



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 01:03 AM UTC

PDB ID : 2GI4 / pdb_00002gi4
Title : Solution Structure of the Low Molecular Weight Protein Tyrosine Phosphatase from *Campylobacter jejuni*.
Authors : Tolkatchev, D.; Shaykhutdinov, R.; Xu, P.; Ni, F.
Deposited on : 2006-03-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

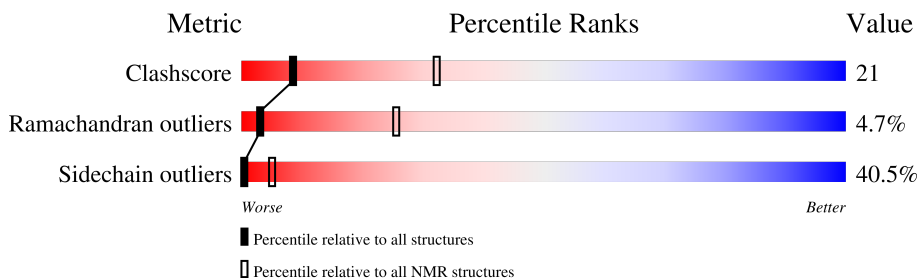
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	156	 29% 58% 9% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:1-A:150 (150)	0.89	3

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2526 atoms, of which 1263 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called possible phosphotyrosine protein phosphatase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	156	2526	806	1263	213	235	9	0

There are 5 discrepancies between the modelled and reference sequences:

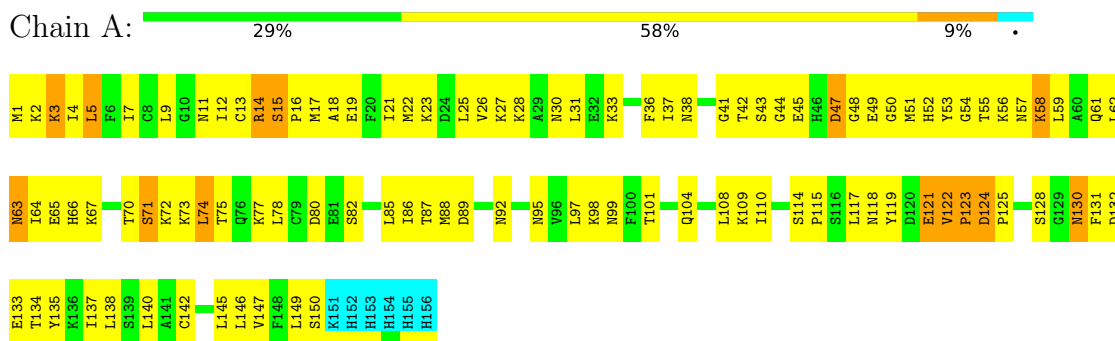
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	HIS	-	expression tag	GB 6968691
A	153	HIS	-	expression tag	GB 6968691
A	154	HIS	-	expression tag	GB 6968691
A	155	HIS	-	expression tag	GB 6968691
A	156	HIS	-	expression tag	GB 6968691

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: possible phosphotyrosine protein phosphatase

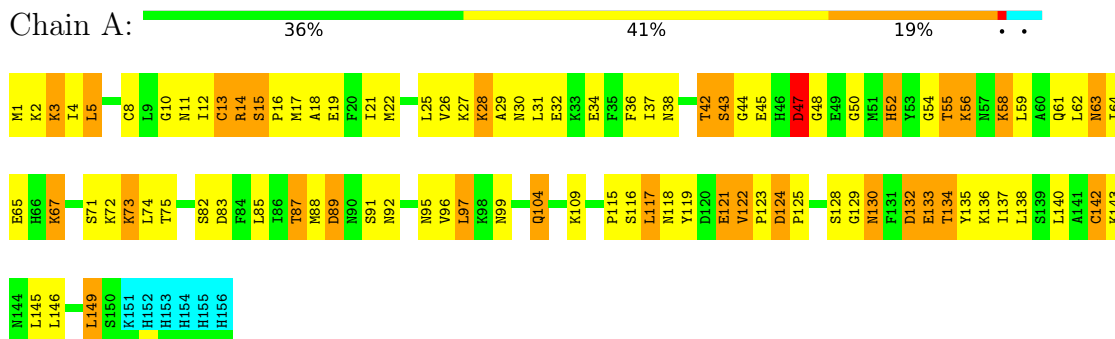


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

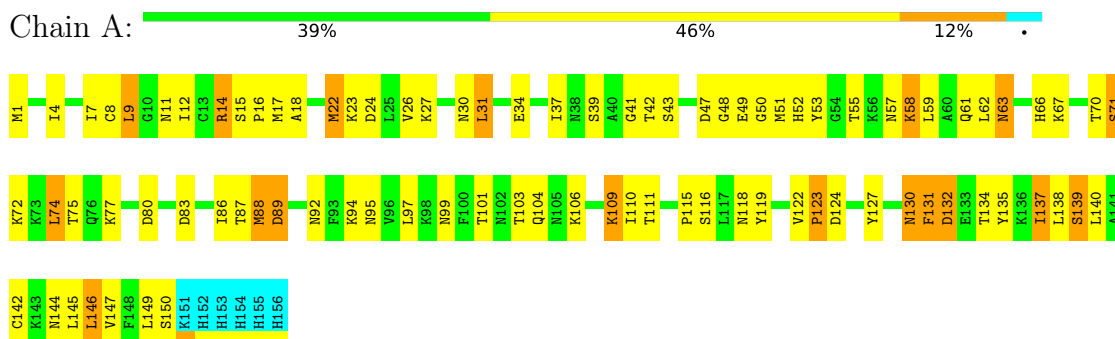
4.2.1 Score per residue for model 1

- Molecule 1: possible phosphotyrosine protein phosphatase



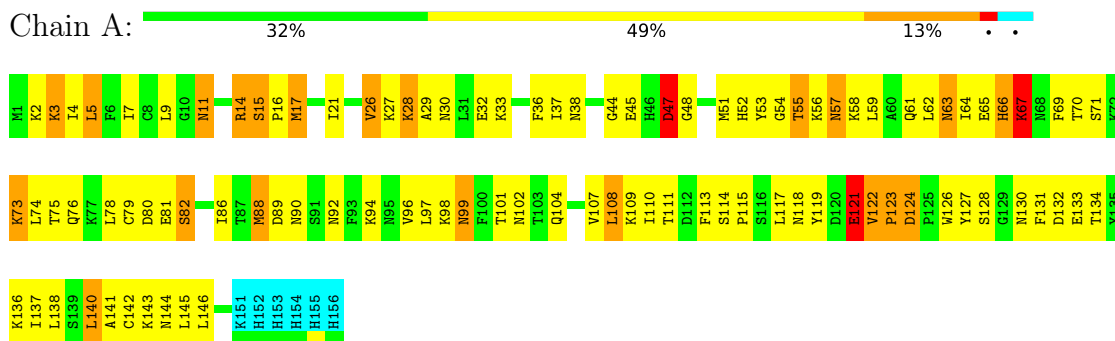
4.2.2 Score per residue for model 2

- Molecule 1: possible phosphotyrosine protein phosphatase



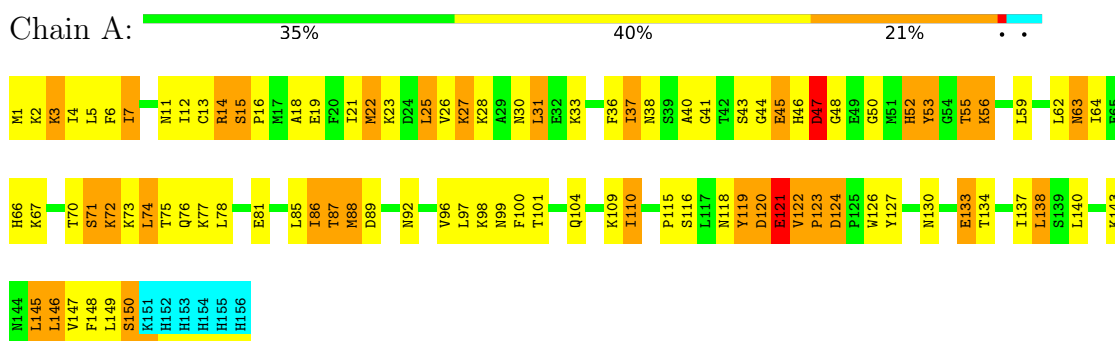
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: possible phosphotyrosine protein phosphatase



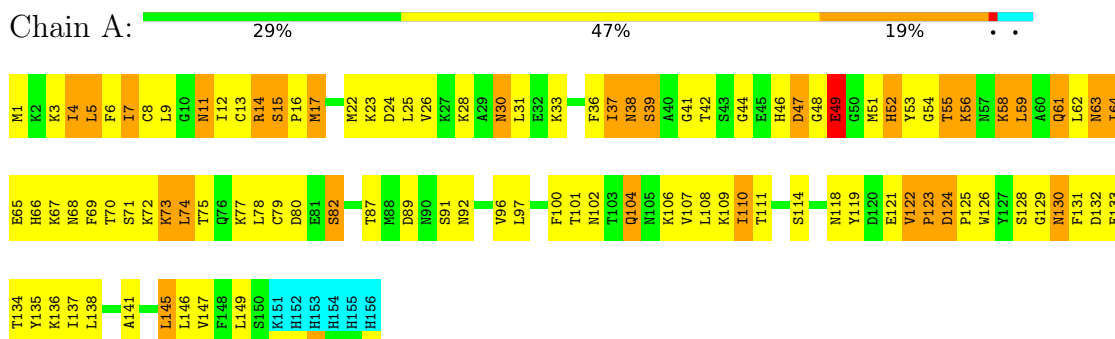
4.2.4 Score per residue for model 4

- Molecule 1: possible phosphotyrosine protein phosphatase



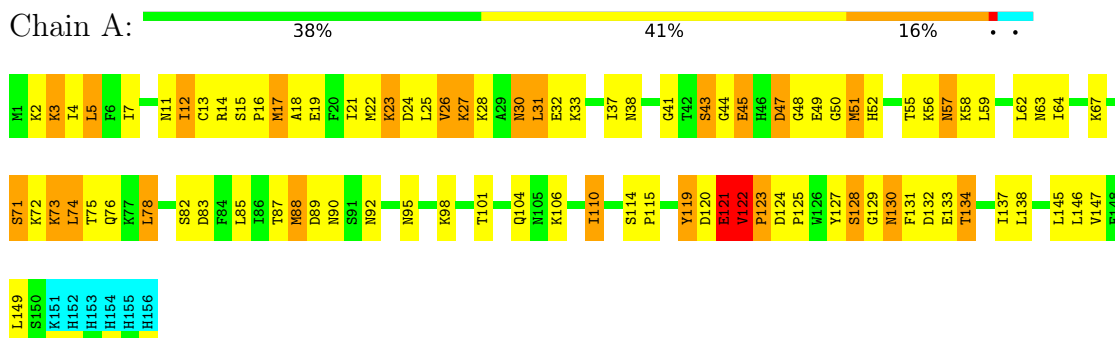
4.2.5 Score per residue for model 5

- Molecule 1: possible phosphotyrosine protein phosphatase



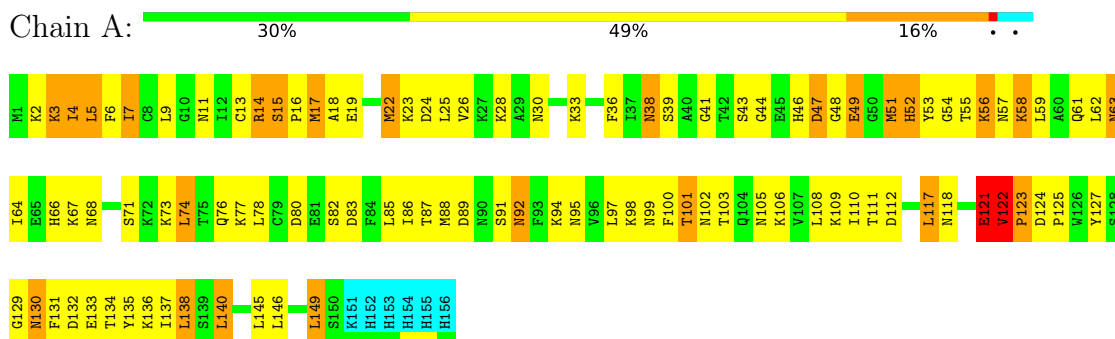
4.2.6 Score per residue for model 6

- Molecule 1: possible phosphotyrosine protein phosphatase



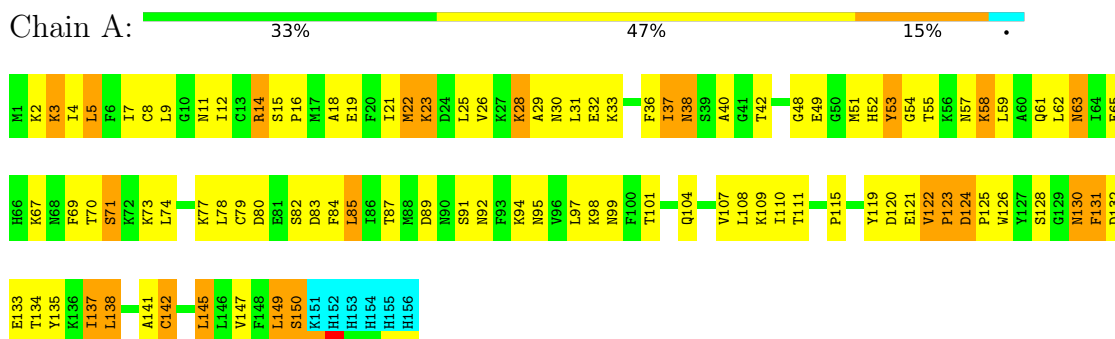
4.2.7 Score per residue for model 7

- Molecule 1: possible phosphotyrosine protein phosphatase



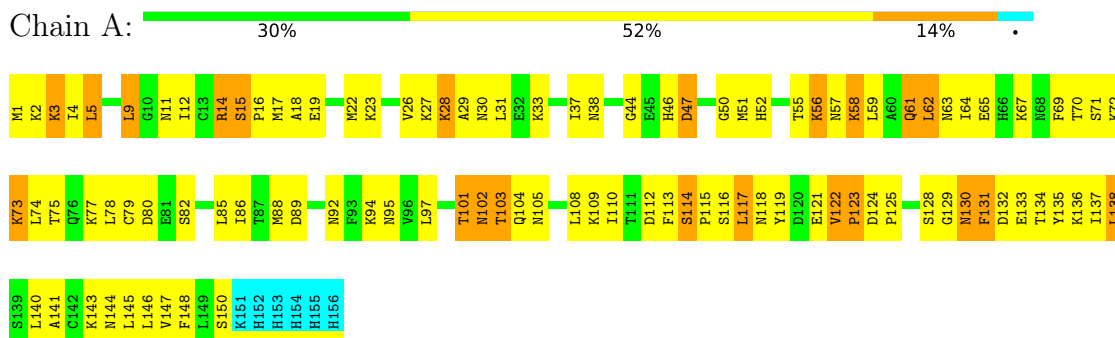
4.2.8 Score per residue for model 8

- Molecule 1: possible phosphotyrosine protein phosphatase



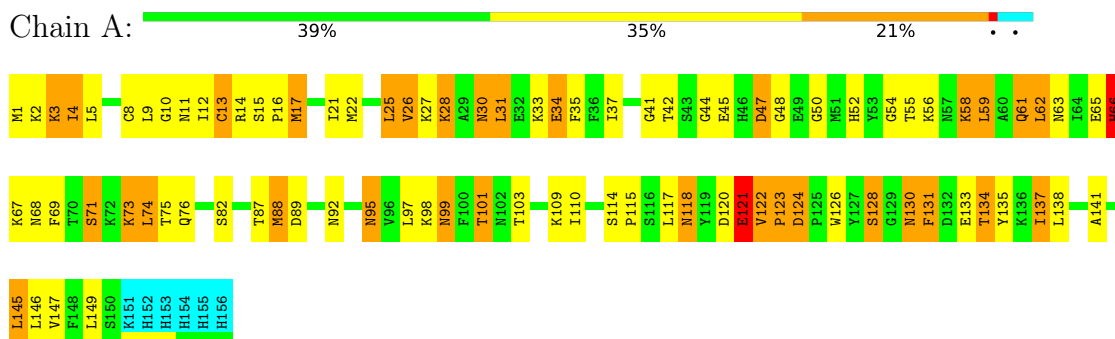
4.2.9 Score per residue for model 9

- Molecule 1: possible phosphotyrosine protein phosphatase



4.2.10 Score per residue for model 10

- Molecule 1: possible phosphotyrosine protein phosphatase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Simulated annealing using torsion angle and Cartesian dynamics*.

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.0

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1203	1210	1207	52±7
All	All	12030	12100	12070	515

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HD21	1:A:137:ILE:HG23	0.77	1.55	10	1
1:A:44:GLY:HA3	1:A:73:LYS:HB3	0.76	1.54	7	7
1:A:123:PRO:HB3	1:A:137:ILE:HG13	0.76	1.56	5	5
1:A:61:GLN:HB3	1:A:62:LEU:HD13	0.76	1.58	9	2
1:A:18:ALA:HA	1:A:21:ILE:HG12	0.76	1.57	6	3
1:A:48:GLY:HA3	1:A:71:SER:HA	0.74	1.60	6	9
1:A:89:ASP:HB2	1:A:92:ASN:HB2	0.74	1.57	6	10
1:A:59:LEU:HA	1:A:63:ASN:HB2	0.73	1.60	7	8
1:A:27:LYS:HA	1:A:31:LEU:HB2	0.72	1.61	6	2
1:A:11:ASN:HA	1:A:15:SER:HB3	0.72	1.62	10	6
1:A:64:ILE:HG21	1:A:67:LYS:HD3	0.70	1.62	3	1
1:A:55:THR:HA	1:A:134:THR:HG21	0.70	1.61	10	2
1:A:130:ASN:ND2	1:A:133:GLU:H	0.69	1.86	8	1
1:A:21:ILE:HG13	1:A:22:MET:N	0.69	2.03	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:MET:HG3	1:A:110:ILE:HB	0.68	1.66	2	2
1:A:4:ILE:HG12	1:A:149:LEU:HD11	0.68	1.66	2	1
1:A:4:ILE:HG21	1:A:149:LEU:HD13	0.68	1.64	5	2
1:A:14:ARG:HB3	1:A:122:VAL:HB	0.66	1.68	6	2
1:A:26:VAL:HA	1:A:30:ASN:HB2	0.65	1.67	10	2
1:A:7:ILE:HG12	1:A:74:LEU:HD13	0.65	1.68	4	4
1:A:14:ARG:HA	1:A:138:LEU:HD21	0.65	1.67	7	2
1:A:53:TYR:O	1:A:124:ASP:HB2	0.64	1.93	5	3
1:A:58:LYS:HE2	1:A:135:TYR:HB2	0.64	1.69	9	1
1:A:13:CYS:O	1:A:55:THR:HG21	0.64	1.92	1	2
1:A:123:PRO:HG3	1:A:137:ILE:HG13	0.63	1.69	2	2
1:A:14:ARG:HB3	1:A:122:VAL:HG13	0.63	1.69	4	3
1:A:58:LYS:HG3	1:A:135:TYR:HB2	0.63	1.70	8	3
1:A:18:ALA:O	1:A:22:MET:HB2	0.63	1.94	4	4
1:A:13:CYS:SG	1:A:122:VAL:HG11	0.62	2.34	1	2
1:A:58:LYS:HE3	1:A:135:TYR:HB2	0.62	1.71	1	2
1:A:27:LYS:HA	1:A:31:LEU:HD23	0.62	1.71	10	1
1:A:97:LEU:HG	1:A:104:GLN:HG3	0.62	1.71	1	1
1:A:17:MET:HE3	1:A:55:THR:HB	0.62	1.71	5	1
1:A:4:ILE:HG21	1:A:149:LEU:HD12	0.62	1.70	7	1
1:A:109:LYS:HB2	1:A:111:THR:HG22	0.61	1.71	5	1
1:A:55:THR:N	1:A:134:THR:HG21	0.61	2.10	4	6
1:A:123:PRO:HB3	1:A:133:GLU:HG3	0.61	1.73	8	2
1:A:125:PRO:HD3	1:A:131:PHE:HA	0.61	1.73	9	2
1:A:14:ARG:HB3	1:A:123:PRO:HD2	0.60	1.72	10	1
1:A:12:ILE:HG22	1:A:50:GLY:H	0.60	1.57	2	2
1:A:3:LYS:HB3	1:A:82:SER:HA	0.60	1.74	3	6
1:A:3:LYS:HG2	1:A:36:PHE:HB2	0.60	1.72	1	1
1:A:17:MET:HE1	1:A:58:LYS:HD3	0.60	1.72	1	1
1:A:17:MET:HA	1:A:67:LYS:HG2	0.59	1.75	7	1
1:A:133:GLU:O	1:A:137:ILE:HG12	0.58	1.98	10	9
1:A:21:ILE:HG13	1:A:22:MET:H	0.58	1.58	4	2
1:A:33:LYS:O	1:A:34:GLU:HB3	0.58	1.97	10	1
1:A:130:ASN:HD22	1:A:131:PHE:N	0.58	1.97	6	4
1:A:4:ILE:HD12	1:A:149:LEU:HD21	0.58	1.75	10	1
1:A:55:THR:HB	1:A:134:THR:HG21	0.58	1.74	8	1
1:A:102:ASN:HA	1:A:104:GLN:HE21	0.57	1.59	5	1
1:A:4:ILE:HG23	1:A:86:ILE:HD13	0.57	1.76	9	1
1:A:14:ARG:HB2	1:A:138:LEU:HD11	0.57	1.75	1	1
1:A:21:ILE:HD11	1:A:142:CYS:SG	0.56	2.40	8	1
1:A:130:ASN:HD22	1:A:132:ASP:H	0.56	1.42	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:LEU:N	1:A:62:LEU:HD22	0.56	2.15	10	1
1:A:3:LYS:HB2	1:A:82:SER:HA	0.56	1.77	6	2
1:A:62:LEU:HD22	1:A:62:LEU:H	0.56	1.59	10	1
1:A:54:GLY:HA2	1:A:131:PHE:HB3	0.56	1.76	10	2
1:A:123:PRO:HG2	1:A:134:THR:HA	0.55	1.77	2	2
1:A:11:ASN:HB3	1:A:48:GLY:N	0.55	2.17	2	2
1:A:11:ASN:HA	1:A:15:SER:OG	0.54	2.03	4	3
1:A:134:THR:O	1:A:138:LEU:HB2	0.54	2.02	8	7
1:A:121:GLU:O	1:A:122:VAL:HG22	0.54	2.01	8	3
1:A:14:ARG:HG2	1:A:122:VAL:HG22	0.54	1.79	10	1
1:A:125:PRO:HA	1:A:129:GLY:H	0.54	1.62	1	2
1:A:15:SER:N	1:A:16:PRO:HD2	0.54	2.18	2	7
1:A:26:VAL:O	1:A:30:ASN:N	0.54	2.41	6	4
1:A:12:ILE:HG22	1:A:49:GLU:HB2	0.54	1.79	6	2
1:A:62:LEU:H	1:A:62:LEU:HD22	0.53	1.62	9	1
1:A:11:ASN:HB2	1:A:47:ASP:HB3	0.53	1.80	1	2
1:A:132:ASP:O	1:A:135:TYR:HB3	0.53	2.04	1	1
1:A:52:HIS:O	1:A:56:LYS:HB2	0.53	2.04	1	2
1:A:109:LYS:HD2	1:A:111:THR:HB	0.53	1.79	2	1
1:A:8:CYS:HB2	1:A:15:SER:HB2	0.53	1.81	10	1
1:A:12:ILE:HA	1:A:50:GLY:HA2	0.52	1.80	2	3
1:A:88:MET:HA	1:A:110:ILE:HB	0.52	1.80	6	1
1:A:33:LYS:O	1:A:34:GLU:CB	0.52	2.56	10	1
1:A:14:ARG:O	1:A:138:LEU:HD11	0.52	2.05	10	3
1:A:64:ILE:HG22	1:A:66:HIS:H	0.52	1.65	4	3
1:A:14:ARG:HD3	1:A:88:MET:HE3	0.52	1.82	9	1
1:A:55:THR:O	1:A:59:LEU:HG	0.52	2.04	7	4
1:A:11:ASN:HA	1:A:15:SER:CB	0.52	2.35	6	9
1:A:7:ILE:HG12	1:A:74:LEU:HD22	0.52	1.80	6	1
1:A:8:CYS:SG	1:A:15:SER:HB2	0.52	2.45	1	1
1:A:134:THR:HG22	1:A:138:LEU:HD22	0.52	1.82	1	1
1:A:130:ASN:ND2	1:A:133:GLU:N	0.52	2.58	8	1
1:A:114:SER:HB3	1:A:117:LEU:HB3	0.51	1.81	3	1
1:A:119:TYR:HE2	1:A:122:VAL:H	0.51	1.48	4	3
1:A:62:LEU:HD22	1:A:62:LEU:N	0.51	2.19	9	1
1:A:17:MET:O	1:A:21:ILE:HG12	0.51	2.06	1	1
1:A:37:ILE:HD13	1:A:37:ILE:N	0.51	2.20	8	2
1:A:4:ILE:HG13	1:A:149:LEU:HD11	0.51	1.82	7	1
1:A:4:ILE:HG12	1:A:149:LEU:HD13	0.51	1.81	8	1
1:A:86:ILE:HD13	1:A:145:LEU:HD11	0.51	1.82	2	2
1:A:26:VAL:O	1:A:30:ASN:HB2	0.51	2.05	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LEU:HA	1:A:63:ASN:HD22	0.51	1.66	2	3
1:A:17:MET:SD	1:A:21:ILE:HD11	0.51	2.46	3	2
1:A:27:LYS:HE2	1:A:31:LEU:HD22	0.51	1.83	4	1
1:A:28:LYS:HG3	1:A:29:ALA:N	0.51	2.21	3	2
1:A:88:MET:HB3	1:A:110:ILE:HD13	0.51	1.81	3	1
1:A:19:GLU:O	1:A:23:LYS:HB2	0.51	2.05	6	3
1:A:12:ILE:HB	1:A:52:HIS:HB2	0.51	1.83	9	1
1:A:88:MET:HG2	1:A:119:TYR:OH	0.50	2.05	9	1
1:A:52:HIS:H	1:A:55:THR:HB	0.50	1.66	7	2
1:A:117:LEU:HD21	1:A:137:ILE:HA	0.50	1.82	9	2
1:A:57:ASN:OD1	1:A:131:PHE:HB3	0.50	2.06	6	1
1:A:56:LYS:HG3	1:A:57:ASN:N	0.50	2.22	9	2
1:A:130:ASN:CG	1:A:131:PHE:N	0.50	2.70	8	1
1:A:59:LEU:HB3	1:A:64:ILE:O	0.49	2.07	9	4
1:A:10:GLY:O	1:A:12:ILE:HG23	0.49	2.07	10	1
1:A:141:ALA:O	1:A:145:LEU:HB2	0.49	2.07	8	3
1:A:87:THR:O	1:A:109:LYS:HA	0.49	2.07	7	2
1:A:3:LYS:HE3	1:A:83:ASP:HB2	0.49	1.84	6	1
1:A:130:ASN:ND2	1:A:132:ASP:H	0.49	2.05	6	1
1:A:10:GLY:O	1:A:47:ASP:HA	0.49	2.06	10	2
1:A:15:SER:O	1:A:19:GLU:HB2	0.49	2.08	1	3
1:A:145:LEU:O	1:A:149:LEU:HB3	0.49	2.07	8	2
1:A:123:PRO:O	1:A:127:TYR:HB2	0.49	2.08	4	4
1:A:96:VAL:HA	1:A:99:ASN:HB2	0.49	1.83	3	1
1:A:18:ALA:HA	1:A:21:ILE:CG1	0.49	2.37	4	3
1:A:88:MET:HE2	1:A:110:ILE:HD12	0.49	1.83	4	1
1:A:13:CYS:HB3	1:A:122:VAL:HG11	0.48	1.85	4	2
1:A:125:PRO:HA	1:A:129:GLY:N	0.48	2.23	1	1
1:A:5:LEU:HG	1:A:38:ASN:HD22	0.48	1.68	7	1
1:A:22:MET:O	1:A:26:VAL:HG13	0.48	2.07	7	2
1:A:141:ALA:O	1:A:145:LEU:HB3	0.48	2.08	5	2
1:A:12:ILE:H	1:A:12:ILE:HD13	0.48	1.66	6	1
1:A:16:PRO:O	1:A:19:GLU:HB3	0.48	2.08	6	3
1:A:5:LEU:HD21	1:A:78:LEU:HD23	0.48	1.84	6	1
1:A:3:LYS:HG2	1:A:36:PHE:HB3	0.48	1.85	7	1
1:A:12:ILE:O	1:A:52:HIS:HB2	0.48	2.08	4	1
1:A:59:LEU:HD12	1:A:63:ASN:HD22	0.48	1.69	10	1
1:A:138:LEU:O	1:A:142:CYS:HB2	0.48	2.08	1	2
1:A:11:ASN:H	1:A:47:ASP:HB3	0.48	1.68	3	1
1:A:13:CYS:C	1:A:16:PRO:HD2	0.48	2.34	4	1
1:A:143:LYS:O	1:A:147:VAL:HG23	0.48	2.09	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LYS:HD3	1:A:135:TYR:HB2	0.48	1.85	5	1
1:A:5:LEU:HD12	1:A:82:SER:HB2	0.48	1.86	1	1
1:A:86:ILE:HG12	1:A:108:LEU:HD13	0.48	1.85	3	1
1:A:96:VAL:HG13	1:A:100:PHE:HD2	0.48	1.69	4	1
1:A:22:MET:O	1:A:26:VAL:HG23	0.48	2.09	8	2
1:A:89:ASP:HB3	1:A:121:GLU:HG2	0.48	1.85	1	2
1:A:17:MET:HE1	1:A:135:TYR:HA	0.48	1.83	2	1
1:A:4:ILE:HB	1:A:37:ILE:HG22	0.48	1.86	4	1
1:A:120:ASP:O	1:A:121:GLU:C	0.48	2.56	10	2
1:A:5:LEU:HG	1:A:38:ASN:OD1	0.48	2.09	8	1
1:A:123:PRO:HB3	1:A:137:ILE:CG1	0.47	2.38	10	2
1:A:124:ASP:OD1	1:A:126:TRP:HB3	0.47	2.10	10	5
1:A:11:ASN:HA	1:A:15:SER:HG	0.47	1.69	3	2
1:A:44:GLY:HA3	1:A:73:LYS:HB2	0.47	1.86	4	1
1:A:122:VAL:HG13	1:A:123:PRO:HD2	0.47	1.87	9	2
1:A:25:LEU:O	1:A:28:LYS:HG3	0.47	2.10	10	2
1:A:55:THR:H	1:A:134:THR:HG21	0.47	1.70	4	1
1:A:51:MET:HB2	1:A:56:LYS:HB2	0.47	1.86	6	1
1:A:26:VAL:HB	1:A:30:ASN:HB2	0.47	1.86	1	1
1:A:109:LYS:HG3	1:A:112:ASP:HB2	0.47	1.85	7	1
1:A:26:VAL:CA	1:A:30:ASN:HB2	0.47	2.38	8	1
1:A:38:ASN:ND2	1:A:38:ASN:N	0.47	2.62	8	1
1:A:11:ASN:CB	1:A:47:ASP:HB3	0.47	2.40	10	2
1:A:130:ASN:HD22	1:A:132:ASP:N	0.47	2.06	3	3
1:A:5:LEU:HD12	1:A:82:SER:HB3	0.47	1.87	3	1
1:A:14:ARG:NH2	1:A:110:ILE:HG13	0.47	2.24	8	1
1:A:110:ILE:O	1:A:114:SER:HB3	0.47	2.10	9	1
1:A:88:MET:HG2	1:A:89:ASP:N	0.47	2.25	6	1
1:A:3:LYS:CB	1:A:82:SER:HA	0.47	2.40	8	7
1:A:87:THR:HG22	1:A:92:ASN:HB3	0.46	1.87	4	1
1:A:4:ILE:CD1	1:A:149:LEU:HD21	0.46	2.39	10	1
1:A:117:LEU:HD13	1:A:137:ILE:HD13	0.46	1.86	7	1
1:A:14:ARG:HG3	1:A:15:SER:N	0.46	2.25	5	4
1:A:128:SER:HB2	1:A:133:GLU:HG3	0.46	1.85	10	1
1:A:42:THR:HB	1:A:92:ASN:HD21	0.46	1.69	1	1
1:A:110:ILE:O	1:A:114:SER:N	0.46	2.48	5	1
1:A:17:MET:HB3	1:A:138:LEU:HG	0.46	1.87	7	1
1:A:41:GLY:O	1:A:74:LEU:HB3	0.46	2.11	6	5
1:A:101:THR:C	1:A:103:THR:H	0.46	2.19	2	4
1:A:28:LYS:HD3	1:A:29:ALA:HB2	0.46	1.86	1	1
1:A:87:THR:O	1:A:88:MET:HB2	0.46	2.10	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ILE:HD13	1:A:37:ILE:H	0.46	1.69	8	2
1:A:86:ILE:HG21	1:A:145:LEU:HD21	0.46	1.85	4	1
1:A:30:ASN:O	1:A:35:PHE:HB2	0.46	2.10	10	1
1:A:14:ARG:NH2	1:A:88:MET:HB3	0.46	2.25	4	1
1:A:146:LEU:O	1:A:150:SER:HB2	0.46	2.10	4	1
1:A:58:LYS:NZ	1:A:61:GLN:HE21	0.46	2.08	5	1
1:A:145:LEU:O	1:A:149:LEU:HG	0.46	2.10	6	1
1:A:17:MET:SD	1:A:59:LEU:HD11	0.46	2.51	10	1
1:A:142:CYS:O	1:A:146:LEU:HB2	0.45	2.11	2	2
1:A:18:ALA:HB2	1:A:138:LEU:HD11	0.45	1.86	4	2
1:A:141:ALA:HA	1:A:144:ASN:ND2	0.45	2.26	9	1
1:A:6:PHE:O	1:A:39:SER:HA	0.45	2.11	7	2
1:A:128:SER:HB3	1:A:133:GLU:OE1	0.45	2.12	6	1
1:A:6:PHE:CE1	1:A:145:LEU:HD21	0.45	2.46	7	1
1:A:12:ILE:HG21	1:A:49:GLU:HB2	0.45	1.88	5	1
1:A:95:ASN:O	1:A:99:ASN:HB2	0.45	2.11	1	2
1:A:9:LEU:HG	1:A:92:ASN:HD22	0.45	1.71	2	1
1:A:8:CYS:O	1:A:41:GLY:HA2	0.45	2.12	5	1
1:A:58:LYS:O	1:A:61:GLN:HB2	0.45	2.11	9	1
1:A:43:SER:HB2	1:A:45:GLU:HG3	0.45	1.89	1	1
1:A:96:VAL:O	1:A:100:PHE:HB2	0.45	2.12	5	1
1:A:16:PRO:HG3	1:A:50:GLY:O	0.45	2.11	6	1
1:A:110:ILE:HG21	1:A:119:TYR:CZ	0.45	2.47	9	1
1:A:113:PHE:HD2	1:A:144:ASN:HB3	0.45	1.72	3	1
1:A:130:ASN:ND2	1:A:133:GLU:HG2	0.45	2.27	3	1
1:A:130:ASN:HB3	1:A:133:GLU:HG2	0.45	1.88	5	1
1:A:5:LEU:HG	1:A:38:ASN:HB2	0.44	1.89	6	1
1:A:44:GLY:HA2	1:A:47:ASP:HB2	0.44	1.89	10	1
1:A:43:SER:HB3	1:A:45:GLU:HG3	0.44	1.88	6	1
1:A:149:LEU:HG	1:A:150:SER:N	0.44	2.26	8	1
1:A:14:ARG:NH2	1:A:88:MET:HB2	0.44	2.28	3	1
1:A:85:LEU:O	1:A:107:VAL:HA	0.44	2.12	8	1
1:A:12:ILE:C	1:A:16:PRO:HG3	0.44	2.38	9	1
1:A:14:ARG:HG2	1:A:122:VAL:HG12	0.44	1.89	6	1
1:A:130:ASN:HD21	1:A:132:ASP:N	0.44	2.10	8	1
1:A:44:GLY:HA3	1:A:73:LYS:CB	0.44	2.35	7	1
1:A:13:CYS:HA	1:A:52:HIS:HB2	0.43	1.89	6	1
1:A:16:PRO:HG2	1:A:50:GLY:HA2	0.43	1.89	1	1
1:A:11:ASN:C	1:A:16:PRO:HD3	0.43	2.38	9	1
1:A:7:ILE:HD11	1:A:85:LEU:HD12	0.43	1.90	7	1
1:A:9:LEU:HD13	1:A:9:LEU:O	0.43	2.13	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:MET:SD	1:A:110:ILE:HD13	0.43	2.54	10	1
1:A:125:PRO:HA	1:A:129:GLY:CA	0.43	2.44	5	3
1:A:24:ASP:O	1:A:27:LYS:HG3	0.43	2.13	6	1
1:A:134:THR:O	1:A:138:LEU:HD12	0.43	2.14	6	1
1:A:55:THR:HG23	1:A:134:THR:HG21	0.43	1.89	1	1
1:A:11:ASN:HB2	1:A:48:GLY:N	0.43	2.29	6	1
1:A:128:SER:HB2	1:A:133:GLU:CD	0.43	2.39	8	1
1:A:11:ASN:HB2	1:A:47:ASP:C	0.43	2.38	9	1
1:A:17:MET:HE3	1:A:138:LEU:HD13	0.42	1.91	6	1
1:A:11:ASN:HB3	1:A:47:ASP:C	0.42	2.38	4	1
1:A:135:TYR:O	1:A:139:SER:HB2	0.42	2.13	2	1
1:A:119:TYR:HE2	1:A:122:VAL:N	0.42	2.11	4	1
1:A:123:PRO:HG3	1:A:137:ILE:HB	0.42	1.90	6	1
1:A:66:HIS:NE2	1:A:69:PHE:HB2	0.42	2.28	10	1
1:A:64:ILE:C	1:A:66:HIS:H	0.42	2.21	4	2
1:A:55:THR:CA	1:A:134:THR:HG21	0.42	2.45	5	1
1:A:64:ILE:O	1:A:66:HIS:N	0.42	2.52	5	1
1:A:59:LEU:HD13	1:A:67:LYS:HD3	0.42	1.91	7	1
1:A:15:SER:HB3	1:A:16:PRO:HD3	0.42	1.91	8	1
1:A:16:PRO:HG3	1:A:50:GLY:HA2	0.42	1.92	10	1
1:A:13:CYS:O	1:A:16:PRO:HD2	0.42	2.14	1	1
1:A:22:MET:O	1:A:26:VAL:HG22	0.42	2.15	4	1
1:A:26:VAL:HA	1:A:30:ASN:ND2	0.42	2.30	7	1
1:A:61:GLN:C	1:A:62:LEU:HD13	0.42	2.39	10	1
1:A:59:LEU:HD23	1:A:63:ASN:CB	0.42	2.44	6	2
1:A:136:LYS:O	1:A:140:LEU:HB2	0.42	2.14	3	2
1:A:6:PHE:HB2	1:A:38:ASN:O	0.42	2.14	4	1
1:A:55:THR:HG23	1:A:134:THR:HB	0.42	1.91	4	1
1:A:16:PRO:HB2	1:A:51:MET:HE2	0.42	1.91	8	1
1:A:110:ILE:HD11	1:A:141:ALA:HB1	0.42	1.91	5	1
1:A:54:GLY:O	1:A:57:ASN:HB3	0.42	2.14	7	1
1:A:85:LEU:C	1:A:86:ILE:HD12	0.42	2.39	9	1
1:A:117:LEU:O	1:A:118:ASN:C	0.42	2.63	1	2
1:A:123:PRO:CG	1:A:134:THR:HA	0.42	2.45	10	1
1:A:17:MET:HG3	1:A:55:THR:HG23	0.41	1.92	7	1
1:A:121:GLU:O	1:A:127:TYR:CD2	0.41	2.73	7	1
1:A:7:ILE:HA	1:A:40:ALA:O	0.41	2.15	8	1
1:A:54:GLY:C	1:A:134:THR:HG21	0.41	2.40	3	1
1:A:110:ILE:HG13	1:A:114:SER:OG	0.41	2.15	10	1
1:A:18:ALA:O	1:A:22:MET:HG3	0.41	2.15	1	1
1:A:27:LYS:HA	1:A:31:LEU:HB3	0.41	1.90	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:LYS:HA	1:A:36:PHE:O	0.41	2.15	8	1
1:A:130:ASN:ND2	1:A:132:ASP:N	0.41	2.69	8	1
1:A:5:LEU:HB2	1:A:82:SER:OG	0.41	2.16	9	1
1:A:17:MET:HG2	1:A:138:LEU:HD23	0.41	1.93	1	1
1:A:54:GLY:HA3	1:A:124:ASP:HA	0.41	1.92	1	1
1:A:123:PRO:HG2	1:A:134:THR:HG22	0.41	1.92	3	1
1:A:5:LEU:HG	1:A:38:ASN:ND2	0.41	2.30	5	1
1:A:52:HIS:O	1:A:56:LYS:HG3	0.41	2.15	5	1
1:A:23:LYS:O	1:A:26:VAL:HG22	0.41	2.16	7	1
1:A:28:LYS:HE3	1:A:29:ALA:HB2	0.41	1.91	9	1
1:A:48:GLY:CA	1:A:71:SER:HA	0.41	2.46	10	1
1:A:5:LEU:HB2	1:A:82:SER:CB	0.41	2.46	3	2
1:A:40:ALA:CB	1:A:72:LYS:HB3	0.41	2.46	4	1
1:A:11:ASN:HB2	1:A:47:ASP:CA	0.41	2.45	6	1
1:A:130:ASN:HD22	1:A:131:PHE:H	0.41	1.58	6	1
1:A:11:ASN:HA	1:A:15:SER:HB2	0.41	1.91	7	1
1:A:61:GLN:HB3	1:A:62:LEU:CD1	0.41	2.39	10	1
1:A:55:THR:CG2	1:A:56:LYS:N	0.41	2.84	3	1
1:A:3:LYS:NZ	1:A:81:GLU:HB3	0.41	2.31	4	1
1:A:59:LEU:CA	1:A:63:ASN:HB2	0.40	2.45	5	1
1:A:145:LEU:O	1:A:149:LEU:HB2	0.40	2.15	2	1
1:A:85:LEU:HB3	1:A:107:VAL:HG22	0.40	1.93	8	1
1:A:3:LYS:C	1:A:4:ILE:HD13	0.40	2.41	10	1
1:A:17:MET:O	1:A:21:ILE:HG13	0.40	2.15	3	1
1:A:15:SER:N	1:A:16:PRO:CD	0.40	2.85	4	1
1:A:7:ILE:HB	1:A:87:THR:HG22	0.40	1.93	2	1
1:A:57:ASN:CG	1:A:131:PHE:HB3	0.40	2.42	3	1
1:A:2:LYS:HD3	1:A:84:PHE:HE2	0.40	1.76	8	1
1:A:54:GLY:HA2	1:A:131:PHE:CA	0.40	2.46	8	1
1:A:58:LYS:HE2	1:A:135:TYR:CB	0.40	2.43	9	1
1:A:101:THR:C	1:A:103:THR:N	0.40	2.80	2	1
1:A:4:ILE:CG2	1:A:149:LEU:HD13	0.40	2.41	5	1
1:A:74:LEU:HD21	1:A:100:PHE:HZ	0.40	1.77	7	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	149/156 (96%)	118±3 (80±2%)	24±4 (16±2%)	7±2 (5±1%)	3	25
All	All	1490/1560 (96%)	1185 (80%)	235 (16%)	70 (5%)	3	25

All 19 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	122	VAL	10
1	A	123	PRO	10
1	A	115	PRO	8
1	A	63	ASN	7
1	A	121	GLU	6
1	A	47	ASP	5
1	A	53	TYR	5
1	A	118	ASN	4
1	A	67	LYS	2
1	A	45	GLU	2
1	A	49	GLU	2
1	A	65	GLU	2
1	A	51	MET	1
1	A	68	ASN	1
1	A	150	SER	1
1	A	50	GLY	1
1	A	102	ASN	1
1	A	34	GLU	1
1	A	66	HIS	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	138/144 (96%)	82±5 (59±4%)	56±5 (41±4%)	0	5
All	All	1380/1440 (96%)	821 (59%)	559 (41%)	0	5

All 120 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	62	LEU	10
1	A	74	LEU	10
1	A	124	ASP	10
1	A	5	LEU	9
1	A	37	ILE	9
1	A	58	LYS	9
1	A	67	LYS	9
1	A	97	LEU	9
1	A	130	ASN	9
1	A	3	LYS	8
1	A	14	ARG	8
1	A	28	LYS	8
1	A	47	ASP	8
1	A	52	HIS	8
1	A	61	GLN	8
1	A	75	THR	8
1	A	104	GLN	8
1	A	146	LEU	8
1	A	101	THR	8
1	A	2	LYS	7
1	A	25	LEU	7
1	A	73	LYS	7
1	A	109	LYS	7
1	A	121	GLU	7
1	A	9	LEU	7
1	A	31	LEU	7
1	A	33	LYS	7
1	A	78	LEU	7
1	A	1	MET	6
1	A	15	SER	6
1	A	38	ASN	6
1	A	56	LYS	6
1	A	72	LYS	6
1	A	87	THR	6
1	A	119	TYR	6
1	A	128	SER	6
1	A	140	LEU	6
1	A	22	MET	6
1	A	51	MET	6
1	A	70	THR	6
1	A	71	SER	6
1	A	77	LYS	6
1	A	80	ASP	6

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Mol	Chain	Res	Type	Models (Total)
1	A	88	MET	6
1	A	95	ASN	6
1	A	99	ASN	6
1	A	17	MET	6
1	A	98	LYS	6
1	A	4	ILE	5
1	A	42	THR	5
1	A	43	SER	5
1	A	23	LYS	5
1	A	94	LYS	5
1	A	131	PHE	5
1	A	76	GLN	5
1	A	108	LEU	5
1	A	32	GLU	4
1	A	55	THR	4
1	A	65	GLU	4
1	A	83	ASP	4
1	A	85	LEU	4
1	A	91	SER	4
1	A	116	SER	4
1	A	149	LEU	4
1	A	57	ASN	4
1	A	106	LYS	4
1	A	7	ILE	4
1	A	27	LYS	4
1	A	69	PHE	4
1	A	79	CYS	4
1	A	46	HIS	4
1	A	110	ILE	4
1	A	138	LEU	4
1	A	145	LEU	4
1	A	13	CYS	3
1	A	117	LEU	3
1	A	134	THR	3
1	A	136	LYS	3
1	A	143	LYS	3
1	A	24	ASP	3
1	A	66	HIS	3
1	A	118	ASN	3
1	A	137	ILE	3
1	A	150	SER	3
1	A	26	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	A	36	PHE	3
1	A	45	GLU	3
1	A	102	ASN	3
1	A	111	THR	3
1	A	120	ASP	3
1	A	30	ASN	3
1	A	49	GLU	3
1	A	34	GLU	2
1	A	89	ASP	2
1	A	132	ASP	2
1	A	133	GLU	2
1	A	142	CYS	2
1	A	8	CYS	2
1	A	39	SER	2
1	A	11	ASN	2
1	A	82	SER	2
1	A	90	ASN	2
1	A	107	VAL	2
1	A	148	PHE	2
1	A	59	LEU	2
1	A	68	ASN	2
1	A	12	ILE	2
1	A	114	SER	2
1	A	122	VAL	2
1	A	105	ASN	2
1	A	96	VAL	1
1	A	139	SER	1
1	A	144	ASN	1
1	A	81	GLU	1
1	A	86	ILE	1
1	A	64	ILE	1
1	A	92	ASN	1
1	A	103	THR	1
1	A	112	ASP	1
1	A	113	PHE	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided