Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 01:27 PM EST

PDB ID	:	2FM4
Title	:	NMR structure of the phosphoryl carrier domain of pyruvate phosphate dikinase
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Deposited on	:	2006-01-06

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

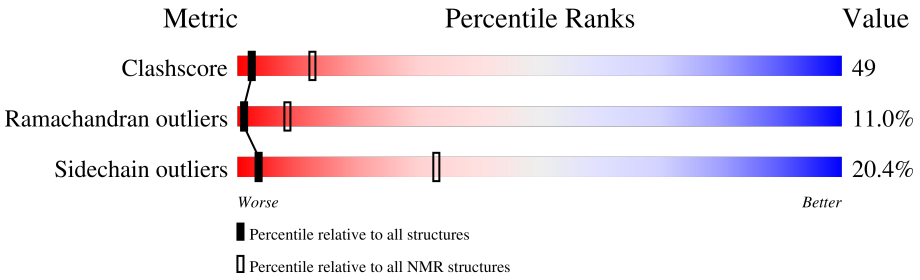
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	128	25% 55% 12% • 7%

2 Ensemble composition and analysis (i)

This entry contains 11 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:390-A:508 (119)	0.48	5

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 5, 6, 7, 10
2	2, 3, 8, 9
Single-model clusters	11

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1818 atoms, of which 902 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Pyruvate, phosphate dikinase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	128	1818	567	902	157	186	6	0

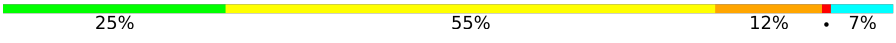
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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: Pyruvate, phosphate dikinase

Chain A:



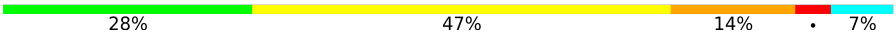
4.2 Scores per residue for each member of the ensemble

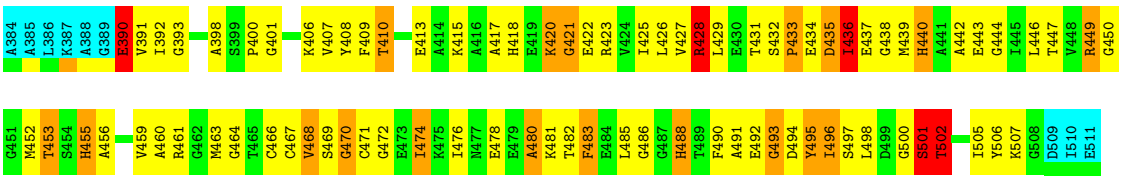
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Pyruvate, phosphate dikinase

Chain A:

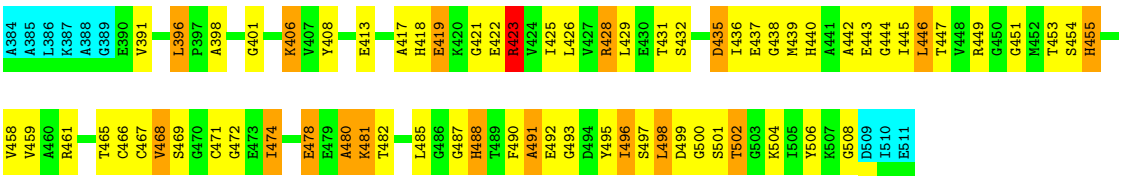




4.2.2 Score per residue for model 2

• Molecule 1: Pyruvate, phosphate dikinase

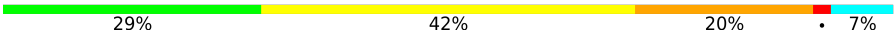
Chain A:

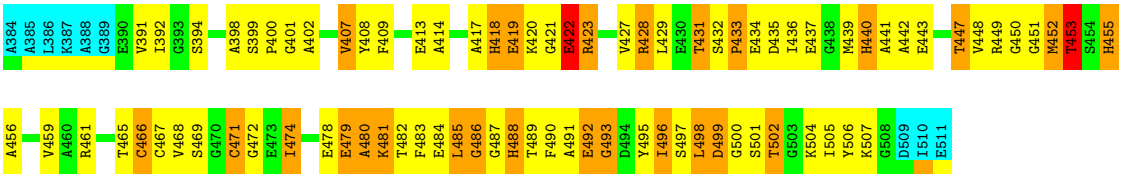


4.2.3 Score per residue for model 3

• Molecule 1: Pyruvate, phosphate dikinase

Chain A:

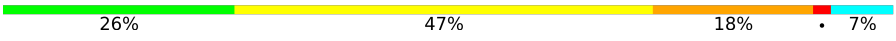


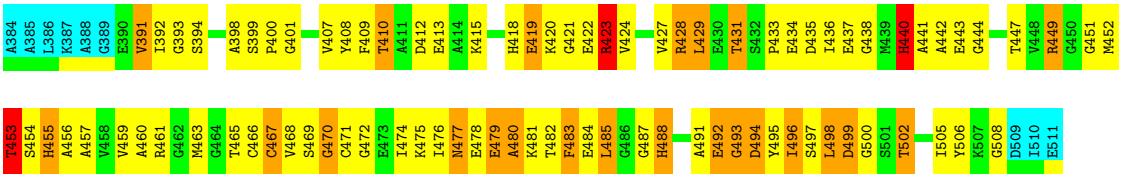


4.2.4 Score per residue for model 4

• Molecule 1: Pyruvate, phosphate dikinase

Chain A:

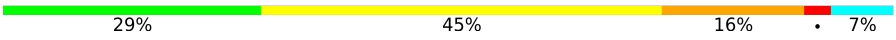


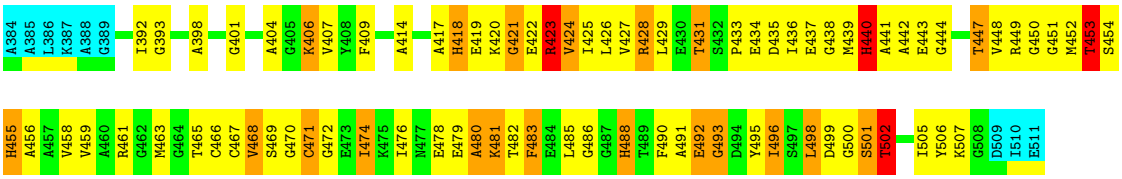


4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Pyruvate, phosphate dikinase

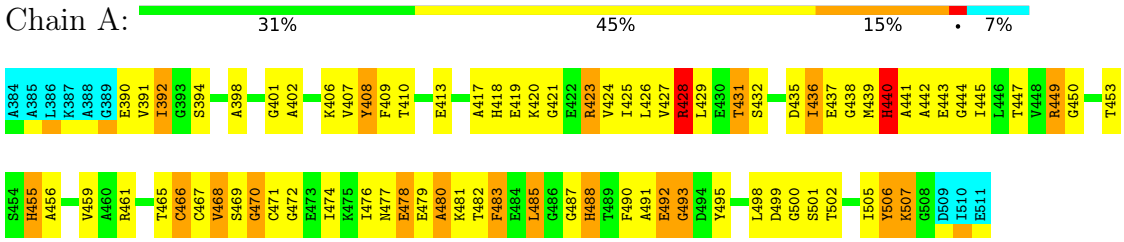
Chain A:





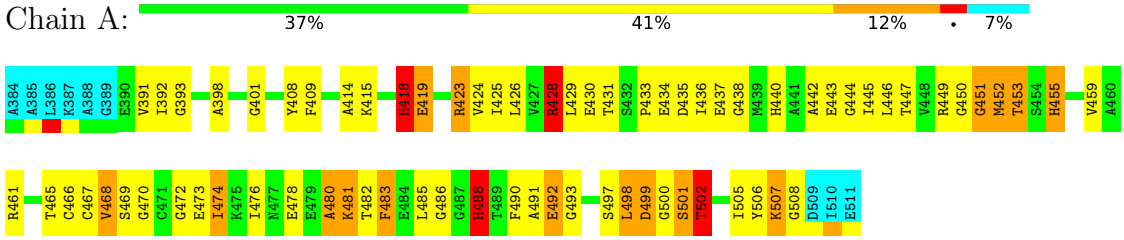
4.2.6 Score per residue for model 6

• Molecule 1: Pyruvate, phosphate dikinase



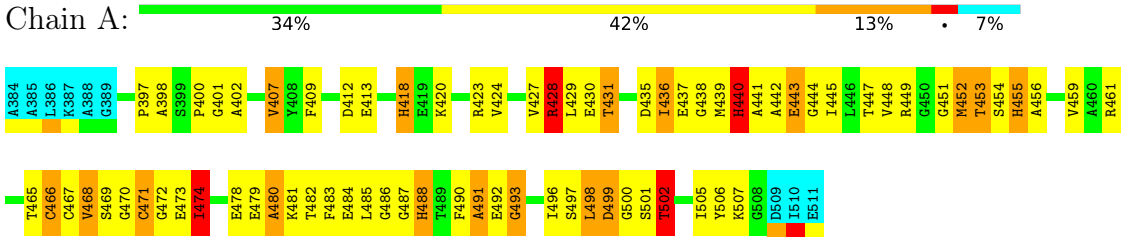
4.2.7 Score per residue for model 7

• Molecule 1: Pyruvate, phosphate dikinase



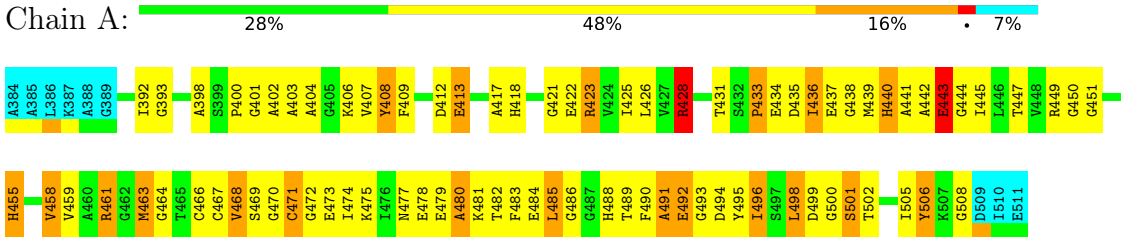
4.2.8 Score per residue for model 8

• Molecule 1: Pyruvate, phosphate dikinase



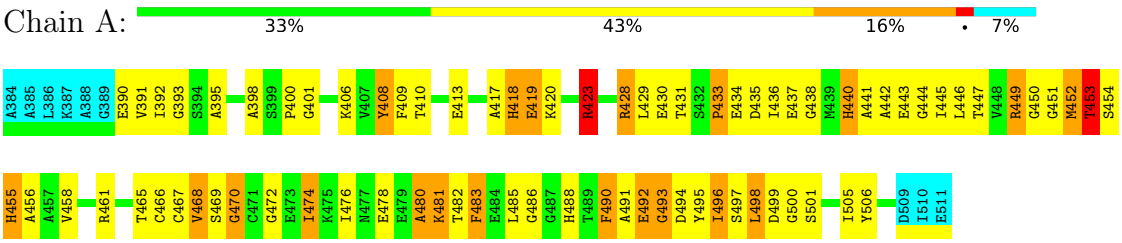
4.2.9 Score per residue for model 9

• Molecule 1: Pyruvate, phosphate dikinase



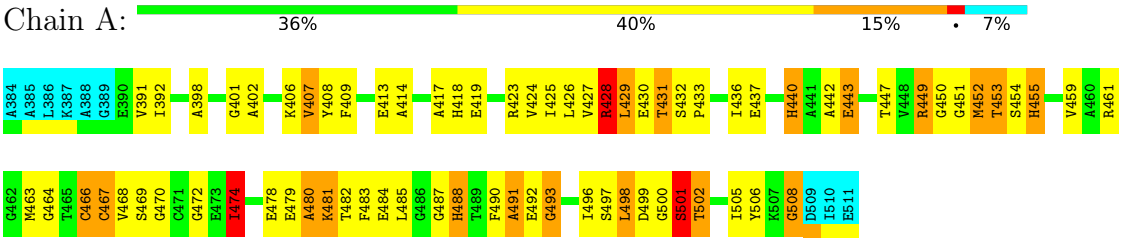
4.2.10 Score per residue for model 10

• Molecule 1: Pyruvate, phosphate dikinase



4.2.11 Score per residue for model 11

• Molecule 1: Pyruvate, phosphate dikinase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry simulated annealing*.

Of the 25 calculated structures, 11 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.0
X-PLOR	refinement	3.0

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.18±0.01	4±0/867 (0.5± 0.0%)	1.14±0.01	0±0/1168 (0.0± 0.0%)
All	All	1.18	44/9537 (0.5%)	1.14	0/12848 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	3.9±0.3
All	All	0	43

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	488	HIS	CG-ND1	-7.31	1.22	1.38	6	11
1	A	418	HIS	CG-ND1	-6.29	1.25	1.38	3	11
1	A	440	HIS	CG-ND1	-6.21	1.25	1.38	11	11
1	A	455	HIS	CG-ND1	-6.20	1.25	1.38	5	11

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	423	ARG	Sidechain	11
1	A	428	ARG	Sidechain	11
1	A	461	ARG	Sidechain	11
1	A	449	ARG	Sidechain	10

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	854	839	839	84±8
All	All	9394	9229	9229	921

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 49.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:498:LEU:H	1:A:498:LEU:HD23	0.94	1.22	6	1
1:A:485:LEU:HD23	1:A:486:GLY:N	0.92	1.79	7	3
1:A:483:PHE:CD2	1:A:491:ALA:HB2	0.92	2.00	3	4
1:A:498:LEU:HD12	1:A:499:ASP:N	0.85	1.85	7	8
1:A:429:LEU:H	1:A:429:LEU:HD23	0.84	1.33	4	1
1:A:436:ILE:HG23	1:A:437:GLU:H	0.84	1.32	3	2
1:A:428:ARG:O	1:A:447:THR:HG22	0.82	1.74	3	8
1:A:496:ILE:O	1:A:496:ILE:HD13	0.80	1.76	9	2
1:A:436:ILE:HG23	1:A:437:GLU:N	0.79	1.92	3	8
1:A:482:THR:HA	1:A:491:ALA:HB3	0.78	1.53	3	5
1:A:496:ILE:HD12	1:A:497:SER:N	0.78	1.92	1	1
1:A:436:ILE:HD11	1:A:440:HIS:NE2	0.78	1.94	3	1
1:A:485:LEU:HD23	1:A:485:LEU:O	0.78	1.78	4	2
1:A:440:HIS:ND1	1:A:441:ALA:N	0.78	2.32	8	4
1:A:402:ALA:N	1:A:466:CYS:SG	0.78	2.57	9	5
1:A:498:LEU:HD23	1:A:498:LEU:N	0.77	1.95	6	1
1:A:476:ILE:HG23	1:A:482:THR:O	0.77	1.80	5	6
1:A:392:ILE:HD12	1:A:485:LEU:HD21	0.76	1.58	6	2
1:A:498:LEU:HD12	1:A:498:LEU:C	0.76	2.00	7	4
1:A:391:VAL:CG2	1:A:506:TYR:CE2	0.75	2.68	11	6
1:A:496:ILE:HD12	1:A:496:ILE:C	0.75	2.01	1	1
1:A:429:LEU:H	1:A:429:LEU:CD2	0.74	1.94	4	1
1:A:501:SER:O	1:A:502:THR:HG23	0.74	1.83	5	2
1:A:424:VAL:O	1:A:442:ALA:HB1	0.73	1.83	11	1
1:A:409:PHE:CD2	1:A:481:LYS:NZ	0.73	2.56	1	1
1:A:485:LEU:HD23	1:A:486:GLY:H	0.72	1.44	7	3
1:A:396:LEU:N	1:A:396:LEU:CD2	0.72	2.53	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:474:ILE:HG23	1:A:483:PHE:CB	0.72	2.15	3	6
1:A:465:THR:HG22	1:A:466:CYS:H	0.69	1.46	5	2
1:A:391:VAL:CG2	1:A:506:TYR:CD2	0.68	2.76	6	6
1:A:431:THR:HG21	1:A:456:ALA:HB2	0.68	1.63	6	2
1:A:436:ILE:CG2	1:A:437:GLU:N	0.68	2.56	8	10
1:A:474:ILE:HG23	1:A:483:PHE:HB2	0.67	1.63	3	6
1:A:392:ILE:CD1	1:A:485:LEU:HD21	0.67	2.20	6	1
1:A:478:GLU:C	1:A:480:ALA:H	0.67	1.93	11	11
1:A:496:ILE:HD12	1:A:496:ILE:H	0.67	1.50	3	2
1:A:423:ARG:N	1:A:423:ARG:HE	0.66	1.87	4	1
1:A:471:CYS:SG	1:A:485:LEU:HD22	0.66	2.31	5	1
1:A:401:GLY:O	1:A:500:GLY:N	0.66	2.29	11	9
1:A:408:TYR:CE1	1:A:413:GLU:OE2	0.66	2.49	4	2
1:A:398:ALA:HB3	1:A:467:CYS:O	0.66	1.91	6	11
1:A:406:LYS:CD	1:A:406:LYS:N	0.65	2.60	11	1
1:A:440:HIS:ND1	1:A:440:HIS:C	0.65	2.49	4	4
1:A:455:HIS:O	1:A:459:VAL:HG23	0.65	1.91	2	10
1:A:494:ASP:CG	1:A:495:TYR:N	0.65	2.50	10	3
1:A:491:ALA:O	1:A:493:GLY:N	0.65	2.30	11	11
1:A:402:ALA:C	1:A:466:CYS:SG	0.65	2.75	3	1
1:A:414:ALA:HB1	1:A:441:ALA:HB1	0.65	1.67	5	1
1:A:458:VAL:CG1	1:A:459:VAL:N	0.65	2.59	9	1
1:A:408:TYR:CZ	1:A:414:ALA:HB2	0.64	2.28	7	2
1:A:401:GLY:N	1:A:500:GLY:O	0.64	2.31	5	11
1:A:408:TYR:CE2	1:A:426:LEU:CD1	0.64	2.81	7	2
1:A:431:THR:OG1	1:A:455:HIS:CD2	0.64	2.50	10	1
1:A:483:PHE:CE2	1:A:490:PHE:CG	0.63	2.86	10	1
1:A:499:ASP:N	1:A:499:ASP:OD1	0.63	2.30	7	1
1:A:391:VAL:HG23	1:A:506:TYR:CE1	0.63	2.28	4	1
1:A:496:ILE:HD13	1:A:496:ILE:C	0.63	2.13	9	1
1:A:414:ALA:HB1	1:A:441:ALA:CB	0.63	2.23	5	2
1:A:451:GLY:N	1:A:469:SER:OG	0.63	2.31	8	5
1:A:440:HIS:CG	1:A:441:ALA:N	0.63	2.66	5	3
1:A:478:GLU:C	1:A:480:ALA:N	0.62	2.51	9	11
1:A:505:ILE:C	1:A:506:TYR:CD1	0.62	2.72	10	2
1:A:423:ARG:N	1:A:423:ARG:NE	0.62	2.47	4	1
1:A:435:ASP:OD1	1:A:439:MET:SD	0.62	2.57	1	1
1:A:506:TYR:CD1	1:A:507:LYS:N	0.62	2.67	8	2
1:A:392:ILE:CG1	1:A:393:GLY:N	0.62	2.63	1	4
1:A:443:GLU:H	1:A:443:GLU:CD	0.62	1.98	3	2
1:A:460:ALA:HB1	1:A:467:CYS:SG	0.62	2.34	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:431:THR:CG2	1:A:456:ALA:HB2	0.62	2.24	4	6
1:A:401:GLY:C	1:A:466:CYS:SG	0.62	2.78	1	4
1:A:403:ALA:HB1	1:A:443:GLU:OE2	0.62	1.94	9	1
1:A:487:GLY:C	1:A:488:HIS:CD2	0.61	2.73	2	1
1:A:407:VAL:HG21	1:A:483:PHE:CE1	0.61	2.30	4	1
1:A:436:ILE:HG22	1:A:437:GLU:N	0.61	2.10	9	3
1:A:485:LEU:O	1:A:487:GLY:N	0.61	2.34	3	1
1:A:408:TYR:CZ	1:A:413:GLU:OE1	0.61	2.53	10	1
1:A:431:THR:OG1	1:A:432:SER:N	0.61	2.31	11	2
1:A:452:MET:C	1:A:453:THR:HG23	0.61	2.16	3	1
1:A:404:ALA:HB1	1:A:495:TYR:OH	0.61	1.96	5	2
1:A:436:ILE:CG2	1:A:437:GLU:H	0.60	2.09	5	5
1:A:483:PHE:CE2	1:A:491:ALA:HB2	0.60	2.30	3	3
1:A:499:ASP:OD1	1:A:500:GLY:N	0.60	2.33	6	1
1:A:429:LEU:CD2	1:A:429:LEU:N	0.60	2.63	4	1
1:A:391:VAL:HG23	1:A:506:TYR:CD2	0.60	2.32	6	2
1:A:465:THR:CG2	1:A:466:CYS:N	0.60	2.64	4	1
1:A:418:HIS:ND1	1:A:419:GLU:OE1	0.59	2.35	3	1
1:A:471:CYS:SG	1:A:485:LEU:HD13	0.59	2.38	2	1
1:A:408:TYR:CE1	1:A:413:GLU:OE1	0.59	2.56	3	2
1:A:436:ILE:CD1	1:A:440:HIS:NE2	0.59	2.66	3	1
1:A:442:ALA:C	1:A:444:GLY:H	0.59	2.01	7	9
1:A:465:THR:HG22	1:A:466:CYS:N	0.59	2.10	4	2
1:A:436:ILE:HD12	1:A:440:HIS:NE2	0.59	2.12	9	1
1:A:479:GLU:O	1:A:480:ALA:HB2	0.58	1.97	3	1
1:A:485:LEU:HD23	1:A:485:LEU:C	0.58	2.18	4	2
1:A:409:PHE:CD2	1:A:481:LYS:CD	0.58	2.86	4	2
1:A:478:GLU:O	1:A:480:ALA:N	0.58	2.37	6	11
1:A:482:THR:HG22	1:A:491:ALA:HA	0.58	1.74	10	5
1:A:417:ALA:O	1:A:421:GLY:N	0.58	2.35	9	4
1:A:391:VAL:HG22	1:A:506:TYR:CD2	0.58	2.32	11	3
1:A:449:ARG:CG	1:A:450:GLY:N	0.58	2.67	11	1
1:A:506:TYR:CD1	1:A:506:TYR:N	0.58	2.71	6	2
1:A:422:GLU:C	1:A:423:ARG:HE	0.58	2.02	4	1
1:A:396:LEU:N	1:A:396:LEU:HD23	0.58	2.13	2	1
1:A:429:LEU:HD23	1:A:429:LEU:N	0.58	2.05	4	1
1:A:498:LEU:N	1:A:498:LEU:CD2	0.58	2.66	6	1
1:A:478:GLU:H	1:A:478:GLU:CD	0.58	2.01	8	1
1:A:408:TYR:CD1	1:A:413:GLU:CD	0.58	2.77	2	1
1:A:471:CYS:SG	1:A:485:LEU:HD11	0.57	2.40	8	1
1:A:451:GLY:C	1:A:453:THR:H	0.57	2.01	3	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:407:VAL:CG1	1:A:491:ALA:C	0.57	2.73	8	1
1:A:413:GLU:N	1:A:413:GLU:OE1	0.57	2.37	8	1
1:A:468:VAL:CG1	1:A:469:SER:N	0.57	2.68	11	10
1:A:440:HIS:C	1:A:442:ALA:N	0.57	2.55	11	4
1:A:494:ASP:CG	1:A:495:TYR:H	0.57	2.02	10	2
1:A:471:CYS:SG	1:A:474:ILE:HD12	0.57	2.40	9	2
1:A:392:ILE:HD13	1:A:490:PHE:CZ	0.57	2.35	1	1
1:A:474:ILE:O	1:A:474:ILE:HG22	0.57	2.00	3	4
1:A:435:ASP:O	1:A:438:GLY:N	0.56	2.38	2	9
1:A:442:ALA:O	1:A:444:GLY:N	0.56	2.36	10	9
1:A:454:SER:O	1:A:458:VAL:HG23	0.56	2.00	10	1
1:A:390:GLU:N	1:A:390:GLU:CD	0.56	2.59	10	1
1:A:450:GLY:C	1:A:452:MET:H	0.56	2.04	7	1
1:A:430:GLU:OE2	1:A:431:THR:N	0.56	2.36	10	1
1:A:391:VAL:HG13	1:A:505:ILE:O	0.56	2.00	11	2
1:A:428:ARG:H	1:A:447:THR:HG22	0.56	1.61	11	3
1:A:482:THR:HG22	1:A:491:ALA:O	0.56	2.01	3	1
1:A:483:PHE:CE1	1:A:490:PHE:O	0.56	2.58	11	3
1:A:409:PHE:O	1:A:410:THR:HG23	0.56	2.01	4	3
1:A:396:LEU:HD23	1:A:396:LEU:H	0.56	1.61	2	1
1:A:409:PHE:CE2	1:A:481:LYS:NZ	0.56	2.73	9	1
1:A:473:GLU:N	1:A:473:GLU:CD	0.56	2.59	7	1
1:A:483:PHE:CD1	1:A:490:PHE:O	0.55	2.59	11	3
1:A:454:SER:OG	1:A:455:HIS:N	0.55	2.38	8	1
1:A:392:ILE:HG21	1:A:490:PHE:CZ	0.55	2.37	1	1
1:A:449:ARG:O	1:A:470:GLY:N	0.55	2.39	6	4
1:A:450:GLY:C	1:A:469:SER:OG	0.55	2.45	7	7
1:A:428:ARG:O	1:A:447:THR:CG2	0.55	2.55	5	7
1:A:505:ILE:CG1	1:A:506:TYR:N	0.55	2.69	3	4
1:A:409:PHE:CE1	1:A:481:LYS:O	0.55	2.60	6	2
1:A:437:GLU:CD	1:A:438:GLY:H	0.55	2.04	7	1
1:A:409:PHE:CD2	1:A:427:VAL:O	0.55	2.60	11	1
1:A:483:PHE:CD2	1:A:491:ALA:CB	0.54	2.87	11	3
1:A:435:ASP:O	1:A:439:MET:N	0.54	2.39	6	4
1:A:408:TYR:O	1:A:409:PHE:CD1	0.54	2.61	11	1
1:A:407:VAL:O	1:A:408:TYR:CG	0.54	2.61	1	1
1:A:433:PRO:O	1:A:435:ASP:N	0.54	2.41	5	6
1:A:409:PHE:N	1:A:409:PHE:CD1	0.54	2.75	7	2
1:A:392:ILE:CG1	1:A:393:GLY:H	0.54	2.15	10	3
1:A:451:GLY:O	1:A:453:THR:N	0.54	2.41	4	7
1:A:409:PHE:CD2	1:A:481:LYS:CE	0.54	2.91	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:409:PHE:CZ	1:A:427:VAL:HG11	0.54	2.37	5	2
1:A:408:TYR:C	1:A:409:PHE:CD1	0.54	2.81	7	2
1:A:417:ALA:O	1:A:420:LYS:N	0.54	2.41	1	3
1:A:407:VAL:HG11	1:A:492:GLU:N	0.54	2.17	9	1
1:A:490:PHE:C	1:A:490:PHE:CD1	0.54	2.81	11	2
1:A:450:GLY:O	1:A:452:MET:N	0.54	2.41	7	1
1:A:498:LEU:C	1:A:498:LEU:CD1	0.54	2.69	7	1
1:A:407:VAL:HB	1:A:492:GLU:H	0.53	1.63	3	1
1:A:407:VAL:CG1	1:A:492:GLU:N	0.53	2.71	9	1
1:A:439:MET:SD	1:A:459:VAL:HG11	0.53	2.42	1	2
1:A:408:TYR:CD1	1:A:413:GLU:OE2	0.53	2.61	2	1
1:A:477:ASN:CB	1:A:482:THR:OG1	0.53	2.57	4	1
1:A:487:GLY:O	1:A:488:HIS:CD2	0.53	2.61	11	6
1:A:437:GLU:CG	1:A:438:GLY:N	0.53	2.72	7	1
1:A:483:PHE:CD1	1:A:483:PHE:N	0.53	2.76	5	6
1:A:482:THR:HA	1:A:491:ALA:CB	0.52	2.33	8	4
1:A:430:GLU:CD	1:A:431:THR:H	0.52	2.06	10	1
1:A:505:ILE:CG2	1:A:506:TYR:N	0.52	2.71	10	1
1:A:436:ILE:O	1:A:439:MET:N	0.52	2.43	1	4
1:A:506:TYR:CZ	1:A:507:LYS:O	0.52	2.62	5	1
1:A:431:THR:O	1:A:455:HIS:NE2	0.52	2.41	10	1
1:A:497:SER:N	1:A:506:TYR:O	0.52	2.42	4	4
1:A:391:VAL:HG22	1:A:506:TYR:CE2	0.52	2.40	10	2
1:A:482:THR:HG22	1:A:491:ALA:H	0.52	1.65	11	4
1:A:448:VAL:HG22	1:A:474:ILE:HB	0.52	1.82	3	2
1:A:451:GLY:C	1:A:453:THR:N	0.52	2.62	4	6
1:A:401:GLY:O	1:A:466:CYS:SG	0.52	2.67	2	3
1:A:484:GLU:OE1	1:A:485:LEU:N	0.52	2.42	3	1
1:A:418:HIS:O	1:A:418:HIS:ND1	0.52	2.42	7	1
1:A:407:VAL:O	1:A:408:TYR:CD2	0.52	2.63	1	2
1:A:498:LEU:HD13	1:A:505:ILE:CG1	0.52	2.34	10	1
1:A:449:ARG:CG	1:A:450:GLY:H	0.51	2.17	11	2
1:A:408:TYR:CE1	1:A:425:ILE:O	0.51	2.63	11	1
1:A:407:VAL:CG2	1:A:408:TYR:N	0.51	2.73	11	1
1:A:413:GLU:O	1:A:417:ALA:N	0.51	2.42	6	2
1:A:442:ALA:C	1:A:444:GLY:N	0.51	2.64	6	8
1:A:435:ASP:OD1	1:A:435:ASP:C	0.51	2.49	1	2
1:A:488:HIS:CG	1:A:490:PHE:CZ	0.51	2.99	7	1
1:A:448:VAL:HG22	1:A:474:ILE:HD12	0.51	1.82	8	1
1:A:452:MET:O	1:A:453:THR:HG23	0.51	2.06	1	1
1:A:483:PHE:CZ	1:A:490:PHE:CD1	0.51	2.99	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:491:ALA:O	1:A:492:GLU:C	0.50	2.48	3	3
1:A:429:LEU:HD12	1:A:429:LEU:H	0.50	1.65	5	2
1:A:429:LEU:O	1:A:449:ARG:CG	0.50	2.59	6	2
1:A:482:THR:HG22	1:A:491:ALA:CA	0.50	2.37	6	2
1:A:483:PHE:CE2	1:A:490:PHE:CB	0.50	2.94	10	1
1:A:409:PHE:CE1	1:A:481:LYS:CD	0.50	2.94	11	1
1:A:419:GLU:C	1:A:421:GLY:H	0.50	2.10	4	1
1:A:431:THR:HG22	1:A:456:ALA:HB2	0.50	1.84	4	1
1:A:428:ARG:O	1:A:447:THR:CB	0.50	2.60	5	6
1:A:408:TYR:CE2	1:A:426:LEU:HD13	0.50	2.41	7	1
1:A:482:THR:HG22	1:A:491:ALA:CB	0.50	2.37	6	3
1:A:409:PHE:CD2	1:A:481:LYS:HE2	0.50	2.42	6	2
1:A:390:GLU:N	1:A:390:GLU:OE2	0.50	2.45	10	1
1:A:484:GLU:CD	1:A:484:GLU:C	0.49	2.66	4	1
1:A:471:CYS:SG	1:A:485:LEU:CD2	0.49	3.00	5	1
1:A:408:TYR:CE2	1:A:426:LEU:HD12	0.49	2.41	11	2
1:A:406:LYS:O	1:A:425:ILE:N	0.49	2.36	11	1
1:A:446:LEU:CD2	1:A:498:LEU:HD22	0.49	2.37	2	1
1:A:490:PHE:CB	1:A:507:LYS:HZ1	0.49	2.19	8	1
1:A:433:PRO:C	1:A:435:ASP:N	0.49	2.64	5	4
1:A:479:GLU:O	1:A:480:ALA:CB	0.49	2.60	3	1
1:A:419:GLU:C	1:A:421:GLY:N	0.49	2.66	4	2
1:A:443:GLU:OE1	1:A:443:GLU:C	0.49	2.50	9	1
1:A:455:HIS:O	1:A:459:VAL:CG2	0.49	2.60	2	9
1:A:463:MET:SD	1:A:463:MET:O	0.49	2.70	4	1
1:A:430:GLU:CD	1:A:431:THR:N	0.49	2.66	10	1
1:A:425:ILE:HG22	1:A:426:LEU:N	0.49	2.23	6	5
1:A:409:PHE:CZ	1:A:427:VAL:CG1	0.49	2.96	4	3
1:A:477:ASN:OD1	1:A:489:THR:CG2	0.49	2.60	9	1
1:A:490:PHE:CZ	1:A:507:LYS:NZ	0.49	2.76	6	1
1:A:475:LYS:NZ	1:A:484:GLU:OE2	0.49	2.46	9	1
1:A:506:TYR:CG	1:A:507:LYS:N	0.49	2.81	5	1
1:A:495:TYR:CD1	1:A:495:TYR:N	0.49	2.81	2	2
1:A:419:GLU:CA	1:A:419:GLU:OE1	0.49	2.59	7	1
1:A:492:GLU:CG	1:A:492:GLU:O	0.48	2.61	1	2
1:A:409:PHE:CD2	1:A:481:LYS:HD3	0.48	2.42	4	2
1:A:452:MET:O	1:A:453:THR:CB	0.48	2.61	8	2
1:A:496:ILE:HA	1:A:508:GLY:H	0.48	1.68	9	1
1:A:432:SER:OG	1:A:435:ASP:CG	0.48	2.50	3	1
1:A:495:TYR:CD1	1:A:496:ILE:N	0.48	2.81	5	1
1:A:505:ILE:HG22	1:A:506:TYR:N	0.48	2.23	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:463:MET:SD	1:A:463:MET:C	0.48	2.92	9	2
1:A:471:CYS:SG	1:A:485:LEU:CD1	0.48	3.02	2	1
1:A:409:PHE:CD2	1:A:481:LYS:HD2	0.48	2.43	5	2
1:A:392:ILE:HD11	1:A:505:ILE:HG21	0.48	1.83	5	1
1:A:431:THR:HG21	1:A:456:ALA:CB	0.48	2.39	1	1
1:A:417:ALA:C	1:A:419:GLU:N	0.47	2.67	2	3
1:A:498:LEU:HD13	1:A:505:ILE:HG12	0.47	1.85	10	2
1:A:484:GLU:CD	1:A:489:THR:OG1	0.47	2.53	3	1
1:A:392:ILE:HG13	1:A:393:GLY:N	0.47	2.24	1	6
1:A:417:ALA:O	1:A:422:GLU:N	0.47	2.41	2	1
1:A:482:THR:HG22	1:A:491:ALA:N	0.47	2.25	3	5
1:A:409:PHE:CB	1:A:481:LYS:HZ3	0.47	2.23	1	1
1:A:483:PHE:CZ	1:A:490:PHE:CB	0.47	2.97	1	1
1:A:429:LEU:N	1:A:429:LEU:HD23	0.47	2.24	2	2
1:A:507:LYS:HE3	1:A:507:LYS:H	0.47	1.70	6	1
1:A:409:PHE:CE1	1:A:481:LYS:HD3	0.47	2.45	11	1
1:A:483:PHE:CZ	1:A:490:PHE:HB3	0.47	2.45	1	1
1:A:501:SER:C	1:A:502:THR:OG1	0.47	2.53	1	1
1:A:422:GLU:O	1:A:423:ARG:NE	0.47	2.42	5	1
1:A:497:SER:O	1:A:506:TYR:N	0.47	2.45	11	3
1:A:401:GLY:H	1:A:500:GLY:CA	0.47	2.23	7	3
1:A:455:HIS:O	1:A:459:VAL:N	0.47	2.40	7	1
1:A:450:GLY:C	1:A:452:MET:N	0.47	2.69	7	1
1:A:407:VAL:HG11	1:A:491:ALA:C	0.47	2.29	8	1
1:A:494:ASP:OD1	1:A:495:TYR:N	0.47	2.41	1	1
1:A:397:PRO:HG3	1:A:502:THR:O	0.47	2.10	8	1
1:A:484:GLU:OE2	1:A:485:LEU:N	0.46	2.48	11	1
1:A:480:ALA:O	1:A:481:LYS:CB	0.46	2.63	11	3
1:A:498:LEU:HD12	1:A:499:ASP:O	0.46	2.10	11	4
1:A:418:HIS:CD2	1:A:418:HIS:O	0.46	2.68	8	1
1:A:474:ILE:HG22	1:A:483:PHE:HB2	0.46	1.85	8	1
1:A:410:THR:OG1	1:A:413:GLU:OE1	0.46	2.33	1	1
1:A:485:LEU:C	1:A:485:LEU:CD2	0.46	2.82	4	2
1:A:507:LYS:CD	1:A:507:LYS:N	0.46	2.79	6	1
1:A:421:GLY:C	1:A:422:GLU:CG	0.46	2.83	3	3
1:A:452:MET:C	1:A:453:THR:CG2	0.46	2.84	3	1
1:A:436:ILE:HD13	1:A:459:VAL:CG1	0.46	2.40	4	1
1:A:406:LYS:CB	1:A:406:LYS:NZ	0.46	2.79	2	1
1:A:496:ILE:HD12	1:A:496:ILE:N	0.46	2.23	3	1
1:A:401:GLY:O	1:A:500:GLY:CA	0.46	2.64	1	6
1:A:427:VAL:HG22	1:A:446:LEU:O	0.46	2.10	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:440:HIS:C	1:A:442:ALA:H	0.46	2.14	11	1
1:A:391:VAL:HG23	1:A:506:TYR:CE2	0.46	2.44	3	3
1:A:490:PHE:CD1	1:A:490:PHE:C	0.46	2.89	2	1
1:A:455:HIS:ND1	1:A:455:HIS:N	0.46	2.64	10	2
1:A:409:PHE:CD1	1:A:481:LYS:HB3	0.46	2.46	4	3
1:A:446:LEU:HD11	1:A:471:CYS:SG	0.46	2.51	1	1
1:A:483:PHE:CE2	1:A:490:PHE:HB2	0.45	2.46	5	2
1:A:496:ILE:C	1:A:496:ILE:CD1	0.45	2.78	9	2
1:A:401:GLY:H	1:A:500:GLY:HA3	0.45	1.71	11	5
1:A:480:ALA:O	1:A:481:LYS:CG	0.45	2.64	11	2
1:A:409:PHE:CE1	1:A:481:LYS:HB3	0.45	2.46	7	3
1:A:506:TYR:CE1	1:A:507:LYS:O	0.45	2.69	5	1
1:A:452:MET:C	1:A:453:THR:OG1	0.45	2.54	10	3
1:A:406:LYS:N	1:A:406:LYS:HD3	0.45	2.25	11	1
1:A:442:ALA:O	1:A:443:GLU:C	0.45	2.54	3	1
1:A:403:ALA:HB1	1:A:443:GLU:CD	0.45	2.31	9	1
1:A:435:ASP:O	1:A:436:ILE:C	0.45	2.55	7	6
1:A:496:ILE:N	1:A:496:ILE:CD1	0.45	2.79	3	1
1:A:485:LEU:CD2	1:A:486:GLY:N	0.45	2.76	8	2
1:A:485:LEU:CD2	1:A:486:GLY:H	0.45	2.21	9	1
1:A:409:PHE:CE2	1:A:427:VAL:CG1	0.45	2.99	1	1
1:A:474:ILE:CG2	1:A:483:PHE:HB2	0.45	2.42	4	3
1:A:440:HIS:O	1:A:442:ALA:N	0.45	2.50	3	3
1:A:409:PHE:CZ	1:A:481:LYS:O	0.45	2.70	4	2
1:A:490:PHE:CE1	1:A:507:LYS:NZ	0.45	2.84	6	1
1:A:409:PHE:CD1	1:A:481:LYS:HD2	0.45	2.47	11	1
1:A:436:ILE:HG22	1:A:437:GLU:H	0.45	1.68	9	3
1:A:500:GLY:O	1:A:501:SER:CB	0.45	2.62	9	2
1:A:460:ALA:O	1:A:464:GLY:N	0.45	2.49	1	1
1:A:406:LYS:N	1:A:406:LYS:HD2	0.45	2.27	5	1
1:A:407:VAL:HG11	1:A:483:PHE:HZ	0.45	1.71	5	1
1:A:507:LYS:NZ	1:A:507:LYS:HB2	0.45	2.27	6	1
1:A:408:TYR:CE1	1:A:413:GLU:HG2	0.45	2.47	9	1
1:A:427:VAL:HG21	1:A:483:PHE:CE2	0.45	2.48	3	1
1:A:440:HIS:CE1	1:A:463:MET:SD	0.44	3.10	1	1
1:A:468:VAL:HG13	1:A:469:SER:N	0.44	2.26	3	9
1:A:391:VAL:HG23	1:A:506:TYR:CD1	0.44	2.47	4	1
1:A:395:ALA:HB3	1:A:468:VAL:HG13	0.44	1.88	10	1
1:A:418:HIS:HB2	1:A:441:ALA:HB1	0.44	1.89	10	1
1:A:491:ALA:C	1:A:493:GLY:N	0.44	2.69	3	2
1:A:485:LEU:HG	1:A:486:GLY:N	0.44	2.26	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:484:GLU:OE2	1:A:489:THR:OG1	0.44	2.36	3	1
1:A:490:PHE:CZ	1:A:507:LYS:HG2	0.44	2.47	6	1
1:A:505:ILE:HG13	1:A:506:TYR:N	0.44	2.27	7	3
1:A:435:ASP:OD1	1:A:436:ILE:N	0.44	2.51	1	1
1:A:392:ILE:HD11	1:A:505:ILE:CG2	0.44	2.43	5	1
1:A:437:GLU:CD	1:A:438:GLY:N	0.44	2.70	7	1
1:A:425:ILE:CG2	1:A:426:LEU:N	0.44	2.81	1	2
1:A:391:VAL:HG22	1:A:505:ILE:O	0.44	2.12	4	1
1:A:450:GLY:O	1:A:470:GLY:N	0.44	2.51	5	1
1:A:409:PHE:CG	1:A:481:LYS:HE2	0.44	2.48	6	1
1:A:499:ASP:OD2	1:A:506:TYR:CE1	0.44	2.71	7	1
1:A:445:ILE:HD12	1:A:467:CYS:SG	0.44	2.53	6	2
1:A:408:TYR:CE1	1:A:413:GLU:CG	0.44	3.00	9	1
1:A:418:HIS:CD2	1:A:418:HIS:C	0.44	2.91	8	1
1:A:409:PHE:CZ	1:A:427:VAL:HB	0.43	2.48	1	1
1:A:433:PRO:C	1:A:435:ASP:H	0.43	2.17	9	2
1:A:437:GLU:HG2	1:A:438:GLY:N	0.43	2.28	7	1
1:A:408:TYR:C	1:A:410:THR:H	0.43	2.16	6	1
1:A:408:TYR:CD1	1:A:425:ILE:O	0.43	2.71	7	2
1:A:483:PHE:CD2	1:A:490:PHE:HB3	0.43	2.49	10	1
1:A:423:ARG:C	1:A:424:VAL:CG2	0.43	2.87	5	3
1:A:424:VAL:N	1:A:443:GLU:OE2	0.43	2.48	8	1
1:A:506:TYR:N	1:A:506:TYR:CD1	0.43	2.87	7	1
1:A:483:PHE:CE2	1:A:490:PHE:HB3	0.43	2.48	10	1
1:A:500:GLY:C	1:A:501:SER:OG	0.43	2.52	11	1
1:A:392:ILE:HD13	1:A:490:PHE:CE2	0.43	2.48	1	1
1:A:406:LYS:HE3	1:A:495:TYR:CD2	0.43	2.48	1	1
1:A:488:HIS:CG	1:A:490:PHE:CE1	0.43	3.06	7	1
1:A:392:ILE:O	1:A:486:GLY:CA	0.43	2.67	9	1
1:A:391:VAL:HG12	1:A:392:ILE:N	0.43	2.28	11	2
1:A:490:PHE:CE1	1:A:507:LYS:HD2	0.43	2.49	7	1
1:A:458:VAL:HG12	1:A:459:VAL:N	0.43	2.26	9	1
1:A:454:SER:O	1:A:458:VAL:N	0.43	2.41	5	2
1:A:407:VAL:CG2	1:A:427:VAL:HG23	0.43	2.44	8	1
1:A:401:GLY:C	1:A:466:CYS:HG	0.43	2.15	10	1
1:A:391:VAL:CG1	1:A:392:ILE:N	0.42	2.82	11	2
1:A:496:ILE:HG22	1:A:507:LYS:CG	0.42	2.44	5	1
1:A:428:ARG:N	1:A:447:THR:HG22	0.42	2.27	8	1
1:A:423:ARG:HE	1:A:423:ARG:H	0.42	1.57	10	1
1:A:408:TYR:C	1:A:410:THR:N	0.42	2.72	6	1
1:A:408:TYR:CZ	1:A:426:LEU:HD13	0.42	2.50	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:496:ILE:HD12	1:A:497:SER:CA	0.42	2.43	1	1
1:A:419:GLU:O	1:A:421:GLY:N	0.42	2.53	4	1
1:A:487:GLY:O	1:A:488:HIS:CG	0.42	2.72	3	1
1:A:454:SER:H	1:A:457:ALA:HB3	0.42	1.74	4	1
1:A:481:LYS:HB2	1:A:492:GLU:CB	0.42	2.45	4	2
1:A:488:HIS:HB3	1:A:490:PHE:CZ	0.42	2.49	7	1
1:A:507:LYS:HE3	1:A:507:LYS:N	0.42	2.29	6	1
1:A:446:LEU:CD1	1:A:468:VAL:CG1	0.42	2.98	10	2
1:A:449:ARG:HG2	1:A:450:GLY:N	0.42	2.30	11	1
1:A:498:LEU:HB3	1:A:505:ILE:HG23	0.42	1.91	6	1
1:A:483:PHE:CE2	1:A:491:ALA:CB	0.42	3.03	11	1
1:A:417:ALA:O	1:A:419:GLU:N	0.42	2.53	5	2
1:A:481:LYS:HB3	1:A:492:GLU:CG	0.42	2.45	2	1
1:A:490:PHE:CD1	1:A:507:LYS:NZ	0.42	2.86	3	1
1:A:434:GLU:CG	1:A:435:ASP:N	0.42	2.83	4	1
1:A:465:THR:OG1	1:A:466:CYS:N	0.42	2.53	7	1
1:A:496:ILE:HG13	1:A:497:SER:N	0.42	2.28	10	1
1:A:429:LEU:CB	1:A:430:GLU:OE2	0.42	2.67	11	1
1:A:485:LEU:O	1:A:486:GLY:C	0.42	2.58	3	1
1:A:478:GLU:O	1:A:479:GLU:C	0.42	2.59	5	3
1:A:453:THR:O	1:A:453:THR:CG2	0.42	2.68	6	1
1:A:454:SER:O	1:A:455:HIS:C	0.41	2.58	4	2
1:A:428:ARG:C	1:A:430:GLU:H	0.41	2.16	8	1
1:A:392:ILE:CG2	1:A:490:PHE:CZ	0.41	3.03	5	1
1:A:482:THR:CB	1:A:491:ALA:HA	0.41	2.44	7	1
1:A:483:PHE:CE1	1:A:490:PHE:CE1	0.41	3.08	11	1
1:A:401:GLY:H	1:A:500:GLY:C	0.41	2.19	2	1
1:A:501:SER:O	1:A:502:THR:CG2	0.41	2.65	5	1
1:A:436:ILE:O	1:A:437:GLU:C	0.41	2.58	1	1
1:A:492:GLU:O	1:A:492:GLU:CD	0.41	2.59	1	2
1:A:506:TYR:CE2	1:A:507:LYS:O	0.41	2.73	1	1
1:A:409:PHE:CG	1:A:481:LYS:HD2	0.41	2.50	3	1
1:A:422:GLU:O	1:A:423:ARG:CB	0.41	2.67	5	1
1:A:409:PHE:CG	1:A:481:LYS:HD3	0.41	2.50	7	1
1:A:490:PHE:CD2	1:A:507:LYS:HE3	0.41	2.51	8	1
1:A:463:MET:HG3	1:A:464:GLY:N	0.41	2.30	9	2
1:A:445:ILE:CG2	1:A:467:CYS:SG	0.41	3.08	10	1
1:A:417:ALA:O	1:A:418:HIS:C	0.41	2.58	3	3
1:A:490:PHE:CG	1:A:507:LYS:NZ	0.41	2.74	3	1
1:A:412:ASP:N	1:A:412:ASP:OD1	0.41	2.52	8	1
1:A:406:LYS:NZ	1:A:406:LYS:HB2	0.41	2.29	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:407:VAL:HG21	1:A:483:PHE:CZ	0.41	2.50	4	1
1:A:409:PHE:CE2	1:A:481:LYS:CE	0.41	3.03	9	1
1:A:445:ILE:HD12	1:A:445:ILE:N	0.41	2.31	9	1
1:A:495:TYR:N	1:A:495:TYR:CD1	0.41	2.89	3	1
1:A:466:CYS:SG	1:A:500:GLY:N	0.41	2.93	4	1
1:A:406:LYS:N	1:A:406:LYS:CD	0.41	2.83	5	1
1:A:429:LEU:O	1:A:449:ARG:N	0.41	2.51	7	1
1:A:403:ALA:CB	1:A:443:GLU:OE2	0.41	2.67	9	1
1:A:409:PHE:CG	1:A:481:LYS:CD	0.41	3.04	10	1
1:A:406:LYS:HD3	1:A:406:LYS:H	0.41	1.76	11	1
1:A:436:ILE:HG13	1:A:440:HIS:NE2	0.41	2.31	11	1
1:A:390:GLU:O	1:A:391:VAL:C	0.41	2.59	1	1
1:A:422:GLU:O	1:A:423:ARG:C	0.41	2.60	2	1
1:A:474:ILE:HG23	1:A:485:LEU:HB2	0.41	1.93	2	1
1:A:482:THR:HG22	1:A:491:ALA:HB1	0.41	1.91	6	1
1:A:419:GLU:O	1:A:419:GLU:CD	0.41	2.59	7	1
1:A:476:ILE:HG21	1:A:481:LYS:NZ	0.41	2.31	7	1
1:A:473:GLU:O	1:A:474:ILE:C	0.41	2.59	8	1
1:A:440:HIS:O	1:A:441:ALA:C	0.41	2.58	9	1
1:A:454:SER:HG	1:A:455:HIS:CE1	0.41	2.33	10	1
1:A:392:ILE:HG21	1:A:490:PHE:CE1	0.41	2.51	1	1
1:A:450:GLY:C	1:A:469:SER:HG	0.41	2.19	5	1
1:A:409:PHE:CE2	1:A:481:LYS:HD3	0.41	2.51	7	1
1:A:408:TYR:CD1	1:A:413:GLU:HG3	0.41	2.51	10	1
1:A:455:HIS:O	1:A:456:ALA:C	0.41	2.60	10	1
1:A:409:PHE:CD1	1:A:409:PHE:N	0.40	2.89	1	1
1:A:420:LYS:NZ	1:A:420:LYS:HB3	0.40	2.31	3	1
1:A:437:GLU:HA	1:A:440:HIS:CD2	0.40	2.52	6	1
1:A:499:ASP:CB	1:A:504:LYS:O	0.40	2.70	3	1
1:A:419:GLU:CD	1:A:419:GLU:C	0.40	2.78	7	1
1:A:404:ALA:CB	1:A:495:TYR:OH	0.40	2.70	9	1
1:A:409:PHE:CD2	1:A:481:LYS:HG2	0.40	2.51	10	1
1:A:436:ILE:HG13	1:A:440:HIS:CE1	0.40	2.51	10	1
1:A:409:PHE:O	1:A:410:THR:CG2	0.40	2.69	1	1
1:A:414:ALA:HB1	1:A:441:ALA:HB3	0.40	1.92	3	1
1:A:406:LYS:HD2	1:A:406:LYS:H	0.40	1.77	5	1
1:A:407:VAL:HG12	1:A:408:TYR:N	0.40	2.31	9	1
1:A:409:PHE:CD2	1:A:481:LYS:HE3	0.40	2.51	6	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	119/128 (93%)	86±5 (72±4%)	20±3 (17±3%)	13±2 (11±2%)	1 8
All	All	1309/1408 (93%)	944 (72%)	221 (17%)	144 (11%)	1 8

All 27 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	472	GLY	11
1	A	480	ALA	11
1	A	443	GLU	10
1	A	501	SER	10
1	A	502	THR	9
1	A	492	GLU	9
1	A	470	GLY	8
1	A	493	GLY	8
1	A	474	ILE	7
1	A	452	MET	7
1	A	400	PRO	6
1	A	433	PRO	6
1	A	434	GLU	6
1	A	453	THR	6
1	A	423	ARG	4
1	A	491	ALA	4
1	A	479	GLU	4
1	A	481	LYS	3
1	A	508	GLY	3
1	A	390	GLU	2
1	A	421	GLY	2
1	A	451	GLY	2
1	A	465	THR	2
1	A	436	ILE	1
1	A	394	SER	1
1	A	422	GLU	1
1	A	486	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	85/90 (94%)	68±4 (80±5%)	17±4 (20±5%)	3 33
All	All	935/990 (94%)	744 (80%)	191 (20%)	3 33

All 65 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	498	LEU	10
1	A	496	ILE	9
1	A	502	THR	9
1	A	431	THR	9
1	A	468	VAL	8
1	A	453	THR	7
1	A	428	ARG	6
1	A	483	PHE	6
1	A	419	GLU	6
1	A	471	CYS	6
1	A	429	LEU	5
1	A	406	LYS	5
1	A	420	LYS	4
1	A	436	ILE	4
1	A	407	VAL	4
1	A	466	CYS	4
1	A	485	LEU	4
1	A	499	ASP	4
1	A	440	HIS	4
1	A	415	LYS	3
1	A	432	SER	3
1	A	488	HIS	3
1	A	474	ILE	3
1	A	423	ARG	3
1	A	481	LYS	3
1	A	408	TYR	3
1	A	410	THR	2
1	A	435	ASP	2
1	A	501	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	445	ILE	2
1	A	465	THR	2
1	A	478	GLU	2
1	A	399	SER	2
1	A	447	THR	2
1	A	394	SER	2
1	A	412	ASP	2
1	A	467	CYS	2
1	A	477	ASN	2
1	A	424	VAL	2
1	A	463	MET	2
1	A	506	TYR	2
1	A	507	LYS	2
1	A	443	GLU	2
1	A	390	GLU	1
1	A	495	TYR	1
1	A	396	LEU	1
1	A	446	LEU	1
1	A	504	LYS	1
1	A	422	GLU	1
1	A	391	VAL	1
1	A	475	LYS	1
1	A	479	GLU	1
1	A	494	ASP	1
1	A	392	ILE	1
1	A	492	GLU	1
1	A	418	HIS	1
1	A	430	GLU	1
1	A	484	GLU	1
1	A	497	SER	1
1	A	505	ILE	1
1	A	413	GLU	1
1	A	458	VAL	1
1	A	461	ARG	1
1	A	473	GLU	1
1	A	490	PHE	1

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 monosaccharides 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