Full wwPDB NMR Structure Validation Report (i)

Feb 23, 2022 – 07:55 AM EST

PDB ID	:	1X5B
Title	:	The solution structure of the VHS domain of human Signal transducing adaptor molecule 2
Authors	:	Tochio, N.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-05-15

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:

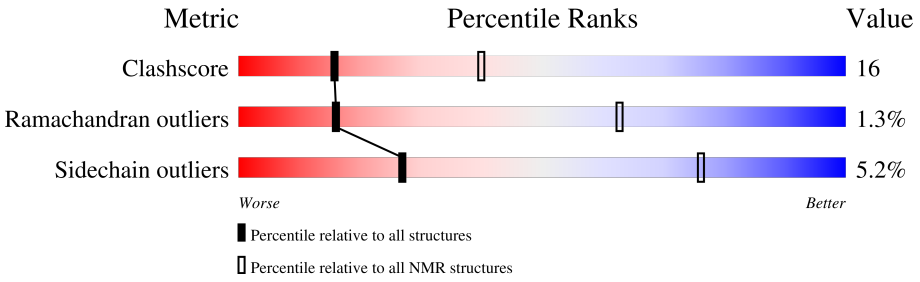
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	163	63% 21% • 15%

2 Ensemble composition and analysis (i)

This entry contains 20 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:14-A:151 (138)	0.28	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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2467 atoms, of which 1234 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called signal transducing adaptor molecule 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	163	2467	773	1234	209	240	11	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP O75886
A	2	SER	-	cloning artifact	UNP O75886
A	3	SER	-	cloning artifact	UNP O75886
A	4	GLY	-	cloning artifact	UNP O75886
A	5	SER	-	cloning artifact	UNP O75886
A	6	SER	-	cloning artifact	UNP O75886
A	7	GLY	-	cloning artifact	UNP O75886
A	158	SER	-	cloning artifact	UNP O75886
A	159	GLY	-	cloning artifact	UNP O75886
A	160	PRO	-	cloning artifact	UNP O75886
A	161	SER	-	cloning artifact	UNP O75886
A	162	SER	-	cloning artifact	UNP O75886
A	163	GLY	-	cloning artifact	UNP O75886

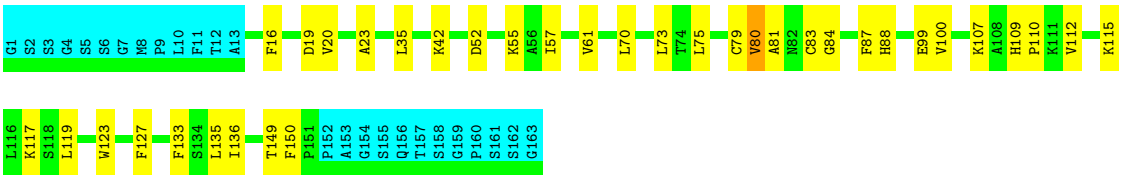
4 Residue-property plots (i)

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: signal transducing adaptor molecule 2

Chain A: 63% 21% • 15%



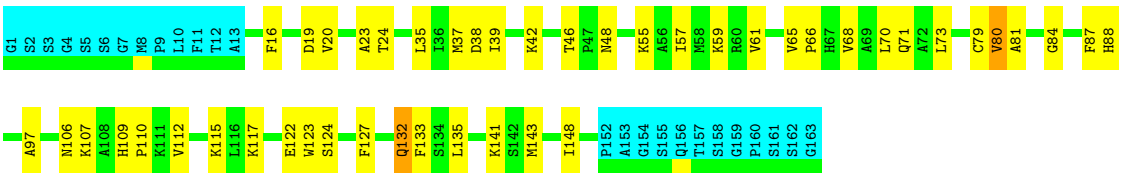
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: signal transducing adaptor molecule 2

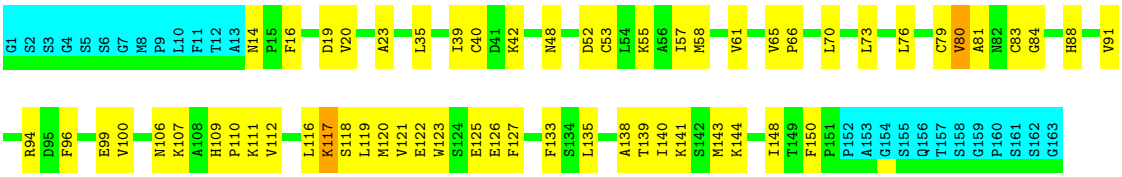
Chain A: 56% 27% • 15%



4.2.2 Score per residue for model 2

• Molecule 1: signal transducing adaptor molecule 2

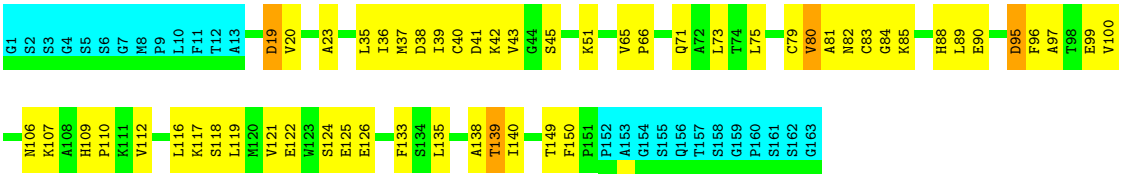
Chain A: 48% 35% • 15%



4.2.3 Score per residue for model 3

- Molecule 1: signal transducing adaptor molecule 2

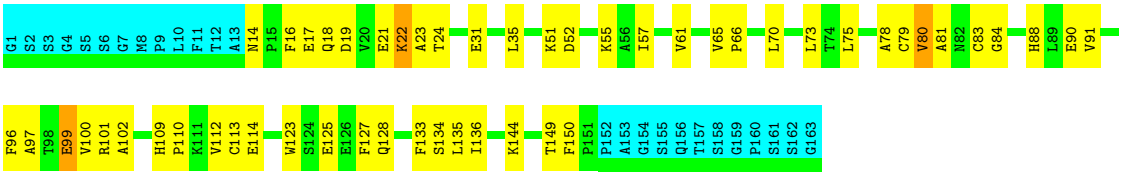
Chain A: 51% 31% • 15%



4.2.4 Score per residue for model 4

- Molecule 1: signal transducing adaptor molecule 2

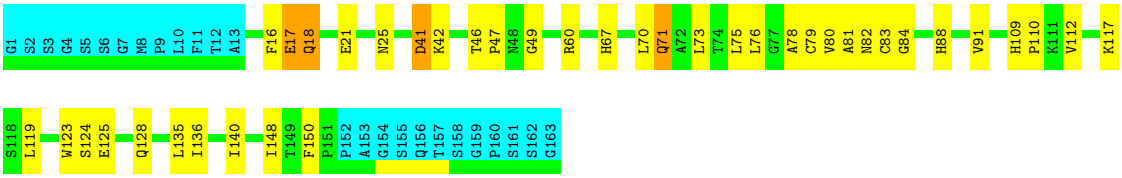
Chain A: 53% 30% • 15%



4.2.5 Score per residue for model 5

- Molecule 1: signal transducing adaptor molecule 2

Chain A: 60% 22% • 15%



4.2.6 Score per residue for model 6

- Molecule 1: signal transducing adaptor molecule 2

Chain A: 55% 28% •• 15%

G1 S2 S3 G4 S5 S6 G7 M8 P9 L10 F11 T12 A13 F16 E17 Q18 D19 A23 T24 N25 E26 Y27 L35 I36 M37 D38 D52 I57 V61 V65 P66 L70 L73 T74 L75 A78 C79 V80 A81 N82 C83 G84 F87 H88 L89 E90 E99

V103 N106 K107 A108 H109 P110 K111 V112 C113 E114 K115 L116 E122 E126 Q132 F133 S134 L135 A138 K141 S142 I148 P152 A153 G154 S155 Q156 T157 S158 G159 P160 S161 S162 G163

4.2.7 Score per residue for model 7

- Molecule 1: signal transducing adaptor molecule 2

Chain A: 55% 28% • 15%

G1 S2 S3 G4 S5 S6 G7 M8 P9 L10 F11 T12 A13 E17 Q18 K22 A23 N28 D32 L35 I36 M37 D38 T46 A50 L54 K55 A56 I57 V61 L73 T74 L75 A78 C79 N82 C83 G84 K85 I86 F87 H88 L89 E90 E99 V103

V112 C113 E114 K115 L116 K117 S118 L119 M120 V121 E125 E126 F127 Q128 K129 D130 F133 S134 L135 I136 I140 K144 T149 F150 P151 P152 A153 G154 S155 Q156 T157 S158 G159 P160 S161 S162 G163

4.2.8 Score per residue for model 8

- Molecule 1: signal transducing adaptor molecule 2

Chain A: 58% 26% • 15%

G1 S2 S3 G4 S5 S6 G7 M8 P9 L10 F11 T12 A13 N14 P15 F16 E17 Q18 A23 T24 N25 E26 Y27 D32 W33 S34 L35 I36 K42 D52 K55 K64 V68 L73 T74 L75 C79 V80 A81 H88 S93 R94 D95 F96 E99 V100 I104

K107 A108 H109 P110 K115 L116 L119 F127 D130 F133 S134 L135 I136 T149 F150 P151 P152 A153 G154 S155 Q156 T157 S158 G159 P160 S161 S162 G163

4.2.9 Score per residue for model 9

- Molecule 1: signal transducing adaptor molecule 2

Chain A: 60% 21% • 15%

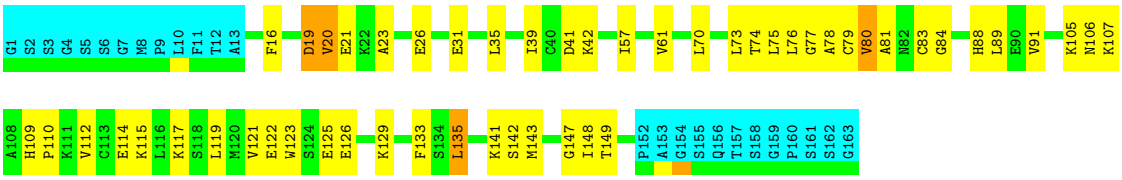
G1 S2 S3 G4 S5 S6 G7 M8 P9 L10 F11 T12 A13 E17 Q18 D19 V20 A23 T24 N25 E26 Y27 L35 I36 I39 N48 G49 A50 K51 D52 K55 R60 V65 P66 L70 Q71 A72 L73 T74 L75 C79 V80 A81 N82 C83 F87 E99

A102 N106 K107 A108 H109 P110 K111 V112 L119 E122 W123 E126 F127 Q128 K129 T149 F150 P151 P152 A153 G154 S155 Q156 T157 S158 G159 P160 S161 S162 G163

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: signal transducing adaptor molecule 2

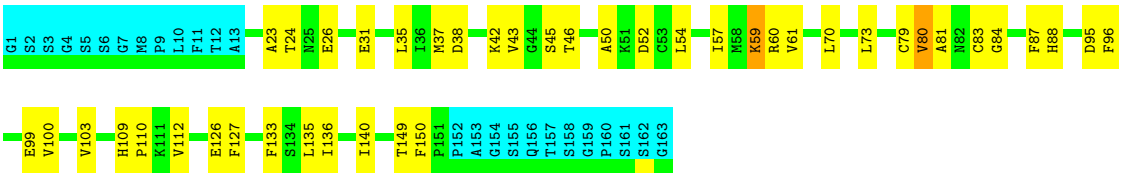
Chain A: 53% 29% • 15%



4.2.11 Score per residue for model 11

- Molecule 1: signal transducing adaptor molecule 2

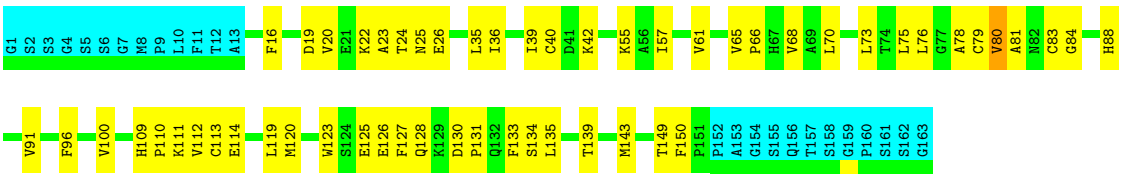
Chain A: 58% 25% • 15%



4.2.12 Score per residue for model 12

- Molecule 1: signal transducing adaptor molecule 2

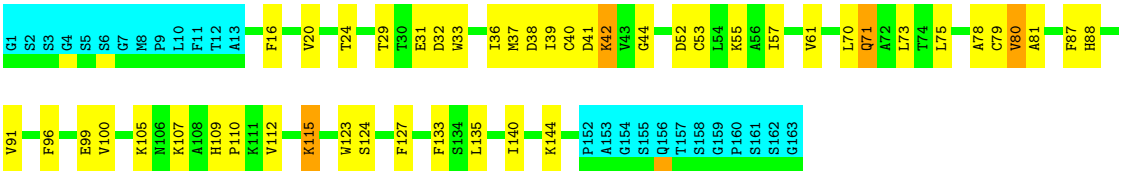
Chain A: 51% 33% • 15%



4.2.13 Score per residue for model 13

- Molecule 1: signal transducing adaptor molecule 2

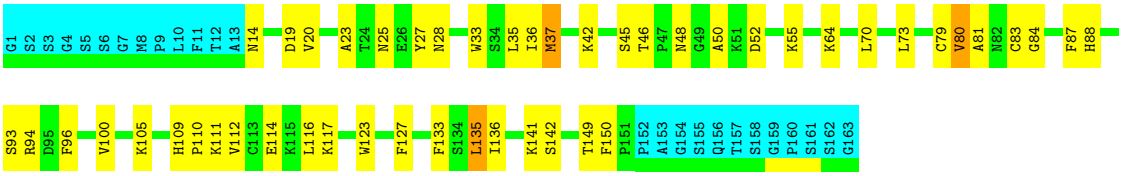
Chain A: 56% 26% • 15%



4.2.14 Score per residue for model 14

- Molecule 1: signal transducing adaptor molecule 2

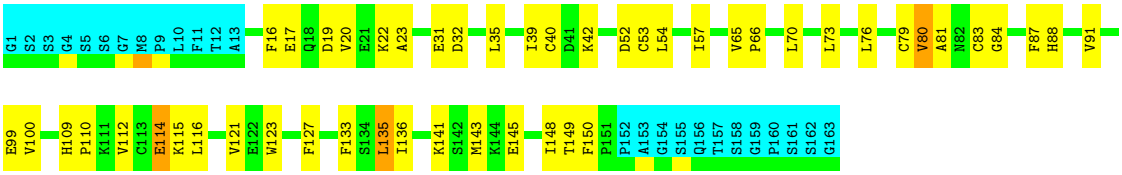
Chain A: 55% 28% • 15%



4.2.15 Score per residue for model 15

- Molecule 1: signal transducing adaptor molecule 2

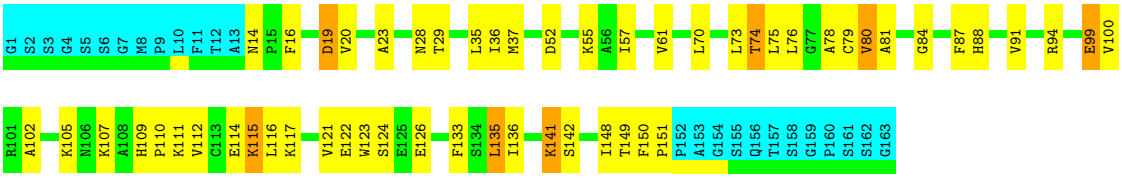
Chain A: 55% 28% • 15%



4.2.16 Score per residue for model 16

- Molecule 1: signal transducing adaptor molecule 2

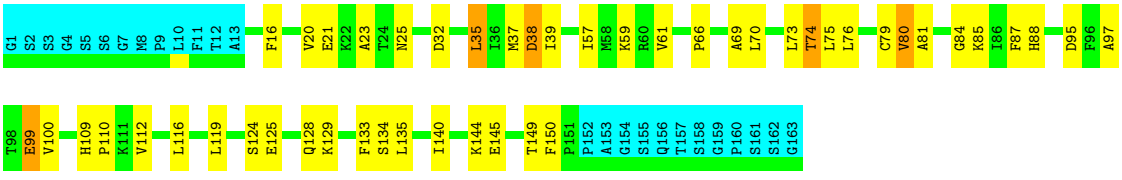
Chain A: 51% 29% • 15%



4.2.17 Score per residue for model 17

- Molecule 1: signal transducing adaptor molecule 2

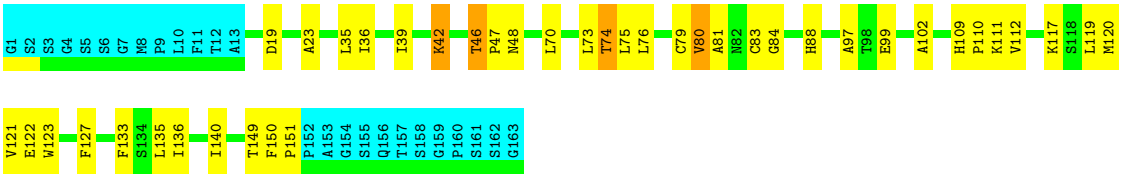
Chain A: 55% 26% • 15%



4.2.18 Score per residue for model 18

• Molecule 1: signal transducing adaptor molecule 2

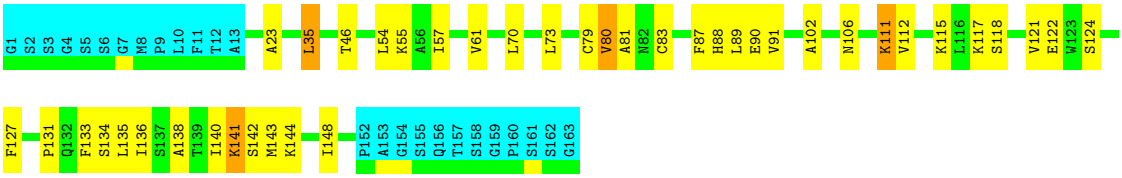
Chain A: 60% 23% • 15%



4.2.19 Score per residue for model 19

• Molecule 1: signal transducing adaptor molecule 2

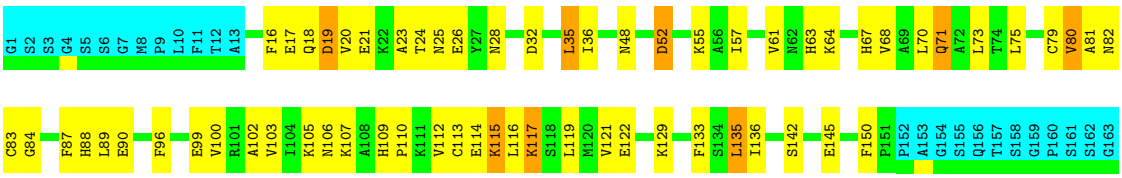
Chain A: 60% 23% • 15%



4.2.20 Score per residue for model 20

• Molecule 1: signal transducing adaptor molecule 2

Chain A: 46% 34% 5% 15%



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 least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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	1080	1094	1090	35±5
All	All	21600	21880	21800	703

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:HD11	1:A:112:VAL:HG13	1.06	1.26	5	19
1:A:23:ALA:HB2	1:A:35:LEU:HD23	0.95	1.33	7	8
1:A:23:ALA:HB2	1:A:35:LEU:HD12	0.92	1.38	3	4
1:A:54:LEU:HD22	1:A:90:GLU:CD	0.91	1.86	19	1
1:A:57:ILE:O	1:A:61:VAL:HG23	0.86	1.68	20	13
1:A:100:VAL:HG13	1:A:116:LEU:HD21	0.86	1.45	14	6
1:A:24:THR:O	1:A:68:VAL:HG13	0.81	1.74	1	3
1:A:127:PHE:CD2	1:A:133:PHE:CE1	0.79	2.70	1	1
1:A:99:GLU:O	1:A:103:VAL:HG23	0.79	1.78	20	4
1:A:135:LEU:HD23	1:A:136:ILE:N	0.77	1.93	15	10
1:A:97:ALA:HB2	1:A:135:LEU:HD21	0.76	1.58	17	3
1:A:36:ILE:HG23	1:A:75:LEU:CD1	0.74	2.13	16	9
1:A:70:LEU:HA	1:A:73:LEU:HD12	0.73	1.59	12	14
1:A:88:HIS:CE1	1:A:127:PHE:CZ	0.72	2.78	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:LEU:O	1:A:35:LEU:HD23	0.72	1.85	10	1
1:A:16:PHE:O	1:A:20:VAL:HG23	0.71	1.84	13	6
1:A:117:LYS:O	1:A:121:VAL:HG23	0.71	1.85	10	3
1:A:36:ILE:HG23	1:A:75:LEU:HD13	0.71	1.61	16	4
1:A:70:LEU:HD21	1:A:111:LYS:HG2	0.71	1.62	12	2
1:A:135:LEU:C	1:A:135:LEU:HD23	0.70	2.07	14	10
1:A:73:LEU:CD1	1:A:112:VAL:HG13	0.69	2.13	12	5
1:A:96:PHE:O	1:A:100:VAL:HG23	0.67	1.90	14	3
1:A:91:VAL:CG1	1:A:123:TRP:CZ3	0.66	2.78	4	7
1:A:136:ILE:HG22	1:A:140:ILE:HD11	0.66	1.67	18	2
1:A:23:ALA:HB2	1:A:35:LEU:HD22	0.66	1.66	9	4
1:A:135:LEU:HD23	1:A:135:LEU:C	0.66	2.09	15	7
1:A:23:ALA:CB	1:A:35:LEU:HD23	0.65	2.21	8	5
1:A:96:PHE:CE2	1:A:100:VAL:HG21	0.64	2.28	2	5
1:A:31:GLU:OE2	1:A:74:THR:HG21	0.63	1.92	10	1
1:A:136:ILE:HG22	1:A:140:ILE:CD1	0.63	2.23	18	1
1:A:91:VAL:HG11	1:A:123:TRP:CZ3	0.62	2.29	4	2
1:A:70:LEU:HG	1:A:112:VAL:HG22	0.61	1.71	4	4
1:A:80:VAL:HG13	1:A:88:HIS:CD2	0.61	2.30	16	7
1:A:73:LEU:HD11	1:A:112:VAL:CG1	0.60	2.17	11	10
1:A:84:GLY:O	1:A:88:HIS:CD2	0.60	2.55	6	16
1:A:149:THR:O	1:A:150:PHE:CD2	0.60	2.55	16	1
1:A:149:THR:O	1:A:150:PHE:CD1	0.60	2.55	3	11
1:A:25:ASN:OD1	1:A:27:TYR:CD2	0.60	2.55	8	1
1:A:88:HIS:CE1	1:A:127:PHE:CE1	0.59	2.91	18	5
1:A:54:LEU:HD22	1:A:90:GLU:OE2	0.59	1.98	19	1
1:A:126:GLU:OE1	1:A:127:PHE:CE2	0.59	2.56	12	2
1:A:33:TRP:HA	1:A:36:ILE:HD12	0.59	1.74	14	3
1:A:148:ILE:H	1:A:148:ILE:HD12	0.58	1.57	6	1
1:A:100:VAL:HG11	1:A:120:MET:SD	0.58	2.37	12	1
1:A:88:HIS:CE1	1:A:127:PHE:CE2	0.58	2.92	15	1
1:A:140:ILE:HG22	1:A:144:LYS:HD2	0.57	1.73	7	3
1:A:121:VAL:HG21	1:A:151:PRO:O	0.57	1.99	18	1
1:A:70:LEU:HD11	1:A:111:LYS:HG2	0.57	1.77	19	2
1:A:80:VAL:HG22	1:A:87:PHE:CE1	0.57	2.34	16	5
1:A:132:GLN:OE1	1:A:133:PHE:CD2	0.57	2.58	1	1
1:A:74:THR:CG2	1:A:75:LEU:N	0.57	2.67	16	3
1:A:19:ASP:HB3	1:A:39:ILE:HD11	0.56	1.77	2	2
1:A:57:ILE:HG12	1:A:75:LEU:HD23	0.55	1.77	6	1
1:A:23:ALA:CA	1:A:35:LEU:HD23	0.55	2.31	8	4
1:A:36:ILE:HG23	1:A:75:LEU:HD12	0.55	1.79	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:HD11	1:A:111:LYS:HD2	0.54	1.79	9	1
1:A:119:LEU:O	1:A:123:TRP:CD2	0.54	2.60	18	2
1:A:90:GLU:CD	1:A:90:GLU:N	0.54	2.60	6	1
1:A:80:VAL:HG21	1:A:123:TRP:CZ2	0.54	2.37	1	3
1:A:76:LEU:HD23	1:A:119:LEU:HD13	0.54	1.78	2	5
1:A:141:LYS:CG	1:A:142:SER:N	0.53	2.71	10	5
1:A:115:LYS:HD2	1:A:119:LEU:HD11	0.53	1.80	7	1
1:A:124:SER:OG	1:A:140:ILE:HD12	0.53	2.04	17	1
1:A:100:VAL:CG1	1:A:116:LEU:HD21	0.52	2.28	14	2
1:A:23:ALA:HA	1:A:35:LEU:HD23	0.52	1.81	6	2
1:A:35:LEU:CD1	1:A:39:ILE:HD11	0.52	2.34	3	1
1:A:73:LEU:HD13	1:A:115:LYS:CG	0.51	2.34	7	2
1:A:132:GLN:OE1	1:A:133:PHE:N	0.51	2.44	1	1
1:A:65:VAL:HG13	1:A:66:PRO:HD2	0.50	1.82	2	8
1:A:14:ASN:ND2	1:A:52:ASP:OD1	0.50	2.44	8	3
1:A:113:CYS:SG	1:A:114:GLU:N	0.50	2.85	7	3
1:A:50:ALA:HB1	1:A:87:PHE:HA	0.50	1.82	14	4
1:A:94:ARG:CZ	1:A:135:LEU:HD12	0.50	2.36	16	2
1:A:117:LYS:HB2	1:A:150:PHE:CD2	0.50	2.41	18	2
1:A:79:CYS:O	1:A:83:CYS:N	0.50	2.45	7	15
1:A:113:CYS:O	1:A:116:LEU:N	0.50	2.45	20	2
1:A:82:ASN:OD1	1:A:83:CYS:N	0.50	2.45	7	1
1:A:79:CYS:O	1:A:81:ALA:N	0.50	2.45	2	19
1:A:28:ASN:ND2	1:A:32:ASP:OD1	0.50	2.45	20	1
1:A:125:GLU:O	1:A:128:GLN:CG	0.50	2.60	17	1
1:A:127:PHE:CD2	1:A:133:PHE:CZ	0.50	2.99	1	1
1:A:125:GLU:OE1	1:A:128:GLN:NE2	0.50	2.45	5	2
1:A:41:ASP:O	1:A:44:GLY:N	0.49	2.45	13	1
1:A:125:GLU:O	1:A:128:GLN:NE2	0.49	2.45	12	1
1:A:75:LEU:O	1:A:78:ALA:HB3	0.49	2.07	4	7
1:A:148:ILE:HD12	1:A:148:ILE:N	0.49	2.22	5	1
1:A:25:ASN:OD1	1:A:27:TYR:CE2	0.49	2.66	8	1
1:A:35:LEU:HD23	1:A:35:LEU:C	0.49	2.26	10	1
1:A:19:ASP:O	1:A:22:LYS:N	0.49	2.45	15	2
1:A:136:ILE:CG2	1:A:140:ILE:HD11	0.49	2.37	18	1
1:A:41:ASP:OD1	1:A:42:LYS:N	0.49	2.45	13	2
1:A:102:ALA:O	1:A:106:ASN:ND2	0.49	2.45	19	1
1:A:54:LEU:O	1:A:57:ILE:N	0.49	2.45	19	3
1:A:143:MET:O	1:A:148:ILE:HD13	0.49	2.08	15	4
1:A:100:VAL:HG13	1:A:116:LEU:CD2	0.49	2.38	17	1
1:A:80:VAL:HG11	1:A:123:TRP:CE2	0.49	2.42	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:VAL:HG11	1:A:123:TRP:CZ2	0.48	2.43	10	1
1:A:100:VAL:HG13	1:A:116:LEU:HD11	0.48	1.85	2	1
1:A:138:ALA:O	1:A:140:ILE:N	0.48	2.46	2	2
1:A:39:ILE:O	1:A:42:LYS:CG	0.48	2.61	18	1
1:A:57:ILE:HG21	1:A:76:LEU:HB2	0.48	1.84	10	2
1:A:77:GLY:HA3	1:A:119:LEU:HD21	0.48	1.84	10	1
1:A:121:VAL:HG21	1:A:151:PRO:HG2	0.48	1.86	16	1
1:A:80:VAL:HG13	1:A:88:HIS:NE2	0.48	2.23	19	1
1:A:90:GLU:OE1	1:A:90:GLU:C	0.47	2.53	19	1
1:A:21:GLU:O	1:A:25:ASN:N	0.47	2.47	17	3
1:A:117:LYS:HG3	1:A:150:PHE:CE2	0.47	2.43	2	1
1:A:109:HIS:CE1	1:A:111:LYS:HB3	0.47	2.44	16	3
1:A:67:HIS:O	1:A:71:GLN:NE2	0.47	2.47	20	1
1:A:95:ASP:CG	1:A:96:PHE:N	0.47	2.67	3	1
1:A:121:VAL:O	1:A:124:SER:N	0.47	2.48	19	2
1:A:106:ASN:O	1:A:107:LYS:C	0.47	2.52	9	6
1:A:135:LEU:O	1:A:138:ALA:N	0.47	2.47	19	1
1:A:109:HIS:CD2	1:A:110:PRO:HD2	0.47	2.45	1	7
1:A:40:CYS:SG	1:A:41:ASP:N	0.47	2.88	3	2
1:A:88:HIS:HB3	1:A:133:PHE:CE1	0.47	2.44	4	12
1:A:78:ALA:O	1:A:82:ASN:ND2	0.47	2.47	7	1
1:A:100:VAL:CG1	1:A:120:MET:SD	0.47	3.02	12	1
1:A:125:GLU:CG	1:A:126:GLU:N	0.47	2.78	10	2
1:A:88:HIS:HB3	1:A:133:PHE:CZ	0.47	2.45	18	3
1:A:96:PHE:CE2	1:A:100:VAL:CG2	0.47	2.98	2	2
1:A:122:GLU:O	1:A:126:GLU:CB	0.47	2.62	16	3
1:A:140:ILE:O	1:A:144:LYS:CD	0.47	2.63	19	1
1:A:35:LEU:CD2	1:A:39:ILE:HD11	0.47	2.40	9	1
1:A:135:LEU:C	1:A:135:LEU:CD2	0.47	2.81	15	2
1:A:122:GLU:HG3	1:A:123:TRP:CD1	0.46	2.45	10	2
1:A:96:PHE:CZ	1:A:100:VAL:CG2	0.46	2.98	2	1
1:A:133:PHE:O	1:A:135:LEU:N	0.46	2.49	17	4
1:A:60:ARG:HB3	1:A:72:ALA:HB2	0.46	1.86	9	1
1:A:39:ILE:O	1:A:42:LYS:N	0.46	2.48	2	3
1:A:144:LYS:HE3	1:A:150:PHE:CD1	0.46	2.46	2	1
1:A:73:LEU:HD13	1:A:115:LYS:HG2	0.46	1.87	7	1
1:A:88:HIS:HB3	1:A:133:PHE:CE2	0.46	2.46	1	2
1:A:125:GLU:CD	1:A:126:GLU:N	0.46	2.69	3	1
1:A:88:HIS:O	1:A:90:GLU:N	0.46	2.49	7	3
1:A:138:ALA:O	1:A:141:LYS:N	0.46	2.49	2	2
1:A:70:LEU:HD21	1:A:111:LYS:HG3	0.46	1.88	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ASN:OD1	1:A:27:TYR:CD1	0.46	2.69	9	3
1:A:37:MET:SD	1:A:37:MET:N	0.46	2.89	14	1
1:A:135:LEU:CD2	1:A:136:ILE:N	0.46	2.74	15	2
1:A:48:ASN:O	1:A:52:ASP:CG	0.46	2.55	20	1
1:A:38:ASP:C	1:A:41:ASP:OD2	0.45	2.55	13	1
1:A:51:LYS:CE	1:A:90:GLU:OE1	0.45	2.64	4	1
1:A:88:HIS:O	1:A:91:VAL:N	0.45	2.50	5	1
1:A:80:VAL:CG2	1:A:87:PHE:CE1	0.45	2.99	6	1
1:A:80:VAL:HG22	1:A:87:PHE:CD1	0.45	2.47	16	1
1:A:143:MET:O	1:A:148:ILE:CD1	0.45	2.64	15	3
1:A:124:SER:OG	1:A:140:ILE:CD1	0.45	2.65	5	3
1:A:25:ASN:CG	1:A:27:TYR:CD2	0.45	2.90	8	1
1:A:87:PHE:C	1:A:87:PHE:CD1	0.45	2.90	19	2
1:A:73:LEU:O	1:A:119:LEU:HD11	0.45	2.12	9	2
1:A:37:MET:O	1:A:38:ASP:C	0.45	2.55	17	5
1:A:73:LEU:CB	1:A:115:LYS:HG2	0.45	2.42	7	2
1:A:149:THR:C	1:A:150:PHE:CD1	0.45	2.91	14	1
1:A:116:LEU:O	1:A:117:LYS:C	0.44	2.55	2	2
1:A:124:SER:OG	1:A:140:ILE:HD13	0.44	2.11	5	1
1:A:126:GLU:CD	1:A:127:PHE:CE2	0.44	2.91	7	1
1:A:23:ALA:N	1:A:35:LEU:HD23	0.44	2.26	8	1
1:A:127:PHE:CB	1:A:133:PHE:CG	0.44	3.00	15	1
1:A:19:ASP:OD2	1:A:42:LYS:NZ	0.44	2.50	1	1
1:A:67:HIS:O	1:A:71:GLN:CD	0.44	2.55	5	1
1:A:73:LEU:HB3	1:A:115:LYS:CG	0.44	2.43	13	2
1:A:125:GLU:O	1:A:128:GLN:CD	0.44	2.56	12	1
1:A:113:CYS:O	1:A:114:GLU:C	0.44	2.55	6	1
1:A:17:GLU:O	1:A:18:GLN:C	0.44	2.55	8	2
1:A:48:ASN:OD1	1:A:48:ASN:C	0.44	2.55	14	1
1:A:109:HIS:CG	1:A:110:PRO:HD2	0.44	2.48	4	15
1:A:141:LYS:HG3	1:A:142:SER:N	0.44	2.26	10	1
1:A:122:GLU:O	1:A:126:GLU:CG	0.44	2.66	9	1
1:A:79:CYS:C	1:A:81:ALA:N	0.44	2.71	19	16
1:A:46:THR:HG23	1:A:47:PRO:HD2	0.44	1.88	5	1
1:A:24:THR:O	1:A:25:ASN:C	0.44	2.55	12	1
1:A:24:THR:HG22	1:A:71:GLN:HB3	0.44	1.89	13	1
1:A:18:GLN:O	1:A:22:LYS:CD	0.44	2.66	4	1
1:A:93:SER:O	1:A:94:ARG:C	0.44	2.55	14	2
1:A:99:GLU:O	1:A:103:VAL:CG2	0.44	2.61	20	1
1:A:39:ILE:O	1:A:40:CYS:C	0.44	2.56	12	4
1:A:127:PHE:HB2	1:A:133:PHE:CG	0.44	2.47	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:GLU:CG	1:A:123:TRP:N	0.44	2.81	18	1
1:A:119:LEU:O	1:A:122:GLU:CG	0.44	2.66	20	1
1:A:126:GLU:OE2	1:A:127:PHE:CZ	0.44	2.71	7	1
1:A:122:GLU:HG3	1:A:123:TRP:N	0.44	2.28	18	2
1:A:126:GLU:OE1	1:A:127:PHE:CZ	0.43	2.71	12	1
1:A:43:VAL:HG11	1:A:83:CYS:SG	0.43	2.53	11	1
1:A:144:LYS:HE2	1:A:150:PHE:CD1	0.43	2.47	4	1
1:A:41:ASP:O	1:A:42:LYS:C	0.43	2.57	5	3
1:A:46:THR:HG22	1:A:49:GLY:N	0.43	2.27	5	1
1:A:35:LEU:C	1:A:35:LEU:CD2	0.43	2.86	10	1
1:A:16:PHE:O	1:A:19:ASP:CG	0.43	2.56	16	1
1:A:114:GLU:OE2	1:A:115:LYS:N	0.43	2.51	15	1
1:A:121:VAL:O	1:A:122:GLU:C	0.43	2.57	19	3
1:A:96:PHE:O	1:A:99:GLU:N	0.43	2.52	4	1
1:A:90:GLU:CD	1:A:91:VAL:N	0.43	2.72	19	1
1:A:125:GLU:HG3	1:A:126:GLU:N	0.43	2.29	10	1
1:A:123:TRP:O	1:A:124:SER:C	0.43	2.55	1	2
1:A:42:LYS:O	1:A:45:SER:N	0.43	2.51	3	3
1:A:80:VAL:O	1:A:88:HIS:NE2	0.43	2.51	14	2
1:A:14:ASN:ND2	1:A:52:ASP:CG	0.43	2.72	16	1
1:A:37:MET:O	1:A:39:ILE:N	0.43	2.51	17	3
1:A:109:HIS:CE1	1:A:111:LYS:CB	0.43	3.01	9	1
1:A:148:ILE:HG22	1:A:150:PHE:CE2	0.43	2.49	16	1
1:A:76:LEU:O	1:A:80:VAL:HG23	0.43	2.14	2	2
1:A:118:SER:OG	1:A:119:LEU:N	0.43	2.52	3	1
1:A:14:ASN:ND2	1:A:52:ASP:O	0.43	2.52	4	1
1:A:127:PHE:HB3	1:A:133:PHE:CG	0.43	2.48	11	2
1:A:128:GLN:O	1:A:129:LYS:C	0.43	2.57	9	1
1:A:123:TRP:O	1:A:127:PHE:N	0.43	2.52	14	1
1:A:117:LYS:HG2	1:A:150:PHE:CE1	0.43	2.49	16	1
1:A:87:PHE:CE1	1:A:91:VAL:CG2	0.42	3.02	13	1
1:A:21:GLU:O	1:A:24:THR:N	0.42	2.52	4	1
1:A:18:GLN:CD	1:A:18:GLN:C	0.42	2.77	5	1
1:A:126:GLU:HG3	1:A:127:PHE:N	0.42	2.29	11	2
1:A:16:PHE:CD1	1:A:53:CYS:SG	0.42	3.10	2	1
1:A:117:LYS:O	1:A:120:MET:N	0.42	2.53	18	2
1:A:125:GLU:CD	1:A:128:GLN:NE2	0.42	2.72	5	1
1:A:60:ARG:CB	1:A:72:ALA:HB2	0.42	2.44	9	1
1:A:91:VAL:HG11	1:A:123:TRP:CE3	0.42	2.49	4	2
1:A:28:ASN:O	1:A:29:THR:C	0.42	2.58	16	1
1:A:138:ALA:C	1:A:140:ILE:N	0.42	2.71	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ALA:O	1:A:106:ASN:CG	0.42	2.58	9	2
1:A:26:GLU:HB3	1:A:68:VAL:HG23	0.42	1.92	12	1
1:A:19:ASP:OD2	1:A:35:LEU:HD11	0.42	2.15	18	1
1:A:52:ASP:O	1:A:53:CYS:C	0.42	2.58	2	2
1:A:70:LEU:HD21	1:A:111:LYS:CG	0.42	2.41	12	1
1:A:132:GLN:OE1	1:A:133:PHE:CG	0.42	2.71	1	1
1:A:88:HIS:C	1:A:90:GLU:N	0.42	2.73	7	2
1:A:114:GLU:HG3	1:A:115:LYS:N	0.42	2.30	20	3
1:A:117:LYS:HB2	1:A:150:PHE:CD1	0.42	2.48	20	1
1:A:85:LYS:HA	1:A:88:HIS:CG	0.42	2.50	3	3
1:A:63:HIS:O	1:A:64:LYS:C	0.42	2.58	20	1
1:A:73:LEU:HD13	1:A:115:LYS:HB3	0.42	1.91	1	1
1:A:133:PHE:O	1:A:134:SER:C	0.42	2.58	4	1
1:A:20:VAL:O	1:A:23:ALA:N	0.42	2.52	10	1
1:A:16:PHE:O	1:A:19:ASP:N	0.41	2.52	20	1
1:A:79:CYS:O	1:A:80:VAL:C	0.41	2.59	16	7
1:A:16:PHE:O	1:A:18:GLN:N	0.41	2.52	5	1
1:A:99:GLU:O	1:A:102:ALA:HB3	0.41	2.15	16	2
1:A:18:GLN:HG3	1:A:19:ASP:N	0.41	2.30	6	2
1:A:24:THR:OG1	1:A:60:ARG:NE	0.41	2.53	11	1
1:A:127:PHE:HB2	1:A:133:PHE:CD2	0.41	2.49	13	1
1:A:19:ASP:O	1:A:20:VAL:C	0.41	2.59	10	7
1:A:104:ILE:O	1:A:107:LYS:N	0.41	2.53	8	1
1:A:70:LEU:O	1:A:73:LEU:N	0.41	2.53	10	1
1:A:131:PRO:O	1:A:134:SER:CB	0.41	2.69	12	2
1:A:125:GLU:CD	1:A:125:GLU:C	0.41	2.79	7	1
1:A:95:ASP:O	1:A:99:GLU:CD	0.41	2.59	17	1
1:A:35:LEU:HD13	1:A:35:LEU:O	0.41	2.16	3	1
1:A:16:PHE:O	1:A:17:GLU:C	0.41	2.59	4	5
1:A:16:PHE:CD2	1:A:53:CYS:SG	0.41	3.14	13	1
1:A:37:MET:C	1:A:39:ILE:N	0.41	2.73	13	1
1:A:42:LYS:O	1:A:43:VAL:C	0.41	2.58	3	1
1:A:101:ARG:HG3	1:A:102:ALA:N	0.41	2.31	4	1
1:A:54:LEU:O	1:A:56:ALA:N	0.41	2.54	7	1
1:A:23:ALA:N	1:A:35:LEU:CD2	0.41	2.84	8	1
1:A:117:LYS:HB3	1:A:150:PHE:CD2	0.41	2.51	14	1
1:A:90:GLU:OE1	1:A:91:VAL:N	0.41	2.54	19	1
1:A:117:LYS:O	1:A:118:SER:C	0.41	2.59	2	2
1:A:51:LYS:CD	1:A:90:GLU:CD	0.41	2.89	3	1
1:A:96:PHE:O	1:A:97:ALA:C	0.41	2.60	4	1
1:A:21:GLU:OE2	1:A:60:ARG:NH2	0.41	2.54	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:LEU:CD2	1:A:39:ILE:CD1	0.41	2.99	10	1
1:A:59:LYS:HG3	1:A:60:ARG:N	0.41	2.29	11	1
1:A:127:PHE:CD1	1:A:133:PHE:CE2	0.41	3.09	15	1
1:A:142:SER:O	1:A:145:GLU:CG	0.41	2.69	20	1
1:A:132:GLN:HG3	1:A:133:PHE:N	0.41	2.30	6	1
1:A:28:ASN:ND2	1:A:32:ASP:OD2	0.41	2.54	7	1
1:A:82:ASN:O	1:A:83:CYS:C	0.40	2.60	6	2
1:A:139:THR:O	1:A:143:MET:SD	0.40	2.80	12	1
1:A:66:PRO:O	1:A:69:ALA:N	0.40	2.54	17	1
1:A:88:HIS:O	1:A:89:LEU:C	0.40	2.60	10	3
1:A:16:PHE:CE1	1:A:42:LYS:HB3	0.40	2.52	8	1
1:A:54:LEU:HA	1:A:57:ILE:HD12	0.40	1.94	15	1
1:A:97:ALA:HB1	1:A:139:THR:HG21	0.40	1.94	3	1
1:A:129:LYS:O	1:A:130:ASP:C	0.40	2.60	7	1
1:A:111:LYS:O	1:A:114:GLU:OE2	0.40	2.40	14	1
1:A:19:ASP:OD1	1:A:19:ASP:N	0.40	2.55	15	1
1:A:135:LEU:HD23	1:A:136:ILE:CA	0.40	2.45	15	1
1:A:46:THR:HG22	1:A:47:PRO:HD2	0.40	1.93	18	1
1:A:87:PHE:CD1	1:A:87:PHE:C	0.40	2.95	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	138/163 (85%)	112±4 (81±3%)	24±4 (18±3%)	2±1 (1±0%)	16	63
All	All	2760/3260 (85%)	2234 (81%)	490 (18%)	36 (1%)	16	63

All 13 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	80	VAL	19
1	A	89	LEU	3
1	A	139	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	20	VAL	2
1	A	31	GLU	2
1	A	117	LYS	1
1	A	17	GLU	1
1	A	107	LYS	1
1	A	64	LYS	1
1	A	147	GLY	1
1	A	28	ASN	1
1	A	38	ASP	1
1	A	134	SER	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	122/139 (88%)	116±2 (95±2%)	6±2 (5±2%)	27 76
All	All	2440/2780 (88%)	2314 (95%)	126 (5%)	27 76

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	55	LYS	11
1	A	99	GLU	11
1	A	46	THR	6
1	A	115	LYS	6
1	A	71	GLN	5
1	A	19	ASP	5
1	A	52	ASP	5
1	A	107	LYS	5
1	A	105	LYS	5
1	A	135	LEU	5
1	A	48	ASN	4
1	A	141	LYS	4
1	A	26	GLU	4
1	A	32	ASP	4
1	A	129	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	59	LYS	3
1	A	74	THR	3
1	A	35	LEU	3
1	A	117	LYS	2
1	A	82	ASN	2
1	A	95	ASP	2
1	A	22	LYS	2
1	A	31	GLU	2
1	A	17	GLU	2
1	A	130	ASP	2
1	A	111	LYS	2
1	A	42	LYS	2
1	A	37	MET	2
1	A	145	GLU	2
1	A	132	GLN	1
1	A	58	MET	1
1	A	18	GLN	1
1	A	41	ASP	1
1	A	38	ASP	1
1	A	60	ARG	1
1	A	21	GLU	1
1	A	149	THR	1
1	A	29	THR	1
1	A	64	LYS	1
1	A	114	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