



Full wwPDB NMR Structure Validation Report

(i)

Dec 13, 2023 – 07:54 PM EST

PDB ID : 2JQX

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 (i) symbol.

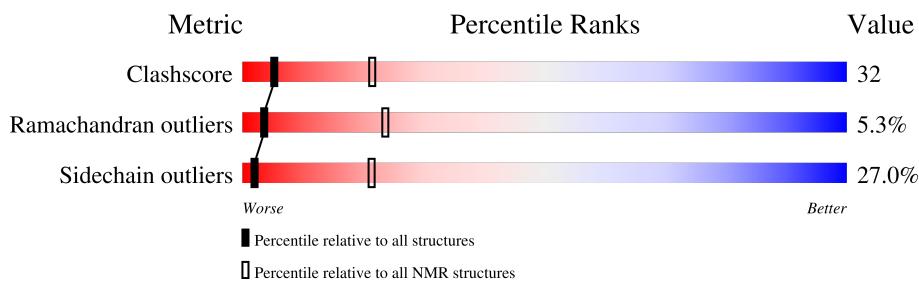
The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	723		37%	51%	11% .

2 Ensemble composition and analysis

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

3 Entry composition [\(i\)](#)

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
			Total	C	H	N	O	S	
1	A	723	11282	3543	5627	1015	1068	29	0

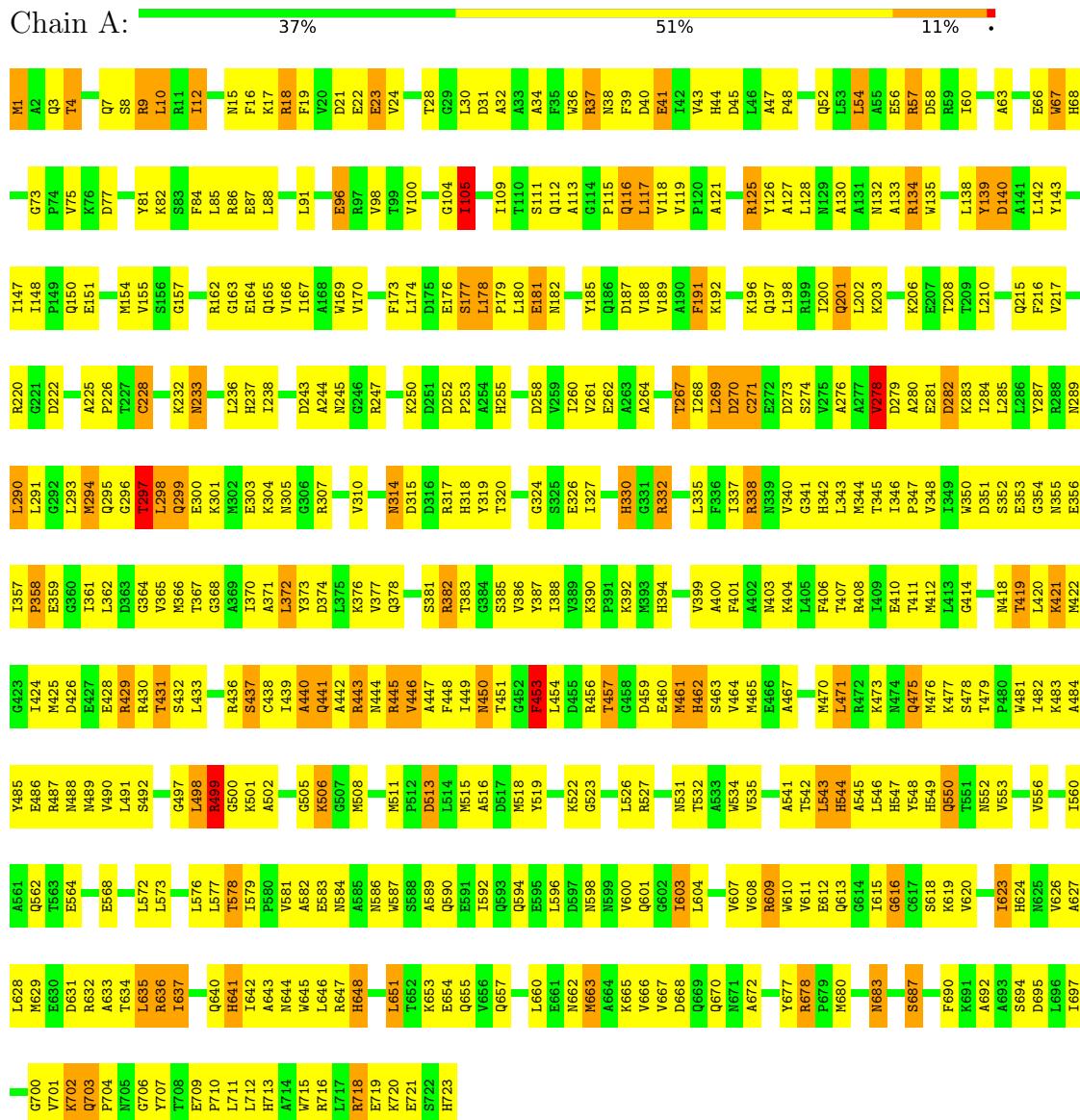
There is a discrepancy between the modelled and reference sequences:

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 i

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 [\(i\)](#)

6.1 Standard geometry [\(i\)](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	5655	5627	5610	359
All	All	5655	5627	5610	359

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 32.

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: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
1:A:449:ILE:HG21	1:A:489:ASN:ND2	0.75	1.97

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:672:ALA:HB1	1:A:677:TYR:CE2	0.75	2.16
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:31:ASP:CG	1:A:34:ALA:HB3	0.71	2.04
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: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: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: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:116:GLN:CD	1:A:451:THR:HG23	0.65	2.12
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
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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: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
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:174:LEU:HD23	1:A:185:TYR:CE2	0.54	2.37
1:A:135:TRP:CD1	1:A:260:ILE:HG21	0.54	2.37
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:303:GLU:CD	1:A:620:VAL:HG12	0.53	2.24
1:A:581:VAL:HG23	1:A:581:VAL:O	0.53	2.03
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: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: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: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:456:ARG:HH21	1:A:457:THR:HG23	0.51	1.64
1:A:278:VAL:HG22	1:A:282:ASP:CG	0.51	2.25
1:A:147:ILE:HD12	1:A:543:LEU:HD11	0.51	1.80
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: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:142:LEU:C	1:A:148:ILE:HG22	0.49	2.28
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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: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: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:85:LEU:HD13	1:A:85:LEU:C	0.47	2.29
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
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:343:LEU:HD12	1:A:343:LEU:C	0.47	2.30
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:660:LEU:HD13	1:A:660:LEU:O	0.46	2.10
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:552:ASN:O	1:A:556:VAL:HG23	0.46	2.10
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:390:LYS:O	1:A:422:MET:HE1	0.46	2.11
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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: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:526:LEU:HD22	1:A:548:TYR:CE1	0.45	2.47
1:A:526:LEU:O	1:A:553:VAL:HG12	0.45	2.12
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
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:646:LEU:HD13	1:A:646:LEU:C	0.44	2.32
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:433:LEU:HD13	1:A:433:LEU:C	0.43	2.34
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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: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
1:A:4:THR:HG1	1:A:12:ILE:C	0.42	2.18
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:N	1:A:450:ASN:OD1	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:459:ASP:CA	1:A:636:ARG:NH1	0.42	2.82
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: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:660:LEU:HD13	1:A:660:LEU:C	0.42	2.35
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:280:ALA:C	1:A:284:ILE:HD12	0.41	2.35
1:A:454:LEU:HD22	1:A:637:ILE:CG2	0.41	2.41
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:276:ALA:HB2	1:A:709:GLU:CD	0.41	2.36
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:139:TYR:CD1	1:A:139:TYR:C	0.41	2.94
1:A:177:SER:H	1:A:177:SER:HG	0.41	1.46
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
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: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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:680:MET:N	1:A:680:MET:CE	0.41	2.84
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
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: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:294:MET:CE	1:A:382:ARG:NH1	0.40	2.84
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:220:ARG:NH1	1:A:228:CYS:HG	0.40	2.13
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: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:451:THR:HG22	1:A:505:GLY:C	0.40	2.36
1:A:456:ARG:CD	1:A:485:TYR:CE1	0.40	3.05

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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 (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	721/723 (100%)	596 (83%)	87 (12%)	38 (5%)	3 23
All	All	721/723 (100%)	596 (83%)	87 (12%)	38 (5%)	3 23

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

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Mol	Chain	Res	Type
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
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 [\(i\)](#)

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	599/599 (100%)	437 (73%)	162 (27%)	2 21
All	All	599/599 (100%)	437 (73%)	162 (27%)	2 21

All 162 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	3	GLN

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Mol	Chain	Res	Type
1	A	4	THR
1	A	9	ARG
1	A	10	LEU
1	A	12	ILE
1	A	17	LYS
1	A	18	ARG
1	A	19	PHE
1	A	23	GLU
1	A	37	ARG
1	A	38	ASN
1	A	41	GLU
1	A	52	GLN
1	A	54	LEU
1	A	56	GLU
1	A	57	ARG
1	A	58	ASP
1	A	66	GLU
1	A	67	TRP
1	A	82	LYS
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	140	ASP
1	A	143	TYR
1	A	151	GLU
1	A	154	MET
1	A	164	GLU
1	A	165	GLN
1	A	176	GLU
1	A	177	SER
1	A	178	LEU
1	A	181	GLU
1	A	191	PHE
1	A	192	LYS
1	A	196	LYS

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	201	GLN
1	A	203	LYS
1	A	206	LYS
1	A	228	CYS
1	A	233	ASN
1	A	243	ASP
1	A	245	ASN
1	A	247	ARG
1	A	250	LYS
1	A	267	THR
1	A	269	LEU
1	A	274	SER
1	A	278	VAL
1	A	281	GLU
1	A	282	ASP
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	362	LEU
1	A	366	MET
1	A	372	LEU
1	A	382	ARG
1	A	392	LYS
1	A	401	PHE
1	A	408	ARG

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Mol	Chain	Res	Type
1	A	410	GLU
1	A	412	MET
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	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
1	A	461	MET
1	A	462	HIS
1	A	463	SER
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	550	GLN
1	A	562	GLN

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Mol	Chain	Res	Type
1	A	564	GLU
1	A	578	THR
1	A	590	GLN
1	A	594	GLN
1	A	598	ASN
1	A	601	GLN
1	A	603	ILE
1	A	609	ARG
1	A	618	SER
1	A	623	ILE
1	A	629	MET
1	A	635	LEU
1	A	636	ARG
1	A	637	ILE
1	A	641	HIS
1	A	648	HIS
1	A	651	LEU
1	A	653	LYS
1	A	654	GLU
1	A	655	GLN
1	A	657	GLN
1	A	663	MET
1	A	665	LYS
1	A	668	ASP
1	A	670	GLN
1	A	678	ARG
1	A	683	ASN
1	A	687	SER
1	A	702	LYS
1	A	703	GLN
1	A	712	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 monosaccharides 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 [\(i\)](#)

No chemical shift data were provided