
1:A:642:GLN:CD	1:A:694:PHE:CE2	0.50	2.85	6	3
1:A:555:GLU:O	1:A:559:GLU:CG	0.50	2.60	16	2
1:A:616:LEU:HD13	1:A:616:LEU:O	0.50	2.06	19	2
1:A:606:VAL:CG2	1:A:610:HIS:NE2	0.49	2.75	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:603:LYS:NZ	1:A:661:ASP:OD2	0.49	2.45	8	1
1:A:644:GLN:CD	1:A:644:GLN:N	0.49	2.65	12	1
1:A:646:MET:O	1:A:646:MET:SD	0.49	2.70	19	1
1:A:623:ALA:HB1	1:A:702:LEU:HB3	0.49	1.84	15	2
1:A:561:LEU:CD1	1:A:561:LEU:C	0.49	2.75	7	2
1:A:635:LEU:N	1:A:635:LEU:CD2	0.49	2.74	4	1
1:A:561:LEU:HD13	1:A:561:LEU:O	0.49	2.07	20	2
1:A:617:LEU:HD23	1:A:647:GLU:OE2	0.49	2.07	4	2
1:A:635:LEU:N	1:A:635:LEU:HD22	0.49	2.22	4	1
1:A:642:GLN:NE2	1:A:694:PHE:CZ	0.49	2.80	7	1
1:A:614:HIS:CE1	1:A:618:GLU:OE2	0.49	2.66	5	1
1:A:635:LEU:HD22	1:A:635:LEU:N	0.49	2.21	11	1
1:A:609:VAL:O	1:A:613:VAL:CG2	0.49	2.61	5	2
1:A:649:VAL:O	1:A:652:THR:OG1	0.49	2.30	1	2
1:A:563:ARG:NH2	1:A:566:GLN:OE1	0.49	2.44	2	1
1:A:563:ARG:NH1	1:A:564:LEU:CD1	0.49	2.76	13	1
1:A:660:LEU:CD1	1:A:660:LEU:C	0.48	2.79	18	2
1:A:610:HIS:CE1	1:A:650:TYR:CZ	0.48	3.01	14	1
1:A:565:GLN:NE2	1:A:692:ALA:CB	0.48	2.76	10	1
1:A:670:THR:OG1	1:A:671:LEU:N	0.48	2.45	20	1
1:A:557:ALA:HB1	1:A:703:PHE:CZ	0.48	2.43	20	1
1:A:568:VAL:O	1:A:572:VAL:HG13	0.48	2.08	1	1
1:A:572:VAL:CG1	1:A:681:SER:OG	0.48	2.62	20	1
1:A:698:ASN:O	1:A:702:LEU:CB	0.48	2.62	5	3
1:A:573:ALA:O	1:A:577:ASP:N	0.48	2.42	9	5
1:A:564:LEU:HD23	1:A:616:LEU:HA	0.48	1.86	16	2
1:A:674:LEU:HD12	1:A:674:LEU:N	0.48	2.24	2	2
1:A:564:LEU:CD2	1:A:619:PHE:CD1	0.48	2.97	7	1
1:A:646:MET:SD	1:A:687:ASP:OD2	0.48	2.71	7	1
1:A:563:ARG:NH2	1:A:566:GLN:CD	0.47	2.67	2	1
1:A:563:ARG:NH2	1:A:566:GLN:HE22	0.47	2.07	2	1
1:A:654:VAL:O	1:A:658:GLN:N	0.47	2.42	14	3
1:A:645:LYS:C	1:A:645:LYS:CD	0.47	2.82	9	1
1:A:560:THR:OG1	1:A:619:PHE:CE2	0.47	2.62	17	1
1:A:656:HIS:C	1:A:656:HIS:CD2	0.47	2.85	2	1
1:A:557:ALA:CB	1:A:703:PHE:CZ	0.47	2.98	20	5
1:A:614:HIS:CE1	1:A:618:GLU:CD	0.47	2.88	12	2
1:A:613:VAL:HG13	1:A:614:HIS:N	0.47	2.25	7	5
1:A:564:LEU:O	1:A:568:VAL:CG2	0.47	2.62	20	3
1:A:602:LEU:HD23	1:A:660:LEU:HD11	0.47	1.86	16	1
1:A:698:ASN:N	1:A:698:ASN:OD1	0.47	2.48	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:681:SER:O	1:A:685:PRO:CG	0.46	2.62	11	5
1:A:654:VAL:O	1:A:658:GLN:CG	0.46	2.63	6	3
1:A:641:ARG:CG	1:A:642:GLN:N	0.46	2.78	8	1
1:A:697:GLY:C	1:A:698:ASN:HD22	0.46	2.13	3	1
1:A:613:VAL:CG2	1:A:650:TYR:OH	0.46	2.64	6	1
1:A:679:ALA:O	1:A:682:ARG:NH1	0.46	2.48	19	1
1:A:686:GLU:OE1	1:A:690:GLN:NE2	0.46	2.48	15	1
1:A:616:LEU:HD22	1:A:688:ALA:HB1	0.46	1.88	14	2
1:A:564:LEU:CD1	1:A:564:LEU:N	0.46	2.79	20	1
1:A:610:HIS:CA	1:A:650:TYR:OH	0.46	2.63	18	4
1:A:614:HIS:CE1	1:A:618:GLU:OE1	0.46	2.68	12	1
1:A:702:LEU:HD23	1:A:703:PHE:CE2	0.46	2.46	16	1
1:A:613:VAL:CG1	1:A:650:TYR:CZ	0.46	2.99	6	2
1:A:606:VAL:CG2	1:A:610:HIS:CE1	0.45	2.99	11	1
1:A:698:ASN:OD1	1:A:702:LEU:HD11	0.45	2.11	4	1
1:A:677:LEU:O	1:A:677:LEU:HD13	0.45	2.12	7	1
1:A:602:LEU:O	1:A:606:VAL:HG12	0.45	2.11	11	2
1:A:557:ALA:CB	1:A:703:PHE:CE1	0.45	2.99	9	2
1:A:567:GLY:O	1:A:571:THR:CG2	0.45	2.63	1	1
1:A:695:LEU:CD1	1:A:702:LEU:CD2	0.45	2.95	14	1
1:A:676:ARG:O	1:A:680:CYS:SG	0.45	2.70	14	2
1:A:613:VAL:HG21	1:A:684:VAL:HG11	0.45	1.88	15	3
1:A:572:VAL:HG21	1:A:685:PRO:HG3	0.45	1.89	16	2
1:A:635:LEU:N	1:A:635:LEU:CD1	0.45	2.80	15	2
1:A:571:THR:O	1:A:574:HIS:CE1	0.45	2.69	4	1
1:A:560:THR:HG23	1:A:561:LEU:N	0.45	2.26	9	2
1:A:613:VAL:HG12	1:A:650:TYR:CZ	0.45	2.47	2	1
1:A:555:GLU:N	1:A:555:GLU:OE1	0.45	2.42	15	1
1:A:698:ASN:OD1	1:A:702:LEU:HD21	0.45	2.12	12	1
1:A:637:ALA:HB1	1:A:641:ARG:HE	0.45	1.72	3	1
1:A:575:LEU:HD13	1:A:575:LEU:O	0.45	2.11	14	1
1:A:646:MET:HG3	1:A:691:LEU:HD11	0.45	1.87	15	1
1:A:674:LEU:N	1:A:674:LEU:CD2	0.45	2.79	6	1
1:A:615:GLU:OE1	1:A:618:GLU:OE2	0.45	2.35	3	1
1:A:564:LEU:N	1:A:564:LEU:CD1	0.44	2.79	16	1
1:A:636:HIS:O	1:A:640:SER:N	0.44	2.39	8	1
1:A:635:LEU:H	1:A:635:LEU:CD2	0.44	2.23	3	1
1:A:621:ARG:CD	1:A:621:ARG:C	0.44	2.85	8	5
1:A:642:GLN:NE2	1:A:642:GLN:C	0.44	2.71	19	1
1:A:636:HIS:O	1:A:640:SER:CB	0.44	2.66	8	1
1:A:695:LEU:C	1:A:695:LEU:CD1	0.44	2.84	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:606:VAL:CG1	1:A:607:ALA:N	0.44	2.80	6	3
1:A:566:GLN:N	1:A:566:GLN:NE2	0.44	2.66	5	1
1:A:561:LEU:CD2	1:A:561:LEU:C	0.44	2.86	8	1
1:A:561:LEU:O	1:A:565:GLN:OE1	0.44	2.36	18	1
1:A:684:VAL:O	1:A:688:ALA:N	0.44	2.47	4	2
1:A:621:ARG:C	1:A:621:ARG:CD	0.44	2.86	16	6
1:A:564:LEU:HD23	1:A:615:GLU:O	0.44	2.12	8	1
1:A:670:THR:HG23	1:A:671:LEU:N	0.44	2.28	20	1
1:A:695:LEU:O	1:A:698:ASN:OD1	0.44	2.36	19	1
1:A:640:SER:O	1:A:644:GLN:OE1	0.43	2.36	12	1
1:A:602:LEU:HD13	1:A:660:LEU:HD11	0.43	1.89	14	1
1:A:600:GLN:CG	1:A:601:ASP:N	0.43	2.81	15	1
1:A:649:VAL:HG23	1:A:650:TYR:N	0.43	2.28	6	1
1:A:617:LEU:HD11	1:A:646:MET:CB	0.43	2.43	16	1
1:A:623:ALA:HB1	1:A:702:LEU:HD21	0.43	1.88	13	1
1:A:681:SER:O	1:A:685:PRO:HD2	0.43	2.13	5	1
1:A:554:LEU:CD1	1:A:699:ALA:HB1	0.43	2.44	14	2
1:A:565:GLN:NE2	1:A:692:ALA:HB2	0.43	2.28	10	1
1:A:614:HIS:CD2	1:A:617:LEU:HD12	0.43	2.49	17	1
1:A:606:VAL:CG2	1:A:607:ALA:N	0.43	2.81	2	3
1:A:575:LEU:HD12	1:A:605:ALA:HB1	0.43	1.91	4	1
1:A:681:SER:O	1:A:685:PRO:HD3	0.43	2.13	15	2
1:A:635:LEU:O	1:A:639:LEU:N	0.43	2.43	3	1
1:A:562:ALA:O	1:A:566:GLN:OE1	0.43	2.37	5	1
1:A:561:LEU:HD23	1:A:561:LEU:O	0.43	2.13	8	1
1:A:674:LEU:N	1:A:674:LEU:HD22	0.43	2.29	6	1
1:A:578:LEU:HD11	1:A:601:ASP:CG	0.43	2.33	13	1
1:A:599:VAL:HG23	1:A:660:LEU:CD2	0.42	2.43	5	1
1:A:635:LEU:HD13	1:A:697:GLY:C	0.42	2.35	19	1
1:A:694:PHE:O	1:A:698:ASN:OD1	0.42	2.37	10	3
1:A:613:VAL:CG1	1:A:650:TYR:OH	0.42	2.68	2	1
1:A:635:LEU:CD1	1:A:697:GLY:O	0.42	2.68	19	1
1:A:648:ASP:O	1:A:652:THR:OG1	0.42	2.36	20	1
1:A:643:LEU:C	1:A:643:LEU:HD23	0.42	2.35	7	1
1:A:565:GLN:CA	1:A:565:GLN:NE2	0.42	2.83	3	1
1:A:635:LEU:HD13	1:A:697:GLY:O	0.42	2.14	5	1
1:A:698:ASN:OD1	1:A:702:LEU:CD1	0.42	2.68	4	1
1:A:684:VAL:N	1:A:685:PRO:CD	0.42	2.83	14	4
1:A:703:PHE:CD1	1:A:703:PHE:N	0.42	2.88	11	1
1:A:672:ASP:CG	1:A:673:ASP:N	0.42	2.73	18	1
1:A:674:LEU:N	1:A:674:LEU:CD1	0.42	2.83	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:636:HIS:NE2	1:A:702:LEU:CD2	0.42	2.83	11	1
1:A:642:GLN:NE2	1:A:645:LYS:NZ	0.42	2.68	1	1
1:A:617:LEU:HD13	1:A:647:GLU:OE1	0.42	2.15	17	1
1:A:644:GLN:CG	1:A:645:LYS:N	0.42	2.83	1	1
1:A:610:HIS:O	1:A:613:VAL:HG12	0.41	2.15	17	1
1:A:570:THR:O	1:A:574:HIS:CE1	0.41	2.73	1	1
1:A:565:GLN:NE2	1:A:616:LEU:CD1	0.41	2.83	3	1
1:A:617:LEU:HD23	1:A:647:GLU:CD	0.41	2.35	3	1
1:A:639:LEU:CD1	1:A:698:ASN:HD22	0.41	2.28	2	1
1:A:635:LEU:HD23	1:A:697:GLY:O	0.41	2.15	15	1
1:A:574:HIS:NE2	1:A:605:ALA:HB1	0.41	2.30	5	1
1:A:613:VAL:CB	1:A:650:TYR:CZ	0.41	3.03	6	1
1:A:566:GLN:HG3	1:A:567:GLY:N	0.41	2.31	9	1
1:A:653:LEU:HD21	1:A:680:CYS:HB2	0.41	1.91	12	1
1:A:639:LEU:CD1	1:A:698:ASN:ND2	0.41	2.83	12	1
1:A:553:GLU:N	1:A:553:GLU:CD	0.41	2.73	7	1
1:A:606:VAL:HG13	1:A:607:ALA:N	0.41	2.29	1	1
1:A:558:VAL:O	1:A:562:ALA:HB2	0.41	2.16	15	1
1:A:568:VAL:O	1:A:571:THR:OG1	0.41	2.37	13	1
1:A:617:LEU:O	1:A:621:ARG:CB	0.41	2.69	5	1
1:A:560:THR:HG23	1:A:563:ARG:NH2	0.41	2.30	19	1
1:A:564:LEU:CD2	1:A:619:PHE:CD2	0.41	3.04	10	1
1:A:700:SER:O	1:A:704:ARG:C	0.41	2.60	20	1
1:A:563:ARG:NH1	1:A:563:ARG:CB	0.41	2.84	12	1
1:A:613:VAL:CG2	1:A:650:TYR:CZ	0.41	3.02	4	1
1:A:610:HIS:CE1	1:A:654:VAL:HG21	0.41	2.51	4	1
1:A:557:ALA:O	1:A:561:LEU:HD12	0.41	2.15	11	1
1:A:575:LEU:CD2	1:A:575:LEU:C	0.41	2.89	8	1
1:A:645:LYS:HG3	1:A:646:MET:N	0.41	2.31	9	1
1:A:700:SER:O	1:A:704:ARG:CA	0.40	2.69	19	1
1:A:676:ARG:NH1	1:A:676:ARG:CB	0.40	2.84	14	1
1:A:600:GLN:H	1:A:600:GLN:CD	0.40	2.19	11	1
1:A:616:LEU:CD2	1:A:688:ALA:HB1	0.40	2.46	15	1
1:A:694:PHE:O	1:A:698:ASN:CG	0.40	2.60	6	1
1:A:695:LEU:CD2	1:A:695:LEU:N	0.40	2.85	19	1
1:A:646:MET:SD	1:A:691:LEU:HD22	0.40	2.57	2	1
1:A:622:SER:O	1:A:625:SER:OG	0.40	2.37	14	1
1:A:555:GLU:O	1:A:558:VAL:HG22	0.40	2.16	13	1
1:A:642:GLN:OE1	1:A:694:PHE:CG	0.40	2.75	11	1
1:A:563:ARG:CB	1:A:563:ARG:NH1	0.40	2.84	6	1
1:A:700:SER:C	1:A:701:LEU:HD12	0.40	2.36	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:554:LEU:HG	1:A:555:GLU:N	0.40	2.32	4	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	117/163 (72%)	114±1 (98±1%)	2±1 (2±1%)	1±1 (1±1%)	34	78
All	All	2340/3260 (72%)	2283 (98%)	42 (2%)	15 (1%)	34	78

All 5 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	704	ARG	5
1	A	661	ASP	4
1	A	553	GLU	3
1	A	670	THR	2
1	A	625	SER	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	97/130 (75%)	87±2 (90±2%)	10±2 (10±2%)	14	58
All	All	1940/2600 (75%)	1742 (90%)	198 (10%)	14	58

All 47 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	ARG	18
1	A	698	ASN	12
1	A	617	LEU	12
1	A	638	LYS	12
1	A	560	THR	11
1	A	609	VAL	11
1	A	558	VAL	10
1	A	684	VAL	10
1	A	602	LEU	7
1	A	619	PHE	6
1	A	646	MET	6
1	A	576	LEU	6
1	A	680	CYS	5
1	A	645	LYS	5
1	A	689	LYS	4
1	A	616	LEU	4
1	A	561	LEU	4
1	A	635	LEU	4
1	A	643	LEU	3
1	A	563	ARG	3
1	A	656	HIS	3
1	A	615	GLU	3
1	A	614	HIS	3
1	A	660	LEU	2
1	A	641	ARG	2
1	A	636	HIS	2
1	A	695	LEU	2
1	A	670	THR	2
1	A	574	HIS	2
1	A	559	GLU	2
1	A	682	ARG	2
1	A	704	ARG	2
1	A	613	VAL	2
1	A	701	LEU	2
1	A	575	LEU	2
1	A	673	ASP	1
1	A	650	TYR	1
1	A	634	THR	1
1	A	639	LEU	1
1	A	642	GLN	1
1	A	671	LEU	1
1	A	696	HIS	1
1	A	565	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	603	LYS	1
1	A	681	SER	1
1	A	686	GLU	1
1	A	610	HIS	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](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 7 Chemical shift validation

No chemical shift data were provided