Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 12:12 PM EST

PDB ID	:	2COE
Title	:	Solution structure of BRCT domain of terminal deoxynucleotidyltransferase
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Deposited on	:	2005-05-17

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

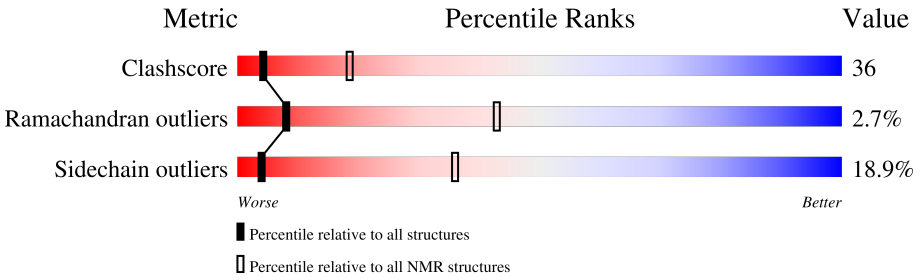
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	120	27% 45% • 24%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 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:24-A:114 (91)	0.24	6

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 11 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1809 atoms, of which 908 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called deoxynucleotidyltransferase, terminal variant.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	120	1809	559	908	158	179	5	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P04053
A	2	SER	-	cloning artifact	UNP P04053
A	3	SER	-	cloning artifact	UNP P04053
A	4	GLY	-	cloning artifact	UNP P04053
A	5	SER	-	cloning artifact	UNP P04053
A	6	SER	-	cloning artifact	UNP P04053
A	7	GLY	-	cloning artifact	UNP P04053
A	115	SER	-	cloning artifact	UNP P04053
A	116	GLY	-	cloning artifact	UNP P04053
A	117	PRO	-	cloning artifact	UNP P04053
A	118	SER	-	cloning artifact	UNP P04053
A	119	SER	-	cloning artifact	UNP P04053
A	120	GLY	-	cloning artifact	UNP P04053

4 Residue-property plots (i)

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: deoxynucleotidyltransferase, terminal variant

Chain A: 27% 45% • 24%

G1 S2 S3 G4 S5 S6 G7 T8 G9 A10 L11 M12 A13 S14 S15 P16 Q17 D18 I19 K20 F21 Q22 D23 L24 V25 I28 L29 E30 K31 K32 M33 G34 R37 R38 A39 L40 L41 M42 E43 L44 A45 R46 R47 K48 G49 F50 R51 V52 E53 N54 E55 L56 S57 D58 S59 V60 T61 H62

I63 V64 A65 E66 N67 N68 S69 D72 V73 L74 E75 W76 L77 Q80 K81 V82 Q83 V84 S85 P88 E89 L90 L91 D92 V93 S94 W95 L96 I97 E98 C99 I100 G101 A102 G103 K104 P105 V106 E107 K111 H112 Q113 L114 S115 G116 P117 S118 S119 G120

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: deoxynucleotidyltransferase, terminal variant

Chain A: 28% 37% 11% 24%

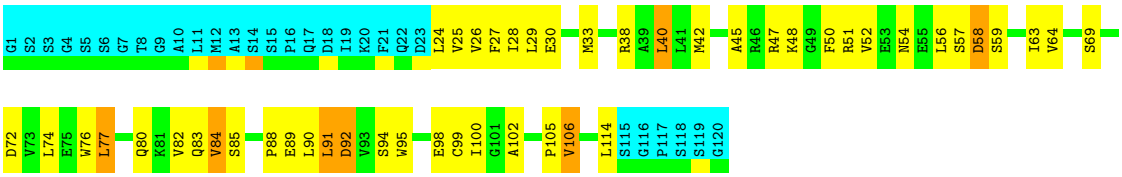
G1 S2 S3 G4 S5 S6 G7 T8 G9 A10 L11 M12 A13 S14 S15 P16 Q17 D18 I19 K20 F21 Q22 D23 L24 I28 L29 E30 K31 K32 M33 G34 R37 R38 A39 L40 L41 M42 E43 R46 R47 K48 G49 F50 N54 E55 L56 S57 D58 S59 V60 T61 H62 I63 V64 A65 E66

N67 D72 V73 L74 E75 W76 L77 Q80 K81 V82 Q83 V84 S85 P88 E89 L90 L91 D92 V93 S94 W95 L96 I97 E98 C99 I100 G101 A102 G103 K104 P105 V106 E107 G110 K111 H112 Q113 L114 S115 G116 P117 S118 S119 G120

4.2.2 Score per residue for model 2

• Molecule 1: deoxynucleotidyltransferase, terminal variant

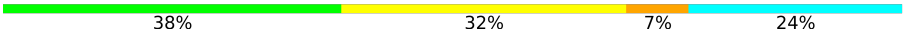
Chain A: 36% 34% 6% 24%

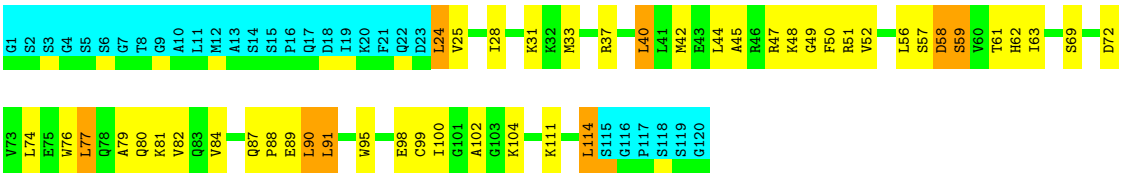


4.2.3 Score per residue for model 3

- Molecule 1: deoxynucleotidyltransferase, terminal variant

Chain A:

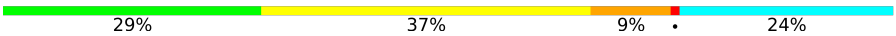




4.2.4 Score per residue for model 4

- Molecule 1: deoxynucleotidyltransferase, terminal variant

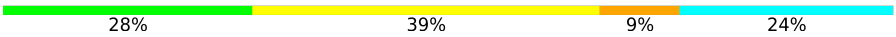
Chain A:

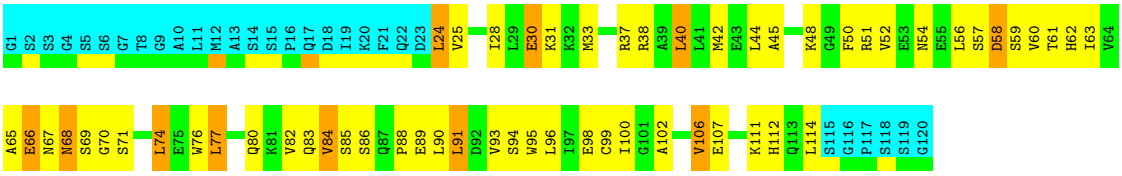


4.2.5 Score per residue for model 5

- Molecule 1: deoxynucleotidyltransferase, terminal variant

Chain A:





4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: deoxynucleotidyltransferase, terminal variant

Chain A: 33% 34% 8% 24%

G1 S2 S3 G4 S5 S6 G7 T8 G9 A10 L11 M12 A13 S14 S15 P16 Q17 D18 I19 K20 F21 Q22 D23 L24 V25 I28 L29 E30 K31 K32 M33 L40 L41 M42 A45 R46 R47 K48 G49 V52 L56 S57 D58 S59 V60 T61 H62 I63 V64 A65 E66 N67 N68 S69 G70

S71 D72 V73 L74 E75 W76 L77 Q80 K81 V82 Q83 V84 S85 P88 E89 L90 L91 W95 E98 C99 I100 G101 A102 G103 K104 P105 V106 E107 M108 T109 Q113 L114 S115 G116 P117 S118 S119 G120

4.2.7 Score per residue for model 7

- Molecule 1: deoxynucleotidyltransferase, terminal variant

Chain A: 31% 36% 8% • 24%

G1 S2 S3 G4 S5 S6 G7 T8 G9 A10 L11 M12 A13 S14 S15 P16 Q17 D18 I19 K20 F21 Q22 D23 L24 V25 V26 F27 I28 L29 E30 K31 K32 M33 G34 R37 R38 A39 L40 L41 M42 E43 L44 A45 R46 R47 K48 G49 F50 R51 V52 L56 S57 D58 S59 V60 T61 H62 I63

V64 A65 E66 N67 N68 S69 D72 V73 L74 L77 V82 Q83 V84 E89 L90 L91 D92 V93 S94 W95 L96 I97 E98 C99 I100 G101 A102 G103 K104 P105 V106 E107 M108 K111 H112 Q113 L114 S115 G116 P117 S118 S119 G120

4.2.8 Score per residue for model 8

- Molecule 1: deoxynucleotidyltransferase, terminal variant

Chain A: 30% 35% 11% 24%

G1 S2 S3 G4 S5 S6 G7 T8 G9 A10 L11 M12 A13 S14 S15 P16 Q17 D18 I19 K20 F21 Q22 D23 L24 V25 I28 K31 K32 M33 R37 R38 A39 L40 L41 M42 E43 L44 K48 G49 F50 R51 V52 E53 N54 E55 L56 S57 D58 S59 V60 T61 H62 I63 E66

S69 D72 W76 L77 Q80 K81 V82 Q83 V84 S85 S86 Q87 P88 E89 L90 L91 D92 V93 S94 W95 L96 I97 E98 C99 I100 G101 A102 P105 V106 E107 M108 T109 G110 K111 H112 Q113 L114 S115 G116 P117 S118 S119 G120

4.2.9 Score per residue for model 9

- Molecule 1: deoxynucleotidyltransferase, terminal variant

Chain A: 23% 44% 8% • 24%

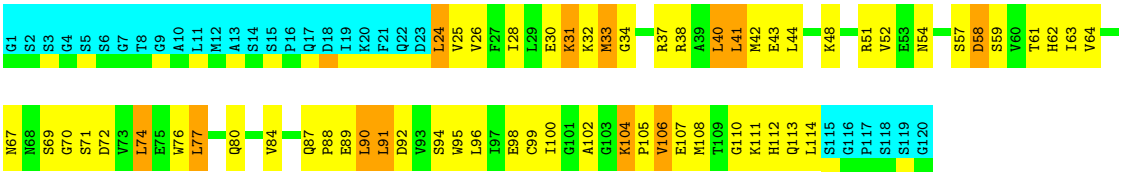
G1 S2 S3 G4 S5 S6 G7 T8 G9 A10 L11 M12 A13 S14 S15 P16 Q17 D18 I19 K20 F21 Q22 D23 L24 V25 I28 L29 E30 K31 K32 M33 G34 T35 T36 R37 R38 A39 L40 L41 M42 E43 L44 A45 R46 R47 K48 G49 F50 R51 V52 E53 N54 E55 L56 S57 D58 S59 V60 T61

H62 I63 E66 N67 N68 S69 G70 S71 D72 V73 L74 E75 W76 L77 Q80 K81 V82 Q83 V84 S85 S86 Q87 P88 E89 L90 L91 D92 V93 S94 W95 L96 I97 E98 C99 I100 G101 A102 G103 K104 P105 V106 E107 G110 K111 H112 Q113 L114 S115 G116 P117 S118 S119 G120

4.2.10 Score per residue for model 10

- Molecule 1: deoxynucleotidyltransferase, terminal variant

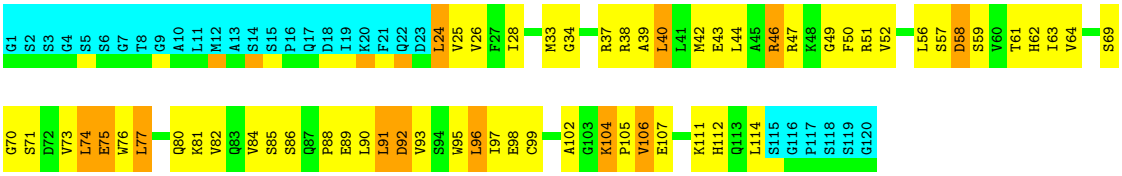
Chain A: 26% 40% 10% 24%



4.2.11 Score per residue for model 11

- Molecule 1: deoxynucleotidyltransferase, terminal variant

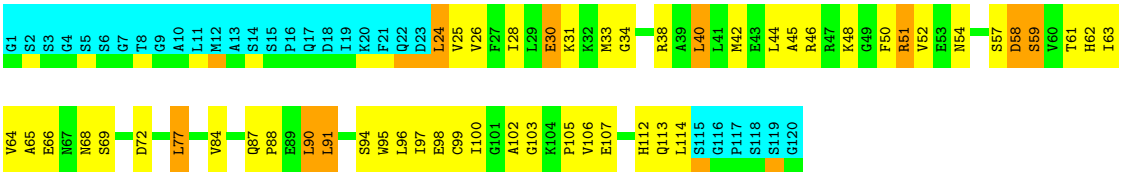
Chain A: 26% 40% 10% 24%



4.2.12 Score per residue for model 12

- Molecule 1: deoxynucleotidyltransferase, terminal variant

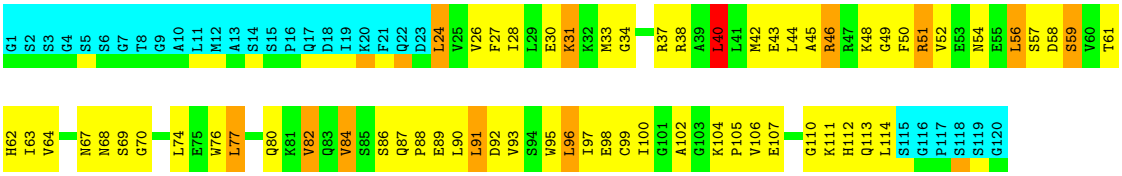
Chain A: 32% 36% 8% 24%



4.2.13 Score per residue for model 13

- Molecule 1: deoxynucleotidyltransferase, terminal variant

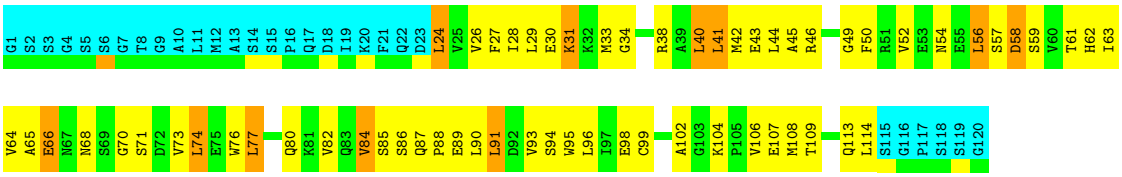
Chain A: 22% 43% 9% • 24%



4.2.14 Score per residue for model 14

• Molecule 1: deoxynucleotidyltransferase, terminal variant

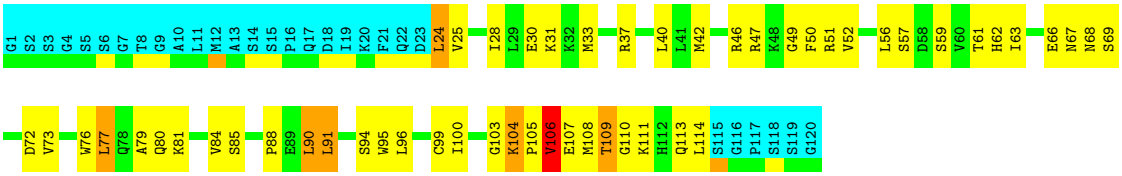
Chain A: 24% 42% 9% 24%



4.2.15 Score per residue for model 15

• Molecule 1: deoxynucleotidyltransferase, terminal variant

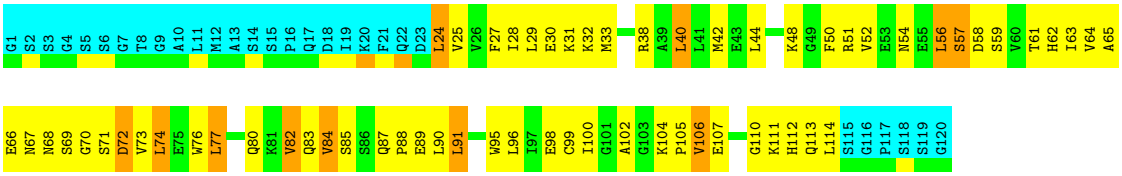
Chain A: 32% 38% 5% • 24%



4.2.16 Score per residue for model 16

• Molecule 1: deoxynucleotidyltransferase, terminal variant

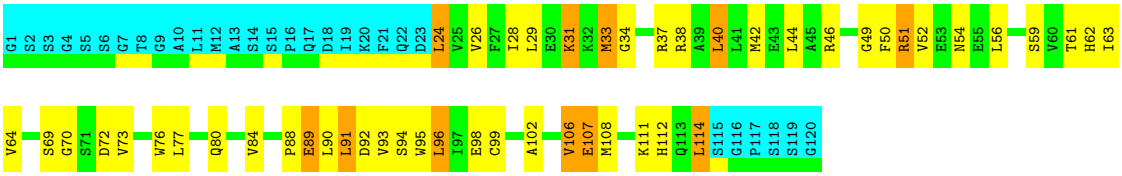
Chain A: 23% 43% 9% 24%



4.2.17 Score per residue for model 17

• Molecule 1: deoxynucleotidyltransferase, terminal variant

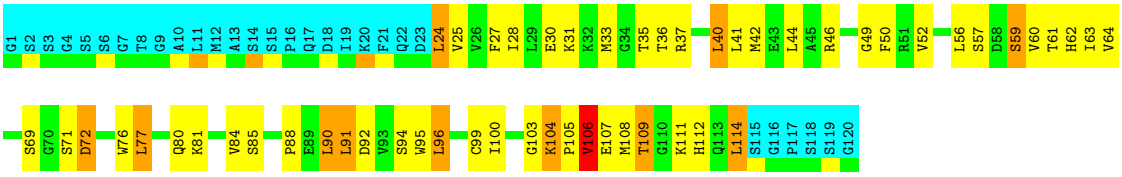
Chain A: 34% 32% 9% 24%



4.2.18 Score per residue for model 18

- Molecule 1: deoxynucleotidyltransferase, terminal variant

Chain A: 31% 35% 9% • 24%



4.2.19 Score per residue for model 19

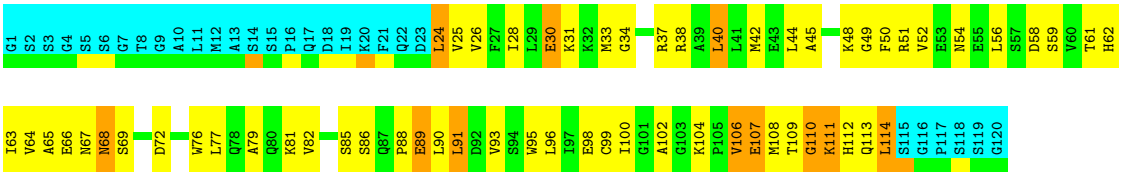
- Molecule 1: deoxynucleotidyltransferase, terminal variant

Chain A: 27% 42% 8% 24%

4.2.20 Score per residue for model 20

- Molecule 1: deoxynucleotidyltransferase, terminal variant

Chain A: 25% 42% 9% 24%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function,structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	1.07
CYANA	refinement	1.07

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	714	737	737	52±8
All	All	14280	14740	14740	1039

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:C	1:A:91:LEU:HD13	0.95	1.81	17	1
1:A:24:LEU:HD11	1:A:50:PHE:CD1	0.90	2.02	20	1
1:A:40:LEU:HD13	1:A:41:LEU:N	0.89	1.83	10	4
1:A:89:GLU:OE2	1:A:91:LEU:HD11	0.86	1.69	7	1
1:A:56:LEU:HD22	1:A:57:SER:N	0.85	1.86	19	4
1:A:89:GLU:CD	1:A:91:LEU:HD11	0.84	1.91	7	1
1:A:56:LEU:HD23	1:A:82:VAL:CG1	0.83	2.03	11	9
1:A:28:ILE:HD11	1:A:96:LEU:CD2	0.83	2.03	15	8
1:A:68:ASN:O	1:A:114:LEU:HD22	0.82	1.75	16	5
1:A:65:ALA:HB1	1:A:68:ASN:OD1	0.81	1.76	6	5
1:A:56:LEU:HD12	1:A:76:TRP:CH2	0.78	2.14	8	1
1:A:56:LEU:HD13	1:A:82:VAL:CG2	0.78	2.10	9	1
1:A:28:ILE:HD12	1:A:42:MET:HG2	0.77	1.55	12	1
1:A:56:LEU:HD13	1:A:82:VAL:HG22	0.77	1.57	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:LEU:HB3	1:A:82:VAL:HG11	0.76	1.57	8	1
1:A:107:GLU:HG3	1:A:109:THR:HG23	0.76	1.56	15	5
1:A:24:LEU:HD22	1:A:62:HIS:CE1	0.76	2.15	8	16
1:A:28:ILE:HD12	1:A:42:MET:HG3	0.76	1.57	11	19
1:A:56:LEU:HD13	1:A:82:VAL:HB	0.74	1.59	14	1
1:A:63:ILE:HD12	1:A:88:PRO:HG2	0.74	1.59	16	19
1:A:91:LEU:HD13	1:A:95:TRP:CD2	0.73	2.19	2	17
1:A:73:VAL:HB	1:A:90:LEU:HD13	0.73	1.60	16	3
1:A:28:ILE:HD11	1:A:96:LEU:HD21	0.72	1.61	15	6
1:A:28:ILE:HD12	1:A:42:MET:CG	0.72	2.14	3	12
1:A:99:CYS:SG	1:A:106:VAL:HG22	0.71	2.24	2	12
1:A:89:GLU:HB3	1:A:91:LEU:HD11	0.71	1.61	17	1
1:A:58:ASP:HA	1:A:84:VAL:HG23	0.69	1.63	10	5
1:A:48:LYS:HE2	1:A:100:ILE:HG23	0.69	1.65	2	3
1:A:25:VAL:HG22	1:A:51:ARG:HD3	0.69	1.63	15	3
1:A:56:LEU:O	1:A:82:VAL:HG21	0.68	1.88	19	3
1:A:56:LEU:HD13	1:A:82:VAL:CG1	0.68	2.19	8	1
1:A:24:LEU:HD11	1:A:50:PHE:CE1	0.68	2.23	20	1
1:A:40:LEU:CD2	1:A:44:LEU:HD21	0.68	2.19	10	3
1:A:24:LEU:HD12	1:A:50:PHE:CE1	0.67	2.24	15	6
1:A:42:MET:CB	1:A:52:VAL:HG11	0.67	2.19	6	11
1:A:59:SER:O	1:A:61:THR:HG23	0.67	1.89	10	16
1:A:30:GLU:O	1:A:31:LYS:C	0.67	2.33	9	14
1:A:40:LEU:HD12	1:A:41:LEU:HD22	0.66	1.66	18	3
1:A:73:VAL:HG11	1:A:90:LEU:HD22	0.66	1.66	14	2
1:A:56:LEU:HD13	1:A:82:VAL:HG11	0.65	1.66	8	1
1:A:76:TRP:CD1	1:A:80:GLN:NE2	0.65	2.65	16	3
1:A:95:TRP:CD1	1:A:106:VAL:HG23	0.64	2.28	8	15
1:A:91:LEU:HD13	1:A:91:LEU:N	0.64	2.06	17	1
1:A:56:LEU:HD22	1:A:56:LEU:C	0.64	2.12	16	4
1:A:91:LEU:HD21	1:A:108:MET:SD	0.64	2.33	10	3
1:A:90:LEU:HB3	1:A:114:LEU:HD23	0.64	1.69	12	7
1:A:56:LEU:HD23	1:A:82:VAL:HG11	0.64	1.69	4	9
1:A:74:LEU:C	1:A:74:LEU:HD12	0.64	2.14	11	3
1:A:89:GLU:C	1:A:90:LEU:HD23	0.63	2.13	9	6
1:A:56:LEU:C	1:A:82:VAL:HG21	0.63	2.14	8	1
1:A:50:PHE:O	1:A:52:VAL:HG23	0.62	1.94	13	2
1:A:61:THR:OG1	1:A:62:HIS:CE1	0.62	2.52	7	9
1:A:107:GLU:CG	1:A:109:THR:HG23	0.62	2.23	15	3
1:A:45:ALA:HB3	1:A:52:VAL:HG21	0.62	1.69	19	7
1:A:96:LEU:HD13	1:A:100:ILE:CD1	0.62	2.25	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:C	1:A:114:LEU:HD12	0.61	2.13	5	6
1:A:25:VAL:HG22	1:A:51:ARG:CD	0.61	2.25	11	2
1:A:29:LEU:CD1	1:A:76:TRP:CE2	0.61	2.83	14	1
1:A:96:LEU:HD13	1:A:100:ILE:HD11	0.61	1.72	18	1
1:A:42:MET:HB3	1:A:52:VAL:HG11	0.61	1.73	6	9
1:A:89:GLU:O	1:A:91:LEU:HD22	0.60	1.95	17	1
1:A:76:TRP:CZ2	1:A:80:GLN:CD	0.60	2.75	10	5
1:A:76:TRP:CZ2	1:A:80:GLN:OE1	0.60	2.55	2	4
1:A:89:GLU:OE1	1:A:91:LEU:HD21	0.60	1.97	7	1
1:A:62:HIS:CD2	1:A:89:GLU:OE1	0.59	2.56	17	2
1:A:91:LEU:CD1	1:A:95:TRP:CE3	0.58	2.86	18	7
1:A:76:TRP:CE2	1:A:80:GLN:NE2	0.58	2.71	3	6
1:A:91:LEU:HD13	1:A:95:TRP:CE3	0.58	2.34	18	4
1:A:95:TRP:CE2	1:A:99:CYS:SG	0.58	2.96	18	18
1:A:56:LEU:HD22	1:A:76:TRP:CH2	0.58	2.34	17	7
1:A:89:GLU:C	1:A:90:LEU:HD13	0.57	2.20	10	1
1:A:90:LEU:O	1:A:114:LEU:HD22	0.57	1.99	17	2
1:A:91:LEU:O	1:A:114:LEU:HD21	0.57	2.00	18	1
1:A:56:LEU:CD2	1:A:57:SER:N	0.57	2.68	16	4
1:A:90:LEU:HD13	1:A:90:LEU:N	0.57	2.15	10	1
1:A:25:VAL:HG21	1:A:59:SER:O	0.56	2.00	8	12
1:A:107:GLU:O	1:A:112:HIS:CE1	0.56	2.58	13	10
1:A:40:LEU:CD1	1:A:41:LEU:N	0.56	2.66	6	4
1:A:66:GLU:CB	1:A:93:VAL:HG11	0.56	2.30	14	2
1:A:90:LEU:CD1	1:A:90:LEU:N	0.56	2.68	12	2
1:A:40:LEU:CD1	1:A:41:LEU:HD22	0.55	2.31	18	3
1:A:76:TRP:CE2	1:A:80:GLN:CD	0.55	2.80	9	8
1:A:58:ASP:HA	1:A:84:VAL:HG12	0.55	1.79	2	8
1:A:65:ALA:CB	1:A:68:ASN:OD1	0.55	2.53	6	3
1:A:56:LEU:HB3	1:A:82:VAL:HG21	0.55	1.77	14	1
1:A:24:LEU:HB2	1:A:62:HIS:CE1	0.55	2.36	20	1
1:A:42:MET:O	1:A:52:VAL:HG21	0.55	2.02	6	6
1:A:74:LEU:CD2	1:A:90:LEU:CD1	0.55	2.85	14	1
1:A:46:ARG:CG	1:A:52:VAL:HG13	0.55	2.31	12	1
1:A:27:PHE:CE1	1:A:76:TRP:CH2	0.54	2.96	14	1
1:A:91:LEU:HD12	1:A:95:TRP:CE3	0.54	2.37	19	8
1:A:95:TRP:CD2	1:A:99:CYS:SG	0.54	3.00	2	8
1:A:46:ARG:HG3	1:A:52:VAL:HG13	0.54	1.79	12	1
1:A:74:LEU:CD2	1:A:90:LEU:HD11	0.54	2.32	14	2
1:A:56:LEU:HD22	1:A:80:GLN:HG3	0.54	1.78	17	2
1:A:92:ASP:HA	1:A:114:LEU:HD21	0.54	1.79	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:C	1:A:114:LEU:HD22	0.54	2.23	17	7
1:A:56:LEU:CD2	1:A:82:VAL:CG1	0.54	2.85	4	9
1:A:90:LEU:HD23	1:A:90:LEU:N	0.54	2.18	9	3
1:A:95:TRP:CD1	1:A:99:CYS:SG	0.54	3.01	18	1
1:A:71:SER:HA	1:A:74:LEU:HD23	0.54	1.77	5	3
1:A:89:GLU:O	1:A:91:LEU:CD2	0.53	2.57	17	1
1:A:56:LEU:C	1:A:56:LEU:CD2	0.53	2.76	16	4
1:A:90:LEU:N	1:A:90:LEU:HD13	0.53	2.19	12	1
1:A:26:VAL:O	1:A:52:VAL:HG13	0.53	2.04	20	1
1:A:25:VAL:HG13	1:A:51:ARG:O	0.52	2.04	20	2
1:A:105:PRO:O	1:A:106:VAL:O	0.52	2.27	18	2
1:A:106:VAL:HG13	1:A:107:GLU:N	0.52	2.19	15	2
1:A:24:LEU:HD22	1:A:62:HIS:HE1	0.52	1.65	18	16
1:A:45:ALA:HB2	1:A:96:LEU:HD11	0.52	1.81	20	1
1:A:80:GLN:HB3	1:A:82:VAL:HG12	0.52	1.81	8	1
1:A:48:LYS:CE	1:A:100:ILE:HG23	0.52	2.35	10	5
1:A:65:ALA:HB1	1:A:68:ASN:CG	0.52	2.25	7	2
1:A:76:TRP:CZ2	1:A:80:GLN:HG3	0.52	2.39	16	5
1:A:90:LEU:C	1:A:114:LEU:CD2	0.52	2.78	10	7
1:A:27:PHE:CE2	1:A:76:TRP:CH2	0.52	2.98	13	1
1:A:95:TRP:NE1	1:A:106:VAL:HG23	0.51	2.20	17	4
1:A:81:LYS:CG	1:A:81:LYS:O	0.51	2.57	18	3
1:A:62:HIS:CG	1:A:95:TRP:CH2	0.51	2.97	17	1
1:A:25:VAL:CG2	1:A:59:SER:O	0.51	2.58	16	12
1:A:48:LYS:HE3	1:A:100:ILE:HG23	0.51	1.83	10	9
1:A:56:LEU:CD2	1:A:82:VAL:HG11	0.51	2.35	2	5
1:A:92:ASP:N	1:A:114:LEU:HD11	0.51	2.21	17	1
1:A:66:GLU:N	1:A:68:ASN:OD1	0.51	2.44	12	5
1:A:28:ILE:CD1	1:A:96:LEU:CD2	0.50	2.87	15	2
1:A:98:GLU:O	1:A:102:ALA:CB	0.50	2.59	17	6
1:A:32:LYS:CE	1:A:67:ASN:O	0.50	2.59	10	1
1:A:24:LEU:CB	1:A:62:HIS:CE1	0.50	2.94	20	1
1:A:42:MET:SD	1:A:52:VAL:CG1	0.50	2.99	11	9
1:A:56:LEU:CD1	1:A:82:VAL:HG11	0.50	2.35	8	1
1:A:29:LEU:HD21	1:A:31:LYS:HG3	0.50	1.82	9	1
1:A:114:LEU:H	1:A:114:LEU:HD22	0.50	1.65	12	6
1:A:98:GLU:O	1:A:102:ALA:N	0.50	2.43	3	18
1:A:63:ILE:CD1	1:A:77:LEU:CD2	0.50	2.89	7	1
1:A:24:LEU:CD1	1:A:50:PHE:CE1	0.50	2.94	15	1
1:A:104:LYS:CB	1:A:105:PRO:CD	0.50	2.90	15	2
1:A:84:VAL:O	1:A:85:SER:CB	0.50	2.60	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:THR:OG1	1:A:111:LYS:CG	0.50	2.60	8	1
1:A:91:LEU:HD23	1:A:113:GLN:HG2	0.50	1.84	10	1
1:A:26:VAL:CG1	1:A:64:VAL:CG2	0.50	2.90	12	2
1:A:62:HIS:CD2	1:A:95:TRP:CH2	0.50	2.99	17	1
1:A:63:ILE:CD1	1:A:77:LEU:HD21	0.50	2.36	5	6
1:A:24:LEU:HG	1:A:62:HIS:CE1	0.50	2.42	14	2
1:A:40:LEU:CD1	1:A:44:LEU:HD21	0.49	2.37	16	13
1:A:76:TRP:CH2	1:A:80:GLN:HG3	0.49	2.43	14	5
1:A:26:VAL:HG13	1:A:64:VAL:HG23	0.49	1.85	7	6
1:A:24:LEU:HD12	1:A:50:PHE:CD1	0.49	2.42	15	4
1:A:40:LEU:HD21	1:A:44:LEU:HD21	0.49	1.85	10	2
1:A:66:GLU:O	1:A:67:ASN:CB	0.49	2.60	20	5
1:A:66:GLU:HB2	1:A:93:VAL:HG11	0.48	1.84	8	3
1:A:104:LYS:HB2	1:A:105:PRO:HD2	0.48	1.85	18	2
1:A:24:LEU:CD1	1:A:50:PHE:CD1	0.48	2.89	20	1
1:A:73:VAL:HG12	1:A:77:LEU:HD12	0.48	1.85	15	1
1:A:91:LEU:N	1:A:91:LEU:CD1	0.48	2.76	17	1
1:A:26:VAL:HG13	1:A:64:VAL:CG2	0.48	2.38	12	4
1:A:95:TRP:CZ2	1:A:108:MET:HE3	0.48	2.43	17	1
1:A:107:GLU:OE2	1:A:109:THR:CG2	0.48	2.62	18	1
1:A:70:GLY:O	1:A:74:LEU:N	0.48	2.45	11	3
1:A:74:LEU:O	1:A:77:LEU:N	0.48	2.47	14	10
1:A:93:VAL:HG22	1:A:97:ILE:HG13	0.48	1.85	13	2
1:A:38:ARG:NH2	1:A:54:ASN:O	0.47	2.47	9	10
1:A:50:PHE:CE2	1:A:99:CYS:HB3	0.47	2.44	12	5
1:A:71:SER:O	1:A:74:LEU:N	0.47	2.48	11	4
1:A:90:LEU:O	1:A:91:LEU:HD13	0.47	2.09	17	1
1:A:82:VAL:HG22	1:A:83:GLN:N	0.47	2.24	2	3
1:A:39:ALA:O	1:A:43:GLU:N	0.47	2.47	4	2
1:A:66:GLU:HB2	1:A:93:VAL:HG21	0.47	1.86	14	3
1:A:56:LEU:HD12	1:A:60:VAL:HG21	0.47	1.86	5	3
1:A:69:SER:O	1:A:72:ASP:N	0.47	2.48	16	15
1:A:104:LYS:HB2	1:A:105:PRO:CD	0.47	2.39	18	2
1:A:89:GLU:OE1	1:A:108:MET:CE	0.47	2.63	7	1
1:A:96:LEU:CD1	1:A:100:ILE:HD11	0.47	2.39	18	1
1:A:28:ILE:HD11	1:A:96:LEU:CD1	0.47	2.40	1	1
1:A:45:ALA:O	1:A:48:LYS:N	0.47	2.48	2	4
1:A:107:GLU:O	1:A:112:HIS:ND1	0.47	2.48	20	12
1:A:70:GLY:N	1:A:114:LEU:CB	0.47	2.78	10	3
1:A:34:GLY:O	1:A:38:ARG:CB	0.46	2.64	9	12
1:A:110:GLY:O	1:A:113:GLN:N	0.46	2.48	8	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:HD22	1:A:114:LEU:H	0.46	1.70	2	2
1:A:89:GLU:CG	1:A:91:LEU:HD11	0.46	2.39	7	1
1:A:57:SER:O	1:A:84:VAL:HG23	0.46	2.10	19	1
1:A:66:GLU:CB	1:A:93:VAL:CG1	0.46	2.93	14	1
1:A:40:LEU:HD13	1:A:40:LEU:C	0.46	2.29	6	2
1:A:26:VAL:HG11	1:A:96:LEU:CD2	0.46	2.41	4	4
1:A:64:VAL:HG21	1:A:96:LEU:HB2	0.46	1.86	17	2
1:A:40:LEU:HD22	1:A:44:LEU:CD2	0.46	2.41	18	3
1:A:76:TRP:NE1	1:A:80:GLN:NE2	0.46	2.64	5	4
1:A:65:ALA:C	1:A:68:ASN:OD1	0.46	2.54	7	2
1:A:37:ARG:O	1:A:41:LEU:N	0.46	2.48	19	2
1:A:40:LEU:O	1:A:43:GLU:N	0.46	2.49	19	5
1:A:89:GLU:CD	1:A:91:LEU:HD21	0.46	2.31	7	1
1:A:99:CYS:O	1:A:103:GLY:N	0.46	2.47	18	3
1:A:98:GLU:C	1:A:100:ILE:N	0.46	2.69	3	4
1:A:65:ALA:HB1	1:A:68:ASN:HB2	0.46	1.87	16	2
1:A:95:TRP:NE1	1:A:99:CYS:SG	0.45	2.89	18	1
1:A:111:LYS:HE3	1:A:112:HIS:CD2	0.45	2.46	4	1
1:A:73:VAL:CB	1:A:90:LEU:HD13	0.45	2.37	16	1
1:A:56:LEU:CD1	1:A:76:TRP:CH2	0.45	2.95	8	1
1:A:56:LEU:CB	1:A:82:VAL:HG11	0.45	2.37	8	1
1:A:94:SER:OG	1:A:95:TRP:N	0.45	2.50	7	1
1:A:38:ARG:NH2	1:A:54:ASN:OD1	0.45	2.50	12	1
1:A:61:THR:OG1	1:A:62:HIS:ND1	0.45	2.49	18	3
1:A:46:ARG:O	1:A:49:GLY:N	0.45	2.49	18	10
1:A:75:GLU:HG3	1:A:76:TRP:N	0.45	2.26	11	1
1:A:26:VAL:HG11	1:A:96:LEU:HD13	0.45	1.89	14	1
1:A:70:GLY:O	1:A:74:LEU:HD23	0.45	2.12	16	2
1:A:66:GLU:OE1	1:A:67:ASN:ND2	0.45	2.49	16	1
1:A:92:ASP:CG	1:A:114:LEU:CD1	0.45	2.85	4	1
1:A:40:LEU:HD13	1:A:41:LEU:CA	0.45	2.41	10	4
1:A:76:TRP:CE2	1:A:80:GLN:CG	0.45	3.00	8	2
1:A:108:MET:SD	1:A:113:GLN:NE2	0.45	2.90	8	3
1:A:50:PHE:O	1:A:52:VAL:N	0.45	2.50	2	1
1:A:84:VAL:C	1:A:86:SER:N	0.45	2.71	14	2
1:A:29:LEU:N	1:A:64:VAL:O	0.44	2.47	7	2
1:A:38:ARG:CG	1:A:42:MET:SD	0.44	3.05	20	7
1:A:27:PHE:CE1	1:A:56:LEU:N	0.44	2.85	19	4
1:A:67:ASN:O	1:A:68:ASN:C	0.44	2.54	5	1
1:A:86:SER:O	1:A:87:GLN:C	0.44	2.55	9	4
1:A:70:GLY:O	1:A:90:LEU:HD23	0.44	2.12	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:GLU:HB2	1:A:93:VAL:CG1	0.44	2.43	1	2
1:A:63:ILE:HD12	1:A:77:LEU:HD21	0.44	1.89	8	6
1:A:92:ASP:C	1:A:94:SER:N	0.44	2.71	10	3
1:A:63:ILE:CD1	1:A:88:PRO:HG2	0.44	2.43	19	5
1:A:30:GLU:OE2	1:A:34:GLY:N	0.44	2.50	9	1
1:A:91:LEU:CD1	1:A:95:TRP:CD2	0.44	3.01	5	4
1:A:69:SER:O	1:A:70:GLY:C	0.44	2.55	5	5
1:A:93:VAL:O	1:A:96:LEU:N	0.44	2.50	5	1
1:A:66:GLU:O	1:A:68:ASN:ND2	0.44	2.51	7	2
1:A:30:GLU:O	1:A:33:MET:N	0.44	2.51	9	1
1:A:92:ASP:CA	1:A:114:LEU:HD11	0.43	2.43	18	2
1:A:42:MET:SD	1:A:52:VAL:HG12	0.43	2.53	11	1
1:A:76:TRP:CZ3	1:A:77:LEU:HD22	0.43	2.48	9	1
1:A:95:TRP:CD1	1:A:106:VAL:CG2	0.43	3.01	2	5
1:A:29:LEU:HD11	1:A:76:TRP:CD1	0.43	2.48	14	1
1:A:90:LEU:N	1:A:90:LEU:CD1	0.43	2.81	15	2
1:A:89:GLU:OE1	1:A:108:MET:SD	0.43	2.77	7	1
1:A:84:VAL:O	1:A:86:SER:N	0.43	2.51	14	1
1:A:98:GLU:O	1:A:102:ALA:HB3	0.43	2.12	17	3
1:A:46:ARG:HG3	1:A:52:VAL:CG1	0.43	2.42	12	1
1:A:92:ASP:O	1:A:94:SER:N	0.43	2.51	17	1
1:A:66:GLU:HB2	1:A:93:VAL:CG2	0.43	2.44	5	1
1:A:66:GLU:O	1:A:68:ASN:OD1	0.42	2.37	5	1
1:A:74:LEU:C	1:A:74:LEU:CD1	0.42	2.85	11	3
1:A:40:LEU:CD2	1:A:44:LEU:CD2	0.42	2.93	18	2
1:A:45:ALA:HB3	1:A:52:VAL:CG2	0.42	2.43	19	1
1:A:83:GLN:C	1:A:85:SER:N	0.42	2.71	19	1
1:A:81:LYS:O	1:A:81:LYS:CG	0.42	2.67	4	3
1:A:113:GLN:O	1:A:114:LEU:C	0.42	2.58	12	4
1:A:90:LEU:N	1:A:90:LEU:HD23	0.42	2.28	17	1
1:A:92:ASP:O	1:A:93:VAL:C	0.42	2.58	17	1
1:A:42:MET:HG2	1:A:52:VAL:CG1	0.42	2.44	14	3
1:A:29:LEU:O	1:A:30:GLU:C	0.42	2.58	2	2
1:A:71:SER:C	1:A:73:VAL:N	0.42	2.73	11	1
1:A:76:TRP:O	1:A:79:ALA:HB3	0.42	2.15	20	3
1:A:28:ILE:CD1	1:A:42:MET:HG3	0.42	2.44	4	1
1:A:95:TRP:O	1:A:99:CYS:SG	0.42	2.78	15	5
1:A:42:MET:CG	1:A:52:VAL:HG11	0.42	2.45	18	2
1:A:96:LEU:O	1:A:97:ILE:C	0.42	2.57	19	3
1:A:90:LEU:CB	1:A:114:LEU:HD23	0.42	2.45	10	1
1:A:64:VAL:HG13	1:A:93:VAL:HA	0.42	1.91	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:PRO:C	1:A:106:VAL:O	0.42	2.58	18	2
1:A:96:LEU:O	1:A:100:ILE:N	0.41	2.50	15	1
1:A:95:TRP:CE2	1:A:108:MET:HE3	0.41	2.49	17	1
1:A:114:LEU:HD13	1:A:114:LEU:N	0.41	2.29	18	1
1:A:100:ILE:O	1:A:103:GLY:N	0.41	2.53	19	1
1:A:48:LYS:NZ	1:A:100:ILE:O	0.41	2.51	16	1
1:A:83:GLN:O	1:A:85:SER:N	0.41	2.53	19	1
1:A:42:MET:SD	1:A:53:GLU:O	0.41	2.78	8	1
1:A:76:TRP:CE2	1:A:80:GLN:HG3	0.41	2.51	8	1
1:A:76:TRP:NE1	1:A:80:GLN:CD	0.41	2.73	9	1
1:A:28:ILE:CD1	1:A:41:LEU:HB3	0.41	2.45	10	2
1:A:56:LEU:HD11	1:A:77:LEU:HD23	0.41	1.92	13	1
1:A:27:PHE:O	1:A:64:VAL:N	0.41	2.49	18	2
1:A:70:GLY:N	1:A:114:LEU:HB3	0.41	2.31	14	1
1:A:83:GLN:O	1:A:84:VAL:C	0.41	2.59	16	2
1:A:104:LYS:CB	1:A:105:PRO:HD2	0.41	2.45	15	2
1:A:69:SER:O	1:A:71:SER:N	0.41	2.53	9	2
1:A:24:LEU:CD2	1:A:50:PHE:CD1	0.41	3.04	14	1
1:A:31:LYS:HE3	1:A:76:TRP:CD1	0.41	2.51	17	1
1:A:82:VAL:HG22	1:A:82:VAL:O	0.41	2.16	19	1
1:A:108:MET:O	1:A:109:THR:C	0.41	2.59	20	1
1:A:94:SER:O	1:A:95:TRP:C	0.41	2.60	2	1
1:A:37:ARG:O	1:A:38:ARG:C	0.41	2.59	5	3
1:A:69:SER:C	1:A:71:SER:N	0.41	2.73	9	2
1:A:42:MET:CG	1:A:52:VAL:CG1	0.41	2.99	11	1
1:A:98:GLU:O	1:A:99:CYS:C	0.40	2.59	1	2
1:A:29:LEU:CD2	1:A:31:LYS:HG3	0.40	2.45	9	1
1:A:35:THR:O	1:A:36:THR:C	0.40	2.60	18	2
1:A:26:VAL:HG11	1:A:96:LEU:HD23	0.40	1.93	4	1
1:A:110:GLY:O	1:A:111:LYS:C	0.40	2.59	20	1
1:A:38:ARG:O	1:A:42:MET:SD	0.40	2.80	1	1
1:A:40:LEU:O	1:A:41:LEU:C	0.40	2.60	19	1
1:A:98:GLU:O	1:A:100:ILE:N	0.40	2.54	3	1
1:A:74:LEU:HD12	1:A:74:LEU:O	0.40	2.16	11	1
1:A:84:VAL:O	1:A:85:SER:C	0.40	2.60	14	1
1:A:91:LEU:CD2	1:A:113:GLN:NE2	0.40	2.85	20	1
1:A:38:ARG:O	1:A:42:MET:CG	0.40	2.70	1	1
1:A:40:LEU:HD11	1:A:44:LEU:HD21	0.40	1.92	7	1
1:A:64:VAL:CG1	1:A:93:VAL:HA	0.40	2.46	20	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	91/120 (76%)	73±3 (80±3%)	16±3 (17±3%)	2±1 (3±1%)	8 43
All	All	1820/2400 (76%)	1454 (80%)	316 (17%)	50 (3%)	8 43

All 10 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	33	MET	19
1	A	106	VAL	16
1	A	40	LEU	4
1	A	110	GLY	3
1	A	51	ARG	2
1	A	109	THR	2
1	A	86	SER	1
1	A	82	VAL	1
1	A	31	LYS	1
1	A	84	VAL	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	80/101 (79%)	65±2 (81±3%)	15±2 (19±3%)	4 36
All	All	1600/2020 (79%)	1297 (81%)	303 (19%)	4 36

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	24	LEU	20
1	A	40	LEU	20
1	A	77	LEU	20
1	A	91	LEU	20
1	A	111	LYS	16
1	A	58	ASP	14
1	A	104	LYS	13
1	A	84	VAL	12
1	A	57	SER	12
1	A	85	SER	11
1	A	31	LYS	10
1	A	37	ARG	10
1	A	96	LEU	9
1	A	90	LEU	9
1	A	114	LEU	8
1	A	89	GLU	8
1	A	59	SER	7
1	A	94	SER	7
1	A	72	ASP	6
1	A	56	LEU	6
1	A	47	ARG	5
1	A	92	ASP	5
1	A	51	ARG	5
1	A	87	GLN	5
1	A	74	LEU	5
1	A	54	ASN	4
1	A	66	GLU	4
1	A	68	ASN	4
1	A	67	ASN	3
1	A	30	GLU	3
1	A	41	LEU	3
1	A	32	LYS	3
1	A	46	ARG	3
1	A	82	VAL	3
1	A	33	MET	2
1	A	86	SER	2
1	A	106	VAL	2
1	A	107	GLU	2
1	A	81	LYS	1
1	A	75	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 (i)

No chemical shift data were provided