



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2022 – 01:38 PM EST

PDB ID : 2H25
Title : Solution Structure of Maltose Binding Protein complexed with beta-cyclodextrin
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Deposited on : 2006-05-18

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 following versions of software and data (see [references ⓘ](#)) 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

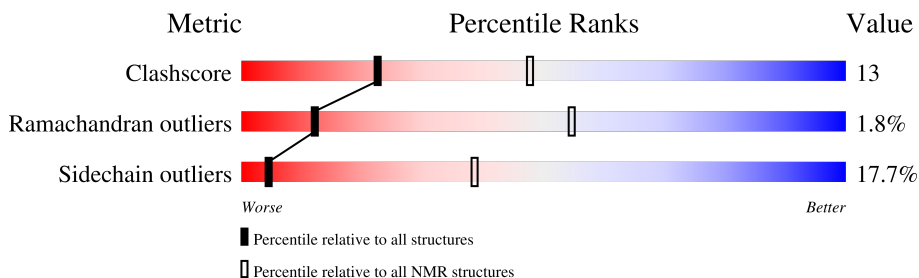
1 Overall quality at a glance

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	370	 71% 27% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 10 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:2-A:370 (369)	0.81	10

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5735 atoms, of which 2858 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	370	5735	1851	2858	469	551	6	0

There is a discrepancy between the modelled and reference sequences:

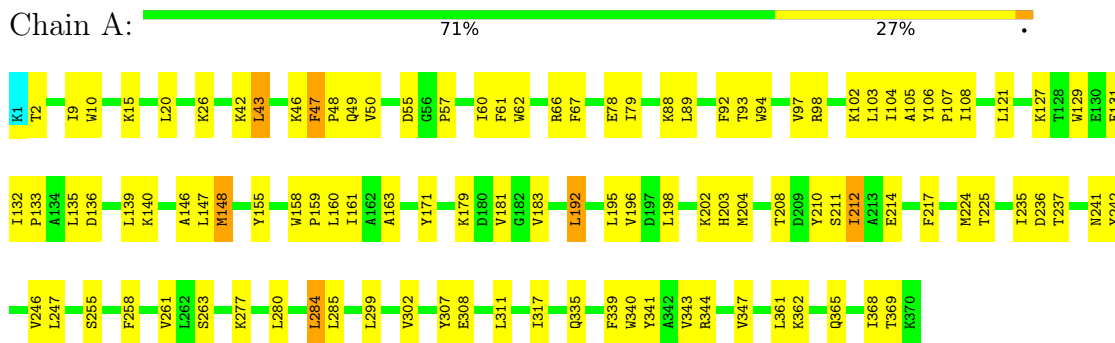
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	THR	ILE	conflict	UNP P0AEX9

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: Maltose-binding periplasmic protein

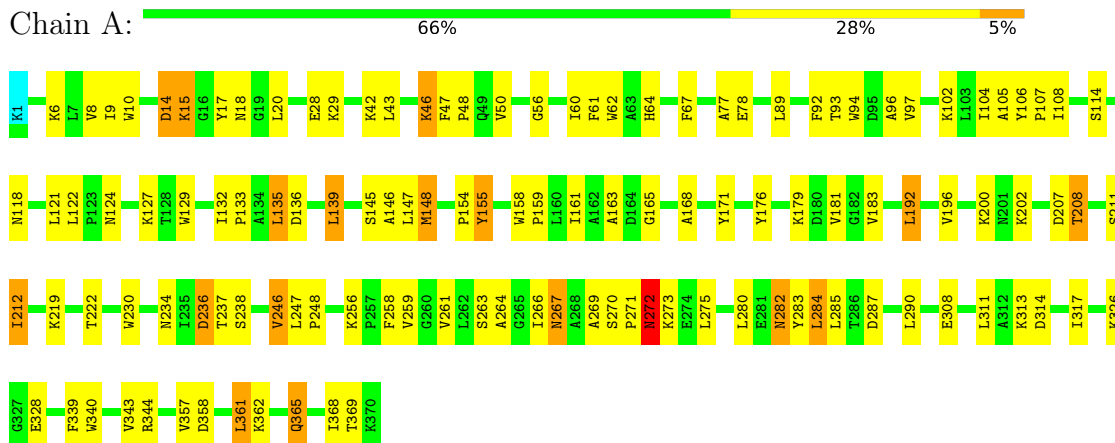


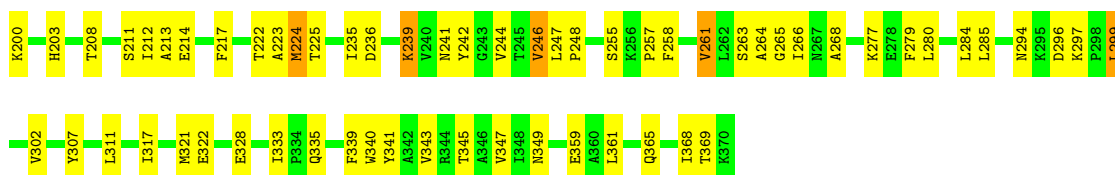
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

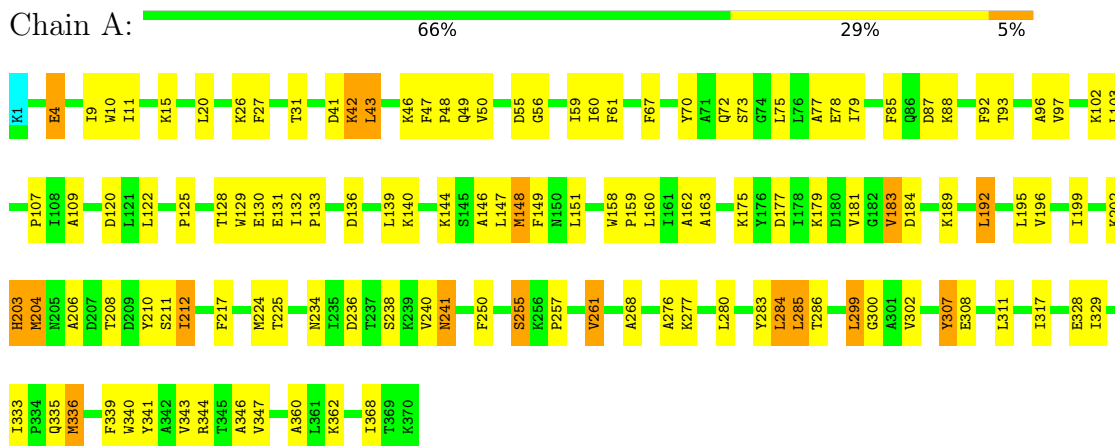
- Molecule 1: Maltose-binding periplasmic protein





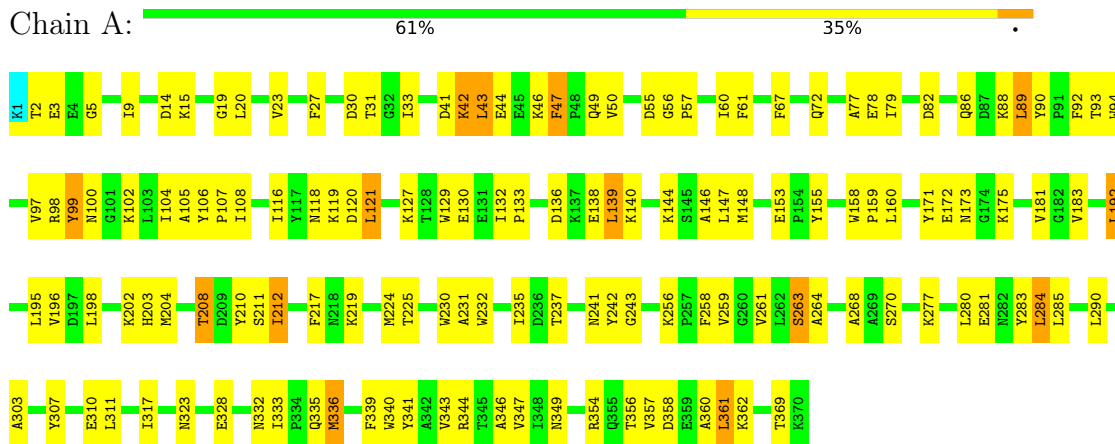
4.2.5 Score per residue for model 5

- Molecule 1: Maltose-binding periplasmic protein



4.2.6 Score per residue for model 6

- Molecule 1: Maltose-binding periplasmic protein



4.2.7 Score per residue for model 7

- Molecule 1: Maltose-binding periplasmic protein



5 Refinement protocol and experimental data overview

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

Of the 40 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	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2868	2843	2840	72±6
All	All	28680	28430	28400	721

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:280:LEU:HD22	1:A:284:LEU:HD22	0.84	1.48	3	2
1:A:51:ALA:HB1	1:A:75:LEU:HD22	0.83	1.49	4	2
1:A:183:VAL:HG12	1:A:361:LEU:CD2	0.83	2.03	1	2
1:A:280:LEU:HD23	1:A:284:LEU:HD22	0.81	1.53	1	5
1:A:161:ILE:HG21	1:A:192:LEU:HD12	0.81	1.50	4	1
1:A:169:PHE:CE2	1:A:333:ILE:HD11	0.80	2.11	4	2
1:A:92:PHE:CE1	1:A:93:THR:HG23	0.80	2.11	6	2
1:A:125:PRO:CB	1:A:245:THR:HG21	0.79	2.07	3	1
1:A:129:TRP:CE3	1:A:132:ILE:HD12	0.79	2.12	1	8
1:A:46:LYS:O	1:A:50:VAL:HG22	0.79	1.78	8	6
1:A:192:LEU:O	1:A:196:VAL:HG23	0.77	1.79	1	10
1:A:67:PHE:CD2	1:A:105:ALA:HB2	0.77	2.15	7	1
1:A:9:ILE:HG21	1:A:20:LEU:HD21	0.77	1.55	9	3
1:A:183:VAL:HG12	1:A:361:LEU:HD22	0.76	1.57	6	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:192:LEU:HD12	1:A:357:VAL:HG22	0.76	1.58	10	1
1:A:339:PHE:CE1	1:A:343:VAL:HG21	0.76	2.15	9	5
1:A:161:ILE:HD13	1:A:192:LEU:HD12	0.76	1.55	7	3
1:A:116:ILE:HD12	1:A:227:ASN:HB2	0.75	1.58	3	2
1:A:112:ALA:HB3	1:A:320:THR:HG23	0.75	1.59	9	1
1:A:135:LEU:HD23	1:A:139:LEU:HD12	0.75	1.58	1	1
1:A:343:VAL:O	1:A:347:VAL:HG23	0.75	1.81	6	7
1:A:9:ILE:HG21	1:A:20:LEU:CD2	0.74	2.12	4	5
1:A:183:VAL:HG12	1:A:361:LEU:HD23	0.74	1.57	1	1
1:A:209:ASP:OD2	1:A:212:ILE:HD11	0.74	1.81	3	2
1:A:183:VAL:O	1:A:361:LEU:HD13	0.73	1.82	6	1
1:A:339:PHE:O	1:A:343:VAL:HG23	0.73	1.83	6	7
1:A:181:VAL:CG1	1:A:183:VAL:HG23	0.73	2.13	7	2
1:A:157:THR:O	1:A:161:ILE:HD12	0.73	1.84	10	1
1:A:43:LEU:HD11	1:A:62:TRP:CZ3	0.73	2.19	3	1
1:A:227:ASN:ND2	1:A:231:ALA:HB2	0.72	1.98	2	1
1:A:147:LEU:HD12	1:A:224:MET:CB	0.72	2.14	10	1
1:A:365:GLN:O	1:A:369:THR:HG22	0.72	1.85	1	1
1:A:280:LEU:HD23	1:A:284:LEU:CD2	0.72	2.14	5	2
1:A:89:LEU:HD12	1:A:94:TRP:CZ2	0.72	2.20	10	4
1:A:235:ILE:HG21	1:A:242:TYR:CD1	0.72	2.20	2	4
1:A:59:ILE:HD13	1:A:280:LEU:HD21	0.72	1.62	3	2
1:A:106:TYR:OH	1:A:266:ILE:HD11	0.71	1.85	1	1
1:A:280:LEU:HD22	1:A:284:LEU:CD2	0.71	2.13	3	1
1:A:105:ALA:HB1	1:A:263:SER:HB2	0.70	1.63	6	5
1:A:64:HIS:CD2	1:A:96:ALA:HB1	0.70	2.21	2	1
1:A:97:VAL:HB	1:A:105:ALA:HB3	0.70	1.62	9	2
1:A:285:LEU:CD2	1:A:304:LEU:HD13	0.69	2.18	9	2
1:A:77:ALA:HB2	1:A:267:ASN:O	0.69	1.87	1	1
1:A:79:ILE:HD11	1:A:103:LEU:CB	0.69	2.18	7	5
1:A:181:VAL:HG12	1:A:183:VAL:HG23	0.68	1.64	7	3
1:A:339:PHE:CZ	1:A:343:VAL:HG21	0.68	2.23	10	6
1:A:115:LEU:HD11	1:A:147:LEU:HD11	0.68	1.66	3	1
1:A:116:ILE:HG22	1:A:217:PHE:CZ	0.68	2.24	4	1
1:A:232:TRP:HA	1:A:235:ILE:HD12	0.68	1.65	6	1
1:A:158:TRP:CE2	1:A:162:ALA:HB2	0.67	2.24	5	1
1:A:169:PHE:CD2	1:A:333:ILE:HD11	0.67	2.24	7	1
1:A:131:GLU:O	1:A:135:LEU:HD12	0.67	1.89	7	2
1:A:311:LEU:O	1:A:317:ILE:HD12	0.67	1.89	1	3
1:A:346:ALA:HB1	1:A:360:ALA:HB1	0.67	1.65	2	3
1:A:159:PRO:O	1:A:163:ALA:HB2	0.67	1.90	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:MET:HB2	1:A:208:THR:HG21	0.66	1.66	5	2
1:A:11:ILE:HD11	1:A:15:LYS:HD3	0.66	1.65	5	1
1:A:365:GLN:HA	1:A:368:ILE:HD12	0.66	1.68	9	1
1:A:94:TRP:CZ3	1:A:103:LEU:HD11	0.66	2.26	7	1
1:A:333:ILE:HD12	1:A:335:GLN:HB2	0.66	1.68	6	3
1:A:60:ILE:HD11	1:A:62:TRP:CE3	0.66	2.26	7	3
1:A:139:LEU:HD13	1:A:146:ALA:HA	0.66	1.68	5	5
1:A:106:TYR:CE1	1:A:266:ILE:HD12	0.65	2.26	4	1
1:A:259:VAL:HG23	1:A:328:GLU:O	0.65	1.90	6	1
1:A:217:PHE:CG	1:A:225:THR:HG21	0.65	2.27	8	3
1:A:304:LEU:HD23	1:A:307:TYR:HB2	0.64	1.69	9	2
1:A:77:ALA:HB2	1:A:268:ALA:HA	0.64	1.70	5	4
1:A:122:LEU:HD22	1:A:223:ALA:HB1	0.64	1.68	2	1
1:A:50:VAL:O	1:A:53:THR:HG22	0.63	1.93	2	1
1:A:285:LEU:HD23	1:A:304:LEU:HD13	0.63	1.69	8	1
1:A:311:LEU:HB3	1:A:317:ILE:HG21	0.63	1.71	10	10
1:A:122:LEU:CD2	1:A:223:ALA:HB1	0.63	2.24	2	1
1:A:19:GLY:O	1:A:23:VAL:HG23	0.63	1.94	6	2
1:A:339:PHE:CE2	1:A:368:ILE:HD13	0.62	2.29	5	1
1:A:280:LEU:CD2	1:A:284:LEU:HD22	0.62	2.24	3	5
1:A:105:ALA:HB1	1:A:263:SER:HB3	0.62	1.69	4	1
1:A:234:ASN:OD1	1:A:235:ILE:HG23	0.62	1.93	7	1
1:A:79:ILE:HD11	1:A:103:LEU:HB3	0.61	1.70	3	5
1:A:77:ALA:HB2	1:A:268:ALA:CA	0.61	2.26	5	2
1:A:109:ALA:HB2	1:A:299:LEU:HD12	0.61	1.71	5	1
1:A:108:ILE:HD13	1:A:284:LEU:O	0.61	1.95	8	1
1:A:213:ALA:HB1	1:A:225:THR:HG23	0.61	1.73	2	1
1:A:47:PHE:CE2	1:A:60:ILE:HG21	0.61	2.31	5	1
1:A:302:VAL:HG21	1:A:307:TYR:HB3	0.60	1.73	2	3
1:A:161:ILE:CD1	1:A:192:LEU:HD12	0.60	2.26	7	1
1:A:135:LEU:CD2	1:A:139:LEU:HD12	0.60	2.26	1	1
1:A:136:ASP:OD1	1:A:146:ALA:HB3	0.60	1.96	1	1
1:A:147:LEU:HD11	1:A:226:ILE:HG13	0.60	1.73	8	1
1:A:64:HIS:CD2	1:A:261:VAL:HG12	0.60	2.31	9	3
1:A:181:VAL:HG21	1:A:365:GLN:HA	0.60	1.73	10	2
1:A:104:ILE:HD12	1:A:104:ILE:O	0.60	1.95	4	4
1:A:147:LEU:HD12	1:A:224:MET:HB3	0.60	1.71	10	1
1:A:85:PHE:CZ	1:A:285:LEU:HD22	0.60	2.31	7	2
1:A:64:HIS:ND1	1:A:261:VAL:HG12	0.59	2.12	2	1
1:A:116:ILE:HD12	1:A:227:ASN:CB	0.59	2.27	3	1
1:A:139:LEU:HD22	1:A:223:ALA:HB2	0.59	1.73	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:164:ASP:OD2	1:A:190:ALA:HB3	0.59	1.98	2	1
1:A:198:LEU:HD13	1:A:204:MET:CE	0.59	2.28	8	1
1:A:183:VAL:CG1	1:A:361:LEU:HD22	0.59	2.26	6	4
1:A:160:LEU:CD2	1:A:195:LEU:HD13	0.59	2.27	6	2
1:A:148:MET:CG	1:A:213:ALA:HB2	0.58	2.28	2	1
1:A:110:VAL:HG13	1:A:260:GLY:O	0.58	1.98	2	1
1:A:132:ILE:HD13	1:A:147:LEU:HD22	0.58	1.75	2	4
1:A:300:GLY:O	1:A:311:LEU:HD13	0.58	1.99	5	2
1:A:2:THR:HG22	1:A:55:ASP:O	0.58	1.98	6	1
1:A:148:MET:SD	1:A:208:THR:HG23	0.58	2.39	3	1
1:A:115:LEU:HD11	1:A:147:LEU:CD1	0.57	2.30	3	2
1:A:151:LEU:CD2	1:A:195:LEU:HD21	0.57	2.29	9	1
1:A:129:TRP:CZ2	1:A:160:LEU:HD13	0.57	2.35	6	1
1:A:109:ALA:CB	1:A:299:LEU:HD22	0.57	2.30	8	2
1:A:97:VAL:CG1	1:A:105:ALA:HB3	0.57	2.30	8	3
1:A:92:PHE:CD1	1:A:93:THR:HG23	0.57	2.35	6	1
1:A:160:LEU:HD11	1:A:194:PHE:CD2	0.56	2.34	10	2
1:A:192:LEU:HD23	1:A:196:VAL:CG2	0.56	2.30	4	1
1:A:109:ALA:HB2	1:A:299:LEU:CD1	0.56	2.30	5	1
1:A:9:ILE:HD12	1:A:9:ILE:N	0.56	2.14	7	1
1:A:311:LEU:CB	1:A:317:ILE:HG21	0.56	2.30	6	2
1:A:108:ILE:HD12	1:A:284:LEU:HD23	0.56	1.77	10	1
1:A:129:TRP:CH2	1:A:160:LEU:HD13	0.56	2.36	3	1
1:A:339:PHE:CE2	1:A:343:VAL:HG21	0.56	2.36	1	4
1:A:307:TYR:CE2	1:A:311:LEU:HD11	0.56	2.36	7	3
1:A:154:PRO:CB	1:A:343:VAL:HG12	0.55	2.31	1	1
1:A:195:LEU:HA	1:A:198:LEU:HD12	0.55	1.78	8	1
1:A:23:VAL:HG12	1:A:279:PHE:CZ	0.55	2.35	4	1
1:A:196:VAL:HG12	1:A:200:LYS:HD2	0.55	1.76	4	2
1:A:108:ILE:CG2	1:A:290:LEU:HD21	0.55	2.31	9	1
1:A:9:ILE:HD12	1:A:37:VAL:HG22	0.55	1.78	8	1
1:A:108:ILE:HD12	1:A:262:LEU:O	0.55	2.02	7	1
1:A:168:ALA:HB2	1:A:339:PHE:CZ	0.55	2.36	1	1
1:A:105:ALA:HB1	1:A:263:SER:CB	0.55	2.32	3	4
1:A:365:GLN:O	1:A:369:THR:HG23	0.55	2.02	3	5
1:A:181:VAL:HG11	1:A:368:ILE:HD12	0.55	1.79	4	1
1:A:92:PHE:CE1	1:A:93:THR:HG22	0.55	2.37	5	4
1:A:181:VAL:HG11	1:A:368:ILE:HD13	0.54	1.79	1	1
1:A:160:LEU:HD23	1:A:195:LEU:HD13	0.54	1.79	9	1
1:A:178:ILE:HG21	1:A:335:GLN:OE1	0.53	2.03	8	1
1:A:147:LEU:HD12	1:A:224:MET:HB2	0.53	1.79	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:LEU:HD22	1:A:224:MET:SD	0.53	2.42	5	1
1:A:9:ILE:HD13	1:A:20:LEU:HD12	0.53	1.79	2	2
1:A:27:PHE:CE1	1:A:31:THR:HG21	0.53	2.39	8	2
1:A:217:PHE:CD2	1:A:225:THR:HG21	0.53	2.39	9	3
1:A:125:PRO:HB2	1:A:245:THR:HG21	0.53	1.77	3	1
1:A:345:THR:HG22	1:A:349:ASN:OD1	0.53	2.03	4	1
1:A:235:ILE:HG21	1:A:242:TYR:CE1	0.53	2.39	6	2
1:A:302:VAL:HG21	1:A:307:TYR:CD2	0.53	2.39	4	2
1:A:59:ILE:HD11	1:A:276:ALA:HB1	0.53	1.80	5	1
1:A:236:ASP:O	1:A:237:THR:HG23	0.52	2.03	10	1
1:A:147:LEU:HD13	1:A:224:MET:HB2	0.52	1.80	4	1
1:A:208:THR:HA	1:A:212:ILE:HD12	0.52	1.80	7	4
1:A:115:LEU:HD22	1:A:248:PRO:HD3	0.52	1.79	9	1
1:A:114:SER:HB3	1:A:244:VAL:HG13	0.52	1.82	4	1
1:A:97:VAL:HG23	1:A:103:LEU:CD2	0.52	2.35	7	1
1:A:64:HIS:HD2	1:A:261:VAL:HG12	0.52	1.64	1	2
1:A:272:ASN:ND2	1:A:275:LEU:HD12	0.52	2.20	1	2
1:A:106:TYR:HB2	1:A:264:ALA:HB3	0.52	1.80	4	1
1:A:181:VAL:HG12	1:A:183:VAL:H	0.52	1.65	9	4
1:A:107:PRO:HB3	1:A:261:VAL:HG21	0.52	1.82	2	3
1:A:97:VAL:O	1:A:97:VAL:HG23	0.51	2.04	5	1
1:A:79:ILE:HD11	1:A:103:LEU:HB2	0.51	1.82	5	3
1:A:59:ILE:HG21	1:A:280:LEU:HD11	0.51	1.82	7	1
1:A:2:THR:HG23	1:A:57:PRO:HA	0.51	1.83	2	1
1:A:149:PHE:CZ	1:A:195:LEU:HD11	0.51	2.40	5	1
1:A:11:ILE:HD11	1:A:15:LYS:CD	0.51	2.35	5	1
1:A:148:MET:SD	1:A:222:THR:HG21	0.51	2.45	4	4
1:A:98:ARG:HB3	1:A:103:LEU:HD23	0.51	1.82	2	1
1:A:109:ALA:O	1:A:261:VAL:HG12	0.51	2.06	5	3
1:A:47:PHE:CE2	1:A:60:ILE:HD12	0.51	2.41	2	1
1:A:89:LEU:HD13	1:A:94:TRP:CZ2	0.51	2.41	3	3
1:A:301:ALA:HB2	1:A:321:MET:CG	0.51	2.36	3	1
1:A:120:ASP:HB3	1:A:121:LEU:HD23	0.51	1.82	6	1
1:A:342:ALA:HB1	1:A:364:ALA:HA	0.51	1.83	9	1
1:A:64:HIS:CB	1:A:96:ALA:HB1	0.50	2.36	1	1
1:A:302:VAL:HG11	1:A:307:TYR:CD2	0.50	2.41	4	3
1:A:60:ILE:HD11	1:A:62:TRP:HE3	0.50	1.65	8	1
1:A:151:LEU:HD21	1:A:195:LEU:HD21	0.50	1.82	9	1
1:A:343:VAL:HG12	1:A:347:VAL:CG2	0.50	2.36	9	1
1:A:92:PHE:HB2	1:A:329:ILE:HD11	0.50	1.82	5	1
1:A:339:PHE:CD2	1:A:368:ILE:HD12	0.50	2.42	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:PHE:CZ	1:A:198:LEU:HD11	0.50	2.42	3	1
1:A:155:TYR:CD1	1:A:258:PHE:CE2	0.50	3.00	2	1
1:A:155:TYR:CZ	1:A:340:TRP:CH2	0.50	3.00	8	2
1:A:61:PHE:CE2	1:A:264:ALA:HB2	0.50	2.41	6	1
1:A:61:PHE:CE2	1:A:284:LEU:HD21	0.50	2.41	6	1
1:A:149:PHE:O	1:A:208:THR:HG22	0.50	2.07	7	1
1:A:108:ILE:HG23	1:A:285:LEU:CD2	0.50	2.37	1	1
1:A:155:TYR:CE1	1:A:340:TRP:CH2	0.50	3.00	2	1
1:A:92:PHE:CE2	1:A:93:THR:HG23	0.50	2.42	4	2
1:A:110:VAL:HG22	1:A:261:VAL:HG13	0.50	1.83	4	1
1:A:339:PHE:CD2	1:A:368:ILE:HD13	0.50	2.42	5	1
1:A:158:TRP:CD1	1:A:258:PHE:CZ	0.50	3.00	9	2
1:A:158:TRP:CD1	1:A:258:PHE:CE2	0.50	3.00	6	2
1:A:283:TYR:O	1:A:286:THR:HG22	0.50	2.07	3	1
1:A:155:TYR:CE1	1:A:258:PHE:CD1	0.50	3.00	10	1
1:A:78:GLU:HA	1:A:104:ILE:HG22	0.49	1.84	6	1
1:A:155:TYR:CZ	1:A:258:PHE:CE1	0.49	3.00	1	1
1:A:155:TYR:CD2	1:A:258:PHE:CD2	0.49	3.00	1	2
1:A:155:TYR:CD2	1:A:258:PHE:CE2	0.49	3.00	4	1
1:A:155:TYR:CZ	1:A:258:PHE:CD1	0.49	3.00	3	1
1:A:158:TRP:N	1:A:159:PRO:HD2	0.49	2.22	7	5
1:A:85:PHE:O	1:A:89:LEU:HD12	0.49	2.08	7	1
1:A:60:ILE:HG22	1:A:265:GLY:O	0.49	2.07	4	1
1:A:59:ILE:HG21	1:A:280:LEU:HD21	0.49	1.85	8	1
1:A:194:PHE:CZ	1:A:250:PHE:CE1	0.49	3.01	3	1
1:A:213:ALA:O	1:A:225:THR:HG21	0.49	2.08	4	1
1:A:139:LEU:HD22	1:A:145:SER:O	0.49	2.07	1	1
1:A:155:TYR:CZ	1:A:340:TRP:CZ2	0.49	3.00	1	1
1:A:158:TRP:N	1:A:159:PRO:CD	0.49	2.76	5	7
1:A:108:ILE:O	1:A:303:ALA:HB3	0.49	2.07	6	1
1:A:194:PHE:CD1	1:A:250:PHE:CZ	0.49	3.00	3	1
1:A:171:TYR:CE2	1:A:176:TYR:CE2	0.49	3.00	8	1
1:A:132:ILE:N	1:A:133:PRO:CD	0.48	2.76	8	7
1:A:238:SER:HB3	1:A:240:VAL:HG23	0.48	1.85	5	2
1:A:108:ILE:HG22	1:A:290:LEU:HD21	0.48	1.85	9	2
1:A:103:LEU:O	1:A:104:ILE:HG23	0.48	2.08	10	5
1:A:27:PHE:CD2	1:A:283:TYR:CE1	0.48	3.01	6	1
1:A:94:TRP:CH2	1:A:103:LEU:HD11	0.48	2.43	7	1
1:A:155:TYR:CE1	1:A:258:PHE:CD2	0.48	3.00	6	1
1:A:60:ILE:CG1	1:A:61:PHE:N	0.48	2.77	7	10
1:A:132:ILE:N	1:A:133:PRO:HD2	0.48	2.23	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:GLY:HA3	1:A:188:ALA:HB2	0.48	1.86	3	1
1:A:163:ALA:HB2	1:A:255:SER:HA	0.48	1.84	10	1
1:A:357:VAL:CG1	1:A:358:ASP:N	0.48	2.77	1	2
1:A:11:ILE:HD11	1:A:15:LYS:HE3	0.48	1.83	2	1
1:A:76:LEU:HD13	1:A:104:ILE:HD13	0.48	1.85	4	1
1:A:90:TYR:CD1	1:A:92:PHE:CZ	0.48	3.01	6	1
1:A:90:TYR:CZ	1:A:321:MET:HE2	0.48	2.44	2	1
1:A:121:LEU:HD11	1:A:223:ALA:HA	0.48	1.85	4	1
1:A:43:LEU:HD12	1:A:47:PHE:CD1	0.48	2.43	6	1
1:A:155:TYR:CE1	1:A:258:PHE:CG	0.48	3.01	6	1
1:A:40:PRO:HG2	1:A:43:LEU:HD22	0.48	1.86	2	2
1:A:115:LEU:CD1	1:A:147:LEU:HD11	0.48	2.38	3	1
1:A:266:ILE:HD11	1:A:280:LEU:HD12	0.48	1.84	9	1
1:A:345:THR:HG22	1:A:349:ASN:ND2	0.48	2.23	9	1
1:A:97:VAL:HG21	1:A:107:PRO:CG	0.48	2.38	10	1
1:A:90:TYR:CD1	1:A:92:PHE:CE2	0.48	3.02	6	1
1:A:166:GLY:CA	1:A:188:ALA:HB2	0.47	2.39	2	1
1:A:183:VAL:O	1:A:188:ALA:HB3	0.47	2.09	3	2
1:A:151:LEU:HD13	1:A:206:ALA:HA	0.47	1.87	5	1
1:A:79:ILE:HG21	1:A:106:TYR:CE1	0.47	2.44	6	2
1:A:160:LEU:HD21	1:A:194:PHE:HB3	0.47	1.86	8	1
1:A:89:LEU:HD23	1:A:303:ALA:HB1	0.47	1.84	3	1
1:A:37:VAL:HG12	1:A:39:HIS:CE1	0.47	2.44	8	1
1:A:2:THR:HG23	1:A:2:THR:O	0.47	2.09	3	2
1:A:261:VAL:O	1:A:261:VAL:HG13	0.47	2.09	7	1
1:A:343:VAL:HG12	1:A:347:VAL:HG23	0.47	1.86	9	1
1:A:183:VAL:O	1:A:361:LEU:HD22	0.47	2.09	8	1
1:A:194:PHE:CE1	1:A:250:PHE:CE1	0.47	3.02	3	1
1:A:136:ASP:HA	1:A:146:ALA:HB2	0.47	1.86	7	3
1:A:151:LEU:HD21	1:A:195:LEU:HD11	0.47	1.85	10	1
1:A:64:HIS:NE2	1:A:329:ILE:HG22	0.47	2.25	2	1
1:A:192:LEU:HD22	1:A:357:VAL:HG23	0.47	1.87	1	1
1:A:155:TYR:CE1	1:A:258:PHE:CZ	0.47	3.03	2	1
1:A:154:PRO:CG	1:A:343:VAL:HG12	0.47	2.40	1	1
1:A:171:TYR:CD2	1:A:176:TYR:CZ	0.47	3.03	8	1
1:A:115:LEU:HD12	1:A:225:THR:O	0.46	2.10	3	1
1:A:199:ILE:HG23	1:A:204:MET:O	0.46	2.10	9	3
1:A:97:VAL:HG11	1:A:107:PRO:CG	0.46	2.40	7	1
1:A:10:TRP:CE3	1:A:43:LEU:HD13	0.46	2.45	1	1
1:A:96:ALA:HB2	1:A:329:ILE:HG21	0.46	1.86	7	1
1:A:139:LEU:HD13	1:A:139:LEU:H	0.46	1.70	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:VAL:HG12	1:A:183:VAL:CG2	0.46	2.41	1	2
1:A:47:PHE:CZ	1:A:60:ILE:HG21	0.46	2.45	3	1
1:A:116:ILE:HG22	1:A:217:PHE:CE2	0.46	2.45	4	1
1:A:97:VAL:CG2	1:A:103:LEU:HD22	0.46	2.40	7	1
1:A:198:LEU:HD13	1:A:204:MET:HE2	0.46	1.86	8	1
1:A:161:ILE:HG12	1:A:192:LEU:HD12	0.46	1.88	8	1
1:A:77:ALA:HB2	1:A:267:ASN:C	0.46	2.31	1	1
1:A:92:PHE:CE1	1:A:93:THR:CG2	0.46	2.99	8	4
1:A:78:GLU:CG	1:A:79:ILE:N	0.46	2.79	8	2
1:A:290:LEU:HD13	1:A:307:TYR:CD2	0.46	2.46	10	1
1:A:148:MET:HG3	1:A:213:ALA:HB2	0.46	1.87	2	1
1:A:166:GLY:HA2	1:A:188:ALA:HB2	0.46	1.87	2	1
1:A:27:PHE:CD2	1:A:283:TYR:CD1	0.46	3.04	6	1
1:A:139:LEU:HD22	1:A:139:LEU:N	0.46	2.25	8	2
1:A:49:GLN:CG	1:A:50:VAL:N	0.45	2.79	4	8
1:A:42:LYS:C	1:A:43:LEU:HD23	0.45	2.32	4	1
1:A:210:TYR:CD1	1:A:211:SER:N	0.45	2.84	10	1
1:A:151:LEU:HD22	1:A:195:LEU:HD21	0.45	1.88	10	2
1:A:92:PHE:CE2	1:A:93:THR:CG2	0.45	2.99	4	2
1:A:47:PHE:N	1:A:48:PRO:CD	0.45	2.79	9	5
1:A:89:LEU:CD1	1:A:94:TRP:CZ2	0.45	2.99	4	2
1:A:160:LEU:HD11	1:A:194:PHE:CE2	0.45	2.46	10	1
1:A:10:TRP:CE3	1:A:43:LEU:CD1	0.45	3.00	2	1
1:A:5:GLY:O	1:A:33:ILE:HG23	0.45	2.12	6	1
1:A:109:ALA:HB2	1:A:299:LEU:HD13	0.45	1.88	7	1
1:A:40:PRO:O	1:A:43:LEU:HD22	0.45	2.11	2	1
1:A:70:TYR:O	1:A:75:LEU:HD12	0.45	2.12	5	1
1:A:194:PHE:CE2	1:A:198:LEU:HD11	0.45	2.47	7	3
1:A:286:THR:HG23	1:A:289:GLY:HA3	0.45	1.89	3	1
1:A:116:ILE:HG23	1:A:242:TYR:HB2	0.45	1.88	4	1
1:A:94:TRP:CZ3	1:A:103:LEU:CD1	0.45	2.98	7	1
1:A:44:GLU:CG	1:A:62:TRP:CH2	0.45	3.00	8	1
1:A:92:PHE:CD1	1:A:93:THR:N	0.45	2.85	3	3
1:A:217:PHE:CD2	1:A:225:THR:CG2	0.45	3.00	9	1
1:A:10:TRP:CG	1:A:57:PRO:CG	0.45	3.00	10	1
1:A:17:TYR:CD1	1:A:18:ASN:N	0.45	2.85	10	4
1:A:213:ALA:CB	1:A:225:THR:HG23	0.45	2.42	2	1
1:A:47:PHE:CB	1:A:48:PRO:HD3	0.45	2.42	3	2
1:A:109:ALA:CB	1:A:299:LEU:HD13	0.45	2.41	7	1
1:A:47:PHE:CE2	1:A:57:PRO:CG	0.44	2.99	6	1
1:A:235:ILE:HG21	1:A:242:TYR:HD1	0.44	1.65	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:ILE:HD12	1:A:81:PRO:HD3	0.44	1.89	7	1
1:A:339:PHE:CE1	1:A:343:VAL:CG2	0.44	3.00	10	4
1:A:90:TYR:CZ	1:A:321:MET:CE	0.44	3.00	2	1
1:A:157:THR:HG21	1:A:347:VAL:HG11	0.44	1.87	4	1
1:A:129:TRP:CZ3	1:A:132:ILE:HD12	0.44	2.47	5	1
1:A:147:LEU:HB2	1:A:224:MET:HE2	0.44	1.89	6	1
1:A:61:PHE:N	1:A:61:PHE:CD1	0.44	2.85	10	2
1:A:106:TYR:CE1	1:A:264:ALA:HB3	0.44	2.47	1	1
1:A:171:TYR:CD1	1:A:176:TYR:CZ	0.44	3.06	1	1
1:A:105:ALA:HB1	1:A:263:SER:OG	0.44	2.11	10	1
1:A:47:PHE:CE2	1:A:60:ILE:CG2	0.44	3.00	5	1
1:A:198:LEU:HD23	1:A:202:LYS:HG3	0.43	1.89	6	1
1:A:282:ASN:O	1:A:283:TYR:CG	0.43	2.71	1	1
1:A:149:PHE:CZ	1:A:204:MET:CE	0.43	3.01	2	1
1:A:49:GLN:HG3	1:A:50:VAL:HG13	0.43	1.90	9	3
1:A:366:THR:HG22	1:A:370:LYS:HG2	0.43	1.90	8	1
1:A:193:THR:OG1	1:A:357:VAL:HG21	0.43	2.13	10	1
1:A:272:ASN:CG	1:A:275:LEU:HD12	0.43	2.33	1	1
1:A:90:TYR:CB	1:A:92:PHE:CE2	0.43	3.00	3	1
1:A:307:TYR:CE2	1:A:311:LEU:CD1	0.43	3.01	7	2
1:A:117:TYR:CD1	1:A:245:THR:HG22	0.43	2.48	8	1
1:A:121:LEU:HD12	1:A:139:LEU:CD2	0.43	2.43	10	1
1:A:10:TRP:CD2	1:A:57:PRO:CG	0.43	3.01	7	1
1:A:90:TYR:CE2	1:A:305:LYS:CG	0.43	3.01	7	1
1:A:107:PRO:O	1:A:285:LEU:HD21	0.43	2.13	7	1
1:A:192:LEU:C	1:A:192:LEU:HD13	0.43	2.34	10	1
1:A:217:PHE:CD1	1:A:218:ASN:N	0.43	2.86	2	1
1:A:33:ILE:HG21	1:A:275:LEU:HD13	0.43	1.89	9	1
1:A:20:LEU:HD11	1:A:284:LEU:HD21	0.43	1.90	2	1
1:A:106:TYR:CE1	1:A:266:ILE:CD1	0.43	3.00	4	1
1:A:42:LYS:O	1:A:43:LEU:HD23	0.43	2.14	10	4
1:A:258:PHE:CD1	1:A:330:MET:CG	0.43	3.02	7	1
1:A:230:TRP:CD1	1:A:231:ALA:N	0.43	2.86	6	1
1:A:125:PRO:CG	1:A:245:THR:HG21	0.43	2.43	3	1
1:A:361:LEU:HD23	1:A:361:LEU:N	0.43	2.28	6	1
1:A:10:TRP:CE3	1:A:43:LEU:HD12	0.43	2.49	2	1
1:A:96:ALA:CB	1:A:261:VAL:HG21	0.43	2.44	5	1
1:A:42:LYS:O	1:A:43:LEU:HG	0.43	2.14	6	1
1:A:308:GLU:O	1:A:312:ALA:HB2	0.42	2.14	3	1
1:A:364:ALA:O	1:A:368:ILE:HD12	0.42	2.14	3	1
1:A:155:TYR:CD1	1:A:258:PHE:CD2	0.42	3.07	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:VAL:HG21	1:A:107:PRO:HD3	0.42	1.90	9	1
1:A:59:ILE:HD13	1:A:280:LEU:CD2	0.42	2.42	3	1
1:A:79:ILE:HG22	1:A:106:TYR:OH	0.42	2.14	3	2
1:A:108:ILE:HA	1:A:285:LEU:HD21	0.42	1.90	6	1
1:A:202:LYS:O	1:A:203:HIS:CG	0.42	2.72	6	2
1:A:329:ILE:HG22	1:A:330:MET:N	0.42	2.29	8	1
1:A:129:TRP:CZ3	1:A:160:LEU:HD13	0.42	2.49	3	1
1:A:160:LEU:HD11	1:A:250:PHE:CE1	0.42	2.49	5	1
1:A:283:TYR:CD1	1:A:283:TYR:N	0.42	2.87	5	1
1:A:85:PHE:CD2	1:A:89:LEU:CD1	0.42	3.02	7	1
1:A:104:ILE:C	1:A:104:ILE:HD12	0.42	2.35	10	1
1:A:155:TYR:CE2	1:A:258:PHE:CG	0.42	3.07	1	1
1:A:121:LEU:HD12	1:A:122:LEU:HB2	0.42	1.92	4	1
1:A:64:HIS:HE2	1:A:329:ILE:HG22	0.42	1.73	2	1
1:A:116:ILE:HG23	1:A:243:GLY:O	0.42	2.14	6	1
1:A:147:LEU:HD21	1:A:226:ILE:HD11	0.42	1.91	8	1
1:A:176:TYR:CD1	1:A:176:TYR:N	0.42	2.87	1	2
1:A:59:ILE:HG22	1:A:60:ILE:N	0.42	2.29	4	2
1:A:217:PHE:CG	1:A:225:THR:CG2	0.42	3.00	8	1
1:A:246:VAL:CG2	1:A:247:LEU:N	0.42	2.83	10	5
1:A:97:VAL:O	1:A:103:LEU:HD23	0.42	2.13	3	1
1:A:178:ILE:HG21	1:A:335:GLN:NE2	0.42	2.30	3	1
1:A:183:VAL:CG1	1:A:184:ASP:N	0.42	2.83	8	3
1:A:86:GLN:HG2	1:A:94:TRP:CZ2	0.42	2.49	7	1
1:A:301:ALA:HB2	1:A:320:THR:HB	0.42	1.91	7	1
1:A:90:TYR:CG	1:A:92:PHE:CZ	0.42	3.08	6	1
1:A:256:LYS:N	1:A:257:PRO:CD	0.42	2.83	7	1
1:A:118:ASN:HB3	1:A:121:LEU:HD12	0.42	1.90	9	1
1:A:168:ALA:HB1	1:A:339:PHE:CE1	0.42	2.50	10	1
1:A:53:THR:HG23	1:A:55:ASP:HB2	0.42	1.92	8	1
1:A:311:LEU:HB2	1:A:317:ILE:HG21	0.41	1.92	6	1
1:A:79:ILE:O	1:A:80:THR:HG23	0.41	2.15	10	1
1:A:209:ASP:O	1:A:213:ALA:CB	0.41	2.68	3	1
1:A:369:THR:O	1:A:369:THR:HG23	0.41	2.14	6	1
1:A:357:VAL:HG12	1:A:361:LEU:CD1	0.41	2.45	8	1
1:A:79:ILE:HG21	1:A:106:TYR:CZ	0.41	2.51	8	1
1:A:10:TRP:CG	1:A:57:PRO:HG2	0.41	2.50	10	1
1:A:47:PHE:N	1:A:48:PRO:HD2	0.41	2.30	1	1
1:A:78:GLU:OE1	1:A:104:ILE:HG22	0.41	2.15	9	1
1:A:210:TYR:OH	1:A:230:TRP:CZ2	0.41	2.74	9	1
1:A:222:THR:HG21	1:A:225:THR:HB	0.41	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ILE:N	1:A:9:ILE:CD1	0.41	2.84	7	1
1:A:78:GLU:O	1:A:79:ILE:CG2	0.41	2.69	7	1
1:A:88:LYS:O	1:A:304:LEU:HD12	0.41	2.15	8	1
1:A:2:THR:HG21	1:A:271:PRO:HD2	0.41	1.92	9	1
1:A:122:LEU:HD21	1:A:124:ASN:O	0.41	2.15	1	1
1:A:171:TYR:CD1	1:A:176:TYR:CE2	0.41	3.09	1	1
1:A:133:PRO:HB3	1:A:198:LEU:HD21	0.41	1.91	2	1
1:A:192:LEU:CD2	1:A:357:VAL:HG22	0.41	2.45	3	1
1:A:122:LEU:HD21	1:A:125:PRO:HA	0.41	1.93	5	1
1:A:99:TYR:CE1	1:A:332:ASN:OD1	0.41	2.74	6	1
1:A:171:TYR:CD2	1:A:175:LYS:O	0.41	2.74	6	1
1:A:172:GLU:CG	1:A:173:ASN:N	0.41	2.83	6	1
1:A:97:VAL:CG2	1:A:103:LEU:CD2	0.41	2.99	7	1
1:A:259:VAL:HG23	1:A:328:GLU:C	0.41	2.37	1	1
1:A:150:ASN:OD1	1:A:156:PHE:CG	0.41	2.74	2	1
1:A:150:ASN:OD1	1:A:156:PHE:CD2	0.41	2.74	9	1
1:A:171:TYR:CE1	1:A:174:GLY:O	0.40	2.74	4	1
1:A:246:VAL:HG11	1:A:322:GLU:CD	0.40	2.36	4	1
1:A:336:MET:O	1:A:340:TRP:CD1	0.40	2.74	5	2
1:A:203:HIS:O	1:A:203:HIS:CD2	0.40	2.75	10	1
1:A:155:TYR:CZ	1:A:258:PHE:CZ	0.40	3.10	1	1
1:A:47:PHE:CZ	1:A:57:PRO:CG	0.40	3.05	3	1
1:A:90:TYR:HB3	1:A:92:PHE:CE2	0.40	2.51	3	1
1:A:117:TYR:CE2	1:A:243:GLY:O	0.40	2.75	3	1
1:A:129:TRP:CD1	1:A:248:PRO:O	0.40	2.74	9	1
1:A:230:TRP:O	1:A:230:TRP:CD1	0.40	2.74	1	1
1:A:147:LEU:HD12	1:A:224:MET:C	0.40	2.37	3	1
1:A:282:ASN:O	1:A:283:TYR:CD1	0.40	2.75	3	1
1:A:181:VAL:CG1	1:A:183:VAL:CG2	0.40	2.99	4	1
1:A:149:PHE:CE1	1:A:195:LEU:HD11	0.40	2.51	5	1
1:A:133:PRO:HG3	1:A:198:LEU:HD21	0.40	1.93	7	1
1:A:337:SER:O	1:A:341:TYR:CE2	0.40	2.74	7	1
1:A:62:TRP:O	1:A:67:PHE:CE2	0.40	2.74	9	1
1:A:64:HIS:CG	1:A:261:VAL:HG12	0.40	2.50	9	1
1:A:135:LEU:HD23	1:A:139:LEU:CD1	0.40	2.45	10	1
1:A:282:ASN:ND2	1:A:282:ASN:N	0.40	2.70	1	1
1:A:210:TYR:CD2	1:A:214:GLU:OE2	0.40	2.75	3	1
1:A:10:TRP:CD2	1:A:57:PRO:HG2	0.40	2.50	7	1
1:A:171:TYR:CZ	1:A:174:GLY:O	0.40	2.74	2	1
1:A:62:TRP:CD1	1:A:66:ARG:CB	0.40	3.04	4	1
1:A:60:ILE:HD11	1:A:62:TRP:CZ3	0.40	2.50	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:TRP:CH2	1:A:103:LEU:CD1	0.40	3.05	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	368/370 (99%)	328±4 (89±1%)	33±5 (9±1%)	7±2 (2±1%)	12	54
All	All	3680/3700 (99%)	3283 (89%)	329 (9%)	68 (2%)	12	54

All 32 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	284	LEU	8
1	A	236	ASP	6
1	A	104	ILE	6
1	A	56	GLY	4
1	A	257	PRO	4
1	A	285	LEU	3
1	A	331	PRO	3
1	A	41	ASP	3
1	A	107	PRO	3
1	A	248	PRO	2
1	A	241	ASN	2
1	A	16	GLY	2
1	A	208	THR	2
1	A	57	PRO	2
1	A	14	ASP	1
1	A	15	LYS	1
1	A	165	GLY	1
1	A	269	ALA	1
1	A	271	PRO	1
1	A	272	ASN	1
1	A	220	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	97	VAL	1
1	A	239	LYS	1
1	A	4	GLU	1
1	A	203	HIS	1
1	A	255	SER	1
1	A	69	GLY	1
1	A	166	GLY	1
1	A	3	GLU	1
1	A	221	GLU	1
1	A	237	THR	1
1	A	354	ARG	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	296/297 (100%)	244±5 (82±2%)	52±5 (18±2%)	4	38
All	All	2960/2970 (100%)	2435 (82%)	525 (18%)	4	38

All 172 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	148	MET	10
1	A	212	ILE	10
1	A	211	SER	9
1	A	192	LEU	8
1	A	43	LEU	8
1	A	46	LYS	7
1	A	102	LYS	7
1	A	127	LYS	7
1	A	47	PHE	7
1	A	140	LYS	7
1	A	277	LYS	7
1	A	15	LYS	6
1	A	42	LYS	6
1	A	67	PHE	6

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Mol	Chain	Res	Type	Models (Total)
1	A	78	GLU	6
1	A	139	LEU	6
1	A	179	LYS	6
1	A	263	SER	6
1	A	308	GLU	6
1	A	344	ARG	6
1	A	362	LYS	6
1	A	26	LYS	6
1	A	98	ARG	6
1	A	204	MET	6
1	A	341	TYR	6
1	A	210	TYR	6
1	A	6	LYS	5
1	A	62	TRP	5
1	A	121	LEU	5
1	A	135	LEU	5
1	A	202	LYS	5
1	A	219	LYS	5
1	A	246	VAL	5
1	A	314	ASP	5
1	A	55	ASP	5
1	A	66	ARG	5
1	A	214	GLU	5
1	A	111	GLU	5
1	A	131	GLU	5
1	A	261	VAL	5
1	A	88	LYS	5
1	A	14	ASP	4
1	A	114	SER	4
1	A	207	ASP	4
1	A	237	THR	4
1	A	128	THR	4
1	A	170	LYS	4
1	A	285	LEU	4
1	A	175	LYS	4
1	A	255	SER	4
1	A	370	LYS	4
1	A	142	LYS	4
1	A	241	ASN	4
1	A	359	GLU	4
1	A	10	TRP	4
1	A	82	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	28	GLU	3
1	A	29	LYS	3
1	A	155	TYR	3
1	A	236	ASP	3
1	A	256	LYS	3
1	A	270	SER	3
1	A	273	LYS	3
1	A	365	GLN	3
1	A	87	ASP	3
1	A	95	ASP	3
1	A	307	TYR	3
1	A	328	GLU	3
1	A	354	ARG	3
1	A	44	GLU	3
1	A	58	ASP	3
1	A	119	LYS	3
1	A	144	LYS	3
1	A	172	GLU	3
1	A	286	THR	3
1	A	297	LYS	3
1	A	31	THR	3
1	A	80	THR	3
1	A	89	LEU	3
1	A	203	HIS	3
1	A	239	LYS	3
1	A	299	LEU	3
1	A	335	GLN	3
1	A	72	GLN	3
1	A	130	GLU	3
1	A	183	VAL	3
1	A	189	LYS	3
1	A	336	MET	3
1	A	281	GLU	3
1	A	118	ASN	2
1	A	200	LYS	2
1	A	208	THR	2
1	A	234	ASN	2
1	A	238	SER	2
1	A	267	ASN	2
1	A	287	ASP	2
1	A	290	LEU	2
1	A	326	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	361	LEU	2
1	A	2	THR	2
1	A	251	LYS	2
1	A	306	SER	2
1	A	20	LEU	2
1	A	99	TYR	2
1	A	120	ASP	2
1	A	253	GLN	2
1	A	224	MET	2
1	A	296	ASP	2
1	A	73	SER	2
1	A	136	ASP	2
1	A	177	ASP	2
1	A	3	GLU	2
1	A	86	GLN	2
1	A	138	GLU	2
1	A	153	GLU	2
1	A	310	GLU	2
1	A	49	GLN	2
1	A	83	LYS	2
1	A	147	LEU	2
1	A	352	SER	2
1	A	8	VAL	1
1	A	272	ASN	1
1	A	282	ASN	1
1	A	313	LYS	1
1	A	41	ASP	1
1	A	122	LEU	1
1	A	284	LEU	1
1	A	316	ARG	1
1	A	358	ASP	1
1	A	18	ASN	1
1	A	39	HIS	1
1	A	65	ASP	1
1	A	93	THR	1
1	A	227	ASN	1
1	A	274	GLU	1
1	A	304	LEU	1
1	A	320	THR	1
1	A	322	GLU	1
1	A	366	THR	1
1	A	25	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	64	HIS	1
1	A	145	SER	1
1	A	294	ASN	1
1	A	321	MET	1
1	A	4	GLU	1
1	A	30	ASP	1
1	A	100	ASN	1
1	A	323	ASN	1
1	A	349	ASN	1
1	A	356	THR	1
1	A	27	PHE	1
1	A	85	PHE	1
1	A	367	ARG	1
1	A	34	LYS	1
1	A	171	TYR	1
1	A	242	TYR	1
1	A	345	THR	1
1	A	355	GLN	1
1	A	45	GLU	1
1	A	156	PHE	1
1	A	157	THR	1
1	A	185	ASN	1
1	A	193	THR	1
1	A	247	LEU	1
1	A	337	SER	1
1	A	22	GLU	1
1	A	164	ASP	1
1	A	197	ASP	1
1	A	198	LEU	1
1	A	221	GLU	1
1	A	233	SER	1
1	A	291	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided