



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:04 am GMT

PDB ID : 2RM6
Title : Glutathione peroxidase-type tryparedoxin peroxidase, reduced form
Authors : Melchers, J.; Feher, K.; Diechtierow, M.; Krauth-Siegel, L.; Muhle-Goll, C.
Deposited on : 2007-10-09

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

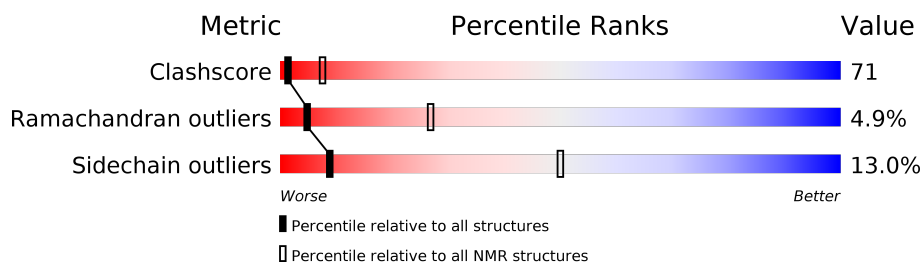
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	167	<div> <div>20%</div> <div>39%</div> <div>10%</div> <div>•</div> <div>31%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:13-A:43, A:52-A:76, A:100-A:111, A:116-A:126, A:137-A:172 (115)	0.21	13

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 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 7, 8, 9, 11, 13, 14, 15, 18, 19, 20
2	6, 12, 16
3	4, 17
Single-model clusters	10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2621 atoms, of which 1309 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Glutathione peroxidase-like protein.

Mol	Chain	Residues	Atoms						Trace
1	A	167	Total	C	H	N	O	S	0
			2621	848	1309	213	246	5	

There are 6 discrepancies between the modelled and reference sequences:

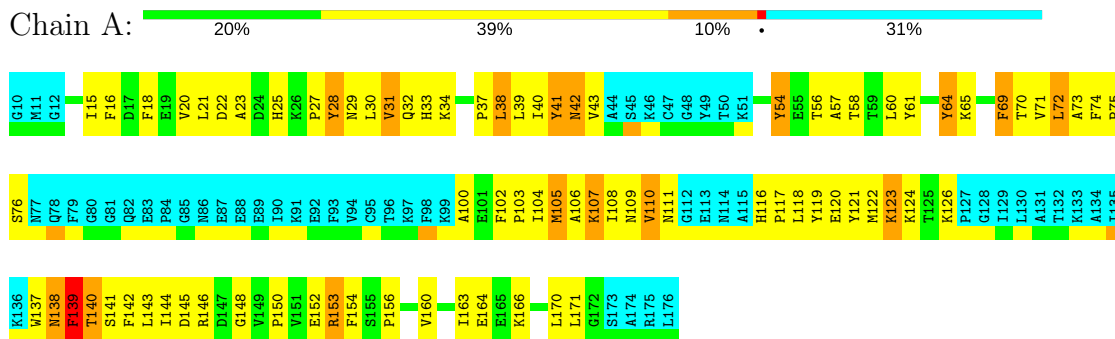
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	EXPRESSION TAG	UNP Q869A5
A	11	MET	-	EXPRESSION TAG	UNP Q869A5
A	12	GLY	-	EXPRESSION TAG	UNP Q869A5
A	59	THR	ALA	SEE REMARK 999	UNP Q869A5
A	76	SER	CYS	ENGINEERED	UNP Q869A5
A	86	ASN	THR	SEE REMARK 999	UNP Q869A5

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Glutathione peroxidase-like protein

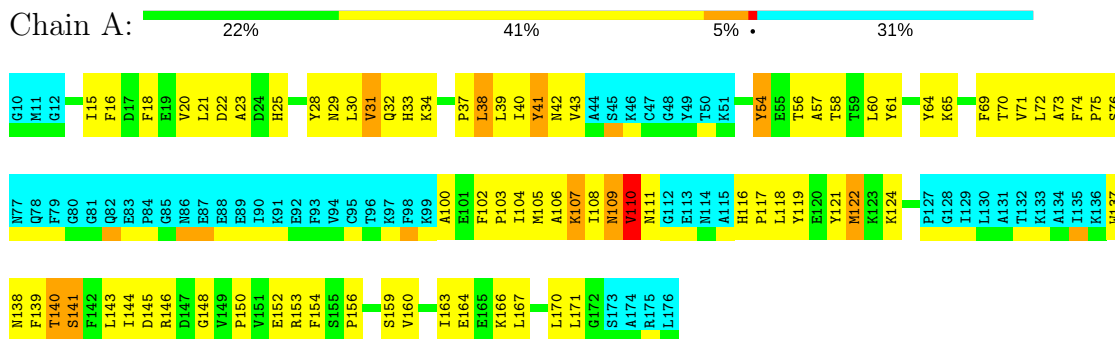


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

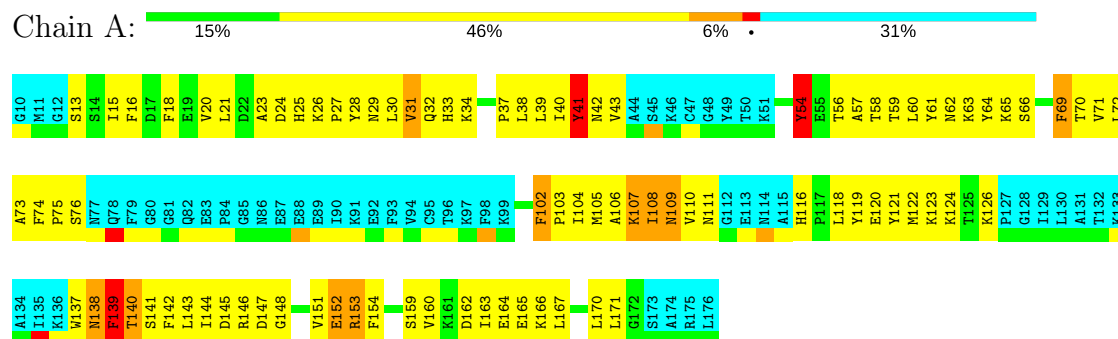
4.2.1 Score per residue for model 1

- Molecule 1: Glutathione peroxidase-like protein



4.2.2 Score per residue for model 2

- Molecule 1: Glutathione peroxidase-like protein



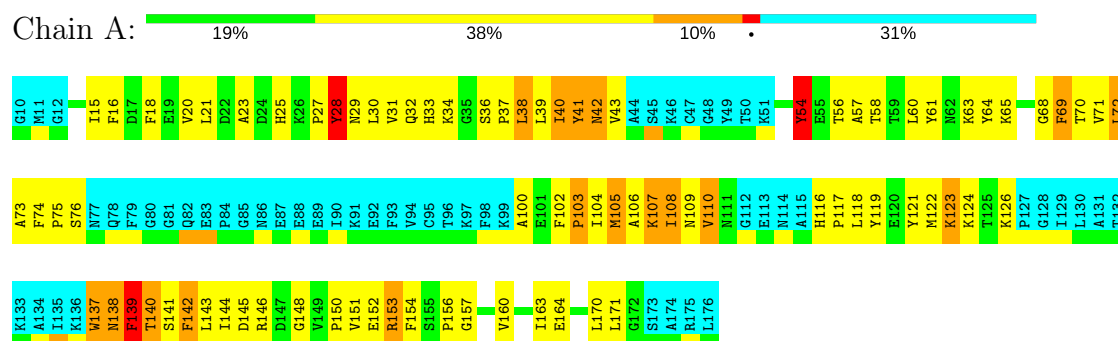
4.2.3 Score per residue for model 3

- Molecule 1: Glutathione peroxidase-like protein



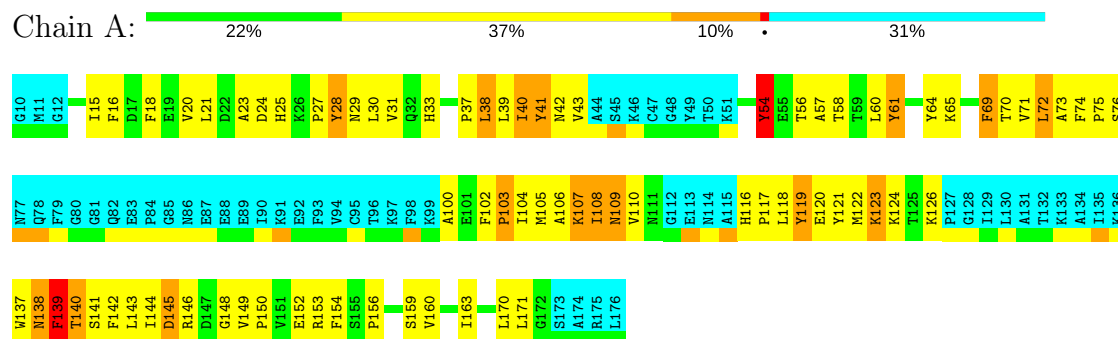
4.2.4 Score per residue for model 4

- Molecule 1: Glutathione peroxidase-like protein



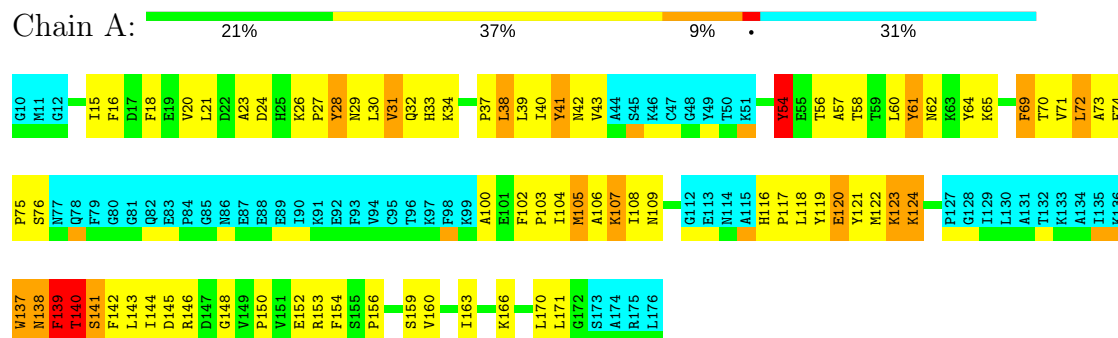
4.2.5 Score per residue for model 5

- Molecule 1: Glutathione peroxidase-like protein



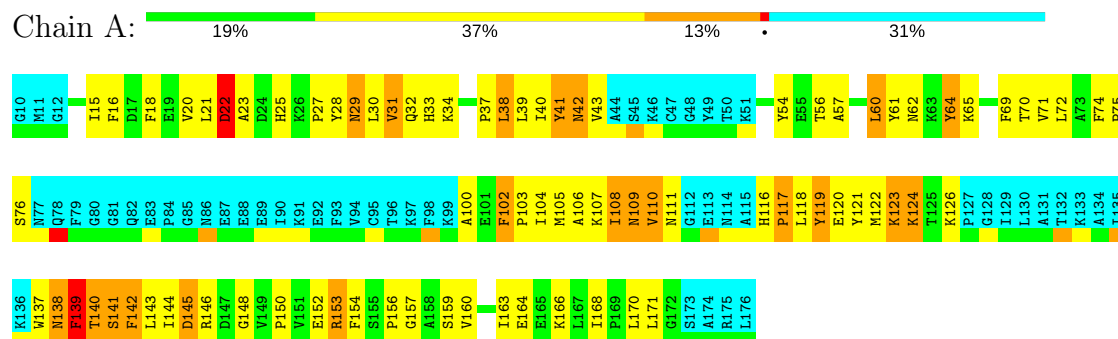
4.2.6 Score per residue for model 6

- Molecule 1: Glutathione peroxidase-like protein



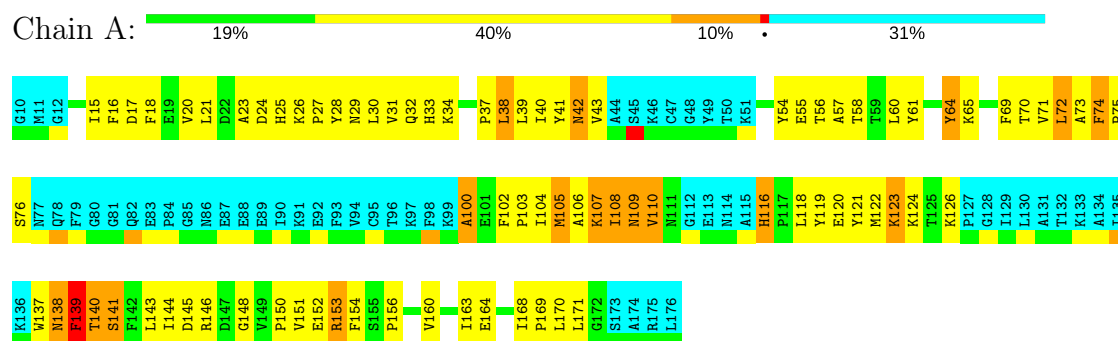
4.2.7 Score per residue for model 7

- Molecule 1: Glutathione peroxidase-like protein



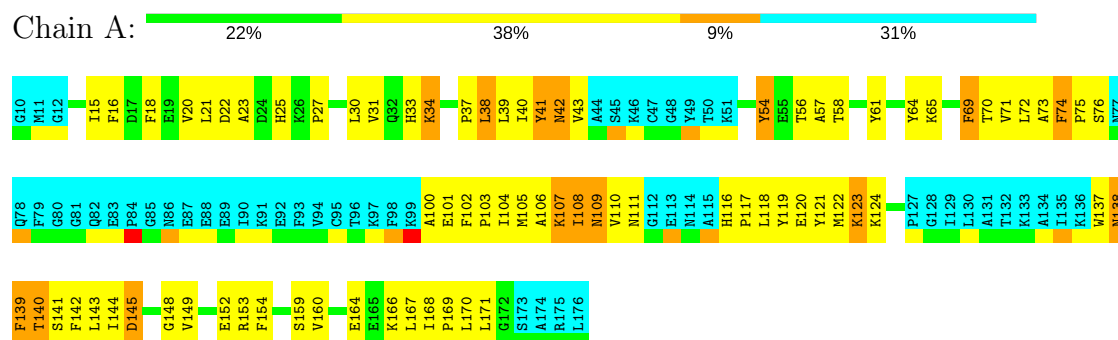
4.2.8 Score per residue for model 8

- Molecule 1: Glutathione peroxidase-like protein



4.2.9 Score per residue for model 9

- Molecule 1: Glutathione peroxidase-like protein



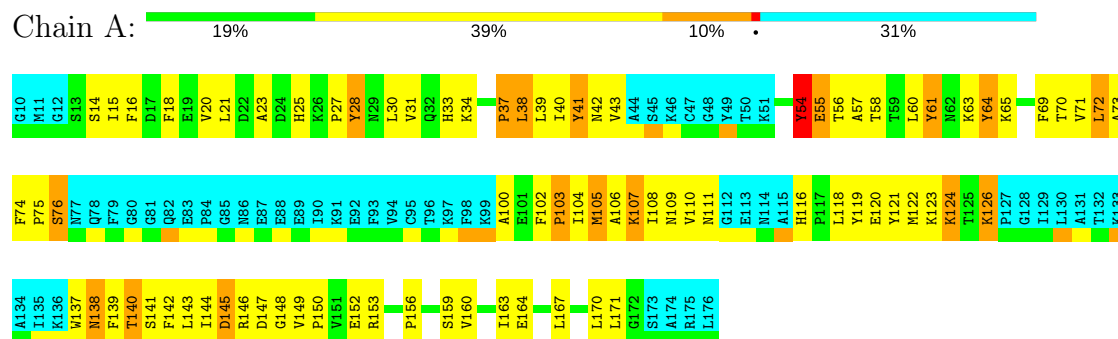
4.2.10 Score per residue for model 10

- Molecule 1: Glutathione peroxidase-like protein



4.2.11 Score per residue for model 11

- Molecule 1: Glutathione peroxidase-like protein



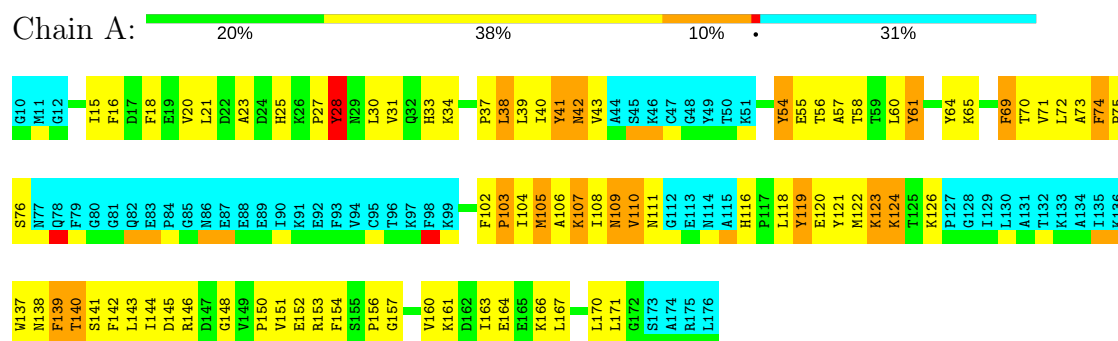
4.2.12 Score per residue for model 12

- Molecule 1: Glutathione peroxidase-like protein



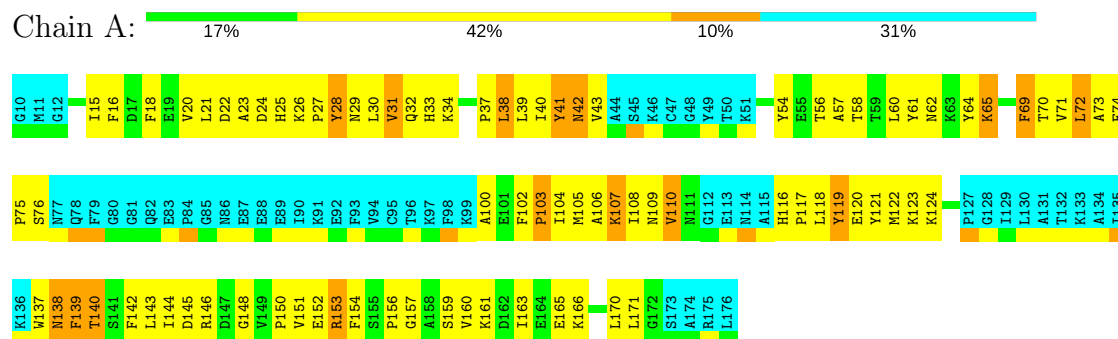
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Glutathione peroxidase-like protein



4.2.14 Score per residue for model 14

- Molecule 1: Glutathione peroxidase-like protein



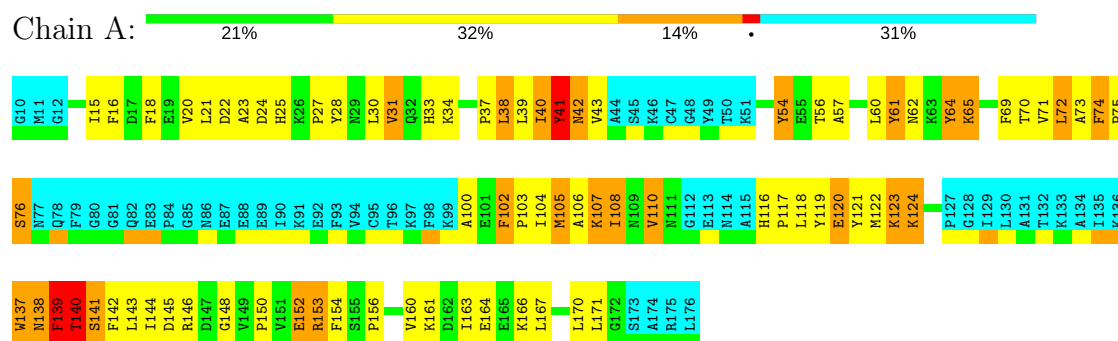
4.2.15 Score per residue for model 15

- Molecule 1: Glutathione peroxidase-like protein



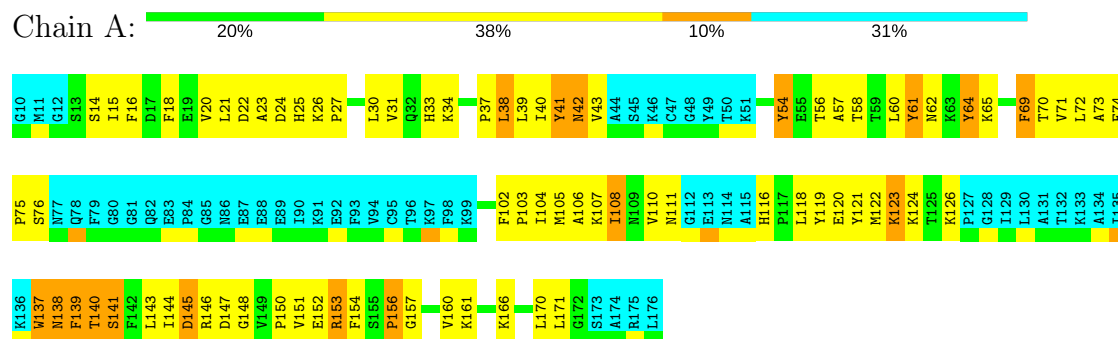
4.2.16 Score per residue for model 16

- Molecule 1: Glutathione peroxidase-like protein



4.2.17 Score per residue for model 17

- Molecule 1: Glutathione peroxidase-like protein



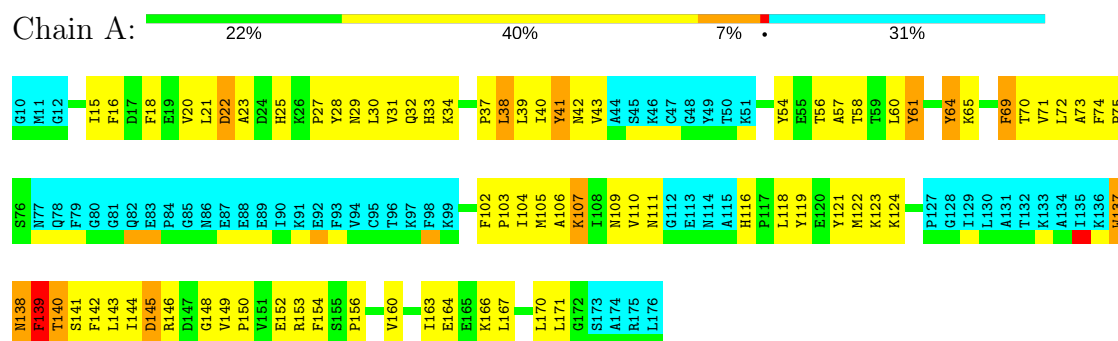
4.2.18 Score per residue for model 18

- Molecule 1: Glutathione peroxidase-like protein



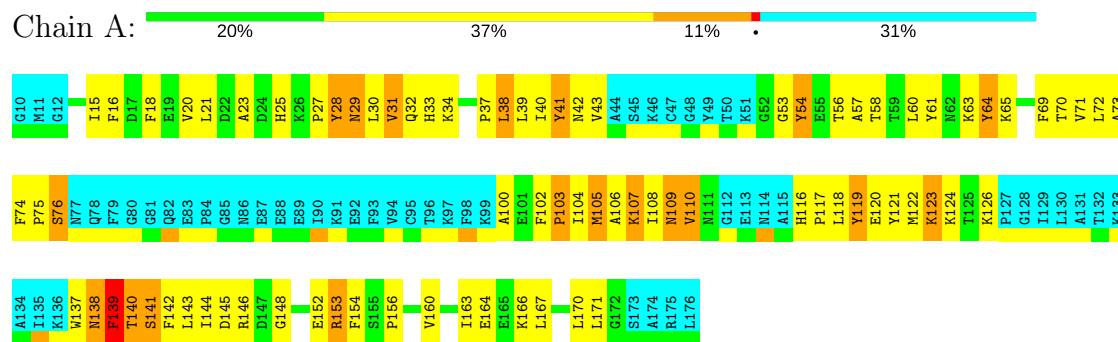
4.2.19 Score per residue for model 19

- Molecule 1: Glutathione peroxidase-like protein



4.2.20 Score per residue for model 20

- Molecule 1: Glutathione peroxidase-like protein



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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
ARIA	structure solution	1.2
ARIA	refinement	1.2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	0.88±0.13	6±3/953 (0.7±0.3%)	0.70±0.03	0±0/1296 (0.0±0.0%)
All	All	0.89	126/19060 (0.7%)	0.70	0/25920 (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	0.5±0.6
All	All	0	9

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	139	PHE	CE1-CZ	11.65	1.59	1.37	19	8
1	A	28	TYR	CE1-CZ	11.62	1.53	1.38	5	6
1	A	28	TYR	CE2-CZ	-11.53	1.23	1.38	5	6
1	A	54	TYR	CE1-CZ	10.80	1.52	1.38	15	12
1	A	54	TYR	CE2-CZ	-10.77	1.24	1.38	15	12
1	A	64	TYR	CE2-CZ	10.74	1.52	1.38	19	11
1	A	64	TYR	CE1-CZ	-10.50	1.24	1.38	19	11
1	A	69	PHE	CE2-CZ	9.55	1.55	1.37	5	12
1	A	139	PHE	CE2-CZ	-9.52	1.19	1.37	19	8
1	A	41	TYR	CE2-CZ	-9.46	1.26	1.38	16	1
1	A	69	PHE	CE1-CZ	-8.56	1.21	1.37	5	12
1	A	41	TYR	CE1-CZ	8.52	1.49	1.38	16	1
1	A	74	PHE	CE1-CZ	7.83	1.52	1.37	16	6
1	A	61	TYR	CE1-CZ	-6.61	1.29	1.38	15	8
1	A	74	PHE	CE2-CZ	-6.50	1.25	1.37	16	4
1	A	61	TYR	CE2-CZ	5.83	1.46	1.38	15	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	142	PHE	CE1-CZ	5.25	1.47	1.37	4	1

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	119	TYR	Sidechain	5
1	A	142	PHE	Sidechain	2
1	A	41	TYR	Sidechain	1
1	A	139	PHE	Sidechain	1

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	925	920	917	131±8
All	All	18500	18400	18340	2617

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 71.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ALA:HB1	1:A:71:VAL:HG11	1.01	1.30	12	20
1:A:40:ILE:HG22	1:A:119:TYR:OH	1.01	1.56	20	18
1:A:39:LEU:HB3	1:A:41:TYR:HE1	0.98	1.15	20	19
1:A:33:HIS:CE1	1:A:70:THR:HB	0.88	2.03	3	20
1:A:73:ALA:HB3	1:A:104:ILE:HD12	0.88	1.41	12	11
1:A:39:LEU:HB3	1:A:41:TYR:CE1	0.87	2.05	20	20
1:A:62:ASN:HA	1:A:65:LYS:HG3	0.86	1.45	2	2
1:A:110:VAL:HA	1:A:119:TYR:OH	0.86	1.71	15	2
1:A:16:PHE:HB3	1:A:31:VAL:HG12	0.84	1.48	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:PRO:HG2	1:A:107:LYS:HB3	0.82	1.50	16	10
1:A:15:ILE:HD12	1:A:30:LEU:HD21	0.81	1.52	13	12
1:A:74:PHE:CE1	1:A:105:MET:HG3	0.81	2.10	3	6
1:A:61:TYR:CD1	1:A:70:THR:HA	0.81	2.10	17	20
1:A:74:PHE:CG	1:A:105:MET:HG2	0.80	2.11	14	9
1:A:21:LEU:O	1:A:105:MET:HB3	0.79	1.78	3	8
1:A:108:ILE:HG13	1:A:116:HIS:CB	0.78	2.08	5	10
1:A:15:ILE:HB	1:A:118:LEU:HD11	0.77	1.54	20	20
1:A:18:PHE:HE2	1:A:121:TYR:HB2	0.77	1.40	16	15
1:A:38:LEU:HB2	1:A:70:THR:HG22	0.77	1.56	9	20
1:A:43:VAL:HA	1:A:139:PHE:HA	0.77	1.56	20	8
1:A:71:VAL:O	1:A:102:PHE:HB3	0.77	1.80	8	4
1:A:43:VAL:O	1:A:75:PRO:HA	0.77	1.79	2	16
1:A:33:HIS:HB2	1:A:38:LEU:HD22	0.77	1.57	2	2
1:A:18:PHE:CE2	1:A:121:TYR:HB2	0.76	2.16	16	19
1:A:43:VAL:HG11	1:A:73:ALA:HB1	0.75	1.59	17	13
1:A:74:PHE:HD2	1:A:108:ILE:HD12	0.75	1.38	7	5
1:A:141:SER:O	1:A:153:ARG:HA	0.75	1.80	20	8
1:A:37:PRO:HG3	1:A:170:LEU:HB3	0.75	1.58	11	16
1:A:72:LEU:H	1:A:72:LEU:HD12	0.75	1.42	16	5
1:A:15:ILE:HB	1:A:118:LEU:CD1	0.74	2.13	17	20
1:A:24:ASP:HB2	1:A:26:LYS:HE2	0.74	1.59	14	5
1:A:21:LEU:O	1:A:105:MET:HB2	0.74	1.83	10	10
1:A:151:VAL:HG13	1:A:152:GLU:HG2	0.74	1.58	8	1
1:A:40:ILE:HG23	1:A:72:LEU:HB2	0.74	1.58	9	6
1:A:16:PHE:CE2	1:A:34:LYS:HG2	0.74	2.18	11	15
1:A:75:PRO:HB2	1:A:107:LYS:HG2	0.73	1.60	9	2
1:A:15:ILE:HG23	1:A:150:PRO:HD3	0.73	1.60	10	15
1:A:118:LEU:HG	1:A:122:MET:HE3	0.73	1.59	6	11
1:A:75:PRO:O	1:A:107:LYS:HB2	0.73	1.83	2	11
1:A:20:VAL:HG13	1:A:74:PHE:HZ	0.72	1.43	16	16
1:A:137:TRP:HB3	1:A:156:PRO:HG3	0.72	1.62	3	13
1:A:56:THR:HG21	1:A:163:ILE:HD12	0.72	1.61	7	7
1:A:21:LEU:HB3	1:A:25:HIS:HA	0.72	1.62	7	7
1:A:40:ILE:HG23	1:A:72:LEU:HD13	0.72	1.61	12	5
1:A:143:LEU:HB3	1:A:152:GLU:HB2	0.72	1.61	3	19
1:A:15:ILE:HG21	1:A:122:MET:HE1	0.72	1.62	9	1
1:A:37:PRO:HG3	1:A:170:LEU:CB	0.72	2.15	3	20
1:A:72:LEU:HA	1:A:103:PRO:HB2	0.71	1.59	10	1
1:A:33:HIS:CB	1:A:38:LEU:HD22	0.71	2.15	7	2
1:A:108:ILE:HG13	1:A:110:VAL:HG22	0.71	1.61	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ALA:HA	1:A:106:ALA:HA	0.71	1.62	13	15
1:A:74:PHE:CD2	1:A:119:TYR:HE2	0.70	2.04	8	3
1:A:20:VAL:HG13	1:A:74:PHE:CZ	0.70	2.20	18	20
1:A:108:ILE:HG13	1:A:116:HIS:HB2	0.70	1.62	4	9
1:A:57:ALA:CB	1:A:71:VAL:HG11	0.70	2.17	19	19
1:A:26:LYS:HE2	1:A:26:LYS:HA	0.70	1.61	18	2
1:A:28:TYR:OH	1:A:103:PRO:HB3	0.69	1.86	6	3
1:A:73:ALA:HB3	1:A:104:ILE:HG13	0.69	1.63	16	4
1:A:16:PHE:HB3	1:A:31:VAL:HG13	0.69	1.64	2	9
1:A:16:PHE:HB3	1:A:31:VAL:CG1	0.69	2.15	3	7
1:A:16:PHE:CE1	1:A:31:VAL:HA	0.69	2.22	9	14
1:A:105:MET:HG3	1:A:106:ALA:N	0.69	2.03	15	2
1:A:33:HIS:HB2	1:A:38:LEU:HD13	0.69	1.61	11	18
1:A:28:TYR:CE2	1:A:72:LEU:HD23	0.69	2.22	16	5
1:A:143:LEU:HD23	1:A:152:GLU:HB2	0.69	1.65	16	1
1:A:38:LEU:O	1:A:144:ILE:HB	0.69	1.88	16	20
1:A:74:PHE:CD1	1:A:105:MET:HG2	0.69	2.23	14	7
1:A:37:PRO:HG2	1:A:171:LEU:HD23	0.69	1.65	11	20
1:A:24:ASP:HB2	1:A:26:LYS:HG2	0.69	1.64	8	1
1:A:39:LEU:HD23	1:A:69:PHE:CE1	0.68	2.23	12	13
1:A:23:ALA:HA	1:A:106:ALA:N	0.68	2.04	12	20
1:A:31:VAL:HG12	1:A:34:LYS:HE2	0.68	1.64	6	1
1:A:72:LEU:HA	1:A:103:PRO:HG2	0.68	1.66	4	9
1:A:28:TYR:CE2	1:A:72:LEU:HD21	0.68	2.24	18	3
1:A:41:TYR:CE1	1:A:71:VAL:HG13	0.67	2.23	12	18
1:A:106:ALA:O	1:A:107:LYS:HG2	0.67	1.89	19	13
1:A:120:GLU:O	1:A:124:LYS:HB3	0.67	1.89	13	12
1:A:31:VAL:HG12	1:A:34:LYS:HG3	0.67	1.67	10	8
1:A:37:PRO:HD3	1:A:146:ARG:HG2	0.67	1.66	14	18
1:A:40:ILE:HD12	1:A:122:MET:CE	0.67	2.19	15	10
1:A:140:THR:HA	1:A:154:PHE:O	0.66	1.90	17	14
1:A:108:ILE:HG13	1:A:116:HIS:HB3	0.66	1.67	9	3
1:A:42:ASN:HB3	1:A:110:VAL:HG11	0.66	1.66	15	1
1:A:16:PHE:CE2	1:A:148:GLY:HA3	0.66	2.26	19	18
1:A:74:PHE:CE1	1:A:105:MET:HB3	0.66	2.26	6	8
1:A:75:PRO:HD2	1:A:107:LYS:HA	0.66	1.68	12	6
1:A:25:HIS:CD2	1:A:106:ALA:HB3	0.66	2.26	19	5
1:A:23:ALA:HA	1:A:106:ALA:CA	0.65	2.21	20	17
1:A:61:TYR:CE1	1:A:65:LYS:HB3	0.65	2.26	13	17
1:A:16:PHE:CD1	1:A:30:LEU:HG	0.65	2.25	2	14
1:A:21:LEU:HB2	1:A:105:MET:HE1	0.65	1.68	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ASN:HD21	1:A:142:PHE:HE2	0.65	1.31	5	1
1:A:16:PHE:CD1	1:A:31:VAL:HA	0.64	2.27	5	17
1:A:62:ASN:HA	1:A:65:LYS:HE2	0.64	1.67	7	1
1:A:151:VAL:HG23	1:A:152:GLU:HG2	0.64	1.70	12	4
1:A:56:THR:HA	1:A:160:VAL:HG22	0.64	1.67	12	17
1:A:41:TYR:CD1	1:A:71:VAL:HG13	0.63	2.28	8	20
1:A:108:ILE:HD11	1:A:110:VAL:HG13	0.63	1.69	16	5
1:A:75:PRO:O	1:A:107:LYS:HE2	0.63	1.93	10	1
1:A:143:LEU:HD11	1:A:170:LEU:HD12	0.63	1.70	2	19
1:A:61:TYR:CZ	1:A:65:LYS:HD2	0.63	2.28	10	5
1:A:73:ALA:HB3	1:A:104:ILE:CD1	0.63	2.23	15	10
1:A:42:ASN:ND2	1:A:140:THR:HB	0.63	2.09	10	3
1:A:20:VAL:O	1:A:27:PRO:HA	0.63	1.93	18	7
1:A:42:ASN:OD1	1:A:76:SER:HB2	0.63	1.94	12	1
1:A:15:ILE:CD1	1:A:144:ILE:HG21	0.62	2.23	5	20
1:A:37:PRO:HG3	1:A:170:LEU:HB2	0.62	1.71	16	13
1:A:72:LEU:HD23	1:A:103:PRO:HB2	0.62	1.71	15	2
1:A:74:PHE:CZ	1:A:105:MET:HG3	0.62	2.30	1	2
1:A:28:TYR:HE2	1:A:72:LEU:HD23	0.62	1.52	16	5
1:A:75:PRO:HG2	1:A:107:LYS:HD2	0.62	1.70	10	1
1:A:143:LEU:HD22	1:A:166:LYS:HB3	0.62	1.70	3	8
1:A:61:TYR:O	1:A:65:LYS:HG2	0.62	1.94	11	14
1:A:74:PHE:CD2	1:A:108:ILE:HD12	0.62	2.29	5	5
1:A:43:VAL:HG12	1:A:139:PHE:CG	0.62	2.30	5	3
1:A:61:TYR:CE1	1:A:70:THR:HA	0.61	2.30	12	18
1:A:43:VAL:HG23	1:A:139:PHE:CD1	0.61	2.30	10	9
1:A:42:ASN:HB2	1:A:110:VAL:HG11	0.61	1.69	7	3
1:A:56:THR:HG23	1:A:160:VAL:HA	0.61	1.72	7	8
1:A:102:PHE:HB2	1:A:103:PRO:HD2	0.61	1.71	7	9
1:A:22:ASP:HA	1:A:105:MET:HE2	0.61	1.71	17	3
1:A:40:ILE:HD12	1:A:122:MET:HE1	0.61	1.72	7	5
1:A:100:ALA:H	1:A:104:ILE:HD13	0.61	1.55	16	1
1:A:43:VAL:HG13	1:A:75:PRO:HA	0.61	1.72	10	6
1:A:43:VAL:HB	1:A:139:PHE:CE1	0.61	2.31	19	2
1:A:38:LEU:CB	1:A:70:THR:HG22	0.61	2.25	9	20
1:A:143:LEU:HD23	1:A:152:GLU:HG3	0.61	1.71	12	4
1:A:143:LEU:HD23	1:A:152:GLU:CG	0.61	2.26	18	10
1:A:41:TYR:HB3	1:A:139:PHE:O	0.60	1.97	6	11
1:A:40:ILE:HG13	1:A:144:ILE:HG13	0.60	1.72	18	12
1:A:39:LEU:O	1:A:71:VAL:HA	0.60	1.97	10	19
1:A:39:LEU:HD12	1:A:141:SER:HB3	0.60	1.72	11	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:TYR:HB2	1:A:69:PHE:HD2	0.60	1.56	3	19
1:A:71:VAL:O	1:A:102:PHE:HB2	0.60	1.96	12	8
1:A:74:PHE:HD2	1:A:108:ILE:HD13	0.59	1.56	20	1
1:A:56:THR:HA	1:A:160:VAL:CG2	0.59	2.27	12	17
1:A:42:ASN:CB	1:A:110:VAL:HG11	0.59	2.26	15	2
1:A:108:ILE:HG13	1:A:110:VAL:HG13	0.59	1.72	1	1
1:A:70:THR:CG2	1:A:72:LEU:HG	0.59	2.28	17	8
1:A:119:TYR:O	1:A:123:LYS:HG3	0.59	1.97	20	7
1:A:43:VAL:HG12	1:A:139:PHE:HA	0.59	1.72	16	3
1:A:61:TYR:CE2	1:A:103:PRO:HD3	0.59	2.33	14	10
1:A:43:VAL:HG23	1:A:139:PHE:CD2	0.59	2.32	4	1
1:A:33:HIS:CB	1:A:38:LEU:HD13	0.59	2.27	11	16
1:A:61:TYR:HD1	1:A:70:THR:HA	0.59	1.56	10	3
1:A:126:LYS:HG2	1:A:153:ARG:NH2	0.59	2.12	7	3
1:A:37:PRO:O	1:A:69:PHE:HA	0.59	1.97	9	20
1:A:120:GLU:HA	1:A:123:LYS:HD2	0.59	1.74	13	2
1:A:20:VAL:HG21	1:A:30:LEU:HD13	0.59	1.74	12	10
1:A:43:VAL:HG23	1:A:139:PHE:HB3	0.59	1.73	8	3
1:A:42:ASN:OD1	1:A:140:THR:HB	0.59	1.98	9	6
1:A:70:THR:OG1	1:A:103:PRO:HG2	0.58	1.98	10	10
1:A:76:SER:HB2	1:A:110:VAL:HG23	0.58	1.75	2	2
1:A:74:PHE:CE1	1:A:105:MET:HG2	0.58	2.33	10	1
1:A:75:PRO:HG2	1:A:107:LYS:HG2	0.58	1.75	14	1
1:A:20:VAL:HG23	1:A:30:LEU:HB2	0.58	1.74	7	1
1:A:108:ILE:HD12	1:A:110:VAL:HG22	0.58	1.74	13	1
1:A:73:ALA:O	1:A:104:ILE:HA	0.58	1.98	8	7
1:A:23:ALA:HA	1:A:105:MET:C	0.58	2.18	6	13
1:A:43:VAL:CG1	1:A:73:ALA:HB1	0.58	2.28	3	11
1:A:126:LYS:HG2	1:A:153:ARG:HH22	0.58	1.57	17	3
1:A:121:TYR:HA	1:A:124:LYS:HE2	0.57	1.74	10	1
1:A:118:LEU:O	1:A:122:MET:HG2	0.57	1.99	9	1
1:A:75:PRO:CB	1:A:107:LYS:HG2	0.57	2.29	9	2
1:A:76:SER:HA	1:A:110:VAL:HG23	0.57	1.74	15	1
1:A:25:HIS:CD2	1:A:106:ALA:HB1	0.57	2.33	3	10
1:A:20:VAL:HG23	1:A:30:LEU:HD22	0.57	1.77	10	1
1:A:71:VAL:O	1:A:103:PRO:HD2	0.57	1.99	9	9
1:A:15:ILE:HG21	1:A:122:MET:HE2	0.57	1.77	19	5
1:A:105:MET:HG3	1:A:107:LYS:H	0.57	1.60	4	4
1:A:21:LEU:HD23	1:A:27:PRO:HA	0.57	1.76	16	16
1:A:60:LEU:HB3	1:A:69:PHE:HE2	0.57	1.59	4	19
1:A:37:PRO:O	1:A:69:PHE:HD1	0.56	1.83	20	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ASN:OD1	1:A:76:SER:HB3	0.56	1.99	4	2
1:A:126:LYS:HG2	1:A:151:VAL:HA	0.56	1.76	10	1
1:A:18:PHE:CD2	1:A:118:LEU:HA	0.56	2.36	8	17
1:A:56:THR:OG1	1:A:159:SER:HA	0.56	2.00	2	10
1:A:38:LEU:HA	1:A:69:PHE:CD1	0.56	2.35	18	18
1:A:18:PHE:HE2	1:A:121:TYR:CB	0.56	2.14	9	6
1:A:75:PRO:O	1:A:107:LYS:HG2	0.56	2.01	14	1
1:A:16:PHE:CE1	1:A:30:LEU:HG	0.56	2.35	7	7
1:A:31:VAL:CG1	1:A:34:LYS:HE2	0.56	2.30	6	1
1:A:58:THR:HA	1:A:102:PHE:CD1	0.56	2.36	10	11
1:A:138:ASN:HB2	1:A:156:PRO:CB	0.56	2.31	10	5
1:A:144:ILE:HG22	1:A:148:GLY:HA2	0.55	1.78	11	15
1:A:75:PRO:O	1:A:107:LYS:HA	0.55	2.01	9	3
1:A:39:LEU:HB2	1:A:69:PHE:CZ	0.55	2.37	10	12
1:A:41:TYR:CE1	1:A:141:SER:HB3	0.55	2.37	20	2
1:A:62:ASN:HA	1:A:65:LYS:CG	0.55	2.31	16	2
1:A:116:HIS:CE1	1:A:118:LEU:HB3	0.55	2.36	15	4
1:A:154:PHE:HZ	1:A:166:LYS:HB2	0.55	1.60	10	10
1:A:61:TYR:CD2	1:A:102:PHE:HA	0.55	2.37	18	18
1:A:43:VAL:HA	1:A:139:PHE:CA	0.55	2.29	18	3
1:A:15:ILE:HD13	1:A:40:ILE:HD11	0.55	1.78	11	9
1:A:16:PHE:HD1	1:A:30:LEU:HG	0.55	1.60	2	2
1:A:31:VAL:CG1	1:A:34:LYS:HG3	0.55	2.32	12	5
1:A:108:ILE:HD12	1:A:116:HIS:HB3	0.55	1.77	20	1
1:A:144:ILE:CG2	1:A:148:GLY:HA2	0.55	2.32	3	14
1:A:42:ASN:HD21	1:A:140:THR:HB	0.55	1.61	2	3
1:A:37:PRO:HG2	1:A:171:LEU:CD2	0.55	2.31	16	20
1:A:41:TYR:OH	1:A:163:ILE:HD13	0.54	2.02	20	5
1:A:72:LEU:HD23	1:A:103:PRO:CB	0.54	2.32	10	1
1:A:42:ASN:N	1:A:42:ASN:HD22	0.54	2.00	3	1
1:A:126:LYS:HB3	1:A:153:ARG:NH2	0.54	2.17	12	2
1:A:73:ALA:HB2	1:A:102:PHE:CE2	0.54	2.36	19	1
1:A:64:TYR:HB2	1:A:69:PHE:CD2	0.54	2.37	18	18
1:A:20:VAL:HG12	1:A:28:TYR:HB3	0.54	1.80	8	7
1:A:74:PHE:CD1	1:A:105:MET:HB3	0.54	2.38	6	6
1:A:15:ILE:HD11	1:A:38:LEU:HD11	0.54	1.79	1	3
1:A:137:TRP:HB2	1:A:140:THR:OG1	0.54	2.02	14	5
1:A:21:LEU:HB2	1:A:105:MET:SD	0.54	2.42	10	2
1:A:145:ASP:HA	1:A:170:LEU:HD13	0.54	1.80	7	4
1:A:110:VAL:HG13	1:A:119:TYR:CE2	0.54	2.38	15	1
1:A:74:PHE:CD1	1:A:105:MET:HG3	0.54	2.38	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:TYR:CD2	1:A:102:PHE:HB3	0.54	2.38	19	14
1:A:72:LEU:CA	1:A:103:PRO:HG2	0.53	2.33	4	4
1:A:60:LEU:HD21	1:A:164:GLU:HG3	0.53	1.79	2	3
1:A:164:GLU:HA	1:A:167:LEU:HB3	0.53	1.80	2	10
1:A:29:ASN:HD21	1:A:31:VAL:HG22	0.53	1.63	19	2
1:A:43:VAL:HG23	1:A:75:PRO:HA	0.53	1.81	6	3
1:A:40:ILE:CG2	1:A:119:TYR:OH	0.53	2.46	20	3
1:A:126:LYS:HD2	1:A:150:PRO:HB2	0.53	1.80	10	1
1:A:102:PHE:CE2	1:A:104:ILE:HD11	0.53	2.38	5	7
1:A:29:ASN:ND2	1:A:31:VAL:HG23	0.53	2.19	2	1
1:A:65:LYS:HA	1:A:69:PHE:O	0.53	2.03	9	18
1:A:43:VAL:HG23	1:A:139:PHE:CE1	0.53	2.38	15	3
1:A:145:ASP:OD1	1:A:149:VAL:HG12	0.53	2.04	11	4
1:A:39:LEU:HD12	1:A:141:SER:OG	0.53	2.04	12	1
1:A:15:ILE:HG23	1:A:150:PRO:CD	0.53	2.31	10	9
1:A:63:LYS:HE3	1:A:64:TYR:CE2	0.53	2.39	3	6
1:A:16:PHE:CZ	1:A:34:LYS:HG2	0.53	2.39	12	2
1:A:75:PRO:O	1:A:107:LYS:HE3	0.53	2.02	16	1
1:A:76:SER:HA	1:A:108:ILE:O	0.53	2.03	20	2
1:A:18:PHE:CE2	1:A:121:TYR:CB	0.53	2.92	8	14
1:A:22:ASP:HA	1:A:105:MET:CE	0.52	2.34	1	2
1:A:138:ASN:HB2	1:A:156:PRO:HB3	0.52	1.81	17	2
1:A:38:LEU:HD23	1:A:38:LEU:N	0.52	2.20	5	11
1:A:73:ALA:HB2	1:A:102:PHE:HE2	0.52	1.63	19	1
1:A:154:PHE:CE2	1:A:163:ILE:HA	0.52	2.39	8	9
1:A:75:PRO:CG	1:A:107:LYS:HB3	0.52	2.28	16	2
1:A:43:VAL:CA	1:A:139:PHE:HA	0.52	2.30	18	2
1:A:58:THR:N	1:A:102:PHE:HE1	0.52	2.02	2	3
1:A:41:TYR:CD2	1:A:139:PHE:HD2	0.52	2.22	11	6
1:A:53:GLY:HA2	1:A:56:THR:HB	0.52	1.80	20	1
1:A:38:LEU:N	1:A:38:LEU:HD23	0.52	2.20	4	7
1:A:56:THR:CG2	1:A:163:ILE:HD12	0.52	2.33	7	11
1:A:29:ASN:OD1	1:A:32:GLN:HB3	0.52	2.05	18	7
1:A:121:TYR:HA	1:A:124:LYS:HG2	0.52	1.81	18	2
1:A:160:VAL:O	1:A:164:GLU:HG3	0.51	2.06	8	7
1:A:126:LYS:HB2	1:A:126:LYS:NZ	0.51	2.20	10	1
1:A:42:ASN:ND2	1:A:76:SER:HB2	0.51	2.20	13	1
1:A:152:GLU:OE1	1:A:152:GLU:HA	0.51	2.05	16	1
1:A:73:ALA:HB3	1:A:104:ILE:HG12	0.51	1.82	2	3
1:A:119:TYR:HA	1:A:122:MET:HB2	0.51	1.83	2	9
1:A:39:LEU:HD23	1:A:141:SER:HB3	0.51	1.83	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:HG	1:A:122:MET:CE	0.51	2.36	14	7
1:A:122:MET:HG3	1:A:150:PRO:HG3	0.51	1.83	12	3
1:A:110:VAL:HA	1:A:119:TYR:HH	0.51	1.64	7	1
1:A:137:TRP:HB3	1:A:156:PRO:CG	0.51	2.36	1	2
1:A:116:HIS:CE1	1:A:118:LEU:H	0.51	2.24	18	17
1:A:22:ASP:HA	1:A:105:MET:SD	0.51	2.46	7	3
1:A:138:ASN:O	1:A:140:THR:N	0.50	2.44	19	11
1:A:61:TYR:HD2	1:A:101:GLU:O	0.50	1.90	9	1
1:A:168:ILE:N	1:A:169:PRO:HD2	0.50	2.22	8	2
1:A:33:HIS:CE1	1:A:70:THR:CB	0.50	2.91	12	7
1:A:29:ASN:O	1:A:32:GLN:HG2	0.50	2.06	10	8
1:A:69:PHE:HB2	1:A:171:LEU:HD21	0.50	1.84	4	18
1:A:116:HIS:ND1	1:A:118:LEU:HB3	0.50	2.22	4	5
1:A:39:LEU:HD23	1:A:69:PHE:HE1	0.50	1.66	10	3
1:A:29:ASN:ND2	1:A:31:VAL:HG22	0.50	2.22	19	1
1:A:20:VAL:HG22	1:A:118:LEU:HD22	0.50	1.83	15	9
1:A:20:VAL:CG2	1:A:30:LEU:HB2	0.50	2.36	20	9
1:A:121:TYR:O	1:A:124:LYS:HG2	0.50	2.05	20	3
1:A:108:ILE:HB	1:A:116:HIS:HB2	0.50	1.84	9	2
1:A:58:THR:HA	1:A:102:PHE:CE1	0.50	2.42	9	4
1:A:74:PHE:CD2	1:A:105:MET:HG2	0.50	2.41	8	6
1:A:122:MET:SD	1:A:144:ILE:HD11	0.50	2.47	14	8
1:A:76:SER:CB	1:A:110:VAL:HG23	0.50	2.36	12	2
1:A:28:TYR:CE2	1:A:103:PRO:HB3	0.50	2.42	13	2
1:A:40:ILE:HD12	1:A:122:MET:HE3	0.50	1.82	20	2
1:A:74:PHE:CD2	1:A:108:ILE:HD13	0.50	2.42	1	2
1:A:72:LEU:HA	1:A:103:PRO:O	0.50	2.07	6	6
1:A:43:VAL:CG2	1:A:139:PHE:HB3	0.49	2.37	18	1
1:A:18:PHE:CD1	1:A:117:PRO:HB2	0.49	2.42	6	3
1:A:108:ILE:CG1	1:A:110:VAL:HG22	0.49	2.36	20	1
1:A:121:TYR:O	1:A:124:LYS:HG3	0.49	2.06	7	1
1:A:52:GLY:O	1:A:55:GLU:HG3	0.49	2.07	10	1
1:A:154:PHE:CG	1:A:163:ILE:HG12	0.49	2.43	16	6
1:A:108:ILE:CD1	1:A:110:VAL:HG13	0.49	2.36	9	4
1:A:24:ASP:O	1:A:25:HIS:HB2	0.49	2.07	2	8
1:A:54:TYR:HA	1:A:139:PHE:CZ	0.49	2.42	10	4
1:A:40:ILE:HG23	1:A:72:LEU:CB	0.49	2.38	20	3
1:A:28:TYR:CZ	1:A:103:PRO:HB3	0.49	2.41	6	2
1:A:160:VAL:HG12	1:A:164:GLU:OE2	0.49	2.07	2	4
1:A:110:VAL:HG12	1:A:119:TYR:CD2	0.49	2.43	9	1
1:A:105:MET:HG3	1:A:107:LYS:N	0.49	2.23	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:PHE:CD2	1:A:119:TYR:HE1	0.49	2.26	12	3
1:A:39:LEU:HD23	1:A:69:PHE:CZ	0.49	2.43	12	2
1:A:41:TYR:HD2	1:A:139:PHE:HD1	0.48	1.51	4	1
1:A:72:LEU:CD2	1:A:103:PRO:HB2	0.48	2.38	2	2
1:A:20:VAL:CG1	1:A:74:PHE:HZ	0.48	2.18	1	2
1:A:39:LEU:CB	1:A:41:TYR:HE1	0.48	2.12	2	9
1:A:16:PHE:HA	1:A:30:LEU:HD23	0.48	1.85	15	7
1:A:102:PHE:HB2	1:A:103:PRO:CD	0.48	2.39	19	2
1:A:42:ASN:ND2	1:A:110:VAL:HB	0.48	2.24	13	1
1:A:119:TYR:HA	1:A:122:MET:CG	0.48	2.38	15	2
1:A:154:PHE:CZ	1:A:163:ILE:HA	0.48	2.43	19	5
1:A:37:PRO:CD	1:A:146:ARG:HG2	0.48	2.39	14	1
1:A:142:PHE:HA	1:A:152:GLU:O	0.48	2.09	9	3
1:A:126:LYS:HE2	1:A:151:VAL:C	0.48	2.29	10	1
1:A:122:MET:HB3	1:A:142:PHE:CZ	0.48	2.43	2	1
1:A:41:TYR:HD2	1:A:139:PHE:HD2	0.48	1.51	11	3
1:A:110:VAL:HA	1:A:119:TYR:CZ	0.48	2.44	7	2
1:A:108:ILE:CG1	1:A:110:VAL:HG13	0.48	2.39	1	1
1:A:38:LEU:HG	1:A:144:ILE:HB	0.48	1.86	1	3
1:A:58:THR:HA	1:A:102:PHE:HE1	0.47	1.69	1	4
1:A:15:ILE:CD1	1:A:40:ILE:HD11	0.47	2.39	11	6
1:A:143:LEU:HD23	1:A:152:GLU:HG2	0.47	1.84	10	4
1:A:21:LEU:HA	1:A:28:TYR:H	0.47	1.68	10	1
1:A:60:LEU:HD21	1:A:160:VAL:HA	0.47	1.86	7	1
1:A:57:ALA:HA	1:A:71:VAL:HG21	0.47	1.85	7	1
1:A:15:ILE:CG2	1:A:150:PRO:HD3	0.47	2.38	4	5
1:A:74:PHE:CZ	1:A:105:MET:HG2	0.47	2.45	10	1
1:A:126:LYS:HB2	1:A:126:LYS:HZ3	0.47	1.68	10	1
1:A:42:ASN:O	1:A:139:PHE:HA	0.47	2.09	8	1
1:A:41:TYR:CE2	1:A:57:ALA:HB2	0.47	2.44	8	1
1:A:74:PHE:CD2	1:A:119:TYR:CE2	0.47	2.95	8	1
1:A:39:LEU:HB2	1:A:69:PHE:HZ	0.47	1.69	10	1
1:A:39:LEU:HD22	1:A:143:LEU:HA	0.47	1.85	1	5
1:A:20:VAL:O	1:A:21:LEU:HD23	0.47	2.09	1	2
1:A:15:ILE:HG21	1:A:122:MET:HE3	0.47	1.85	10	1
1:A:161:LYS:O	1:A:165:GLU:HG2	0.47	2.08	14	1
1:A:138:ASN:HB3	1:A:156:PRO:HB3	0.47	1.87	5	1
1:A:23:ALA:C	1:A:106:ALA:HB2	0.47	2.29	19	1
1:A:41:TYR:CE1	1:A:71:VAL:HG22	0.47	2.45	9	1
1:A:42:ASN:HD21	1:A:76:SER:HB2	0.47	1.70	13	1
1:A:74:PHE:HA	1:A:105:MET:HB3	0.47	1.85	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:O	1:A:122:MET:HG3	0.47	2.10	4	5
1:A:121:TYR:HA	1:A:124:LYS:HD2	0.47	1.87	20	1
1:A:70:THR:OG1	1:A:103:PRO:HG3	0.47	2.09	15	5
1:A:23:ALA:CA	1:A:106:ALA:HA	0.47	2.36	13	3
1:A:140:THR:OG1	1:A:156:PRO:HD3	0.47	2.10	4	4
1:A:126:LYS:HE3	1:A:151:VAL:O	0.47	2.09	13	3
1:A:61:TYR:CE2	1:A:102:PHE:HA	0.47	2.45	7	6
1:A:16:PHE:CE2	1:A:148:GLY:CA	0.47	2.97	19	5
1:A:153:ARG:CZ	1:A:153:ARG:HB3	0.47	2.39	17	2
1:A:16:PHE:CB	1:A:31:VAL:HG12	0.47	2.32	3	1
1:A:40:ILE:HG23	1:A:72:LEU:HD12	0.47	1.87	14	1
1:A:76:SER:OG	1:A:110:VAL:HG23	0.47	2.09	20	1
1:A:61:TYR:CE2	1:A:65:LYS:HD2	0.46	2.45	10	1
1:A:15:ILE:HG12	1:A:148:GLY:O	0.46	2.10	11	9
1:A:41:TYR:N	1:A:41:TYR:CD1	0.46	2.83	2	3
1:A:42:ASN:HB3	1:A:119:TYR:CE2	0.46	2.45	11	1
1:A:42:ASN:HD22	1:A:110:VAL:HB	0.46	1.70	8	1
1:A:43:VAL:HG13	1:A:75:PRO:CA	0.46	2.40	10	3
1:A:145:ASP:CG	1:A:146:ARG:N	0.46	2.68	17	4
1:A:76:SER:HB2	1:A:110:VAL:CG2	0.46	2.40	11	2
1:A:100:ALA:HB1	1:A:102:PHE:CE2	0.46	2.46	20	1
1:A:121:TYR:HA	1:A:124:LYS:CD	0.46	2.40	20	1
1:A:64:TYR:C	1:A:69:PHE:HB3	0.46	2.31	10	4
1:A:43:VAL:CG2	1:A:139:PHE:CE1	0.46	2.98	15	1
1:A:102:PHE:CE1	1:A:104:ILE:HD11	0.46	2.46	13	1
1:A:105:MET:SD	1:A:107:LYS:N	0.46	2.88	2	1
1:A:39:LEU:N	1:A:69:PHE:CE1	0.46	2.84	7	13
1:A:42:ASN:HB2	1:A:110:VAL:CG2	0.46	2.41	2	1
1:A:15:ILE:HB	1:A:118:LEU:HD12	0.46	1.85	7	1
1:A:142:PHE:CD1	1:A:153:ARG:HB2	0.46	2.46	11	3
1:A:14:SER:HB3	1:A:147:ASP:O	0.46	2.11	3	3
1:A:15:ILE:HD11	1:A:144:ILE:HG21	0.46	1.87	13	6
1:A:144:ILE:CD1	1:A:150:PRO:HB3	0.46	2.41	10	1
1:A:138:ASN:HB3	1:A:156:PRO:CB	0.45	2.41	5	1
1:A:15:ILE:HD12	1:A:30:LEU:HD11	0.45	1.88	10	1
1:A:42:ASN:HB3	1:A:110:VAL:HB	0.45	1.88	8	1
1:A:74:PHE:CD2	1:A:119:TYR:CE1	0.45	3.04	12	6
1:A:52:GLY:O	1:A:55:GLU:HG2	0.45	2.11	3	1
1:A:22:ASP:O	1:A:106:ALA:HB2	0.45	2.12	9	2
1:A:38:LEU:HB2	1:A:70:THR:CG2	0.45	2.37	17	2
1:A:61:TYR:CD2	1:A:102:PHE:CB	0.45	3.00	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HD12	1:A:141:SER:CB	0.45	2.42	7	8
1:A:58:THR:CA	1:A:102:PHE:HE1	0.45	2.25	2	3
1:A:75:PRO:HD2	1:A:107:LYS:N	0.45	2.27	18	1
1:A:139:PHE:O	1:A:140:THR:C	0.45	2.55	8	8
1:A:39:LEU:N	1:A:69:PHE:HE1	0.45	2.10	12	6
1:A:100:ALA:HB1	1:A:102:PHE:CE1	0.45	2.46	11	2
1:A:42:ASN:HB2	1:A:110:VAL:CG1	0.45	2.41	7	1
1:A:137:TRP:O	1:A:138:ASN:O	0.45	2.35	19	3
1:A:40:ILE:HG12	1:A:72:LEU:CD1	0.45	2.42	3	5
1:A:126:LYS:HG3	1:A:150:PRO:HB2	0.45	1.88	11	1
1:A:31:VAL:HG12	1:A:34:LYS:CG	0.45	2.41	10	3
1:A:42:ASN:HB2	1:A:110:VAL:HG21	0.45	1.88	2	1
1:A:61:TYR:CD1	1:A:65:LYS:HB3	0.44	2.47	6	5
1:A:106:ALA:O	1:A:107:LYS:HB3	0.44	2.11	11	2
1:A:72:LEU:HD12	1:A:72:LEU:N	0.44	2.20	16	1
1:A:58:THR:HA	1:A:102:PHE:CD2	0.44	2.47	13	2
1:A:111:ASN:N	1:A:119:TYR:OH	0.44	2.49	7	1
1:A:33:HIS:HB3	1:A:38:LEU:HD22	0.44	1.85	7	1
1:A:105:MET:SD	1:A:106:ALA:N	0.44	2.91	16	3
1:A:41:TYR:CD1	1:A:41:TYR:N	0.44	2.84	15	3
1:A:102:PHE:CB	1:A:103:PRO:HD2	0.44	2.39	7	1
1:A:118:LEU:O	1:A:121:TYR:HB3	0.44	2.12	17	2
1:A:15:ILE:CG2	1:A:122:MET:HE2	0.44	2.42	19	3
1:A:105:MET:CG	1:A:107:LYS:H	0.44	2.25	4	1
1:A:20:VAL:O	1:A:28:TYR:N	0.44	2.50	4	5
1:A:37:PRO:HD3	1:A:146:ARG:CG	0.44	2.42	18	1
1:A:102:PHE:O	1:A:104:ILE:HD12	0.44	2.12	19	2
1:A:54:TYR:HB3	1:A:55:GLU:OE2	0.44	2.12	11	1
1:A:21:LEU:HB3	1:A:25:HIS:CA	0.44	2.39	7	1
1:A:144:ILE:HD13	1:A:150:PRO:HB3	0.44	1.89	10	1
1:A:16:PHE:CG	1:A:31:VAL:HG13	0.44	2.48	10	1
1:A:100:ALA:HB3	1:A:104:ILE:HD11	0.44	1.90	7	3
1:A:105:MET:SD	1:A:108:ILE:HG23	0.44	2.53	16	3
1:A:39:LEU:HD23	1:A:141:SER:CB	0.44	2.43	17	2
1:A:29:ASN:HD21	1:A:32:GLN:NE2	0.44	2.11	7	1
1:A:41:TYR:HA	1:A:141:SER:HA	0.43	1.89	16	1
1:A:70:THR:HG23	1:A:72:LEU:HG	0.43	1.88	17	1
1:A:15:ILE:HD13	1:A:144:ILE:HG21	0.43	1.88	3	4
1:A:75:PRO:HG2	1:A:107:LYS:CG	0.43	2.42	14	1
1:A:42:ASN:HB2	1:A:110:VAL:CB	0.43	2.43	11	1
1:A:60:LEU:CD2	1:A:160:VAL:HG13	0.43	2.42	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:THR:HG21	1:A:72:LEU:HG	0.43	1.90	17	1
1:A:142:PHE:HA	1:A:153:ARG:HA	0.43	1.90	16	2
1:A:56:THR:HG22	1:A:60:LEU:HD12	0.43	1.90	16	1
1:A:73:ALA:C	1:A:74:PHE:HD1	0.43	2.17	16	1
1:A:40:ILE:HG22	1:A:119:TYR:HH	0.43	1.63	20	1
1:A:153:ARG:HB3	1:A:153:ARG:CZ	0.43	2.43	7	4
1:A:108:ILE:H	1:A:108:ILE:HD13	0.43	1.72	16	1
1:A:105:MET:C	1:A:107:LYS:H	0.43	2.17	15	2
1:A:20:VAL:HG12	1:A:21:LEU:N	0.43	2.29	16	5
1:A:42:ASN:OD1	1:A:110:VAL:HB	0.43	2.14	4	1
1:A:105:MET:CG	1:A:106:ALA:N	0.43	2.82	10	2
1:A:109:ASN:C	1:A:109:ASN:HD22	0.43	2.16	10	1
1:A:41:TYR:O	1:A:73:ALA:HA	0.43	2.14	11	1
1:A:108:ILE:HD12	1:A:108:ILE:O	0.43	2.13	6	1
1:A:75:PRO:HG3	1:A:104:ILE:CG2	0.43	2.44	20	1
1:A:43:VAL:HG23	1:A:139:PHE:CE2	0.42	2.49	4	1
1:A:25:HIS:CE1	1:A:106:ALA:HB1	0.42	2.48	18	1
1:A:126:LYS:HD2	1:A:151:VAL:O	0.42	2.14	2	1
1:A:76:SER:HB3	1:A:110:VAL:HG23	0.42	1.90	16	1
1:A:74:PHE:HD2	1:A:108:ILE:CD1	0.42	2.19	17	1
1:A:56:THR:HG23	1:A:160:VAL:CA	0.42	2.43	7	1
1:A:42:ASN:HB2	1:A:110:VAL:HB	0.42	1.90	11	1
1:A:40:ILE:HG13	1:A:144:ILE:CG1	0.42	2.42	6	1
1:A:28:TYR:CE2	1:A:72:LEU:HD22	0.42	2.50	14	1
1:A:20:VAL:CG1	1:A:21:LEU:N	0.42	2.82	5	6
1:A:20:VAL:HG11	1:A:28:TYR:HD2	0.42	1.73	18	1
1:A:143:LEU:HB3	1:A:152:GLU:CB	0.42	2.44	16	1
1:A:54:TYR:HA	1:A:139:PHE:CE2	0.42	2.49	16	1
1:A:15:ILE:CG2	1:A:122:MET:HE3	0.42	2.45	10	1
1:A:15:ILE:HG21	1:A:144:ILE:HD12	0.42	1.91	1	1
1:A:39:LEU:HD13	1:A:69:PHE:CZ	0.42	2.49	17	4
1:A:105:MET:HA	1:A:105:MET:HE2	0.42	1.90	9	1
1:A:122:MET:HG2	1:A:142:PHE:CG	0.42	2.49	6	3
1:A:20:VAL:CG1	1:A:74:PHE:CZ	0.42	2.99	19	1
1:A:21:LEU:HD12	1:A:25:HIS:CD2	0.42	2.49	10	1
1:A:74:PHE:CD1	1:A:105:MET:CB	0.42	3.02	15	1
1:A:61:TYR:CD1	1:A:65:LYS:HG2	0.42	2.49	2	1
1:A:39:LEU:HG	1:A:143:LEU:HA	0.42	1.90	16	1
1:A:73:ALA:CB	1:A:104:ILE:HD12	0.42	2.40	17	1
1:A:39:LEU:HD13	1:A:142:PHE:O	0.42	2.15	20	2
1:A:26:LYS:HA	1:A:26:LYS:CE	0.42	2.40	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:ILE:CG1	1:A:116:HIS:HB3	0.42	2.43	9	1
1:A:61:TYR:O	1:A:65:LYS:N	0.42	2.52	16	1
1:A:31:VAL:HB	1:A:34:LYS:NZ	0.41	2.30	16	1
1:A:164:GLU:O	1:A:168:ILE:HG13	0.41	2.15	7	1
1:A:23:ALA:HB2	1:A:104:ILE:O	0.41	2.15	1	1
1:A:31:VAL:HB	1:A:34:LYS:CE	0.41	2.45	4	1
1:A:39:LEU:HD13	1:A:69:PHE:CE1	0.41	2.50	4	1
1:A:123:LYS:HA	1:A:126:LYS:O	0.41	2.14	12	1
1:A:73:ALA:HB3	1:A:104:ILE:CG1	0.41	2.45	1	1
1:A:40:ILE:CG2	1:A:72:LEU:HD13	0.41	2.40	16	2
1:A:121:TYR:CD1	1:A:124:LYS:HE3	0.41	2.50	8	1
1:A:109:ASN:HD22	1:A:109:ASN:C	0.41	2.18	9	1
1:A:137:TRP:HA	1:A:137:TRP:CE3	0.41	2.50	8	1
1:A:116:HIS:O	1:A:119:TYR:N	0.41	2.53	4	3
1:A:28:TYR:HE2	1:A:72:LEU:HD11	0.41	1.75	18	1
1:A:29:ASN:O	1:A:29:ASN:ND2	0.41	2.54	5	1
1:A:123:LYS:HD3	1:A:124:LYS:N	0.41	2.30	6	1
1:A:28:TYR:HE2	1:A:72:LEU:HD21	0.41	1.74	20	1
1:A:43:VAL:HG12	1:A:139:PHE:CD1	0.41	2.50	5	2
1:A:69:PHE:HB2	1:A:171:LEU:CD2	0.41	2.45	16	1
1:A:43:VAL:HG23	1:A:75:PRO:CA	0.41	2.46	16	1
1:A:138:ASN:CG	1:A:139:PHE:H	0.41	2.19	19	1
1:A:108:ILE:CG1	1:A:116:HIS:HB2	0.41	2.40	4	1
1:A:39:LEU:CD1	1:A:143:LEU:HA	0.41	2.46	4	1
1:A:40:ILE:HD12	1:A:122:MET:HE2	0.41	1.92	10	1
1:A:61:TYR:HB2	1:A:71:VAL:HB	0.41	1.91	9	1
1:A:22:ASP:HB3	1:A:26:LYS:HE3	0.41	1.92	14	1
1:A:28:TYR:HE2	1:A:72:LEU:CD2	0.41	2.28	1	1
1:A:74:PHE:HD2	1:A:108:ILE:HD11	0.41	1.75	6	1
1:A:100:ALA:N	1:A:104:ILE:HD12	0.41	2.31	3	1
1:A:30:LEU:HD11	1:A:38:LEU:HD11	0.41	1.93	7	1
1:A:31:VAL:HG12	1:A:34:LYS:HD3	0.41	1.92	2	3
1:A:42:ASN:N	1:A:42:ASN:ND2	0.41	2.66	3	1
1:A:75:PRO:HD2	1:A:107:LYS:CA	0.41	2.43	12	1
1:A:162:ASP:O	1:A:165:GLU:HG2	0.41	2.16	2	1
1:A:31:VAL:HB	1:A:34:LYS:HE2	0.41	1.91	19	1
1:A:39:LEU:CD2	1:A:143:LEU:HA	0.40	2.47	1	1
1:A:102:PHE:HB3	1:A:103:PRO:CD	0.40	2.46	8	1
1:A:42:ASN:HB3	1:A:110:VAL:CB	0.40	2.45	8	1
1:A:60:LEU:HD21	1:A:164:GLU:CG	0.40	2.46	8	1
1:A:108:ILE:HG12	1:A:109:ASN:O	0.40	2.17	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:ALA:HB3	1:A:102:PHE:CD2	0.40	2.52	1	1
1:A:154:PHE:CE2	1:A:166:LYS:HG3	0.40	2.51	14	1
1:A:71:VAL:HG12	1:A:102:PHE:CD2	0.40	2.51	12	1
1:A:110:VAL:HG23	1:A:110:VAL:O	0.40	2.17	5	1
1:A:116:HIS:CE1	1:A:118:LEU:CB	0.40	3.05	11	1
1:A:110:VAL:O	1:A:111:ASN:HB2	0.40	2.16	13	1
1:A:31:VAL:HB	1:A:34:LYS:HE3	0.40	1.91	13	1
1:A:59:THR:HA	1:A:62:ASN:ND2	0.40	2.31	2	1
1:A:36:SER:HB2	1:A:68:GLY:HA3	0.40	1.93	4	1
1:A:139:PHE:N	1:A:156:PRO:HB3	0.40	2.31	11	1
1:A:20:VAL:HG22	1:A:74:PHE:HZ	0.40	1.76	3	1
1:A:121:TYR:HD1	1:A:124:LYS:HE3	0.40	1.76	14	1
1:A:72:LEU:HD22	1:A:105:MET:CE	0.40	2.47	19	1

6.3 Torsion angles

6.3.1 Protein backbone

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	115/167 (69%)	95±3 (83±2%)	14±3 (12±2%)	6±1 (5±1%)	5	27
All	All	2300/3340 (69%)	1903 (83%)	284 (12%)	113 (5%)	5	27

All 14 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	138	ASN	20
1	A	140	THR	20
1	A	107	LYS	16
1	A	139	PHE	16
1	A	76	SER	12
1	A	117	PRO	10
1	A	103	PRO	8
1	A	110	VAL	2
1	A	109	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	22	ASP	2
1	A	37	PRO	2
1	A	156	PRO	1
1	A	100	ALA	1
1	A	157	GLY	1

6.3.2 Protein sidechains ⓘ

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	102/141 (72%)	89±4 (87±4%)	13±4 (13±4%)	9	50
All	All	2040/2820 (72%)	1774 (87%)	266 (13%)	9	50

All 40 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	145	ASP	20
1	A	123	LYS	19
1	A	38	LEU	19
1	A	41	TYR	17
1	A	54	TYR	16
1	A	153	ARG	14
1	A	110	VAL	12
1	A	108	ILE	11
1	A	42	ASN	11
1	A	72	LEU	11
1	A	31	VAL	10
1	A	105	MET	10
1	A	109	ASN	9
1	A	141	SER	9
1	A	28	TYR	7
1	A	124	LYS	6
1	A	139	PHE	6
1	A	137	TRP	6
1	A	161	LYS	6
1	A	62	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	55	GLU	4
1	A	40	ILE	4
1	A	120	GLU	4
1	A	29	ASN	3
1	A	102	PHE	3
1	A	65	LYS	3
1	A	66	SER	3
1	A	60	LEU	2
1	A	140	THR	2
1	A	122	MET	2
1	A	152	GLU	2
1	A	126	LYS	2
1	A	22	ASP	2
1	A	19	GLU	1
1	A	138	ASN	1
1	A	107	LYS	1
1	A	34	LYS	1
1	A	17	ASP	1
1	A	116	HIS	1
1	A	147	ASP	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 carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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