Full wwPDB NMR Structure Validation Report (i)

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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
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:

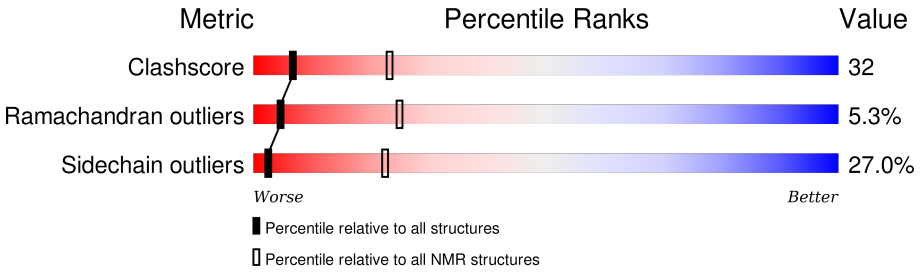
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	723	37% 51% 11% .

2 Ensemble composition and analysis (i)

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
			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:

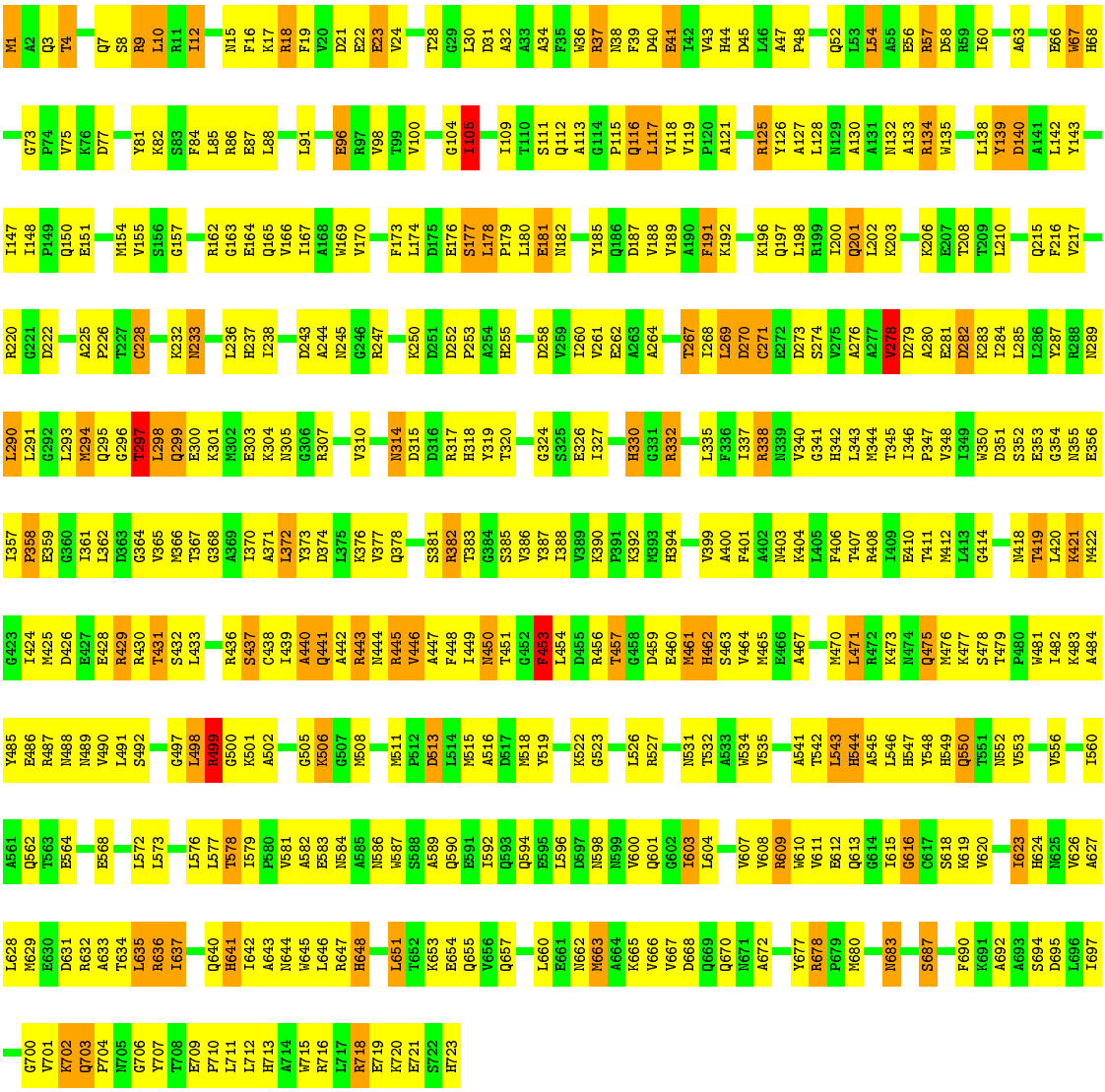
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	ENGINEERED	UNP P37330

4 Residue-property plots (i)

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: Malate synthase G

Chain A:



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. 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	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:592:ILE:HG21	1:A:651:LEU:CD2	0.68	2.18
1:A:174:LEU:HD23	1:A:185:TYR:CD2	0.68	2.24
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:O	1:A:433:LEU:HD13	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:198:LEU:HD22	1:A:210:LEU:CD1	0.63	2.21
1:A:39:PHE:O	1:A:43:VAL:HG23	0.63	1.93
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:603:ILE:HG22	1:A:635:LEU:CG	0.62	2.24

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:296:GLY:O	1:A:297:THR:HG23	0.62	1.94
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:626:VAL:HG12	1:A:628:LEU:HD13	0.62	1.72
1:A:341:GLY:O	1:A:361:ILE:HG22	0.62	1.95
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:424:ILE:CG2	1:A:447:ALA:HB1	0.60	2.23
1:A:43:VAL:O	1:A:47:ALA:HB2	0.60	1.95
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:498:LEU:HD13	1:A:502:ALA:CB	0.59	2.27
1:A:217:VAL:HG21	1:A:232:LYS:HB2	0.59	1.73
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:236:LEU:HD12	1:A:548:TYR:HB2	0.56	1.77
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: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:433:LEU:HD21	1:A:577:LEU:HD22	0.55	1.79
1:A:57:ARG:O	1:A:60:ILE:HG22	0.55	2.02
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:388:ILE:HD13	1:A:406:PHE:CE1	0.54	2.37
1:A:135:TRP:CD1	1:A:260:ILE:HG21	0.54	2.37
1:A:611:VAL:HG12	1:A:719:GLU:CG	0.54	2.32
1:A:573:LEU:O	1:A:577:LEU:HD23	0.54	2.03
1:A:287:TYR:OH	1:A:291:LEU:HD22	0.54	2.03
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:O	1:A:581:VAL:HG23	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:465:MET:SD	1:A:701:VAL:HG12	0.52	2.44
1:A:269:LEU:CD1	1:A:293:LEU:HD11	0.52	2.34
1:A:163:GLY:O	1:A:167:ILE:HG23	0.52	2.04
1:A:135:TRP:CH2	1:A:237:HIS:CD2	0.52	2.97
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:198:LEU:HD13	1:A:216:PHE:CE1	0.50	2.41
1:A:148:ILE:O	1:A:148:ILE:HG23	0.50	2.06
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:642:ILE:CG2	1:A:697:ILE:HG23	0.50	2.37
1:A:439:ILE:HD11	1:A:449:ILE:HD11	0.50	1.83
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:643:ALA:HB2	1:A:697:ILE:O	0.49	2.08

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:388:ILE:HD13	1:A:406:PHE:HE1	0.49	1.68
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:449:ILE:N	1:A:449:ILE:HD12	0.48	2.23
1:A:400:ALA:HB1	1:A:404:LYS:HE2	0.48	1.85
1:A:446:VAL:CG1	1:A:448:PHE:CE2	0.48	2.97
1:A:269:LEU:HD13	1:A:293:LEU:HD11	0.48	1.84
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:662:ASN:O	1:A:666:VAL:HG23	0.47	2.09
1:A:383:THR:HG23	1:A:385:SER:O	0.47	2.08
1:A:694:SER:HA	1:A:697:ILE:HD12	0.47	1.85
1:A:202:LEU:HD21	1:A:208:THR:HG21	0.47	1.86
1:A:634:THR:O	1:A:637:ILE:HG22	0.47	2.09
1:A:471:LEU:HG	1:A:582:ALA:HB2	0.47	1.85
1:A:222:ASP:OD2	1:A:225:ALA:HB3	0.47	2.09
1:A:491:LEU:HD23	1:A:560:ILE:CG2	0.47	2.39
1:A:85:LEU:HD13	1:A:85:LEU:C	0.47	2.29
1:A:343:LEU:HD12	1:A:343:LEU:C	0.47	2.30
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:319:TYR:O	1:A:327:ILE:HG22	0.46	2.10
1:A:607:VAL:O	1:A:611:VAL:HG23	0.46	2.10
1:A:118:VAL:CG2	1:A:453:PHE:CE2	0.46	2.98
1:A:552:ASN:O	1:A:556:VAL:HG23	0.46	2.10
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:169:TRP:N	1:A:169:TRP:CE3	0.46	2.83
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:713:HIS:CD2	1:A:716:ARG:NH1	0.46	2.84
1:A:442:ALA:HB2	1:A:446:VAL:CG2	0.46	2.41
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:OE1	1:A:22:GLU:N	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:148:ILE:HG12	1:A:166:VAL:HG22	0.45	1.87
1:A:75:VAL:CG1	1:A:81:TYR:CD2	0.45	3.00
1:A:133:ALA:HB3	1:A:264:ALA:HB3	0.45	1.86
1:A:39:PHE:CE1	1:A:43:VAL:CG2	0.45	2.99
1:A:337:ILE:N	1:A:387:TYR:O	0.45	2.50
1:A:294:MET:CE	1:A:373:TYR:CD1	0.45	2.99
1:A:709:GLU:N	1:A:710:PRO:CD	0.45	2.79
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: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:646:LEU:C	1:A:646:LEU:HD13	0.44	2.32
1:A:451:THR:O	1:A:453:PHE:CE2	0.44	2.71
1:A:75:VAL:CG2	1:A:579:ILE:HD11	0.44	2.42
1:A:623:ILE:HG23	1:A:624:HIS:N	0.44	2.27
1:A:340:VAL:HG23	1:A:340:VAL:O	0.44	2.13
1:A:461:MET:O	1:A:465:MET:N	0.44	2.51
1:A:287:TYR:HE1	1:A:291:LEU:HD13	0.44	1.71
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: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:462:HIS:CG	1:A:640:GLN:NE2	0.44	2.86
1:A:600:VAL:O	1:A:604:LEU:N	0.43	2.51
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:32:ALA:O	1:A:36:TRP:CG	0.43	2.71
1:A:433:LEU:HD13	1:A:433:LEU:C	0.43	2.34
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:54:LEU:HD13	1:A:54:LEU:O	0.43	2.13
1:A:9:ARG:CZ	1:A:40:ASP:CB	0.43	2.97
1:A:139:TYR:CE2	1:A:140:ASP:OD1	0.43	2.72
1:A:701:VAL:HG23	1:A:702:LYS:N	0.43	2.29

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
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:448:PHE:CD1	1:A:498:LEU:CD2	0.43	3.00
1:A:135:TRP:CH2	1:A:237:HIS:NE2	0.43	2.87
1:A:105:ILE:HG22	1:A:109:ILE:HG23	0.43	1.90
1:A:644:ASN:OD1	1:A:645:TRP:CD1	0.43	2.72
1:A:350:TRP:CE2	1:A:354:GLY:CA	0.43	3.01
1:A:683:ASN:ND2	1:A:718:ARG:NH2	0.43	2.66
1:A:357:ILE:N	1:A:358:PRO:CD	0.43	2.82
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:543:LEU:HD12	1:A:547:HIS:HE1	0.42	1.72
1:A:456:ARG:HD2	1:A:485:TYR:CE1	0.42	2.49
1:A:187:ASP:OD2	1:A:202:LEU:HD13	0.42	2.14
1:A:454:LEU:HD13	1:A:634:THR:HA	0.42	1.91
1:A:372:LEU:HD22	1:A:376:LYS:CD	0.42	2.44
1:A:342:HIS:CE1	1:A:709:GLU:OE1	0.42	2.73
1:A:4:THR:HG1	1:A:12:ILE:C	0.42	2.18
1:A:450:ASN:N	1:A:450:ASN:OD1	0.42	2.53
1:A:84:PHE:O	1:A:88:LEU:HD12	0.42	2.14
1:A:424:ILE:HG23	1:A:447:ALA:CB	0.42	2.32
1:A:330:HIS:CD2	1:A:332:ARG:CZ	0.42	3.02
1:A:63:ALA:O	1:A:67:TRP:CD2	0.42	2.73
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:338:ARG:NH2	1:A:364:GLY:HA2	0.42	2.30
1:A:173:PHE:CD2	1:A:546:LEU:HD22	0.42	2.50
1:A:424:ILE:HD13	1:A:438:CYS:HB3	0.42	1.91
1:A:478:SER:CB	1:A:637:ILE:HD11	0.42	2.45
1:A:451:THR:OG1	1:A:453:PHE:CE2	0.42	2.72
1:A:660:LEU:HD13	1:A:660:LEU:C	0.42	2.35
1:A:18:ARG:NH1	1:A:22:GLU:CB	0.42	2.83
1:A:462:HIS:NE2	1:A:703:GLN:NE2	0.42	2.67
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:337:ILE:HG22	1:A:338:ARG:N	0.42	2.29
1:A:253:PRO:O	1:A:255:HIS:CE1	0.42	2.73
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:188:VAL:CG1	1:A:200:ILE:CG2	0.41	2.97
1:A:454:LEU:HD22	1:A:637:ILE:CG2	0.41	2.41

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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:181:GLU:OE1	1:A:181:GLU:CA	0.41	2.68
1:A:641:HIS:O	1:A:645:TRP:CD2	0.41	2.73
1:A:636:ARG:NH1	1:A:706:GLY:O	0.41	2.53
1:A:711:LEU:O	1:A:715:TRP:CD1	0.41	2.73
1:A:692:ALA:HB2	1:A:715:TRP:CG	0.41	2.50
1:A:436:ARG:CZ	1:A:497:GLY:CA	0.41	2.98
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:215:GLN:O	1:A:217:VAL:HG23	0.41	2.14
1:A:338:ARG:O	1:A:388:ILE:HG23	0.41	2.15
1:A:180:LEU:CD2	1:A:185:TYR:CE1	0.41	3.04
1:A:318:HIS:O	1:A:319:TYR:CD1	0.41	2.74
1:A:584:ASN:OD1	1:A:648:HIS:CD2	0.41	2.73
1:A:139:TYR:CD1	1:A:139:TYR:C	0.41	2.94
1:A:350:TRP:CZ3	1:A:356:GLU:O	0.41	2.73
1:A:41:GLU:HA	1:A:44:HIS:CE1	0.41	2.51
1:A:271:CYS:CB	1:A:632:ARG:CZ	0.41	2.99
1:A:177:SER:HG	1:A:177:SER:H	0.41	1.46
1:A:177:SER:CB	1:A:550:GLN:NE2	0.41	2.84
1:A:481:TRP:O	1:A:484:ALA:HB3	0.41	2.15
1:A:236:LEU:CB	1:A:549:HIS:CD2	0.41	3.04
1:A:75:VAL:CG2	1:A:579:ILE:CD1	0.41	2.98
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:300:GLU:O	1:A:310:VAL:N	0.41	2.53
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:611:VAL:HG12	1:A:719:GLU:CB	0.41	2.46
1:A:642:ILE:CG2	1:A:697:ILE:CG2	0.41	2.99
1:A:32:ALA:O	1:A:36:TRP:CD2	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:135:TRP:CH2	1:A:260:ILE:O	0.41	2.74
1:A:584:ASN:OD1	1:A:648:HIS:CG	0.41	2.73
1:A:482:ILE:HG23	1:A:483:LYS:N	0.41	2.29
1:A:471:LEU:HD23	1:A:471:LEU:H	0.41	1.75
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:465:MET:O	1:A:647:ARG:NH2	0.41	2.54
1:A:457:THR:CG2	1:A:479:THR:CG2	0.41	2.99
1:A:77:ASP:OD2	1:A:81:TYR:CD1	0.41	2.74

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:134:ARG:CZ	1:A:330:HIS:O	0.41	2.69
1:A:462:HIS:CE1	1:A:700:GLY:O	0.41	2.73
1:A:267:THR:O	1:A:268:ILE:HD13	0.41	2.16
1:A:680:MET:N	1:A:680:MET:CE	0.41	2.84
1:A:719:GLU:OE2	1:A:723:HIS:CD2	0.41	2.74
1:A:276:ALA:HB3	1:A:713:HIS:CD2	0.41	2.46
1:A:488:ASN:O	1:A:492:SER:CB	0.41	2.69
1:A:236:LEU:O	1:A:549:HIS:CE1	0.41	2.74
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:541:ALA:O	1:A:544:HIS:CD2	0.41	2.73
1:A:464:VAL:HG21	1:A:581:VAL:HG12	0.41	1.92
1:A:631:ASP:OD2	1:A:633:ALA:HB3	0.41	2.15
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:318:HIS:CD2	1:A:326:GLU:OE2	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:377:VAL:HG23	1:A:378:GLN:N	0.41	2.31
1:A:608:VAL:O	1:A:612:GLU:N	0.40	2.54
1:A:109:ILE:HD11	1:A:448:PHE:CZ	0.40	2.48
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:641:HIS:ND1	1:A:645:TRP:CH2	0.40	2.89
1:A:481:TRP:CZ2	1:A:578:THR:O	0.40	2.74
1:A:132:ASN:CB	1:A:314:ASN:ND2	0.40	2.84
1:A:368:GLY:O	1:A:371:ALA:HB3	0.40	2.16
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:299:GLN:N	1:A:299:GLN:NE2	0.40	2.69
1:A:220:ARG:NH1	1:A:228:CYS:HG	0.40	2.13
1:A:443:ARG:N	1:A:443:ARG:NE	0.40	2.69
1:A:662:ASN:ND2	1:A:663:MET:CE	0.40	2.84
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:15:ASN:ND2	1:A:16:PHE:N	0.40	2.69
1:A:273:ASP:OD2	1:A:707:TYR:CD2	0.40	2.74
1:A:488:ASN:ND2	1:A:489:ASN:ND2	0.40	2.70
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:491:LEU:HD23	1:A:560:ILE:HG22	0.40	1.91
1:A:128:LEU:CD2	1:A:132:ASN:ND2	0.40	2.85
1:A:273:ASP:OD1	1:A:342:HIS:CE1	0.40	2.74
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:289:ASN:ND2	1:A:290:LEU:N	0.40	2.69
1:A:150:GLN:CA	1:A:150:GLN:OE1	0.40	2.70
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%)	4 25
All	All	721/723 (100%)	596 (83%)	87 (12%)	38 (5%)	4 25

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

Mol	Chain	Res	Type
1	A	278	VAL
1	A	315	ASP
1	A	330	HIS
1	A	8	SER
1	A	105	ILE
1	A	305	ASN
1	A	616	GLY
1	A	500	GLY
1	A	381	SER
1	A	704	PRO
1	A	270	ASP
1	A	506	LYS
1	A	155	VAL
1	A	297	THR
1	A	111	SER

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Mol	Chain	Res	Type
1	A	279	ASP
1	A	355	ASN
1	A	358	PRO
1	A	440	ALA
1	A	446	VAL
1	A	687	SER
1	A	426	ASP
1	A	226	PRO
1	A	271	CYS
1	A	179	PRO
1	A	511	MET
1	A	298	LEU
1	A	419	THR
1	A	347	PRO
1	A	583	GLU
1	A	444	ASN
1	A	157	GLY
1	A	414	GLY
1	A	30	LEU
1	A	182	ASN
1	A	499	ARG
1	A	453	PHE
1	A	513	ASP

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 22
All	All	599/599 (100%)	437 (73%)	162 (27%)	2 22

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	247	ARG
1	A	278	VAL

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Mol	Chain	Res	Type
1	A	635	LEU
1	A	299	GLN
1	A	54	LEU
1	A	609	ARG
1	A	623	ILE
1	A	651	LEU
1	A	429	ARG
1	A	401	PHE
1	A	470	MET
1	A	718	ARG
1	A	527	ARG
1	A	140	ASP
1	A	590	GLN
1	A	421	LYS
1	A	501	LYS
1	A	233	ASN
1	A	508	MET
1	A	206	LYS
1	A	143	TYR
1	A	637	ILE
1	A	335	LEU
1	A	598	ASN
1	A	462	HIS
1	A	441	GLN
1	A	52	GLN
1	A	1	MET
1	A	332	ARG
1	A	362	LEU
1	A	243	ASP
1	A	457	THR
1	A	653	LYS
1	A	298	LEU
1	A	420	LEU
1	A	67	TRP
1	A	294	MET
1	A	203	LYS
1	A	178	LEU
1	A	176	GLU
1	A	191	PHE
1	A	428	GLU
1	A	430	ARG
1	A	37	ARG

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Mol	Chain	Res	Type
1	A	477	LYS
1	A	57	ARG
1	A	139	TYR
1	A	382	ARG
1	A	87	GLU
1	A	338	ARG
1	A	475	GLN
1	A	307	ARG
1	A	712	LEU
1	A	134	ARG
1	A	655	GLN
1	A	636	ARG
1	A	192	LYS
1	A	66	GLU
1	A	703	GLN
1	A	443	ARG
1	A	629	MET
1	A	282	ASP
1	A	550	GLN
1	A	518	MET
1	A	657	GLN
1	A	603	ILE
1	A	437	SER
1	A	285	LEU
1	A	721	GLU
1	A	542	THR
1	A	18	ARG
1	A	9	ARG
1	A	267	THR
1	A	4	THR
1	A	498	LEU
1	A	499	ARG
1	A	425	MET
1	A	112	GLN
1	A	702	LYS
1	A	412	MET
1	A	578	THR
1	A	408	ARG
1	A	648	HIS
1	A	304	LYS
1	A	197	GLN
1	A	17	LYS

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Mol	Chain	Res	Type
1	A	82	LYS
1	A	366	MET
1	A	317	ARG
1	A	105	ILE
1	A	450	ASN
1	A	543	LEU
1	A	181	GLU
1	A	151	GLU
1	A	177	SER
1	A	290	LEU
1	A	314	ASN
1	A	126	TYR
1	A	453	PHE
1	A	654	GLU
1	A	678	ARG
1	A	432	SER
1	A	522	LYS
1	A	196	LYS
1	A	116	GLN
1	A	460	GLU
1	A	58	ASP
1	A	274	SER
1	A	3	GLN
1	A	687	SER
1	A	19	PHE
1	A	201	GLN
1	A	117	LEU
1	A	12	ILE
1	A	431	THR
1	A	154	MET
1	A	410	GLU
1	A	473	LYS
1	A	359	GLU
1	A	670	GLN
1	A	445	ARG
1	A	56	GLU
1	A	476	MET
1	A	10	LEU
1	A	641	HIS
1	A	245	ASN
1	A	23	GLU
1	A	683	ASN

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Mol	Chain	Res	Type
1	A	392	LYS
1	A	295	GLN
1	A	38	ASN
1	A	515	MET
1	A	471	LEU
1	A	544	HIS
1	A	297	THR
1	A	564	GLU
1	A	250	LYS
1	A	345	THR
1	A	461	MET
1	A	164	GLU
1	A	562	GLN
1	A	344	MET
1	A	352	SER
1	A	665	LYS
1	A	594	GLN
1	A	165	GLN
1	A	96	GLU
1	A	463	SER
1	A	668	ASP
1	A	283	LYS
1	A	269	LEU
1	A	281	GLU
1	A	41	GLU
1	A	125	ARG
1	A	601	GLN
1	A	618	SER
1	A	513	ASP
1	A	720	LYS
1	A	372	LEU
1	A	663	MET
1	A	487	ARG
1	A	228	CYS

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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