



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 10:59 PM UTC

PDB ID : 1CMZ / pdb_00001cmz
Title : SOLUTION STRUCTURE OF GAIP (GALPHA INTERACTING PROTEIN): A REGULATOR OF G PROTEIN SIGNALING
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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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

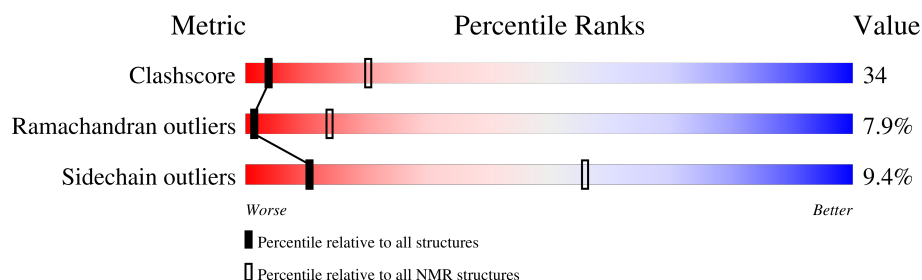
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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)	0.63	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:

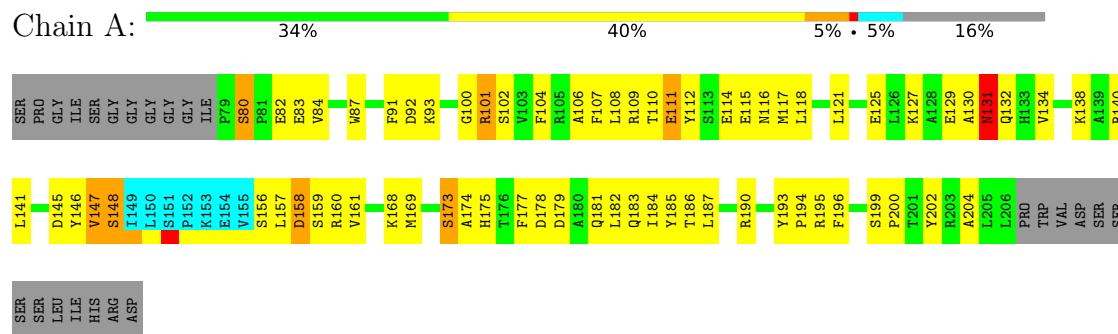
Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	GLN	SEE REMARK 999	UNP P49795
A	69	PRO	PRO	SEE REMARK 999	UNP P49795
A	70	GLY	LEU	SEE REMARK 999	UNP P49795
A	71	ILE	PRO	SEE REMARK 999	UNP P49795
A	72	SER	SER	SEE REMARK 999	UNP P49795
A	73	GLY	CYS	SEE REMARK 999	UNP P49795
A	74	GLY	GLU	SEE REMARK 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 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

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

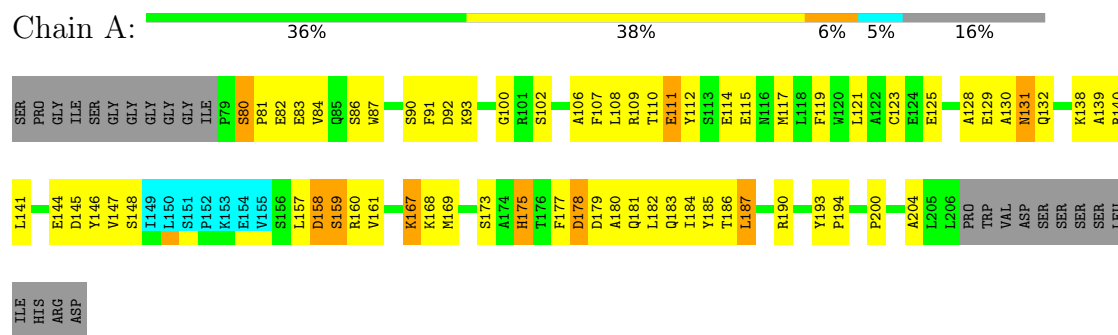


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

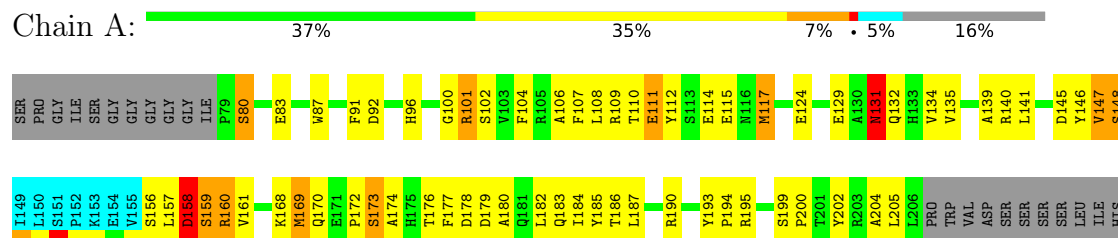
- Molecule 1: PROTEIN (GAIP (G-ALPHA INTERACTING) PROTEIN)



ASP

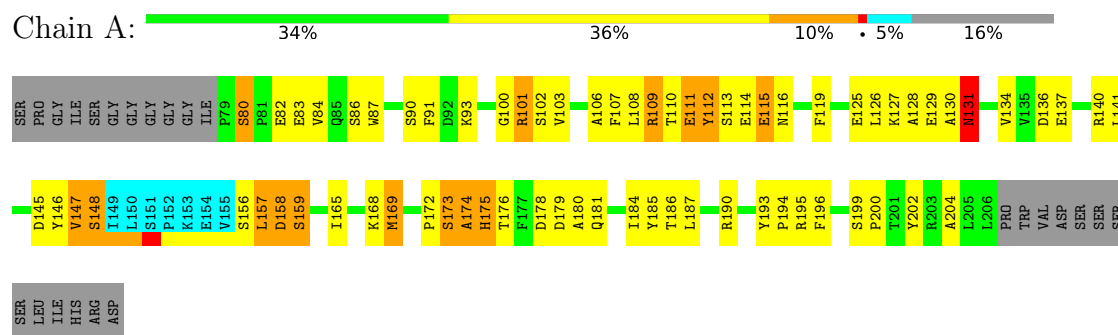
4.2.9 Score per residue for model 9

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

ARG
ASP

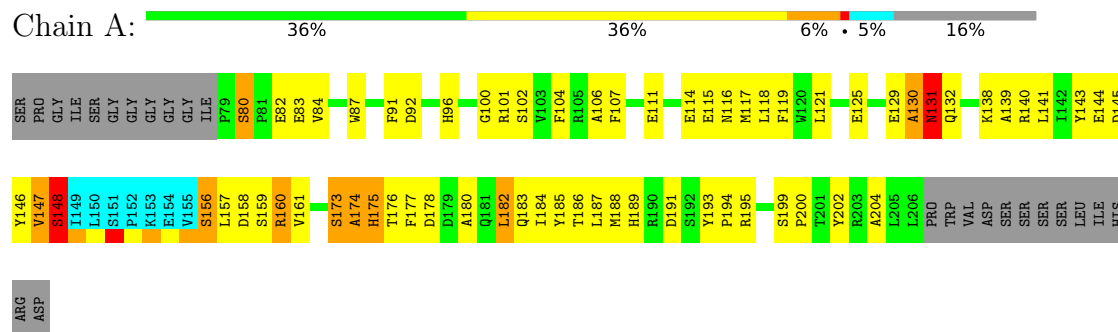
4.2.10 Score per residue for model 10

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

SER
LEU
ILE
HIS
ARG
ASP

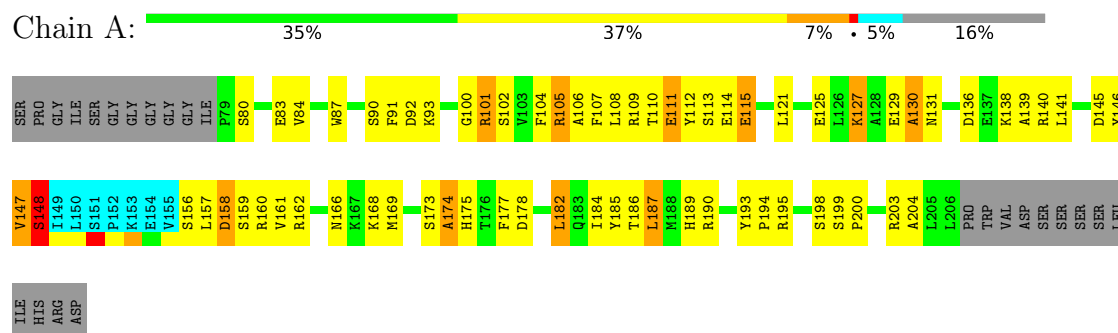
4.2.11 Score per residue for model 11 (medoid)

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

ARG
ASP

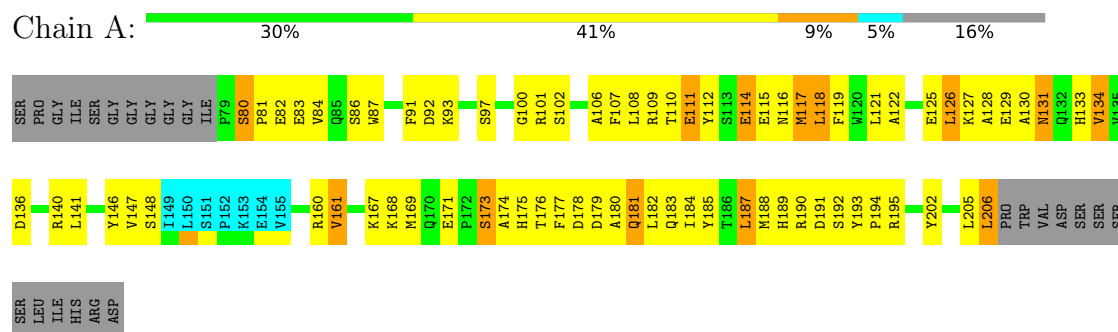
4.2.12 Score per residue for model 12

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



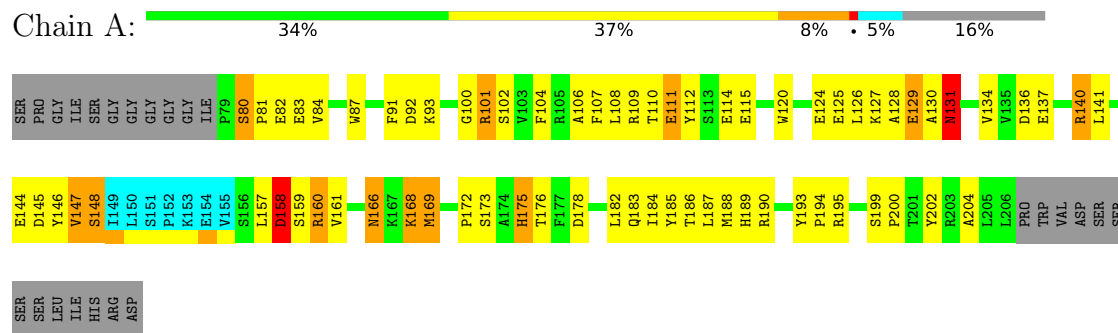
4.2.13 Score per residue for model 13

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



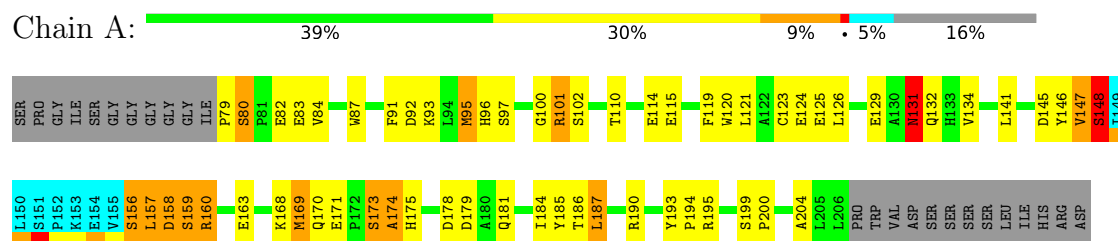
4.2.14 Score per residue for model 14

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



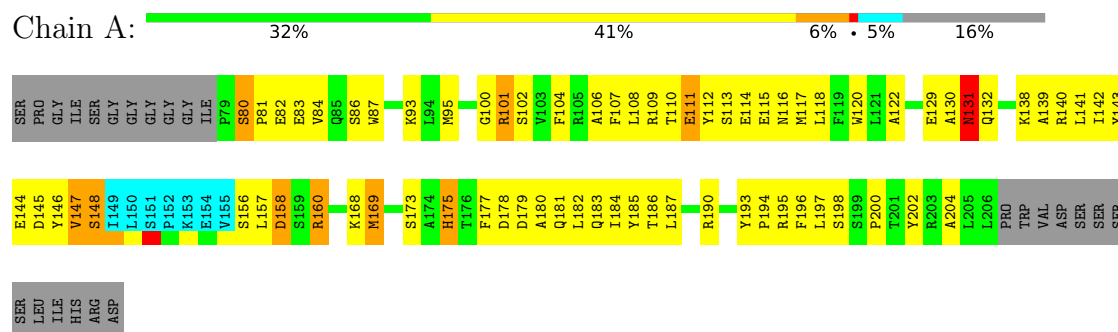
4.2.15 Score per residue for model 15

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



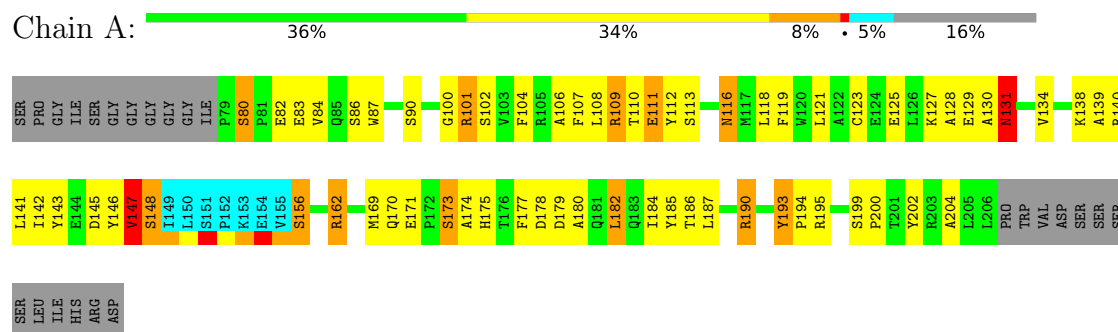
4.2.16 Score per residue for model 16

- 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)

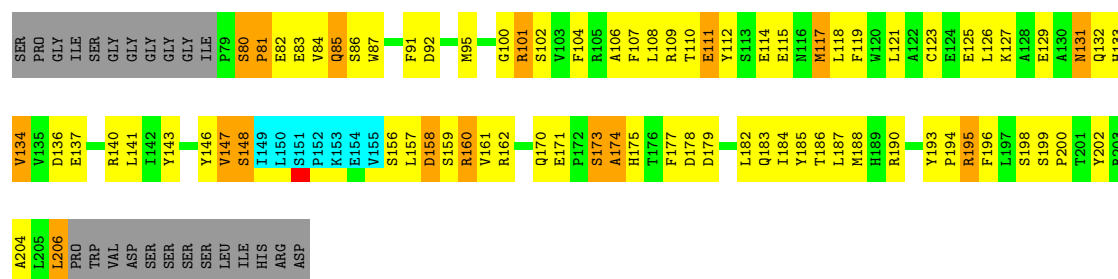




4.2.19 Score per residue for model 19

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

Chain A: 28% 41% 11% 5% 16%



4.2.20 Score per residue for model 20

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

Chain A: 35% 37% 7% 5% 16%



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	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.49±0.01	0±0/1023 (0.0± 0.0%)	1.20±0.01	0±0/1382 (0.0± 0.0%)
All	All	1.49	0/20460 (0.0%)	1.20	5/27640 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	196	PHE	CA-CB-CG	-5.49	108.31	113.80	6	5

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	998	955	955	67±8
All	All	19960	19100	19100	1345

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:LEU:HD23	1:A:182:LEU:C	0.68	2.14	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ASN:HD22	1:A:131:ASN:H	0.66	1.32	11	3
1:A:83:GLU:O	1:A:87:TRP:CG	0.63	2.52	10	20
1:A:131:ASN:ND2	1:A:131:ASN:H	0.62	1.92	15	11
1:A:189:HIS:NE2	1:A:193:TYR:CZ	0.62	2.67	4	2
1:A:131:ASN:HD22	1:A:131:ASN:N	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:114:GLU:CD	1:A:114:GLU:H	0.59	2.05	14	1
1:A:123:CYS:SG	1:A:181:GLN:NE2	0.58	2.76	18	1
1:A:129:GLU:O	1:A:130:ALA:HB3	0.58	1.98	17	3
1:A:111:GLU:O	1:A:112:TYR:CG	0.58	2.56	12	5
1:A:131:ASN:H	1:A:131:ASN:HD22	0.58	1.41	13	8
1:A:114:GLU:CD	1:A:115:GLU:N	0.57	2.62	7	1
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:120:TRP:NE1	1:A:181:GLN:HE21	0.57	1.97	16	2
1:A:133:HIS:CD2	1:A:134:VAL:N	0.57	2.73	19	2
1:A:189:HIS:CE1	1:A:190:ARG:HH21	0.57	2.17	13	1
1:A:189:HIS:CD2	1:A:193:TYR:CE1	0.56	2.93	6	1
1:A:131:ASN:ND2	1:A:131:ASN:N	0.56	2.53	13	9
1:A:129:GLU:CD	1:A:130:ALA:N	0.56	2.63	6	1
1:A:137:GLU:H	1:A:137:GLU:CD	0.56	2.09	18	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:115:GLU:H	1:A:115:GLU:CD	0.56	2.09	15	3
1:A:200:PRO:O	1:A:204:ALA:HB2	0.55	2.01	4	18
1:A:110:THR:C	1:A:112:TYR:H	0.55	2.09	10	17
1:A:140:ARG:O	1:A:144:GLU:N	0.55	2.39	2	5
1:A:115:GLU:CD	1:A:115:GLU:N	0.55	2.65	12	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:174:ALA:O	1:A:176:THR:N	0.54	2.41	10	3
1:A:129:GLU:C	1:A:131:ASN:ND2	0.54	2.66	2	6
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	10	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:GLU:N	1:A:114:GLU:OE2	0.54	2.40	7	1
1:A:89:GLN:NE2	1:A:93:LYS:NZ	0.54	2.56	18	1
1:A:159:SER:OG	1:A:160:ARG:N	0.53	2.41	4	5
1:A:92:ASP:CG	1:A:93:LYS:N	0.53	2.67	2	6
1:A:128:ALA:O	1:A:130:ALA:N	0.53	2.41	10	3
1:A:91:PHE:CD1	1:A:185:TYR:OH	0.53	2.61	15	9
1:A:110:THR:OG1	1:A:111:GLU:N	0.53	2.41	19	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:129:GLU:C	1:A:131:ASN:HD22	0.53	2.12	6	4
1:A:129:GLU:CD	1:A:130:ALA:H	0.53	2.12	6	1
1:A:117:MET:C	1:A:117:MET:SD	0.53	2.91	19	2
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:121:LEU:O	1:A:125:GLU:N	0.53	2.42	19	8
1:A:98:PRO:O	1:A:101:ARG:NH1	0.53	2.42	6	1
1:A:114:GLU:CD	1:A:114:GLU:N	0.53	2.67	13	3
1:A:175:HIS:H	1:A:175:HIS:CD2	0.53	2.22	7	1
1:A:165:ILE:HD12	1:A:165:ILE:N	0.53	2.18	10	1
1:A:116:ASN:N	1:A:116:ASN:OD1	0.53	2.41	20	1
1:A:200:PRO:O	1:A:204:ALA:N	0.53	2.42	2	9
1:A:145:ASP:OD2	1:A:146:TYR:CZ	0.53	2.62	8	6
1:A:197:LEU:O	1:A:203:ARG:NH2	0.53	2.41	3	1
1:A:79:PRO:N	1:A:83:GLU:OE1	0.53	2.42	15	2
1:A:111:GLU:C	1:A:112:TYR:CD2	0.53	2.87	6	5
1:A:179:ASP:OD1	1:A:180:ALA:N	0.53	2.42	7	6
1:A:184:ILE:O	1:A:187:LEU:N	0.52	2.42	18	12
1:A:136:ASP:OD1	1:A:140:ARG:NH2	0.52	2.42	3	3
1:A:107:PHE:CE2	1:A:111:GLU:OE2	0.52	2.62	11	1
1:A:145:ASP:OD1	1:A:146:TYR:CE1	0.52	2.62	12	2
1:A:181:GLN:O	1:A:181:GLN:NE2	0.52	2.43	10	1
1:A:145:ASP:OD1	1:A:146:TYR:CZ	0.52	2.62	12	1
1:A:120:TRP:CZ3	1:A:124:GLU:OE1	0.52	2.62	20	2
1:A:143:TYR:OH	1:A:162:ARG:NH2	0.52	2.42	17	1
1:A:162:ARG:HH11	1:A:162:ARG:CG	0.52	2.18	17	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:166:ASN:HD22	1:A:166:ASN:N	0.52	2.02	14	2
1:A:129:GLU:N	1:A:129:GLU:OE1	0.52	2.41	14	1
1:A:146:TYR:O	1:A:147:VAL:C	0.52	2.53	18	18
1:A:145:ASP:OD2	1:A:146:TYR:CE2	0.52	2.62	16	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:PRO:N	1:A:83:GLU:CD	0.52	2.68	6	1
1:A:105:ARG:NH1	1:A:105:ARG:CG	0.52	2.73	12	3
1:A:129:GLU:OE2	1:A:130:ALA:N	0.52	2.42	6	1
1:A:80:SER:C	1:A:82:GLU:H	0.52	2.13	1	15
1:A:114:GLU:O	1:A:117:MET:N	0.52	2.43	6	5
1:A:82:GLU:N	1:A:82:GLU:OE1	0.52	2.42	2	1
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:140:ARG:NH1	1:A:140:ARG:CG	0.52	2.72	1	7
1:A:175:HIS:CD2	1:A:178:ASP:OD1	0.52	2.62	3	1
1:A:162:ARG:NH1	1:A:162:ARG:CG	0.52	2.72	7	1
1:A:175:HIS:O	1:A:175:HIS:CD2	0.52	2.62	15	1
1:A:158:ASP:OD2	1:A:162:ARG:NH2	0.52	2.43	19	1
1:A:82:GLU:N	1:A:82:GLU:CD	0.52	2.68	2	1
1:A:136:ASP:OD2	1:A:140:ARG:NH2	0.52	2.43	13	3
1:A:111:GLU:OE1	1:A:195:ARG:NH2	0.52	2.42	11	1
1:A:160:ARG:CG	1:A:160:ARG:NH1	0.52	2.72	16	2
1:A:114:GLU:OE2	1:A:115:GLU:N	0.52	2.42	13	1
1:A:120:TRP:CH2	1:A:124:GLU:OE1	0.52	2.62	14	1
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:175:HIS:ND1	1:A:175:HIS:C	0.52	2.66	11	1
1:A:191:ASP:O	1:A:195:ARG:NH1	0.52	2.42	11	1
1:A:109:ARG:NH1	1:A:109:ARG:CG	0.52	2.73	18	3
1:A:195:ARG:NH1	1:A:195:ARG:CG	0.52	2.72	7	3
1:A:116:ASN:HD21	1:A:184:ILE:CG2	0.52	2.18	17	1
1:A:120:TRP:CD1	1:A:181:GLN:HE22	0.52	2.23	4	1
1:A:110:THR:O	1:A:112:TYR:CD2	0.52	2.63	13	1
1:A:137:GLU:OE2	1:A:140:ARG:NH2	0.52	2.42	20	1
1:A:111:GLU:C	1:A:112:TYR:CG	0.51	2.88	16	9
1:A:157:LEU:HD22	1:A:157:LEU:N	0.51	2.20	11	1
1:A:162:ARG:CG	1:A:162:ARG:HH11	0.51	2.18	7	1
1:A:131:ASN:N	1:A:131:ASN:ND2	0.51	2.57	11	1
1:A:137:GLU:CD	1:A:140:ARG:NH2	0.51	2.68	20	1
1:A:140:ARG:CG	1:A:140:ARG:HH11	0.51	2.18	1	8
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:100:GLY:C	1:A:102:SER:N	0.51	2.68	6	20
1:A:174:ALA:C	1:A:176:THR:N	0.51	2.68	10	3
1:A:120:TRP:CZ2	1:A:124:GLU:OE2	0.51	2.63	14	1
1:A:177:PHE:O	1:A:178:ASP:C	0.51	2.53	7	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:LEU:O	1:A:162:ARG:NH2	0.51	2.43	4	1
1:A:203:ARG:NH1	1:A:203:ARG:CG	0.51	2.73	6	1
1:A:102:SER:OG	1:A:103:VAL:N	0.51	2.43	10	2
1:A:129:GLU:C	1:A:131:ASN:H	0.51	2.14	19	11
1:A:195:ARG:CG	1:A:195:ARG:HH11	0.51	2.18	4	4
1:A:110:THR:C	1:A:112:TYR:N	0.51	2.69	14	16
1:A:80:SER:N	1:A:83:GLU:OE1	0.51	2.43	9	2
1:A:119:PHE:C	1:A:119:PHE:CD1	0.51	2.88	10	1
1:A:129:GLU:C	1:A:131:ASN:N	0.51	2.68	18	11
1:A:119:PHE:O	1:A:181:GLN:NE2	0.51	2.44	13	1
1:A:83:GLU:N	1:A:83:GLU:CD	0.50	2.69	9	9
1:A:147:VAL:O	1:A:148:SER:C	0.50	2.53	6	5
1:A:80:SER:O	1:A:82:GLU:N	0.50	2.44	13	14
1:A:202:TYR:C	1:A:202:TYR:CD1	0.50	2.88	9	6
1:A:189:HIS:O	1:A:189:HIS:ND1	0.50	2.41	14	1
1:A:175:HIS:CE1	1:A:178:ASP:CB	0.50	2.94	18	1
1:A:115:GLU:CD	1:A:115:GLU:H	0.50	2.14	5	2
1:A:190:ARG:O	1:A:190:ARG:NE	0.50	2.42	6	1
1:A:168:LYS:NZ	1:A:176:THR:OG1	0.50	2.42	14	1
1:A:125:GLU:C	1:A:127:LYS:N	0.50	2.69	14	6
1:A:85:GLN:CD	1:A:85:GLN:N	0.50	2.69	19	1
1:A:169:MET:SD	1:A:169:MET:O	0.50	2.69	8	7
1:A:105:ARG:NH2	1:A:114:GLU:OE2	0.50	2.45	12	2
1:A:182:LEU:C	1:A:182:LEU:HD13	0.50	2.32	11	1
1:A:85:GLN:N	1:A:85:GLN:OE1	0.50	2.44	19	1
1:A:101:ARG:NH1	1:A:101:ARG:CG	0.50	2.73	6	1
1:A:160:ARG:NH1	1:A:160:ARG:CG	0.50	2.72	15	2
1:A:190:ARG:NH1	1:A:190:ARG:CG	0.50	2.72	17	2
1:A:101:ARG:CG	1:A:101:ARG:HH11	0.50	2.19	6	1
1:A:115:GLU:CG	1:A:116:ASN:N	0.50	2.75	8	1
1:A:96:HIS:O	1:A:96:HIS:ND1	0.50	2.44	15	2
1:A:190:ARG:O	1:A:194:PRO:CG	0.49	2.60	7	13
1:A:173:SER:C	1:A:175:HIS:H	0.49	2.15	12	5
1:A:179:ASP:OD1	1:A:179:ASP:N	0.49	2.45	7	2
1:A:125:GLU:C	1:A:127:LYS:H	0.49	2.13	14	3
1:A:120:TRP:CD1	1:A:181:GLN:HE21	0.49	2.25	16	2
1:A:145:ASP:OD1	1:A:146:TYR:CD2	0.49	2.65	16	1
1:A:173:SER:OG	1:A:175:HIS:NE2	0.49	2.44	1	1
1:A:195:ARG:CG	1:A:195:ARG:NH1	0.49	2.72	4	1
1:A:177:PHE:O	1:A:181:GLN:N	0.49	2.37	3	1
1:A:109:ARG:CG	1:A:109:ARG:HH11	0.49	2.21	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:ASP:O	1:A:96:HIS:N	0.49	2.42	11	1
1:A:196:PHE:O	1:A:198:SER:N	0.49	2.46	16	1
1:A:168:LYS:O	1:A:170:GLN:N	0.49	2.46	15	3
1:A:119:PHE:O	1:A:123:CYS:SG	0.49	2.71	1	4
1:A:169:MET:C	1:A:169:MET:SD	0.49	2.96	3	1
1:A:80:SER:C	1:A:82:GLU:N	0.49	2.69	13	15
1:A:174:ALA:C	1:A:176:THR:H	0.49	2.16	20	3
1:A:157:LEU:O	1:A:158:ASP:CB	0.49	2.61	1	6
1:A:167:LYS:CB	1:A:167:LYS:NZ	0.49	2.76	8	2
1:A:175:HIS:CD2	1:A:178:ASP:OD2	0.49	2.66	14	1
1:A:189:HIS:ND1	1:A:189:HIS:O	0.49	2.45	8	2
1:A:173:SER:OG	1:A:175:HIS:CE1	0.49	2.65	16	1
1:A:109:ARG:HH11	1:A:109:ARG:CG	0.49	2.19	3	2
1:A:147:VAL:O	1:A:148:SER:O	0.49	2.31	19	17
1:A:123:CYS:SG	1:A:181:GLN:CD	0.49	2.96	5	1
1:A:105:ARG:CG	1:A:105:ARG:HH11	0.49	2.21	7	3
1:A:114:GLU:CD	1:A:115:GLU:H	0.49	2.16	7	1
1:A:171:GLU:N	1:A:171:GLU:CD	0.49	2.71	13	1
1:A:190:ARG:CG	1:A:190:ARG:HH11	0.48	2.20	17	1
1:A:170:GLN:O	1:A:171:GLU:C	0.48	2.55	2	2
1:A:109:ARG:CG	1:A:109:ARG:NH1	0.48	2.72	3	2
1:A:129:GLU:CA	1:A:131:ASN:ND2	0.48	2.77	2	3
1:A:162:ARG:O	1:A:166:ASN:ND2	0.48	2.47	3	1
1:A:120:TRP:O	1:A:123:CYS:SG	0.48	2.69	18	2
1:A:114:GLU:O	1:A:116:ASN:N	0.48	2.46	10	2
1:A:160:ARG:CG	1:A:161:VAL:N	0.48	2.76	13	1
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:124:GLU:OE1	1:A:127:LYS:NZ	0.48	2.42	8	1
1:A:181:GLN:CG	1:A:182:LEU:N	0.48	2.77	8	1
1:A:114:GLU:OE1	1:A:114:GLU:N	0.48	2.41	14	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:196:PHE:C	1:A:198:SER:H	0.48	2.16	16	1
1:A:159:SER:O	1:A:161:VAL:N	0.47	2.48	20	7
1:A:196:PHE:C	1:A:198:SER:N	0.47	2.68	16	5
1:A:129:GLU:OE1	1:A:129:GLU:CA	0.47	2.62	14	1
1:A:140:ARG:CG	1:A:140:ARG:NH1	0.47	2.72	14	1
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:159:SER:C	1:A:161:VAL:N	0.47	2.69	20	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:GLU:O	1:A:113:SER:N	0.47	2.46	10	2
1:A:108:LEU:O	1:A:109:ARG:C	0.47	2.57	9	17
1:A:203:ARG:CG	1:A:203:ARG:HH11	0.47	2.22	6	1
1:A:133:HIS:CG	1:A:134:VAL:N	0.47	2.83	19	2
1:A:202:TYR:CD1	1:A:202:TYR:C	0.47	2.92	17	6
1:A:96:HIS:ND1	1:A:96:HIS:N	0.47	2.62	9	2
1:A:173:SER:C	1:A:175:HIS:N	0.47	2.69	15	3
1:A:136:ASP:CG	1:A:140:ARG:NH2	0.47	2.72	3	2
1:A:79:PRO:CD	1:A:83:GLU:OE2	0.47	2.62	7	1
1:A:189:HIS:ND1	1:A:193:TYR:CE1	0.47	2.83	8	1
1:A:170:GLN:N	1:A:170:GLN:CD	0.47	2.73	9	1
1:A:174:ALA:O	1:A:175:HIS:ND1	0.47	2.48	12	1
1:A:109:ARG:C	1:A:109:ARG:CD	0.47	2.88	6	2
1:A:157:LEU:N	1:A:157:LEU:CD2	0.47	2.78	11	1
1:A:182:LEU:C	1:A:182:LEU:CD2	0.47	2.85	2	1
1:A:182:LEU:C	1:A:182:LEU:CD1	0.47	2.88	11	5
1:A:157:LEU:HD13	1:A:158:ASP:N	0.47	2.25	15	1
1:A:110:THR:O	1:A:112:TYR:CD1	0.47	2.68	17	2
1:A:178:ASP:CG	1:A:179:ASP:H	0.47	2.18	18	1
1:A:184:ILE:C	1:A:186:THR:N	0.46	2.72	9	11
1:A:143:TYR:CD1	1:A:143:TYR:O	0.46	2.67	6	2
1:A:96:HIS:CG	1:A:96:HIS:O	0.46	2.69	5	1
1:A:123:CYS:SG	1:A:124:GLU:N	0.46	2.88	8	1
1:A:107:PHE:CZ	1:A:111:GLU:OE1	0.46	2.68	7	1
1:A:157:LEU:O	1:A:158:ASP:CG	0.46	2.58	16	4
1:A:171:GLU:N	1:A:171:GLU:OE2	0.46	2.49	13	1
1:A:178:ASP:CG	1:A:179:ASP:N	0.46	2.73	18	1
1:A:137:GLU:CD	1:A:140:ARG:HH21	0.46	2.18	20	1
1:A:114:GLU:O	1:A:115:GLU:C	0.46	2.58	19	15
1:A:194:PRO:C	1:A:195:ARG:HE	0.46	2.18	19	1
1:A:173:SER:OG	1:A:174:ALA:N	0.46	2.48	7	2
1:A:206:LEU:C	1:A:206:LEU:CD1	0.46	2.89	7	3
1:A:189:HIS:CE1	1:A:190:ARG:NH2	0.46	2.83	12	2
1:A:97:SER:C	1:A:101:ARG:HH21	0.46	2.19	2	1
1:A:175:HIS:N	1:A:175:HIS:ND1	0.46	2.64	2	2
1:A:111:GLU:O	1:A:112:TYR:C	0.46	2.59	7	4
1:A:173:SER:OG	1:A:175:HIS:CD2	0.46	2.68	1	1
1:A:105:ARG:HH21	1:A:118:LEU:CD2	0.46	2.23	7	1
1:A:116:ASN:OD1	1:A:184:ILE:CG2	0.46	2.64	13	2
1:A:168:LYS:NZ	1:A:176:THR:CB	0.46	2.79	14	1
1:A:143:TYR:CE1	1:A:147:VAL:HG11	0.46	2.46	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:SER:O	1:A:174:ALA:O	0.46	2.34	20	3
1:A:114:GLU:C	1:A:116:ASN:N	0.46	2.72	10	2
1:A:196:PHE:CD1	1:A:196:PHE:C	0.45	2.94	10	1
1:A:92:ASP:OD1	1:A:92:ASP:N	0.45	2.49	5	3
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:206:LEU:C	1:A:206:LEU:HD23	0.45	2.35	6	1
1:A:146:TYR:C	1:A:148:SER:N	0.45	2.74	11	2
1:A:95:MET:HE1	1:A:117:MET:SD	0.45	2.51	4	1
1:A:106:ALA:O	1:A:107:PHE:C	0.45	2.59	6	19
1:A:140:ARG:O	1:A:141:LEU:C	0.45	2.60	9	19
1:A:156:SER:O	1:A:157:LEU:C	0.45	2.59	10	1
1:A:199:SER:C	1:A:203:ARG:HH12	0.45	2.19	12	1
1:A:156:SER:OG	1:A:187:LEU:CD1	0.45	2.64	15	1
1:A:168:LYS:C	1:A:170:GLN:N	0.45	2.74	15	1
1:A:193:TYR:N	1:A:194:PRO:HD2	0.45	2.27	17	19
1:A:121:LEU:O	1:A:122:ALA:C	0.45	2.59	13	3
1:A:184:ILE:O	1:A:185:TYR:C	0.45	2.60	11	12
1:A:159:SER:O	1:A:160:ARG:C	0.45	2.60	20	10
1:A:115:GLU:N	1:A:115:GLU:OE2	0.45	2.49	5	2
1:A:143:TYR:C	1:A:143:TYR:CD1	0.45	2.94	11	1
1:A:137:GLU:CD	1:A:137:GLU:N	0.45	2.73	18	1
1:A:100:GLY:O	1:A:101:ARG:C	0.45	2.60	18	17
1:A:141:LEU:N	1:A:141:LEU:CD2	0.45	2.80	4	4
1:A:157:LEU:O	1:A:158:ASP:O	0.45	2.35	8	1
1:A:177:PHE:O	1:A:179:ASP:N	0.45	2.50	1	1
1:A:141:LEU:O	1:A:141:LEU:HD23	0.45	2.11	20	2
1:A:168:LYS:O	1:A:169:MET:C	0.44	2.60	13	14
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:117:MET:O	1:A:118:LEU:C	0.44	2.60	16	5
1:A:141:LEU:HD12	1:A:141:LEU:N	0.44	2.27	17	2
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:189:HIS:ND1	1:A:189:HIS:C	0.44	2.75	11	2
1:A:129:GLU:O	1:A:130:ALA:C	0.44	2.61	6	5
1:A:175:HIS:CD2	1:A:175:HIS:N	0.44	2.84	7	1
1:A:86:SER:OG	1:A:93:LYS:CD	0.44	2.65	16	2
1:A:131:ASN:H	1:A:131:ASN:ND2	0.44	2.10	7	1
1:A:92:ASP:O	1:A:93:LYS:C	0.44	2.61	15	8
1:A:141:LEU:N	1:A:141:LEU:HD22	0.44	2.27	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:120:TRP:NE1	1:A:181:GLN:NE2	0.44	2.65	15	1
1:A:91:PHE:O	1:A:92:ASP:C	0.44	2.60	13	9
1:A:181:GLN:CD	1:A:181:GLN:C	0.44	2.86	1	4
1:A:200:PRO:O	1:A:204:ALA:CB	0.44	2.66	1	4
1:A:128:ALA:O	1:A:129:GLU:C	0.44	2.59	14	3
1:A:192:SER:O	1:A:196:PHE:CB	0.44	2.66	20	5
1:A:124:GLU:CD	1:A:124:GLU:C	0.44	2.86	9	1
1:A:111:GLU:C	1:A:113:SER:N	0.44	2.75	10	2
1:A:177:PHE:O	1:A:180:ALA:N	0.44	2.50	1	2
1:A:173:SER:O	1:A:174:ALA:HB2	0.44	2.13	9	1
1:A:114:GLU:CD	1:A:114:GLU:O	0.44	2.61	15	1
1:A:182:LEU:O	1:A:183:GLN:C	0.44	2.60	6	13
1:A:98:PRO:N	1:A:101:ARG:HH21	0.44	2.10	2	1
1:A:206:LEU:C	1:A:206:LEU:CD2	0.44	2.90	6	1
1:A:115:GLU:O	1:A:116:ASN:C	0.44	2.61	7	2
1:A:138:LYS:O	1:A:139:ALA:C	0.44	2.61	2	9
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:175:HIS:CD2	1:A:175:HIS:C	0.44	2.95	13	1
1:A:157:LEU:O	1:A:158:ASP:OD1	0.44	2.35	15	2
1:A:82:GLU:O	1:A:86:SER:OG	0.43	2.36	17	4
1:A:175:HIS:O	1:A:178:ASP:OD2	0.43	2.36	3	2
1:A:158:ASP:O	1:A:159:SER:CB	0.43	2.64	4	1
1:A:158:ASP:O	1:A:159:SER:OG	0.43	2.36	20	3
1:A:124:GLU:CD	1:A:124:GLU:O	0.43	2.61	15	2
1:A:146:TYR:O	1:A:148:SER:O	0.43	2.37	13	2
1:A:174:ALA:O	1:A:175:HIS:C	0.43	2.61	10	1
1:A:170:GLN:C	1:A:171:GLU:CD	0.43	2.87	17	2
1:A:129:GLU:CG	1:A:130:ALA:H	0.43	2.25	6	1
1:A:95:MET:SD	1:A:185:TYR:OH	0.43	2.77	7	1
1:A:114:GLU:OE1	1:A:114:GLU:C	0.43	2.61	19	2
1:A:145:ASP:OD1	1:A:145:ASP:O	0.43	2.36	12	1
1:A:144:GLU:CD	1:A:144:GLU:C	0.43	2.86	18	1
1:A:175:HIS:ND1	1:A:175:HIS:N	0.43	2.67	19	1
1:A:132:GLN:O	1:A:132:GLN:CD	0.43	2.61	20	1
1:A:128:ALA:O	1:A:129:GLU:CD	0.43	2.62	5	2
1:A:114:GLU:CD	1:A:114:GLU:C	0.43	2.87	4	2
1:A:92:ASP:CG	1:A:93:LYS:H	0.43	2.19	20	2
1:A:130:ALA:O	1:A:131:ASN:O	0.43	2.36	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:ASP:O	1:A:145:ASP:OD1	0.43	2.37	4	6
1:A:158:ASP:O	1:A:159:SER:O	0.43	2.37	5	2
1:A:118:LEU:O	1:A:122:ALA:N	0.43	2.41	16	1
1:A:129:GLU:OE1	1:A:134:VAL:O	0.43	2.37	18	1
1:A:166:ASN:OD1	1:A:166:ASN:O	0.43	2.36	20	1
1:A:118:LEU:O	1:A:119:PHE:C	0.43	2.61	18	6
1:A:178:ASP:O	1:A:179:ASP:C	0.43	2.61	15	7
1:A:175:HIS:O	1:A:178:ASP:OD1	0.43	2.37	18	1
1:A:175:HIS:NE2	1:A:178:ASP:OD1	0.43	2.51	3	1
1:A:157:LEU:O	1:A:158:ASP:C	0.43	2.61	10	1
1:A:135:VAL:O	1:A:139:ALA:CB	0.43	2.67	9	1
1:A:188:MET:O	1:A:189:HIS:C	0.43	2.61	14	2
1:A:115:GLU:OE2	1:A:116:ASN:N	0.43	2.52	2	1
1:A:116:ASN:OD1	1:A:116:ASN:C	0.43	2.61	8	3
1:A:172:PRO:O	1:A:173:SER:OG	0.43	2.33	6	1
1:A:187:LEU:O	1:A:187:LEU:HD23	0.43	2.14	6	2
1:A:124:GLU:OE2	1:A:181:GLN:OE1	0.43	2.37	8	1
1:A:158:ASP:O	1:A:158:ASP:OD1	0.43	2.37	11	1
1:A:163:GLU:CD	1:A:163:GLU:C	0.43	2.87	15	1
1:A:113:SER:O	1:A:113:SER:OG	0.43	2.37	17	1
1:A:100:GLY:C	1:A:102:SER:H	0.42	2.21	7	11
1:A:137:GLU:CD	1:A:137:GLU:C	0.42	2.87	5	1
1:A:144:GLU:O	1:A:148:SER:OG	0.42	2.36	11	2
1:A:141:LEU:N	1:A:141:LEU:CD1	0.42	2.81	17	2
1:A:162:ARG:O	1:A:166:ASN:CG	0.42	2.62	12	1
1:A:157:LEU:C	1:A:158:ASP:OD1	0.42	2.62	14	1
1:A:168:LYS:HZ2	1:A:176:THR:CB	0.42	2.27	14	1
1:A:128:ALA:C	1:A:129:GLU:CD	0.42	2.87	1	4
1:A:195:ARG:O	1:A:196:PHE:C	0.42	2.62	16	4
1:A:141:LEU:O	1:A:145:ASP:CG	0.42	2.62	11	5
1:A:191:ASP:OD1	1:A:195:ARG:NH2	0.42	2.52	13	1
1:A:131:ASN:O	1:A:132:GLN:CD	0.42	2.62	19	1
1:A:170:GLN:O	1:A:171:GLU:CD	0.42	2.62	19	1
1:A:171:GLU:O	1:A:171:GLU:CD	0.42	2.62	3	1
1:A:132:GLN:O	1:A:132:GLN:NE2	0.42	2.52	4	1
1:A:98:PRO:O	1:A:102:SER:OG	0.42	2.38	6	1
1:A:125:GLU:O	1:A:129:GLU:OE1	0.42	2.37	7	1
1:A:80:SER:O	1:A:83:GLU:OE1	0.42	2.38	10	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:181:GLN:CD	1:A:181:GLN:O	0.42	2.62	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:LEU:HD12	1:A:129:GLU:OE2	0.42	2.15	18	1
1:A:179:ASP:OD1	1:A:179:ASP:C	0.42	2.62	19	1
1:A:127:LYS:C	1:A:129:GLU:H	0.42	2.23	2	1
1:A:105:ARG:NH2	1:A:118:LEU:CD2	0.42	2.83	7	1
1:A:82:GLU:O	1:A:86:SER:CB	0.42	2.67	13	2
1:A:186:THR:CG2	1:A:190:ARG:NH2	0.42	2.82	15	1
1:A:145:ASP:CG	1:A:146:TYR:CD2	0.42	2.98	16	1
1:A:173:SER:O	1:A:173:SER:OG	0.42	2.31	20	1
1:A:125:GLU:O	1:A:126:LEU:C	0.42	2.62	18	2
1:A:144:GLU:C	1:A:148:SER:OG	0.42	2.63	11	1
1:A:113:SER:C	1:A:115:GLU:OE2	0.42	2.62	12	1
1:A:115:GLU:C	1:A:115:GLU:CD	0.42	2.86	2	1
1:A:125:GLU:O	1:A:128:ALA:N	0.42	2.41	10	1
1:A:114:GLU:O	1:A:114:GLU:OE2	0.42	2.37	11	1
1:A:160:ARG:CD	1:A:160:ARG:C	0.42	2.92	15	1
1:A:136:ASP:O	1:A:137:GLU:C	0.42	2.62	10	5
1:A:181:GLN:C	1:A:181:GLN:OE1	0.42	2.63	15	2
1:A:130:ALA:O	1:A:131:ASN:CG	0.42	2.62	12	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:178:ASP:O	1:A:182:LEU:N	0.42	2.49	17	1
1:A:129:GLU:CG	1:A:130:ALA:N	0.42	2.83	6	1
1:A:143:TYR:CD1	1:A:143:TYR:C	0.42	2.96	6	2
1:A:195:ARG:O	1:A:199:SER:OG	0.42	2.36	14	2
1:A:184:ILE:HG22	1:A:188:MET:SD	0.42	2.55	19	1
1:A:105:ARG:NH2	1:A:118:LEU:HD23	0.41	2.30	7	1
1:A:124:GLU:OE2	1:A:124:GLU:O	0.41	2.38	9	1
1:A:133:HIS:CD2	1:A:133:HIS:H	0.41	2.32	13	1
1:A:170:GLN:O	1:A:171:GLU:OE2	0.41	2.38	19	2
1:A:131:ASN:O	1:A:132:GLN:OE1	0.41	2.37	19	1
1:A:175:HIS:CE1	1:A:178:ASP:CG	0.41	2.98	18	1
1:A:83:GLU:CD	1:A:83:GLU:H	0.41	2.23	19	1
1:A:184:ILE:CG2	1:A:185:TYR:N	0.41	2.84	4	1
1:A:127:LYS:NZ	1:A:127:LYS:CB	0.41	2.83	12	1
1:A:175:HIS:O	1:A:178:ASP:CG	0.41	2.63	10	1
1:A:174:ALA:C	1:A:175:HIS:ND1	0.41	2.78	12	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: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:105:ARG:NH1	1:A:114:GLU:OE1	0.41	2.54	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:SER:O	1:A:174:ALA:C	0.41	2.62	11	2
1:A:157:LEU:C	1:A:158:ASP:CG	0.41	2.88	9	2
1:A:120:TRP:HE1	1:A:181:GLN:HE21	0.41	1.58	16	1
1:A:146:TYR:O	1:A:147:VAL:CG2	0.41	2.68	19	1
1:A:95:MET:C	1:A:97:SER:H	0.41	2.24	15	1
1:A:188:MET:O	1:A:192:SER:OG	0.40	2.34	13	1
1:A:115:GLU:OE1	1:A:146:TYR:OH	0.40	2.36	14	1
1:A:175:HIS:O	1:A:175:HIS:CG	0.40	2.73	15	1
1:A:82:GLU:O	1:A:83:GLU:C	0.40	2.63	19	1
1:A:116:ASN:OD1	1:A:116:ASN:N	0.40	2.53	5	2
1:A:175:HIS:C	1:A:175:HIS:ND1	0.40	2.80	10	1
1:A:199:SER:C	1:A:203:ARG:NH1	0.40	2.80	12	1
1:A:138:LYS:C	1:A:140:ARG:N	0.40	2.78	17	1
1:A:159:SER:O	1:A:162:ARG:N	0.40	2.52	2	1
1:A:95:MET:SD	1:A:185:TYR:CE1	0.40	3.14	7	1
1:A:189:HIS:CD2	1:A:190:ARG:NH2	0.40	2.89	13	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%)	16±2 (14±2%)	9±2 (8±2%)	1	14
All	All	2380/3040 (78%)	1863 (78%)	330 (14%)	187 (8%)	1	14

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	111	GLU	17
1	A	131	ASN	17
1	A	101	ARG	17
1	A	147	VAL	16

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Mol	Chain	Res	Type	Models (Total)
1	A	158	ASP	15
1	A	173	SER	14
1	A	156	SER	11
1	A	81	PRO	9
1	A	132	GLN	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	178	ASP	1
1	A	112	TYR	1
1	A	115	GLU	1
1	A	157	LEU	1
1	A	129	GLU	1
1	A	197	LEU	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±3 (91±2%)	10±3 (9±2%)	10	56
All	All	2180/2680 (81%)	1976 (91%)	204 (9%)	10	56

All 50 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	84	VAL	16
1	A	131	ASN	16
1	A	104	PHE	12
1	A	187	LEU	11
1	A	134	VAL	10
1	A	169	MET	8

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Mol	Chain	Res	Type	Models (Total)
1	A	167	LYS	6
1	A	109	ARG	6
1	A	118	LEU	6
1	A	160	ARG	6
1	A	90	SER	5
1	A	158	ASP	5
1	A	182	LEU	5
1	A	95	MET	4
1	A	126	LEU	4
1	A	115	GLU	3
1	A	193	TYR	3
1	A	132	GLN	3
1	A	138	LYS	3
1	A	184	ILE	3
1	A	105	ARG	3
1	A	206	LEU	3
1	A	117	MET	3
1	A	148	SER	3
1	A	110	THR	2
1	A	166	ASN	2
1	A	176	THR	2
1	A	195	ARG	2
1	A	203	ARG	2
1	A	129	GLU	2
1	A	114	GLU	2
1	A	162	ARG	2
1	A	175	HIS	2
1	A	205	LEU	2
1	A	140	ARG	2
1	A	116	ASN	2
1	A	82	GLU	1
1	A	121	LEU	1
1	A	96	HIS	1
1	A	101	ARG	1
1	A	127	LYS	1
1	A	161	VAL	1
1	A	181	GLN	1
1	A	168	LYS	1
1	A	157	LEU	1
1	A	147	VAL	1
1	A	190	ARG	1
1	A	85	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	156	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided