



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 05:17 PM UTC

PDB ID : 2JQX / pdb_00002jqx
Title : Solution structure of Malate Synthase G from joint refinement against NMR and SAXS data
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Deposited on : 2007-06-13

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

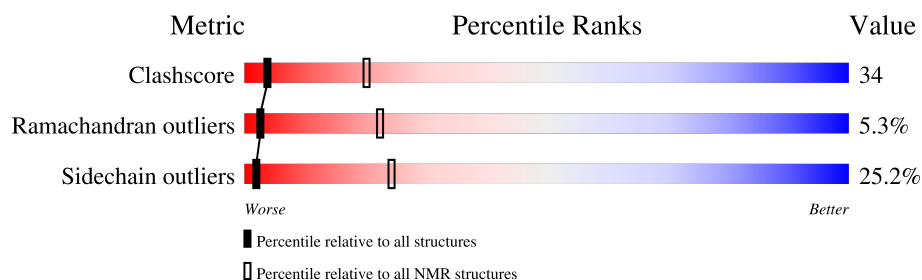
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

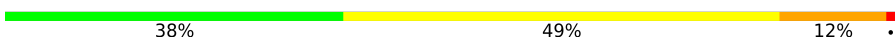
The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	723	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11282 atoms, of which 5627 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Malate synthase G.

Mol	Chain	Residues	Atoms						Trace
1	A	723	Total	C	H	N	O	S	0
			11282	3543	5627	1015	1068	29	

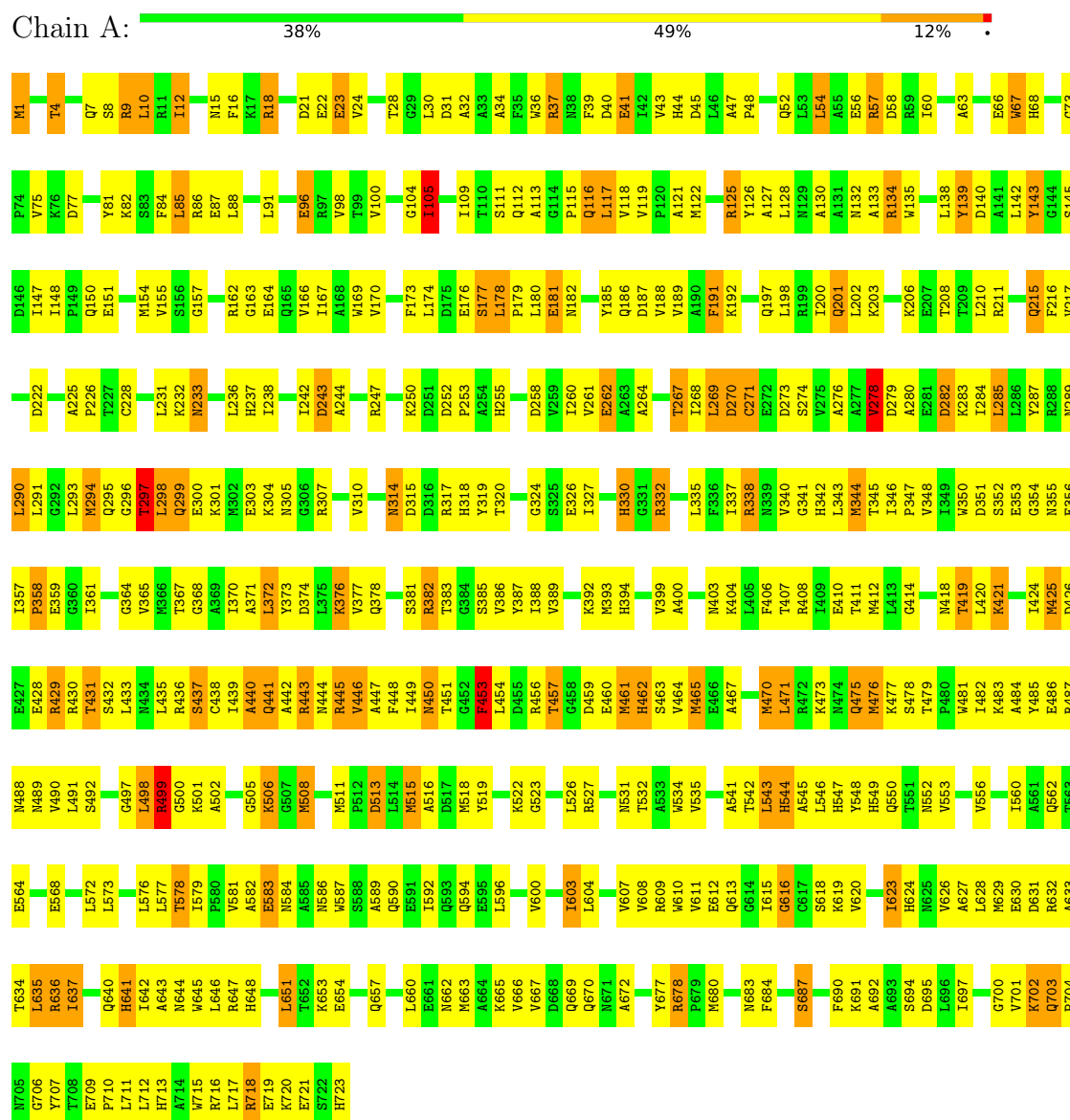
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P37330

4 Residue-property plots

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

• Molecule 1: Malate synthase G



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing/Cartesian molecular dynamics*.

Of the 5 calculated structures, 1 were deposited, based on the following criterion: *closest to the average*.

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

Software name	Classification	Version
CNS	refinement	1.0

No chemical shift data was provided.

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	5655	5627	5610	387
All	All	5655	5627	5610	387

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:117:LEU:HD12	1:A:535:VAL:HG23	0.94	1.34
1:A:604:LEU:HD22	1:A:667:VAL:HG11	0.93	1.36
1:A:643:ALA:HB1	1:A:701:VAL:HG13	0.92	1.39
1:A:198:LEU:HD22	1:A:210:LEU:HD11	0.91	1.43
1:A:276:ALA:HB3	1:A:713:HIS:CG	0.89	2.02
1:A:98:VAL:HG11	1:A:439:ILE:HG22	0.88	1.43
1:A:592:ILE:HG21	1:A:651:LEU:HD21	0.87	1.43
1:A:424:ILE:HG23	1:A:447:ALA:HB1	0.86	1.46
1:A:109:ILE:HD11	1:A:448:PHE:CE2	0.85	2.06
1:A:604:LEU:CD2	1:A:667:VAL:HG11	0.79	2.08
1:A:39:PHE:CE1	1:A:365:VAL:HG11	0.79	2.12
1:A:663:MET:O	1:A:667:VAL:HG23	0.78	1.78
1:A:31:ASP:CG	1:A:34:ALA:HB3	0.76	2.04
1:A:162:ARG:O	1:A:166:VAL:HG23	0.76	1.81
1:A:604:LEU:HD21	1:A:690:PHE:CD2	0.76	2.15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:449:ILE:HG21	1:A:489:ASN:ND2	0.75	1.97
1:A:672:ALA:HB1	1:A:677:TYR:CE2	0.75	2.16
1:A:294:MET:HE2	1:A:382:ARG:NH1	0.74	1.97
1:A:464:VAL:O	1:A:470:MET:HE1	0.74	1.81
1:A:167:ILE:HG21	1:A:252:ASP:HB3	0.74	1.57
1:A:32:ALA:HB1	1:A:36:TRP:CZ2	0.74	2.17
1:A:10:LEU:HD23	1:A:12:ILE:HD12	0.74	1.58
1:A:166:VAL:O	1:A:170:VAL:HG23	0.74	1.83
1:A:276:ALA:HB1	1:A:710:PRO:HA	0.73	1.60
1:A:611:VAL:HG12	1:A:719:GLU:HG2	0.73	1.60
1:A:596:LEU:O	1:A:600:VAL:HG23	0.72	1.84
1:A:117:LEU:HD12	1:A:535:VAL:CG2	0.72	2.13
1:A:142:LEU:HD23	1:A:147:ILE:HG21	0.72	1.62
1:A:238:ILE:HG23	1:A:549:HIS:CE1	0.72	2.20
1:A:680:MET:HE1	1:A:684:PHE:CD2	0.71	2.20
1:A:603:ILE:O	1:A:607:VAL:HG23	0.71	1.86
1:A:498:LEU:HD13	1:A:502:ALA:HB3	0.71	1.61
1:A:104:GLY:O	1:A:419:THR:HG22	0.70	1.84
1:A:646:LEU:HD13	1:A:646:LEU:O	0.70	1.87
1:A:116:GLN:CD	1:A:451:THR:HG23	0.70	2.12
1:A:374:ASP:OD2	1:A:386:VAL:HG23	0.69	1.88
1:A:119:VAL:CG2	1:A:269:LEU:HD23	0.69	2.18
1:A:393:MET:HE1	1:A:441:GLN:HG2	0.69	1.61
1:A:189:VAL:HG22	1:A:201:GLN:O	0.69	1.87
1:A:367:THR:HA	1:A:370:ILE:HD12	0.68	1.64
1:A:174:LEU:HD23	1:A:185:TYR:CD2	0.68	2.24
1:A:592:ILE:HG21	1:A:651:LEU:CD2	0.68	2.18
1:A:448:PHE:CD1	1:A:498:LEU:HD21	0.68	2.22
1:A:454:LEU:HD22	1:A:637:ILE:HG21	0.68	1.64
1:A:399:VAL:HG11	1:A:437:SER:O	0.68	1.89
1:A:294:MET:HE1	1:A:373:TYR:CD1	0.68	2.24
1:A:643:ALA:CB	1:A:701:VAL:HG13	0.68	2.18
1:A:180:LEU:HD13	1:A:208:THR:HG21	0.67	1.66
1:A:439:ILE:HG21	1:A:498:LEU:HA	0.67	1.65
1:A:604:LEU:HD22	1:A:667:VAL:CG1	0.66	2.18
1:A:418:ASN:OD1	1:A:419:THR:HG23	0.66	1.91
1:A:433:LEU:HD13	1:A:433:LEU:O	0.65	1.90
1:A:98:VAL:HG22	1:A:440:ALA:HA	0.65	1.68
1:A:337:ILE:HG13	1:A:386:VAL:HG13	0.65	1.68
1:A:138:LEU:HD13	1:A:261:VAL:HG21	0.64	1.69
1:A:451:THR:HG22	1:A:506:LYS:N	0.64	2.07
1:A:457:THR:HG22	1:A:479:THR:CG2	0.64	2.23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:39:PHE:O	1:A:43:VAL:HG23	0.63	1.93
1:A:198:LEU:HD22	1:A:210:LEU:CD1	0.63	2.21
1:A:680:MET:N	1:A:680:MET:HE2	0.63	2.08
1:A:125:ARG:CZ	1:A:615:ILE:HD12	0.63	2.24
1:A:23:GLU:OE1	1:A:24:VAL:HG23	0.63	1.92
1:A:296:GLY:O	1:A:297:THR:HG23	0.62	1.94
1:A:603:ILE:HG22	1:A:635:LEU:CG	0.62	2.24
1:A:188:VAL:HG13	1:A:200:ILE:CG2	0.62	2.24
1:A:407:THR:O	1:A:411:THR:HG23	0.62	1.94
1:A:341:GLY:O	1:A:361:ILE:HG22	0.62	1.95
1:A:626:VAL:HG12	1:A:628:LEU:HD13	0.62	1.72
1:A:47:ALA:HB3	1:A:48:PRO:HD3	0.61	1.71
1:A:117:LEU:CD1	1:A:535:VAL:HG23	0.61	2.19
1:A:478:SER:HB3	1:A:637:ILE:HD11	0.60	1.73
1:A:287:TYR:CZ	1:A:291:LEU:HD22	0.60	2.32
1:A:43:VAL:O	1:A:47:ALA:HB2	0.60	1.95
1:A:424:ILE:CG2	1:A:447:ALA:HB1	0.60	2.23
1:A:28:THR:HB	1:A:372:LEU:HD13	0.60	1.74
1:A:486:GLU:O	1:A:490:VAL:HG23	0.59	1.97
1:A:178:LEU:HD12	1:A:178:LEU:O	0.59	1.96
1:A:217:VAL:HG21	1:A:232:LYS:HB2	0.59	1.73
1:A:498:LEU:HD13	1:A:502:ALA:CB	0.59	2.27
1:A:603:ILE:HG22	1:A:635:LEU:CD1	0.58	2.28
1:A:346:ILE:O	1:A:348:VAL:HG23	0.58	1.98
1:A:303:GLU:CD	1:A:620:VAL:HG12	0.58	2.24
1:A:603:ILE:HG22	1:A:635:LEU:HD12	0.57	1.76
1:A:10:LEU:HD12	1:A:351:ASP:HA	0.57	1.74
1:A:119:VAL:HG21	1:A:127:ALA:HB2	0.57	1.77
1:A:262:GLU:O	1:A:545:ALA:HB2	0.57	1.99
1:A:116:GLN:OE1	1:A:451:THR:HG23	0.57	2.00
1:A:464:VAL:CG2	1:A:581:VAL:HG12	0.57	2.30
1:A:39:PHE:CD1	1:A:365:VAL:HG11	0.57	2.35
1:A:526:LEU:HD21	1:A:547:HIS:CB	0.57	2.30
1:A:568:GLU:O	1:A:572:LEU:HD13	0.57	1.99
1:A:119:VAL:HG21	1:A:269:LEU:HD23	0.56	1.75
1:A:287:TYR:CE1	1:A:291:LEU:HD13	0.56	2.35
1:A:471:LEU:HD23	1:A:471:LEU:N	0.56	2.15
1:A:180:LEU:HD11	1:A:188:VAL:CG2	0.56	2.30
1:A:187:ASP:OD2	1:A:202:LEU:HD22	0.56	2.00
1:A:236:LEU:HD12	1:A:548:TYR:HB2	0.56	1.77
1:A:117:LEU:HD22	1:A:130:ALA:HB2	0.56	1.75
1:A:589:ALA:HA	1:A:592:ILE:HD12	0.56	1.78

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:278:VAL:HG22	1:A:282:ASP:CG	0.56	2.25
1:A:24:VAL:O	1:A:28:THR:HG23	0.55	2.01
1:A:276:ALA:HB3	1:A:713:HIS:ND1	0.55	2.15
1:A:451:THR:HG21	1:A:534:TRP:N	0.55	2.15
1:A:343:LEU:HB3	1:A:361:ILE:HG23	0.55	1.78
1:A:461:MET:SD	1:A:470:MET:HE2	0.55	2.42
1:A:619:LYS:HB3	1:A:627:ALA:HB1	0.55	1.77
1:A:138:LEU:CD1	1:A:261:VAL:HG21	0.55	2.31
1:A:456:ARG:NH2	1:A:457:THR:HG23	0.55	2.15
1:A:31:ASP:OD2	1:A:34:ALA:HB3	0.55	2.02
1:A:57:ARG:O	1:A:60:ILE:HG22	0.55	2.02
1:A:433:LEU:HD21	1:A:577:LEU:HD22	0.55	1.79
1:A:12:ILE:N	1:A:12:ILE:HD13	0.55	2.17
1:A:663:MET:HA	1:A:663:MET:HE3	0.55	1.79
1:A:174:LEU:HD23	1:A:185:TYR:CE2	0.54	2.37
1:A:122:MET:HE1	1:A:282:ASP:O	0.54	2.01
1:A:135:TRP:CD1	1:A:260:ILE:HG21	0.54	2.37
1:A:142:LEU:C	1:A:148:ILE:HG22	0.54	2.28
1:A:388:ILE:HD13	1:A:406:PHE:CE1	0.54	2.37
1:A:287:TYR:OH	1:A:291:LEU:HD22	0.54	2.03
1:A:573:LEU:O	1:A:577:LEU:HD23	0.54	2.03
1:A:611:VAL:HG12	1:A:719:GLU:CG	0.54	2.32
1:A:86:ARG:HG2	1:A:91:LEU:HD13	0.53	1.81
1:A:603:ILE:HG22	1:A:635:LEU:HG	0.53	1.78
1:A:543:LEU:HD12	1:A:547:HIS:CE1	0.53	2.39
1:A:118:VAL:HG22	1:A:453:PHE:CE2	0.52	2.39
1:A:269:LEU:CD1	1:A:293:LEU:HD11	0.52	2.34
1:A:465:MET:SD	1:A:701:VAL:HG12	0.52	2.44
1:A:85:LEU:HD13	1:A:85:LEU:C	0.52	2.29
1:A:135:TRP:CH2	1:A:237:HIS:CD2	0.52	2.97
1:A:163:GLY:O	1:A:167:ILE:HG23	0.52	2.04
1:A:581:VAL:HG23	1:A:581:VAL:O	0.52	2.03
1:A:616:GLY:HA2	1:A:620:VAL:HG11	0.52	1.82
1:A:73:GLY:O	1:A:581:VAL:HG21	0.52	2.05
1:A:662:ASN:ND2	1:A:663:MET:HE1	0.52	2.19
1:A:343:LEU:HD12	1:A:343:LEU:C	0.52	2.30
1:A:100:VAL:HG22	1:A:442:ALA:HB1	0.51	1.81
1:A:188:VAL:HG13	1:A:200:ILE:HG23	0.51	1.83
1:A:344:MET:HE2	1:A:344:MET:HA	0.51	1.81
1:A:389:VAL:O	1:A:425:MET:HE3	0.51	2.05
1:A:456:ARG:HH21	1:A:457:THR:HG23	0.51	1.64
1:A:147:ILE:HD12	1:A:543:LEU:HD11	0.51	1.80

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:188:VAL:HG11	1:A:191:PHE:CE2	0.51	2.40
1:A:626:VAL:CG1	1:A:628:LEU:HD13	0.51	2.35
1:A:148:ILE:HG23	1:A:148:ILE:O	0.50	2.06
1:A:198:LEU:HD13	1:A:216:PHE:CE1	0.50	2.41
1:A:135:TRP:CZ3	1:A:237:HIS:CE1	0.50	2.99
1:A:125:ARG:NE	1:A:615:ILE:HD12	0.50	2.22
1:A:280:ALA:O	1:A:284:ILE:HD12	0.50	2.07
1:A:100:VAL:HA	1:A:442:ALA:HB1	0.50	1.83
1:A:439:ILE:HD11	1:A:449:ILE:HD11	0.50	1.83
1:A:642:ILE:CG2	1:A:697:ILE:HG23	0.50	2.37
1:A:145:SER:HA	1:A:515:MET:HE3	0.49	1.84
1:A:167:ILE:HD13	1:A:252:ASP:CB	0.49	2.37
1:A:39:PHE:CE1	1:A:43:VAL:HG21	0.49	2.42
1:A:412:MET:HE3	1:A:412:MET:HA	0.49	1.84
1:A:200:ILE:HB	1:A:208:THR:HG23	0.49	1.84
1:A:388:ILE:HD13	1:A:406:PHE:HE1	0.49	1.68
1:A:643:ALA:HB2	1:A:697:ILE:O	0.49	2.08
1:A:238:ILE:HG23	1:A:549:HIS:NE2	0.49	2.22
1:A:442:ALA:HB2	1:A:446:VAL:HG23	0.49	1.83
1:A:531:ASN:OD1	1:A:532:THR:HG23	0.49	2.08
1:A:98:VAL:HG22	1:A:440:ALA:CA	0.49	2.36
1:A:646:LEU:HD13	1:A:646:LEU:C	0.49	2.32
1:A:412:MET:HE3	1:A:412:MET:CA	0.49	2.37
1:A:412:MET:HE3	1:A:412:MET:N	0.49	2.22
1:A:663:MET:HE3	1:A:663:MET:CA	0.49	2.38
1:A:121:ALA:HB2	1:A:270:ASP:HA	0.48	1.84
1:A:167:ILE:HG21	1:A:252:ASP:CB	0.48	2.36
1:A:457:THR:HG22	1:A:479:THR:HG21	0.48	1.86
1:A:276:ALA:HB1	1:A:710:PRO:CA	0.48	2.36
1:A:433:LEU:HD13	1:A:433:LEU:C	0.48	2.34
1:A:400:ALA:HB1	1:A:404:LYS:HE2	0.48	1.85
1:A:449:ILE:N	1:A:449:ILE:HD12	0.48	2.23
1:A:269:LEU:HD13	1:A:293:LEU:HD11	0.48	1.84
1:A:446:VAL:CG1	1:A:448:PHE:CE2	0.48	2.97
1:A:592:ILE:CG2	1:A:651:LEU:HD21	0.48	2.27
1:A:301:LYS:O	1:A:615:ILE:HD11	0.47	2.08
1:A:424:ILE:N	1:A:448:PHE:O	0.47	2.47
1:A:672:ALA:HB1	1:A:677:TYR:CD2	0.47	2.43
1:A:383:THR:HG23	1:A:385:SER:O	0.47	2.08
1:A:662:ASN:O	1:A:666:VAL:HG23	0.47	2.09
1:A:202:LEU:HD21	1:A:208:THR:HG21	0.47	1.86
1:A:222:ASP:OD2	1:A:225:ALA:HB3	0.47	2.09

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:471:LEU:HG	1:A:582:ALA:HB2	0.47	1.85
1:A:491:LEU:HD23	1:A:560:ILE:CG2	0.47	2.39
1:A:634:THR:O	1:A:637:ILE:HG22	0.47	2.09
1:A:694:SER:HA	1:A:697:ILE:HD12	0.47	1.85
1:A:660:LEU:HD13	1:A:660:LEU:C	0.47	2.35
1:A:476:MET:HE3	1:A:476:MET:HA	0.47	1.86
1:A:319:TYR:O	1:A:327:ILE:HG22	0.46	2.10
1:A:479:THR:O	1:A:482:ILE:HG22	0.46	2.10
1:A:534:TRP:HZ2	1:A:629:MET:HE1	0.46	1.69
1:A:660:LEU:HD13	1:A:660:LEU:O	0.46	2.10
1:A:280:ALA:C	1:A:284:ILE:HD12	0.46	2.35
1:A:118:VAL:CG2	1:A:453:PHE:CE2	0.46	2.98
1:A:607:VAL:O	1:A:611:VAL:HG23	0.46	2.10
1:A:276:ALA:HB2	1:A:709:GLU:CD	0.46	2.36
1:A:552:ASN:O	1:A:556:VAL:HG23	0.46	2.10
1:A:139:TYR:CD1	1:A:139:TYR:C	0.46	2.94
1:A:169:TRP:N	1:A:169:TRP:CE3	0.46	2.83
1:A:244:ALA:HB2	1:A:255:HIS:HB3	0.46	1.86
1:A:105:ILE:HG22	1:A:109:ILE:CG2	0.46	2.41
1:A:198:LEU:CD1	1:A:216:PHE:CE1	0.46	2.99
1:A:320:THR:HG22	1:A:324:GLY:O	0.46	2.11
1:A:442:ALA:HB2	1:A:446:VAL:CG2	0.46	2.41
1:A:713:HIS:CD2	1:A:716:ARG:NH1	0.46	2.84
1:A:115:PRO:CD	1:A:544:HIS:CE1	0.45	3.00
1:A:544:HIS:CD2	1:A:545:ALA:N	0.45	2.85
1:A:22:GLU:N	1:A:22:GLU:OE1	0.45	2.49
1:A:68:HIS:ND1	1:A:581:VAL:HG11	0.45	2.26
1:A:135:TRP:CD1	1:A:260:ILE:CG2	0.45	2.99
1:A:75:VAL:CG1	1:A:81:TYR:CD2	0.45	3.00
1:A:148:ILE:HG12	1:A:166:VAL:HG22	0.45	1.87
1:A:451:THR:HG22	1:A:505:GLY:C	0.45	2.36
1:A:39:PHE:CE1	1:A:43:VAL:CG2	0.45	2.99
1:A:133:ALA:HB3	1:A:264:ALA:HB3	0.45	1.86
1:A:294:MET:CE	1:A:373:TYR:CD1	0.45	2.99
1:A:337:ILE:N	1:A:387:TYR:O	0.45	2.50
1:A:122:MET:HE1	1:A:285:LEU:HB2	0.45	1.88
1:A:519:TYR:CD1	1:A:519:TYR:C	0.45	2.95
1:A:526:LEU:O	1:A:553:VAL:HG12	0.45	2.12
1:A:526:LEU:HD22	1:A:548:TYR:CE1	0.45	2.47
1:A:709:GLU:N	1:A:710:PRO:CD	0.45	2.79
1:A:75:VAL:HG13	1:A:81:TYR:CD2	0.44	2.47
1:A:586:ASN:O	1:A:587:TRP:CE3	0.44	2.70

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:338:ARG:O	1:A:338:ARG:NE	0.44	2.50
1:A:475:GLN:NE2	1:A:645:TRP:CZ2	0.44	2.85
1:A:198:LEU:CD1	1:A:216:PHE:CZ	0.44	2.99
1:A:442:ALA:CB	1:A:446:VAL:HG23	0.44	2.41
1:A:75:VAL:CG2	1:A:579:ILE:HD11	0.44	2.42
1:A:340:VAL:HG23	1:A:340:VAL:O	0.44	2.13
1:A:451:THR:O	1:A:453:PHE:CE2	0.44	2.71
1:A:623:ILE:HG23	1:A:624:HIS:N	0.44	2.27
1:A:287:TYR:HE1	1:A:291:LEU:HD13	0.44	1.71
1:A:461:MET:O	1:A:465:MET:N	0.44	2.51
1:A:130:ALA:O	1:A:264:ALA:HB3	0.44	2.13
1:A:238:ILE:HG22	1:A:261:VAL:HG12	0.44	1.88
1:A:462:HIS:CG	1:A:640:GLN:NE2	0.44	2.86
1:A:608:VAL:HG13	1:A:609:ARG:N	0.44	2.28
1:A:644:ASN:O	1:A:648:HIS:CD2	0.44	2.70
1:A:109:ILE:HD13	1:A:421:LYS:HD3	0.43	1.90
1:A:462:HIS:CE1	1:A:703:GLN:CG	0.43	3.01
1:A:600:VAL:O	1:A:604:LEU:N	0.43	2.51
1:A:32:ALA:O	1:A:36:TRP:CG	0.43	2.71
1:A:21:ASP:OD1	1:A:22:GLU:N	0.43	2.51
1:A:113:ALA:HB1	1:A:548:TYR:CE2	0.43	2.49
1:A:9:ARG:CZ	1:A:40:ASP:CB	0.43	2.97
1:A:54:LEU:HD13	1:A:54:LEU:O	0.43	2.13
1:A:139:TYR:CE2	1:A:140:ASP:OD1	0.43	2.72
1:A:113:ALA:CB	1:A:548:TYR:CE2	0.43	3.02
1:A:178:LEU:HD23	1:A:233:ASN:CB	0.43	2.44
1:A:701:VAL:HG23	1:A:702:LYS:N	0.43	2.29
1:A:135:TRP:CH2	1:A:237:HIS:NE2	0.43	2.87
1:A:448:PHE:CD1	1:A:498:LEU:CD2	0.43	3.00
1:A:105:ILE:HG22	1:A:109:ILE:HG23	0.43	1.90
1:A:350:TRP:CE2	1:A:354:GLY:CA	0.43	3.01
1:A:357:ILE:N	1:A:358:PRO:CD	0.43	2.82
1:A:644:ASN:OD1	1:A:645:TRP:CD1	0.43	2.72
1:A:683:ASN:ND2	1:A:718:ARG:NH2	0.43	2.66
1:A:442:ALA:CB	1:A:446:VAL:CG2	0.43	2.97
1:A:498:LEU:O	1:A:499:ARG:CB	0.43	2.66
1:A:143:TYR:CD1	1:A:143:TYR:C	0.42	2.96
1:A:456:ARG:HD2	1:A:485:TYR:CE1	0.42	2.49
1:A:543:LEU:HD12	1:A:547:HIS:HE1	0.42	1.72
1:A:187:ASP:OD2	1:A:202:LEU:HD13	0.42	2.14
1:A:372:LEU:HD22	1:A:376:LYS:CD	0.42	2.44
1:A:454:LEU:HD13	1:A:634:THR:HA	0.42	1.91

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:7:GLN:CD	1:A:36:TRP:CG	0.42	2.97
1:A:84:PHE:O	1:A:88:LEU:HD12	0.42	2.14
1:A:342:HIS:CE1	1:A:709:GLU:OE1	0.42	2.73
1:A:450:ASN:OD1	1:A:450:ASN:N	0.42	2.53
1:A:63:ALA:O	1:A:67:TRP:CD2	0.42	2.73
1:A:330:HIS:CD2	1:A:332:ARG:CZ	0.42	3.02
1:A:424:ILE:HG23	1:A:447:ALA:CB	0.42	2.32
1:A:680:MET:HE2	1:A:680:MET:CA	0.42	2.45
1:A:459:ASP:CA	1:A:636:ARG:NH1	0.42	2.82
1:A:677:TYR:CD1	1:A:677:TYR:C	0.42	2.97
1:A:147:ILE:CD1	1:A:543:LEU:HD11	0.42	2.45
1:A:173:PHE:CD2	1:A:546:LEU:HD22	0.42	2.50
1:A:338:ARG:NH2	1:A:364:GLY:HA2	0.42	2.30
1:A:18:ARG:NH1	1:A:22:GLU:CB	0.42	2.83
1:A:44:HIS:CE1	1:A:353:GLU:OE2	0.42	2.73
1:A:122:MET:HE1	1:A:285:LEU:CB	0.42	2.45
1:A:403:ASN:ND2	1:A:445:ARG:CG	0.42	2.83
1:A:424:ILE:HD13	1:A:438:CYS:HB3	0.42	1.91
1:A:451:THR:OG1	1:A:453:PHE:CE2	0.42	2.72
1:A:462:HIS:NE2	1:A:703:GLN:NE2	0.42	2.67
1:A:478:SER:CB	1:A:637:ILE:HD11	0.42	2.45
1:A:253:PRO:O	1:A:255:HIS:CE1	0.42	2.73
1:A:337:ILE:HG22	1:A:338:ARG:N	0.42	2.29
1:A:464:VAL:O	1:A:467:ALA:HB3	0.42	2.14
1:A:278:VAL:O	1:A:278:VAL:CG1	0.42	2.68
1:A:1:MET:HB3	1:A:4:THR:HG22	0.41	1.91
1:A:181:GLU:CA	1:A:181:GLU:OE1	0.41	2.68
1:A:188:VAL:CG1	1:A:200:ILE:CG2	0.41	2.97
1:A:374:ASP:C	1:A:377:VAL:HG22	0.41	2.40
1:A:454:LEU:HD22	1:A:637:ILE:CG2	0.41	2.41
1:A:620:VAL:HG23	1:A:630:GLU:CD	0.41	2.40
1:A:139:TYR:CD2	1:A:258:ASP:CG	0.41	2.99
1:A:436:ARG:CZ	1:A:497:GLY:CA	0.41	2.98
1:A:636:ARG:NH1	1:A:706:GLY:O	0.41	2.53
1:A:641:HIS:O	1:A:645:TRP:CD2	0.41	2.73
1:A:692:ALA:HB2	1:A:715:TRP:CG	0.41	2.50
1:A:711:LEU:O	1:A:715:TRP:CD1	0.41	2.73
1:A:215:GLN:O	1:A:217:VAL:HG23	0.41	2.14
1:A:424:ILE:CG1	1:A:448:PHE:O	0.41	2.69
1:A:41:GLU:HA	1:A:44:HIS:CE1	0.41	2.51
1:A:177:SER:CB	1:A:550:GLN:NE2	0.41	2.84
1:A:180:LEU:CD2	1:A:185:TYR:CE1	0.41	3.04

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:210:LEU:O	1:A:211:ARG:C	0.41	2.63
1:A:271:CYS:CB	1:A:632:ARG:CZ	0.41	2.99
1:A:318:HIS:O	1:A:319:TYR:CD1	0.41	2.74
1:A:338:ARG:O	1:A:388:ILE:HG23	0.41	2.15
1:A:350:TRP:CZ3	1:A:356:GLU:O	0.41	2.73
1:A:481:TRP:O	1:A:484:ALA:HB3	0.41	2.15
1:A:584:ASN:OD1	1:A:648:HIS:CD2	0.41	2.73
1:A:75:VAL:CG2	1:A:579:ILE:CD1	0.41	2.98
1:A:236:LEU:CB	1:A:549:HIS:CD2	0.41	3.04
1:A:300:GLU:O	1:A:310:VAL:N	0.41	2.53
1:A:350:TRP:CE2	1:A:354:GLY:HA3	0.41	2.51
1:A:441:GLN:C	1:A:443:ARG:H	0.41	2.23
1:A:695:ASP:OD2	1:A:715:TRP:CZ2	0.41	2.74
1:A:32:ALA:O	1:A:36:TRP:CD2	0.41	2.74
1:A:135:TRP:CH2	1:A:260:ILE:O	0.41	2.74
1:A:372:LEU:HD22	1:A:376:LYS:HD3	0.41	1.93
1:A:464:VAL:HG21	1:A:581:VAL:CG1	0.41	2.46
1:A:584:ASN:OD1	1:A:648:HIS:CG	0.41	2.73
1:A:611:VAL:HG12	1:A:719:GLU:CB	0.41	2.46
1:A:612:GLU:O	1:A:723:HIS:CE1	0.41	2.74
1:A:612:GLU:O	1:A:678:ARG:CZ	0.41	2.68
1:A:642:ILE:CG2	1:A:697:ILE:CG2	0.41	2.99
1:A:139:TYR:CE2	1:A:258:ASP:CG	0.41	2.98
1:A:139:TYR:CE2	1:A:258:ASP:OD2	0.41	2.74
1:A:394:HIS:CE1	1:A:431:THR:OG1	0.41	2.74
1:A:471:LEU:HD23	1:A:471:LEU:H	0.41	1.75
1:A:482:ILE:HG23	1:A:483:LYS:N	0.41	2.29
1:A:77:ASP:OD2	1:A:81:TYR:CD1	0.41	2.74
1:A:134:ARG:CZ	1:A:330:HIS:O	0.41	2.69
1:A:267:THR:O	1:A:268:ILE:HD13	0.41	2.16
1:A:457:THR:CG2	1:A:479:THR:CG2	0.41	2.99
1:A:462:HIS:CE1	1:A:700:GLY:O	0.41	2.73
1:A:465:MET:O	1:A:647:ARG:NH2	0.41	2.54
1:A:7:GLN:OE1	1:A:36:TRP:CE3	0.41	2.74
1:A:189:VAL:O	1:A:255:HIS:CD2	0.41	2.74
1:A:236:LEU:O	1:A:549:HIS:CE1	0.41	2.74
1:A:276:ALA:HB3	1:A:713:HIS:CD2	0.41	2.46
1:A:464:VAL:HG21	1:A:581:VAL:HG12	0.41	1.92
1:A:488:ASN:O	1:A:492:SER:CB	0.41	2.69
1:A:541:ALA:O	1:A:544:HIS:CD2	0.41	2.73
1:A:631:ASP:OD2	1:A:633:ALA:HB3	0.41	2.15
1:A:719:GLU:OE2	1:A:723:HIS:CD2	0.41	2.74

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:9:ARG:NH2	1:A:37:ARG:NH1	0.41	2.68
1:A:44:HIS:CD2	1:A:45:ASP:N	0.41	2.89
1:A:96:GLU:O	1:A:436:ARG:NH1	0.41	2.54
1:A:242:ILE:C	1:A:243:ASP:CG	0.41	2.89
1:A:318:HIS:CD2	1:A:326:GLU:OE2	0.41	2.74
1:A:377:VAL:HG23	1:A:378:GLN:N	0.41	2.31
1:A:439:ILE:O	1:A:441:GLN:N	0.41	2.54
1:A:543:LEU:O	1:A:547:HIS:CE1	0.41	2.74
1:A:109:ILE:HD11	1:A:448:PHE:CZ	0.40	2.48
1:A:132:ASN:CB	1:A:314:ASN:ND2	0.40	2.84
1:A:191:PHE:CD1	1:A:191:PHE:N	0.40	2.89
1:A:368:GLY:O	1:A:371:ALA:HB3	0.40	2.16
1:A:481:TRP:CZ2	1:A:578:THR:O	0.40	2.74
1:A:608:VAL:O	1:A:612:GLU:N	0.40	2.54
1:A:641:HIS:ND1	1:A:645:TRP:CH2	0.40	2.89
1:A:299:GLN:N	1:A:299:GLN:NE2	0.40	2.69
1:A:443:ARG:N	1:A:443:ARG:NE	0.40	2.69
1:A:483:LYS:HA	1:A:508:MET:HE3	0.40	1.92
1:A:604:LEU:O	1:A:608:VAL:HG12	0.40	2.16
1:A:609:ARG:O	1:A:613:GLN:CB	0.40	2.69
1:A:15:ASN:ND2	1:A:16:PHE:N	0.40	2.69
1:A:252:ASP:OD1	1:A:252:ASP:O	0.40	2.38
1:A:330:HIS:CE1	1:A:382:ARG:O	0.40	2.74
1:A:429:ARG:CZ	1:A:576:LEU:O	0.40	2.69
1:A:662:ASN:ND2	1:A:663:MET:CE	0.40	2.84
1:A:128:LEU:CD2	1:A:132:ASN:ND2	0.40	2.85
1:A:273:ASP:OD2	1:A:707:TYR:CD2	0.40	2.74
1:A:456:ARG:CD	1:A:485:TYR:CE1	0.40	3.05
1:A:488:ASN:ND2	1:A:489:ASN:ND2	0.40	2.70
1:A:491:LEU:HD23	1:A:560:ILE:HG22	0.40	1.91
1:A:150:GLN:OE1	1:A:150:GLN:CA	0.40	2.70
1:A:273:ASP:OD1	1:A:342:HIS:CE1	0.40	2.74
1:A:289:ASN:ND2	1:A:290:LEU:N	0.40	2.69
1:A:516:ALA:HA	1:A:519:TYR:CD2	0.40	2.52
1:A:519:TYR:O	1:A:523:GLY:N	0.40	2.54
1:A:610:TRP:CE3	1:A:610:TRP:O	0.40	2.74

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	721/723 (100%)	596 (83%)	87 (12%)	38 (5%)	2	22
All	All	721/723 (100%)	596 (83%)	87 (12%)	38 (5%)	2	22

All 38 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	8	SER
1	A	30	LEU
1	A	105	ILE
1	A	111	SER
1	A	155	VAL
1	A	157	GLY
1	A	179	PRO
1	A	182	ASN
1	A	226	PRO
1	A	270	ASP
1	A	271	CYS
1	A	278	VAL
1	A	279	ASP
1	A	297	THR
1	A	298	LEU
1	A	305	ASN
1	A	315	ASP
1	A	330	HIS
1	A	347	PRO
1	A	355	ASN
1	A	358	PRO
1	A	381	SER
1	A	414	GLY
1	A	419	THR
1	A	426	ASP
1	A	440	ALA
1	A	444	ASN

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Mol	Chain	Res	Type
1	A	446	VAL
1	A	453	PHE
1	A	499	ARG
1	A	500	GLY
1	A	506	LYS
1	A	511	MET
1	A	513	ASP
1	A	583	GLU
1	A	616	GLY
1	A	687	SER
1	A	704	PRO

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	599/599 (100%)	448 (75%)	151 (25%)	2	24
All	All	599/599 (100%)	448 (75%)	151 (25%)	2	24

All 151 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	THR
1	A	9	ARG
1	A	10	LEU
1	A	12	ILE
1	A	18	ARG
1	A	23	GLU
1	A	37	ARG
1	A	41	GLU
1	A	52	GLN
1	A	54	LEU
1	A	56	GLU
1	A	57	ARG
1	A	58	ASP

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Mol	Chain	Res	Type
1	A	66	GLU
1	A	67	TRP
1	A	82	LYS
1	A	85	LEU
1	A	87	GLU
1	A	96	GLU
1	A	105	ILE
1	A	112	GLN
1	A	116	GLN
1	A	117	LEU
1	A	125	ARG
1	A	126	TYR
1	A	134	ARG
1	A	139	TYR
1	A	143	TYR
1	A	151	GLU
1	A	154	MET
1	A	164	GLU
1	A	176	GLU
1	A	177	SER
1	A	178	LEU
1	A	181	GLU
1	A	186	GLN
1	A	191	PHE
1	A	192	LYS
1	A	197	GLN
1	A	201	GLN
1	A	203	LYS
1	A	206	LYS
1	A	215	GLN
1	A	228	CYS
1	A	231	LEU
1	A	233	ASN
1	A	243	ASP
1	A	247	ARG
1	A	250	LYS
1	A	262	GLU
1	A	267	THR
1	A	269	LEU
1	A	274	SER
1	A	278	VAL
1	A	282	ASP

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Mol	Chain	Res	Type
1	A	283	LYS
1	A	285	LEU
1	A	290	LEU
1	A	294	MET
1	A	295	GLN
1	A	297	THR
1	A	298	LEU
1	A	299	GLN
1	A	304	LYS
1	A	307	ARG
1	A	314	ASN
1	A	317	ARG
1	A	332	ARG
1	A	335	LEU
1	A	338	ARG
1	A	344	MET
1	A	345	THR
1	A	352	SER
1	A	359	GLU
1	A	372	LEU
1	A	376	LYS
1	A	382	ARG
1	A	392	LYS
1	A	408	ARG
1	A	410	GLU
1	A	420	LEU
1	A	421	LYS
1	A	425	MET
1	A	428	GLU
1	A	429	ARG
1	A	430	ARG
1	A	431	THR
1	A	432	SER
1	A	435	LEU
1	A	437	SER
1	A	441	GLN
1	A	443	ARG
1	A	445	ARG
1	A	450	ASN
1	A	453	PHE
1	A	457	THR
1	A	460	GLU

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Mol	Chain	Res	Type
1	A	461	MET
1	A	462	HIS
1	A	463	SER
1	A	465	MET
1	A	470	MET
1	A	471	LEU
1	A	473	LYS
1	A	475	GLN
1	A	476	MET
1	A	477	LYS
1	A	487	ARG
1	A	498	LEU
1	A	499	ARG
1	A	501	LYS
1	A	508	MET
1	A	513	ASP
1	A	515	MET
1	A	518	MET
1	A	522	LYS
1	A	527	ARG
1	A	542	THR
1	A	543	LEU
1	A	544	HIS
1	A	562	GLN
1	A	564	GLU
1	A	578	THR
1	A	583	GLU
1	A	590	GLN
1	A	594	GLN
1	A	603	ILE
1	A	618	SER
1	A	623	ILE
1	A	635	LEU
1	A	636	ARG
1	A	637	ILE
1	A	641	HIS
1	A	651	LEU
1	A	653	LYS
1	A	654	GLU
1	A	657	GLN
1	A	665	LYS
1	A	669	GLN

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Mol	Chain	Res	Type
1	A	670	GLN
1	A	678	ARG
1	A	687	SER
1	A	691	LYS
1	A	702	LYS
1	A	703	GLN
1	A	712	LEU
1	A	717	LEU
1	A	718	ARG
1	A	720	LYS
1	A	721	GLU

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 oligosaccharides 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