Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 05:09 PM BST

PDB ID	:	1TOZ
Title	:	NMR structure of the human NOTCH-1 ligand binding region
Authors	:	Hambleton, S.; Valeyev, N.Y.; Muranyi, A.; Knott, V.; Werner, J.M.; Mcmichael, A.J.; Handford, P.A.; Downing, A.K.
Deposited on	:	2004-06-15

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

The following versions of software and data (see references (1)) were used in the production of this report:

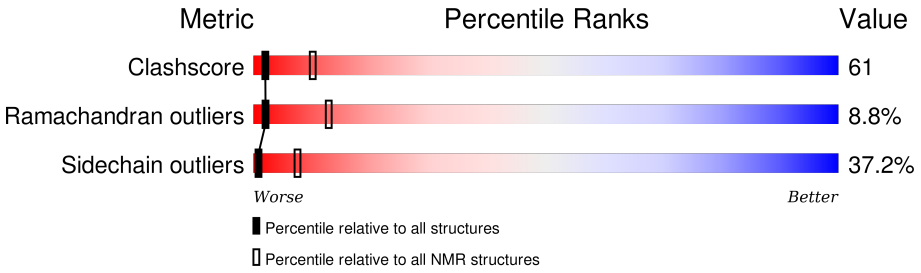
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	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	116	17% 53% 20% • 9%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 9 as representative, based on the following criterion: *fewest violations*.

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:412-A:489 (78)	0.53	2
2	A:490-A:517 (28)	0.57	13

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

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

The models can be grouped into 5 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1638 atoms, of which 774 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Neurogenic locus notch homolog protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	116	Total	C	H	N	O	S	0
			1638	516	774	148	181	19	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	477	ILE	MET	ENGINEERED	UNP P46531

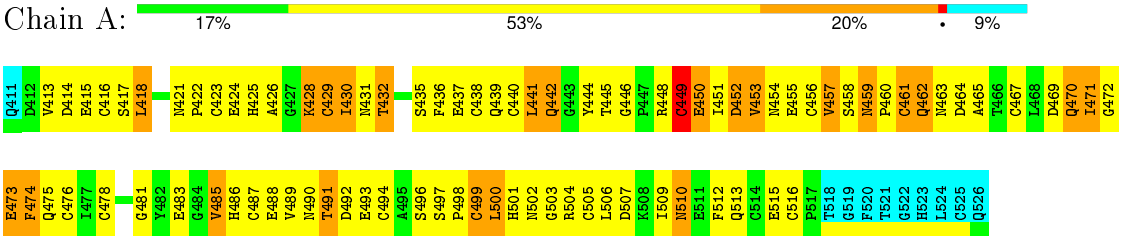
4 Residue-property plots

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: Neurogenic locus notch homolog protein 1

Chain A:



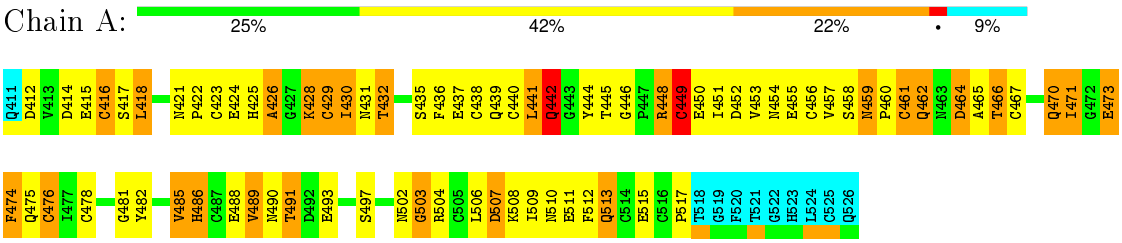
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Neurogenic locus notch homolog protein 1

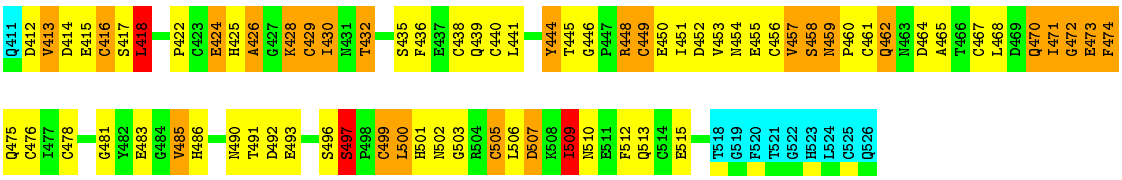
Chain A:



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Neurogenic locus notch homolog protein 1

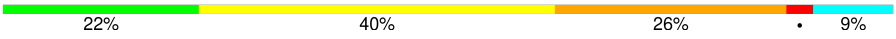
Chain A:

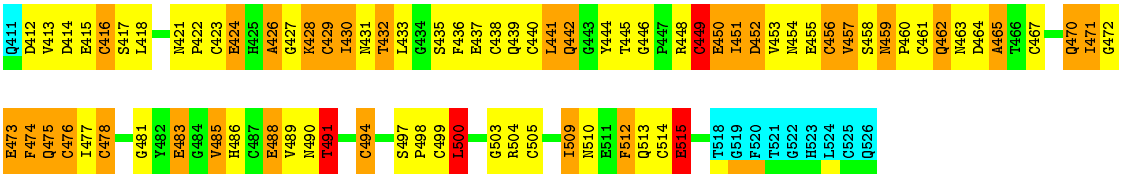


4.2.3 Score per residue for model 3

• Molecule 1: Neurogenic locus notch homolog protein 1

Chain A:

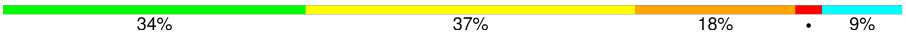


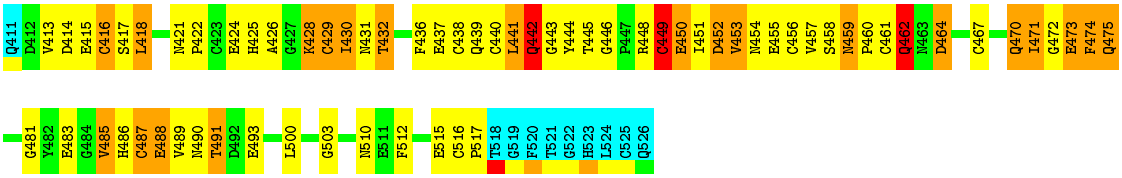


4.2.4 Score per residue for model 4

• Molecule 1: Neurogenic locus notch homolog protein 1

Chain A:

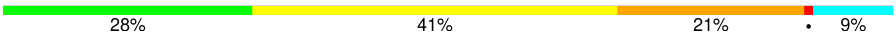


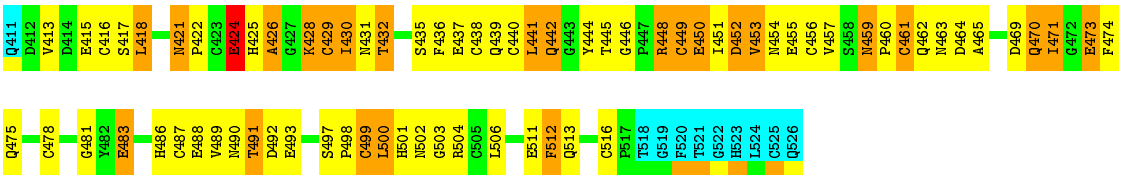


4.2.5 Score per residue for model 5

• Molecule 1: Neurogenic locus notch homolog protein 1

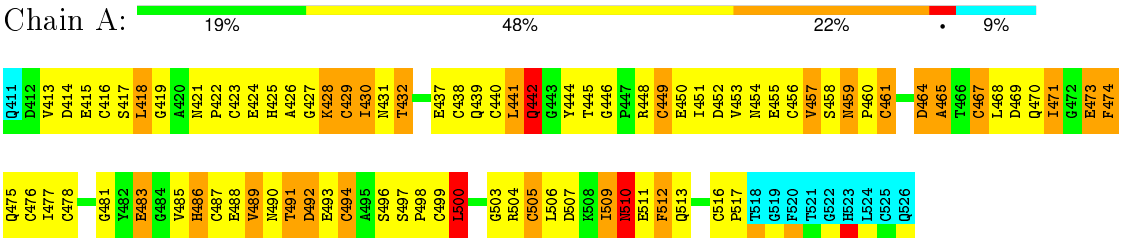
Chain A:





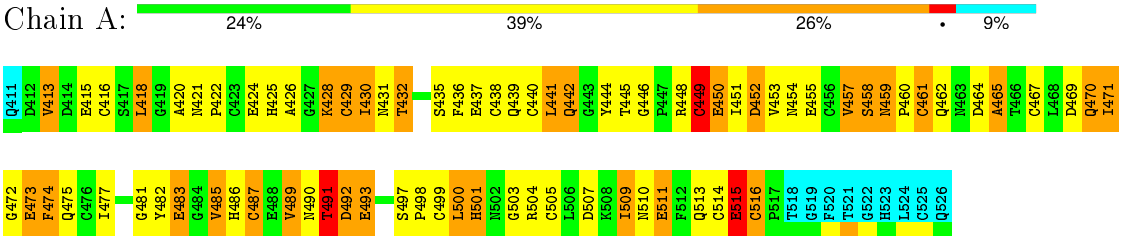
4.2.6 Score per residue for model 6

• Molecule 1: Neurogenic locus notch homolog protein 1



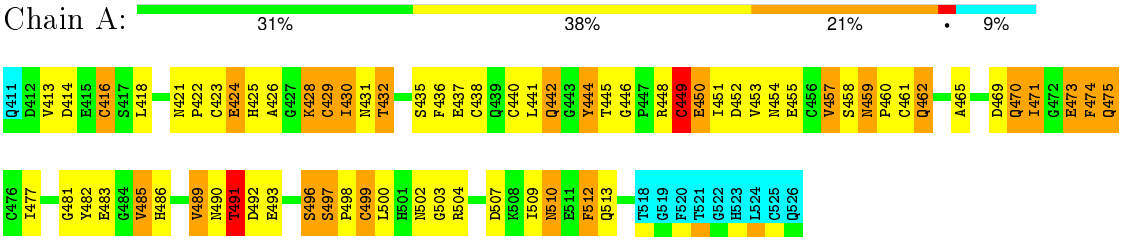
4.2.7 Score per residue for model 7

- Molecule 1: Neurogenic locus notch homolog protein 1



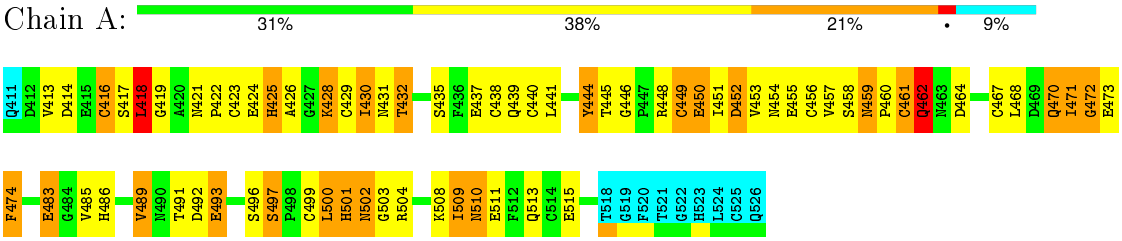
4.2.8 Score per residue for model 8

- Molecule 1: Neurogenic locus notch homolog protein 1



4.2.9 Score per residue for model 9

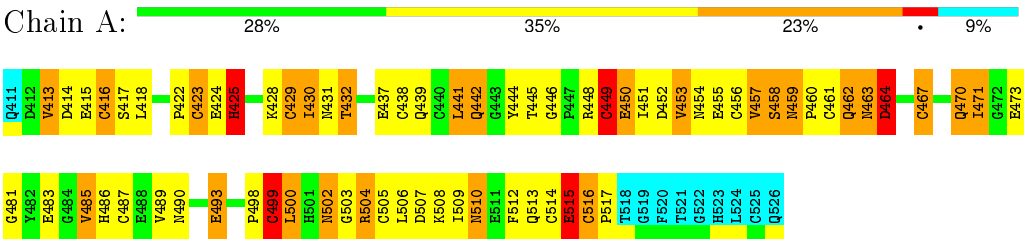
- Molecule 1: Neurogenic locus notch homolog protein 1



4.2.10 Score per residue for model 10

• Molecule 1: Neurogenic locus notch homolog protein 1

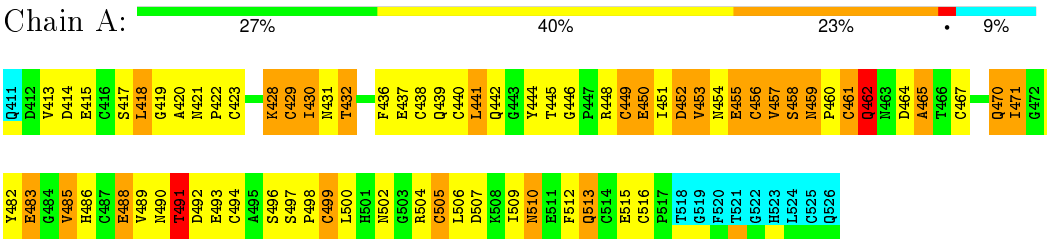
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Neurogenic locus notch homolog protein 1

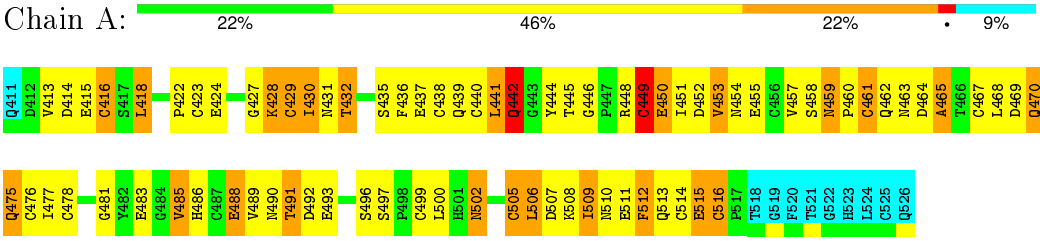
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Neurogenic locus notch homolog protein 1

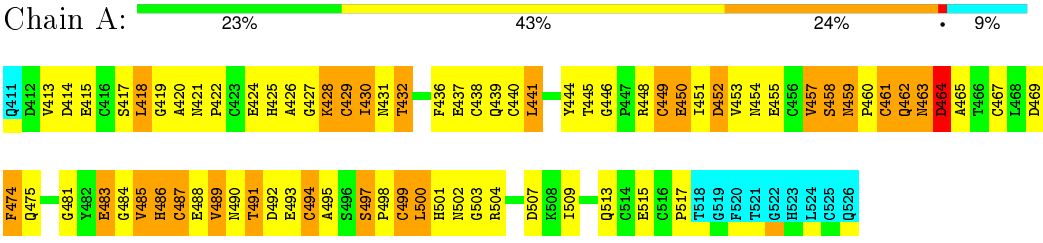
Chain A:



4.2.13 Score per residue for model 13

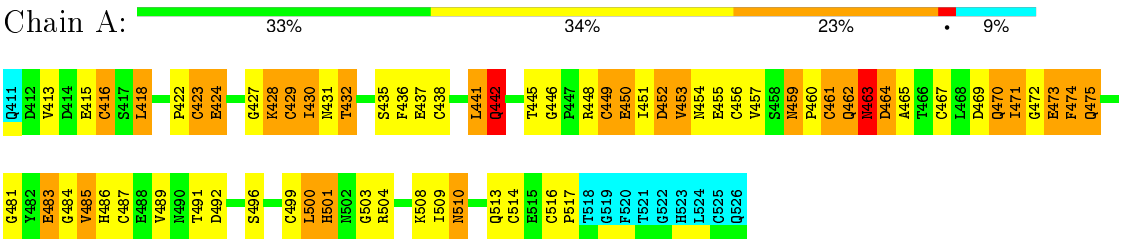
• Molecule 1: Neurogenic locus notch homolog protein 1

Chain A:



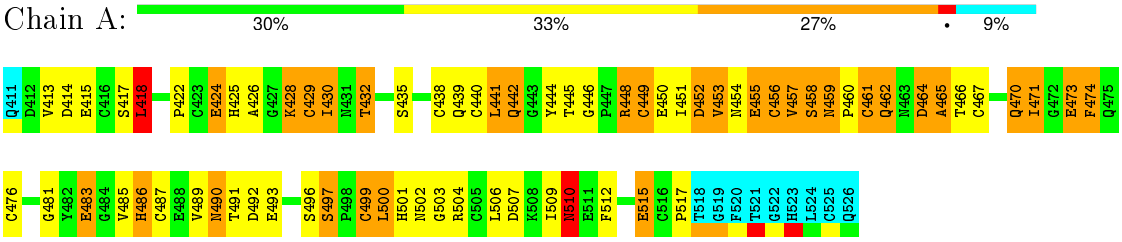
4.2.14 Score per residue for model 14

• Molecule 1: Neurogenic locus notch homolog protein 1



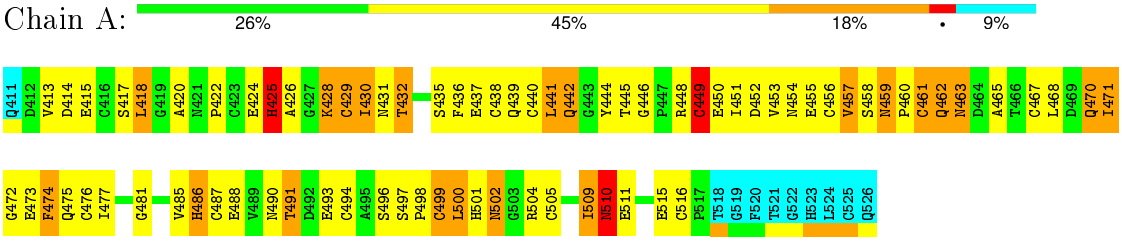
4.2.15 Score per residue for model 15

• Molecule 1: Neurogenic locus notch homolog protein 1



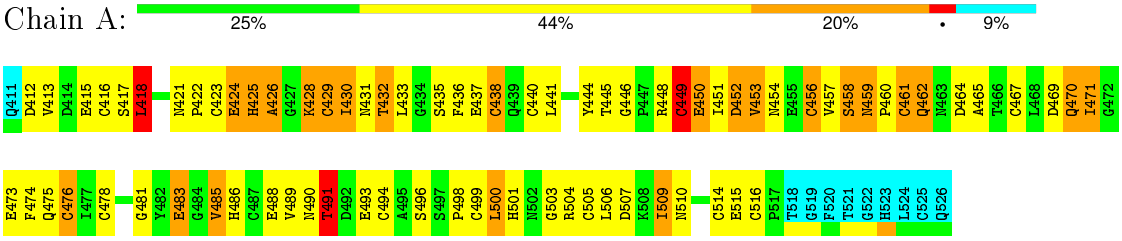
4.2.16 Score per residue for model 16

• Molecule 1: Neurogenic locus notch homolog protein 1



4.2.17 Score per residue for model 17

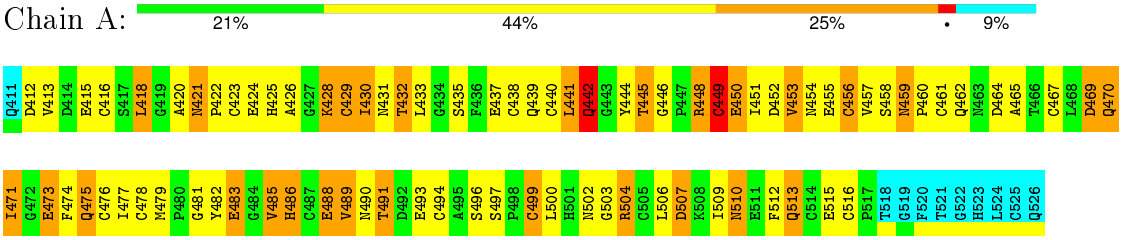
• Molecule 1: Neurogenic locus notch homolog protein 1



4.2.18 Score per residue for model 18

• Molecule 1: Neurogenic locus notch homolog protein 1

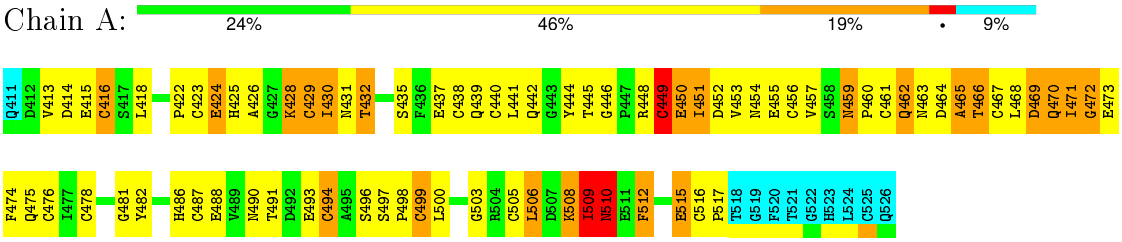
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Neurogenic locus notch homolog protein 1

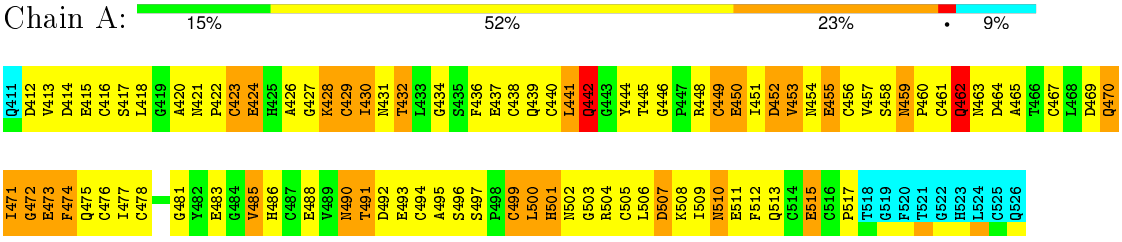
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Neurogenic locus notch homolog protein 1

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 600 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
CYANA	structure solution	1.0.6
CYANA	refinement	1.0.6

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	789	707	693	90±10
All	All	15780	14140	13860	1800

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 61.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:445:THR:HG23	1:A:451:ILE:HG22	1.01	1.22	18	15
1:A:441:LEU:HD13	1:A:441:LEU:O	0.99	1.58	11	4
1:A:499:CYS:SG	1:A:505:CYS:SG	0.97	2.61	3	3
1:A:445:THR:CG2	1:A:451:ILE:HG22	0.94	1.92	12	15
1:A:426:ALA:HB3	1:A:444:TYR:OH	0.93	1.62	9	14
1:A:445:THR:N	1:A:451:ILE:O	0.92	2.02	18	20
1:A:450:GLU:C	1:A:451:ILE:HD12	0.92	1.85	6	13
1:A:454:ASN:O	1:A:457:VAL:HG22	0.91	1.64	19	9
1:A:500:LEU:C	1:A:500:LEU:HD23	0.88	1.89	2	1
1:A:461:CYS:HB3	1:A:465:ALA:HB3	0.87	1.44	6	10
1:A:500:LEU:HD22	1:A:500:LEU:O	0.84	1.72	7	2
1:A:454:ASN:O	1:A:457:VAL:HG13	0.83	1.72	14	6
1:A:489:VAL:HA	1:A:509:ILE:HG22	0.80	1.52	7	2
1:A:441:LEU:HD11	1:A:444:TYR:CE1	0.79	2.12	11	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:446:GLY:CA	1:A:451:ILE:HB	0.78	2.09	5	20
1:A:429:CYS:C	1:A:430:ILE:HD13	0.77	1.99	1	19
1:A:483:GLU:O	1:A:489:VAL:HG22	0.77	1.80	8	6
1:A:461:CYS:SG	1:A:487:CYS:SG	0.76	2.83	15	5
1:A:461:CYS:CB	1:A:465:ALA:HB3	0.76	2.11	6	5
1:A:454:ASN:ND2	1:A:457:VAL:HG23	0.76	1.95	11	4
1:A:427:GLY:HA2	1:A:441:LEU:HD23	0.74	1.57	6	6
1:A:430:ILE:HD13	1:A:430:ILE:N	0.74	1.98	5	8
1:A:430:ILE:N	1:A:430:ILE:HD13	0.73	1.99	20	11
1:A:441:LEU:CD1	1:A:444:TYR:CD1	0.72	2.72	5	7
1:A:485:VAL:HG13	1:A:486:HIS:CD2	0.71	2.20	20	8
1:A:412:ASP:HB2	1:A:433:LEU:HD23	0.71	1.59	3	3
1:A:485:VAL:CG1	1:A:486:HIS:CD2	0.71	2.74	7	7
1:A:413:VAL:CG2	1:A:418:LEU:HD11	0.71	2.15	5	4
1:A:490:ASN:O	1:A:491:THR:HG22	0.71	1.86	18	2
1:A:413:VAL:HG22	1:A:418:LEU:HD11	0.70	1.63	5	4
1:A:477:ILE:N	1:A:477:ILE:HD12	0.70	2.01	6	1
1:A:441:LEU:CD1	1:A:444:TYR:CE1	0.69	2.75	11	2
1:A:445:THR:HG23	1:A:451:ILE:CG2	0.69	2.18	4	15
1:A:446:GLY:N	1:A:451:ILE:HB	0.68	2.02	9	19
1:A:415:GLU:HA	1:A:418:LEU:HD12	0.68	1.64	5	17
1:A:489:VAL:HG11	1:A:507:ASP:CG	0.68	2.09	17	2
1:A:465:ALA:HB1	1:A:476:CYS:HB2	0.67	1.65	20	5
1:A:441:LEU:HD12	1:A:442:GLN:NE2	0.67	2.04	3	2
1:A:451:ILE:CD1	1:A:451:ILE:N	0.67	2.57	3	4
1:A:489:VAL:CA	1:A:509:ILE:HG22	0.67	2.20	7	1
1:A:459:ASN:O	1:A:474:PHE:CE2	0.66	2.49	15	3
1:A:451:ILE:N	1:A:451:ILE:CD1	0.66	2.58	19	3
1:A:459:ASN:N	1:A:460:PRO:HD3	0.66	2.05	3	20
1:A:430:ILE:HD11	1:A:439:GLN:HG3	0.65	1.69	20	8
1:A:450:GLU:O	1:A:451:ILE:HD13	0.65	1.92	16	6
1:A:509:ILE:HD12	1:A:509:ILE:O	0.64	1.91	7	2
1:A:425:HIS:CE1	1:A:471:ILE:HG21	0.64	2.28	7	1
1:A:423:CYS:O	1:A:424:GLU:C	0.64	2.36	20	2
1:A:450:GLU:N	1:A:450:GLU:CD	0.64	2.51	14	4
1:A:425:HIS:O	1:A:426:ALA:HB2	0.64	1.92	17	3
1:A:428:LYS:HE3	1:A:430:ILE:HD12	0.64	1.70	11	5
1:A:450:GLU:O	1:A:451:ILE:HD12	0.64	1.93	11	7
1:A:500:LEU:CD2	1:A:501:HIS:CD2	0.63	2.81	2	2
1:A:448:ARG:O	1:A:449:CYS:CB	0.63	2.45	6	20
1:A:500:LEU:HD22	1:A:500:LEU:C	0.63	2.14	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:464:ASP:O	1:A:465:ALA:HB2	0.63	1.94	7	7
1:A:474:PHE:C	1:A:474:PHE:CD1	0.63	2.71	9	3
1:A:500:LEU:HD12	1:A:500:LEU:O	0.63	1.94	15	1
1:A:461:CYS:O	1:A:462:GLN:O	0.63	2.17	13	3
1:A:459:ASN:CB	1:A:474:PHE:CZ	0.62	2.83	17	5
1:A:500:LEU:O	1:A:501:HIS:CG	0.62	2.52	7	1
1:A:459:ASN:O	1:A:474:PHE:CZ	0.61	2.53	1	3
1:A:475:GLN:NE2	1:A:476:CYS:H	0.61	1.93	3	1
1:A:413:VAL:HG12	1:A:415:GLU:OE1	0.61	1.95	5	2
1:A:457:VAL:HG12	1:A:458:SER:N	0.61	2.11	2	9
1:A:422:PRO:O	1:A:424:GLU:N	0.61	2.32	20	9
1:A:494:CYS:SG	1:A:512:PHE:CD1	0.61	2.94	19	2
1:A:441:LEU:C	1:A:441:LEU:HD13	0.60	2.16	5	1
1:A:446:GLY:CA	1:A:451:ILE:HD13	0.60	2.26	10	2
1:A:475:GLN:HE22	1:A:477:ILE:N	0.60	1.94	8	3
1:A:426:ALA:HB3	1:A:444:TYR:CZ	0.60	2.30	3	1
1:A:471:ILE:O	1:A:473:GLU:N	0.60	2.34	19	15
1:A:493:GLU:O	1:A:512:PHE:CD1	0.60	2.55	1	2
1:A:445:THR:OG1	1:A:446:GLY:N	0.60	2.35	15	20
1:A:512:PHE:CD1	1:A:512:PHE:O	0.60	2.55	5	1
1:A:426:ALA:O	1:A:444:TYR:CZ	0.60	2.55	1	6
1:A:497:SER:OG	1:A:512:PHE:CD2	0.60	2.55	15	2
1:A:441:LEU:HD11	1:A:444:TYR:CD1	0.59	2.32	16	3
1:A:491:THR:HG23	1:A:492:ASP:N	0.59	2.13	7	1
1:A:428:LYS:CE	1:A:430:ILE:HD12	0.59	2.27	12	5
1:A:459:ASN:HB2	1:A:474:PHE:CZ	0.59	2.33	17	5
1:A:512:PHE:CD1	1:A:512:PHE:C	0.59	2.75	12	2
1:A:462:GLN:O	1:A:463:ASN:CB	0.59	2.50	14	3
1:A:461:CYS:SG	1:A:465:ALA:CB	0.59	2.90	16	6
1:A:441:LEU:CD1	1:A:441:LEU:N	0.58	2.66	15	3
1:A:500:LEU:CD2	1:A:501:HIS:CG	0.58	2.85	13	1
1:A:428:LYS:O	1:A:438:CYS:HA	0.58	1.99	8	15
1:A:441:LEU:CD1	1:A:442:GLN:NE2	0.58	2.66	4	5
1:A:474:PHE:CD1	1:A:474:PHE:C	0.58	2.76	4	9
1:A:448:ARG:N	1:A:450:GLU:OE1	0.58	2.37	15	6
1:A:441:LEU:HD22	1:A:441:LEU:O	0.58	1.99	16	2
1:A:461:CYS:SG	1:A:465:ALA:HB3	0.58	2.39	5	3
1:A:441:LEU:HD13	1:A:442:GLN:NE2	0.58	2.12	4	3
1:A:430:ILE:N	1:A:437:GLU:O	0.58	2.36	17	16
1:A:459:ASN:N	1:A:460:PRO:CD	0.58	2.67	3	15
1:A:500:LEU:O	1:A:500:LEU:HD13	0.58	1.99	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:450:GLU:HG2	1:A:451:ILE:CD1	0.57	2.28	14	5
1:A:500:LEU:HD22	1:A:501:HIS:CG	0.57	2.33	13	1
1:A:500:LEU:O	1:A:501:HIS:CB	0.57	2.52	7	4
1:A:416:CYS:SG	1:A:436:PHE:CD1	0.57	2.97	3	4
1:A:451:ILE:N	1:A:451:ILE:HD12	0.57	2.15	8	1
1:A:430:ILE:CD1	1:A:430:ILE:N	0.57	2.66	14	9
1:A:441:LEU:CD1	1:A:444:TYR:CG	0.57	2.88	16	3
1:A:512:PHE:C	1:A:512:PHE:CD1	0.57	2.78	8	1
1:A:485:VAL:HG12	1:A:486:HIS:CD2	0.57	2.34	14	6
1:A:462:GLN:NE2	1:A:462:GLN:O	0.57	2.38	14	1
1:A:428:LYS:O	1:A:439:GLN:N	0.57	2.36	9	16
1:A:471:ILE:O	1:A:471:ILE:CD1	0.57	2.53	11	7
1:A:501:HIS:CD2	1:A:502:ASN:N	0.57	2.73	9	2
1:A:459:ASN:ND2	1:A:459:ASN:N	0.56	2.53	6	6
1:A:494:CYS:SG	1:A:512:PHE:CE1	0.56	2.98	3	1
1:A:471:ILE:CD1	1:A:471:ILE:O	0.56	2.54	6	13
1:A:489:VAL:HG12	1:A:509:ILE:HG23	0.56	1.77	7	1
1:A:463:ASN:O	1:A:464:ASP:CB	0.56	2.53	10	3
1:A:506:LEU:O	1:A:512:PHE:CD2	0.56	2.58	6	1
1:A:424:GLU:O	1:A:425:HIS:CD2	0.56	2.58	8	1
1:A:459:ASN:N	1:A:459:ASN:ND2	0.56	2.53	2	14
1:A:415:GLU:O	1:A:420:ALA:HB3	0.56	2.00	11	6
1:A:424:GLU:O	1:A:425:HIS:CG	0.56	2.59	8	2
1:A:425:HIS:NE2	1:A:471:ILE:CG2	0.56	2.68	10	2
1:A:441:LEU:HD23	1:A:442:GLN:NE2	0.56	2.16	18	2
1:A:500:LEU:C	1:A:500:LEU:HD22	0.56	2.21	13	1
1:A:453:VAL:CG2	1:A:454:ASN:N	0.55	2.70	2	18
1:A:426:ALA:HB2	1:A:471:ILE:HG21	0.55	1.78	13	4
1:A:454:ASN:O	1:A:457:VAL:CG1	0.55	2.53	14	4
1:A:512:PHE:CG	1:A:512:PHE:O	0.55	2.59	19	2
1:A:500:LEU:CD2	1:A:500:LEU:O	0.55	2.51	7	2
1:A:500:LEU:C	1:A:500:LEU:CD2	0.55	2.66	2	1
1:A:497:SER:OG	1:A:512:PHE:CE2	0.55	2.59	15	2
1:A:490:ASN:H	1:A:490:ASN:ND2	0.55	1.99	20	1
1:A:422:PRO:CG	1:A:450:GLU:CD	0.55	2.75	17	1
1:A:454:ASN:O	1:A:457:VAL:CG2	0.55	2.54	9	8
1:A:454:ASN:HB3	1:A:457:VAL:CG1	0.55	2.32	14	10
1:A:490:ASN:O	1:A:491:THR:CG2	0.55	2.55	18	2
1:A:477:ILE:N	1:A:477:ILE:CD1	0.55	2.70	6	1
1:A:423:CYS:O	1:A:426:ALA:N	0.54	2.39	18	1
1:A:470:GLN:N	1:A:473:GLU:O	0.54	2.39	5	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:451:ILE:HD12	1:A:451:ILE:N	0.54	2.18	17	6
1:A:422:PRO:HG3	1:A:436:PHE:CE1	0.54	2.37	1	5
1:A:418:LEU:N	1:A:418:LEU:HD23	0.54	2.17	9	1
1:A:423:CYS:O	1:A:424:GLU:CG	0.54	2.55	18	1
1:A:414:ASP:O	1:A:417:SER:N	0.54	2.36	15	9
1:A:506:LEU:HD23	1:A:508:LYS:CE	0.54	2.32	1	1
1:A:471:ILE:O	1:A:472:GLY:C	0.54	2.45	19	5
1:A:457:VAL:CG1	1:A:458:SER:N	0.54	2.70	7	10
1:A:455:GLU:HB2	1:A:474:PHE:CD1	0.54	2.38	18	3
1:A:471:ILE:HD12	1:A:471:ILE:O	0.54	2.02	6	13
1:A:500:LEU:O	1:A:500:LEU:HD23	0.54	2.02	2	1
1:A:436:PHE:CD1	1:A:436:PHE:C	0.54	2.81	12	5
1:A:454:ASN:HB3	1:A:457:VAL:HG13	0.54	1.80	20	8
1:A:488:GLU:O	1:A:509:ILE:HG23	0.54	2.02	6	1
1:A:466:THR:CG2	1:A:466:THR:O	0.53	2.56	1	1
1:A:441:LEU:N	1:A:441:LEU:CD1	0.53	2.71	10	1
1:A:459:ASN:HB2	1:A:474:PHE:CE2	0.53	2.38	17	5
1:A:426:ALA:CB	1:A:471:ILE:CG2	0.53	2.87	2	4
1:A:430:ILE:N	1:A:430:ILE:CD1	0.53	2.68	18	7
1:A:506:LEU:HD23	1:A:515:GLU:HG3	0.53	1.80	19	1
1:A:488:GLU:O	1:A:509:ILE:CG2	0.53	2.57	1	5
1:A:441:LEU:HD13	1:A:441:LEU:C	0.53	2.23	11	1
1:A:453:VAL:HG22	1:A:454:ASN:N	0.53	2.19	2	12
1:A:456:CYS:HB3	1:A:474:PHE:CD1	0.53	2.38	16	2
1:A:426:ALA:O	1:A:444:TYR:CE2	0.53	2.62	9	5
1:A:489:VAL:HG21	1:A:507:ASP:CG	0.53	2.24	8	3
1:A:490:ASN:O	1:A:491:THR:O	0.53	2.26	7	13
1:A:448:ARG:CB	1:A:450:GLU:OE1	0.53	2.57	12	1
1:A:418:LEU:HD23	1:A:418:LEU:N	0.52	2.19	6	2
1:A:422:PRO:CB	1:A:450:GLU:OE1	0.52	2.57	4	2
1:A:445:THR:O	1:A:449:CYS:HA	0.52	2.04	12	14
1:A:441:LEU:HD13	1:A:444:TYR:CD1	0.52	2.38	11	6
1:A:470:GLN:CB	1:A:473:GLU:O	0.52	2.57	17	6
1:A:422:PRO:C	1:A:424:GLU:N	0.52	2.63	17	17
1:A:438:CYS:SG	1:A:450:GLU:CB	0.52	2.97	17	8
1:A:461:CYS:O	1:A:462:GLN:CB	0.52	2.57	15	10
1:A:426:ALA:CB	1:A:471:ILE:HG21	0.52	2.34	6	4
1:A:425:HIS:CE1	1:A:471:ILE:CG2	0.52	2.92	7	3
1:A:471:ILE:CD1	1:A:473:GLU:CD	0.52	2.78	19	2
1:A:471:ILE:O	1:A:471:ILE:HD12	0.52	2.05	13	7
1:A:446:GLY:HA2	1:A:451:ILE:CG1	0.52	2.34	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:421:ASN:C	1:A:421:ASN:ND2	0.52	2.63	18	1
1:A:422:PRO:O	1:A:424:GLU:CG	0.52	2.58	10	3
1:A:446:GLY:HA2	1:A:451:ILE:HB	0.52	1.82	5	7
1:A:441:LEU:HD12	1:A:442:GLN:HE21	0.52	1.64	12	2
1:A:488:GLU:OE2	1:A:509:ILE:HD13	0.52	2.05	3	1
1:A:474:PHE:CD1	1:A:475:GLN:N	0.52	2.77	20	8
1:A:455:GLU:CB	1:A:474:PHE:CD1	0.52	2.93	18	2
1:A:446:GLY:HA3	1:A:451:ILE:HD13	0.51	1.80	10	2
1:A:483:GLU:O	1:A:489:VAL:HB	0.51	2.06	12	8
1:A:459:ASN:HB3	1:A:474:PHE:CZ	0.51	2.41	19	1
1:A:462:GLN:O	1:A:463:ASN:OD1	0.51	2.28	14	1
1:A:448:ARG:C	1:A:450:GLU:OE2	0.51	2.49	16	3
1:A:475:GLN:C	1:A:475:GLN:CD	0.51	2.69	16	2
1:A:450:GLU:OE2	1:A:451:ILE:CD1	0.51	2.58	4	2
1:A:485:VAL:CG1	1:A:486:HIS:NE2	0.51	2.74	7	2
1:A:445:THR:HG23	1:A:446:GLY:N	0.51	2.21	3	20
1:A:426:ALA:CB	1:A:471:ILE:HG22	0.51	2.35	20	2
1:A:425:HIS:O	1:A:426:ALA:CB	0.51	2.58	17	3
1:A:491:THR:HG23	1:A:493:GLU:OE1	0.51	2.06	9	1
1:A:498:PRO:O	1:A:500:LEU:N	0.50	2.41	7	4
1:A:426:ALA:CB	1:A:444:TYR:OH	0.50	2.59	18	1
1:A:501:HIS:O	1:A:517:PRO:CB	0.50	2.59	15	1
1:A:456:CYS:CB	1:A:474:PHE:CD1	0.50	2.94	16	2
1:A:450:GLU:C	1:A:451:ILE:CD1	0.50	2.80	3	2
1:A:512:PHE:N	1:A:512:PHE:CD1	0.50	2.79	11	2
1:A:464:ASP:O	1:A:465:ALA:CB	0.50	2.60	7	3
1:A:496:SER:O	1:A:497:SER:CB	0.50	2.59	2	1
1:A:506:LEU:HD23	1:A:508:LYS:HD3	0.50	1.84	20	1
1:A:489:VAL:HG12	1:A:509:ILE:CG2	0.50	2.37	7	1
1:A:509:ILE:O	1:A:510:ASN:CB	0.50	2.59	14	5
1:A:449:CYS:N	1:A:450:GLU:OE1	0.50	2.45	15	6
1:A:413:VAL:CG1	1:A:415:GLU:OE1	0.50	2.59	5	2
1:A:450:GLU:HG2	1:A:451:ILE:HD12	0.50	1.82	15	3
1:A:444:TYR:CE1	1:A:452:ASP:OD1	0.50	2.65	8	1
1:A:445:THR:HG23	1:A:451:ILE:HB	0.50	1.84	1	3
1:A:500:LEU:HD22	1:A:501:HIS:CB	0.50	2.36	13	1
1:A:506:LEU:HD22	1:A:515:GLU:CD	0.50	2.27	15	1
1:A:475:GLN:NE2	1:A:476:CYS:CA	0.50	2.75	12	1
1:A:444:TYR:CE2	1:A:452:ASP:HB2	0.49	2.42	1	7
1:A:499:CYS:O	1:A:503:GLY:N	0.49	2.43	9	3
1:A:455:GLU:O	1:A:459:ASN:ND2	0.49	2.45	2	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:431:ASN:OD1	1:A:432:THR:N	0.49	2.45	8	17
1:A:432:THR:CB	1:A:435:SER:O	0.49	2.60	7	11
1:A:441:LEU:HD13	1:A:442:GLN:HE21	0.49	1.65	4	2
1:A:494:CYS:HB2	1:A:512:PHE:CD2	0.49	2.42	6	1
1:A:462:GLN:CD	1:A:463:ASN:N	0.49	2.66	13	2
1:A:490:ASN:H	1:A:509:ILE:HG23	0.49	1.65	19	1
1:A:432:THR:OG1	1:A:437:GLU:N	0.49	2.46	9	8
1:A:445:THR:HG22	1:A:451:ILE:O	0.49	2.08	8	1
1:A:423:CYS:O	1:A:424:GLU:CB	0.49	2.60	8	3
1:A:422:PRO:CB	1:A:450:GLU:OE2	0.49	2.61	17	1
1:A:455:GLU:OE2	1:A:455:GLU:N	0.49	2.46	10	2
1:A:482:TYR:CE2	1:A:490:ASN:HB3	0.49	2.42	7	3
1:A:502:ASN:O	1:A:517:PRO:CD	0.49	2.61	1	1
1:A:424:GLU:C	1:A:425:HIS:CD2	0.49	2.86	8	2
1:A:444:TYR:CZ	1:A:452:ASP:HB2	0.48	2.43	17	19
1:A:470:GLN:CA	1:A:473:GLU:O	0.48	2.61	5	7
1:A:471:ILE:HD12	1:A:471:ILE:N	0.48	2.23	3	12
1:A:494:CYS:SG	1:A:512:PHE:CD2	0.48	3.05	6	1
1:A:455:GLU:OE2	1:A:473:GLU:N	0.48	2.46	19	2
1:A:475:GLN:HE21	1:A:477:ILE:HD11	0.48	1.68	7	2
1:A:455:GLU:N	1:A:455:GLU:OE2	0.48	2.47	3	2
1:A:483:GLU:O	1:A:489:VAL:CB	0.48	2.62	12	5
1:A:500:LEU:HD22	1:A:501:HIS:N	0.48	2.23	13	1
1:A:432:THR:HG1	1:A:436:PHE:CA	0.48	2.21	11	5
1:A:471:ILE:N	1:A:471:ILE:HD12	0.48	2.24	2	8
1:A:490:ASN:H	1:A:509:ILE:HG22	0.48	1.68	2	1
1:A:445:THR:HG23	1:A:446:GLY:H	0.48	1.68	7	15
1:A:445:THR:HB	1:A:453:VAL:CG1	0.48	2.38	15	12
1:A:506:LEU:HD23	1:A:508:LYS:HE2	0.48	1.86	1	3
1:A:465:ALA:HB1	1:A:476:CYS:CB	0.48	2.39	16	1
1:A:468:LEU:O	1:A:470:GLN:NE2	0.48	2.47	19	2
1:A:415:GLU:CA	1:A:418:LEU:HD12	0.47	2.36	5	4
1:A:414:ASP:OD2	1:A:417:SER:N	0.47	2.47	20	3
1:A:444:TYR:CE1	1:A:452:ASP:CG	0.47	2.87	8	1
1:A:468:LEU:N	1:A:475:GLN:O	0.47	2.47	19	2
1:A:436:PHE:C	1:A:436:PHE:CD1	0.47	2.88	17	1
1:A:500:LEU:HG	1:A:501:HIS:CD2	0.47	2.44	17	2
1:A:450:GLU:OE1	1:A:451:ILE:HG12	0.47	2.09	9	3
1:A:412:ASP:OD2	1:A:413:VAL:N	0.47	2.47	2	1
1:A:489:VAL:CG2	1:A:489:VAL:O	0.47	2.61	7	1
1:A:460:PRO:HA	1:A:467:CYS:CB	0.47	2.39	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:412:ASP:OD1	1:A:434:GLY:N	0.47	2.48	20	1
1:A:505:CYS:SG	1:A:514:CYS:SG	0.47	3.12	7	1
1:A:450:GLU:N	1:A:450:GLU:OE1	0.47	2.47	3	2
1:A:427:GLY:CA	1:A:441:LEU:HD23	0.47	2.37	3	2
1:A:449:CYS:N	1:A:450:GLU:OE2	0.47	2.48	16	3
1:A:489:VAL:O	1:A:489:VAL:CG2	0.47	2.62	1	3
1:A:482:TYR:CD2	1:A:490:ASN:HA	0.47	2.45	19	1
1:A:441:LEU:HD11	1:A:444:TYR:CZ	0.47	2.44	10	3
1:A:509:ILE:HD12	1:A:509:ILE:H	0.47	1.69	3	1
1:A:493:GLU:N	1:A:493:GLU:OE1	0.47	2.48	6	2
1:A:499:CYS:O	1:A:500:LEU:O	0.47	2.33	16	3
1:A:458:SER:C	1:A:459:ASN:ND2	0.47	2.68	18	4
1:A:444:TYR:CE1	1:A:452:ASP:HB2	0.47	2.45	9	2
1:A:461:CYS:O	1:A:462:GLN:CG	0.47	2.63	12	1
1:A:490:ASN:OD1	1:A:510:ASN:N	0.47	2.47	20	1
1:A:461:CYS:HA	1:A:486:HIS:CD2	0.47	2.45	8	1
1:A:461:CYS:C	1:A:462:GLN:HG3	0.47	2.30	16	1
1:A:512:PHE:CD1	1:A:512:PHE:N	0.46	2.83	1	2
1:A:477:ILE:CG2	1:A:478:CYS:N	0.46	2.78	20	2
1:A:490:ASN:ND2	1:A:509:ILE:CG1	0.46	2.77	15	1
1:A:471:ILE:CD1	1:A:473:GLU:HG2	0.46	2.40	20	1
1:A:422:PRO:HG3	1:A:436:PHE:CZ	0.46	2.45	1	2
1:A:454:ASN:OD1	1:A:457:VAL:N	0.46	2.49	8	5
1:A:463:ASN:ND2	1:A:465:ALA:H	0.46	2.08	13	1
1:A:475:GLN:NE2	1:A:476:CYS:N	0.46	2.63	12	1
1:A:441:LEU:C	1:A:441:LEU:HD22	0.46	2.30	11	2
1:A:442:GLN:N	1:A:442:GLN:NE2	0.46	2.63	5	1
1:A:441:LEU:HD11	1:A:444:TYR:CG	0.46	2.46	16	1
1:A:441:LEU:O	1:A:443:GLY:N	0.46	2.49	4	1
1:A:493:GLU:OE1	1:A:510:ASN:CA	0.46	2.64	7	1
1:A:441:LEU:CD2	1:A:442:GLN:NE2	0.46	2.79	18	2
1:A:504:ARG:O	1:A:515:GLU:N	0.46	2.49	13	4
1:A:432:THR:OG1	1:A:435:SER:O	0.46	2.33	17	9
1:A:493:GLU:OE1	1:A:510:ASN:N	0.46	2.49	7	1
1:A:454:ASN:CB	1:A:457:VAL:HG13	0.46	2.40	20	7
1:A:413:VAL:HG12	1:A:415:GLU:OE2	0.46	2.11	17	1
1:A:483:GLU:O	1:A:489:VAL:O	0.46	2.34	4	1
1:A:450:GLU:OE1	1:A:451:ILE:HD13	0.46	2.11	20	1
1:A:493:GLU:HB3	1:A:512:PHE:CD1	0.46	2.45	15	1
1:A:461:CYS:O	1:A:462:GLN:C	0.46	2.54	16	3
1:A:441:LEU:O	1:A:441:LEU:HD13	0.46	2.11	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:462:GLN:NE2	1:A:464:ASP:OD1	0.46	2.48	4	1
1:A:450:GLU:OE1	1:A:450:GLU:N	0.46	2.48	20	2
1:A:486:HIS:H	1:A:486:HIS:CD2	0.46	2.27	16	1
1:A:454:ASN:OD1	1:A:456:CYS:N	0.46	2.47	14	4
1:A:455:GLU:OE1	1:A:473:GLU:N	0.46	2.49	9	3
1:A:502:ASN:O	1:A:503:GLY:C	0.46	2.54	1	1
1:A:496:SER:O	1:A:497:SER:C	0.46	2.54	9	2
1:A:456:CYS:O	1:A:456:CYS:SG	0.46	2.74	19	3
1:A:440:CYS:SG	1:A:449:CYS:C	0.46	2.94	20	8
1:A:456:CYS:SG	1:A:456:CYS:O	0.45	2.75	17	3
1:A:462:GLN:HG2	1:A:462:GLN:O	0.45	2.11	14	1
1:A:440:CYS:N	1:A:449:CYS:O	0.45	2.49	3	3
1:A:486:HIS:C	1:A:488:GLU:N	0.45	2.68	16	4
1:A:414:ASP:OD2	1:A:416:CYS:SG	0.45	2.74	1	5
1:A:462:GLN:OE1	1:A:463:ASN:ND2	0.45	2.49	19	1
1:A:450:GLU:OE2	1:A:450:GLU:N	0.45	2.49	18	1
1:A:500:LEU:HD22	1:A:501:HIS:CD2	0.45	2.47	7	1
1:A:500:LEU:O	1:A:502:ASN:N	0.45	2.45	13	8
1:A:446:GLY:CA	1:A:451:ILE:CG1	0.45	2.94	7	5
1:A:506:LEU:N	1:A:513:GLN:O	0.45	2.49	11	3
1:A:489:VAL:HG21	1:A:507:ASP:OD1	0.45	2.12	7	1
1:A:413:VAL:HG13	1:A:418:LEU:CD1	0.45	2.41	7	1
1:A:475:GLN:NE2	1:A:475:GLN:O	0.45	2.50	10	1
1:A:460:PRO:O	1:A:461:CYS:HB2	0.45	2.11	13	8
1:A:450:GLU:CD	1:A:451:ILE:CD1	0.45	2.85	20	2
1:A:462:GLN:HE22	1:A:463:ASN:ND2	0.45	2.09	16	1
1:A:502:ASN:C	1:A:502:ASN:ND2	0.45	2.70	16	1
1:A:428:LYS:O	1:A:438:CYS:SG	0.45	2.75	10	15
1:A:508:LYS:O	1:A:510:ASN:N	0.45	2.50	9	2
1:A:462:GLN:NE2	1:A:463:ASN:HB2	0.45	2.26	16	1
1:A:461:CYS:O	1:A:462:GLN:HG3	0.45	2.12	13	3
1:A:473:GLU:OE2	1:A:474:PHE:N	0.45	2.50	3	1
1:A:488:GLU:O	1:A:509:ILE:HG21	0.45	2.12	11	1
1:A:448:ARG:O	1:A:449:CYS:HB2	0.45	2.12	16	2
1:A:509:ILE:O	1:A:510:ASN:ND2	0.45	2.50	16	2
1:A:500:LEU:CD1	1:A:500:LEU:C	0.45	2.85	15	1
1:A:462:GLN:O	1:A:463:ASN:HB3	0.45	2.10	14	1
1:A:426:ALA:HB3	1:A:444:TYR:HH	0.45	1.69	4	1
1:A:475:GLN:NE2	1:A:477:ILE:N	0.45	2.64	8	1
1:A:468:LEU:HD12	1:A:475:GLN:HE21	0.45	1.70	16	1
1:A:462:GLN:O	1:A:463:ASN:ND2	0.45	2.49	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:444:TYR:OH	1:A:471:ILE:HG22	0.45	2.11	7	2
1:A:412:ASP:CG	1:A:432:THR:O	0.45	2.55	3	5
1:A:437:GLU:HG3	1:A:438:CYS:N	0.45	2.27	8	3
1:A:421:ASN:OD1	1:A:425:HIS:N	0.45	2.50	18	1
1:A:446:GLY:CA	1:A:451:ILE:CB	0.45	2.94	7	2
1:A:483:GLU:OE1	1:A:484:GLY:N	0.45	2.50	13	1
1:A:422:PRO:HB2	1:A:450:GLU:CG	0.44	2.42	5	4
1:A:455:GLU:HB3	1:A:474:PHE:CD1	0.44	2.47	11	1
1:A:444:TYR:CD2	1:A:451:ILE:C	0.44	2.91	5	1
1:A:455:GLU:CG	1:A:474:PHE:HB3	0.44	2.42	3	10
1:A:422:PRO:C	1:A:450:GLU:O	0.44	2.56	11	5
1:A:423:CYS:SG	1:A:439:GLN:O	0.44	2.75	6	4
1:A:515:GLU:CG	1:A:516:CYS:N	0.44	2.80	7	2
1:A:452:ASP:C	1:A:452:ASP:OD2	0.44	2.56	2	2
1:A:438:CYS:O	1:A:449:CYS:O	0.44	2.35	6	3
1:A:493:GLU:N	1:A:493:GLU:OE2	0.44	2.49	1	2
1:A:412:ASP:OD2	1:A:431:ASN:OD1	0.44	2.35	20	2
1:A:471:ILE:C	1:A:473:GLU:N	0.44	2.69	12	14
1:A:491:THR:CG2	1:A:492:ASP:N	0.44	2.81	7	1
1:A:510:ASN:O	1:A:511:GLU:CB	0.44	2.65	7	1
1:A:498:PRO:O	1:A:499:CYS:C	0.44	2.55	17	4
1:A:444:TYR:CZ	1:A:452:ASP:CB	0.44	3.00	5	1
1:A:455:GLU:OE2	1:A:473:GLU:CA	0.44	2.65	12	1
1:A:500:LEU:O	1:A:500:LEU:CD1	0.44	2.65	15	1
1:A:432:THR:OG1	1:A:436:PHE:C	0.44	2.56	8	3
1:A:449:CYS:C	1:A:450:GLU:OE2	0.44	2.56	15	5
1:A:490:ASN:N	1:A:490:ASN:OD1	0.44	2.49	3	1
1:A:462:GLN:HG3	1:A:463:ASN:N	0.44	2.27	12	2
1:A:483:GLU:CG	1:A:487:CYS:SG	0.44	3.06	4	1
1:A:492:ASP:OD2	1:A:495:ALA:N	0.44	2.51	20	1
1:A:455:GLU:N	1:A:469:ASP:OD1	0.44	2.51	8	1
1:A:501:HIS:O	1:A:517:PRO:CG	0.44	2.65	15	1
1:A:429:CYS:SG	1:A:429:CYS:O	0.44	2.75	1	4
1:A:475:GLN:NE2	1:A:477:ILE:HD11	0.44	2.28	18	1
1:A:506:LEU:O	1:A:512:PHE:CG	0.44	2.70	6	1
1:A:448:ARG:CD	1:A:450:GLU:OE1	0.43	2.65	1	1
1:A:412:ASP:OD2	1:A:432:THR:O	0.43	2.36	17	2
1:A:499:CYS:O	1:A:503:GLY:O	0.43	2.36	2	9
1:A:491:THR:O	1:A:493:GLU:OE1	0.43	2.36	8	1
1:A:441:LEU:HD13	1:A:441:LEU:N	0.43	2.28	15	1
1:A:436:PHE:O	1:A:436:PHE:CD1	0.43	2.72	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:476:CYS:SG	1:A:476:CYS:O	0.43	2.76	3	1
1:A:498:PRO:O	1:A:500:LEU:HD12	0.43	2.13	7	1
1:A:489:VAL:CG2	1:A:507:ASP:OD2	0.43	2.67	1	1
1:A:456:CYS:CB	1:A:469:ASP:CB	0.43	2.97	19	1
1:A:466:THR:O	1:A:476:CYS:HA	0.43	2.14	15	2
1:A:455:GLU:O	1:A:459:ASN:N	0.43	2.51	12	1
1:A:464:ASP:OD2	1:A:488:GLU:CD	0.43	2.57	6	1
1:A:503:GLY:HA2	1:A:517:PRO:CD	0.43	2.43	10	2
1:A:455:GLU:CB	1:A:474:PHE:HB3	0.43	2.43	11	1
1:A:475:GLN:CD	1:A:475:GLN:C	0.43	2.78	4	2
1:A:438:CYS:SG	1:A:450:GLU:HB3	0.43	2.53	17	2
1:A:470:GLN:CB	1:A:473:GLU:HG3	0.43	2.44	3	1
1:A:498:PRO:O	1:A:499:CYS:O	0.43	2.37	19	1
1:A:507:ASP:CG	1:A:512:PHE:CE1	0.43	2.92	6	1
1:A:441:LEU:N	1:A:441:LEU:HD13	0.43	2.29	16	1
1:A:461:CYS:SG	1:A:461:CYS:O	0.43	2.76	16	1
1:A:515:GLU:OE2	1:A:516:CYS:N	0.43	2.51	7	1
1:A:423:CYS:SG	1:A:428:LYS:O	0.43	2.77	1	3
1:A:498:PRO:O	1:A:499:CYS:HB2	0.43	2.14	3	2
1:A:424:GLU:O	1:A:425:HIS:HB2	0.43	2.14	18	1
1:A:468:LEU:HB2	1:A:475:GLN:CB	0.43	2.43	2	1
1:A:461:CYS:O	1:A:463:ASN:OD1	0.43	2.37	14	1
1:A:431:ASN:OD1	1:A:431:ASN:C	0.43	2.57	11	1
1:A:493:GLU:OE1	1:A:493:GLU:N	0.43	2.51	10	1
1:A:497:SER:O	1:A:505:CYS:SG	0.43	2.77	3	2
1:A:416:CYS:SG	1:A:421:ASN:OD1	0.43	2.77	9	1
1:A:485:VAL:HG12	1:A:486:HIS:CG	0.43	2.48	18	1
1:A:492:ASP:OD1	1:A:495:ALA:HB2	0.43	2.14	13	1
1:A:462:GLN:CG	1:A:463:ASN:N	0.43	2.81	12	2
1:A:416:CYS:SG	1:A:429:CYS:C	0.42	2.97	1	3
1:A:470:GLN:HG3	1:A:473:GLU:CG	0.42	2.44	19	1
1:A:490:ASN:O	1:A:507:ASP:OD1	0.42	2.37	12	1
1:A:441:LEU:CD2	1:A:442:GLN:HG2	0.42	2.44	11	1
1:A:432:THR:HG1	1:A:437:GLU:N	0.42	2.12	8	1
1:A:445:THR:CG2	1:A:451:ILE:O	0.42	2.66	8	1
1:A:423:CYS:O	1:A:424:GLU:HB2	0.42	2.15	8	4
1:A:506:LEU:HD13	1:A:515:GLU:OE2	0.42	2.14	17	1
1:A:432:THR:HG1	1:A:435:SER:C	0.42	2.17	9	1
1:A:454:ASN:OD1	1:A:469:ASP:CB	0.42	2.67	19	1
1:A:464:ASP:O	1:A:465:ALA:C	0.42	2.57	13	1
1:A:422:PRO:CG	1:A:450:GLU:HG3	0.42	2.45	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:489:VAL:CG1	1:A:507:ASP:OD2	0.42	2.67	17	1
1:A:484:GLY:HA3	1:A:489:VAL:CG2	0.42	2.43	14	1
1:A:432:THR:O	1:A:435:SER:O	0.42	2.36	3	4
1:A:456:CYS:HB2	1:A:469:ASP:CB	0.42	2.44	19	1
1:A:448:ARG:N	1:A:448:ARG:CD	0.42	2.83	18	1
1:A:421:ASN:OD1	1:A:429:CYS:SG	0.42	2.77	4	4
1:A:500:LEU:HD23	1:A:501:HIS:CD2	0.42	2.49	2	1
1:A:482:TYR:CD1	1:A:482:TYR:N	0.42	2.88	8	1
1:A:503:GLY:CA	1:A:517:PRO:HD3	0.42	2.45	13	4
1:A:500:LEU:O	1:A:503:GLY:O	0.42	2.37	6	2
1:A:454:ASN:OD1	1:A:456:CYS:CB	0.42	2.66	17	1
1:A:436:PHE:CD1	1:A:436:PHE:O	0.42	2.72	3	2
1:A:503:GLY:CA	1:A:515:GLU:O	0.42	2.67	4	1
1:A:499:CYS:O	1:A:503:GLY:C	0.42	2.58	17	2
1:A:450:GLU:CD	1:A:451:ILE:HD13	0.42	2.35	19	1
1:A:488:GLU:O	1:A:488:GLU:CG	0.42	2.67	13	1
1:A:498:PRO:C	1:A:500:LEU:N	0.42	2.73	16	1
1:A:461:CYS:HB3	1:A:465:ALA:CB	0.42	2.45	15	3
1:A:494:CYS:SG	1:A:497:SER:O	0.42	2.78	13	1
1:A:463:ASN:OD1	1:A:487:CYS:O	0.42	2.38	16	1
1:A:475:GLN:C	1:A:475:GLN:NE2	0.42	2.73	12	1
1:A:505:CYS:SG	1:A:505:CYS:O	0.42	2.78	12	1
1:A:505:CYS:O	1:A:505:CYS:SG	0.42	2.78	11	1
1:A:470:GLN:HG2	1:A:473:GLU:O	0.41	2.15	9	1
1:A:499:CYS:SG	1:A:503:GLY:O	0.41	2.78	19	1
1:A:490:ASN:ND2	1:A:490:ASN:H	0.41	2.12	15	1
1:A:461:CYS:C	1:A:462:GLN:O	0.41	2.58	13	2
1:A:450:GLU:C	1:A:451:ILE:HD13	0.41	2.36	9	1
1:A:490:ASN:O	1:A:507:ASP:OD2	0.41	2.38	2	2
1:A:428:LYS:O	1:A:438:CYS:CA	0.41	2.68	8	1
1:A:461:CYS:O	1:A:462:GLN:NE2	0.41	2.50	16	1
1:A:468:LEU:HA	1:A:468:LEU:HD23	0.41	1.75	2	2
1:A:500:LEU:O	1:A:501:HIS:CD2	0.41	2.73	14	2
1:A:446:GLY:CA	1:A:451:ILE:HG12	0.41	2.46	13	2
1:A:468:LEU:HD23	1:A:468:LEU:HA	0.41	1.80	9	2
1:A:486:HIS:O	1:A:487:CYS:C	0.41	2.59	13	3
1:A:422:PRO:CG	1:A:450:GLU:OE1	0.41	2.68	17	1
1:A:454:ASN:CG	1:A:457:VAL:HG13	0.41	2.36	1	2
1:A:514:CYS:O	1:A:515:GLU:O	0.41	2.39	3	1
1:A:500:LEU:HD12	1:A:500:LEU:HA	0.41	1.82	16	1
1:A:486:HIS:CD2	1:A:486:HIS:N	0.41	2.89	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:475:GLN:NE2	1:A:475:GLN:C	0.41	2.74	10	1
1:A:490:ASN:CG	1:A:507:ASP:OD1	0.41	2.59	10	1
1:A:424:GLU:HB3	1:A:425:HIS:CD2	0.41	2.50	9	2
1:A:421:ASN:CG	1:A:429:CYS:SG	0.41	2.99	5	1
1:A:429:CYS:O	1:A:429:CYS:SG	0.41	2.78	2	1
1:A:423:CYS:SG	1:A:450:GLU:HB3	0.41	2.56	20	1
1:A:489:VAL:HG21	1:A:507:ASP:OD2	0.41	2.15	8	1
1:A:461:CYS:O	1:A:486:HIS:O	0.41	2.39	10	1
1:A:493:GLU:N	1:A:493:GLU:CD	0.41	2.73	10	1
1:A:412:ASP:OD1	1:A:432:THR:O	0.41	2.39	3	2
1:A:422:PRO:CB	1:A:450:GLU:HG3	0.41	2.45	16	2
1:A:424:GLU:C	1:A:425:HIS:CG	0.41	2.94	8	2
1:A:431:ASN:C	1:A:431:ASN:OD1	0.41	2.59	16	1
1:A:422:PRO:O	1:A:424:GLU:HG3	0.41	2.16	10	1
1:A:462:GLN:O	1:A:463:ASN:CG	0.41	2.59	14	1
1:A:455:GLU:OE1	1:A:455:GLU:N	0.41	2.53	14	1
1:A:432:THR:C	1:A:435:SER:O	0.41	2.59	3	1
1:A:421:ASN:ND2	1:A:424:GLU:N	0.41	2.69	3	1
1:A:463:ASN:CG	1:A:464:ASP:N	0.41	2.73	13	1
1:A:498:PRO:C	1:A:499:CYS:SG	0.41	2.99	8	1
1:A:500:LEU:CD2	1:A:500:LEU:C	0.41	2.87	7	1
1:A:515:GLU:CD	1:A:516:CYS:O	0.41	2.59	10	1
1:A:463:ASN:O	1:A:465:ALA:N	0.41	2.50	3	1
1:A:414:ASP:C	1:A:416:CYS:N	0.41	2.75	9	2
1:A:428:LYS:HD2	1:A:430:ILE:CD1	0.41	2.46	12	1
1:A:438:CYS:SG	1:A:450:GLU:HB2	0.41	2.56	12	1
1:A:490:ASN:O	1:A:491:THR:C	0.41	2.59	5	1
1:A:470:GLN:CG	1:A:473:GLU:O	0.41	2.69	20	1
1:A:461:CYS:SG	1:A:485:VAL:O	0.41	2.79	13	2
1:A:478:CYS:SG	1:A:482:TYR:O	0.41	2.79	18	1
1:A:442:GLN:H	1:A:442:GLN:NE2	0.41	2.14	5	1
1:A:490:ASN:ND2	1:A:490:ASN:N	0.41	2.69	20	1
1:A:428:LYS:HE2	1:A:430:ILE:HD12	0.40	1.93	17	1
1:A:464:ASP:OD1	1:A:488:GLU:OE1	0.40	2.39	1	1
1:A:460:PRO:HA	1:A:467:CYS:SG	0.40	2.55	19	1
1:A:488:GLU:O	1:A:488:GLU:OE1	0.40	2.40	4	1
1:A:492:ASP:C	1:A:493:GLU:OE1	0.40	2.59	6	1
1:A:462:GLN:OE1	1:A:488:GLU:OE1	0.40	2.40	20	1
1:A:464:ASP:CG	1:A:487:CYS:O	0.40	2.59	7	1
1:A:515:GLU:OE2	1:A:516:CYS:O	0.40	2.39	7	1
1:A:477:ILE:HD13	1:A:477:ILE:HA	0.40	1.81	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:489:VAL:CG1	1:A:507:ASP:CG	0.40	2.87	17	1
1:A:469:ASP:C	1:A:469:ASP:OD2	0.40	2.59	17	1
1:A:488:GLU:OE2	1:A:509:ILE:CD1	0.40	2.69	3	1
1:A:422:PRO:O	1:A:450:GLU:O	0.40	2.39	19	1
1:A:469:ASP:OD2	1:A:469:ASP:C	0.40	2.59	18	1
1:A:486:HIS:CD2	1:A:486:HIS:H	0.40	2.33	13	1
1:A:460:PRO:O	1:A:461:CYS:CB	0.40	2.69	6	1
1:A:487:CYS:O	1:A:487:CYS:SG	0.40	2.79	16	1
1:A:500:LEU:O	1:A:501:HIS:HB3	0.40	2.16	9	1
1:A:414:ASP:HB3	1:A:417:SER:CB	0.40	2.46	9	1
1:A:456:CYS:O	1:A:467:CYS:SG	0.40	2.80	10	1
1:A:438:CYS:CB	1:A:450:GLU:HB3	0.40	2.46	17	1
1:A:422:PRO:C	1:A:424:GLU:H	0.40	2.20	14	1
1:A:453:VAL:O	1:A:455:GLU:OE1	0.40	2.39	11	1
1:A:413:VAL:CG1	1:A:418:LEU:HD11	0.40	2.47	7	1
1:A:464:ASP:OD2	1:A:486:HIS:O	0.40	2.40	1	1
1:A:441:LEU:HD22	1:A:442:GLN:HG2	0.40	1.94	11	1
1:A:492:ASP:OD2	1:A:494:CYS:SG	0.40	2.79	11	1
1:A:459:ASN:N	1:A:459:ASN:HD22	0.40	2.13	6	1
1:A:415:GLU:HA	1:A:418:LEU:HG	0.40	1.92	6	1
1:A:426:ALA:CB	1:A:471:ILE:HB	0.40	2.47	8	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	106/116 (91%)	79±3 (75±3%)	17±3 (16±2%)	9±2 (9±1%)	2	13
All	All	2120/2320 (91%)	1585 (75%)	349 (16%)	186 (9%)	2	13

All 27 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	449	CYS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	481	GLY	18
1	A	491	THR	18
1	A	510	ASN	17
1	A	462	GLN	13
1	A	442	GLN	12
1	A	418	LEU	12
1	A	472	GLY	9
1	A	424	GLU	9
1	A	509	ILE	8
1	A	465	ALA	7
1	A	515	GLU	6
1	A	500	LEU	6
1	A	426	ALA	5
1	A	419	GLY	4
1	A	425	HIS	4
1	A	499	CYS	3
1	A	464	ASP	3
1	A	497	SER	3
1	A	450	GLU	2
1	A	476	CYS	1
1	A	423	CYS	1
1	A	511	GLU	1
1	A	501	HIS	1
1	A	517	PRO	1
1	A	503	GLY	1
1	A	463	ASN	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	93/101 (92%)	58±3 (63±3%)	35±3 (37±3%)	1 7
All	All	1860/2020 (92%)	1169 (63%)	691 (37%)	1 7

All 75 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	441	LEU	20
1	A	459	ASN	20
1	A	429	CYS	20
1	A	432	THR	20
1	A	430	ILE	20
1	A	470	GLN	20
1	A	471	ILE	20
1	A	428	LYS	19
1	A	485	VAL	18
1	A	467	CYS	17
1	A	416	CYS	16
1	A	513	GLN	15
1	A	413	VAL	15
1	A	504	ARG	14
1	A	442	GLN	14
1	A	474	PHE	14
1	A	483	GLU	14
1	A	450	GLU	13
1	A	456	CYS	12
1	A	464	ASP	12
1	A	461	CYS	12
1	A	473	GLU	12
1	A	493	GLU	11
1	A	496	SER	11
1	A	449	CYS	11
1	A	516	CYS	11
1	A	452	ASP	11
1	A	497	SER	11
1	A	500	LEU	11
1	A	475	GLN	10
1	A	453	VAL	10
1	A	499	CYS	10
1	A	457	VAL	10
1	A	458	SER	10
1	A	486	HIS	9
1	A	492	ASP	9
1	A	469	ASP	9
1	A	515	GLU	9
1	A	505	CYS	8
1	A	488	GLU	8
1	A	494	CYS	8
1	A	489	VAL	8
1	A	462	GLN	8

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Mol	Chain	Res	Type	Models (Total)
1	A	478	CYS	8
1	A	421	ASN	7
1	A	510	ASN	7
1	A	511	GLU	7
1	A	512	PHE	7
1	A	440	CYS	7
1	A	418	LEU	7
1	A	507	ASP	6
1	A	506	LEU	5
1	A	502	ASN	5
1	A	448	ARG	5
1	A	425	HIS	5
1	A	491	THR	5
1	A	463	ASN	5
1	A	476	CYS	4
1	A	501	HIS	4
1	A	514	CYS	4
1	A	509	ILE	4
1	A	423	CYS	3
1	A	417	SER	3
1	A	508	LYS	3
1	A	455	GLU	3
1	A	444	TYR	3
1	A	487	CYS	3
1	A	451	ILE	2
1	A	490	ASN	2
1	A	466	THR	2
1	A	479	MET	1
1	A	438	CYS	1
1	A	477	ILE	1
1	A	445	THR	1
1	A	424	GLU	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

There are no carbohydrates 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