Full wwPDB NMR Structure Validation Report (i)

Jun 16, 2024 – 06:27 AM EDT

PDB ID	:	1SUY
Title	:	NMR structure of the ThKaiA180C-CIIABD complex (average minimized structure)
Authors	:	Vakonakis, I.; LiWang, A.C.
Deposited on	:	2004-03-26

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.

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

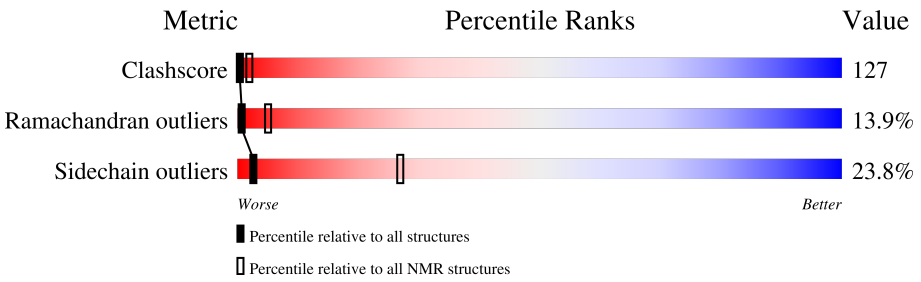
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	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	107	27% 58% 14% •
1	B	107	27% 58% 14% •
2	C	34	• 38% 41% 18%
2	D	34	• 38% 41% 18%

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 (i)

There are 2 unique types of molecules in this entry. The entry contains 4596 atoms, of which 2328 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called circadian clock protein KaiA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	107	1788	561	905	151	166	5	0
1	B	107	1788	561	905	151	166	5	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	CLONING ARTIFACT	UNP Q79V62
A	2	MET	-	CLONING ARTIFACT	UNP Q79V62
A	3	ALA	-	CLONING ARTIFACT	UNP Q79V62
B	201	ALA	-	CLONING ARTIFACT	UNP Q79V62
B	202	MET	-	CLONING ARTIFACT	UNP Q79V62
B	203	ALA	-	CLONING ARTIFACT	UNP Q79V62

- Molecule 2 is a protein called circadian clock protein KaiC.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	C	34	510	152	259	43	54	2	0
2	D	34	510	152	259	43	54	2	0

There are 6 discrepancies between the modelled and reference sequences:

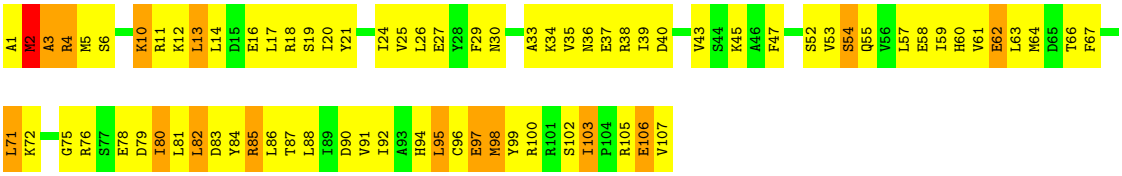
Chain	Residue	Modelled	Actual	Comment	Reference
C	401	ALA	-	CLONING ARTIFACT	UNP Q8RR33
C	402	MET	-	CLONING ARTIFACT	UNP Q8RR33
C	403	ALA	-	CLONING ARTIFACT	UNP Q8RR33
D	501	ALA	-	CLONING ARTIFACT	UNP Q8RR33
D	502	MET	-	CLONING ARTIFACT	UNP Q8RR33
D	503	ALA	-	CLONING ARTIFACT	UNP Q8RR33

4 Residue-property plots (i)

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.

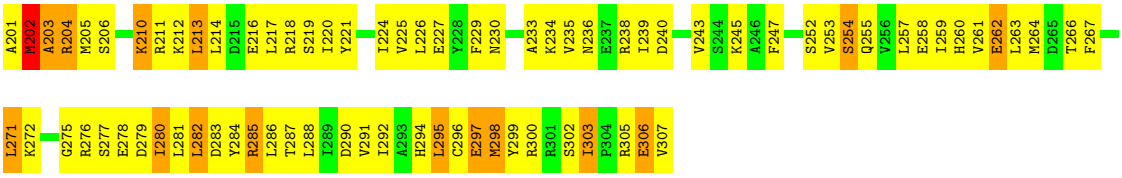
• Molecule 1: circadian clock protein KaiA

Chain A: 27% 58% 14%



• Molecule 1: circadian clock protein KaiA

Chain B: 27% 58% 14%



• Molecule 2: circadian clock protein KaiC

Chain C: 38% 41% 18%

• Molecule 2: circadian clock protein KaiC

Chain D: 38% 41% 18%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Distance geometry, Simulated annealing.*

Of the ? calculated structures, 1 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
XPLOR-NIH	structure solution	2.9.1
XPLOR-NIH	refinement	2.9.1

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	883	905	902	226
1	B	883	905	899	225
2	C	251	259	256	135
2	D	251	259	256	134
All	All	2268	2328	2313	581

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 127.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:85:ARG:NH2	1:B:285:ARG:NH2	1.43	1.63
2:D:524:ILE:O	2:D:526:LYS:N	1.32	1.62
2:D:508:GLY:O	2:D:509:THR:CG2	1.31	1.76
2:C:424:ILE:O	2:C:426:LYS:N	1.30	1.62
1:A:2:MET:O	1:A:2:MET:HE2	1.30	1.22
2:C:408:GLY:O	2:C:409:THR:CG2	1.30	1.76
1:A:106:GLU:O	1:A:107:VAL:HG12	1.28	1.28
1:B:306:GLU:O	1:B:307:VAL:HG12	1.24	1.28
1:B:202:MET:HE2	1:B:202:MET:O	1.23	1.31
2:C:408:GLY:O	2:C:409:THR:HG23	1.21	0.98
2:D:508:GLY:O	2:D:509:THR:HG23	1.20	0.98
2:D:508:GLY:C	2:D:509:THR:HG23	1.16	1.61

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:106:GLU:O	1:A:107:VAL:CG1	1.14	1.95
1:B:202:MET:O	1:B:202:MET:CE	1.13	1.96
2:C:408:GLY:C	2:C:409:THR:HG23	1.12	1.61
1:B:306:GLU:O	1:B:307:VAL:CG1	1.12	1.95
1:A:2:MET:O	1:A:2:MET:CE	1.12	1.96
1:A:106:GLU:OE1	1:A:106:GLU:N	1.12	1.83
1:B:306:GLU:OE1	1:B:306:GLU:N	1.11	1.83
2:C:419:THR:O	2:C:420:GLU:O	1.11	1.68
2:C:434:GLU:N	2:C:434:GLU:OE1	1.11	1.81
2:D:534:GLU:N	2:D:534:GLU:OE1	1.11	1.81
2:D:519:THR:O	2:D:520:GLU:O	1.10	1.68
1:B:266:THR:HG21	2:C:406:ILE:HD12	1.08	1.25
1:B:267:PHE:CZ	2:C:406:ILE:CG2	1.08	2.37
1:B:306:GLU:OE1	1:B:306:GLU:CA	1.08	2.01
1:B:264:MET:SD	1:B:284:TYR:CD2	1.07	2.47
1:A:63:LEU:CD1	2:D:506:ILE:HD13	1.06	1.80
1:A:67:PHE:CZ	2:D:506:ILE:CG2	1.06	2.38
1:A:64:MET:SD	1:A:84:TYR:CD2	1.06	2.48
1:A:67:PHE:CE1	2:D:506:ILE:HG22	1.06	1.85
1:B:263:LEU:CD1	2:C:406:ILE:HD13	1.06	1.79
1:A:106:GLU:OE1	1:A:106:GLU:CA	1.05	2.01
1:B:267:PHE:CE1	2:C:406:ILE:HG22	1.05	1.84
1:B:204:ARG:HG3	1:B:204:ARG:HH11	1.05	1.10
1:B:202:MET:SD	1:B:205:MET:O	1.02	2.18
1:A:66:THR:HG21	2:D:506:ILE:HD12	1.02	1.24
2:C:434:GLU:H	2:C:434:GLU:CD	1.01	1.58
1:A:47:PHE:CD2	1:A:98:MET:SD	1.01	2.53
1:A:2:MET:SD	1:A:5:MET:O	1.01	2.18
1:A:82:LEU:CD1	2:D:519:THR:OG1	1.01	2.09
2:D:534:GLU:H	2:D:534:GLU:CD	1.01	1.58
1:A:29:PHE:HB3	2:D:512:ARG:NH1	1.00	1.71
1:B:247:PHE:CD2	1:B:298:MET:SD	1.00	2.53
1:B:263:LEU:HD12	2:C:406:ILE:HD13	1.00	1.28
1:B:229:PHE:HB3	2:C:412:ARG:NH1	0.99	1.71
1:B:282:LEU:CD1	2:C:419:THR:OG1	0.99	2.10
1:B:202:MET:HE2	1:B:205:MET:N	0.98	1.72
1:A:4:ARG:HG3	1:A:4:ARG:HH11	0.98	1.10
1:A:63:LEU:HD12	2:D:506:ILE:HD13	0.98	1.28
1:B:264:MET:SD	1:B:284:TYR:CG	0.98	2.57
2:C:401:ALA:O	2:C:402:MET:CG	0.98	2.11
2:D:501:ALA:O	2:D:502:MET:CG	0.97	2.11
1:A:97:GLU:HA	1:A:97:GLU:OE1	0.97	1.60

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:64:MET:SD	1:A:84:TYR:CG	0.96	2.57
1:B:297:GLU:CA	1:B:297:GLU:OE1	0.95	2.14
1:A:78:GLU:OE1	2:C:417:GLU:OE2	0.95	1.84
1:A:97:GLU:OE1	1:A:97:GLU:CA	0.95	2.14
2:C:401:ALA:O	2:C:402:MET:HG2	0.95	1.61
1:A:2:MET:CE	1:A:5:MET:N	0.94	2.30
1:B:278:GLU:OE1	2:D:517:GLU:OE2	0.94	1.84
1:B:210:LYS:HE3	2:D:532:GLU:OE1	0.94	1.62
1:B:202:MET:CE	1:B:205:MET:N	0.94	2.30
1:A:10:LYS:HE3	2:C:432:GLU:OE1	0.92	1.64
1:B:297:GLU:OE1	1:B:297:GLU:HA	0.91	1.60
2:D:501:ALA:O	2:D:502:MET:HG2	0.91	1.61
1:A:2:MET:SD	1:A:2:MET:N	0.91	2.44
1:B:306:GLU:C	1:B:307:VAL:HG12	0.91	1.85
1:B:202:MET:HE2	1:B:205:MET:H	0.91	1.23
1:A:106:GLU:C	1:A:107:VAL:HG12	0.91	1.85
1:B:272:LYS:HE3	2:D:517:GLU:OE1	0.90	1.66
1:B:257:LEU:HB3	2:D:522:ALA:HB1	0.90	1.41
1:A:63:LEU:CD1	2:D:506:ILE:CD1	0.90	2.50
1:A:72:LYS:HE3	2:C:417:GLU:OE1	0.90	1.66
1:B:263:LEU:CD1	2:C:406:ILE:CD1	0.90	2.49
2:C:418:LYS:O	2:C:419:THR:O	0.90	1.90
1:A:57:LEU:HB3	2:C:422:ALA:HB1	0.90	1.41
1:A:30:ASN:ND2	1:A:33:ALA:O	0.90	2.05
1:B:230:ASN:ND2	1:B:233:ALA:O	0.90	2.05
2:D:518:LYS:O	2:D:519:THR:O	0.90	1.90
1:A:2:MET:HE2	1:A:5:MET:N	0.89	1.83
1:B:202:MET:SD	1:B:202:MET:N	0.89	2.44
1:B:263:LEU:HD12	2:C:406:ILE:CD1	0.89	1.98
1:B:283:ASP:OD1	1:B:284:TYR:N	0.89	2.06
1:A:30:ASN:CB	1:A:33:ALA:HB3	0.89	1.98
1:A:30:ASN:HD22	1:A:33:ALA:N	0.89	1.66
1:B:230:ASN:HD22	1:B:233:ALA:N	0.89	1.66
2:C:420:GLU:OE1	2:C:420:GLU:N	0.88	2.06
1:A:82:LEU:HD13	2:D:519:THR:OG1	0.88	1.67
1:B:230:ASN:CB	1:B:233:ALA:HB3	0.88	1.98
1:A:83:ASP:OD1	1:A:84:TYR:N	0.88	2.06
2:D:520:GLU:OE1	2:D:520:GLU:N	0.88	2.07
1:B:282:LEU:HD13	2:C:419:THR:OG1	0.87	1.68
1:A:63:LEU:HD12	2:D:506:ILE:CD1	0.87	1.99
1:B:306:GLU:OE1	1:B:306:GLU:HA	0.86	1.69
1:B:230:ASN:ND2	1:B:233:ALA:N	0.86	2.23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:106:GLU:OE1	1:A:106:GLU:HA	0.86	1.69
1:B:298:MET:HG3	1:B:299:TYR:N	0.86	1.85
1:A:2:MET:HE2	1:A:5:MET:H	0.85	1.30
1:A:64:MET:SD	1:A:84:TYR:CB	0.85	2.65
1:B:264:MET:SD	1:B:284:TYR:CB	0.85	2.65
1:A:30:ASN:ND2	1:A:33:ALA:N	0.85	2.23
1:A:14:LEU:HD22	1:A:55:GLN:OE1	0.85	1.71
1:A:98:MET:HG3	1:A:99:TYR:N	0.84	1.85
1:A:100:ARG:HH22	2:D:531:LEU:CD2	0.84	1.85
1:B:254:SER:OG	2:D:529:GLN:HB2	0.84	1.72
1:A:4:ARG:HG3	1:A:4:ARG:NH1	0.84	1.77
2:D:509:THR:N	2:D:510:PRO:CD	0.84	2.40
1:B:214:LEU:HD22	1:B:255:GLN:OE1	0.84	1.71
2:C:409:THR:N	2:C:410:PRO:CD	0.84	2.40
1:A:2:MET:O	1:A:4:ARG:N	0.83	2.11
1:B:202:MET:O	1:B:204:ARG:N	0.83	2.11
1:B:300:ARG:HH22	2:C:431:LEU:CD2	0.82	1.87
1:A:67:PHE:CE1	2:D:506:ILE:CG2	0.82	2.62
1:A:97:GLU:OE1	1:A:97:GLU:O	0.82	1.98
1:B:306:GLU:O	1:B:307:VAL:CB	0.82	2.27
2:C:409:THR:H	2:C:410:PRO:CD	0.82	1.88
1:A:54:SER:OG	2:C:429:GLN:HB2	0.81	1.73
1:A:106:GLU:O	1:A:107:VAL:CB	0.81	2.26
1:B:290:ASP:OD1	2:C:426:LYS:NZ	0.81	2.14
1:B:297:GLU:OE1	1:B:297:GLU:O	0.81	1.98
2:C:408:GLY:O	2:C:409:THR:CB	0.81	2.28
2:D:508:GLY:O	2:D:509:THR:CB	0.81	2.28
2:C:401:ALA:C	2:C:402:MET:HG2	0.80	1.96
1:B:262:GLU:OE1	1:B:262:GLU:HA	0.80	1.77
1:A:62:GLU:OE1	1:A:62:GLU:HA	0.80	1.77
1:A:82:LEU:HD12	2:D:519:THR:OG1	0.80	1.77
2:D:501:ALA:C	2:D:502:MET:HG2	0.79	1.97
2:D:509:THR:H	2:D:510:PRO:CD	0.79	1.88
1:B:204:ARG:HG3	1:B:204:ARG:NH1	0.79	1.76
1:B:210:LYS:CE	2:D:532:GLU:OE1	0.79	2.30
1:B:282:LEU:HD13	2:C:415:VAL:CG1	0.79	2.08
2:C:402:MET:O	2:C:403:ALA:CB	0.79	2.30
1:A:90:ASP:OD1	2:D:526:LYS:NZ	0.79	2.13
1:B:204:ARG:HH11	1:B:204:ARG:CG	0.78	1.91
1:A:86:LEU:HD21	2:D:521:LEU:CA	0.78	2.09
1:B:267:PHE:CE1	2:C:406:ILE:CG2	0.78	2.62
2:D:502:MET:O	2:D:503:ALA:CB	0.78	2.30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:10:LYS:CE	2:C:432:GLU:OE1	0.78	2.32
1:B:203:ALA:C	1:B:204:ARG:HG2	0.78	2.00
1:B:282:LEU:HD23	1:B:283:ASP:N	0.77	1.94
1:A:3:ALA:C	1:A:4:ARG:HG2	0.77	2.00
1:A:82:LEU:HD13	2:D:515:VAL:CG1	0.77	2.08
1:A:82:LEU:HD23	1:A:83:ASP:N	0.77	1.94
2:D:512:ARG:HG3	2:D:513:ILE:N	0.77	1.94
1:B:286:LEU:HD21	2:C:421:LEU:CA	0.77	2.10
1:B:282:LEU:HD12	2:C:419:THR:OG1	0.77	1.78
2:C:412:ARG:HG3	2:C:413:ILE:N	0.77	1.94
1:B:213:LEU:O	1:B:217:LEU:HG	0.77	1.80
1:A:13:LEU:O	1:A:17:LEU:HG	0.76	1.80
1:A:2:MET:CG	1:A:5:MET:O	0.76	2.34
1:A:14:LEU:CD2	1:A:55:GLN:OE1	0.76	2.33
1:A:4:ARG:HH11	1:A:4:ARG:CG	0.76	1.92
1:A:62:GLU:OE1	1:A:62:GLU:CA	0.76	2.34
1:B:287:THR:O	1:B:291:VAL:HG23	0.75	1.81
1:B:262:GLU:OE1	1:B:262:GLU:CA	0.75	2.34
1:A:64:MET:SD	1:A:84:TYR:HB3	0.75	2.21
1:A:3:ALA:O	1:A:4:ARG:HG2	0.74	1.82
1:B:279:ASP:HB3	2:C:415:VAL:CG2	0.74	2.12
1:B:202:MET:CG	1:B:205:MET:O	0.74	2.34
1:B:214:LEU:CD2	1:B:255:GLN:OE1	0.74	2.34
1:B:264:MET:SD	1:B:284:TYR:HB3	0.74	2.21
1:B:203:ALA:O	1:B:204:ARG:HG2	0.74	1.82
1:B:267:PHE:CZ	2:C:406:ILE:HG22	0.74	2.08
1:A:87:THR:O	1:A:91:VAL:HG23	0.73	1.81
1:A:79:ASP:HB3	2:D:515:VAL:CG2	0.73	2.13
1:B:247:PHE:CD2	1:B:299:TYR:CE1	0.73	2.77
2:C:409:THR:N	2:C:410:PRO:HD3	0.73	1.98
2:C:425:ALA:O	2:C:426:LYS:CB	0.73	2.37
1:A:82:LEU:HD13	2:D:515:VAL:HG11	0.72	1.61
2:D:509:THR:N	2:D:510:PRO:HD3	0.72	1.98
2:D:525:ALA:O	2:D:526:LYS:CB	0.72	2.37
1:A:47:PHE:CD2	1:A:99:TYR:CE1	0.72	2.77
1:B:267:PHE:CZ	2:C:406:ILE:HG21	0.72	2.19
1:A:30:ASN:CG	1:A:33:ALA:HB3	0.72	2.04
1:B:230:ASN:CG	1:B:233:ALA:HB3	0.72	2.04
1:B:282:LEU:HD13	2:C:415:VAL:HG11	0.72	1.60
1:B:258:GLU:OE2	2:D:525:ALA:HB2	0.72	1.84
1:A:58:GLU:OE2	2:C:425:ALA:HB2	0.71	1.85
2:D:518:LYS:O	2:D:518:LYS:CG	0.71	2.38

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:C:418:LYS:O	2:C:418:LYS:CG	0.71	2.38
2:D:508:GLY:C	2:D:509:THR:CG2	0.70	2.37
2:D:517:GLU:O	2:D:519:THR:N	0.70	2.25
1:A:67:PHE:CZ	2:D:506:ILE:HG21	0.70	2.20
2:C:417:GLU:O	2:C:419:THR:N	0.70	2.25
2:D:516:ASP:O	2:D:519:THR:HB	0.69	1.87
1:A:86:LEU:HD21	2:D:521:LEU:HA	0.69	1.64
1:B:239:ILE:O	1:B:243:VAL:HG23	0.69	1.88
1:B:267:PHE:CD2	1:B:284:TYR:CZ	0.69	2.81
2:C:416:ASP:O	2:C:419:THR:HB	0.69	1.87
2:C:408:GLY:C	2:C:409:THR:CG2	0.69	2.36
2:C:415:VAL:HB	2:C:419:THR:OG1	0.69	1.88
1:B:300:ARG:HH12	2:C:431:LEU:HD23	0.68	1.48
2:D:518:LYS:O	2:D:519:THR:C	0.68	2.31
1:A:67:PHE:CD2	1:A:84:TYR:CZ	0.68	2.81
1:A:39:ILE:O	1:A:43:VAL:HG23	0.68	1.88
2:D:505:ILE:HG22	2:D:505:ILE:O	0.68	1.89
2:D:515:VAL:HB	2:D:519:THR:OG1	0.68	1.88
1:A:100:ARG:HH12	2:D:531:LEU:HD23	0.68	1.48
2:C:418:LYS:O	2:C:419:THR:C	0.67	2.31
2:C:417:GLU:C	2:C:419:THR:H	0.67	1.93
1:B:282:LEU:HD23	1:B:283:ASP:H	0.66	1.51
1:B:286:LEU:CD2	2:C:421:LEU:O	0.66	2.44
1:A:97:GLU:OE1	1:A:97:GLU:C	0.66	2.33
1:B:297:GLU:OE1	1:B:297:GLU:C	0.66	2.33
2:C:405:ILE:HG22	2:C:405:ILE:O	0.66	1.89
1:A:88:LEU:C	1:A:88:LEU:HD13	0.66	2.11
2:C:409:THR:H	2:C:410:PRO:HD3	0.66	1.50
2:D:518:LYS:O	2:D:518:LYS:HG2	0.66	1.89
1:A:100:ARG:NH2	2:D:531:LEU:CD2	0.66	2.58
1:B:247:PHE:CG	1:B:298:MET:SD	0.66	2.88
1:B:288:LEU:C	1:B:288:LEU:HD13	0.66	2.11
2:D:517:GLU:C	2:D:519:THR:H	0.66	1.93
2:D:524:ILE:C	2:D:526:LYS:N	0.66	2.45
1:A:86:LEU:CD2	2:D:521:LEU:O	0.66	2.43
1:B:286:LEU:HD21	2:C:421:LEU:HA	0.66	1.65
1:A:82:LEU:HD23	1:A:83:ASP:H	0.66	1.51
1:A:47:PHE:CG	1:A:98:MET:SD	0.65	2.88
1:A:85:ARG:CZ	1:B:285:ARG:NH2	0.65	2.47
1:B:305:ARG:C	1:B:306:GLU:OE1	0.65	2.35
1:A:30:ASN:HD22	1:A:33:ALA:H	0.65	1.33
2:C:418:LYS:O	2:C:418:LYS:HG2	0.65	1.89

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:252:SER:OG	2:D:531:LEU:HD23	0.65	1.91
2:D:520:GLU:HG3	2:D:523:ARG:HE	0.64	1.51
2:D:523:ARG:HG2	2:D:524:ILE:N	0.64	2.06
1:B:230:ASN:HD22	1:B:233:ALA:H	0.64	1.33
2:D:519:THR:O	2:D:520:GLU:C	0.64	2.36
1:A:52:SER:OG	2:C:431:LEU:HD23	0.64	1.93
1:A:105:ARG:C	1:A:106:GLU:OE1	0.64	2.35
2:C:420:GLU:HG3	2:C:423:ARG:HE	0.64	1.52
1:A:100:ARG:NH2	2:D:531:LEU:HD21	0.64	2.07
1:B:260:HIS:CE1	1:B:288:LEU:HB2	0.63	2.28
2:C:423:ARG:HG2	2:C:424:ILE:N	0.63	2.06
1:A:3:ALA:C	1:A:4:ARG:CG	0.63	2.66
1:A:60:HIS:CE1	1:A:88:LEU:HB2	0.63	2.28
1:B:253:VAL:HG12	1:B:257:LEU:CG	0.63	2.24
1:B:203:ALA:C	1:B:204:ARG:CG	0.63	2.66
1:A:30:ASN:OD1	1:A:35:VAL:CG2	0.63	2.47
1:A:53:VAL:HG12	1:A:57:LEU:CG	0.62	2.24
1:A:63:LEU:HD11	2:D:506:ILE:HD13	0.62	1.67
1:B:300:ARG:NH2	2:C:431:LEU:HD21	0.62	2.09
2:C:401:ALA:O	2:C:402:MET:CE	0.62	2.47
1:A:43:VAL:HG21	1:A:94:HIS:ND1	0.62	2.09
1:B:230:ASN:OD1	1:B:235:VAL:CG2	0.62	2.47
1:B:243:VAL:HG21	1:B:294:HIS:ND1	0.62	2.10
1:B:202:MET:HG3	1:B:205:MET:O	0.62	1.91
2:D:501:ALA:O	2:D:502:MET:CE	0.62	2.47
1:B:300:ARG:NH2	2:C:431:LEU:CD2	0.62	2.61
1:B:300:ARG:HH12	2:C:431:LEU:CD2	0.62	2.06
2:D:520:GLU:H	2:D:520:GLU:CD	0.61	1.97
2:D:501:ALA:O	2:D:502:MET:SD	0.61	2.58
1:A:4:ARG:NH1	1:A:4:ARG:CG	0.61	2.54
2:D:534:GLU:N	2:D:534:GLU:CD	0.61	2.23
1:A:100:ARG:HH12	2:D:531:LEU:CD2	0.61	2.06
2:C:402:MET:O	2:C:403:ALA:HB3	0.61	1.96
2:D:516:ASP:O	2:D:517:GLU:O	0.61	2.19
1:A:85:ARG:NH2	1:B:285:ARG:CZ	0.61	2.48
1:A:106:GLU:C	1:A:107:VAL:CG1	0.61	2.58
1:B:210:LYS:HE3	2:D:532:GLU:CD	0.61	2.16
1:A:83:ASP:OD1	1:A:84:TYR:CD1	0.61	2.54
1:A:106:GLU:N	1:A:106:GLU:CD	0.61	2.54
1:B:306:GLU:N	1:B:306:GLU:CD	0.61	2.54
2:C:401:ALA:O	2:C:402:MET:SD	0.61	2.58
2:D:522:ALA:O	2:D:524:ILE:N	0.61	2.34

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:292:ILE:O	1:B:295:LEU:HD23	0.60	1.96
1:A:92:ILE:O	1:A:95:LEU:HD23	0.60	1.96
2:C:422:ALA:O	2:C:424:ILE:N	0.60	2.34
1:A:10:LYS:HE3	2:C:432:GLU:CD	0.60	2.17
1:A:2:MET:SD	1:A:5:MET:C	0.60	2.80
2:D:502:MET:O	2:D:503:ALA:HB3	0.60	1.95
1:B:283:ASP:OD1	1:B:284:TYR:CD1	0.60	2.54
2:C:413:ILE:HG23	2:C:415:VAL:HG13	0.60	1.74
2:D:509:THR:H	2:D:510:PRO:HD3	0.60	1.51
1:A:100:ARG:HH22	2:D:531:LEU:HD21	0.60	1.55
1:B:263:LEU:HD11	2:C:406:ILE:HD13	0.59	1.66
2:D:517:GLU:C	2:D:519:THR:N	0.59	2.55
1:A:4:ARG:N	1:A:4:ARG:HD2	0.59	2.12
2:C:416:ASP:O	2:C:417:GLU:O	0.59	2.19
2:D:513:ILE:HG23	2:D:515:VAL:HG13	0.59	1.74
1:B:292:ILE:HA	1:B:295:LEU:CD2	0.59	2.28
2:D:512:ARG:HG3	2:D:513:ILE:H	0.59	1.58
1:A:58:GLU:OE1	2:C:429:GLN:OE1	0.59	2.21
1:B:204:ARG:N	1:B:204:ARG:HD2	0.59	2.12
2:C:419:THR:O	2:C:420:GLU:C	0.59	2.36
1:B:202:MET:SD	1:B:205:MET:C	0.59	2.80
1:A:67:PHE:CG	1:A:84:TYR:OH	0.58	2.56
1:B:300:ARG:HH22	2:C:431:LEU:HD21	0.58	1.58
1:A:67:PHE:CZ	2:D:506:ILE:HG22	0.58	2.09
1:A:85:ARG:CG	1:A:85:ARG:HH11	0.58	2.12
1:A:92:ILE:HA	1:A:95:LEU:CD2	0.58	2.28
1:B:267:PHE:CG	1:B:284:TYR:OH	0.58	2.55
1:B:285:ARG:CG	1:B:285:ARG:HH11	0.58	2.11
1:B:258:GLU:OE1	2:D:529:GLN:OE1	0.58	2.21
2:C:412:ARG:HG3	2:C:413:ILE:H	0.58	1.58
2:D:526:LYS:HG2	2:D:528:MET:CE	0.58	2.29
1:A:30:ASN:HB2	1:A:33:ALA:HB3	0.58	1.76
1:A:78:GLU:OE1	2:C:417:GLU:CG	0.57	2.52
2:C:420:GLU:H	2:C:420:GLU:CD	0.57	1.97
1:B:253:VAL:HG12	1:B:257:LEU:CD1	0.57	2.29
1:B:278:GLU:OE1	2:D:517:GLU:CG	0.57	2.52
2:C:401:ALA:O	2:C:402:MET:CB	0.57	2.52
1:A:16:GLU:O	1:A:20:ILE:HG13	0.57	2.00
1:A:53:VAL:HG12	1:A:57:LEU:CD1	0.57	2.29
1:B:247:PHE:CE2	1:B:299:TYR:CD1	0.57	2.93
2:D:501:ALA:O	2:D:502:MET:CB	0.57	2.52
1:B:216:GLU:O	1:B:220:ILE:HG13	0.57	2.00

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:221:TYR:HA	1:B:224:ILE:HD12	0.57	1.76
2:C:426:LYS:HG2	2:C:428:MET:CE	0.56	2.29
1:A:2:MET:HG3	1:A:5:MET:O	0.56	1.91
1:B:272:LYS:CE	2:D:517:GLU:OE1	0.56	2.49
1:A:47:PHE:CE2	1:A:99:TYR:CD1	0.56	2.93
1:A:57:LEU:CB	2:C:422:ALA:HB1	0.56	2.26
1:B:285:ARG:NH1	1:B:285:ARG:HG3	0.56	2.16
1:B:229:PHE:CB	2:C:412:ARG:NH1	0.56	2.61
2:C:424:ILE:C	2:C:426:LYS:N	0.56	2.45
1:B:282:LEU:CD1	2:C:415:VAL:HG11	0.56	2.31
1:A:21:TYR:HA	1:A:24:ILE:HD12	0.56	1.77
1:B:204:ARG:N	1:B:204:ARG:CD	0.56	2.68
1:B:211:ARG:HD2	1:B:211:ARG:O	0.56	2.01
2:C:428:MET:O	2:C:430:ASP:N	0.55	2.35
1:A:11:ARG:HD2	1:A:11:ARG:O	0.55	2.01
1:A:30:ASN:ND2	1:A:33:ALA:CA	0.55	2.69
2:C:417:GLU:C	2:C:419:THR:N	0.55	2.55
1:B:287:THR:O	1:B:291:VAL:CG2	0.55	2.53
1:A:39:ILE:HG22	1:A:94:HIS:ND1	0.55	2.16
1:B:204:ARG:NH1	1:B:204:ARG:CG	0.55	2.54
2:D:528:MET:O	2:D:530:ASP:N	0.55	2.35
1:B:267:PHE:CD2	1:B:284:TYR:CE2	0.55	2.94
1:A:67:PHE:CD2	1:A:84:TYR:CE2	0.55	2.94
1:B:278:GLU:OE1	2:D:517:GLU:CD	0.55	2.45
2:D:517:GLU:O	2:D:519:THR:HG22	0.55	2.02
1:B:230:ASN:ND2	1:B:233:ALA:CA	0.55	2.69
1:B:230:ASN:HB2	1:B:233:ALA:HB3	0.55	1.76
2:C:417:GLU:O	2:C:419:THR:HG22	0.55	2.02
1:A:82:LEU:CD1	2:D:515:VAL:HG11	0.55	2.31
1:A:4:ARG:N	1:A:4:ARG:CD	0.54	2.68
1:A:85:ARG:NH1	1:A:85:ARG:HG3	0.54	2.15
2:D:533:SER:HA	2:D:534:GLU:OE1	0.54	2.02
1:A:20:ILE:CD1	1:A:45:LYS:CE	0.54	2.86
1:B:224:ILE:HG12	1:B:238:ARG:CB	0.54	2.33
1:B:239:ILE:HG22	1:B:294:HIS:ND1	0.54	2.16
1:A:53:VAL:O	1:A:57:LEU:HG	0.54	2.03
1:B:253:VAL:O	1:B:257:LEU:HG	0.54	2.03
1:B:254:SER:OG	2:D:529:GLN:CB	0.54	2.52
1:A:53:VAL:HG12	1:A:57:LEU:HD11	0.54	1.78
1:A:86:LEU:CD2	2:D:521:LEU:HA	0.54	2.31
1:A:71:LEU:CD1	1:A:71:LEU:N	0.54	2.71
1:B:202:MET:HE2	1:B:204:ARG:N	0.54	2.18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:54:SER:OG	1:A:55:GLN:N	0.54	2.41
1:B:280:ILE:HD13	2:C:410:PRO:HA	0.54	1.80
1:A:24:ILE:HG12	1:A:38:ARG:CB	0.53	2.33
1:A:82:LEU:CD2	1:A:83:ASP:N	0.53	2.71
1:B:282:LEU:CD1	2:C:415:VAL:CG1	0.53	2.85
1:B:253:VAL:HG12	1:B:257:LEU:HD11	0.53	1.78
1:B:286:LEU:CD2	2:C:421:LEU:HA	0.53	2.33
1:A:54:SER:OG	2:C:429:GLN:CB	0.53	2.53
1:B:253:VAL:HG12	1:B:257:LEU:HG	0.53	1.80
1:A:80:ILE:HD13	2:D:510:PRO:HA	0.53	1.81
1:B:271:LEU:CD1	1:B:271:LEU:N	0.53	2.71
1:A:2:MET:HE2	1:A:4:ARG:N	0.53	2.17
1:A:87:THR:O	1:A:91:VAL:CG2	0.53	2.53
1:A:95:LEU:O	1:A:98:MET:CG	0.53	2.57
1:B:220:ILE:CD1	1:B:245:LYS:CE	0.53	2.86
2:C:433:SER:HA	2:C:434:GLU:OE1	0.53	2.02
2:D:519:THR:C	2:D:520:GLU:O	0.53	2.46
1:B:266:THR:CG2	2:C:406:ILE:HD12	0.53	2.18
1:B:306:GLU:C	1:B:307:VAL:CG1	0.53	2.58
1:B:227:GLU:O	1:B:230:ASN:OD1	0.53	2.27
1:B:254:SER:OG	1:B:255:GLN:N	0.53	2.41
1:A:57:LEU:HB3	2:C:422:ALA:CB	0.52	2.26
1:A:82:LEU:HD22	2:D:515:VAL:HG11	0.52	1.80
1:B:227:GLU:CD	1:B:238:ARG:HE	0.52	2.08
1:B:282:LEU:CD2	1:B:283:ASP:N	0.52	2.71
1:A:63:LEU:HD11	2:D:506:ILE:CD1	0.52	2.32
1:B:295:LEU:HG	1:B:296:CYS:N	0.52	2.16
1:A:2:MET:O	1:A:3:ALA:C	0.52	2.47
1:B:295:LEU:O	1:B:298:MET:CG	0.52	2.57
1:A:60:HIS:ND1	1:A:88:LEU:HB2	0.52	2.19
1:A:72:LYS:CE	2:C:417:GLU:OE1	0.52	2.49
1:A:80:ILE:CD1	2:D:512:ARG:HG2	0.52	2.35
1:A:78:GLU:OE1	2:C:417:GLU:CD	0.52	2.45
1:B:280:ILE:CD1	2:C:412:ARG:HG2	0.52	2.35
1:A:57:LEU:O	2:C:422:ALA:HB3	0.52	2.03
1:A:82:LEU:CD1	2:D:515:VAL:CG1	0.52	2.85
1:B:202:MET:CE	1:B:204:ARG:C	0.52	2.78
1:B:260:HIS:ND1	1:B:288:LEU:HB2	0.52	2.19
1:A:86:LEU:CD2	2:D:521:LEU:CA	0.52	2.85
1:B:285:ARG:CG	1:B:285:ARG:NH1	0.52	2.70
1:B:257:LEU:O	2:D:522:ALA:HB3	0.52	2.03
1:A:53:VAL:HG12	1:A:57:LEU:HG	0.51	1.80

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:95:LEU:HG	1:A:96:CYS:N	0.51	2.16
1:A:39:ILE:O	1:A:43:VAL:CG2	0.51	2.59
1:B:257:LEU:HB3	2:D:522:ALA:CB	0.51	2.26
1:B:286:LEU:CD2	2:C:421:LEU:CA	0.51	2.87
1:A:2:MET:CE	1:A:4:ARG:C	0.51	2.78
1:A:27:GLU:CD	1:A:38:ARG:HE	0.51	2.07
1:A:100:ARG:NH1	2:D:531:LEU:CD2	0.51	2.74
1:A:27:GLU:O	1:A:30:ASN:OD1	0.51	2.27
1:B:254:SER:HA	1:B:257:LEU:HD12	0.51	1.82
1:B:263:LEU:HD11	2:C:406:ILE:CD1	0.51	2.31
1:B:276:ARG:HB3	2:C:411:THR:OG1	0.51	2.06
2:C:420:GLU:N	2:C:420:GLU:CD	0.51	2.63
1:B:280:ILE:HD12	2:C:412:ARG:HG2	0.51	1.82
1:B:282:LEU:HD22	2:C:415:VAL:HG11	0.51	1.81
1:B:230:ASN:CG	1:B:233:ALA:O	0.50	2.49
1:A:29:PHE:CB	2:D:512:ARG:NH1	0.50	2.61
1:A:54:SER:HA	1:A:57:LEU:HD12	0.50	1.82
1:A:76:ARG:HB3	2:D:511:THR:OG1	0.50	2.06
1:B:236:ASN:C	1:B:236:ASN:OD1	0.50	2.50
1:A:30:ASN:CG	1:A:33:ALA:O	0.50	2.49
1:A:66:THR:CG2	2:D:506:ILE:HD12	0.50	2.17
2:D:526:LYS:HG2	2:D:528:MET:HE3	0.50	1.83
1:A:29:PHE:HB3	2:D:512:ARG:HH11	0.50	1.62
1:B:202:MET:O	1:B:203:ALA:C	0.50	2.47
1:B:255:GLN:O	1:B:259:ILE:N	0.50	2.38
1:B:201:ALA:O	1:B:202:MET:C	0.49	2.51
1:B:283:ASP:OD2	1:B:284:TYR:CE1	0.49	2.65
1:A:83:ASP:OD2	1:A:84:TYR:CE1	0.49	2.65
2:C:432:GLU:O	2:C:433:SER:O	0.49	2.30
1:A:80:ILE:HD12	2:D:512:ARG:HG2	0.49	1.82
1:B:239:ILE:O	1:B:243:VAL:CG2	0.49	2.59
2:C:405:ILE:O	2:C:405:ILE:CG2	0.49	2.60
1:A:2:MET:HE3	1:A:5:MET:N	0.49	2.19
1:B:290:ASP:OD1	1:B:290:ASP:C	0.49	2.51
1:B:300:ARG:NH1	2:C:431:LEU:CD2	0.49	2.75
1:A:106:GLU:O	1:A:107:VAL:HB	0.49	2.05
1:A:36:ASN:C	1:A:36:ASN:OD1	0.49	2.50
1:A:99:TYR:O	1:A:103:ILE:CG1	0.49	2.61
2:C:422:ALA:C	2:C:424:ILE:N	0.49	2.67
1:A:30:ASN:ND2	1:A:33:ALA:C	0.48	2.66
2:C:416:ASP:O	2:C:419:THR:CB	0.48	2.60
2:D:520:GLU:N	2:D:520:GLU:CD	0.48	2.63

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:2:MET:CE	1:A:5:MET:H	0.48	2.00
1:B:230:ASN:ND2	1:B:233:ALA:C	0.48	2.66
1:A:1:ALA:O	1:A:2:MET:C	0.48	2.51
1:A:67:PHE:CG	1:A:84:TYR:CZ	0.48	3.02
1:B:257:LEU:CB	2:D:522:ALA:HB1	0.48	2.26
2:D:522:ALA:C	2:D:524:ILE:N	0.48	2.67
2:D:532:GLU:O	2:D:533:SER:O	0.48	2.30
1:B:267:PHE:CG	1:B:284:TYR:CZ	0.48	3.02
2:D:503:ALA:O	2:D:505:ILE:N	0.48	2.47
2:D:525:ALA:O	2:D:526:LYS:HB3	0.48	2.09
1:B:299:TYR:O	1:B:303:ILE:CG1	0.47	2.61
2:D:516:ASP:O	2:D:519:THR:CB	0.47	2.60
1:A:25:VAL:HG11	1:A:84:TYR:CE1	0.47	2.44
1:A:26:LEU:HD23	2:D:508:GLY:HA2	0.47	1.85
1:A:67:PHE:O	1:A:71:LEU:HD13	0.47	2.10
2:C:434:GLU:N	2:C:434:GLU:CD	0.47	2.23
1:A:25:VAL:CG1	1:A:84:TYR:CE1	0.47	2.98
1:B:306:GLU:O	1:B:307:VAL:HB	0.47	2.05
1:B:226:LEU:HD23	2:C:408:GLY:HA2	0.47	1.85
1:B:267:PHE:O	1:B:271:LEU:HD13	0.47	2.10
1:A:67:PHE:CD1	1:A:84:TYR:OH	0.47	2.64
1:B:254:SER:O	1:B:258:GLU:HG3	0.47	2.10
2:C:403:ALA:O	2:C:405:ILE:N	0.47	2.47
2:D:520:GLU:HG3	2:D:523:ARG:NE	0.47	2.24
1:A:90:ASP:OD1	1:A:90:ASP:C	0.47	2.51
1:A:47:PHE:CE2	1:A:99:TYR:CE1	0.47	3.03
1:A:66:THR:HG21	2:D:506:ILE:CD1	0.47	2.17
1:A:30:ASN:HB2	1:A:33:ALA:CB	0.47	2.40
1:B:271:LEU:HD23	1:B:278:GLU:HA	0.47	1.87
1:B:247:PHE:CE2	1:B:299:TYR:CE1	0.46	3.03
1:A:53:VAL:O	1:A:57:LEU:CG	0.46	2.64
1:B:225:VAL:HG11	1:B:284:TYR:CE1	0.46	2.45
2:D:508:GLY:O	2:D:509:THR:OG1	0.46	2.32
1:B:202:MET:CE	1:B:205:MET:H	0.46	2.00
1:A:55:GLN:O	1:A:59:ILE:N	0.46	2.38
2:C:416:ASP:O	2:C:417:GLU:C	0.46	2.53
1:A:54:SER:O	1:A:58:GLU:HG3	0.46	2.10
1:A:80:ILE:HG13	1:A:80:ILE:O	0.46	2.09
1:B:225:VAL:CG1	1:B:284:TYR:CE1	0.46	2.98
1:B:253:VAL:CG1	1:B:257:LEU:HD11	0.46	2.40
2:C:408:GLY:O	2:C:409:THR:OG1	0.46	2.32
1:B:271:LEU:N	1:B:271:LEU:HD13	0.46	2.26

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:280:ILE:HG13	1:B:280:ILE:O	0.46	2.09
1:A:20:ILE:CD1	1:A:45:LYS:HE3	0.46	2.41
1:A:57:LEU:O	1:A:61:VAL:HG23	0.46	2.10
1:A:71:LEU:N	1:A:71:LEU:HD13	0.46	2.26
1:B:257:LEU:O	1:B:261:VAL:HG23	0.46	2.10
1:B:253:VAL:O	1:B:257:LEU:CG	0.45	2.64
2:D:502:MET:O	2:D:503:ALA:HB2	0.45	2.10
1:A:53:VAL:CG1	1:A:57:LEU:HD11	0.45	2.40
1:A:71:LEU:HD23	1:A:78:GLU:HA	0.45	1.87
1:B:220:ILE:CD1	1:B:245:LYS:HE3	0.45	2.41
1:A:24:ILE:CG1	1:A:38:ARG:HB3	0.45	2.42
1:B:224:ILE:CG1	1:B:238:ARG:HB3	0.45	2.42
2:D:509:THR:H	2:D:510:PRO:HD2	0.45	1.68
1:B:202:MET:HE2	1:B:204:ARG:C	0.45	2.29
1:B:230:ASN:HB2	1:B:233:ALA:CB	0.45	2.40
1:B:266:THR:HG21	2:C:406:ILE:CD1	0.45	2.18
2:C:425:ALA:O	2:C:426:LYS:HB2	0.45	2.10
2:D:516:ASP:O	2:D:517:GLU:C	0.45	2.53
1:A:86:LEU:HD21	2:D:521:LEU:N	0.45	2.27
1:B:202:MET:HE2	1:B:204:ARG:CA	0.45	2.42
1:B:295:LEU:O	1:B:298:MET:HG2	0.45	2.12
2:C:402:MET:O	2:C:403:ALA:HB2	0.45	2.10
1:B:278:GLU:O	1:B:281:LEU:HB2	0.44	2.12
1:A:47:PHE:CD2	1:A:99:TYR:CD1	0.44	3.05
1:B:284:TYR:O	1:B:288:LEU:N	0.44	2.43
1:B:247:PHE:CD2	1:B:299:TYR:CD1	0.44	3.05
1:A:71:LEU:O	1:A:75:GLY:N	0.44	2.51
2:C:425:ALA:O	2:C:426:LYS:HB3	0.44	2.09
1:A:86:LEU:O	1:A:90:ASP:CB	0.44	2.66
1:B:229:PHE:HB3	2:C:412:ARG:HH11	0.44	1.63
2:D:525:ALA:O	2:D:526:LYS:HB2	0.44	2.10
1:A:78:GLU:O	1:A:81:LEU:HB2	0.43	2.12
1:B:286:LEU:HD21	2:C:421:LEU:N	0.43	2.28
1:B:229:PHE:CE2	1:B:283:ASP:CB	0.43	3.01
1:B:236:ASN:O	1:B:240:ASP:N	0.43	2.42
2:C:420:GLU:HG3	2:C:423:ARG:NE	0.43	2.24
1:A:36:ASN:O	1:A:40:ASP:N	0.43	2.42
1:A:54:SER:CA	1:A:57:LEU:HD12	0.43	2.44
1:B:271:LEU:O	1:B:275:GLY:N	0.43	2.51
1:A:84:TYR:O	1:A:88:LEU:N	0.43	2.42
1:A:100:ARG:O	1:A:103:ILE:HG13	0.43	2.14
2:C:426:LYS:HG2	2:C:428:MET:HE3	0.43	1.89

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:29:PHE:CE2	1:A:83:ASP:CB	0.43	3.01
1:B:286:LEU:O	1:B:290:ASP:CB	0.43	2.66
1:A:67:PHE:CE1	2:D:507:SER:O	0.43	2.72
1:A:95:LEU:O	1:A:98:MET:HG2	0.43	2.12
1:B:254:SER:CA	1:B:257:LEU:HD12	0.43	2.44
1:B:267:PHE:CE1	2:C:407:SER:O	0.43	2.72
1:A:2:MET:HE3	1:A:4:ARG:C	0.43	2.33
1:A:86:LEU:CD2	2:D:521:LEU:C	0.43	2.88
1:B:288:LEU:O	1:B:288:LEU:HD22	0.43	2.13
1:B:299:TYR:O	1:B:303:ILE:HG12	0.42	2.14
1:B:283:ASP:OD1	1:B:284:TYR:CG	0.42	2.72
1:B:288:LEU:C	1:B:288:LEU:CD1	0.42	2.83
2:C:409:THR:H	2:C:410:PRO:HD2	0.42	1.68
1:A:2:MET:CE	1:A:4:ARG:CA	0.42	2.97
1:A:88:LEU:O	1:A:88:LEU:HD22	0.42	2.13
1:B:202:MET:CE	1:B:204:ARG:CA	0.42	2.97
1:B:258:GLU:CD	2:D:525:ALA:HB2	0.42	2.35
2:C:433:SER:CA	2:C:434:GLU:OE1	0.42	2.68
1:A:36:ASN:OD1	1:A:36:ASN:O	0.42	2.38
1:A:55:GLN:O	1:A:59:ILE:HG13	0.42	2.15
1:B:300:ARG:O	1:B:303:ILE:HG13	0.42	2.14
1:A:34:LYS:O	1:A:37:GLU:N	0.42	2.48
1:A:47:PHE:CB	1:A:98:MET:SD	0.42	3.08
1:B:229:PHE:HB3	2:C:412:ARG:HH12	0.42	1.66
1:B:234:LYS:O	1:B:236:ASN:N	0.42	2.53
1:B:253:VAL:C	1:B:257:LEU:HD12	0.42	2.34
1:B:255:GLN:O	1:B:259:ILE:HG13	0.42	2.15
2:D:515:VAL:HB	2:D:519:THR:CB	0.42	2.44
2:D:522:ALA:O	2:D:523:ARG:C	0.42	2.58
1:A:83:ASP:OD1	1:A:84:TYR:CG	0.42	2.73
1:B:234:LYS:O	1:B:235:VAL:C	0.42	2.59
1:A:34:LYS:O	1:A:36:ASN:N	0.41	2.53
1:A:58:GLU:CD	2:C:425:ALA:HB2	0.41	2.36
1:A:99:TYR:O	1:A:103:ILE:HG12	0.41	2.14
1:B:253:VAL:O	1:B:257:LEU:CD1	0.41	2.68
2:C:422:ALA:O	2:C:423:ARG:C	0.41	2.58
1:A:34:LYS:O	1:A:35:VAL:C	0.41	2.59
1:A:53:VAL:C	1:A:57:LEU:HD12	0.41	2.35
1:B:236:ASN:OD1	1:B:236:ASN:O	0.41	2.38
1:B:247:PHE:CB	1:B:298:MET:SD	0.41	3.08
1:B:282:LEU:CD2	2:C:415:VAL:HG11	0.41	2.45
2:C:415:VAL:HB	2:C:419:THR:CB	0.41	2.44

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:262:GLU:OE1	1:B:262:GLU:N	0.41	2.54
2:C:429:GLN:HG2	2:C:429:GLN:O	0.41	2.16
2:D:533:SER:CA	2:D:534:GLU:OE1	0.41	2.68
1:A:2:MET:HE2	1:A:4:ARG:CA	0.41	2.46
1:A:26:LEU:CD2	2:D:508:GLY:HA2	0.41	2.46
1:A:29:PHE:CE2	1:A:83:ASP:HB3	0.41	2.51
1:A:34:LYS:C	1:A:36:ASN:N	0.41	2.74
1:A:53:VAL:O	1:A:57:LEU:CD1	0.41	2.68
1:A:82:LEU:CD2	2:D:515:VAL:HG11	0.41	2.45
1:B:214:LEU:O	1:B:218:ARG:HB2	0.41	2.16
2:D:529:GLN:HG2	2:D:529:GLN:O	0.41	2.16
1:A:100:ARG:CZ	2:D:531:LEU:HD21	0.41	2.46
1:B:286:LEU:CD2	2:C:421:LEU:C	0.41	2.89
1:B:226:LEU:CD2	2:C:408:GLY:HA2	0.40	2.47
1:A:14:LEU:O	1:A:18:ARG:HB2	0.40	2.16
1:B:224:ILE:HG12	1:B:238:ARG:HB3	0.40	1.91
1:B:290:ASP:OD1	1:B:290:ASP:O	0.40	2.39
1:A:30:ASN:CB	1:A:33:ALA:CB	0.40	2.86
2:C:419:THR:C	2:C:420:GLU:O	0.40	2.46
1:A:47:PHE:HB2	1:A:98:MET:SD	0.40	2.56
1:A:90:ASP:OD1	1:A:90:ASP:O	0.40	2.39
1:B:247:PHE:HB2	1:B:298:MET:SD	0.40	2.56
1:B:276:ARG:O	1:B:277:SER:C	0.40	2.59

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	105/107 (98%)	97 (92%)	6 (6%)	2 (2%)	11	53
1	B	105/107 (98%)	97 (92%)	6 (6%)	2 (2%)	11	53
2	C	32/34 (94%)	11 (34%)	4 (12%)	17 (53%)	0	0
2	D	32/34 (94%)	11 (34%)	4 (12%)	17 (53%)	0	0
All	All	274/282 (97%)	216 (79%)	20 (7%)	38 (14%)	1	5

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

Mol	Chain	Res	Type
1	A	2	MET
1	A	3	ALA
1	B	202	MET
1	B	203	ALA
2	C	402	MET
2	C	403	ALA
2	C	404	GLY
2	C	409	THR
2	C	410	PRO
2	C	417	GLU
2	C	418	LYS
2	C	419	THR
2	C	420	GLU
2	C	421	LEU
2	C	423	ARG
2	C	425	ALA
2	C	426	LYS
2	C	429	GLN
2	C	431	LEU
2	C	432	GLU
2	C	433	SER
2	D	502	MET
2	D	503	ALA
2	D	504	GLY
2	D	509	THR
2	D	510	PRO
2	D	517	GLU
2	D	518	LYS
2	D	519	THR
2	D	520	GLU
2	D	521	LEU
2	D	523	ARG
2	D	525	ALA
2	D	526	LYS
2	D	529	GLN
2	D	531	LEU
2	D	532	GLU
2	D	533	SER

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	99/99 (100%)	80 (81%)	19 (19%)	4	35
1	B	99/99 (100%)	80 (81%)	19 (19%)	4	35
2	C	27/27 (100%)	16 (59%)	11 (41%)	0	4
2	D	27/27 (100%)	16 (59%)	11 (41%)	0	4
All	All	252/252 (100%)	192 (76%)	60 (24%)	2	27

All 60 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	2	MET
1	A	4	ARG
1	A	6	SER
1	A	10	LYS
1	A	12	LYS
1	A	13	LEU
1	A	19	SER
1	A	54	SER
1	A	62	GLU
1	A	71	LEU
1	A	80	ILE
1	A	82	LEU
1	A	85	ARG
1	A	95	LEU
1	A	97	GLU
1	A	98	MET
1	A	102	SER
1	A	103	ILE
1	A	106	GLU
1	B	202	MET
1	B	204	ARG
1	B	206	SER
1	B	210	LYS
1	B	212	LYS
1	B	213	LEU

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Mol	Chain	Res	Type
1	B	219	SER
1	B	254	SER
1	B	262	GLU
1	B	271	LEU
1	B	280	ILE
1	B	282	LEU
1	B	285	ARG
1	B	295	LEU
1	B	297	GLU
1	B	298	MET
1	B	302	SER
1	B	303	ILE
1	B	306	GLU
2	C	402	MET
2	C	405	ILE
2	C	411	THR
2	C	412	ARG
2	C	414	SER
2	C	421	LEU
2	C	423	ARG
2	C	431	LEU
2	C	432	GLU
2	C	433	SER
2	C	434	GLU
2	D	502	MET
2	D	505	ILE
2	D	511	THR
2	D	512	ARG
2	D	514	SER
2	D	521	LEU
2	D	523	ARG
2	D	531	LEU
2	D	532	GLU
2	D	533	SER
2	D	534	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