



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 09:31 PM UTC

PDB ID : 2P01 / pdb_00002p01
Title : The structure of receptor-associated protein(RAP)
Authors : Lee, D.; Walsh, J.D.; Migliorini, M.; Yu, P.; Cai, T.; Schwieters, C.D.; Krueger, S.; Strickland, D.K.; Wang, Y.X.
Deposited on : 2007-02-28

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

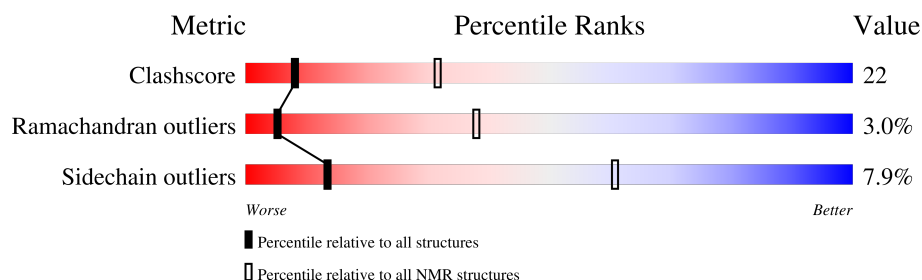
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

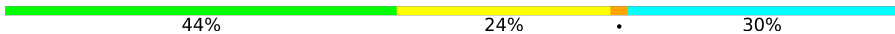
The overall completeness of chemical shifts assignment was not calculated.

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	323	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:20-A:64, A:71-A:90 (65)	0.45	1
2	A:117-A:155, A:189-A:211 (62)	0.60	9
3	A:219-A:317 (99)	1.02	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5325 atoms, of which 2659 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-2-macroglobulin receptor-associated protein.

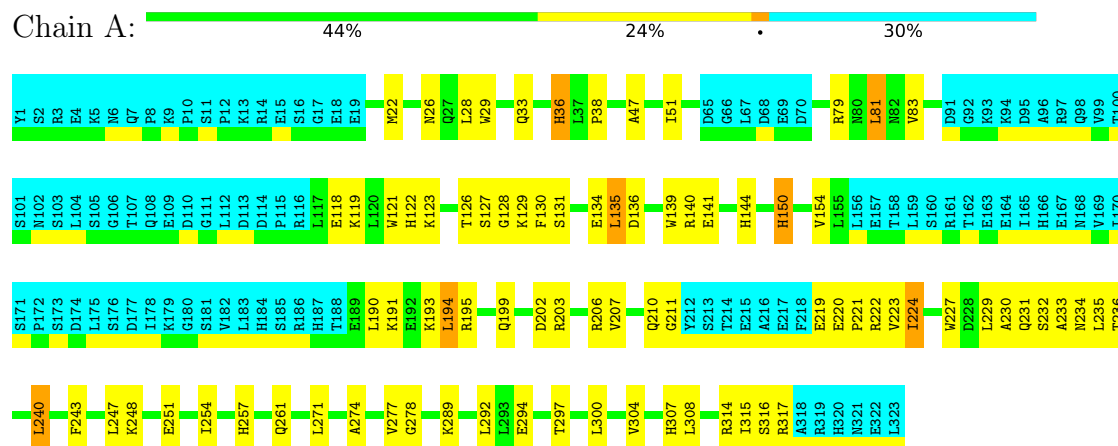
Mol	Chain	Residues	Atoms						Trace
1	A	323	Total	C	H	N	O	S	0
			5325	1655	2659	501	509	1	

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: Alpha-2-macroglobulin receptor-associated protein

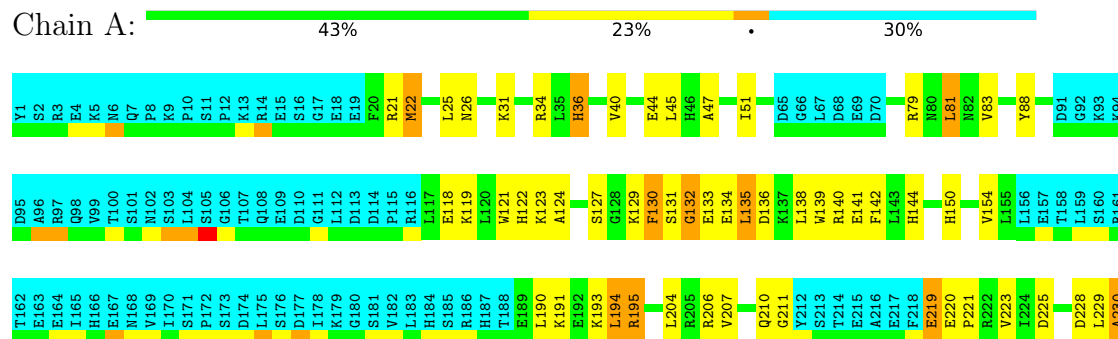


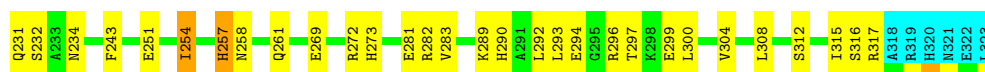
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

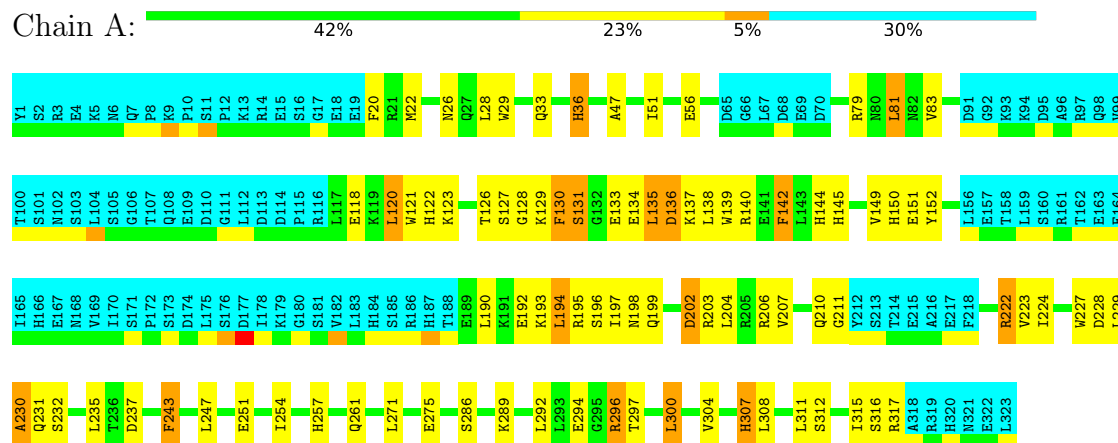
- Molecule 1: Alpha-2-macroglobulin receptor-associated protein





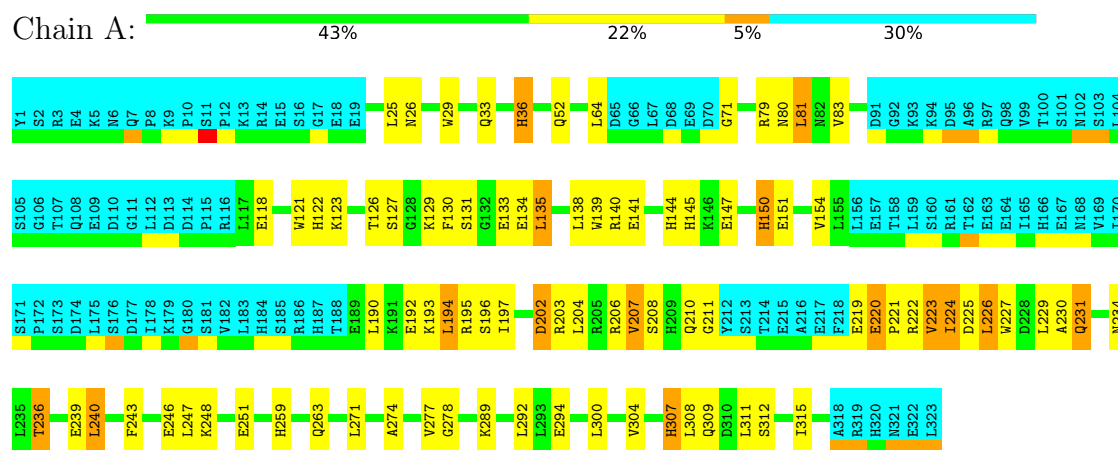
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



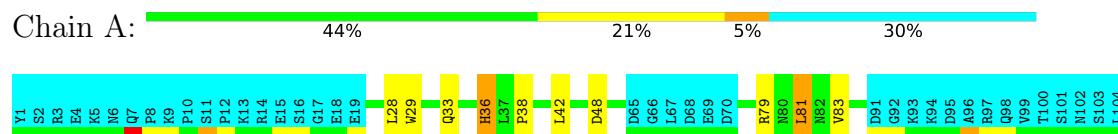
4.2.3 Score per residue for model 3

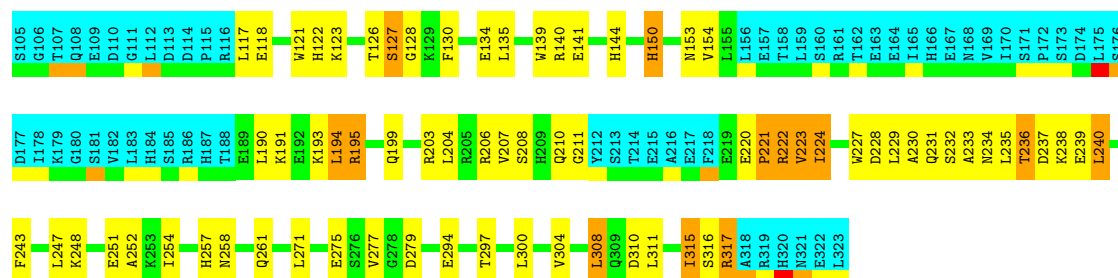
- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



4.2.4 Score per residue for model 4

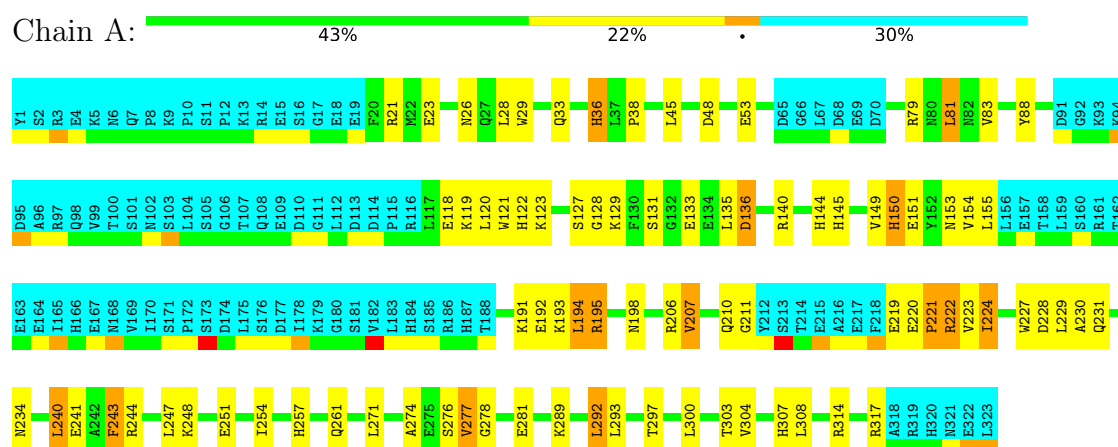
- Molecule 1: Alpha-2-macroglobulin receptor-associated protein





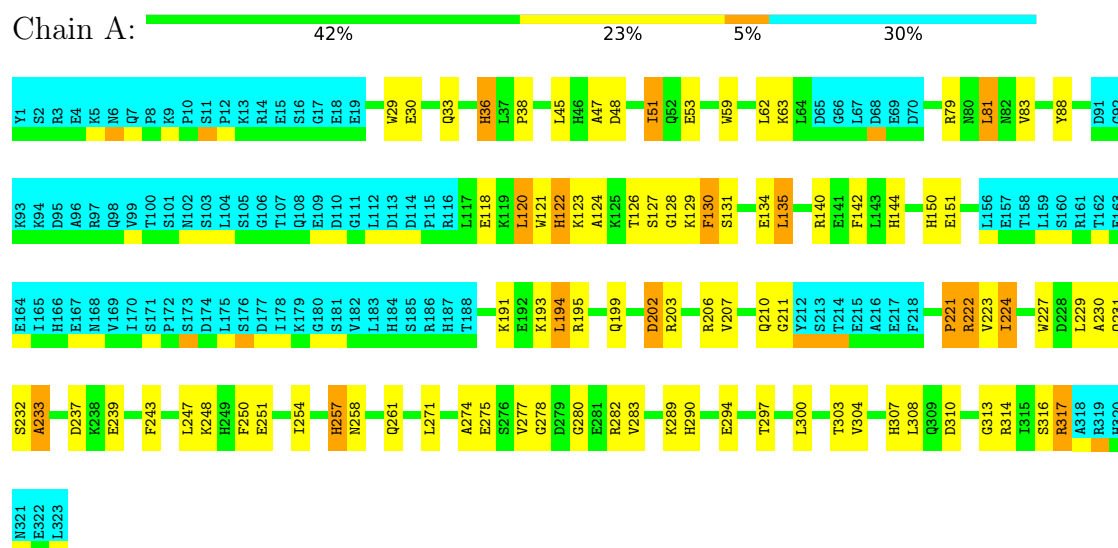
4.2.5 Score per residue for model 5

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



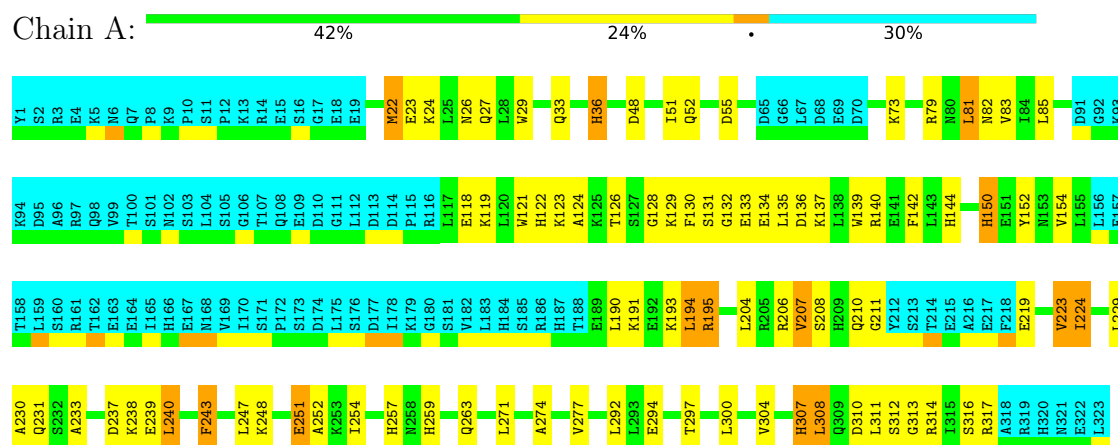
4.2.6 Score per residue for model 6

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



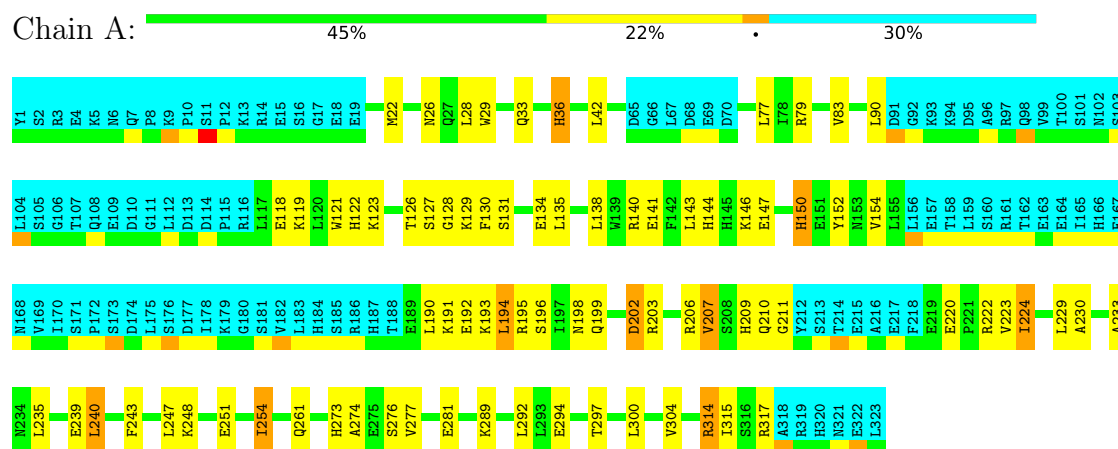
4.2.7 Score per residue for model 7

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



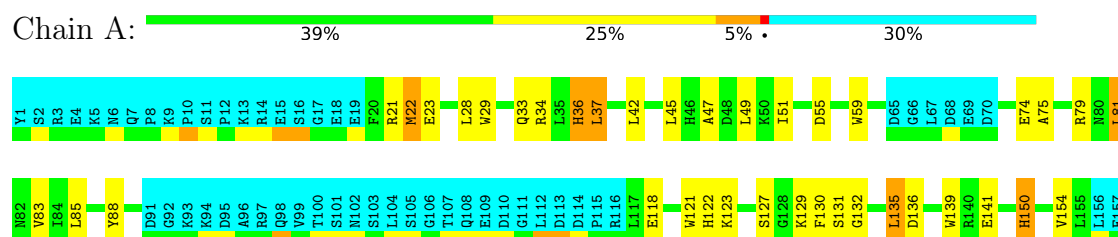
4.2.8 Score per residue for model 8

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



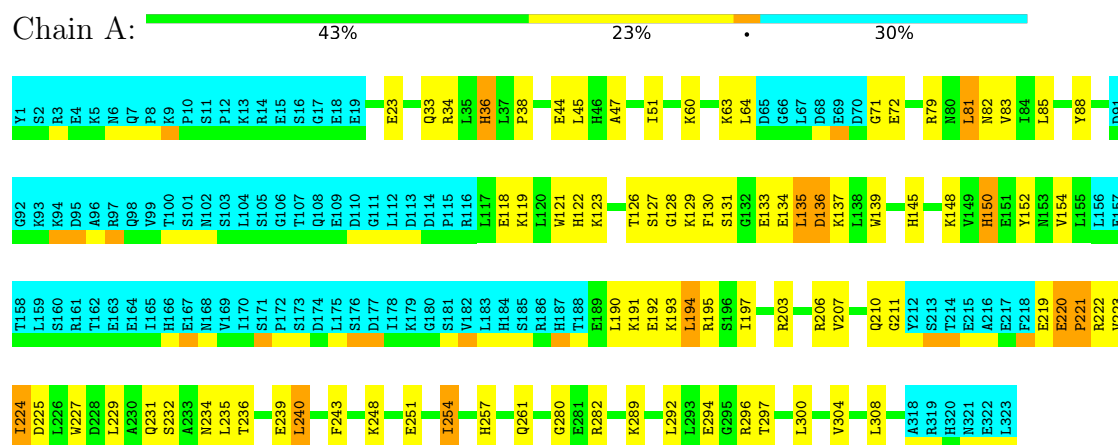
4.2.9 Score per residue for model 9

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



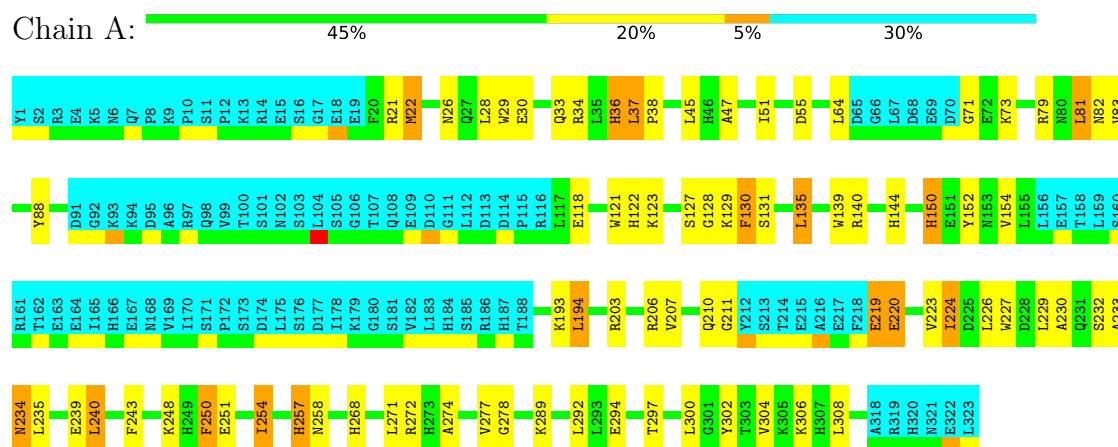
4.2.12 Score per residue for model 12

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



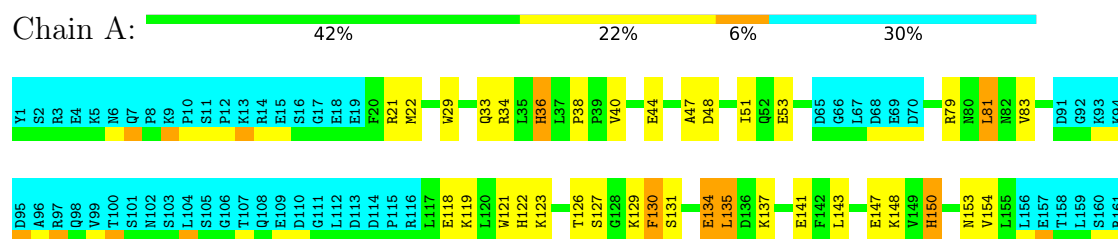
4.2.13 Score per residue for model 13

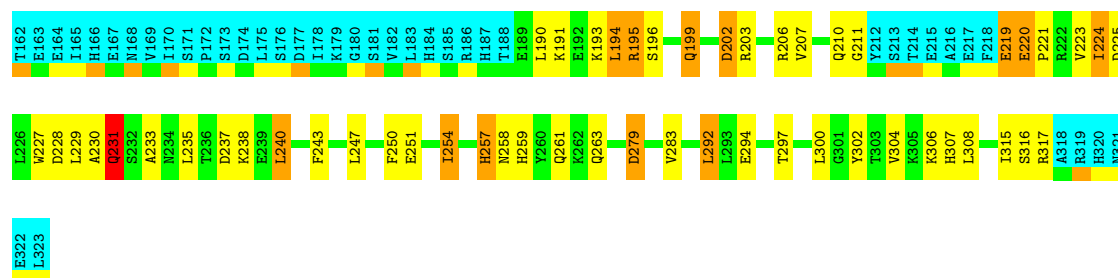
- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



4.2.14 Score per residue for model 14

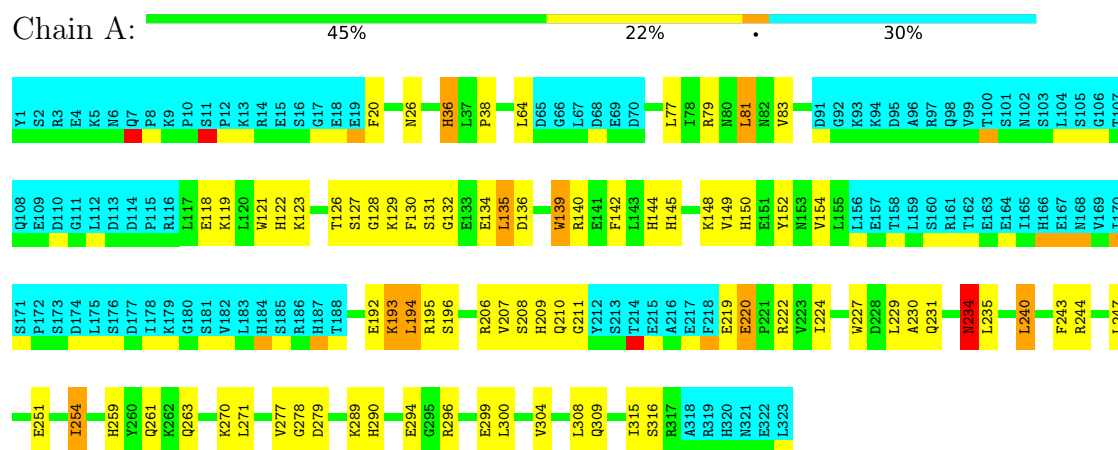
- Molecule 1: Alpha-2-macroglobulin receptor-associated protein





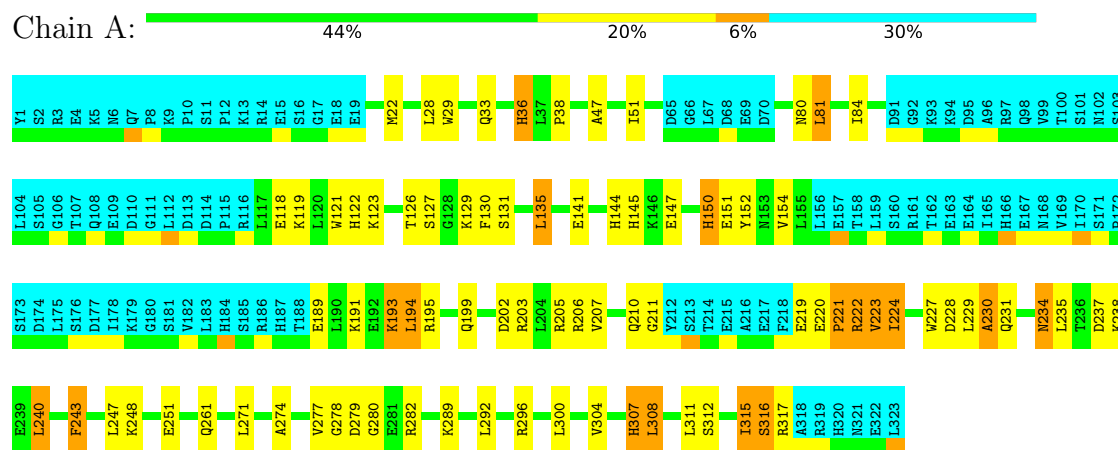
4.2.15 Score per residue for model 15

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



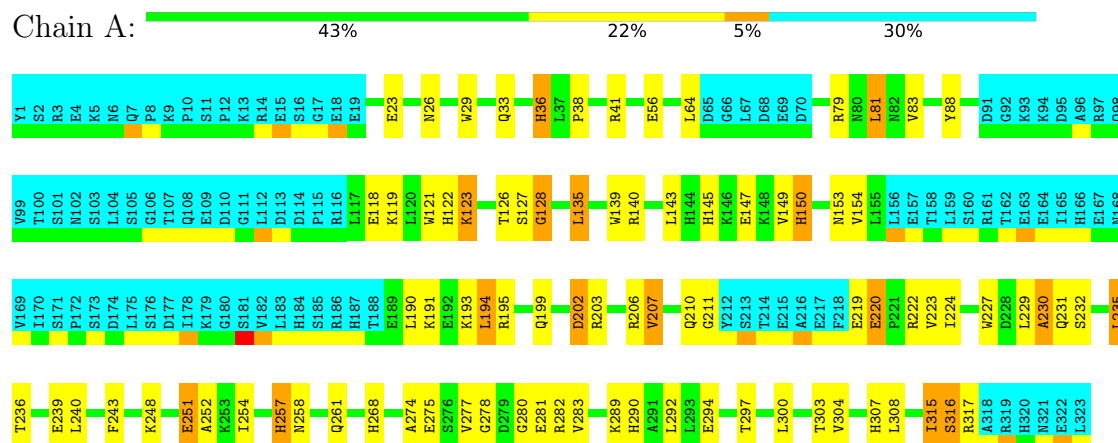
4.2.16 Score per residue for model 16

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



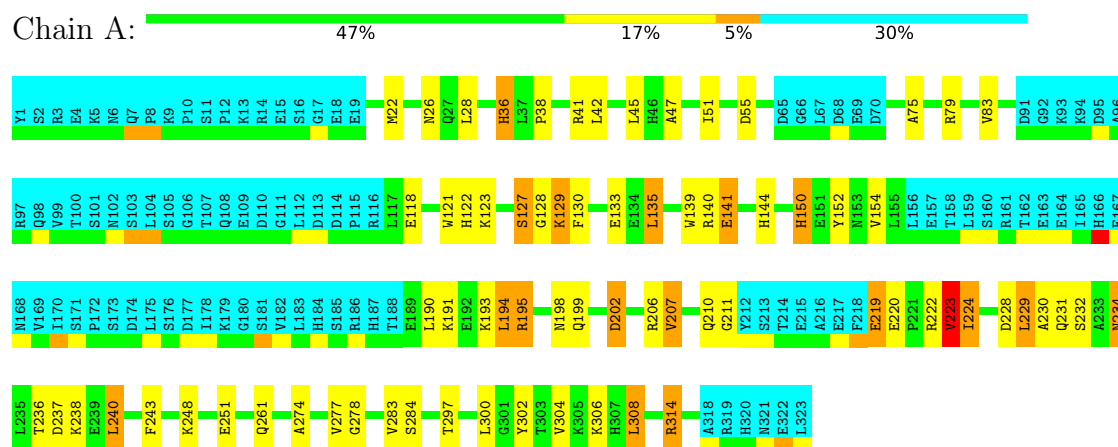
4.2.17 Score per residue for model 17

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



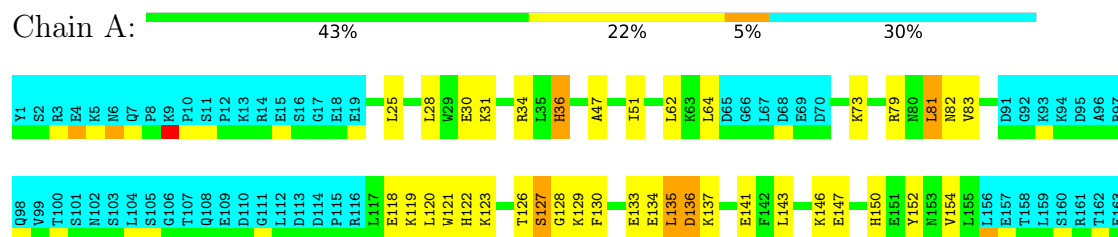
4.2.18 Score per residue for model 18

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



4.2.19 Score per residue for model 19

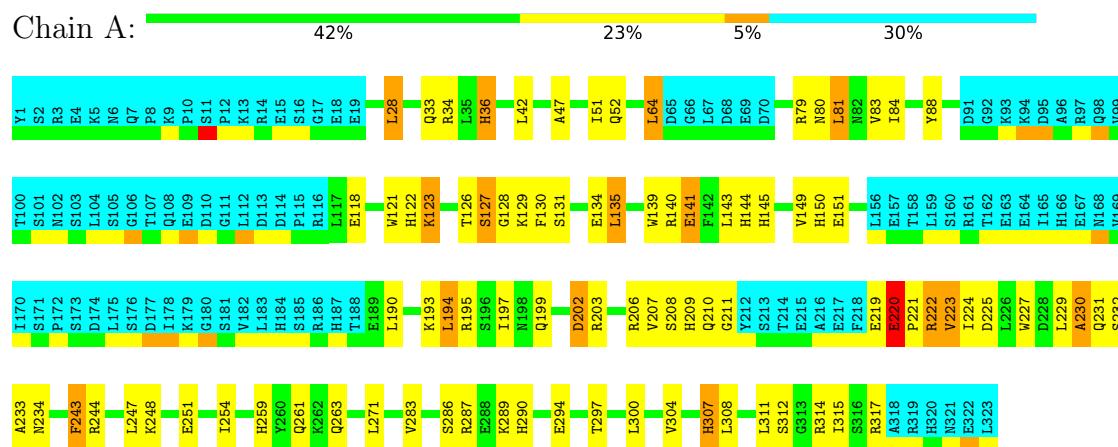
- Molecule 1: Alpha-2-macroglobulin receptor-associated protein





4.2.20 Score per residue for model 20

- Molecule 1: Alpha-2-macroglobulin receptor-associated protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SANS measurement*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *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
X-PLOR	refinement	3

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	0.65±0.01	0±0/1937 (0.0± 0.0%)	1.08±0.01	1±0/2591 (0.0± 0.0%)
All	All	0.65	0/38740 (0.0%)	1.08	15/51820 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	150	HIS	CA-CB-CG	-5.78	108.02	113.80	11	14
1	A	122	HIS	CA-CB-CG	-5.15	108.65	113.80	6	1

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	1901	1946	1946	85±9
All	All	38020	38920	38920	1694

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:GLY:O	1:A:130:PHE:N	1.15	1.76	7	3
1:A:223:VAL:HG13	1:A:224:ILE:H	1.01	1.16	7	8
1:A:141:GLU:O	1:A:144:HIS:ND1	0.93	2.02	16	1
1:A:202:ASP:OD1	1:A:203:ARG:N	0.90	2.03	16	8
1:A:48:ASP:O	1:A:51:ILE:HG22	0.87	1.69	7	1
1:A:134:GLU:H	1:A:134:GLU:CD	0.87	1.77	14	2
1:A:199:GLN:O	1:A:202:ASP:OD1	0.85	1.94	16	2
1:A:124:ALA:HB1	1:A:130:PHE:CG	0.84	2.07	1	1
1:A:230:ALA:O	1:A:235:LEU:HD21	0.82	1.73	19	2
1:A:124:ALA:O	1:A:128:GLY:O	0.82	1.97	7	1
1:A:120:LEU:HD22	1:A:142:PHE:CZ	0.81	2.11	2	1
1:A:153:ASN:OD1	1:A:154:VAL:N	0.80	2.14	4	1
1:A:194:LEU:HD12	1:A:194:LEU:C	0.80	2.01	12	20
1:A:219:GLU:O	1:A:223:VAL:HG11	0.79	1.78	3	1
1:A:129:LYS:O	1:A:131:SER:N	0.79	2.16	9	15
1:A:264:LEU:HD21	1:A:294:GLU:OE1	0.79	1.77	11	1
1:A:62:LEU:C	1:A:62:LEU:HD12	0.78	2.03	11	1
1:A:121:TRP:CE2	1:A:135:LEU:HD13	0.78	2.14	1	12
1:A:223:VAL:HG13	1:A:224:ILE:N	0.77	1.94	7	10
1:A:206:ARG:O	1:A:210:GLN:N	0.77	2.17	6	20
1:A:235:LEU:N	1:A:235:LEU:HD12	0.77	1.95	19	3
1:A:150:HIS:O	1:A:154:VAL:HG23	0.75	1.82	16	17
1:A:220:GLU:O	1:A:223:VAL:HG12	0.75	1.80	16	3
1:A:276:SER:O	1:A:278:GLY:N	0.75	2.19	5	1
1:A:33:GLN:O	1:A:36:HIS:CD2	0.75	2.39	9	7
1:A:274:ALA:O	1:A:277:VAL:HG22	0.75	1.81	7	1
1:A:150:HIS:CD2	1:A:150:HIS:C	0.74	2.66	20	6
1:A:145:HIS:O	1:A:149:VAL:HG22	0.74	1.82	15	2
1:A:231:GLN:O	1:A:240:LEU:HD21	0.73	1.83	15	5
1:A:141:GLU:OE1	1:A:204:LEU:HD21	0.73	1.84	1	5
1:A:79:ARG:O	1:A:83:VAL:HG23	0.72	1.84	2	19
1:A:248:LYS:O	1:A:251:GLU:HG3	0.72	1.84	7	7
1:A:81:LEU:C	1:A:81:LEU:HD13	0.72	2.09	10	1
1:A:26:ASN:OD1	1:A:27:GLN:N	0.72	2.22	7	1
1:A:147:GLU:O	1:A:150:HIS:CD2	0.72	2.42	10	3
1:A:222:ARG:O	1:A:225:ASP:N	0.71	2.23	20	1
1:A:144:HIS:CD2	1:A:145:HIS:N	0.71	2.59	16	1
1:A:23:GLU:H	1:A:23:GLU:CD	0.70	1.94	5	1
1:A:240:LEU:O	1:A:240:LEU:HD13	0.70	1.86	11	12
1:A:207:VAL:O	1:A:211:GLY:N	0.70	2.25	15	19
1:A:271:LEU:C	1:A:271:LEU:HD23	0.70	2.12	9	2
1:A:23:GLU:O	1:A:26:ASN:OD1	0.69	2.11	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:HIS:CD2	1:A:151:GLU:N	0.69	2.61	3	6
1:A:77:LEU:C	1:A:77:LEU:HD23	0.69	2.13	15	1
1:A:128:GLY:C	1:A:130:PHE:N	0.68	2.50	7	5
1:A:233:ALA:H	1:A:235:LEU:HD11	0.68	1.47	19	1
1:A:150:HIS:O	1:A:153:ASN:OD1	0.68	2.11	4	2
1:A:29:TRP:CD1	1:A:33:GLN:HE21	0.68	2.06	5	11
1:A:21:ARG:NH2	1:A:53:GLU:OE2	0.68	2.27	14	2
1:A:124:ALA:HB1	1:A:130:PHE:CD2	0.68	2.23	1	1
1:A:144:HIS:CE1	1:A:145:HIS:CD2	0.68	2.82	16	1
1:A:314:ARG:HE	1:A:314:ARG:N	0.67	1.88	18	1
1:A:118:GLU:OE1	1:A:122:HIS:NE2	0.67	2.26	6	1
1:A:143:LEU:O	1:A:146:LYS:HG2	0.67	1.88	8	2
1:A:23:GLU:N	1:A:23:GLU:OE1	0.67	2.28	17	1
1:A:314:ARG:N	1:A:314:ARG:NE	0.67	2.42	18	1
1:A:119:LYS:O	1:A:123:LYS:HB2	0.66	1.90	8	10
1:A:280:GLY:O	1:A:282:ARG:N	0.66	2.28	11	6
1:A:314:ARG:O	1:A:317:ARG:O	0.66	2.13	7	3
1:A:230:ALA:O	1:A:235:LEU:HD11	0.66	1.91	17	1
1:A:314:ARG:NE	1:A:314:ARG:N	0.66	2.44	11	2
1:A:144:HIS:NE2	1:A:145:HIS:CD2	0.65	2.64	16	1
1:A:228:ASP:O	1:A:231:GLN:CG	0.65	2.44	14	4
1:A:223:VAL:HG11	1:A:308:LEU:HD21	0.65	1.68	10	1
1:A:145:HIS:O	1:A:149:VAL:HG13	0.65	1.91	15	2
1:A:229:LEU:O	1:A:232:SER:N	0.65	2.30	1	7
1:A:42:LEU:C	1:A:42:LEU:HD23	0.65	2.16	4	1
1:A:29:TRP:NE1	1:A:33:GLN:NE2	0.65	2.45	13	9
1:A:229:LEU:C	1:A:231:GLN:H	0.65	1.99	7	4
1:A:45:LEU:HD13	1:A:88:TYR:OH	0.64	1.91	12	5
1:A:274:ALA:O	1:A:277:VAL:HG12	0.64	1.92	16	10
1:A:235:LEU:HD12	1:A:235:LEU:H	0.64	1.51	19	1
1:A:60:LYS:O	1:A:63:LYS:HG2	0.64	1.93	12	1
1:A:315:ILE:HG22	1:A:316:SER:N	0.64	2.05	19	2
1:A:64:LEU:HD13	1:A:64:LEU:O	0.64	1.91	20	1
1:A:315:ILE:O	1:A:317:ARG:N	0.64	2.30	16	4
1:A:224:ILE:HD11	1:A:250:PHE:CE1	0.64	2.28	13	1
1:A:224:ILE:HD11	1:A:250:PHE:CZ	0.64	2.27	13	1
1:A:287:ARG:NH2	1:A:290:HIS:CG	0.64	2.66	11	1
1:A:223:VAL:HG22	1:A:224:ILE:N	0.64	2.08	3	3
1:A:243:PHE:C	1:A:243:PHE:CD1	0.63	2.76	5	16
1:A:223:VAL:CG1	1:A:224:ILE:H	0.63	2.00	7	5
1:A:131:SER:O	1:A:133:GLU:N	0.63	2.31	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:ASP:OD1	1:A:202:ASP:C	0.63	2.40	9	10
1:A:144:HIS:CD2	1:A:144:HIS:C	0.63	2.76	16	1
1:A:221:PRO:O	1:A:222:ARG:CB	0.63	2.47	16	6
1:A:220:GLU:O	1:A:221:PRO:O	0.63	2.15	5	2
1:A:118:GLU:O	1:A:122:HIS:CD2	0.63	2.52	7	20
1:A:150:HIS:O	1:A:154:VAL:CG2	0.63	2.46	18	17
1:A:294:GLU:O	1:A:297:THR:OG1	0.63	2.17	2	11
1:A:26:ASN:OD1	1:A:26:ASN:C	0.62	2.42	7	3
1:A:281:GLU:C	1:A:283:VAL:H	0.62	2.02	1	2
1:A:271:LEU:O	1:A:271:LEU:HD23	0.62	1.93	15	8
1:A:219:GLU:O	1:A:223:VAL:CG1	0.62	2.48	3	1
1:A:314:ARG:N	1:A:314:ARG:HE	0.62	1.91	11	2
1:A:130:PHE:HA	1:A:134:GLU:HG3	0.62	1.71	14	1
1:A:221:PRO:O	1:A:223:VAL:N	0.62	2.33	10	1
1:A:29:TRP:NE1	1:A:33:GLN:HE21	0.61	1.93	13	6
1:A:121:TRP:CE3	1:A:135:LEU:HD22	0.61	2.30	2	15
1:A:257:HIS:HB2	1:A:300:LEU:HD23	0.61	1.72	7	1
1:A:234:ASN:O	1:A:235:LEU:HB2	0.61	1.96	4	2
1:A:194:LEU:C	1:A:194:LEU:CD1	0.61	2.72	5	20
1:A:140:ARG:O	1:A:144:HIS:CG	0.61	2.54	7	11
1:A:296:ARG:HE	1:A:296:ARG:C	0.61	2.04	16	1
1:A:81:LEU:O	1:A:81:LEU:HD13	0.60	1.95	16	17
1:A:292:LEU:O	1:A:292:LEU:HD12	0.60	1.96	19	5
1:A:28:LEU:O	1:A:28:LEU:HD13	0.60	1.96	20	1
1:A:34:ARG:O	1:A:36:HIS:CE1	0.60	2.54	12	5
1:A:75:ALA:HB1	1:A:79:ARG:NH1	0.60	2.11	18	2
1:A:302:TYR:OH	1:A:306:LYS:NZ	0.60	2.34	11	3
1:A:315:ILE:O	1:A:316:SER:C	0.60	2.41	1	8
1:A:277:VAL:HG13	1:A:279:ASP:H	0.60	1.56	16	1
1:A:309:GLN:OE1	1:A:309:GLN:N	0.60	2.35	19	1
1:A:123:LYS:O	1:A:127:SER:CB	0.60	2.49	8	18
1:A:221:PRO:O	1:A:222:ARG:HB2	0.60	1.95	5	2
1:A:251:GLU:OE1	1:A:252:ALA:N	0.60	2.35	17	2
1:A:223:VAL:HG21	1:A:308:LEU:HD11	0.60	1.73	7	1
1:A:62:LEU:C	1:A:62:LEU:CD1	0.59	2.73	11	1
1:A:144:HIS:CG	1:A:145:HIS:N	0.59	2.70	16	1
1:A:307:HIS:NE2	1:A:311:LEU:HD13	0.59	2.12	19	1
1:A:219:GLU:O	1:A:220:GLU:C	0.59	2.45	9	2
1:A:147:GLU:O	1:A:150:HIS:HD2	0.59	1.80	10	3
1:A:207:VAL:O	1:A:211:GLY:CA	0.59	2.50	18	20
1:A:123:LYS:O	1:A:127:SER:OG	0.59	2.20	12	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:275:GLU:OE2	1:A:283:VAL:HG13	0.59	1.97	17	2
1:A:64:LEU:O	1:A:64:LEU:HD23	0.59	1.97	15	4
1:A:230:ALA:O	1:A:233:ALA:N	0.59	2.35	4	2
1:A:131:SER:O	1:A:134:GLU:N	0.59	2.35	1	1
1:A:230:ALA:O	1:A:231:GLN:C	0.58	2.47	3	5
1:A:141:GLU:OE1	1:A:141:GLU:N	0.58	2.36	14	3
1:A:29:TRP:CD1	1:A:33:GLN:NE2	0.58	2.71	17	10
1:A:241:GLU:OE2	1:A:244:ARG:NH2	0.58	2.36	5	1
1:A:22:MET:O	1:A:26:ASN:ND2	0.58	2.37	10	6
1:A:150:HIS:O	1:A:154:VAL:CB	0.58	2.52	4	14
1:A:307:HIS:O	1:A:311:LEU:CB	0.58	2.52	16	5
1:A:239:GLU:N	1:A:239:GLU:OE1	0.58	2.36	4	1
1:A:199:GLN:O	1:A:202:ASP:OD2	0.58	2.21	11	8
1:A:236:THR:H	1:A:239:GLU:CD	0.58	2.06	4	1
1:A:130:PHE:CE1	1:A:134:GLU:OE1	0.58	2.56	2	1
1:A:229:LEU:O	1:A:230:ALA:C	0.58	2.47	14	14
1:A:234:ASN:CG	1:A:235:LEU:H	0.58	2.06	16	2
1:A:283:VAL:CG1	1:A:287:ARG:NH1	0.58	2.66	20	1
1:A:290:HIS:CE1	1:A:294:GLU:OE2	0.57	2.57	1	1
1:A:261:GLN:HE21	1:A:297:THR:CG2	0.57	2.12	4	7
1:A:239:GLU:CD	1:A:240:LEU:N	0.57	2.62	4	1
1:A:280:GLY:C	1:A:282:ARG:H	0.57	2.06	16	1
1:A:257:HIS:NE2	1:A:261:GLN:CD	0.57	2.63	14	1
1:A:237:ASP:N	1:A:239:GLU:OE1	0.57	2.38	4	1
1:A:131:SER:HA	1:A:135:LEU:HD12	0.57	1.76	12	2
1:A:138:LEU:HD13	1:A:141:GLU:OE2	0.57	2.00	8	1
1:A:223:VAL:CG2	1:A:224:ILE:N	0.57	2.66	8	2
1:A:195:ARG:NH1	1:A:199:GLN:HE22	0.57	1.98	11	1
1:A:250:PHE:CE2	1:A:307:HIS:CE1	0.56	2.93	14	1
1:A:136:ASP:CG	1:A:137:LYS:N	0.56	2.62	2	2
1:A:277:VAL:HG13	1:A:278:GLY:N	0.56	2.15	17	10
1:A:220:GLU:O	1:A:222:ARG:N	0.56	2.38	4	3
1:A:62:LEU:HD12	1:A:62:LEU:O	0.56	2.00	11	1
1:A:229:LEU:HD22	1:A:229:LEU:N	0.56	2.15	14	1
1:A:124:ALA:C	1:A:130:PHE:HB2	0.56	2.25	1	1
1:A:133:GLU:N	1:A:133:GLU:OE1	0.56	2.39	2	2
1:A:229:LEU:O	1:A:231:GLN:N	0.56	2.39	7	9
1:A:130:PHE:CG	1:A:134:GLU:OE1	0.56	2.58	6	1
1:A:220:GLU:C	1:A:222:ARG:H	0.56	2.08	12	1
1:A:136:ASP:OD1	1:A:136:ASP:C	0.56	2.48	19	4
1:A:121:TRP:CZ2	1:A:135:LEU:HD13	0.56	2.36	18	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:GLY:O	1:A:130:PHE:CD1	0.56	2.58	20	2
1:A:250:PHE:CZ	1:A:307:HIS:NE2	0.56	2.74	14	1
1:A:152:TYR:CE1	1:A:193:LYS:NZ	0.56	2.67	15	1
1:A:223:VAL:HG23	1:A:224:ILE:N	0.56	2.14	8	1
1:A:21:ARG:C	1:A:22:MET:SD	0.56	2.89	9	4
1:A:195:ARG:NE	1:A:199:GLN:NE2	0.55	2.54	2	1
1:A:276:SER:O	1:A:277:VAL:C	0.55	2.48	5	1
1:A:275:GLU:OE2	1:A:287:ARG:NH2	0.55	2.39	9	1
1:A:231:GLN:CG	1:A:232:SER:N	0.55	2.69	2	3
1:A:223:VAL:CG2	1:A:308:LEU:HD21	0.55	2.31	18	2
1:A:149:VAL:HG13	1:A:150:HIS:N	0.55	2.16	10	2
1:A:314:ARG:O	1:A:315:ILE:O	0.55	2.23	19	1
1:A:31:LYS:O	1:A:34:ARG:HG2	0.55	2.01	1	1
1:A:222:ARG:O	1:A:223:VAL:C	0.55	2.47	20	1
1:A:145:HIS:CE1	1:A:197:ILE:HG23	0.55	2.36	12	4
1:A:237:ASP:OD1	1:A:238:LYS:N	0.55	2.38	4	6
1:A:121:TRP:CD2	1:A:135:LEU:HD22	0.55	2.36	10	7
1:A:129:LYS:C	1:A:131:SER:H	0.55	2.09	12	4
1:A:221:PRO:O	1:A:222:ARG:HB3	0.55	2.00	11	2
1:A:190:LEU:HD23	1:A:193:LYS:NZ	0.55	2.16	19	3
1:A:229:LEU:C	1:A:231:GLN:N	0.55	2.65	7	10
1:A:150:HIS:O	1:A:154:VAL:HB	0.55	2.02	4	2
1:A:227:TRP:CD1	1:A:227:TRP:N	0.55	2.71	2	5
1:A:232:SER:O	1:A:233:ALA:O	0.55	2.24	11	2
1:A:191:LYS:O	1:A:195:ARG:CG	0.55	2.55	18	12
1:A:292:LEU:HD12	1:A:292:LEU:C	0.55	2.26	19	4
1:A:230:ALA:O	1:A:235:LEU:HD12	0.55	2.02	15	3
1:A:204:LEU:O	1:A:207:VAL:HG12	0.55	2.02	7	1
1:A:146:LYS:CG	1:A:147:GLU:N	0.55	2.70	8	2
1:A:141:GLU:O	1:A:144:HIS:CE1	0.55	2.60	16	1
1:A:40:VAL:O	1:A:44:GLU:OE1	0.54	2.25	14	2
1:A:47:ALA:O	1:A:51:ILE:HG12	0.54	2.02	20	10
1:A:269:GLU:OE2	1:A:273:HIS:NE2	0.54	2.40	1	1
1:A:134:GLU:CD	1:A:134:GLU:N	0.54	2.56	14	1
1:A:219:GLU:OE1	1:A:220:GLU:N	0.54	2.39	18	2
1:A:247:LEU:O	1:A:251:GLU:CB	0.54	2.56	14	3
1:A:231:GLN:OE1	1:A:244:ARG:NH2	0.54	2.40	15	1
1:A:234:ASN:ND2	1:A:234:ASN:N	0.54	2.55	18	2
1:A:271:LEU:HD23	1:A:271:LEU:C	0.54	2.28	2	8
1:A:140:ARG:O	1:A:144:HIS:ND1	0.54	2.41	15	2
1:A:145:HIS:O	1:A:149:VAL:HG23	0.54	2.02	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:236:THR:OG1	1:A:239:GLU:OE1	0.54	2.24	4	1
1:A:45:LEU:HD12	1:A:88:TYR:OH	0.54	2.02	6	1
1:A:134:GLU:N	1:A:134:GLU:OE1	0.54	2.35	15	3
1:A:271:LEU:HD23	1:A:271:LEU:O	0.54	2.02	9	2
1:A:149:VAL:CG1	1:A:150:HIS:N	0.54	2.70	10	2
1:A:143:LEU:CD2	1:A:143:LEU:N	0.54	2.71	20	3
1:A:29:TRP:CH2	1:A:42:LEU:HD11	0.54	2.37	9	1
1:A:236:THR:OG1	1:A:239:GLU:HG2	0.54	2.03	11	1
1:A:296:ARG:CD	1:A:296:ARG:C	0.54	2.80	2	1
1:A:234:ASN:C	1:A:235:LEU:HD22	0.54	2.28	12	2
1:A:296:ARG:C	1:A:296:ARG:NE	0.54	2.65	16	1
1:A:81:LEU:C	1:A:81:LEU:CD1	0.54	2.81	10	18
1:A:131:SER:C	1:A:133:GLU:N	0.54	2.65	1	1
1:A:315:ILE:C	1:A:317:ARG:H	0.54	2.10	19	1
1:A:193:LYS:O	1:A:196:SER:OG	0.53	2.25	15	7
1:A:195:ARG:CD	1:A:199:GLN:NE2	0.53	2.71	2	1
1:A:283:VAL:HG13	1:A:284:SER:N	0.53	2.18	9	2
1:A:289:LYS:HD3	1:A:292:LEU:HD23	0.53	1.79	1	10
1:A:290:HIS:NE2	1:A:294:GLU:OE2	0.53	2.41	1	1
1:A:259:HIS:O	1:A:263:GLN:OE1	0.53	2.26	20	7
1:A:303:THR:HG22	1:A:307:HIS:ND1	0.53	2.19	5	2
1:A:139:TRP:CZ3	1:A:142:PHE:CE2	0.53	2.97	11	4
1:A:257:HIS:ND1	1:A:258:ASN:N	0.53	2.56	13	5
1:A:133:GLU:O	1:A:136:ASP:OD2	0.53	2.27	5	4
1:A:268:HIS:NE2	1:A:272:ARG:NE	0.53	2.57	13	1
1:A:227:TRP:CH2	1:A:308:LEU:HD23	0.53	2.39	15	3
1:A:134:GLU:O	1:A:138:LEU:HD23	0.53	2.04	8	1
1:A:37:LEU:HD23	1:A:37:LEU:N	0.53	2.18	9	2
1:A:271:LEU:HD13	1:A:286:SER:CB	0.53	2.34	11	2
1:A:250:PHE:CG	1:A:251:GLU:N	0.53	2.73	13	1
1:A:236:THR:OG1	1:A:239:GLU:CG	0.53	2.56	11	2
1:A:117:LEU:HD12	1:A:117:LEU:N	0.53	2.18	11	2
1:A:120:LEU:O	1:A:120:LEU:HD13	0.53	2.04	6	1
1:A:205:ARG:O	1:A:209:HIS:ND1	0.52	2.42	9	1
1:A:235:LEU:N	1:A:235:LEU:CD2	0.52	2.72	13	2
1:A:281:GLU:C	1:A:283:VAL:N	0.52	2.68	1	2
1:A:137:LYS:O	1:A:141:GLU:OE1	0.52	2.27	10	2
1:A:199:GLN:CD	1:A:199:GLN:C	0.52	2.77	14	1
1:A:261:GLN:NE2	1:A:297:THR:HG21	0.52	2.18	4	6
1:A:296:ARG:NH1	1:A:299:GLU:OE1	0.52	2.42	1	1
1:A:120:LEU:HD22	1:A:142:PHE:CE1	0.52	2.39	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:302:TYR:OH	1:A:306:LYS:CE	0.52	2.58	11	3
1:A:140:ARG:O	1:A:144:HIS:CD2	0.52	2.63	13	8
1:A:206:ARG:O	1:A:210:GLN:CB	0.52	2.57	1	7
1:A:121:TRP:C	1:A:121:TRP:CD1	0.52	2.88	13	12
1:A:250:PHE:C	1:A:250:PHE:CD1	0.52	2.85	13	5
1:A:229:LEU:HD23	1:A:232:SER:OG	0.52	2.04	13	1
1:A:236:THR:N	1:A:239:GLU:CD	0.52	2.67	4	1
1:A:145:HIS:O	1:A:149:VAL:HG12	0.52	2.05	5	2
1:A:315:ILE:O	1:A:315:ILE:HG22	0.52	2.04	8	2
1:A:152:TYR:CE1	1:A:193:LYS:HE3	0.52	2.40	18	2
1:A:128:GLY:C	1:A:130:PHE:H	0.51	2.11	19	3
1:A:261:GLN:NE2	1:A:297:THR:CG2	0.51	2.74	18	8
1:A:134:GLU:O	1:A:137:LYS:CG	0.51	2.58	2	1
1:A:36:HIS:C	1:A:37:LEU:HD23	0.51	2.30	9	1
1:A:194:LEU:HD12	1:A:194:LEU:O	0.51	2.06	11	14
1:A:81:LEU:HD13	1:A:81:LEU:C	0.51	2.30	7	17
1:A:150:HIS:CG	1:A:151:GLU:N	0.51	2.79	2	2
1:A:23:GLU:OE1	1:A:23:GLU:N	0.51	2.37	11	2
1:A:207:VAL:C	1:A:211:GLY:H	0.51	2.13	17	3
1:A:29:TRP:HE1	1:A:33:GLN:NE2	0.51	2.03	13	1
1:A:236:THR:HG1	1:A:239:GLU:CD	0.51	2.13	3	1
1:A:130:PHE:CD1	1:A:134:GLU:OE1	0.51	2.64	6	2
1:A:64:LEU:HD23	1:A:64:LEU:C	0.51	2.31	3	4
1:A:219:GLU:O	1:A:220:GLU:O	0.51	2.29	9	7
1:A:227:TRP:CZ2	1:A:308:LEU:HD23	0.51	2.41	17	6
1:A:129:LYS:C	1:A:131:SER:N	0.51	2.69	12	11
1:A:192:GLU:O	1:A:195:ARG:HG3	0.51	2.06	2	2
1:A:243:PHE:CD1	1:A:243:PHE:C	0.51	2.88	2	3
1:A:220:GLU:O	1:A:223:VAL:CG1	0.51	2.58	3	1
1:A:280:GLY:C	1:A:282:ARG:N	0.51	2.67	16	1
1:A:145:HIS:O	1:A:149:VAL:CG2	0.51	2.59	2	2
1:A:280:GLY:C	1:A:281:GLU:OE1	0.51	2.54	11	1
1:A:251:GLU:O	1:A:254:ILE:CG2	0.51	2.59	8	10
1:A:136:ASP:OD1	1:A:137:LYS:N	0.51	2.44	2	2
1:A:277:VAL:CG1	1:A:278:GLY:N	0.51	2.74	17	9
1:A:240:LEU:HD13	1:A:240:LEU:C	0.50	2.30	11	9
1:A:234:ASN:O	1:A:235:LEU:CB	0.50	2.59	4	2
1:A:195:ARG:O	1:A:199:GLN:OE1	0.50	2.29	8	1
1:A:206:ARG:O	1:A:210:GLN:HG2	0.50	2.06	8	1
1:A:139:TRP:CH2	1:A:142:PHE:CE2	0.50	2.99	15	1
1:A:240:LEU:C	1:A:240:LEU:CD1	0.50	2.85	4	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:PHE:CD2	1:A:307:HIS:CE1	0.50	2.99	14	1
1:A:311:LEU:HD12	1:A:314:ARG:NH2	0.50	2.21	20	1
1:A:196:SER:O	1:A:199:GLN:HG3	0.50	2.06	14	1
1:A:251:GLU:OE1	1:A:251:GLU:C	0.50	2.54	7	6
1:A:30:GLU:OE2	1:A:34:ARG:NH2	0.50	2.44	19	2
1:A:121:TRP:CZ3	1:A:135:LEU:HD22	0.50	2.41	18	4
1:A:190:LEU:HA	1:A:193:LYS:HZ2	0.50	1.67	19	2
1:A:247:LEU:CD2	1:A:247:LEU:N	0.50	2.75	7	2
1:A:235:LEU:HD22	1:A:240:LEU:CD2	0.50	2.36	19	1
1:A:315:ILE:CG2	1:A:316:SER:N	0.50	2.73	19	1
1:A:132:GLY:O	1:A:136:ASP:CG	0.50	2.55	7	5
1:A:223:VAL:CG1	1:A:224:ILE:N	0.50	2.74	12	8
1:A:315:ILE:C	1:A:317:ARG:N	0.50	2.70	19	2
1:A:223:VAL:O	1:A:226:LEU:N	0.50	2.45	3	1
1:A:152:TYR:CD1	1:A:193:LYS:HE3	0.50	2.42	13	1
1:A:271:LEU:HD21	1:A:275:GLU:OE2	0.49	2.07	9	2
1:A:251:GLU:CD	1:A:251:GLU:C	0.49	2.80	9	1
1:A:220:GLU:CA	1:A:220:GLU:OE1	0.49	2.60	20	1
1:A:194:LEU:HG	1:A:195:ARG:N	0.49	2.22	4	19
1:A:271:LEU:C	1:A:271:LEU:CD2	0.49	2.83	9	6
1:A:139:TRP:CZ3	1:A:142:PHE:CD2	0.49	3.00	15	2
1:A:235:LEU:N	1:A:235:LEU:HD22	0.49	2.21	13	1
1:A:228:ASP:O	1:A:231:GLN:NE2	0.49	2.41	2	2
1:A:316:SER:OG	1:A:317:ARG:N	0.49	2.45	2	1
1:A:152:TYR:CD1	1:A:193:LYS:CE	0.49	2.95	11	5
1:A:237:ASP:CG	1:A:238:LYS:N	0.49	2.71	7	2
1:A:281:GLU:O	1:A:283:VAL:N	0.49	2.45	1	2
1:A:235:LEU:N	1:A:235:LEU:CD1	0.49	2.67	19	1
1:A:134:GLU:OE1	1:A:134:GLU:N	0.49	2.38	4	4
1:A:62:LEU:HD12	1:A:63:LYS:N	0.49	2.23	6	1
1:A:313:GLY:O	1:A:316:SER:OG	0.49	2.30	6	2
1:A:221:PRO:O	1:A:225:ASP:CB	0.49	2.61	12	2
1:A:128:GLY:O	1:A:129:LYS:CG	0.49	2.60	18	1
1:A:257:HIS:NE2	1:A:297:THR:O	0.48	2.46	5	1
1:A:248:LYS:O	1:A:251:GLU:CG	0.48	2.60	7	8
1:A:314:ARG:NE	1:A:314:ARG:CA	0.48	2.76	18	2
1:A:223:VAL:HG21	1:A:308:LEU:HD22	0.48	1.84	12	1
1:A:121:TRP:CD1	1:A:121:TRP:C	0.48	2.92	18	6
1:A:307:HIS:O	1:A:311:LEU:HB2	0.48	2.08	16	3
1:A:311:LEU:O	1:A:315:ILE:CG1	0.48	2.61	4	1
1:A:42:LEU:C	1:A:42:LEU:CD2	0.48	2.87	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:223:VAL:HG23	1:A:308:LEU:HD21	0.48	1.85	18	2
1:A:260:TYR:CD2	1:A:293:LEU:HD11	0.48	2.42	10	1
1:A:300:LEU:HD13	1:A:300:LEU:O	0.48	2.09	9	2
1:A:195:ARG:CD	1:A:195:ARG:C	0.48	2.86	5	3
1:A:203:ARG:HE	1:A:207:VAL:HG21	0.48	1.68	13	1
1:A:220:GLU:CB	1:A:221:PRO:CD	0.48	2.92	14	1
1:A:143:LEU:O	1:A:147:GLU:OE1	0.48	2.32	17	1
1:A:64:LEU:C	1:A:64:LEU:CD1	0.48	2.87	20	1
1:A:133:GLU:HA	1:A:136:ASP:OD2	0.48	2.08	5	2
1:A:195:ARG:CZ	1:A:199:GLN:HE22	0.48	2.22	4	1
1:A:243:PHE:O	1:A:247:LEU:HD23	0.48	2.09	20	2
1:A:192:GLU:O	1:A:195:ARG:HG2	0.48	2.08	15	2
1:A:226:LEU:O	1:A:229:LEU:HB2	0.48	2.09	19	2
1:A:308:LEU:O	1:A:312:SER:CB	0.48	2.61	20	5
1:A:279:ASP:O	1:A:283:VAL:HG23	0.48	2.08	14	1
1:A:237:ASP:OD1	1:A:237:ASP:N	0.48	2.45	2	5
1:A:63:LYS:CG	1:A:64:LEU:N	0.48	2.77	12	1
1:A:296:ARG:HG3	1:A:297:THR:N	0.48	2.23	2	1
1:A:153:ASN:CG	1:A:154:VAL:N	0.48	2.71	5	1
1:A:250:PHE:CE2	1:A:307:HIS:NE2	0.48	2.82	14	1
1:A:294:GLU:CD	1:A:294:GLU:C	0.47	2.82	3	5
1:A:194:LEU:CD1	1:A:198:ASN:ND2	0.47	2.77	8	2
1:A:302:TYR:CE1	1:A:306:LYS:NZ	0.47	2.82	18	1
1:A:251:GLU:CD	1:A:252:ALA:N	0.47	2.72	9	2
1:A:308:LEU:O	1:A:312:SER:OG	0.47	2.33	3	4
1:A:191:LYS:O	1:A:195:ARG:CB	0.47	2.63	18	2
1:A:193:LYS:CG	1:A:194:LEU:N	0.47	2.78	9	7
1:A:152:TYR:CD1	1:A:152:TYR:N	0.47	2.83	2	1
1:A:296:ARG:CZ	1:A:299:GLU:OE1	0.47	2.62	1	2
1:A:28:LEU:N	1:A:28:LEU:CD2	0.47	2.77	18	11
1:A:258:ASN:OD1	1:A:258:ASN:C	0.47	2.58	17	4
1:A:237:ASP:OD1	1:A:237:ASP:C	0.47	2.57	6	1
1:A:82:ASN:OD1	1:A:82:ASN:C	0.47	2.58	11	5
1:A:230:ALA:O	1:A:235:LEU:CD1	0.47	2.62	9	2
1:A:141:GLU:O	1:A:144:HIS:CG	0.47	2.66	16	1
1:A:64:LEU:HD13	1:A:64:LEU:C	0.47	2.34	20	1
1:A:122:HIS:CD2	1:A:122:HIS:N	0.47	2.83	17	12
1:A:126:THR:C	1:A:128:GLY:N	0.47	2.72	7	11
1:A:203:ARG:CD	1:A:203:ARG:C	0.47	2.88	12	2
1:A:133:GLU:CG	1:A:134:GLU:N	0.47	2.78	19	1
1:A:311:LEU:O	1:A:315:ILE:HG13	0.46	2.10	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:N	1:A:117:LEU:CD1	0.46	2.78	11	1
1:A:141:GLU:HA	1:A:144:HIS:ND1	0.46	2.25	16	1
1:A:219:GLU:CD	1:A:220:GLU:O	0.46	2.58	20	1
1:A:220:GLU:N	1:A:220:GLU:OE1	0.46	2.49	20	1
1:A:293:LEU:O	1:A:297:THR:OG1	0.46	2.33	11	2
1:A:41:ARG:O	1:A:45:LEU:HD13	0.46	2.10	18	1
1:A:310:ASP:C	1:A:310:ASP:OD1	0.46	2.58	7	2
1:A:130:PHE:O	1:A:135:LEU:N	0.46	2.48	7	1
1:A:225:ASP:O	1:A:228:ASP:HB2	0.46	2.09	14	1
1:A:225:ASP:O	1:A:229:LEU:HD23	0.46	2.09	14	1
1:A:247:LEU:O	1:A:251:GLU:HG2	0.46	2.10	8	2
1:A:150:HIS:HA	1:A:153:ASN:OD1	0.46	2.11	5	1
1:A:137:LYS:O	1:A:141:GLU:CD	0.46	2.59	10	1
1:A:149:VAL:CG1	1:A:153:ASN:ND2	0.46	2.78	11	1
1:A:56:GLU:CD	1:A:56:GLU:C	0.46	2.84	2	1
1:A:273:HIS:O	1:A:276:SER:OG	0.46	2.28	8	1
1:A:229:LEU:N	1:A:229:LEU:CD2	0.46	2.78	14	1
1:A:28:LEU:C	1:A:28:LEU:CD1	0.46	2.88	20	1
1:A:198:ASN:OD1	1:A:198:ASN:C	0.46	2.58	5	2
1:A:191:LYS:O	1:A:195:ARG:HB3	0.46	2.11	18	2
1:A:206:ARG:O	1:A:210:GLN:HG3	0.46	2.11	10	1
1:A:130:PHE:O	1:A:135:LEU:HG	0.46	2.10	13	1
1:A:56:GLU:OE1	1:A:56:GLU:C	0.46	2.59	17	1
1:A:48:ASP:OD1	1:A:48:ASP:C	0.46	2.58	5	4
1:A:236:THR:C	1:A:239:GLU:OE2	0.46	2.59	4	1
1:A:55:ASP:OD1	1:A:55:ASP:C	0.46	2.59	13	3
1:A:189:GLU:O	1:A:193:LYS:CD	0.46	2.64	16	1
1:A:274:ALA:O	1:A:277:VAL:CG1	0.45	2.64	18	6
1:A:55:ASP:OD2	1:A:77:LEU:HD21	0.45	2.12	11	1
1:A:309:GLN:CD	1:A:309:GLN:C	0.45	2.83	15	1
1:A:193:LYS:HG2	1:A:194:LEU:N	0.45	2.26	1	9
1:A:199:GLN:O	1:A:202:ASP:CG	0.45	2.59	2	4
1:A:237:ASP:CG	1:A:238:LYS:H	0.45	2.19	4	2
1:A:289:LYS:NZ	1:A:292:LEU:HD23	0.45	2.26	8	1
1:A:284:SER:O	1:A:288:GLU:OE1	0.45	2.35	11	1
1:A:279:ASP:OD1	1:A:279:ASP:C	0.45	2.60	4	2
1:A:247:LEU:N	1:A:247:LEU:CD2	0.45	2.79	20	5
1:A:224:ILE:HD13	1:A:227:TRP:CZ3	0.45	2.47	11	1
1:A:223:VAL:HG21	1:A:308:LEU:CD2	0.45	2.41	6	1
1:A:85:LEU:CD2	1:A:85:LEU:N	0.45	2.79	7	2
1:A:152:TYR:CE1	1:A:193:LYS:CE	0.45	2.99	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:LEU:O	1:A:141:GLU:HG3	0.45	2.11	8	1
1:A:221:PRO:O	1:A:222:ARG:C	0.45	2.60	10	1
1:A:307:HIS:CD2	1:A:311:LEU:HD13	0.45	2.46	19	1
1:A:315:ILE:O	1:A:317:ARG:HG3	0.45	2.11	19	1
1:A:220:GLU:C	1:A:222:ARG:N	0.45	2.74	12	1
1:A:219:GLU:CD	1:A:219:GLU:O	0.45	2.60	19	1
1:A:194:LEU:CG	1:A:195:ARG:N	0.45	2.80	5	11
1:A:219:GLU:O	1:A:219:GLU:HG2	0.45	2.12	17	2
1:A:236:THR:OG1	1:A:239:GLU:CD	0.45	2.60	19	3
1:A:236:THR:N	1:A:239:GLU:OE2	0.45	2.50	4	1
1:A:74:GLU:CG	1:A:75:ALA:N	0.45	2.80	9	1
1:A:82:ASN:OD1	1:A:82:ASN:O	0.45	2.35	12	5
1:A:192:GLU:CD	1:A:192:GLU:C	0.45	2.84	3	1
1:A:124:ALA:HA	1:A:127:SER:OG	0.45	2.12	6	1
1:A:243:PHE:CD1	1:A:244:ARG:N	0.45	2.86	20	2
1:A:257:HIS:NE2	1:A:261:GLN:NE2	0.45	2.65	14	1
1:A:207:VAL:CG1	1:A:208:SER:N	0.44	2.80	3	2
1:A:251:GLU:O	1:A:254:ILE:HG22	0.44	2.12	7	2
1:A:261:GLN:OE1	1:A:297:THR:HG21	0.44	2.11	6	1
1:A:310:ASP:OD1	1:A:314:ARG:NE	0.44	2.50	10	1
1:A:281:GLU:OE1	1:A:281:GLU:N	0.44	2.50	11	1
1:A:312:SER:O	1:A:316:SER:OG	0.44	2.32	11	1
1:A:143:LEU:N	1:A:143:LEU:HD22	0.44	2.26	17	3
1:A:138:LEU:O	1:A:141:GLU:CG	0.44	2.65	1	2
1:A:134:GLU:O	1:A:138:LEU:HD13	0.44	2.11	3	1
1:A:235:LEU:HD22	1:A:239:GLU:CD	0.44	2.38	8	1
1:A:148:LYS:O	1:A:152:TYR:CD2	0.44	2.69	12	2
1:A:28:LEU:HD13	1:A:28:LEU:C	0.44	2.37	20	1
1:A:219:GLU:CD	1:A:219:GLU:C	0.44	2.85	20	1
1:A:251:GLU:C	1:A:251:GLU:CD	0.44	2.85	4	2
1:A:235:LEU:HD22	1:A:239:GLU:OE2	0.44	2.13	8	1
1:A:192:GLU:O	1:A:195:ARG:CG	0.44	2.65	12	1
1:A:131:SER:O	1:A:132:GLY:C	0.44	2.61	1	1
1:A:145:HIS:ND1	1:A:197:ILE:HG23	0.44	2.27	3	1
1:A:234:ASN:CG	1:A:235:LEU:N	0.44	2.72	16	2
1:A:268:HIS:ND1	1:A:268:HIS:C	0.44	2.75	17	1
1:A:52:GLN:NE2	1:A:80:ASN:HD22	0.44	2.11	3	1
1:A:126:THR:C	1:A:128:GLY:H	0.44	2.20	7	1
1:A:77:LEU:HD12	1:A:77:LEU:N	0.44	2.27	8	1
1:A:20:PHE:N	1:A:26:ASN:OD1	0.44	2.39	2	1
1:A:227:TRP:N	1:A:227:TRP:CD1	0.44	2.84	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLU:CD	1:A:53:GLU:C	0.44	2.85	6	1
1:A:210:GLN:C	1:A:210:GLN:CD	0.44	2.85	10	1
1:A:191:LYS:HA	1:A:194:LEU:HD23	0.44	1.89	12	1
1:A:223:VAL:C	1:A:225:ASP:N	0.43	2.74	3	1
1:A:287:ARG:NH2	1:A:290:HIS:ND1	0.43	2.66	11	1
1:A:277:VAL:HG13	1:A:279:ASP:N	0.43	2.28	4	1
1:A:26:ASN:O	1:A:26:ASN:OD1	0.43	2.36	3	2
1:A:62:LEU:CD2	1:A:73:LYS:NZ	0.43	2.82	10	1
1:A:287:ARG:HH22	1:A:290:HIS:CE1	0.43	2.31	11	1
1:A:144:HIS:NE2	1:A:145:HIS:CG	0.43	2.87	16	1
1:A:62:LEU:CD1	1:A:73:LYS:HZ3	0.43	2.27	19	1
1:A:147:GLU:HG3	1:A:148:LYS:N	0.43	2.27	14	1
1:A:26:ASN:OD1	1:A:26:ASN:O	0.43	2.36	15	1
1:A:222:ARG:HE	1:A:223:VAL:HG23	0.43	1.73	2	1
1:A:289:LYS:O	1:A:290:HIS:C	0.43	2.62	20	5
1:A:119:LYS:CG	1:A:120:LEU:N	0.43	2.81	19	1
1:A:145:HIS:O	1:A:149:VAL:CB	0.43	2.66	2	1
1:A:45:LEU:HD22	1:A:88:TYR:OH	0.43	2.13	12	1
1:A:228:ASP:O	1:A:231:GLN:HG2	0.43	2.10	14	1
1:A:124:ALA:HB1	1:A:130:PHE:CD1	0.43	2.48	1	1
1:A:20:PHE:H	1:A:26:ASN:CG	0.43	2.19	2	1
1:A:145:HIS:O	1:A:149:VAL:HB	0.43	2.14	20	2
1:A:239:GLU:CD	1:A:240:LEU:H	0.43	2.22	4	1
1:A:210:GLN:CG	1:A:211:GLY:N	0.43	2.82	8	1
1:A:134:GLU:O	1:A:137:LYS:HG2	0.43	2.14	2	1
1:A:206:ARG:NH1	1:A:209:HIS:ND1	0.43	2.66	15	1
1:A:269:GLU:OE1	1:A:272:ARG:NH2	0.42	2.52	1	1
1:A:190:LEU:HA	1:A:193:LYS:HD3	0.42	1.89	7	2
1:A:250:PHE:CE2	1:A:311:LEU:HD11	0.42	2.49	9	1
1:A:260:TYR:O	1:A:264:LEU:N	0.42	2.51	9	1
1:A:219:GLU:OE2	1:A:220:GLU:O	0.42	2.37	20	1
1:A:220:GLU:CD	1:A:220:GLU:N	0.42	2.77	3	1
1:A:303:THR:O	1:A:307:HIS:ND1	0.42	2.50	17	2
1:A:25:LEU:HD12	1:A:25:LEU:N	0.42	2.30	1	2
1:A:274:ALA:C	1:A:276:SER:N	0.42	2.75	5	1
1:A:202:ASP:CG	1:A:203:ARG:N	0.42	2.76	11	1
1:A:257:HIS:NE2	1:A:297:THR:HG22	0.42	2.28	11	1
1:A:21:ARG:CZ	1:A:53:GLU:OE2	0.42	2.68	14	1
1:A:25:LEU:N	1:A:25:LEU:CD1	0.42	2.82	19	1
1:A:22:MET:SD	1:A:22:MET:N	0.42	2.93	1	1
1:A:283:VAL:CG1	1:A:284:SER:N	0.42	2.83	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:263:GLN:OE1	1:A:263:GLN:N	0.42	2.53	19	1
1:A:314:ARG:O	1:A:315:ILE:C	0.42	2.62	19	1
1:A:30:GLU:CD	1:A:30:GLU:C	0.42	2.87	6	1
1:A:124:ALA:O	1:A:128:GLY:C	0.42	2.60	7	1
1:A:123:LYS:O	1:A:127:SER:HB3	0.42	2.15	9	2
1:A:146:LYS:HG3	1:A:147:GLU:N	0.42	2.29	8	2
1:A:263:GLN:N	1:A:263:GLN:CD	0.42	2.78	20	1
1:A:223:VAL:O	1:A:224:ILE:C	0.42	2.61	3	1
1:A:235:LEU:HD22	1:A:235:LEU:N	0.42	2.30	12	1
1:A:130:PHE:O	1:A:135:LEU:CG	0.42	2.67	13	1
1:A:130:PHE:O	1:A:135:LEU:CB	0.42	2.68	18	2
1:A:221:PRO:C	1:A:222:ARG:CG	0.42	2.90	4	1
1:A:257:HIS:ND1	1:A:257:HIS:C	0.42	2.76	13	1
1:A:59:TRP:HA	1:A:62:LEU:HD21	0.41	1.92	6	1
1:A:230:ALA:C	1:A:235:LEU:HD12	0.41	2.40	14	1
1:A:55:ASP:OD1	1:A:55:ASP:O	0.41	2.38	13	1
1:A:123:LYS:O	1:A:127:SER:N	0.41	2.53	19	1
1:A:222:ARG:O	1:A:226:LEU:HD13	0.41	2.15	3	1
1:A:151:GLU:O	1:A:155:LEU:CG	0.41	2.68	5	1
1:A:55:ASP:O	1:A:55:ASP:OD1	0.41	2.39	9	1
1:A:230:ALA:O	1:A:232:SER:N	0.41	2.54	18	1
1:A:190:LEU:HD23	1:A:193:LYS:HZ1	0.41	1.74	19	1
1:A:280:GLY:O	1:A:281:GLU:O	0.41	2.38	9	1
1:A:250:PHE:CD2	1:A:251:GLU:N	0.41	2.88	13	1
1:A:240:LEU:O	1:A:240:LEU:CD1	0.41	2.66	16	1
1:A:139:TRP:O	1:A:140:ARG:C	0.41	2.64	20	2
1:A:133:GLU:O	1:A:137:LYS:HG2	0.41	2.16	7	1
1:A:126:THR:O	1:A:127:SER:C	0.41	2.63	3	5
1:A:203:ARG:O	1:A:207:VAL:HG23	0.41	2.15	6	1
1:A:121:TRP:CD2	1:A:135:LEU:CD2	0.41	3.04	9	1
1:A:220:GLU:O	1:A:221:PRO:C	0.41	2.63	10	1
1:A:73:LYS:N	1:A:73:LYS:HD2	0.41	2.30	13	1
1:A:230:ALA:O	1:A:235:LEU:CD2	0.41	2.66	17	1
1:A:310:ASP:O	1:A:311:LEU:C	0.41	2.63	19	1
1:A:80:ASN:O	1:A:84:ILE:HG13	0.41	2.15	20	1
1:A:22:MET:SD	1:A:24:LYS:NZ	0.41	2.83	7	1
1:A:77:LEU:C	1:A:77:LEU:CD2	0.41	2.85	15	1
1:A:152:TYR:CE1	1:A:193:LYS:HD2	0.41	2.50	19	1
1:A:137:LYS:HG3	1:A:138:LEU:N	0.41	2.31	2	1
1:A:261:GLN:HE21	1:A:297:THR:HG21	0.41	1.76	2	1
1:A:64:LEU:C	1:A:64:LEU:CD2	0.41	2.93	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:246:GLU:CG	1:A:247:LEU:N	0.41	2.84	3	1
1:A:23:GLU:CD	1:A:23:GLU:N	0.41	2.68	5	1
1:A:257:HIS:CE1	1:A:261:GLN:OE1	0.41	2.74	14	2
1:A:85:LEU:N	1:A:85:LEU:CD2	0.41	2.84	9	1
1:A:23:GLU:CD	1:A:23:GLU:H	0.41	2.22	12	1
1:A:225:ASP:O	1:A:229:LEU:CD2	0.41	2.69	14	1
1:A:141:GLU:C	1:A:144:HIS:ND1	0.41	2.73	16	1
1:A:206:ARG:O	1:A:210:GLN:HB3	0.41	2.16	20	1
1:A:131:SER:C	1:A:133:GLU:H	0.41	2.23	1	1
1:A:237:ASP:N	1:A:237:ASP:OD1	0.41	2.50	4	1
1:A:227:TRP:O	1:A:230:ALA:HB3	0.41	2.16	17	2
1:A:195:ARG:HG3	1:A:196:SER:N	0.40	2.31	2	1
1:A:203:ARG:HD2	1:A:203:ARG:C	0.40	2.41	4	1
1:A:139:TRP:CH2	1:A:142:PHE:CD2	0.40	3.09	15	1
1:A:228:ASP:OD1	1:A:228:ASP:O	0.40	2.39	16	1
1:A:230:ALA:C	1:A:232:SER:N	0.40	2.77	18	1
1:A:25:LEU:N	1:A:25:LEU:HD12	0.40	2.29	19	1
1:A:309:GLN:O	1:A:312:SER:OG	0.40	2.35	3	1
1:A:21:ARG:HH21	1:A:53:GLU:CD	0.40	2.23	5	1
1:A:51:ILE:CG2	1:A:52:GLN:N	0.40	2.84	7	1
1:A:73:LYS:N	1:A:73:LYS:CD	0.40	2.85	7	1
1:A:195:ARG:CG	1:A:196:SER:N	0.40	2.85	8	1
1:A:128:GLY:O	1:A:129:LYS:C	0.40	2.64	18	1
1:A:271:LEU:HD12	1:A:286:SER:OG	0.40	2.16	2	1
1:A:243:PHE:O	1:A:246:GLU:HG2	0.40	2.17	3	1
1:A:47:ALA:O	1:A:51:ILE:HG13	0.40	2.16	6	1
1:A:239:GLU:O	1:A:239:GLU:CD	0.40	2.64	7	1
1:A:21:ARG:HH21	1:A:53:GLU:CG	0.40	2.29	5	1
1:A:275:GLU:OE2	1:A:283:VAL:CG1	0.40	2.69	6	1
1:A:45:LEU:O	1:A:49:LEU:CD1	0.40	2.70	9	1
1:A:80:ASN:OD1	1:A:84:ILE:HD11	0.40	2.16	16	1
1:A:190:LEU:O	1:A:194:LEU:HB3	0.40	2.17	10	1
1:A:41:ARG:NH2	1:A:88:TYR:CZ	0.40	2.88	17	1
1:A:239:GLU:CD	1:A:239:GLU:O	0.40	2.65	17	1
1:A:271:LEU:CD2	1:A:275:GLU:OE2	0.40	2.68	19	1
1:A:52:GLN:NE2	1:A:80:ASN:ND2	0.40	2.70	20	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	226/323 (70%)	208±3 (92±1%)	12±3 (5±1%)	7±2 (3±1%)	5	38
All	All	4520/6460 (70%)	4153 (92%)	232 (5%)	135 (3%)	5	38

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	36	HIS	20
1	A	130	PHE	13
1	A	222	ARG	13
1	A	38	PRO	12
1	A	230	ALA	10
1	A	221	PRO	8
1	A	220	GLU	7
1	A	234	ASN	7
1	A	219	GLU	6
1	A	223	VAL	6
1	A	233	ALA	6
1	A	281	GLU	5
1	A	128	GLY	4
1	A	315	ILE	4
1	A	129	LYS	3
1	A	316	SER	3
1	A	231	GLN	2
1	A	132	GLY	1
1	A	282	ARG	1
1	A	277	VAL	1
1	A	279	ASP	1
1	A	236	THR	1
1	A	317	ARG	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	201/289 (70%)	185±3 (92±1%)	16±3 (8±1%)	13 61
All	All	4020/5780 (70%)	3703 (92%)	317 (8%)	13 61

All 73 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	194	LEU	20
1	A	304	VAL	20
1	A	300	LEU	19
1	A	224	ILE	18
1	A	81	LEU	17
1	A	240	LEU	16
1	A	135	LEU	14
1	A	254	ILE	14
1	A	36	HIS	13
1	A	202	ASP	10
1	A	257	HIS	9
1	A	139	TRP	9
1	A	207	VAL	7
1	A	308	LEU	7
1	A	195	ARG	6
1	A	223	VAL	6
1	A	243	PHE	6
1	A	22	MET	5
1	A	307	HIS	5
1	A	236	THR	5
1	A	234	ASN	4
1	A	136	ASP	4
1	A	127	SER	4
1	A	120	LEU	3
1	A	315	ILE	3
1	A	292	LEU	3
1	A	42	LEU	3
1	A	314	ARG	3
1	A	235	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	123	LYS	3
1	A	261	GLN	3
1	A	293	LEU	2
1	A	142	PHE	2
1	A	296	ARG	2
1	A	208	SER	2
1	A	317	ARG	2
1	A	251	GLU	2
1	A	209	HIS	2
1	A	37	LEU	2
1	A	88	TYR	2
1	A	220	GLU	2
1	A	193	LYS	2
1	A	64	LEU	2
1	A	141	GLU	2
1	A	131	SER	1
1	A	204	LEU	1
1	A	275	GLU	1
1	A	226	LEU	1
1	A	51	ILE	1
1	A	256	LYS	1
1	A	316	SER	1
1	A	244	ARG	1
1	A	62	LEU	1
1	A	288	GLU	1
1	A	297	THR	1
1	A	44	GLU	1
1	A	250	PHE	1
1	A	134	GLU	1
1	A	199	GLN	1
1	A	231	GLN	1
1	A	247	LEU	1
1	A	270	LYS	1
1	A	294	GLU	1
1	A	26	ASN	1
1	A	203	ARG	1
1	A	222	ARG	1
1	A	133	GLU	1
1	A	229	LEU	1
1	A	31	LYS	1
1	A	309	GLN	1
1	A	311	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	28	LEU	1
1	A	190	LEU	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