Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 01:01 AM BST

PDB ID	:	2LGZ
Title	:	Solution structure of STT3P
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Deposited on	:	2011-08-03

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 (i) symbol.

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

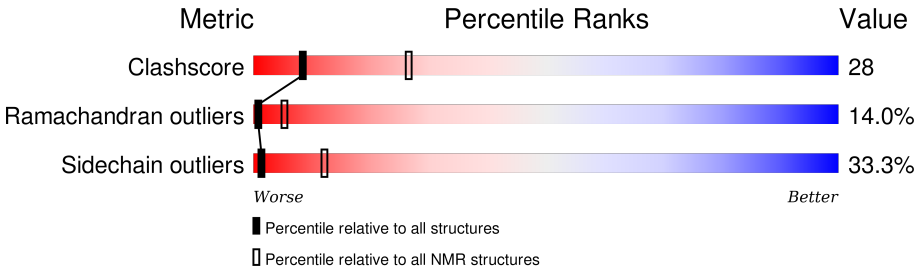
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 36%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	273	16% 53% 7% 23%

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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:21-A:146, A:153-A:166, A:189-A:197, A:202-A:261 (209)	1.52	4

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	4, 5, 7, 8, 10
2	3, 9
3	1, 2
Single-model clusters	6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4340 atoms, of which 2124 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3.

Mol	Chain	Residues	Atoms						Trace
1	A	273	Total	C	H	N	O	S	0
			4340	1395	2124	392	423	6	

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P39007
A	2	GLY	-	EXPRESSION TAG	UNP P39007
A	3	SER	-	EXPRESSION TAG	UNP P39007
A	4	SER	-	EXPRESSION TAG	UNP P39007
A	5	HIS	-	EXPRESSION TAG	UNP P39007
A	6	HIS	-	EXPRESSION TAG	UNP P39007
A	7	HIS	-	EXPRESSION TAG	UNP P39007
A	8	HIS	-	EXPRESSION TAG	UNP P39007
A	9	HIS	-	EXPRESSION TAG	UNP P39007
A	10	HIS	-	EXPRESSION TAG	UNP P39007
A	11	SER	-	EXPRESSION TAG	UNP P39007
A	12	SER	-	EXPRESSION TAG	UNP P39007
A	13	GLY	-	EXPRESSION TAG	UNP P39007
A	14	LEU	-	EXPRESSION TAG	UNP P39007
A	15	VAL	-	EXPRESSION TAG	UNP P39007
A	16	PRO	-	EXPRESSION TAG	UNP P39007
A	17	ARG	-	EXPRESSION TAG	UNP P39007
A	18	GLY	-	EXPRESSION TAG	UNP P39007
A	19	SER	-	EXPRESSION TAG	UNP P39007
A	105	ASN	MET	CONFLICT	UNP P39007
A	145	ASN	MET	CONFLICT	UNP P39007
A	231	ASN	MET	CONFLICT	UNP P39007

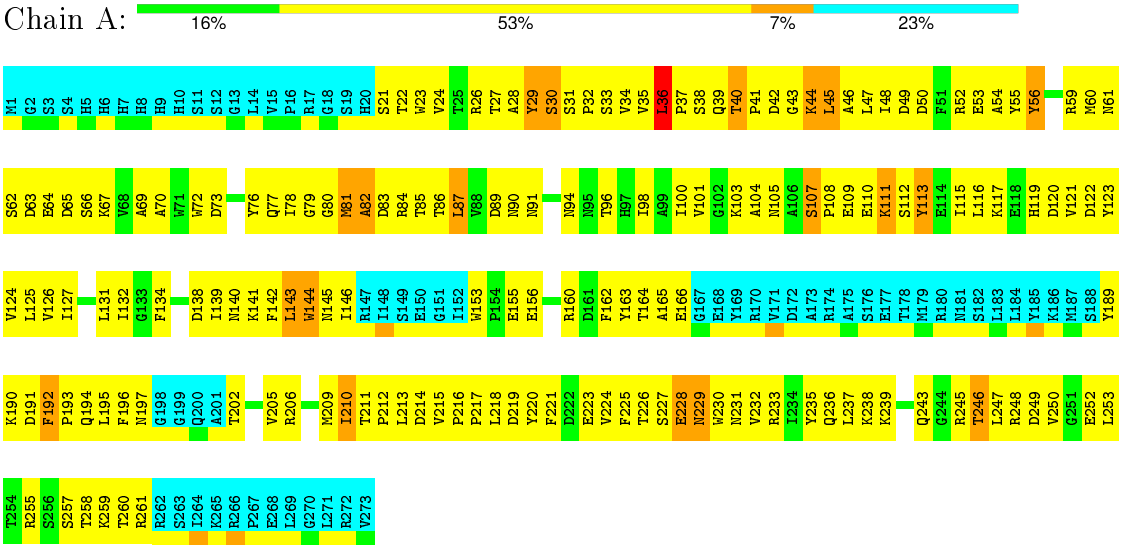
4 Residue-property plots (i)

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: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3

Chain A:



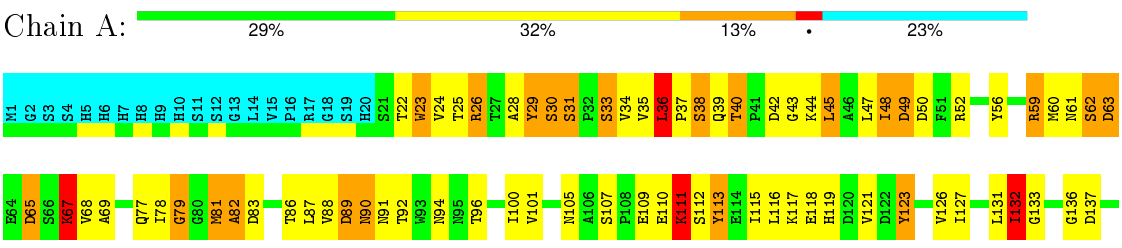
4.2 Scores per residue for each member of the ensemble

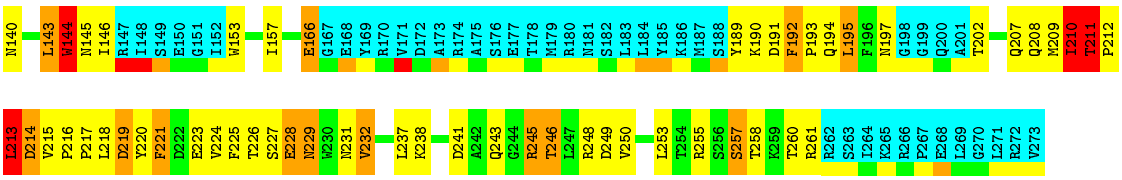
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3

Chain A:

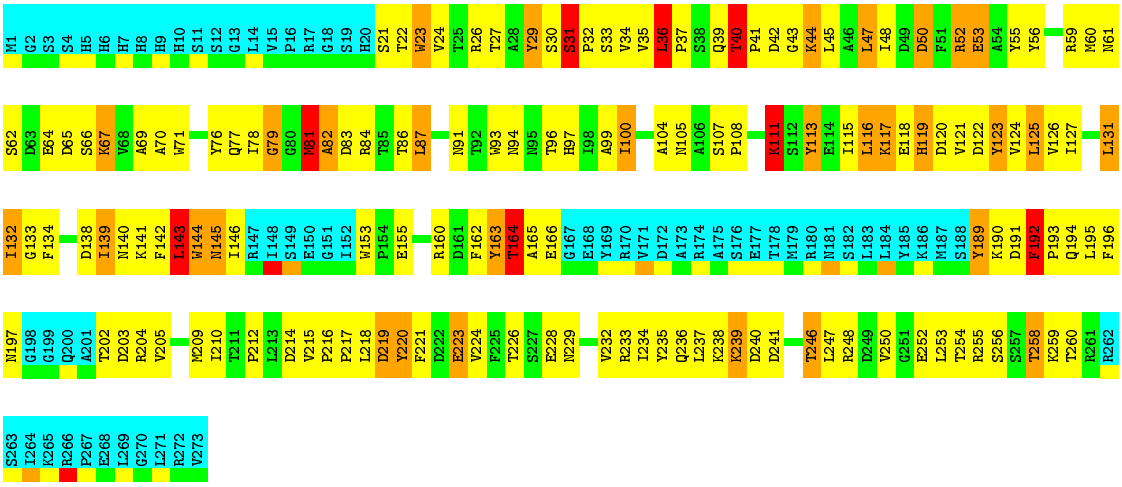




4.2.2 Score per residue for model 2

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3

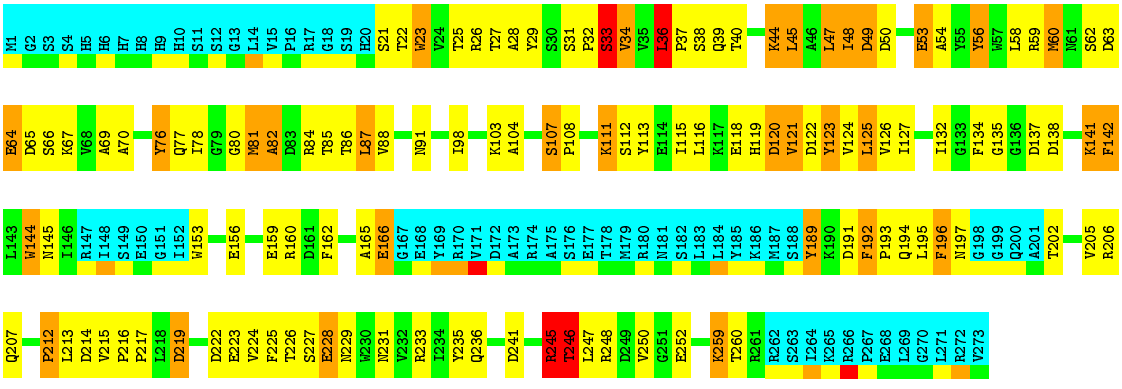
Chain A: 22% 40% 11% • 23%



4.2.3 Score per residue for model 3

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3

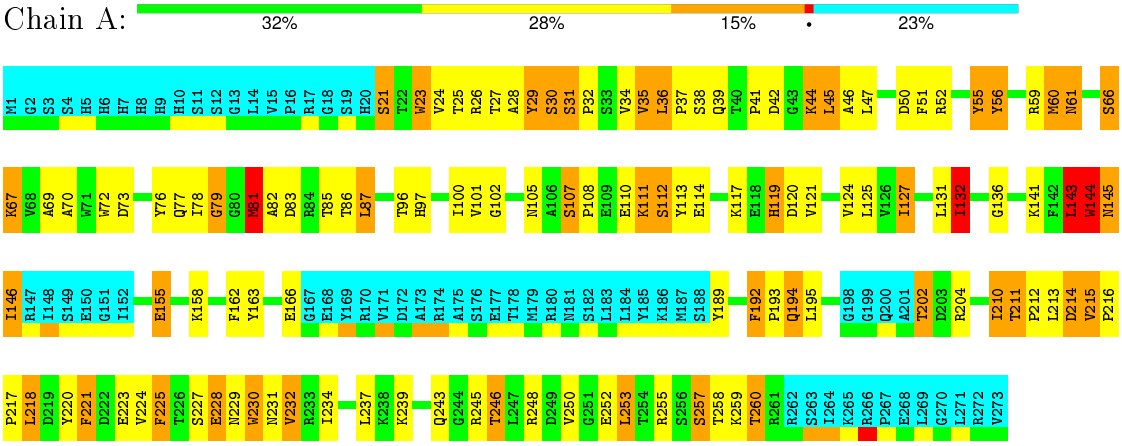
Chain A: 31% 33% 12% • 23%



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3

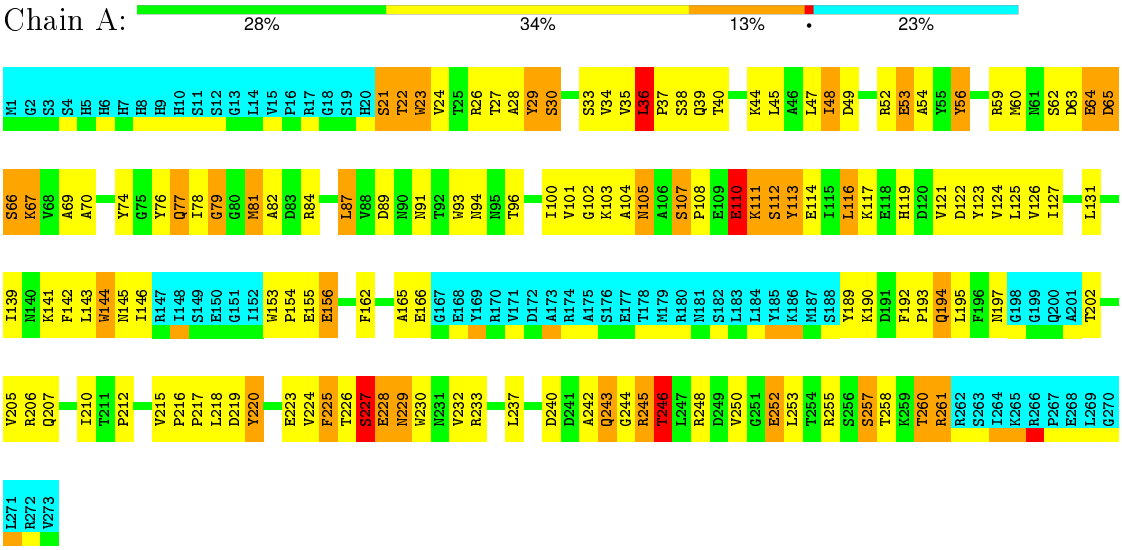
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3

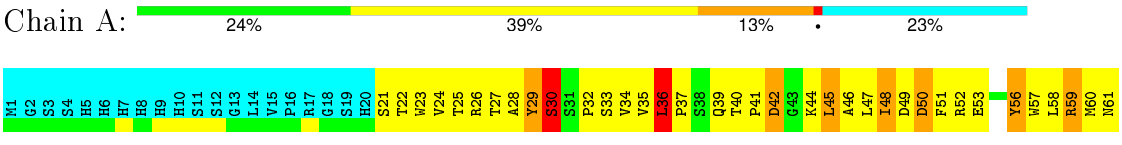
Chain A:

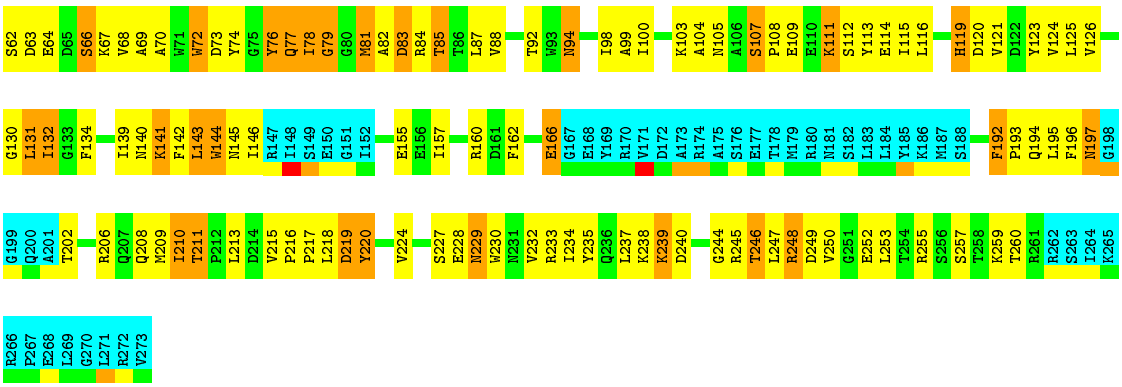


4.2.6 Score per residue for model 6

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3

Chain A:

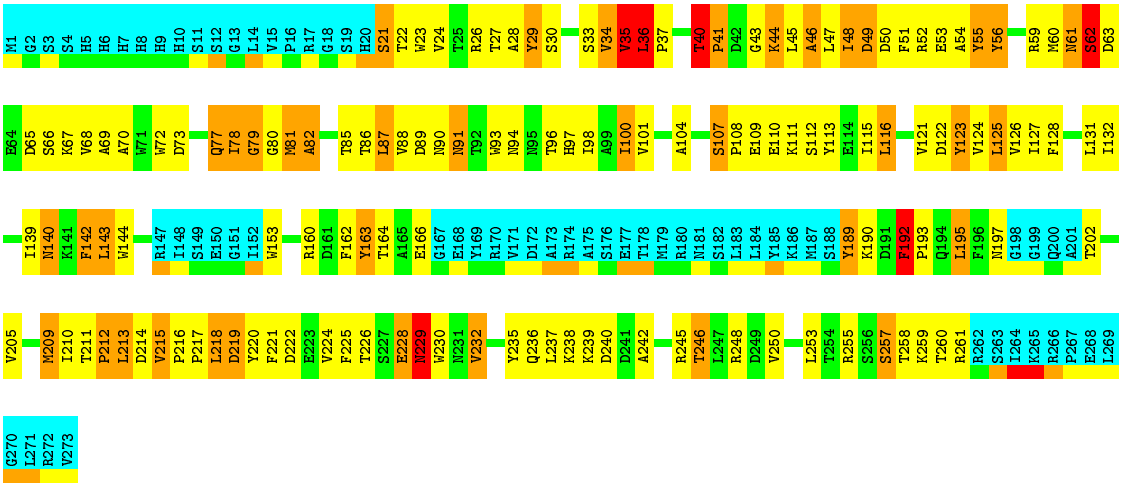




4.2.7 Score per residue for model 7

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3

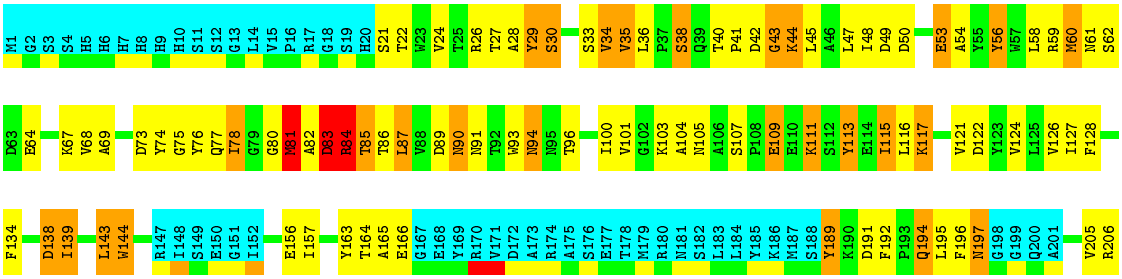
Chain A:

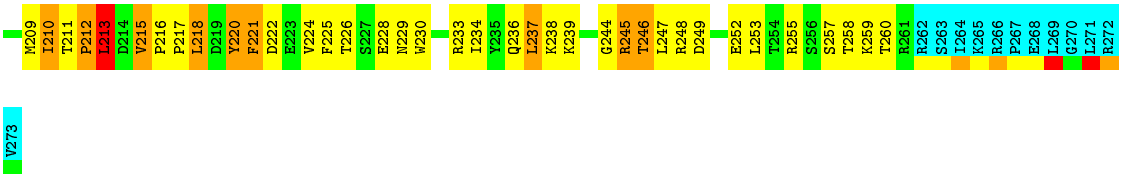


4.2.8 Score per residue for model 8

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3

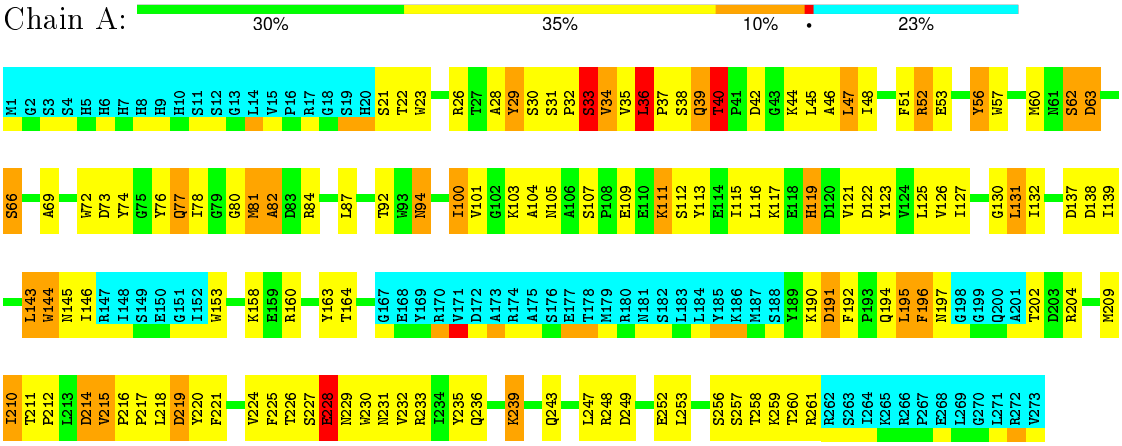
Chain A:





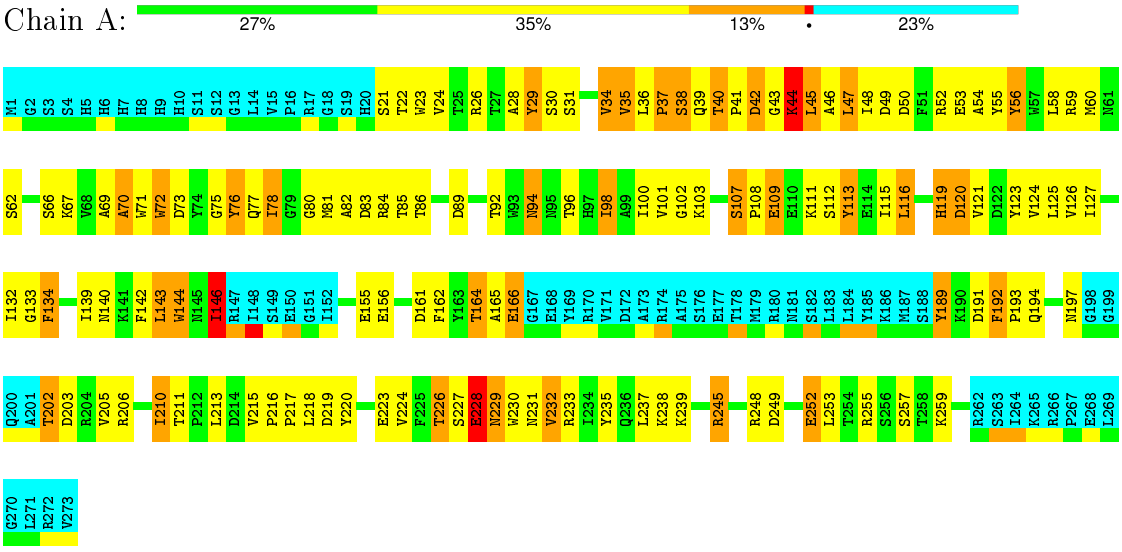
4.2.9 Score per residue for model 9

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



4.2.10 Score per residue for model 10

• Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	3.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2lgz_cs.str
Number of chemical shift lists	1
Total number of shifts	1187
Number of shifts mapped to atoms	1187
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	36%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	1718	1633	1633	94±7
All	All	17180	16330	16330	940

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:ASP:O	1:A:192:PHE:HB2	0.95	1.56	1	2
1:A:45:LEU:HD23	1:A:121:VAL:HG12	0.89	1.45	3	1
1:A:216:PRO:N	1:A:217:PRO:HD2	0.87	1.85	9	7
1:A:45:LEU:HD21	1:A:121:VAL:HG13	0.87	1.44	5	4
1:A:213:LEU:HD13	1:A:218:LEU:HD21	0.81	1.51	1	1
1:A:54:ALA:HB2	1:A:80:GLY:O	0.81	1.74	8	1
1:A:216:PRO:N	1:A:217:PRO:CD	0.80	2.45	9	7
1:A:216:PRO:HG2	1:A:217:PRO:HD3	0.80	1.52	1	7
1:A:22:THR:O	1:A:26:ARG:N	0.79	2.15	8	5
1:A:104:ALA:HB2	1:A:220:TYR:CB	0.79	2.08	5	1
1:A:191:ASP:O	1:A:192:PHE:CB	0.77	2.31	1	3
1:A:107:SER:N	1:A:108:PRO:CD	0.76	2.49	2	1
1:A:126:VAL:HG11	1:A:226:THR:O	0.76	1.81	10	2
1:A:35:VAL:HG11	1:A:116:LEU:HD13	0.76	1.56	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HD11	1:A:99:ALA:HB2	0.75	1.58	6	1
1:A:45:LEU:HD13	1:A:124:VAL:HG21	0.75	1.58	2	1
1:A:69:ALA:O	1:A:72:TRP:N	0.75	2.16	10	1
1:A:110:GLU:O	1:A:111:LYS:CB	0.75	2.34	5	3
1:A:216:PRO:CD	1:A:217:PRO:CD	0.74	2.65	1	7
1:A:36:LEU:HD11	1:A:99:ALA:HB1	0.74	1.59	2	1
1:A:56:TYR:HB3	1:A:72:TRP:CD1	0.74	2.17	10	1
1:A:123:TYR:CE2	1:A:224:VAL:HG13	0.73	2.18	9	1
1:A:54:ALA:HB1	1:A:142:PHE:CB	0.71	2.14	3	2
1:A:210:ILE:HG23	1:A:211:THR:H	0.71	1.45	1	1
1:A:27:THR:HG23	1:A:121:VAL:HG21	0.71	1.63	2	1
1:A:216:PRO:CD	1:A:217:PRO:HD2	0.70	2.16	1	7
1:A:224:VAL:HG12	1:A:228:GLU:HG3	0.70	1.63	1	1
1:A:56:TYR:CD2	1:A:69:ALA:HB1	0.70	2.22	8	5
1:A:214:ASP:O	1:A:215:VAL:O	0.70	2.08	9	1
1:A:216:PRO:CG	1:A:217:PRO:HD3	0.69	2.17	1	7
1:A:195:LEU:HD21	1:A:231:ASN:CG	0.69	2.08	1	1
1:A:119:HIS:CB	1:A:224:VAL:HG22	0.69	2.18	6	1
1:A:104:ALA:HB2	1:A:220:TYR:CG	0.69	2.22	5	1
1:A:24:VAL:O	1:A:28:ALA:HB3	0.68	1.89	6	2
1:A:45:LEU:HD22	1:A:48:ILE:HB	0.68	1.64	6	1
1:A:49:ASP:O	1:A:80:GLY:N	0.68	2.26	8	1
1:A:210:ILE:HG22	1:A:211:THR:HG22	0.68	1.63	4	1
1:A:66:SER:CB	1:A:69:ALA:HB3	0.68	2.19	6	6
1:A:215:VAL:C	1:A:217:PRO:HD2	0.68	2.09	9	7
1:A:33:SER:O	1:A:35:VAL:HG23	0.68	1.88	6	1
1:A:78:ILE:O	1:A:79:GLY:C	0.68	2.33	2	5
1:A:81:MET:O	1:A:82:ALA:HB2	0.67	1.88	7	2
1:A:45:LEU:HD22	1:A:124:VAL:CG2	0.67	2.18	7	1
1:A:23:TRP:CD1	1:A:24:VAL:HG13	0.67	2.24	6	2
1:A:110:GLU:O	1:A:111:LYS:HB2	0.67	1.90	5	1
1:A:125:LEU:HD12	1:A:126:VAL:HG23	0.67	1.65	6	1
1:A:112:SER:HB2	1:A:116:LEU:HD12	0.66	1.67	10	1
1:A:192:PHE:CB	1:A:193:PRO:CD	0.66	2.73	1	5
1:A:28:ALA:O	1:A:29:TYR:C	0.66	2.32	6	9
1:A:209:MET:HA	1:A:232:VAL:HG13	0.66	1.65	6	1
1:A:142:PHE:CE2	1:A:143:LEU:HD23	0.66	2.26	6	1
1:A:56:TYR:C	1:A:56:TYR:CD1	0.66	2.69	8	2
1:A:227:SER:O	1:A:228:GLU:C	0.65	2.34	1	4
1:A:53:GLU:HB3	1:A:80:GLY:N	0.65	2.07	10	3
1:A:242:ALA:O	1:A:243:GLN:C	0.65	2.34	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:O	1:A:36:LEU:C	0.65	2.35	1	1
1:A:233:ARG:HG2	1:A:234:ILE:HD12	0.65	1.69	8	1
1:A:22:THR:HG21	1:A:47:LEU:CB	0.65	2.21	9	2
1:A:87:LEU:HD12	1:A:91:ASN:HA	0.65	1.68	1	2
1:A:68:VAL:HG12	1:A:252:GLU:OE2	0.65	1.92	6	1
1:A:45:LEU:HD23	1:A:48:ILE:HB	0.65	1.69	7	1
1:A:126:VAL:HG21	1:A:227:SER:O	0.64	1.91	6	2
1:A:210:ILE:HG23	1:A:239:LYS:HD2	0.64	1.70	9	1
1:A:119:HIS:HB2	1:A:224:VAL:HG22	0.64	1.69	6	1
1:A:107:SER:CB	1:A:108:PRO:HD2	0.64	2.22	5	6
1:A:246:THR:O	1:A:250:VAL:HG13	0.64	1.92	6	3
1:A:45:LEU:CD2	1:A:121:VAL:HG13	0.64	2.23	5	5
1:A:56:TYR:CD1	1:A:56:TYR:C	0.63	2.72	3	1
1:A:210:ILE:HD11	1:A:235:TYR:CD1	0.63	2.28	6	1
1:A:47:LEU:HD13	1:A:144:TRP:CH2	0.63	2.29	5	1
1:A:24:VAL:HG11	1:A:156:GLU:CB	0.63	2.23	10	1
1:A:230:TRP:O	1:A:234:ILE:HD12	0.63	1.94	6	1
1:A:214:ASP:O	1:A:215:VAL:HG22	0.63	1.93	9	1
1:A:81:MET:CE	1:A:143:LEU:HD23	0.63	2.23	9	1
1:A:34:VAL:HG12	1:A:116:LEU:HD13	0.63	1.71	6	1
1:A:27:THR:O	1:A:121:VAL:HG11	0.63	1.93	6	1
1:A:210:ILE:HG23	1:A:239:LYS:CB	0.62	2.24	6	1
1:A:56:TYR:O	1:A:60:MET:N	0.62	2.32	7	2
1:A:225:PHE:CE2	1:A:247:LEU:HD12	0.62	2.30	3	1
1:A:53:GLU:HB3	1:A:80:GLY:HA3	0.62	1.70	8	1
1:A:225:PHE:O	1:A:232:VAL:HG21	0.62	1.94	4	2
1:A:44:LYS:HD2	1:A:78:ILE:HD11	0.62	1.70	2	1
1:A:48:ILE:HG21	1:A:124:VAL:O	0.62	1.94	8	1
1:A:112:SER:CB	1:A:116:LEU:HD12	0.62	2.23	10	1
1:A:104:ALA:HB2	1:A:219:ASP:HB2	0.62	1.71	9	3
1:A:66:SER:HB2	1:A:69:ALA:HB3	0.62	1.72	6	2
1:A:115:ILE:HD13	1:A:220:TYR:CZ	0.62	2.30	2	1
1:A:29:TYR:CB	1:A:45:LEU:HD13	0.62	2.25	1	1
1:A:72:TRP:NE1	1:A:76:TYR:HB2	0.61	2.09	10	1
1:A:121:VAL:O	1:A:125:LEU:HD23	0.61	1.95	2	2
1:A:126:VAL:HG11	1:A:227:SER:O	0.61	1.95	5	1
1:A:54:ALA:HB1	1:A:142:PHE:HB3	0.61	1.70	10	2
1:A:210:ILE:HD12	1:A:239:LYS:CG	0.61	2.25	2	1
1:A:143:LEU:O	1:A:144:TRP:C	0.61	2.39	8	1
1:A:100:ILE:CD1	1:A:101:VAL:HG13	0.61	2.26	10	2
1:A:47:LEU:HD12	1:A:144:TRP:CZ2	0.61	2.31	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:ILE:HD12	1:A:101:VAL:HG13	0.61	1.73	10	2
1:A:22:THR:HG21	1:A:47:LEU:HB2	0.61	1.71	10	3
1:A:105:ASN:HB2	1:A:116:LEU:HD21	0.61	1.73	1	1
1:A:218:LEU:O	1:A:222:ASP:N	0.61	2.34	8	1
1:A:69:ALA:O	1:A:72:TRP:HE3	0.60	1.79	10	1
1:A:69:ALA:HB1	1:A:72:TRP:CE3	0.60	2.31	6	1
1:A:23:TRP:CZ2	1:A:125:LEU:HD13	0.60	2.31	9	2
1:A:68:VAL:HG13	1:A:252:GLU:OE2	0.60	1.96	8	1
1:A:53:GLU:HA	1:A:72:TRP:CD1	0.60	2.31	10	1
1:A:60:MET:HB3	1:A:69:ALA:HB2	0.60	1.73	8	2
1:A:197:ASN:HB2	1:A:202:THR:HG21	0.60	1.73	3	1
1:A:45:LEU:O	1:A:48:ILE:N	0.60	2.35	7	1
1:A:101:VAL:HG13	1:A:223:GLU:OE1	0.60	1.97	1	1
1:A:28:ALA:HB1	1:A:155:GLU:HG2	0.60	1.74	4	1
1:A:50:ASP:HB3	1:A:144:TRP:CD1	0.60	2.32	8	2
1:A:144:TRP:O	1:A:145:ASN:C	0.60	2.40	2	1
1:A:58:LEU:HD22	1:A:141:LYS:CG	0.59	2.27	6	1
1:A:45:LEU:HG	1:A:48:ILE:HD13	0.59	1.74	1	1
1:A:210:ILE:HD12	1:A:235:TYR:CE1	0.59	2.32	10	1
1:A:69:ALA:HA	1:A:72:TRP:NE1	0.59	2.11	7	1
1:A:122:ASP:HA	1:A:125:LEU:HD22	0.59	1.73	3	1
1:A:127:ILE:HD11	1:A:226:THR:HG22	0.59	1.74	8	1
1:A:112:SER:O	1:A:113:TYR:CB	0.59	2.51	5	1
1:A:35:VAL:HG12	1:A:98:ILE:HG12	0.59	1.73	10	1
1:A:50:ASP:C	1:A:53:GLU:OE2	0.59	2.40	7	1
1:A:60:MET:CB	1:A:69:ALA:HB2	0.59	2.27	3	1
1:A:77:GLN:HG2	1:A:87:LEU:HD22	0.59	1.73	7	1
1:A:195:LEU:O	1:A:196:PHE:C	0.59	2.39	3	2
1:A:58:LEU:HD22	1:A:141:LYS:HG3	0.59	1.74	6	1
1:A:125:LEU:O	1:A:125:LEU:HD12	0.59	1.98	2	2
1:A:189:TYR:CD1	1:A:189:TYR:C	0.58	2.77	4	1
1:A:87:LEU:HD13	1:A:94:ASN:OD1	0.58	1.97	7	1
1:A:45:LEU:HD22	1:A:124:VAL:HG23	0.58	1.75	7	2
1:A:90:ASN:O	1:A:94:ASN:N	0.58	2.37	8	3
1:A:45:LEU:CG	1:A:48:ILE:HD13	0.58	2.29	1	1
1:A:81:MET:O	1:A:82:ALA:CB	0.58	2.51	7	1
1:A:39:GLN:O	1:A:40:THR:HG23	0.58	1.97	2	3
1:A:35:VAL:HG12	1:A:102:GLY:CA	0.58	2.29	4	1
1:A:69:ALA:HB1	1:A:72:TRP:CZ2	0.58	2.33	7	1
1:A:72:TRP:CE3	1:A:73:ASP:N	0.58	2.72	10	2
1:A:76:TYR:CE2	1:A:87:LEU:HD23	0.58	2.34	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:VAL:HG13	1:A:41:PRO:HB3	0.57	1.75	10	1
1:A:80:GLY:O	1:A:81:MET:CB	0.57	2.51	8	3
1:A:45:LEU:HD12	1:A:48:ILE:HG12	0.57	1.75	8	1
1:A:44:LYS:C	1:A:45:LEU:HD12	0.57	2.19	2	1
1:A:65:ASP:HB2	1:A:260:THR:HG22	0.57	1.76	2	1
1:A:81:MET:CE	1:A:143:LEU:HD13	0.57	2.29	2	1
1:A:105:ASN:OD1	1:A:116:LEU:HD21	0.57	1.99	9	1
1:A:24:VAL:HG12	1:A:156:GLU:CG	0.57	2.29	5	1
1:A:43:GLY:O	1:A:44:LYS:C	0.57	2.42	10	3
1:A:45:LEU:HD11	1:A:121:VAL:HG22	0.57	1.75	1	1
1:A:131:LEU:HD13	1:A:136:GLY:C	0.57	2.19	1	1
1:A:56:TYR:OH	1:A:86:THR:HG21	0.57	1.99	4	1
1:A:105:ASN:ND2	1:A:116:LEU:HD11	0.57	2.15	9	1
1:A:125:LEU:HD23	1:A:126:VAL:N	0.57	2.14	3	1
1:A:48:ILE:HD12	1:A:128:PHE:CB	0.57	2.29	8	1
1:A:59:ARG:O	1:A:60:MET:C	0.57	2.42	4	4
1:A:122:ASP:O	1:A:126:VAL:HG23	0.57	1.99	7	3
1:A:213:LEU:HD13	1:A:218:LEU:CD2	0.57	2.27	1	1
1:A:210:ILE:O	1:A:211:THR:O	0.57	2.21	1	1
1:A:232:VAL:HG22	1:A:236:GLN:NE2	0.57	2.14	7	1
1:A:86:THR:C	1:A:87:LEU:HD23	0.57	2.20	1	2
1:A:47:LEU:HD12	1:A:144:TRP:CH2	0.57	2.34	10	1
1:A:127:ILE:HD12	1:A:227:SER:HB3	0.57	1.76	4	1
1:A:69:ALA:HA	1:A:72:TRP:CE2	0.57	2.34	7	1
1:A:93:TRP:CZ3	1:A:260:THR:HG21	0.57	2.35	8	1
1:A:121:VAL:O	1:A:125:LEU:HD12	0.57	1.99	10	1
1:A:107:SER:N	1:A:108:PRO:HD3	0.57	2.15	2	1
1:A:216:PRO:CG	1:A:217:PRO:CD	0.57	2.83	1	7
1:A:23:TRP:CE2	1:A:24:VAL:HG13	0.57	2.34	7	1
1:A:192:PHE:HB3	1:A:193:PRO:HD3	0.56	1.76	4	1
1:A:101:VAL:HG12	1:A:116:LEU:HD21	0.56	1.77	7	1
1:A:225:PHE:CZ	1:A:247:LEU:HD12	0.56	2.34	3	1
1:A:189:TYR:CD1	1:A:189:TYR:N	0.56	2.69	3	1
1:A:113:TYR:O	1:A:116:LEU:HD22	0.56	1.99	2	1
1:A:71:TRP:NE1	1:A:127:ILE:HD13	0.56	2.15	2	1
1:A:58:LEU:HD22	1:A:140:ASN:OD1	0.56	2.00	10	1
1:A:210:ILE:O	1:A:211:THR:HG23	0.56	1.99	6	1
1:A:77:GLN:O	1:A:87:LEU:HD22	0.56	2.00	3	4
1:A:126:VAL:HG11	1:A:228:GLU:O	0.56	2.01	2	2
1:A:45:LEU:HD13	1:A:48:ILE:HG13	0.56	1.76	9	1
1:A:80:GLY:O	1:A:81:MET:HB3	0.56	2.00	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:HG12	1:A:105:ASN:ND2	0.56	2.16	8	1
1:A:45:LEU:HD22	1:A:48:ILE:CB	0.56	2.31	6	1
1:A:195:LEU:HD13	1:A:228:GLU:HA	0.56	1.77	7	1
1:A:233:ARG:CG	1:A:234:ILE:HD12	0.56	2.30	8	1
1:A:26:ARG:CG	1:A:46:ALA:HB3	0.56	2.30	9	2
1:A:49:ASP:O	1:A:53:GLU:OE1	0.56	2.23	7	1
1:A:36:LEU:CB	1:A:37:PRO:CD	0.56	2.82	1	9
1:A:126:VAL:HG13	1:A:189:TYR:CE2	0.56	2.36	2	1
1:A:47:LEU:HD23	1:A:48:ILE:N	0.56	2.16	3	1
1:A:143:LEU:HD23	1:A:143:LEU:N	0.56	2.16	4	1
1:A:142:PHE:O	1:A:143:LEU:HD22	0.55	2.01	7	1
1:A:56:TYR:HD2	1:A:69:ALA:HB1	0.55	1.59	5	1
1:A:26:ARG:HB3	1:A:45:LEU:HD13	0.55	1.78	8	1
1:A:125:LEU:HD21	1:A:189:TYR:O	0.55	2.01	3	1
1:A:220:TYR:O	1:A:224:VAL:HG23	0.55	2.01	5	2
1:A:62:SER:O	1:A:63:ASP:CB	0.55	2.54	1	2
1:A:142:PHE:O	1:A:143:LEU:HD12	0.55	2.00	2	1
1:A:126:VAL:HG11	1:A:229:ASN:HA	0.55	1.78	9	1
1:A:44:LYS:HG2	1:A:124:VAL:HG21	0.55	1.79	8	1
1:A:29:TYR:HB2	1:A:45:LEU:HD21	0.55	1.77	6	1
1:A:192:PHE:HB2	1:A:193:PRO:CD	0.55	2.31	1	1
1:A:22:THR:HG22	1:A:26:ARG:HD3	0.55	1.79	9	1
1:A:100:ILE:HD12	1:A:101:VAL:N	0.55	2.17	10	3
1:A:76:TYR:CD1	1:A:77:GLN:N	0.55	2.75	6	1
1:A:36:LEU:HD11	1:A:99:ALA:CB	0.55	2.29	6	1
1:A:221:PHE:O	1:A:225:PHE:HB3	0.55	2.01	4	1
1:A:26:ARG:NH1	1:A:47:LEU:HD22	0.55	2.16	2	1
1:A:220:TYR:CE1	1:A:224:VAL:HG21	0.55	2.36	9	1
1:A:105:ASN:CG	1:A:116:LEU:HD11	0.55	2.23	9	1
1:A:123:TYR:CD1	1:A:123:TYR:C	0.55	2.81	3	1
1:A:53:GLU:CB	1:A:80:GLY:HA3	0.55	2.31	8	1
1:A:56:TYR:HB2	1:A:72:TRP:CD2	0.54	2.37	6	1
1:A:216:PRO:CD	1:A:217:PRO:HD3	0.54	2.32	9	7
1:A:132:ILE:HG22	1:A:237:LEU:HD23	0.54	1.79	6	1
1:A:45:LEU:HG	1:A:124:VAL:HG23	0.54	1.78	8	1
1:A:27:THR:HG21	1:A:192:PHE:O	0.54	2.02	6	1
1:A:35:VAL:HG13	1:A:102:GLY:HA3	0.54	1.79	5	1
1:A:70:ALA:HB3	1:A:252:GLU:HA	0.54	1.80	10	3
1:A:53:GLU:CB	1:A:80:GLY:N	0.54	2.70	10	1
1:A:119:HIS:CD2	1:A:224:VAL:HG22	0.54	2.38	10	1
1:A:197:ASN:CB	1:A:202:THR:HG21	0.54	2.32	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:246:THR:O	1:A:250:VAL:HG23	0.54	2.03	5	3
1:A:123:TYR:CD2	1:A:124:VAL:HG13	0.54	2.37	2	2
1:A:229:ASN:O	1:A:233:ARG:N	0.54	2.40	6	5
1:A:53:GLU:CD	1:A:53:GLU:H	0.54	2.06	7	1
1:A:260:THR:HG22	1:A:261:ARG:HG3	0.54	1.78	7	1
1:A:116:LEU:HA	1:A:119:HIS:CD2	0.54	2.37	10	1
1:A:192:PHE:CB	1:A:193:PRO:HD3	0.54	2.32	1	4
1:A:133:GLY:CA	1:A:234:ILE:HD13	0.54	2.32	2	1
1:A:23:TRP:CE2	1:A:125:LEU:HD22	0.54	2.37	9	1
1:A:34:VAL:O	1:A:116:LEU:HD13	0.54	2.02	9	1
1:A:38:SER:O	1:A:39:GLN:CB	0.53	2.56	10	1
1:A:66:SER:HB3	1:A:69:ALA:HB3	0.53	1.80	7	3
1:A:65:ASP:CB	1:A:260:THR:HG22	0.53	2.33	2	1
1:A:125:LEU:HD23	1:A:193:PRO:CD	0.53	2.33	4	1
1:A:81:MET:HE2	1:A:143:LEU:HD23	0.53	1.80	9	1
1:A:49:ASP:CB	1:A:78:ILE:HD11	0.53	2.33	5	1
1:A:100:ILE:HD13	1:A:219:ASP:HB3	0.53	1.79	5	1
1:A:48:ILE:HD12	1:A:128:PHE:HB3	0.53	1.79	8	1
1:A:107:SER:CB	1:A:108:PRO:CD	0.53	2.86	5	2
1:A:34:VAL:O	1:A:34:VAL:HG22	0.53	2.04	6	5
1:A:126:VAL:HG22	1:A:233:ARG:HD3	0.53	1.78	6	1
1:A:87:LEU:HD13	1:A:94:ASN:ND2	0.53	2.18	1	1
1:A:73:ASP:HA	1:A:76:TYR:CD2	0.53	2.38	4	1
1:A:192:PHE:HB3	1:A:193:PRO:CD	0.53	2.34	4	1
1:A:58:LEU:HD23	1:A:58:LEU:O	0.53	2.04	10	1
1:A:228:GLU:HG2	1:A:232:VAL:HG12	0.53	1.80	2	1
1:A:112:SER:O	1:A:113:TYR:HB3	0.53	2.03	7	1
1:A:69:ALA:HB1	1:A:72:TRP:CZ3	0.53	2.39	6	1
1:A:210:ILE:HD12	1:A:239:LYS:CD	0.53	2.33	2	1
1:A:125:LEU:HD22	1:A:193:PRO:HG3	0.53	1.81	6	1
1:A:29:TYR:HB3	1:A:45:LEU:HD13	0.52	1.82	1	1
1:A:76:TYR:CD1	1:A:76:TYR:N	0.52	2.76	4	1
1:A:197:ASN:HA	1:A:202:THR:HG21	0.52	1.82	2	1
1:A:215:VAL:HB	1:A:217:PRO:HD2	0.52	1.80	3	7
1:A:227:SER:O	1:A:229:ASN:N	0.52	2.42	1	1
1:A:115:ILE:HD13	1:A:220:TYR:CE1	0.52	2.39	7	2
1:A:55:TYR:O	1:A:59:ARG:N	0.52	2.43	10	3
1:A:47:LEU:O	1:A:47:LEU:HD23	0.52	2.04	6	1
1:A:77:GLN:O	1:A:87:LEU:HD13	0.52	2.04	3	3
1:A:45:LEU:HD13	1:A:48:ILE:CG2	0.52	2.34	6	1
1:A:27:THR:HG21	1:A:192:PHE:C	0.52	2.24	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LEU:HD13	1:A:141:LYS:HB3	0.52	1.82	6	1
1:A:253:LEU:O	1:A:253:LEU:HD23	0.52	2.04	1	5
1:A:69:ALA:O	1:A:70:ALA:C	0.52	2.48	10	1
1:A:29:TYR:O	1:A:30:SER:CB	0.52	2.58	6	2
1:A:35:VAL:O	1:A:36:LEU:HD22	0.52	2.04	4	1
1:A:214:ASP:O	1:A:215:VAL:C	0.52	2.48	4	1
1:A:143:LEU:N	1:A:143:LEU:CD2	0.52	2.72	4	1
1:A:52:ARG:CZ	1:A:124:VAL:HG12	0.52	2.34	2	1
1:A:45:LEU:O	1:A:46:ALA:C	0.52	2.49	7	1
1:A:45:LEU:HD22	1:A:48:ILE:CG2	0.52	2.35	6	1
1:A:165:ALA:HB2	1:A:196:PHE:CE1	0.52	2.40	2	1
1:A:45:LEU:CG	1:A:121:VAL:HG13	0.52	2.35	9	1
1:A:205:VAL:HG23	1:A:228:GLU:CD	0.51	2.26	10	1
1:A:81:MET:HE3	1:A:143:LEU:HD13	0.51	1.82	2	1
1:A:41:PRO:HG2	1:A:78:ILE:HD12	0.51	1.81	8	1
1:A:224:VAL:HG12	1:A:228:GLU:CG	0.51	2.35	1	1
1:A:37:PRO:O	1:A:38:SER:CB	0.51	2.57	1	1
1:A:45:LEU:HD21	1:A:121:VAL:CG1	0.51	2.27	5	3
1:A:123:TYR:OH	1:A:224:VAL:HG22	0.51	2.05	5	1
1:A:56:TYR:CB	1:A:72:TRP:CD2	0.51	2.93	6	1
1:A:240:ASP:OD2	1:A:247:LEU:HD22	0.51	2.06	2	2
1:A:31:SER:N	1:A:40:THR:HG22	0.51	2.20	2	1
1:A:125:LEU:CD1	1:A:126:VAL:HG23	0.51	2.35	6	1
1:A:69:ALA:O	1:A:73:ASP:N	0.51	2.44	9	1
1:A:215:VAL:CB	1:A:217:PRO:HD2	0.51	2.35	3	7
1:A:85:THR:O	1:A:88:VAL:HG22	0.51	2.06	6	1
1:A:195:LEU:HD11	1:A:231:ASN:HB2	0.51	1.81	1	1
1:A:56:TYR:CE2	1:A:69:ALA:HB1	0.51	2.40	2	1
1:A:220:TYR:N	1:A:220:TYR:CD1	0.51	2.76	8	1
1:A:28:ALA:O	1:A:30:SER:N	0.51	2.43	6	3
1:A:142:PHE:CD2	1:A:143:LEU:HD23	0.51	2.40	6	1
1:A:87:LEU:O	1:A:87:LEU:HD13	0.51	2.06	9	1
1:A:87:LEU:O	1:A:87:LEU:HD22	0.51	2.06	9	1
1:A:94:ASN:OD1	1:A:98:ILE:HD12	0.51	2.05	6	2
1:A:45:LEU:HD11	1:A:121:VAL:CG2	0.51	2.35	1	1
1:A:123:TYR:N	1:A:227:SER:HB2	0.51	2.21	1	1
1:A:45:LEU:HD12	1:A:48:ILE:CG1	0.51	2.36	8	1
1:A:50:ASP:HB2	1:A:144:TRP:CD1	0.51	2.41	6	3
1:A:192:PHE:N	1:A:193:PRO:HD2	0.51	2.20	7	2
1:A:56:TYR:HB2	1:A:72:TRP:CZ2	0.51	2.41	7	1
1:A:193:PRO:O	1:A:194:GLN:CB	0.51	2.59	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:HG11	1:A:101:VAL:CG2	0.51	2.35	10	1
1:A:226:THR:HA	1:A:247:LEU:HD12	0.51	1.82	2	1
1:A:44:LYS:HE3	1:A:124:VAL:HG11	0.50	1.83	10	1
1:A:229:ASN:O	1:A:232:VAL:N	0.50	2.44	7	2
1:A:108:PRO:HD2	1:A:111:LYS:HA	0.50	1.82	2	1
1:A:104:ALA:CB	1:A:220:TYR:CB	0.50	2.89	5	1
1:A:96:THR:O	1:A:100:ILE:HG23	0.50	2.07	1	1
1:A:215:VAL:H	1:A:216:PRO:HD2	0.50	1.67	7	2
1:A:87:LEU:HD21	1:A:94:ASN:CB	0.50	2.35	9	1
1:A:125:LEU:HD23	1:A:193:PRO:HD3	0.50	1.83	4	1
1:A:220:TYR:CD1	1:A:220:TYR:N	0.50	2.80	5	1
1:A:49:ASP:OD1	1:A:78:ILE:HD11	0.50	2.07	8	1
1:A:90:ASN:O	1:A:94:ASN:HB2	0.50	2.07	8	1
1:A:34:VAL:CG1	1:A:116:LEU:HD22	0.50	2.36	10	1
1:A:153:TRP:N	1:A:154:PRO:HD2	0.50	2.22	5	1
1:A:81:MET:CE	1:A:82:ALA:HB3	0.49	2.37	1	2
1:A:47:LEU:HD23	1:A:48:ILE:HD13	0.49	1.83	9	1
1:A:131:LEU:HD21	1:A:136:GLY:C	0.49	2.26	4	1
1:A:237:LEU:O	1:A:237:LEU:HD13	0.49	2.08	7	3
1:A:191:ASP:O	1:A:192:PHE:CG	0.49	2.65	3	1
1:A:72:TRP:NE1	1:A:76:TYR:CB	0.49	2.75	6	2
1:A:105:ASN:ND2	1:A:116:LEU:HD23	0.49	2.22	6	1
1:A:26:ARG:CG	1:A:45:LEU:HA	0.49	2.37	1	1
1:A:35:VAL:HG11	1:A:101:VAL:HG23	0.49	1.84	10	1
1:A:126:VAL:HG11	1:A:229:ASN:CA	0.49	2.37	9	1
1:A:34:VAL:HG22	1:A:34:VAL:O	0.49	2.07	3	1
1:A:36:LEU:H	1:A:37:PRO:HD2	0.49	1.68	4	1
1:A:26:ARG:HG3	1:A:46:ALA:HB3	0.49	1.84	9	2
1:A:123:TYR:O	1:A:127:ILE:HG23	0.49	2.06	5	1
1:A:210:ILE:HG23	1:A:239:LYS:HB3	0.49	1.85	6	1
1:A:27:THR:HA	1:A:121:VAL:HG11	0.49	1.84	3	3
1:A:76:TYR:O	1:A:76:TYR:CD1	0.49	2.66	9	1
1:A:58:LEU:O	1:A:58:LEU:HD23	0.49	2.08	3	2
1:A:40:THR:HG22	1:A:98:ILE:HG21	0.49	1.82	3	1
1:A:104:ALA:HB1	1:A:220:TYR:HA	0.49	1.83	8	1
1:A:216:PRO:HD2	1:A:217:PRO:CD	0.48	2.38	6	7
1:A:29:TYR:CD2	1:A:45:LEU:HD22	0.48	2.43	1	1
1:A:130:GLY:O	1:A:131:LEU:C	0.48	2.51	6	1
1:A:111:LYS:CE	1:A:224:VAL:HG21	0.48	2.38	8	1
1:A:35:VAL:O	1:A:37:PRO:N	0.48	2.47	1	1
1:A:120:ASP:O	1:A:124:VAL:HG22	0.48	2.07	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ARG:HG3	1:A:45:LEU:HD12	0.48	1.85	7	1
1:A:41:PRO:O	1:A:42:ASP:CB	0.48	2.62	10	2
1:A:70:ALA:HB1	1:A:97:HIS:ND1	0.48	2.23	7	1
1:A:53:GLU:CB	1:A:76:TYR:HA	0.48	2.39	8	1
1:A:32:PRO:HA	1:A:116:LEU:HD11	0.48	1.85	6	1
1:A:24:VAL:HG12	1:A:156:GLU:CD	0.48	2.28	5	1
1:A:35:VAL:CG1	1:A:116:LEU:HD13	0.48	2.34	8	1
1:A:27:THR:HB	1:A:121:VAL:HG11	0.48	1.85	4	1
1:A:22:THR:HB	1:A:26:ARG:HB3	0.48	1.86	2	1
1:A:56:TYR:HB2	1:A:72:TRP:CE2	0.48	2.43	7	1
1:A:36:LEU:HD11	1:A:103:LYS:HB2	0.48	1.84	3	1
1:A:192:PHE:HB2	1:A:193:PRO:HD3	0.48	1.86	1	1
1:A:205:VAL:HG13	1:A:228:GLU:OE1	0.48	2.08	5	1
1:A:25:THR:O	1:A:25:THR:HG22	0.48	2.09	1	1
1:A:125:LEU:HD21	1:A:193:PRO:HG3	0.48	1.85	7	1
1:A:212:PRO:O	1:A:213:LEU:CB	0.48	2.62	7	1
1:A:40:THR:N	1:A:41:PRO:HD2	0.48	2.23	7	1
1:A:54:ALA:CB	1:A:80:GLY:O	0.48	2.56	8	1
1:A:123:TYR:CZ	1:A:127:ILE:HD11	0.47	2.44	10	1
1:A:82:ALA:O	1:A:83:ASP:CB	0.47	2.60	8	2
1:A:23:TRP:CD2	1:A:24:VAL:HG13	0.47	2.44	10	1
1:A:216:PRO:HD2	1:A:217:PRO:HD2	0.47	1.86	3	6
1:A:215:VAL:O	1:A:218:LEU:HD12	0.47	2.09	6	1
1:A:72:TRP:CE2	1:A:76:TYR:CB	0.47	2.97	6	1
1:A:222:ASP:O	1:A:226:THR:HG23	0.47	2.09	3	1
1:A:33:SER:O	1:A:34:VAL:HG12	0.47	2.09	1	1
1:A:215:VAL:CB	1:A:216:PRO:CD	0.47	2.92	8	3
1:A:205:VAL:HG13	1:A:228:GLU:OE2	0.47	2.09	7	1
1:A:138:ASP:C	1:A:139:ILE:HD12	0.47	2.29	8	1
1:A:94:ASN:ND2	1:A:98:ILE:HD12	0.47	2.23	10	1
1:A:210:ILE:HG23	1:A:210:ILE:O	0.47	2.09	5	2
1:A:85:THR:O	1:A:88:VAL:HG13	0.47	2.10	6	1
1:A:105:ASN:ND2	1:A:113:TYR:H	0.47	2.07	1	1
1:A:53:GLU:OE1	1:A:79:GLY:HA2	0.47	2.09	7	1
1:A:70:ALA:HB1	1:A:97:HIS:CE1	0.47	2.44	7	1
1:A:122:ASP:O	1:A:126:VAL:HG13	0.47	2.09	5	1
1:A:69:ALA:O	1:A:72:TRP:CE3	0.47	2.64	10	1
1:A:53:GLU:HB3	1:A:80:GLY:CA	0.47	2.39	10	2
1:A:34:VAL:CG1	1:A:116:LEU:HD13	0.47	2.39	6	1
1:A:132:ILE:HG22	1:A:237:LEU:CD2	0.47	2.39	6	1
1:A:215:VAL:CG2	1:A:217:PRO:HG2	0.47	2.40	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HD12	1:A:117:LYS:N	0.47	2.24	8	1
1:A:36:LEU:N	1:A:37:PRO:HD2	0.47	2.24	9	5
1:A:49:ASP:O	1:A:53:GLU:OE2	0.47	2.33	7	1
1:A:41:PRO:CG	1:A:78:ILE:HD12	0.47	2.40	8	1
1:A:56:TYR:HB2	1:A:76:TYR:CE2	0.47	2.45	4	1
1:A:210:ILE:HD11	1:A:235:TYR:HD1	0.47	1.70	6	1
1:A:70:ALA:HB1	1:A:255:ARG:CB	0.47	2.39	6	1
1:A:215:VAL:N	1:A:216:PRO:HD2	0.47	2.25	7	3
1:A:34:VAL:HG13	1:A:34:VAL:O	0.47	2.09	4	1
1:A:36:LEU:CD1	1:A:99:ALA:HB1	0.47	2.36	2	1
1:A:115:ILE:HD12	1:A:116:LEU:N	0.47	2.25	7	1
1:A:49:ASP:OD1	1:A:50:ASP:N	0.46	2.48	10	1
1:A:126:VAL:HG11	1:A:229:ASN:C	0.46	2.30	9	1
1:A:40:THR:HG22	1:A:77:GLN:CD	0.46	2.31	9	1
1:A:226:THR:OG1	1:A:247:LEU:HD12	0.46	2.09	9	1
1:A:39:GLN:O	1:A:40:THR:CB	0.46	2.63	10	1
1:A:45:LEU:HD13	1:A:48:ILE:HG21	0.46	1.86	6	1
1:A:28:ALA:HB1	1:A:155:GLU:CG	0.46	2.41	4	1
1:A:127:ILE:HD11	1:A:227:SER:OG	0.46	2.10	9	1
1:A:48:ILE:HG21	1:A:124:VAL:HG11	0.46	1.87	5	1
1:A:71:TRP:NE1	1:A:127:ILE:HD12	0.46	2.26	10	1
1:A:22:THR:O	1:A:23:TRP:C	0.46	2.54	2	3
1:A:104:ALA:HB2	1:A:220:TYR:CD2	0.46	2.45	5	1
1:A:60:MET:CG	1:A:69:ALA:HB2	0.46	2.40	3	1
1:A:27:THR:OG1	1:A:121:VAL:HG11	0.46	2.10	5	1
1:A:119:HIS:O	1:A:123:TYR:HB3	0.46	2.10	2	1
1:A:53:GLU:HB2	1:A:76:TYR:HA	0.46	1.86	3	1
1:A:227:SER:O	1:A:228:GLU:HG3	0.46	2.11	3	1
1:A:86:THR:O	1:A:87:LEU:HD12	0.46	2.11	8	1
1:A:119:HIS:ND1	1:A:119:HIS:C	0.46	2.68	4	2
1:A:24:VAL:HG11	1:A:156:GLU:HB3	0.46	1.87	10	1
1:A:191:ASP:C	1:A:193:PRO:HD2	0.46	2.31	1	1
1:A:42:ASP:O	1:A:78:ILE:HD13	0.46	2.10	4	1
1:A:56:TYR:CB	1:A:76:TYR:CZ	0.46	2.99	4	1
1:A:125:LEU:HD21	1:A:191:ASP:CB	0.46	2.41	9	1
1:A:22:THR:OG1	1:A:47:LEU:HD22	0.46	2.11	9	3
1:A:238:LYS:O	1:A:242:ALA:HB3	0.46	2.11	7	1
1:A:58:LEU:HD11	1:A:141:LYS:HB3	0.46	1.88	3	1
1:A:47:LEU:HD23	1:A:48:ILE:HG12	0.46	1.86	10	1
1:A:31:SER:CB	1:A:32:PRO:HD2	0.46	2.41	4	1
1:A:61:ASN:O	1:A:62:SER:CB	0.46	2.62	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:225:PHE:O	1:A:232:VAL:HG11	0.46	2.10	4	1
1:A:226:THR:HG22	1:A:232:VAL:CG1	0.45	2.40	10	1
1:A:60:MET:O	1:A:69:ALA:HB2	0.45	2.11	1	1
1:A:145:ASN:O	1:A:146:ILE:HD12	0.45	2.10	4	1
1:A:126:VAL:HG21	1:A:226:THR:O	0.45	2.11	5	1
1:A:44:LYS:HB3	1:A:121:VAL:HG22	0.45	1.88	3	1
1:A:22:THR:HG22	1:A:26:ARG:HE	0.45	1.71	10	1
1:A:131:LEU:HD23	1:A:132:ILE:N	0.45	2.26	2	1
1:A:123:TYR:O	1:A:127:ILE:HD13	0.45	2.11	7	1
1:A:50:ASP:HA	1:A:80:GLY:CA	0.45	2.42	8	1
1:A:26:ARG:HG2	1:A:45:LEU:HA	0.45	1.89	8	1
1:A:29:TYR:HB2	1:A:45:LEU:HD13	0.45	1.88	1	1
1:A:22:THR:O	1:A:26:ARG:HB2	0.45	2.11	3	1
1:A:227:SER:O	1:A:228:GLU:CB	0.45	2.64	3	1
1:A:100:ILE:CD1	1:A:219:ASP:HB3	0.45	2.41	7	3
1:A:56:TYR:CD1	1:A:72:TRP:CE3	0.45	3.05	9	1
1:A:113:TYR:O	1:A:115:ILE:HD13	0.45	2.11	8	1
1:A:42:ASP:HB3	1:A:78:ILE:HG21	0.45	1.88	4	1
1:A:104:ALA:CB	1:A:219:ASP:HB2	0.45	2.42	2	1
1:A:105:ASN:CB	1:A:116:LEU:HD21	0.45	2.42	1	1
1:A:212:PRO:O	1:A:213:LEU:HD12	0.45	2.12	7	1
1:A:143:LEU:HD12	1:A:144:TRP:CZ3	0.45	2.47	1	2
1:A:123:TYR:CE2	1:A:124:VAL:HG13	0.45	2.47	7	1
1:A:131:LEU:C	1:A:132:ILE:HD12	0.45	2.31	6	1
1:A:36:LEU:CB	1:A:37:PRO:HD3	0.45	2.41	1	2
1:A:42:ASP:CB	1:A:78:ILE:HG21	0.45	2.42	4	1
1:A:59:ARG:NH2	1:A:68:VAL:HG21	0.45	2.27	7	1
1:A:209:MET:O	1:A:235:TYR:CG	0.45	2.70	7	1
1:A:75:GLY:O	1:A:78:ILE:HG12	0.45	2.11	8	1
1:A:29:TYR:HB2	1:A:45:LEU:CD2	0.45	2.42	6	1
1:A:31:SER:CB	1:A:32:PRO:CD	0.45	2.95	2	1
1:A:47:LEU:HD13	1:A:144:TRP:CZ2	0.45	2.46	5	1
1:A:45:LEU:CD2	1:A:121:VAL:HG12	0.45	2.32	3	1
1:A:246:THR:O	1:A:250:VAL:N	0.45	2.50	3	1
1:A:111:LYS:O	1:A:112:SER:C	0.44	2.55	10	1
1:A:236:GLN:OE1	1:A:247:LEU:HD13	0.44	2.12	2	1
1:A:126:VAL:HG21	1:A:228:GLU:O	0.44	2.12	6	1
1:A:116:LEU:HD23	1:A:117:LYS:N	0.44	2.27	2	1
1:A:68:VAL:HG13	1:A:252:GLU:CD	0.44	2.32	8	1
1:A:223:GLU:CG	1:A:224:VAL:N	0.44	2.81	1	1
1:A:53:GLU:OE1	1:A:80:GLY:N	0.44	2.47	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:HD22	1:A:94:ASN:HB3	0.44	1.88	8	1
1:A:246:THR:O	1:A:250:VAL:HG22	0.44	2.12	6	3
1:A:73:ASP:HA	1:A:76:TYR:CG	0.44	2.48	4	1
1:A:81:MET:HE2	1:A:82:ALA:HB3	0.44	1.88	2	1
1:A:56:TYR:HB2	1:A:72:TRP:CH2	0.44	2.48	7	1
1:A:23:TRP:HB2	1:A:125:LEU:HD12	0.44	1.89	3	1
1:A:119:HIS:CG	1:A:120:ASP:N	0.44	2.85	6	1
1:A:42:ASP:CG	1:A:78:ILE:HG21	0.44	2.33	4	1
1:A:31:SER:N	1:A:32:PRO:HD2	0.44	2.27	2	1
1:A:87:LEU:HD13	1:A:87:LEU:C	0.44	2.33	9	1
1:A:207:GLN:O	1:A:210:ILE:HG22	0.44	2.13	1	1
1:A:26:ARG:HB2	1:A:45:LEU:HA	0.44	1.90	2	1
1:A:105:ASN:C	1:A:108:PRO:HD3	0.44	2.33	2	1
1:A:210:ILE:HG23	1:A:211:THR:N	0.44	2.23	1	1
1:A:228:GLU:HB2	1:A:232:VAL:CG2	0.44	2.43	1	1
1:A:35:VAL:HG12	1:A:102:GLY:C	0.44	2.34	4	1
1:A:43:GLY:O	1:A:44:LYS:CB	0.44	2.65	2	1
1:A:22:THR:HG21	1:A:47:LEU:HD13	0.44	1.90	8	1
1:A:215:VAL:HB	1:A:216:PRO:HD3	0.44	1.90	8	1
1:A:210:ILE:HD12	1:A:239:LYS:HG2	0.44	1.88	2	1
1:A:223:GLU:O	1:A:226:THR:HG22	0.44	2.13	2	2
1:A:220:TYR:O	1:A:224:VAL:HB	0.44	2.13	7	1
1:A:53:GLU:HB2	1:A:79:GLY:HA2	0.44	1.89	5	1
1:A:210:ILE:HG12	1:A:211:THR:HG22	0.44	1.89	8	1
1:A:211:THR:N	1:A:212:PRO:CD	0.43	2.80	4	1
1:A:214:ASP:O	1:A:215:VAL:CG2	0.43	2.64	9	1
1:A:34:VAL:HG22	1:A:116:LEU:CD1	0.43	2.43	5	1
1:A:86:THR:C	1:A:87:LEU:HG	0.43	2.34	8	1
1:A:22:THR:HG22	1:A:26:ARG:NE	0.43	2.28	10	1
1:A:48:ILE:HG12	1:A:124:VAL:HG21	0.43	1.89	6	1
1:A:76:TYR:CE2	1:A:87:LEU:HA	0.43	2.49	6	1
1:A:125:LEU:HD13	1:A:193:PRO:HB3	0.43	1.89	10	1
1:A:101:VAL:HG12	1:A:223:GLU:CG	0.43	2.44	4	1
1:A:130:GLY:O	1:A:131:LEU:CB	0.43	2.66	9	1
1:A:81:MET:HB2	1:A:143:LEU:HB3	0.43	1.89	7	1
1:A:104:ALA:HB2	1:A:220:TYR:HB3	0.43	1.89	5	1
1:A:111:LYS:CG	1:A:111:LYS:O	0.43	2.66	5	1
1:A:103:LYS:O	1:A:107:SER:OG	0.43	2.35	5	1
1:A:48:ILE:CG1	1:A:124:VAL:HG21	0.43	2.43	6	1
1:A:126:VAL:HG22	1:A:233:ARG:CD	0.43	2.44	6	1
1:A:132:ILE:HG21	1:A:248:ARG:NH1	0.43	2.28	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:229:ASN:O	1:A:230:TRP:C	0.43	2.56	7	1
1:A:45:LEU:CG	1:A:124:VAL:HG23	0.43	2.44	8	1
1:A:143:LEU:HD13	1:A:144:TRP:N	0.43	2.29	10	1
1:A:208:GLN:HG3	1:A:232:VAL:HG11	0.43	1.90	6	1
1:A:210:ILE:HG13	1:A:211:THR:N	0.43	2.29	1	1
1:A:24:VAL:HG11	1:A:157:ILE:HG12	0.43	1.90	1	1
1:A:50:ASP:HA	1:A:81:MET:N	0.43	2.27	4	1
1:A:226:THR:O	1:A:227:SER:C	0.43	2.57	10	1
1:A:213:LEU:HD13	1:A:218:LEU:CD1	0.43	2.43	4	1
1:A:47:LEU:HD23	1:A:48:ILE:CD1	0.43	2.43	9	1
1:A:45:LEU:HB3	1:A:48:ILE:HB	0.43	1.91	8	1
1:A:53:GLU:HB2	1:A:79:GLY:CA	0.43	2.44	2	1
1:A:132:ILE:HG23	1:A:132:ILE:O	0.43	2.14	2	1
1:A:69:ALA:CB	1:A:72:TRP:CZ2	0.43	3.01	7	1
1:A:28:ALA:HB3	1:A:155:GLU:OE1	0.43	2.14	5	1
1:A:115:ILE:HD13	1:A:116:LEU:N	0.43	2.29	8	1
1:A:259:LYS:O	1:A:260:THR:HG23	0.43	2.14	8	1
1:A:72:TRP:HB2	1:A:76:TYR:OH	0.43	2.14	4	1
1:A:75:GLY:O	1:A:78:ILE:HD13	0.43	2.13	10	1
1:A:60:MET:O	1:A:62:SER:N	0.43	2.51	7	3
1:A:48:ILE:O	1:A:52:ARG:HG2	0.43	2.14	9	1
1:A:65:ASP:O	1:A:66:SER:C	0.43	2.57	7	1
1:A:120:ASP:O	1:A:124:VAL:HG13	0.43	2.14	10	3
1:A:45:LEU:O	1:A:49:ASP:N	0.43	2.44	7	3
1:A:123:TYR:HB3	1:A:227:SER:HB2	0.43	1.90	9	1
1:A:125:LEU:HD21	1:A:193:PRO:CG	0.43	2.44	7	1
1:A:87:LEU:HD13	1:A:91:ASN:CB	0.43	2.44	8	1
1:A:236:GLN:HE21	1:A:247:LEU:HD13	0.43	1.73	8	1
1:A:232:VAL:CG1	1:A:232:VAL:O	0.42	2.63	10	1
1:A:213:LEU:O	1:A:213:LEU:HD12	0.42	2.13	1	1
1:A:143:LEU:HG	1:A:143:LEU:O	0.42	2.14	4	1
1:A:126:VAL:CG1	1:A:228:GLU:O	0.42	2.67	3	1
1:A:220:TYR:O	1:A:224:VAL:HG22	0.42	2.14	8	1
1:A:56:TYR:CB	1:A:72:TRP:CE2	0.42	3.02	6	1
1:A:33:SER:O	1:A:34:VAL:C	0.42	2.58	9	4
1:A:45:LEU:O	1:A:47:LEU:N	0.42	2.52	7	1
1:A:226:THR:O	1:A:232:VAL:HG11	0.42	2.14	7	1
1:A:22:THR:OG1	1:A:46:ALA:HB3	0.42	2.15	6	1
1:A:107:SER:HB3	1:A:108:PRO:HD2	0.42	1.89	5	1
1:A:50:ASP:HA	1:A:80:GLY:N	0.42	2.29	8	1
1:A:128:PHE:O	1:A:131:LEU:HD23	0.42	2.15	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:C	1:A:116:LEU:HD13	0.42	2.34	3	1
1:A:52:ARG:O	1:A:55:TYR:HB3	0.42	2.15	10	1
1:A:237:LEU:HD13	1:A:237:LEU:C	0.42	2.34	2	1
1:A:123:TYR:CE2	1:A:224:VAL:HG22	0.42	2.49	9	1
1:A:236:GLN:CD	1:A:247:LEU:HD11	0.42	2.35	9	1
1:A:53:GLU:N	1:A:53:GLU:OE2	0.42	2.50	7	1
1:A:226:THR:HG21	1:A:252:GLU:OE1	0.42	2.13	3	1
1:A:119:HIS:CE1	1:A:224:VAL:HG12	0.42	2.50	4	1
1:A:146:ILE:O	1:A:146:ILE:HG22	0.42	2.14	4	1
1:A:165:ALA:HB2	1:A:196:PHE:CZ	0.42	2.49	2	1
1:A:112:SER:O	1:A:113:TYR:HB2	0.42	2.14	5	1
1:A:121:VAL:O	1:A:121:VAL:HG12	0.42	2.14	4	1
1:A:138:ASP:O	1:A:139:ILE:C	0.42	2.58	2	1
1:A:70:ALA:HB3	1:A:252:GLU:O	0.42	2.15	3	2
1:A:35:VAL:HG13	1:A:102:GLY:CA	0.42	2.44	5	1
1:A:26:ARG:HB3	1:A:45:LEU:HA	0.42	1.91	10	1
1:A:116:LEU:HD12	1:A:116:LEU:C	0.42	2.35	6	1
1:A:53:GLU:HB3	1:A:81:MET:HB3	0.42	1.90	6	1
1:A:81:MET:HG3	1:A:82:ALA:N	0.42	2.29	9	1
1:A:54:ALA:HB1	1:A:142:PHE:HB2	0.42	1.90	7	1
1:A:126:VAL:HG21	1:A:232:VAL:CG1	0.42	2.44	10	1
1:A:226:THR:HG22	1:A:232:VAL:HG11	0.42	1.90	10	1
1:A:44:LYS:HG2	1:A:45:LEU:HD12	0.42	1.92	4	1
1:A:228:GLU:O	1:A:229:ASN:HB2	0.42	2.15	5	1
1:A:87:LEU:O	1:A:91:ASN:N	0.42	2.50	8	2
1:A:230:TRP:O	1:A:234:ILE:HD13	0.42	2.15	8	1
1:A:140:ASN:HB2	1:A:143:LEU:HD22	0.42	1.92	1	1
1:A:67:LYS:HD3	1:A:68:VAL:HG23	0.42	1.92	1	1
1:A:192:PHE:N	1:A:193:PRO:CD	0.42	2.83	7	1
1:A:245:ARG:O	1:A:246:THR:HG23	0.42	2.15	3	1
1:A:100:ILE:HD12	1:A:219:ASP:HB3	0.41	1.91	1	1
1:A:132:ILE:O	1:A:132:ILE:HG23	0.41	2.15	4	1
1:A:108:PRO:O	1:A:109:GLU:CB	0.41	2.68	6	1
1:A:33:SER:O	1:A:34:VAL:CG1	0.41	2.67	1	1
1:A:145:ASN:C	1:A:146:ILE:HD12	0.41	2.35	4	1
1:A:125:LEU:HD21	1:A:191:ASP:CG	0.41	2.35	9	1
1:A:228:GLU:HB3	1:A:232:VAL:HB	0.41	1.91	7	1
1:A:220:TYR:CD1	1:A:224:VAL:HG21	0.41	2.50	7	1
1:A:81:MET:HE2	1:A:82:ALA:HB2	0.41	1.91	5	1
1:A:53:GLU:HB3	1:A:80:GLY:HA2	0.41	1.93	10	1
1:A:34:VAL:HA	1:A:41:PRO:CA	0.41	2.45	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:HG21	1:A:102:GLY:CA	0.41	2.45	10	1
1:A:218:LEU:O	1:A:222:ASP:CB	0.41	2.67	7	1
1:A:54:ALA:HB1	1:A:142:PHE:CG	0.41	2.50	3	1
1:A:83:ASP:O	1:A:84:ARG:CB	0.41	2.68	10	1
1:A:48:ILE:O	1:A:48:ILE:HG22	0.41	2.15	10	1
1:A:21:SER:O	1:A:25:THR:N	0.41	2.52	4	1
1:A:230:TRP:O	1:A:234:ILE:HG22	0.41	2.15	4	1
1:A:22:THR:HG21	1:A:47:LEU:CD1	0.41	2.45	8	1
1:A:86:THR:O	1:A:87:LEU:C	0.41	2.59	8	1
1:A:228:GLU:HB2	1:A:232:VAL:HG21	0.41	1.92	9	1
1:A:53:GLU:O	1:A:57:TRP:N	0.41	2.54	9	1
1:A:253:LEU:HD23	1:A:253:LEU:O	0.41	2.15	9	1
1:A:35:VAL:O	1:A:36:LEU:HD12	0.41	2.15	7	1
1:A:104:ALA:HB2	1:A:219:ASP:CB	0.41	2.45	3	1
1:A:84:ARG:C	1:A:86:THR:H	0.41	2.18	8	1
1:A:131:LEU:HD23	1:A:131:LEU:O	0.41	2.16	1	1
1:A:101:VAL:HG11	1:A:119:HIS:NE2	0.41	2.30	9	1
1:A:45:LEU:HD22	1:A:124:VAL:HG21	0.41	1.91	5	1
1:A:100:ILE:O	1:A:220:TYR:CD1	0.41	2.73	5	1
1:A:63:ASP:O	1:A:64:GLU:CB	0.41	2.69	5	1
1:A:54:ALA:O	1:A:58:LEU:CB	0.41	2.67	8	1
1:A:35:VAL:O	1:A:36:LEU:CD2	0.41	2.68	5	1
1:A:88:VAL:HG13	1:A:89:ASP:N	0.41	2.31	1	2
1:A:56:TYR:O	1:A:69:ALA:HB2	0.41	2.16	9	1
1:A:192:PHE:HB3	1:A:193:PRO:HD2	0.41	1.93	3	1
1:A:56:TYR:CE1	1:A:76:TYR:CD2	0.41	3.08	8	2
1:A:85:THR:O	1:A:88:VAL:HG12	0.41	2.16	3	1
1:A:80:GLY:C	1:A:82:ALA:H	0.41	2.19	10	1
1:A:56:TYR:O	1:A:60:MET:CA	0.41	2.69	1	1
1:A:131:LEU:O	1:A:132:ILE:HB	0.41	2.16	1	1
1:A:69:ALA:HB1	1:A:76:TYR:HE2	0.41	1.76	4	1
1:A:105:ASN:O	1:A:111:LYS:C	0.41	2.59	4	1
1:A:43:GLY:O	1:A:44:LYS:HB3	0.41	2.16	2	1
1:A:71:TRP:O	1:A:71:TRP:CD1	0.41	2.74	2	1
1:A:163:TYR:O	1:A:164:THR:HG23	0.41	2.15	2	1
1:A:65:ASP:CG	1:A:66:SER:N	0.41	2.74	5	1
1:A:124:VAL:O	1:A:127:ILE:HG22	0.41	2.16	3	1
1:A:216:PRO:HG2	1:A:221:PHE:CD1	0.41	2.50	8	1
1:A:133:GLY:HA2	1:A:234:ILE:HD13	0.41	1.93	2	1
1:A:56:TYR:CG	1:A:72:TRP:CE3	0.41	3.09	9	1
1:A:52:ARG:NH2	1:A:124:VAL:HG11	0.41	2.31	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:TYR:OH	1:A:101:VAL:HG21	0.41	2.16	5	1
1:A:153:TRP:N	1:A:154:PRO:CD	0.41	2.84	5	1
1:A:212:PRO:HG2	1:A:213:LEU:HD22	0.41	1.92	8	1
1:A:69:ALA:O	1:A:71:TRP:N	0.40	2.54	10	1
1:A:53:GLU:HA	1:A:72:TRP:NE1	0.40	2.31	10	1
1:A:115:ILE:HD12	1:A:115:ILE:C	0.40	2.37	1	1
1:A:46:ALA:O	1:A:50:ASP:OD1	0.40	2.39	4	1
1:A:36:LEU:HB3	1:A:37:PRO:HD3	0.40	1.93	5	1
1:A:44:LYS:HB3	1:A:121:VAL:HG13	0.40	1.93	3	1
1:A:229:ASN:N	1:A:233:ARG:HB3	0.40	2.31	3	1
1:A:245:ARG:O	1:A:246:THR:CB	0.40	2.70	8	1
1:A:126:VAL:HG21	1:A:232:VAL:HG12	0.40	1.94	10	1
1:A:41:PRO:O	1:A:42:ASP:HB3	0.40	2.16	10	1
1:A:76:TYR:O	1:A:77:GLN:C	0.40	2.60	4	1
1:A:143:LEU:HD12	1:A:144:TRP:CH2	0.40	2.52	4	1
1:A:217:PRO:HD2	1:A:220:TYR:CD2	0.40	2.51	4	1
1:A:49:ASP:O	1:A:53:GLU:CD	0.40	2.60	7	1
1:A:123:TYR:N	1:A:123:TYR:CD1	0.40	2.88	5	1
1:A:34:VAL:HG21	1:A:74:TYR:OH	0.40	2.16	8	1
1:A:146:ILE:HD13	1:A:146:ILE:N	0.40	2.32	10	1
1:A:72:TRP:CE2	1:A:76:TYR:HB3	0.40	2.51	6	1
1:A:26:ARG:CD	1:A:46:ALA:HB3	0.40	2.46	4	1
1:A:197:ASN:CA	1:A:202:THR:HG21	0.40	2.47	3	1
1:A:212:PRO:O	1:A:213:LEU:HB2	0.40	2.16	3	1
1:A:215:VAL:HB	1:A:216:PRO:CD	0.40	2.47	8	1
1:A:221:PHE:O	1:A:225:PHE:CG	0.40	2.74	1	1
1:A:71:TRP:CE2	1:A:127:ILE:HD13	0.40	2.51	2	1
1:A:44:LYS:O	1:A:45:LEU:HB2	0.40	2.17	8	1
1:A:28:ALA:HB1	1:A:156:GLU:C	0.40	2.36	8	1
1:A:131:LEU:O	1:A:132:ILE:HD12	0.40	2.17	6	1
1:A:240:ASP:CG	1:A:247:LEU:HD22	0.40	2.37	6	1
1:A:104:ALA:HB1	1:A:220:TYR:HB3	0.40	1.93	7	1
1:A:228:GLU:HB2	1:A:232:VAL:HB	0.40	1.92	5	1
1:A:105:ASN:O	1:A:112:SER:N	0.40	2.51	5	1
1:A:123:TYR:HA	1:A:126:VAL:HG12	0.40	1.93	3	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	209/273 (77%)	144±4 (69±2%)	36±4 (17±2%)	29±2 (14±1%)	1 5
All	All	2090/2730 (77%)	1442 (69%)	355 (17%)	293 (14%)	1 5

All 79 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	144	TRP	9
1	A	194	GLN	9
1	A	67	LYS	9
1	A	29	TYR	8
1	A	36	LEU	8
1	A	111	LYS	8
1	A	228	GLU	8
1	A	82	ALA	7
1	A	132	ILE	7
1	A	139	ILE	7
1	A	212	PRO	7
1	A	192	PHE	7
1	A	44	LYS	6
1	A	257	SER	6
1	A	40	THR	6
1	A	34	VAL	6
1	A	210	ILE	6
1	A	166	GLU	6
1	A	79	GLY	6
1	A	38	SER	5
1	A	112	SER	5
1	A	109	GLU	5
1	A	61	ASN	5
1	A	245	ARG	5
1	A	143	LEU	5
1	A	145	ASN	4
1	A	146	ILE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	134	PHE	4
1	A	165	ALA	4
1	A	30	SER	4
1	A	81	MET	4
1	A	214	ASP	4
1	A	21	SER	4
1	A	35	VAL	4
1	A	197	ASN	4
1	A	42	ASP	4
1	A	195	LEU	3
1	A	62	SER	3
1	A	211	THR	3
1	A	63	ASP	3
1	A	258	THR	3
1	A	33	SER	3
1	A	39	GLN	3
1	A	260	THR	3
1	A	244	GLY	3
1	A	163	TYR	3
1	A	41	PRO	3
1	A	229	ASN	3
1	A	32	PRO	2
1	A	113	TYR	2
1	A	259	LYS	2
1	A	213	LEU	2
1	A	31	SER	2
1	A	133	GLY	2
1	A	85	THR	2
1	A	261	ARG	2
1	A	140	ASN	2
1	A	196	PHE	2
1	A	78	ILE	2
1	A	246	THR	2
1	A	217	PRO	2
1	A	83	ASP	2
1	A	43	GLY	2
1	A	164	THR	2
1	A	66	SER	1
1	A	60	MET	1
1	A	70	ALA	1
1	A	227	SER	1
1	A	64	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	65	ASP	1
1	A	215	VAL	1
1	A	46	ALA	1
1	A	45	LEU	1
1	A	243	GLN	1
1	A	142	PHE	1
1	A	84	ARG	1
1	A	135	GLY	1
1	A	110	GLU	1
1	A	37	PRO	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	186/239 (78%)	124±6 (67±3%)	62±6 (33±3%)	1 12
All	All	1860/2390 (78%)	1241 (67%)	619 (33%)	1 12

All 160 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	248	ARG	10
1	A	81	MET	9
1	A	107	SER	9
1	A	30	SER	8
1	A	246	THR	8
1	A	119	HIS	8
1	A	36	LEU	8
1	A	56	TYR	8
1	A	113	TYR	8
1	A	77	GLN	7
1	A	219	ASP	7
1	A	245	ARG	7
1	A	239	LYS	7
1	A	218	LEU	7
1	A	166	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	255	ARG	7
1	A	162	PHE	7
1	A	259	LYS	6
1	A	52	ARG	6
1	A	143	LEU	6
1	A	47	LEU	6
1	A	117	LYS	6
1	A	21	SER	6
1	A	221	PHE	6
1	A	257	SER	6
1	A	31	SER	6
1	A	84	ARG	6
1	A	87	LEU	6
1	A	220	TYR	6
1	A	94	ASN	6
1	A	96	THR	6
1	A	48	ILE	6
1	A	189	TYR	6
1	A	44	LYS	5
1	A	141	LYS	5
1	A	76	TYR	5
1	A	64	GLU	5
1	A	206	ARG	5
1	A	153	TRP	5
1	A	164	THR	5
1	A	62	SER	5
1	A	40	THR	5
1	A	111	LYS	5
1	A	195	LEU	5
1	A	225	PHE	5
1	A	258	THR	5
1	A	192	PHE	5
1	A	249	ASP	5
1	A	33	SER	5
1	A	190	LYS	5
1	A	238	LYS	5
1	A	23	TRP	5
1	A	123	TYR	5
1	A	115	ILE	5
1	A	60	MET	5
1	A	213	LEU	5
1	A	160	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	144	TRP	5
1	A	83	ASP	5
1	A	209	MET	5
1	A	59	ARG	5
1	A	202	THR	4
1	A	66	SER	4
1	A	51	PHE	4
1	A	116	LEU	4
1	A	49	ASP	4
1	A	103	LYS	4
1	A	125	LEU	4
1	A	45	LEU	4
1	A	260	THR	4
1	A	53	GLU	4
1	A	67	LYS	4
1	A	232	VAL	4
1	A	211	THR	4
1	A	92	THR	4
1	A	131	LEU	4
1	A	89	ASP	4
1	A	253	LEU	4
1	A	237	LEU	4
1	A	231	ASN	4
1	A	155	GLU	4
1	A	78	ILE	4
1	A	85	THR	4
1	A	100	ILE	4
1	A	93	TRP	3
1	A	191	ASP	3
1	A	35	VAL	3
1	A	91	ASN	3
1	A	163	TYR	3
1	A	42	ASP	3
1	A	145	ASN	3
1	A	214	ASP	3
1	A	243	GLN	3
1	A	241	ASP	3
1	A	229	ASN	3
1	A	38	SER	3
1	A	118	GLU	3
1	A	252	GLU	3
1	A	50	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	55	TYR	3
1	A	86	THR	3
1	A	235	TYR	3
1	A	215	VAL	3
1	A	204	ARG	3
1	A	65	ASP	3
1	A	223	GLU	3
1	A	137	ASP	3
1	A	132	ILE	3
1	A	138	ASP	3
1	A	114	GLU	3
1	A	97	HIS	2
1	A	158	LYS	2
1	A	127	ILE	2
1	A	72	TRP	2
1	A	29	TYR	2
1	A	112	SER	2
1	A	157	ILE	2
1	A	90	ASN	2
1	A	240	ASP	2
1	A	110	GLU	2
1	A	228	GLU	2
1	A	26	ARG	2
1	A	207	GLN	2
1	A	203	ASP	2
1	A	39	GLN	2
1	A	233	ARG	2
1	A	256	SER	2
1	A	120	ASP	2
1	A	210	ILE	2
1	A	61	ASN	2
1	A	196	PHE	2
1	A	194	GLN	2
1	A	197	ASN	2
1	A	109	GLU	2
1	A	134	PHE	2
1	A	63	ASP	2
1	A	261	ARG	2
1	A	74	TYR	2
1	A	140	ASN	2
1	A	156	GLU	2
1	A	73	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	230	TRP	1
1	A	208	GLN	1
1	A	159	GLU	1
1	A	161	ASP	1
1	A	57	TRP	1
1	A	24	VAL	1
1	A	98	ILE	1
1	A	236	GLN	1
1	A	226	THR	1
1	A	121	VAL	1
1	A	22	THR	1
1	A	25	THR	1
1	A	146	ILE	1
1	A	142	PHE	1
1	A	254	THR	1
1	A	105	ASN	1
1	A	122	ASP	1
1	A	227	SER	1
1	A	205	VAL	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

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 36% for the well-defined parts and 35% for the entire structure.

7.1 Chemical shift list 1

File name: 2lgz_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1187
Number of shifts mapped to atoms	1187
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	243	0.08 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	227	0.90 ± 0.05	Should be applied
$^{13}C'$	244	-0.05 ± 0.08	None needed (< 0.5 ppm)
^{15}N	235	0.41 ± 0.13	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 36%, i.e. 942 atoms were assigned a chemical shift out of a possible 2631. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	758/1027 (74%)	187/409 (46%)	385/418 (92%)	186/200 (93%)
Sidechain	182/1325 (14%)	0/773 (0%)	182/487 (37%)	0/65 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	2/279 (1%)	1/145 (1%)	0/124 (0%)	1/10 (10%)
Overall	942/2631 (36%)	188/1327 (14%)	567/1029 (55%)	187/275 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 35%, i.e. 1187 atoms were assigned a chemical shift out of a possible 3430. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	958/1343 (71%)	236/535 (44%)	487/546 (89%)	235/262 (90%)
Sidechain	227/1743 (13%)	0/1024 (0%)	227/626 (36%)	0/93 (0%)
Aromatic	2/344 (1%)	1/181 (1%)	0/146 (0%)	1/17 (6%)
Overall	1187/3430 (35%)	237/1740 (14%)	714/1318 (54%)	236/372 (63%)

7.1.4 Statistically unusual chemical shifts (i)

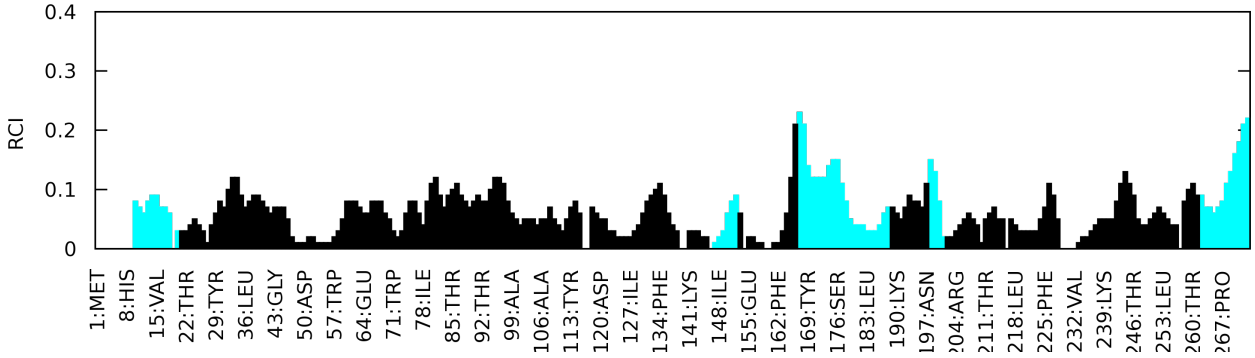
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	230	TRP	HA	11.41	7.28 – 2.08	12.9
1	A	160	ARG	CA	31.54	68.35 – 45.25	-10.9
1	A	27	THR	CB	54.99	78.10 – 61.30	-8.8
1	A	147	ARG	CB	43.89	39.81 – 21.51	7.2
1	A	111	LYS	CB	43.91	41.68 – 23.88	6.3
1	A	55	TYR	CB	27.54	50.05 – 28.55	-5.5

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:


RCI
0.4
0.3
0.2
0.1
0
1:MET
8:HIS
15:VAL
22:THR
29:TYR
36:LEU
43:GLY
50:ASP
57:TRP
64:GLU
71:TRP
78:ILE
85:THR
92:THR
99:ALA
106:ALA
113:TYR
120:ASP
127:ILE
134:PHE
141:LYS
148:ILE
155:GLU
162:PHE
169:TYR
176:SER
183:LEU
190:LYS
197:ASN
204:ARG
211:THR
218:LEU
225:PHE
232:VAL
239:LYS
246:THR
253:LEU
260:THR
267:PRO