



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:09 PM BST

PDB ID : 1CMZ
Title : SOLUTION STRUCTURE OF GAIP (GALPHA INTERACTING PROTEIN): A REGULATOR OF G PROTEIN SIGNALING
Authors : De Alba, E.; De Vries, L.; Farquhar, M.G.; Tjandra, N.
Deposited on : 1999-05-12

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
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

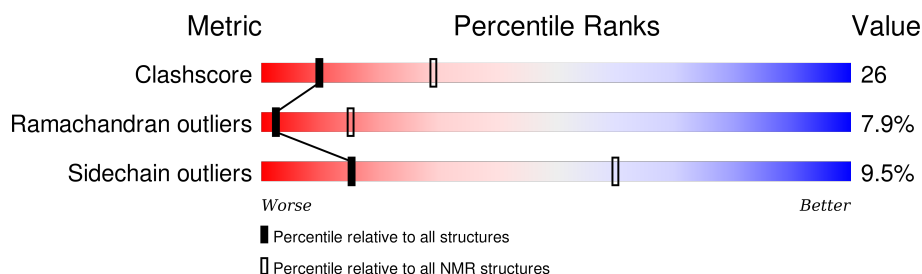
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	152	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models).

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:79-A:148, A:156-A:206 (121)	0.36	11

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 5 single-model clusters were found.

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

3 Entry composition

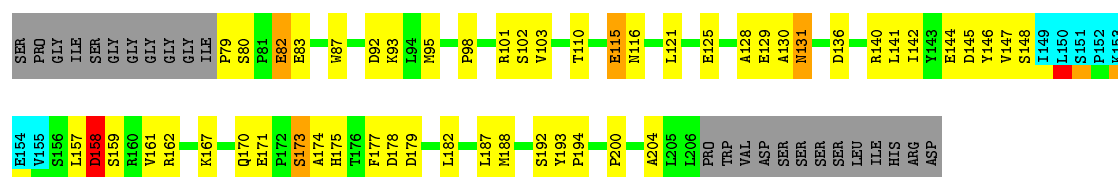
There is only 1 type of molecule in this entry. The entry contains 2069 atoms, of which 1017 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN).

Mol	Chain	Residues	Atoms						Trace
1	A	128	Total	C	H	N	O	S	0
			2069	666	1017	180	201	5	

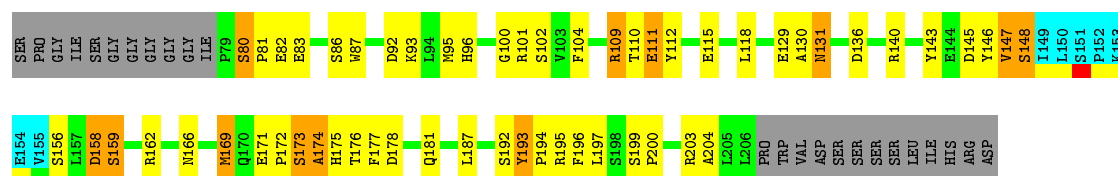
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	GLN	SEE REMARK 999	UNP P49795
A	69	PRO	PRO	SEE REMARK 999	UNP P49795
A	70	GLY	LEU	SEE REMARK 999	UNP P49795
A	71	ILE	PRO	SEE REMARK 999	UNP P49795
A	72	SER	SER	SEE REMARK 999	UNP P49795
A	73	GLY	CYS	SEE REMARK 999	UNP P49795
A	74	GLY	GLU	SEE REMARK 999	UNP P49795
A	75	GLY	VAL	SEE REMARK 999	UNP P49795
A	76	GLY	CYS	SEE REMARK 999	UNP P49795
A	77	GLY	ALA	SEE REMARK 999	UNP P49795
A	78	ILE	THR	SEE REMARK 999	UNP P49795
A	207	PRO	LEU	SEE REMARK 999	UNP P49795
A	208	TRP	GLN	SEE REMARK 999	UNP P49795
A	209	VAL	GLY	SEE REMARK 999	UNP P49795
A	210	ASP	PRO	SEE REMARK 999	UNP P49795
A	212	SER	GLN	SEE REMARK 999	UNP P49795
A	215	LEU	SER	SEE REMARK 999	UNP P49795
A	216	ILE	GLU	SEE REMARK 999	UNP P49795
A	217	HIS	ALA	SEE REMARK 999	UNP P49795
A	218	ARG	-	SEE REMARK 999	UNP P49795
A	219	ASP	-	SEE REMARK 999	UNP P49795



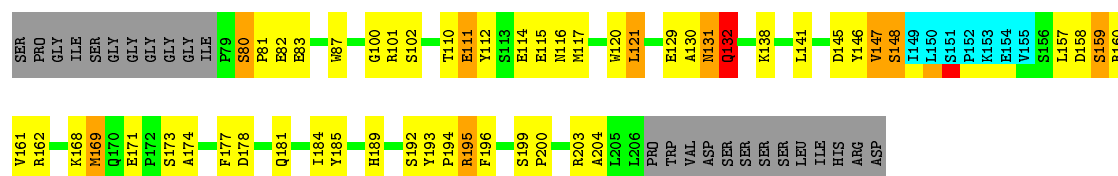
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



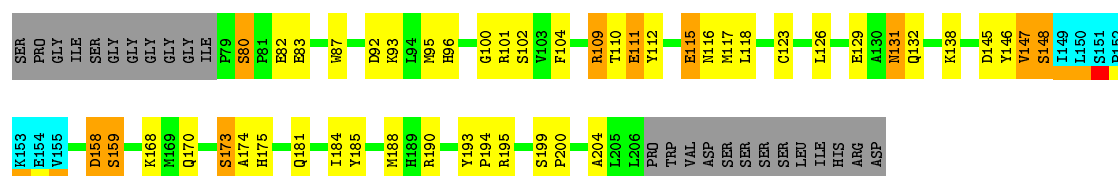
4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



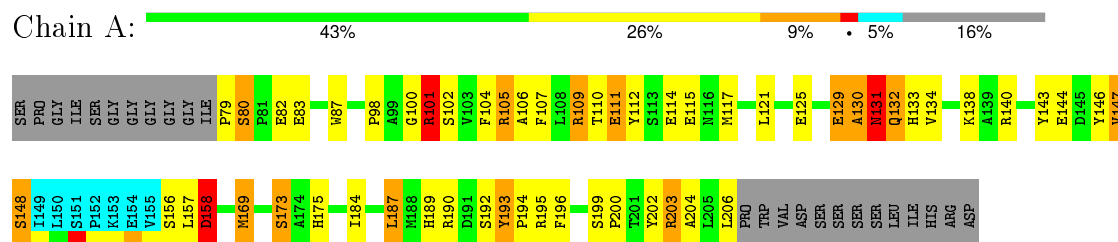
4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



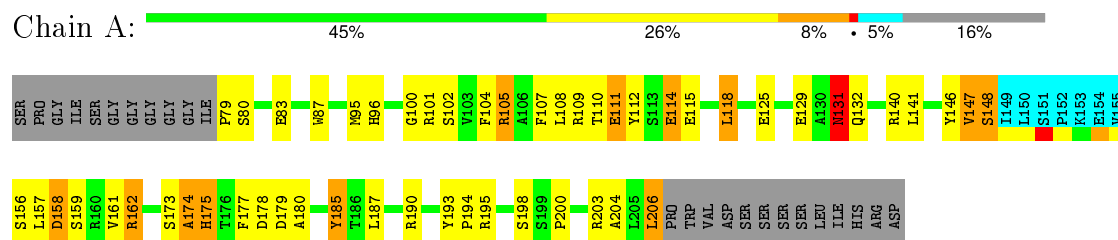
4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



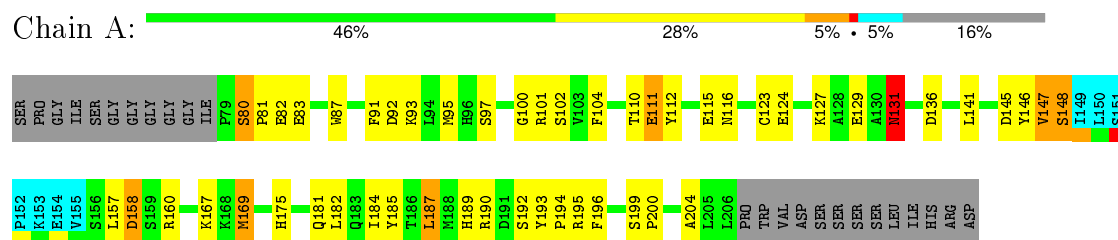
4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



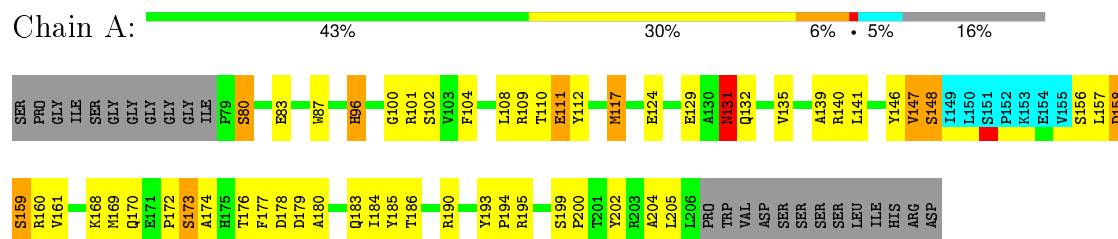
4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



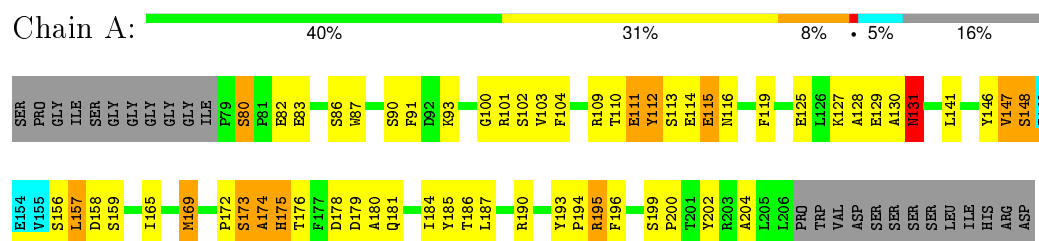
4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



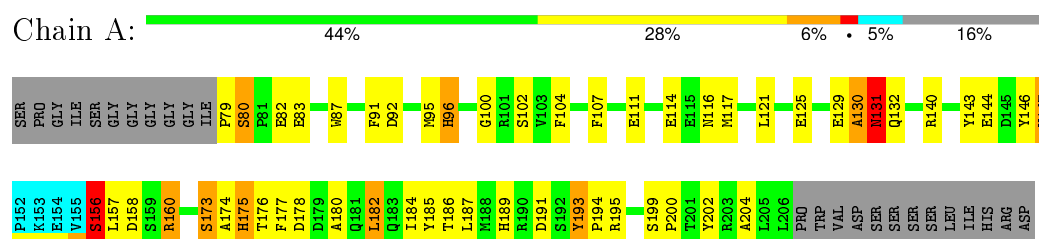
4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



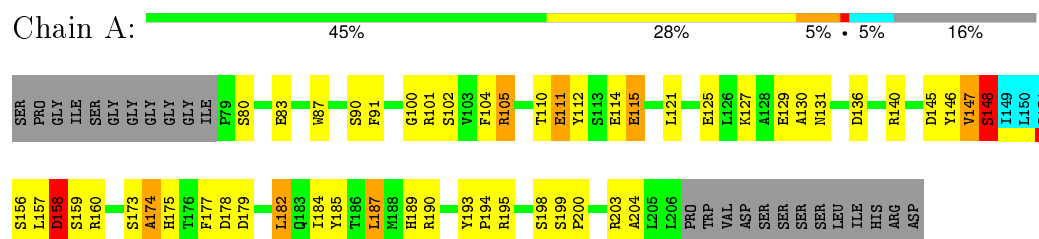
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



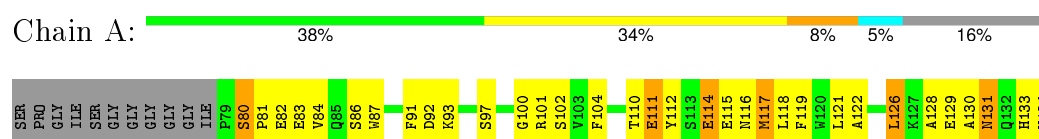
4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



4.2.13 Score per residue for model 13

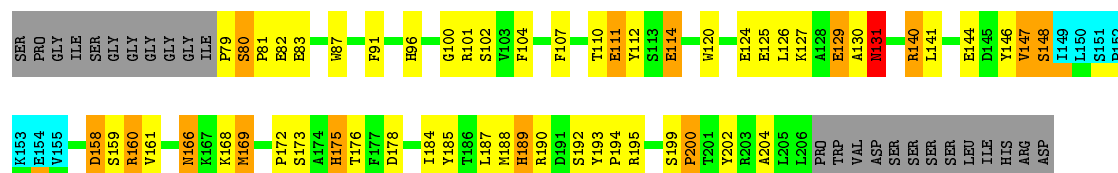
- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)





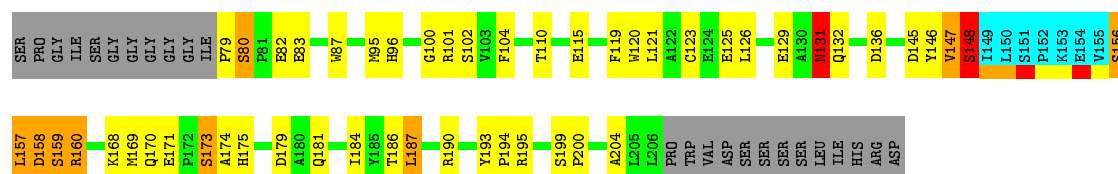
4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



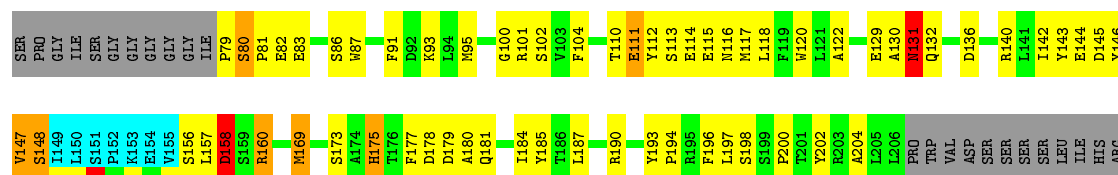
4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



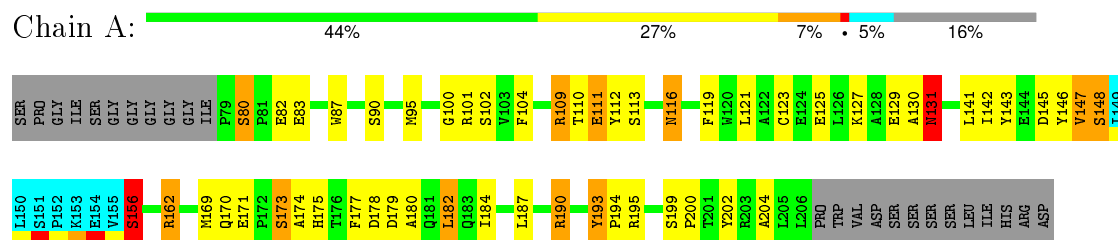
4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



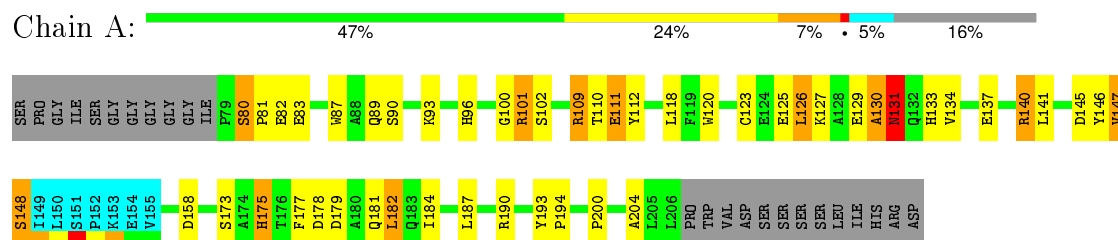
4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



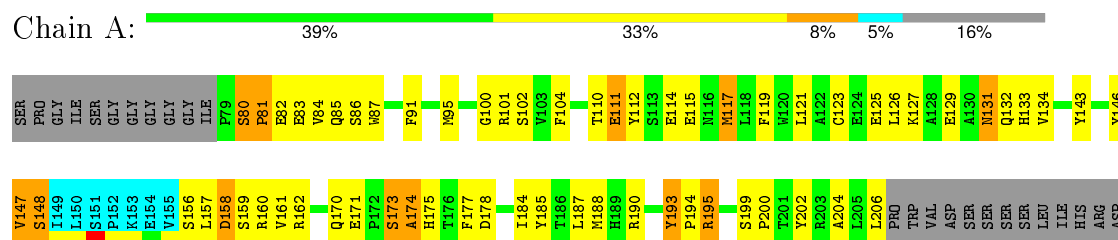
4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



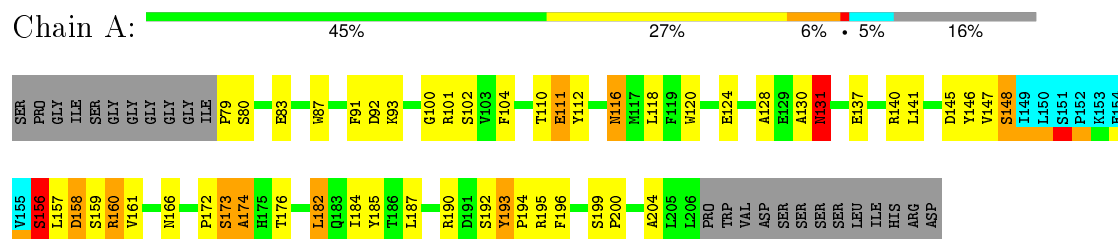
4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING*.

Of the 167 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
NMRPIPE	structure solution	
PIPP	structure solution	
X-PLOR	structure solution	

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)	BMRB entry 4407
Number of chemical shift lists	1
Total number of shifts	1476
Number of shifts mapped to atoms	1476
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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	998	955	955	50±7
All	All	19960	19100	19100	998

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ASN:H	1:A:131:ASN:HD22	0.66	1.32	11	5
1:A:182:LEU:HD23	1:A:182:LEU:C	0.63	2.14	2	1
1:A:83:GLU:O	1:A:87:TRP:CG	0.63	2.52	10	20
1:A:131:ASN:H	1:A:131:ASN:ND2	0.62	1.92	15	6
1:A:131:ASN:ND2	1:A:131:ASN:H	0.62	1.93	17	6
1:A:189:HIS:NE2	1:A:193:TYR:CZ	0.62	2.67	4	2
1:A:131:ASN:N	1:A:131:ASN:HD22	0.61	1.93	11	2
1:A:120:TRP:CD1	1:A:181:GLN:NE2	0.61	2.68	4	1
1:A:189:HIS:NE2	1:A:190:ARG:NH2	0.61	2.48	13	1
1:A:173:SER:O	1:A:175:HIS:N	0.59	2.35	6	9
1:A:95:MET:SD	1:A:185:TYR:CZ	0.59	2.95	7	1
1:A:123:CYS:SG	1:A:181:GLN:NE2	0.58	2.76	18	1
1:A:111:GLU:O	1:A:112:TYR:CG	0.58	2.56	12	5
1:A:129:GLU:O	1:A:130:ALA:HB3	0.58	1.98	17	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ASN:HD22	1:A:131:ASN:H	0.58	1.41	13	6
1:A:129:GLU:O	1:A:131:ASN:ND2	0.57	2.38	3	7
1:A:100:GLY:O	1:A:102:SER:N	0.57	2.37	20	18
1:A:91:PHE:CE2	1:A:185:TYR:CZ	0.57	2.93	8	1
1:A:189:HIS:CE1	1:A:190:ARG:HH21	0.57	2.17	13	1
1:A:133:HIS:CD2	1:A:134:VAL:N	0.57	2.73	19	2
1:A:131:ASN:N	1:A:131:ASN:ND2	0.56	2.53	13	8
1:A:189:HIS:CD2	1:A:193:TYR:CE1	0.56	2.93	6	1
1:A:146:TYR:O	1:A:148:SER:N	0.56	2.39	17	9
1:A:174:ALA:O	1:A:175:HIS:CG	0.56	2.59	10	2
1:A:129:GLU:O	1:A:131:ASN:N	0.56	2.39	6	8
1:A:200:PRO:O	1:A:204:ALA:HB2	0.55	2.01	4	18
1:A:140:ARG:O	1:A:144:GLU:N	0.55	2.39	2	5
1:A:195:ARG:O	1:A:199:SER:N	0.55	2.40	20	14
1:A:193:TYR:N	1:A:194:PRO:CD	0.55	2.70	1	18
1:A:95:MET:SD	1:A:120:TRP:CH2	0.54	3.00	16	1
1:A:95:MET:SD	1:A:120:TRP:CZ3	0.54	3.01	16	1
1:A:114:GLU:CD	1:A:114:GLU:H	0.54	2.05	14	1
1:A:174:ALA:O	1:A:176:THR:N	0.54	2.41	10	3
1:A:114:GLU:OE1	1:A:115:GLU:N	0.54	2.41	7	2
1:A:110:THR:O	1:A:112:TYR:N	0.54	2.41	14	14
1:A:89:GLN:NE2	1:A:93:LYS:NZ	0.54	2.56	18	1
1:A:114:GLU:OE2	1:A:114:GLU:N	0.54	2.40	7	1
1:A:128:ALA:O	1:A:130:ALA:N	0.53	2.41	10	3
1:A:159:SER:OG	1:A:160:ARG:N	0.53	2.41	4	5
1:A:110:THR:OG1	1:A:111:GLU:N	0.53	2.41	13	17
1:A:143:TYR:CZ	1:A:147:VAL:HG11	0.53	2.39	3	1
1:A:81:PRO:O	1:A:85:GLN:NE2	0.53	2.41	19	1
1:A:125:GLU:O	1:A:127:LYS:N	0.53	2.41	18	4
1:A:175:HIS:NE2	1:A:178:ASP:OD2	0.53	2.42	14	1
1:A:114:GLU:CD	1:A:115:GLU:N	0.53	2.62	7	1
1:A:116:ASN:OD1	1:A:116:ASN:N	0.53	2.41	20	2
1:A:121:LEU:O	1:A:125:GLU:N	0.53	2.42	19	8
1:A:175:HIS:CD2	1:A:175:HIS:H	0.53	2.22	7	1
1:A:165:ILE:N	1:A:165:ILE:HD12	0.53	2.18	10	1
1:A:98:PRO:O	1:A:101:ARG:NH1	0.53	2.42	6	1
1:A:200:PRO:O	1:A:204:ALA:N	0.53	2.42	2	9
1:A:179:ASP:OD1	1:A:180:ALA:N	0.53	2.42	9	6
1:A:145:ASP:OD2	1:A:146:TYR:CZ	0.53	2.62	8	6
1:A:79:PRO:N	1:A:83:GLU:OE1	0.53	2.42	15	2
1:A:197:LEU:O	1:A:203:ARG:NH2	0.53	2.41	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:ILE:O	1:A:187:LEU:N	0.52	2.42	18	12
1:A:107:PHE:CE2	1:A:111:GLU:OE2	0.52	2.62	11	1
1:A:136:ASP:OD1	1:A:140:ARG:NH2	0.52	2.42	12	3
1:A:120:TRP:CZ3	1:A:124:GLU:OE1	0.52	2.62	20	2
1:A:162:ARG:CG	1:A:162:ARG:HH11	0.52	2.18	17	1
1:A:143:TYR:OH	1:A:162:ARG:NH2	0.52	2.42	17	1
1:A:145:ASP:OD1	1:A:146:TYR:CE1	0.52	2.62	12	2
1:A:181:GLN:NE2	1:A:181:GLN:O	0.52	2.43	10	1
1:A:145:ASP:OD1	1:A:146:TYR:CZ	0.52	2.62	12	1
1:A:92:ASP:OD1	1:A:93:LYS:N	0.52	2.42	20	5
1:A:145:ASP:O	1:A:146:TYR:CD1	0.52	2.62	3	3
1:A:129:GLU:N	1:A:129:GLU:OE1	0.52	2.41	14	1
1:A:166:ASN:HD22	1:A:166:ASN:N	0.52	2.02	14	1
1:A:124:GLU:OE1	1:A:127:LYS:NZ	0.52	2.42	8	1
1:A:145:ASP:OD2	1:A:146:TYR:CE2	0.52	2.62	16	6
1:A:105:ARG:NH1	1:A:105:ARG:CG	0.52	2.73	12	2
1:A:129:GLU:OE2	1:A:130:ALA:N	0.52	2.42	6	1
1:A:114:GLU:O	1:A:117:MET:N	0.52	2.43	6	5
1:A:198:SER:O	1:A:203:ARG:NH1	0.52	2.42	12	2
1:A:165:ILE:N	1:A:165:ILE:CD1	0.52	2.72	10	1
1:A:82:GLU:N	1:A:82:GLU:OE1	0.52	2.42	2	1
1:A:140:ARG:NH1	1:A:140:ARG:CG	0.52	2.72	1	5
1:A:162:ARG:NH1	1:A:162:ARG:CG	0.52	2.72	7	1
1:A:175:HIS:CD2	1:A:178:ASP:OD1	0.52	2.62	3	1
1:A:158:ASP:OD2	1:A:162:ARG:NH2	0.52	2.43	19	1
1:A:175:HIS:O	1:A:175:HIS:CD2	0.52	2.62	15	1
1:A:160:ARG:CG	1:A:160:ARG:NH1	0.52	2.72	16	3
1:A:160:ARG:CG	1:A:160:ARG:HH11	0.52	2.17	16	2
1:A:86:SER:OG	1:A:93:LYS:NZ	0.52	2.42	16	1
1:A:114:GLU:OE2	1:A:115:GLU:N	0.52	2.42	13	1
1:A:136:ASP:OD2	1:A:140:ARG:NH2	0.52	2.43	13	3
1:A:120:TRP:CH2	1:A:124:GLU:OE1	0.52	2.62	14	1
1:A:111:GLU:OE1	1:A:195:ARG:NH2	0.52	2.42	11	1
1:A:191:ASP:O	1:A:195:ARG:NH1	0.52	2.42	11	1
1:A:116:ASN:HD21	1:A:184:ILE:CG2	0.52	2.18	17	1
1:A:109:ARG:NH1	1:A:109:ARG:CG	0.52	2.73	18	3
1:A:195:ARG:CG	1:A:195:ARG:NH1	0.52	2.72	14	3
1:A:137:GLU:OE2	1:A:140:ARG:NH2	0.52	2.42	20	1
1:A:110:THR:O	1:A:112:TYR:CD2	0.52	2.63	13	1
1:A:137:GLU:H	1:A:137:GLU:CD	0.51	2.09	18	1
1:A:157:LEU:N	1:A:157:LEU:HD22	0.51	2.20	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:GLU:CD	1:A:130:ALA:N	0.51	2.63	6	1
1:A:91:PHE:CD1	1:A:185:TYR:OH	0.51	2.61	19	9
1:A:140:ARG:CG	1:A:140:ARG:NH1	0.51	2.73	3	3
1:A:162:ARG:HH11	1:A:162:ARG:CG	0.51	2.18	7	1
1:A:83:GLU:O	1:A:87:TRP:CD1	0.51	2.64	7	3
1:A:162:ARG:CG	1:A:162:ARG:NH1	0.51	2.72	17	1
1:A:140:ARG:HH11	1:A:140:ARG:CG	0.51	2.18	1	6
1:A:195:ARG:NH1	1:A:195:ARG:CG	0.51	2.72	20	1
1:A:115:GLU:CD	1:A:115:GLU:H	0.51	2.09	15	3
1:A:120:TRP:CZ2	1:A:124:GLU:OE2	0.51	2.63	14	1
1:A:157:LEU:O	1:A:162:ARG:NH2	0.51	2.43	4	1
1:A:203:ARG:CG	1:A:203:ARG:NH1	0.51	2.73	6	1
1:A:195:ARG:HH11	1:A:195:ARG:CG	0.51	2.19	14	2
1:A:195:ARG:CG	1:A:195:ARG:HH11	0.51	2.18	4	2
1:A:105:ARG:CG	1:A:105:ARG:NH1	0.51	2.73	7	1
1:A:102:SER:OG	1:A:103:VAL:N	0.51	2.43	10	2
1:A:110:THR:C	1:A:112:TYR:H	0.51	2.09	10	17
1:A:80:SER:N	1:A:83:GLU:OE1	0.51	2.43	9	2
1:A:119:PHE:O	1:A:181:GLN:NE2	0.51	2.44	13	1
1:A:80:SER:O	1:A:82:GLU:N	0.50	2.44	13	14
1:A:175:HIS:CE1	1:A:178:ASP:CB	0.50	2.94	18	1
1:A:189:HIS:ND1	1:A:189:HIS:O	0.50	2.41	14	3
1:A:115:GLU:N	1:A:115:GLU:CD	0.50	2.65	12	2
1:A:190:ARG:NE	1:A:190:ARG:O	0.50	2.42	6	1
1:A:169:MET:SD	1:A:169:MET:O	0.50	2.69	8	4
1:A:105:ARG:NH2	1:A:114:GLU:OE2	0.50	2.45	12	2
1:A:115:GLU:CD	1:A:115:GLU:N	0.50	2.65	5	2
1:A:85:GLN:OE1	1:A:85:GLN:N	0.50	2.44	19	1
1:A:190:ARG:CG	1:A:190:ARG:NH1	0.50	2.72	17	2
1:A:101:ARG:NH1	1:A:101:ARG:CG	0.50	2.73	6	1
1:A:115:GLU:CG	1:A:116:ASN:N	0.50	2.75	8	1
1:A:101:ARG:HH11	1:A:101:ARG:CG	0.50	2.19	6	1
1:A:96:HIS:O	1:A:96:HIS:ND1	0.50	2.44	15	1
1:A:145:ASP:OD1	1:A:146:TYR:CD2	0.49	2.65	16	1
1:A:190:ARG:O	1:A:194:PRO:CG	0.49	2.60	7	13
1:A:179:ASP:OD1	1:A:179:ASP:N	0.49	2.45	7	1
1:A:109:ARG:CG	1:A:109:ARG:NH1	0.49	2.72	5	2
1:A:173:SER:OG	1:A:175:HIS:NE2	0.49	2.44	1	1
1:A:196:PHE:O	1:A:198:SER:N	0.49	2.46	16	1
1:A:109:ARG:CG	1:A:109:ARG:HH11	0.49	2.21	18	2
1:A:92:ASP:O	1:A:96:HIS:N	0.49	2.42	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:PHE:O	1:A:181:GLN:N	0.49	2.37	3	1
1:A:168:LYS:O	1:A:170:GLN:N	0.49	2.46	15	3
1:A:115:GLU:H	1:A:115:GLU:CD	0.49	2.10	3	2
1:A:129:GLU:C	1:A:131:ASN:ND2	0.49	2.66	2	4
1:A:157:LEU:O	1:A:158:ASP:CB	0.49	2.61	1	6
1:A:175:HIS:CD2	1:A:178:ASP:OD2	0.49	2.66	14	1
1:A:167:LYS:NZ	1:A:167:LYS:CB	0.49	2.76	8	1
1:A:173:SER:OG	1:A:175:HIS:CE1	0.49	2.65	16	1
1:A:92:ASP:CG	1:A:93:LYS:N	0.49	2.67	2	3
1:A:147:VAL:O	1:A:148:SER:O	0.49	2.31	19	17
1:A:109:ARG:HH11	1:A:109:ARG:CG	0.49	2.19	3	2
1:A:105:ARG:CG	1:A:105:ARG:HH11	0.49	2.21	7	1
1:A:190:ARG:CG	1:A:190:ARG:HH11	0.48	2.20	17	1
1:A:117:MET:C	1:A:117:MET:SD	0.48	2.91	19	1
1:A:111:GLU:C	1:A:112:TYR:CD2	0.48	2.87	6	5
1:A:129:GLU:C	1:A:131:ASN:HD22	0.48	2.12	6	3
1:A:119:PHE:O	1:A:123:CYS:SG	0.48	2.71	17	4
1:A:129:GLU:CD	1:A:130:ALA:H	0.48	2.12	6	1
1:A:129:GLU:CA	1:A:131:ASN:ND2	0.48	2.77	2	3
1:A:114:GLU:CD	1:A:114:GLU:N	0.48	2.67	13	2
1:A:120:TRP:O	1:A:123:CYS:SG	0.48	2.69	18	1
1:A:162:ARG:O	1:A:166:ASN:ND2	0.48	2.47	3	1
1:A:160:ARG:CG	1:A:161:VAL:N	0.48	2.76	13	1
1:A:114:GLU:O	1:A:116:ASN:N	0.48	2.46	10	2
1:A:140:ARG:CG	1:A:140:ARG:HH11	0.48	2.21	3	2
1:A:82:GLU:O	1:A:86:SER:N	0.48	2.41	13	2
1:A:117:MET:O	1:A:121:LEU:N	0.48	2.39	4	1
1:A:114:GLU:OE1	1:A:114:GLU:N	0.48	2.41	14	1
1:A:181:GLN:CG	1:A:182:LEU:N	0.48	2.77	8	1
1:A:83:GLU:O	1:A:87:TRP:CD2	0.48	2.66	19	5
1:A:116:ASN:OD1	1:A:117:MET:N	0.48	2.46	11	2
1:A:100:GLY:C	1:A:102:SER:N	0.47	2.68	6	19
1:A:159:SER:O	1:A:161:VAL:N	0.47	2.48	20	7
1:A:129:GLU:OE1	1:A:129:GLU:CA	0.47	2.62	14	1
1:A:105:ARG:HH11	1:A:105:ARG:CG	0.47	2.21	12	2
1:A:146:TYR:O	1:A:147:VAL:C	0.47	2.53	18	17
1:A:129:GLU:O	1:A:130:ALA:CB	0.47	2.62	17	3
1:A:190:ARG:O	1:A:194:PRO:CD	0.47	2.62	8	1
1:A:79:PRO:N	1:A:83:GLU:CD	0.47	2.68	6	1
1:A:111:GLU:O	1:A:113:SER:N	0.47	2.46	10	2
1:A:133:HIS:CG	1:A:134:VAL:N	0.47	2.83	19	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:ARG:CG	1:A:203:ARG:HH11	0.47	2.22	6	1
1:A:96:HIS:ND1	1:A:96:HIS:N	0.47	2.62	9	2
1:A:82:GLU:N	1:A:82:GLU:CD	0.47	2.68	2	1
1:A:166:ASN:N	1:A:166:ASN:HD22	0.47	2.08	3	1
1:A:79:PRO:CD	1:A:83:GLU:OE2	0.47	2.62	7	1
1:A:175:HIS:C	1:A:175:HIS:ND1	0.47	2.66	11	1
1:A:131:ASN:ND2	1:A:131:ASN:N	0.47	2.61	9	3
1:A:129:GLU:C	1:A:131:ASN:N	0.47	2.67	2	9
1:A:189:HIS:ND1	1:A:193:TYR:CE1	0.47	2.83	8	1
1:A:174:ALA:O	1:A:175:HIS:ND1	0.47	2.48	12	1
1:A:157:LEU:N	1:A:157:LEU:CD2	0.47	2.78	11	1
1:A:92:ASP:OD1	1:A:92:ASP:N	0.47	2.48	3	1
1:A:110:THR:O	1:A:112:TYR:CD1	0.47	2.68	17	2
1:A:157:LEU:HD13	1:A:158:ASP:N	0.47	2.25	15	1
1:A:137:GLU:CD	1:A:140:ARG:NH2	0.47	2.68	20	1
1:A:168:LYS:NZ	1:A:176:THR:OG1	0.47	2.42	14	1
1:A:143:TYR:O	1:A:143:TYR:CD1	0.46	2.67	6	2
1:A:80:SER:C	1:A:82:GLU:H	0.46	2.13	1	13
1:A:174:ALA:C	1:A:176:THR:N	0.46	2.68	10	3
1:A:111:GLU:C	1:A:112:TYR:CG	0.46	2.88	12	8
1:A:177:PHE:O	1:A:178:ASP:C	0.46	2.53	7	12
1:A:125:GLU:C	1:A:127:LYS:H	0.46	2.13	14	2
1:A:123:CYS:SG	1:A:124:GLU:N	0.46	2.88	8	1
1:A:96:HIS:CG	1:A:96:HIS:O	0.46	2.69	5	1
1:A:196:PHE:C	1:A:198:SER:N	0.46	2.68	16	1
1:A:129:GLU:C	1:A:131:ASN:H	0.46	2.14	19	8
1:A:171:GLU:N	1:A:171:GLU:OE2	0.46	2.49	13	1
1:A:107:PHE:CZ	1:A:111:GLU:OE1	0.46	2.68	7	1
1:A:119:PHE:CD1	1:A:119:PHE:C	0.46	2.88	10	1
1:A:80:SER:C	1:A:82:GLU:N	0.46	2.69	13	15
1:A:189:HIS:CE1	1:A:190:ARG:NH2	0.46	2.83	12	2
1:A:173:SER:OG	1:A:174:ALA:N	0.46	2.48	7	2
1:A:173:SER:C	1:A:175:HIS:N	0.46	2.69	15	2
1:A:110:THR:C	1:A:112:TYR:N	0.46	2.69	5	13
1:A:175:HIS:N	1:A:175:HIS:ND1	0.46	2.64	2	2
1:A:125:GLU:C	1:A:127:LYS:N	0.46	2.69	14	4
1:A:83:GLU:N	1:A:83:GLU:CD	0.46	2.69	9	4
1:A:116:ASN:OD1	1:A:184:ILE:CG2	0.46	2.64	13	2
1:A:202:TYR:C	1:A:202:TYR:CD1	0.46	2.88	9	7
1:A:173:SER:OG	1:A:175:HIS:CD2	0.46	2.68	1	1
1:A:147:VAL:O	1:A:148:SER:C	0.46	2.53	6	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:LYS:NZ	1:A:176:THR:CB	0.46	2.79	14	1
1:A:105:ARG:HH21	1:A:118:LEU:CD2	0.46	2.23	7	1
1:A:143:TYR:CE1	1:A:147:VAL:HG11	0.46	2.46	19	1
1:A:173:SER:O	1:A:174:ALA:O	0.46	2.34	20	3
1:A:83:GLU:CD	1:A:83:GLU:N	0.46	2.68	10	2
1:A:92:ASP:N	1:A:92:ASP:OD1	0.45	2.49	5	2
1:A:168:LYS:O	1:A:171:GLU:N	0.45	2.43	4	2
1:A:184:ILE:O	1:A:188:MET:SD	0.45	2.74	5	1
1:A:85:GLN:CD	1:A:85:GLN:N	0.45	2.69	19	1
1:A:182:LEU:HD13	1:A:182:LEU:C	0.45	2.32	11	1
1:A:156:SER:OG	1:A:187:LEU:CD1	0.45	2.64	15	1
1:A:193:TYR:N	1:A:194:PRO:HD2	0.45	2.27	17	19
1:A:179:ASP:N	1:A:179:ASP:OD1	0.45	2.47	17	1
1:A:115:GLU:OE2	1:A:115:GLU:N	0.45	2.49	5	1
1:A:173:SER:C	1:A:175:HIS:H	0.45	2.15	12	1
1:A:141:LEU:CD2	1:A:141:LEU:N	0.45	2.80	4	3
1:A:157:LEU:O	1:A:158:ASP:O	0.45	2.35	8	1
1:A:141:LEU:HD23	1:A:141:LEU:O	0.45	2.11	20	2
1:A:177:PHE:O	1:A:179:ASP:N	0.45	2.50	1	1
1:A:114:GLU:N	1:A:114:GLU:CD	0.45	2.70	14	1
1:A:142:ILE:O	1:A:145:ASP:OD1	0.44	2.35	16	3
1:A:188:MET:O	1:A:192:SER:N	0.44	2.41	2	1
1:A:141:LEU:HD12	1:A:141:LEU:N	0.44	2.27	17	1
1:A:82:GLU:O	1:A:86:SER:OG	0.44	2.36	19	3
1:A:96:HIS:N	1:A:96:HIS:ND1	0.44	2.65	11	1
1:A:184:ILE:O	1:A:186:THR:N	0.44	2.50	11	1
1:A:169:MET:SD	1:A:169:MET:C	0.44	2.96	3	1
1:A:86:SER:OG	1:A:93:LYS:CD	0.44	2.65	16	2
1:A:174:ALA:C	1:A:176:THR:H	0.44	2.16	20	2
1:A:175:HIS:CD2	1:A:175:HIS:N	0.44	2.84	7	1
1:A:141:LEU:N	1:A:141:LEU:HD22	0.44	2.27	4	1
1:A:129:GLU:OE2	1:A:131:ASN:ND2	0.44	2.50	11	1
1:A:160:ARG:HH11	1:A:160:ARG:CB	0.44	2.26	11	1
1:A:123:CYS:SG	1:A:181:GLN:CD	0.44	2.96	5	1
1:A:120:TRP:NE1	1:A:181:GLN:NE2	0.44	2.65	15	1
1:A:192:SER:O	1:A:196:PHE:CB	0.44	2.66	20	5
1:A:200:PRO:O	1:A:204:ALA:CB	0.44	2.66	1	4
1:A:171:GLU:N	1:A:171:GLU:CD	0.44	2.71	13	1
1:A:114:GLU:CD	1:A:115:GLU:H	0.44	2.16	7	1
1:A:173:SER:O	1:A:174:ALA:HB2	0.44	2.13	9	1
1:A:177:PHE:O	1:A:180:ALA:N	0.44	2.50	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:GLN:O	1:A:171:GLU:C	0.44	2.55	2	1
1:A:98:PRO:N	1:A:101:ARG:HH21	0.44	2.10	2	1
1:A:157:LEU:O	1:A:158:ASP:OD1	0.44	2.35	20	2
1:A:173:SER:O	1:A:174:ALA:HB3	0.44	2.13	5	3
1:A:160:ARG:HH11	1:A:160:ARG:CG	0.44	2.24	11	1
1:A:158:ASP:O	1:A:159:SER:CB	0.43	2.64	4	1
1:A:175:HIS:O	1:A:178:ASP:OD2	0.43	2.36	3	2
1:A:115:GLU:N	1:A:115:GLU:OE2	0.43	2.51	12	1
1:A:158:ASP:O	1:A:159:SER:OG	0.43	2.36	20	2
1:A:202:TYR:CD1	1:A:202:TYR:C	0.43	2.91	6	2
1:A:146:TYR:O	1:A:148:SER:O	0.43	2.37	13	2
1:A:145:ASP:OD1	1:A:145:ASP:O	0.43	2.36	12	6
1:A:117:MET:SD	1:A:117:MET:C	0.43	2.97	9	1
1:A:95:MET:SD	1:A:185:TYR:OH	0.43	2.77	7	1
1:A:129:GLU:CG	1:A:130:ALA:H	0.43	2.25	6	1
1:A:175:HIS:ND1	1:A:175:HIS:N	0.43	2.67	19	1
1:A:118:LEU:O	1:A:122:ALA:N	0.43	2.41	16	1
1:A:159:SER:C	1:A:161:VAL:N	0.43	2.69	20	7
1:A:166:ASN:O	1:A:166:ASN:OD1	0.43	2.36	20	1
1:A:169:MET:O	1:A:169:MET:SD	0.43	2.77	4	3
1:A:129:GLU:OE1	1:A:134:VAL:O	0.43	2.37	18	1
1:A:130:ALA:O	1:A:131:ASN:O	0.43	2.36	18	6
1:A:145:ASP:O	1:A:145:ASP:OD1	0.43	2.37	5	1
1:A:158:ASP:O	1:A:159:SER:O	0.43	2.37	5	2
1:A:196:PHE:C	1:A:198:SER:H	0.43	2.16	16	1
1:A:175:HIS:O	1:A:178:ASP:OD1	0.43	2.37	18	1
1:A:136:ASP:CG	1:A:140:ARG:NH2	0.43	2.72	3	1
1:A:184:ILE:C	1:A:186:THR:N	0.43	2.72	9	3
1:A:175:HIS:NE2	1:A:178:ASP:OD1	0.43	2.51	3	1
1:A:135:VAL:O	1:A:139:ALA:CB	0.43	2.67	9	1
1:A:168:LYS:HZ2	1:A:176:THR:CB	0.43	2.27	14	1
1:A:113:SER:OG	1:A:113:SER:O	0.43	2.37	17	1
1:A:160:ARG:NH1	1:A:160:ARG:CG	0.43	2.79	14	1
1:A:158:ASP:OD1	1:A:158:ASP:O	0.43	2.37	11	1
1:A:124:GLU:OE2	1:A:181:GLN:OE1	0.43	2.37	8	1
1:A:187:LEU:O	1:A:187:LEU:HD23	0.43	2.14	6	2
1:A:115:GLU:OE2	1:A:116:ASN:N	0.43	2.52	2	1
1:A:141:LEU:CD1	1:A:141:LEU:N	0.42	2.81	17	2
1:A:108:LEU:O	1:A:109:ARG:C	0.42	2.57	9	2
1:A:144:GLU:O	1:A:148:SER:OG	0.42	2.36	11	2
1:A:167:LYS:CB	1:A:167:LYS:NZ	0.42	2.82	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:ASP:OD1	1:A:195:ARG:NH2	0.42	2.52	13	1
1:A:182:LEU:C	1:A:182:LEU:CD1	0.42	2.88	11	4
1:A:132:GLN:O	1:A:132:GLN:NE2	0.42	2.52	4	1
1:A:125:GLU:O	1:A:129:GLU:OE1	0.42	2.37	7	1
1:A:141:LEU:N	1:A:141:LEU:HD12	0.42	2.29	10	1
1:A:98:PRO:O	1:A:102:SER:OG	0.42	2.38	6	1
1:A:170:GLN:CD	1:A:170:GLN:N	0.42	2.73	9	1
1:A:126:LEU:HD12	1:A:129:GLU:OE2	0.42	2.15	18	1
1:A:107:PHE:CE2	1:A:111:GLU:OE1	0.42	2.72	14	1
1:A:168:LYS:CB	1:A:176:THR:OG1	0.42	2.67	14	1
1:A:80:SER:O	1:A:83:GLU:OE1	0.42	2.38	10	1
1:A:173:SER:OG	1:A:173:SER:O	0.42	2.31	20	1
1:A:82:GLU:O	1:A:86:SER:CB	0.42	2.67	13	2
1:A:188:MET:O	1:A:192:SER:OG	0.42	2.35	14	2
1:A:105:ARG:NH2	1:A:118:LEU:CD2	0.42	2.83	7	1
1:A:186:THR:CG2	1:A:190:ARG:NH2	0.42	2.82	15	1
1:A:109:ARG:C	1:A:109:ARG:CD	0.42	2.88	6	1
1:A:114:GLU:O	1:A:115:GLU:C	0.42	2.58	19	6
1:A:178:ASP:CG	1:A:179:ASP:H	0.42	2.18	18	1
1:A:114:GLU:OE2	1:A:114:GLU:O	0.42	2.37	11	1
1:A:125:GLU:O	1:A:128:ALA:N	0.42	2.41	10	1
1:A:178:ASP:O	1:A:182:LEU:N	0.42	2.49	17	1
1:A:93:LYS:O	1:A:97:SER:OG	0.42	2.36	13	1
1:A:126:LEU:HD23	1:A:126:LEU:O	0.42	2.14	13	1
1:A:157:LEU:O	1:A:158:ASP:CG	0.42	2.58	16	3
1:A:141:LEU:N	1:A:141:LEU:CD2	0.42	2.83	13	1
1:A:195:ARG:O	1:A:199:SER:OG	0.42	2.36	14	2
1:A:129:GLU:CG	1:A:130:ALA:N	0.42	2.83	6	1
1:A:184:ILE:HG22	1:A:188:MET:SD	0.42	2.55	19	1
1:A:170:GLN:O	1:A:171:GLU:OE2	0.41	2.38	19	2
1:A:124:GLU:O	1:A:124:GLU:OE2	0.41	2.38	9	1
1:A:133:HIS:CD2	1:A:133:HIS:H	0.41	2.32	13	1
1:A:178:ASP:CG	1:A:179:ASP:N	0.41	2.73	18	1
1:A:105:ARG:NH2	1:A:118:LEU:HD23	0.41	2.30	7	1
1:A:106:ALA:O	1:A:107:PHE:C	0.41	2.59	6	1
1:A:131:ASN:O	1:A:132:GLN:OE1	0.41	2.37	19	1
1:A:96:HIS:ND1	1:A:96:HIS:O	0.41	2.54	18	1
1:A:206:LEU:C	1:A:206:LEU:HD23	0.41	2.35	6	1
1:A:114:GLU:C	1:A:116:ASN:N	0.41	2.72	10	1
1:A:206:LEU:CD1	1:A:206:LEU:C	0.41	2.89	7	2
1:A:184:ILE:CG2	1:A:185:TYR:N	0.41	2.84	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:LYS:CB	1:A:127:LYS:NZ	0.41	2.83	12	1
1:A:111:GLU:O	1:A:112:TYR:C	0.41	2.59	7	1
1:A:133:HIS:CD2	1:A:134:VAL:H	0.41	2.34	19	1
1:A:157:LEU:HD11	1:A:183:GLN:NE2	0.41	2.31	9	1
1:A:105:ARG:NH1	1:A:114:GLU:OE1	0.41	2.54	6	1
1:A:128:ALA:O	1:A:129:GLU:OE2	0.41	2.38	2	1
1:A:143:TYR:CZ	1:A:147:VAL:CG1	0.41	3.03	3	1
1:A:120:TRP:HE1	1:A:181:GLN:HE21	0.41	1.58	16	1
1:A:158:ASP:OD1	1:A:158:ASP:N	0.41	2.53	18	1
1:A:196:PHE:CD1	1:A:196:PHE:C	0.41	2.94	10	1
1:A:146:TYR:O	1:A:147:VAL:CG2	0.41	2.68	19	1
1:A:182:LEU:CD1	1:A:182:LEU:C	0.41	2.89	20	1
1:A:138:LYS:C	1:A:140:ARG:N	0.41	2.74	6	1
1:A:175:HIS:O	1:A:175:HIS:CG	0.41	2.73	15	1
1:A:140:ARG:O	1:A:141:LEU:C	0.40	2.60	7	4
1:A:137:GLU:CD	1:A:137:GLU:N	0.40	2.73	18	1
1:A:156:SER:O	1:A:157:LEU:C	0.40	2.59	10	1
1:A:199:SER:C	1:A:203:ARG:HH12	0.40	2.19	12	1
1:A:121:LEU:O	1:A:122:ALA:C	0.40	2.59	13	1
1:A:116:ASN:N	1:A:116:ASN:OD1	0.40	2.53	5	1
1:A:159:SER:O	1:A:160:ARG:C	0.40	2.60	20	1
1:A:184:ILE:O	1:A:185:TYR:C	0.40	2.60	11	1
1:A:146:TYR:C	1:A:148:SER:N	0.40	2.74	11	2
1:A:189:HIS:CD2	1:A:190:ARG:NH2	0.40	2.89	13	1
1:A:95:MET:SD	1:A:185:TYR:CE1	0.40	3.14	7	1
1:A:143:TYR:CD1	1:A:143:TYR:C	0.40	2.94	11	1
1:A:159:SER:O	1:A:162:ARG:N	0.40	2.52	2	1
1:A:194:PRO:C	1:A:195:ARG:HE	0.40	2.18	19	1
1:A:137:GLU:CD	1:A:140:ARG:HH21	0.40	2.18	20	1
1:A:141:LEU:HD22	1:A:141:LEU:N	0.40	2.32	13	1
1:A:100:GLY:O	1:A:101:ARG:C	0.40	2.60	18	1
1:A:133:HIS:O	1:A:137:GLU:OE1	0.40	2.39	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/152 (78%)	93±2 (78±2%)	17±2 (14±2%)	9±2 (8±2%)	2	15
All	All	2380/3040 (78%)	1863 (78%)	330 (14%)	187 (8%)	2	15

All 23 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	148	SER	18
1	A	101	ARG	17
1	A	111	GLU	17
1	A	131	ASN	17
1	A	147	VAL	16
1	A	158	ASP	15
1	A	173	SER	14
1	A	156	SER	11
1	A	132	GLN	9
1	A	81	PRO	9
1	A	174	ALA	9
1	A	159	SER	7
1	A	130	ALA	7
1	A	175	HIS	6
1	A	172	PRO	5
1	A	169	MET	2
1	A	126	LEU	2
1	A	129	GLU	1
1	A	157	LEU	1
1	A	197	LEU	1
1	A	115	GLU	1
1	A	178	ASP	1
1	A	112	TYR	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/134 (81%)	99±2 (90±2%)	10±2 (10±2%)	15	60
All	All	2180/2680 (81%)	1972 (90%)	208 (10%)	15	60

All 53 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	80	SER	20
1	A	104	PHE	17
1	A	131	ASN	14
1	A	160	ARG	9
1	A	187	LEU	9
1	A	169	MET	8
1	A	158	ASP	8
1	A	95	MET	8
1	A	193	TYR	6
1	A	109	ARG	6
1	A	118	LEU	6
1	A	90	SER	5
1	A	182	LEU	5
1	A	79	PRO	5
1	A	96	HIS	4
1	A	136	ASP	4
1	A	126	LEU	4
1	A	206	LEU	3
1	A	175	HIS	3
1	A	105	ARG	3
1	A	179	ASP	3
1	A	115	GLU	3
1	A	195	ARG	3
1	A	185	TYR	3
1	A	148	SER	3
1	A	156	SER	3
1	A	117	MET	3
1	A	114	GLU	3
1	A	140	ARG	2
1	A	138	LYS	2
1	A	129	GLU	2
1	A	116	ASN	2
1	A	176	THR	2
1	A	132	GLN	2
1	A	84	VAL	2
1	A	203	ARG	2
1	A	205	LEU	2
1	A	162	ARG	2
1	A	184	ILE	2
1	A	110	THR	2
1	A	82	GLU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	157	LEU	1
1	A	101	ARG	1
1	A	200	PRO	1
1	A	166	ASN	1
1	A	121	LEU	1
1	A	161	VAL	1
1	A	181	GLN	1
1	A	190	ARG	1
1	A	167	LYS	1
1	A	189	HIS	1
1	A	171	GLU	1
1	A	97	SER	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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4407

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	1476
Number of shifts mapped to atoms	1476
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	128	-0.42 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	125	-0.03 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	115	1.05 ± 0.20	Should be applied

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 81%, i.e. 1254 atoms were assigned a chemical shift out of a possible 1556. 3 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	464/593 (78%)	232/236 (98%)	121/242 (50%)	111/115 (97%)
Sidechain	674/809 (83%)	423/480 (88%)	243/288 (84%)	8/41 (20%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	116/154 (75%)	62/82 (76%)	52/66 (79%)	2/6 (33%)
Overall	1254/1556 (81%)	717/798 (90%)	416/596 (70%)	121/162 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1330 atoms were assigned a chemical shift out of a possible 1645. 3 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	486/626 (78%)	243/249 (98%)	128/256 (50%)	115/121 (95%)
Sidechain	728/865 (84%)	456/513 (89%)	264/310 (85%)	8/42 (19%)
Aromatic	116/154 (75%)	62/82 (76%)	52/66 (79%)	2/6 (33%)
Overall	1330/1645 (81%)	761/844 (90%)	444/632 (70%)	125/169 (74%)

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	124	GLU	HG3	1.06	3.31 – 1.21	-5.7
1	A	181	GLN	CG	28.13	39.38 – 28.18	-5.0

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:

