Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2K2G
Title	:	Solution structure of the wild-type catalytic domain of human matrix metalloproteinase 12 (MMP-12) in complex with a tight-binding inhibitor
Authors	:	Markus, M.A.; Dwyer, B.; Wolfrom, S.; Li, J.; Li, W.; Malakian, K.; Wilhelm, J.; Tsao, D.H.H.
Deposited on	:	2008-04-01

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 (i) symbol.

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

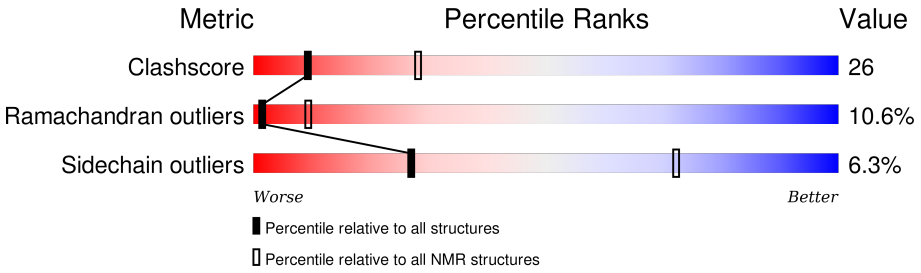
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	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 (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	165	45% 41% • 10%

2 Ensemble composition and analysis

This entry contains 17 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:111-A:185, A:191-A:263 (148)	0.65	5

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

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

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2581 atoms, of which 1256 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	165	2539	831	1240	226	237	5	0

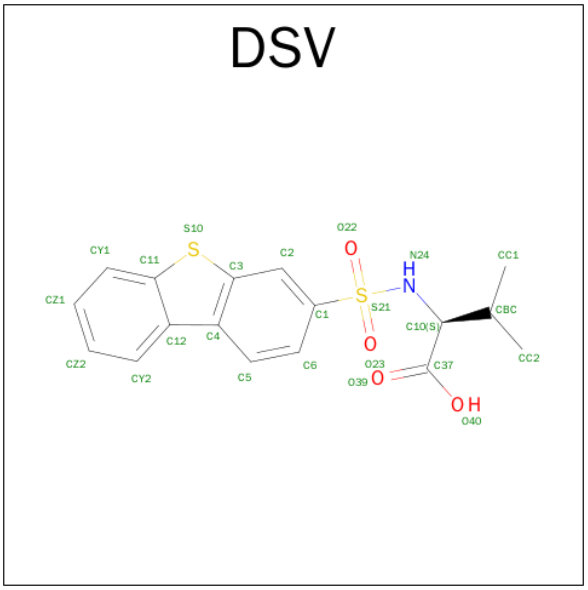
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	MET	-	INITIATING METHIONINE	UNP P39900

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

- Molecule 3 is N-(DIBENZO[B,D]THIOPHEN-3-YLSULFONYL)-L-VALINE (three-letter code: DSV) (formula: $C_{17}H_{17}NO_4S_2$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
3	A	1	40	17	16	1	4	2

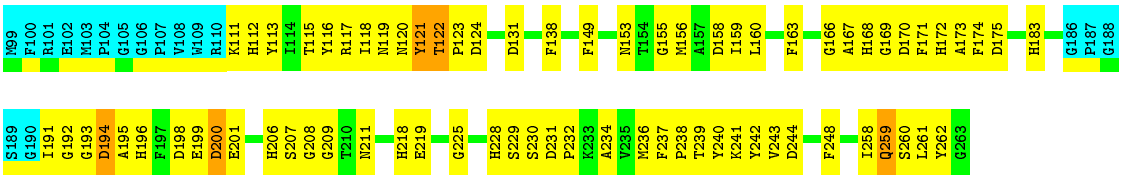
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Macrophage metalloelastase

Chain A:



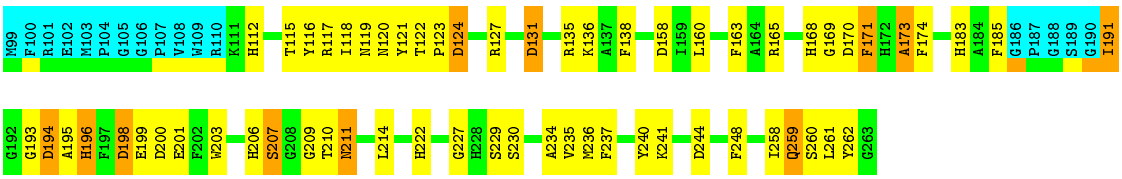
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Macrophage metalloelastase

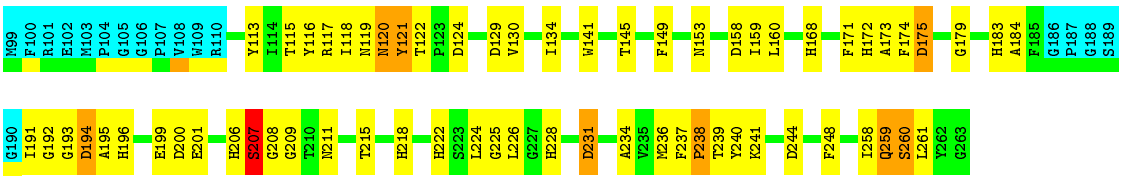
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: Macrophage metalloelastase

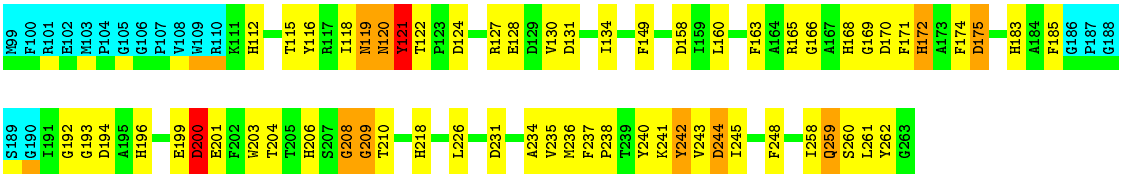
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Macrophage metalloelastase

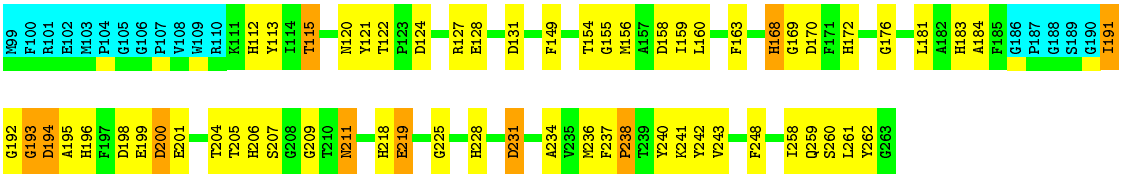
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase

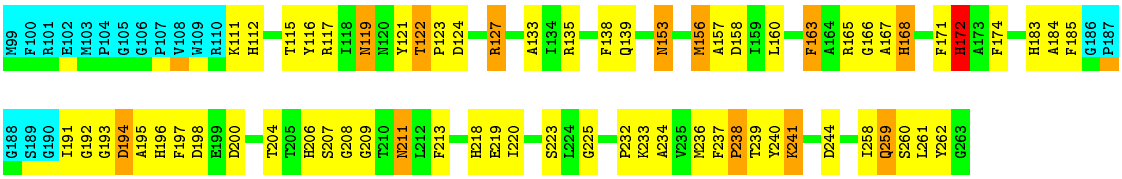
Chain A:



4.2.5 Score per residue for model 5 (medoid)

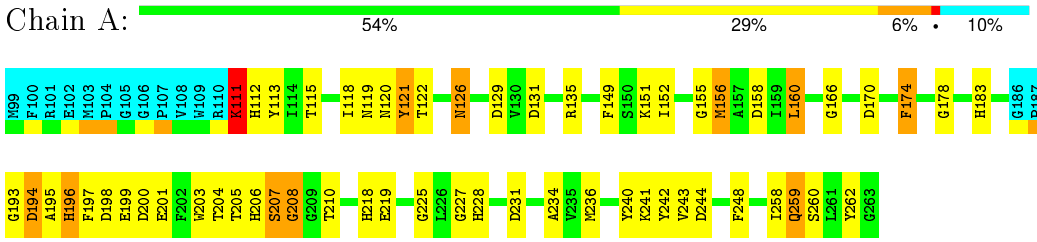
- Molecule 1: Macrophage metalloelastase

Chain A:



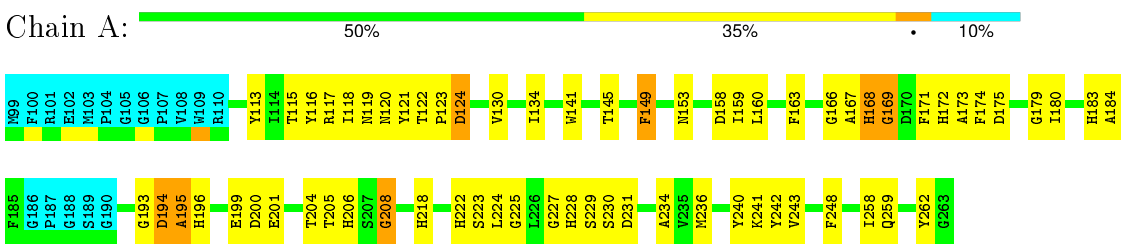
4.2.6 Score per residue for model 6

- Molecule 1: Macrophage metalloelastase



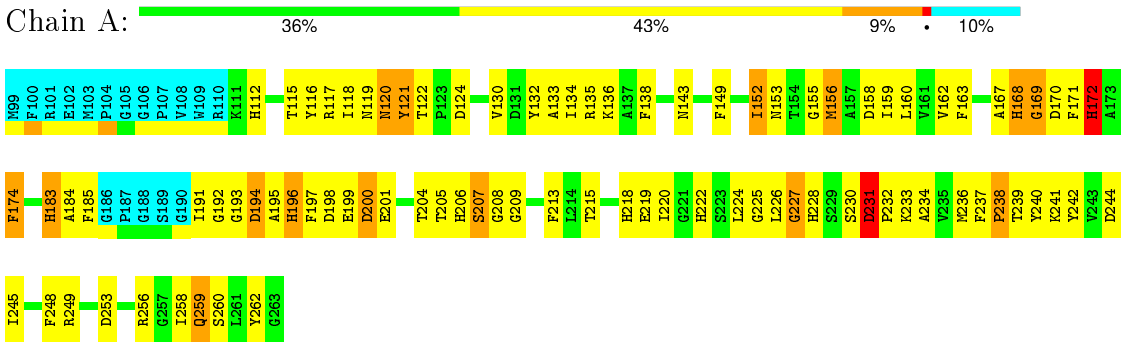
4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



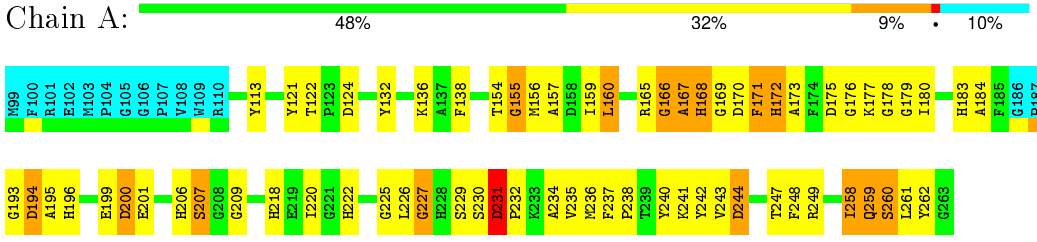
4.2.8 Score per residue for model 8

- Molecule 1: Macrophage metalloelastase



4.2.9 Score per residue for model 9

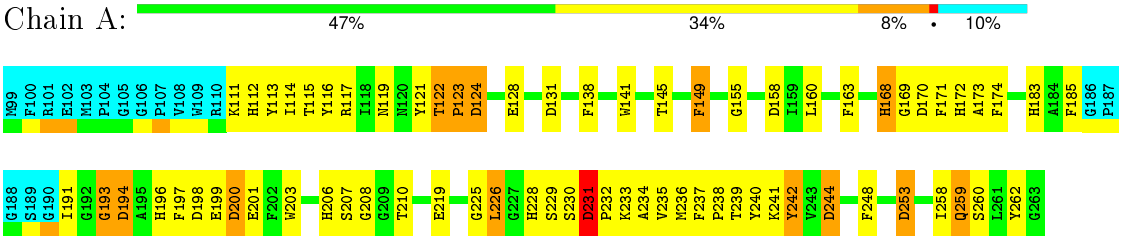
- Molecule 1: Macrophage metalloelastase



4.2.10 Score per residue for model 10

• Molecule 1: Macrophage metalloelastase

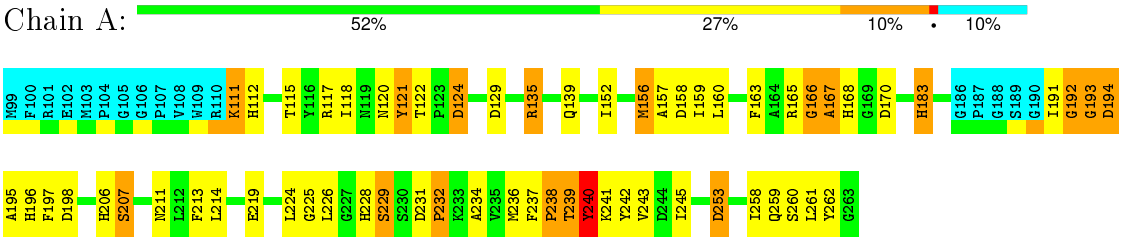
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Macrophage metalloelastase

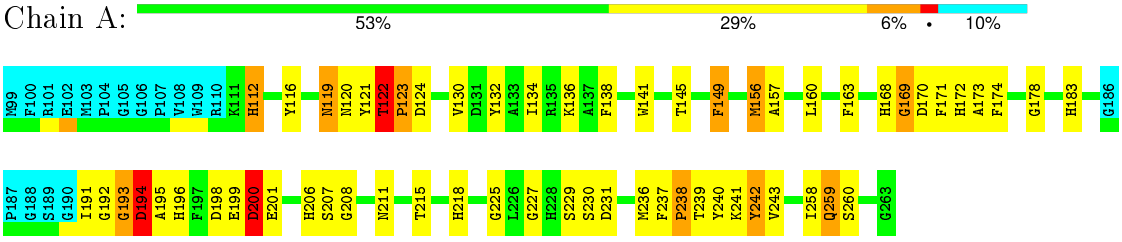
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Macrophage metalloelastase

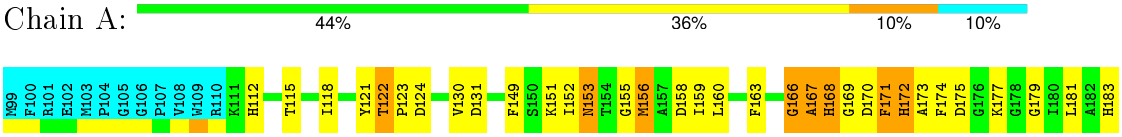
Chain A:

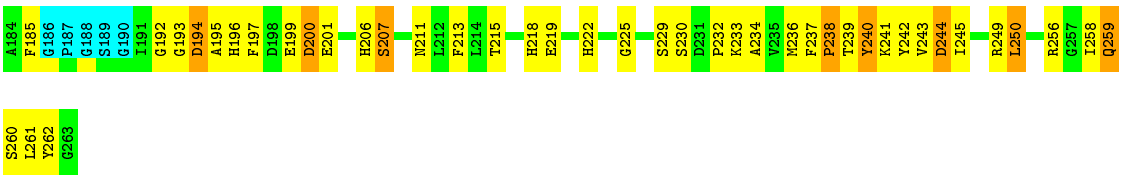


4.2.13 Score per residue for model 13

• Molecule 1: Macrophage metalloelastase

Chain A:

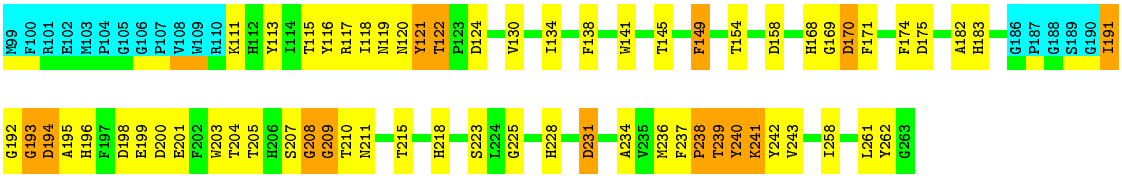




4.2.14 Score per residue for model 14

- Molecule 1: Macrophage metalloelastase

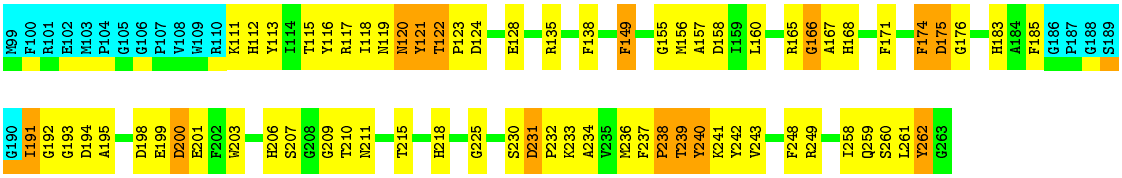
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Macrophage metalloelastase

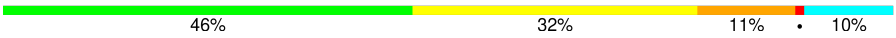
Chain A:

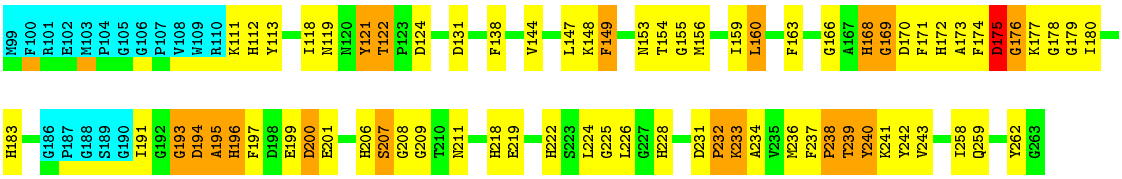


4.2.16 Score per residue for model 16

- Molecule 1: Macrophage metalloelastase

Chain A:

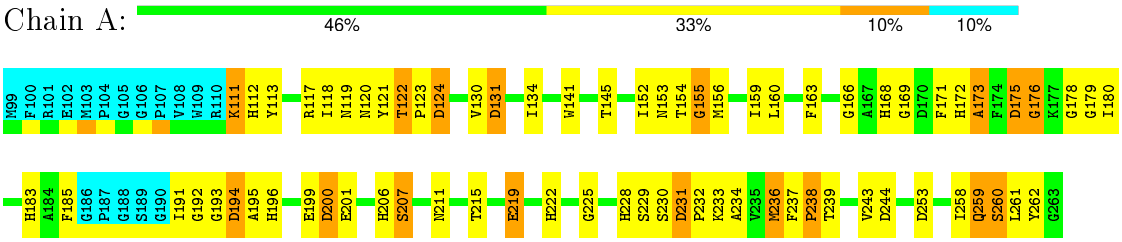




4.2.17 Score per residue for model 17

- Molecule 1: Macrophage metalloelastase

Chain A:


46%
33%
10%
10%
N99 F100 R101 E102 M103 P104 G105 G106 P107 V108 W109 R110 K111 H112 Y113 R117 I118 N119 N120 Y121 T122 P123 D124 V130 D131 I134 W141 T145 I152 N153 T154 G155 M156 I159 L160 F163 G166 A167 H168 G169 D170 F171 H172 A173 F174 D175 G176 K177 G178 G179 I180
H183 A184 F185 G186 P187 G188 S189 G190 I191 G192 G193 D194 A195 H196 E199 D200 E201 H206 S207 N211 T215 E219 H222 G225 H228 S229 S230 D231 P232 K233 A234 V235 M236 F237 P238 T239 V243 D244 D253 I258 Q259 S260 L261 Y262 G263

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing, simulated annealing.*

Of the 100 calculated structures, 17 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
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DSV, ZN

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	1173	1119	1110	61±8
3	A	24	16	16	3±2
All	All	20383	19295	19141	1047

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:241:LYS:O	1:A:243:VAL:HG22	0.79	1.77	3	3
1:A:231:ASP:O	1:A:233:LYS:N	0.75	2.19	16	1
1:A:114:ILE:N	1:A:114:ILE:HD12	0.73	1.98	10	1
1:A:193:GLY:O	1:A:195:ALA:N	0.72	2.23	14	15
1:A:240:TYR:CD1	1:A:240:TYR:N	0.66	2.63	13	2
1:A:242:TYR:CG	1:A:243:VAL:N	0.63	2.67	11	2
1:A:183:HIS:ND1	1:A:184:ALA:N	0.63	2.47	4	3
1:A:171:PHE:CE2	1:A:172:HIS:NE2	0.62	2.67	17	1
1:A:117:ARG:NE	1:A:119:ASN:ND2	0.62	2.47	7	4
1:A:183:HIS:CD2	1:A:184:ALA:N	0.62	2.67	7	2
1:A:168:HIS:CD2	1:A:169:GLY:N	0.62	2.67	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:TYR:CZ	1:A:136:LYS:NZ	0.62	2.68	9	2
1:A:237:PHE:O	1:A:238:PRO:O	0.62	2.16	14	11
1:A:168:HIS:CG	1:A:169:GLY:N	0.62	2.67	4	9
1:A:168:HIS:CE1	1:A:174:PHE:CE1	0.61	2.88	2	1
1:A:168:HIS:CE1	1:A:183:HIS:NE2	0.61	2.67	8	1
1:A:168:HIS:ND1	1:A:174:PHE:CZ	0.61	2.68	15	3
1:A:242:TYR:CD1	1:A:243:VAL:N	0.61	2.68	16	3
1:A:239:THR:O	1:A:241:LYS:N	0.61	2.33	14	4
1:A:121:TYR:N	1:A:121:TYR:CD1	0.61	2.68	16	3
1:A:183:HIS:CG	1:A:184:ALA:N	0.61	2.68	2	4
1:A:168:HIS:CE1	1:A:174:PHE:CZ	0.61	2.88	1	4
1:A:240:TYR:CG	1:A:241:LYS:N	0.61	2.68	6	11
1:A:117:ARG:HE	1:A:119:ASN:ND2	0.61	1.94	7	1
1:A:171:PHE:CZ	1:A:183:HIS:CE1	0.61	2.88	1	1
1:A:118:ILE:HG22	1:A:120:ASN:O	0.60	1.96	6	2
1:A:113:TYR:CE1	1:A:148:LYS:NZ	0.60	2.69	16	1
1:A:228:HIS:CD2	1:A:236:MET:SD	0.60	2.95	14	3
1:A:240:TYR:CD1	1:A:241:LYS:N	0.60	2.70	7	7
1:A:156:MET:SD	1:A:157:ALA:N	0.60	2.75	5	2
1:A:135:ARG:NH2	1:A:136:LYS:NZ	0.60	2.50	1	1
1:A:121:TYR:CD1	1:A:121:TYR:N	0.59	2.70	5	5
1:A:218:HIS:CE1	1:A:236:MET:SD	0.59	2.95	15	1
1:A:236:MET:SD	1:A:237:PHE:N	0.59	2.76	2	10
1:A:228:HIS:NE2	1:A:236:MET:SD	0.59	2.76	7	1
1:A:117:ARG:NE	1:A:119:ASN:HD21	0.59	1.96	17	4
1:A:228:HIS:ND1	1:A:236:MET:SD	0.58	2.76	8	1
1:A:180:ILE:N	1:A:180:ILE:HD12	0.58	2.13	7	1
1:A:152:ILE:HD11	1:A:156:MET:O	0.58	1.98	6	3
1:A:231:ASP:N	1:A:232:PRO:CD	0.58	2.66	11	5
1:A:218:HIS:CE1	1:A:222:HIS:NE2	0.58	2.70	7	1
1:A:218:HIS:CD2	1:A:236:MET:SD	0.58	2.96	12	1
1:A:117:ARG:NH1	1:A:119:ASN:HD21	0.58	1.96	10	1
1:A:154:THR:O	1:A:156:MET:N	0.58	2.37	17	2
1:A:116:TYR:CD1	1:A:138:PHE:CE2	0.57	2.92	12	2
1:A:218:HIS:NE2	1:A:236:MET:SD	0.57	2.77	15	1
1:A:116:TYR:CE1	1:A:138:PHE:CE2	0.57	2.92	12	1
1:A:119:ASN:ND2	1:A:119:ASN:N	0.57	2.53	12	2
1:A:118:ILE:HG21	1:A:121:TYR:CE1	0.57	2.34	1	1
1:A:117:ARG:HE	1:A:119:ASN:HD21	0.57	1.41	2	4
1:A:222:HIS:HE2	1:A:228:HIS:CD2	0.57	2.16	17	1
1:A:168:HIS:CE1	1:A:172:HIS:CD2	0.56	2.93	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:ASN:N	1:A:119:ASN:HD22	0.56	1.98	5	1
1:A:138:PHE:CD1	1:A:149:PHE:CD2	0.56	2.93	8	1
1:A:132:TYR:CE1	1:A:136:LYS:NZ	0.56	2.73	9	1
1:A:149:PHE:CD1	1:A:149:PHE:N	0.56	2.73	15	4
1:A:261:LEU:N	1:A:261:LEU:HD12	0.56	2.16	11	2
1:A:163:PHE:N	1:A:163:PHE:CD1	0.56	2.73	5	6
1:A:206:HIS:CG	1:A:207:SER:N	0.56	2.74	8	4
1:A:206:HIS:CG	1:A:207:SER:H	0.56	2.19	10	2
1:A:119:ASN:HD22	1:A:119:ASN:N	0.56	1.98	12	1
1:A:204:THR:HG22	1:A:205:THR:N	0.56	2.16	14	1
1:A:256:ARG:NH1	1:A:259:GLN:HE22	0.56	1.99	8	1
1:A:163:PHE:CD1	1:A:163:PHE:N	0.56	2.74	16	5
1:A:183:HIS:CE1	1:A:196:HIS:O	0.56	2.59	3	3
1:A:135:ARG:HH22	1:A:136:LYS:NZ	0.56	1.99	1	1
1:A:171:PHE:O	1:A:172:HIS:CG	0.55	2.59	7	1
1:A:171:PHE:O	1:A:173:ALA:N	0.55	2.40	10	5
1:A:229:SER:OG	1:A:230:SER:N	0.55	2.39	7	3
1:A:168:HIS:ND1	1:A:172:HIS:O	0.55	2.39	8	2
1:A:191:ILE:O	1:A:191:ILE:HG23	0.55	2.01	5	2
1:A:149:PHE:N	1:A:149:PHE:CD1	0.55	2.75	14	7
1:A:178:GLY:O	1:A:180:ILE:N	0.55	2.39	17	3
1:A:191:ILE:O	1:A:193:GLY:N	0.55	2.36	11	5
1:A:228:HIS:N	1:A:228:HIS:CD2	0.55	2.74	14	1
1:A:120:ASN:O	1:A:122:THR:N	0.55	2.40	14	1
1:A:222:HIS:CE1	1:A:228:HIS:NE2	0.55	2.74	17	3
1:A:114:ILE:N	1:A:114:ILE:CD1	0.55	2.69	10	1
1:A:228:HIS:CG	1:A:236:MET:SD	0.55	2.99	14	2
1:A:183:HIS:CD2	1:A:196:HIS:O	0.54	2.61	1	5
1:A:111:LYS:O	1:A:112:HIS:ND1	0.54	2.40	5	2
1:A:258:ILE:O	1:A:260:SER:N	0.54	2.41	15	14
1:A:171:PHE:CE2	1:A:172:HIS:CD2	0.54	2.95	17	1
1:A:204:THR:O	1:A:206:HIS:N	0.54	2.41	8	4
1:A:258:ILE:HG23	1:A:259:GLN:N	0.54	2.17	5	12
1:A:171:PHE:CZ	1:A:172:HIS:NE2	0.54	2.76	17	1
1:A:194:ASP:O	1:A:196:HIS:CE1	0.54	2.61	9	12
1:A:174:PHE:CE1	1:A:183:HIS:CE1	0.54	2.96	6	2
1:A:203:TRP:CZ3	1:A:210:THR:HG22	0.54	2.38	15	3
1:A:194:ASP:O	1:A:196:HIS:CD2	0.54	2.61	4	7
1:A:121:TYR:CE2	1:A:131:ASP:OD1	0.54	2.62	3	2
1:A:211:ASN:ND2	1:A:239:THR:OG1	0.53	2.41	13	1
1:A:208:GLY:N	1:A:242:TYR:OH	0.53	2.41	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:199:GLU:O	1:A:201:GLU:N	0.53	2.41	12	15
1:A:194:ASP:O	1:A:196:HIS:NE2	0.53	2.40	7	7
1:A:185:PHE:O	1:A:185:PHE:CG	0.53	2.61	17	1
1:A:207:SER:OG	1:A:208:GLY:N	0.53	2.39	10	2
1:A:183:HIS:O	1:A:183:HIS:CG	0.53	2.60	11	4
1:A:261:LEU:N	1:A:261:LEU:CD1	0.53	2.71	11	1
1:A:153:ASN:HD22	1:A:153:ASN:N	0.53	2.02	13	1
1:A:222:HIS:NE2	1:A:228:HIS:CD2	0.53	2.76	17	1
1:A:185:PHE:CD2	1:A:192:GLY:O	0.53	2.62	17	2
1:A:219:GLU:OE1	1:A:219:GLU:N	0.53	2.42	4	1
1:A:240:TYR:OH	1:A:248:PHE:CE2	0.53	2.62	10	4
1:A:197:PHE:CE2	1:A:219:GLU:OE2	0.53	2.62	8	5
1:A:117:ARG:NH2	1:A:155:GLY:O	0.53	2.42	10	1
1:A:168:HIS:CG	1:A:169:GLY:H	0.53	2.22	12	4
1:A:177:LYS:N	1:A:200:ASP:OD2	0.53	2.42	16	2
1:A:138:PHE:CD1	1:A:149:PHE:CG	0.53	2.97	8	5
1:A:185:PHE:CD1	1:A:192:GLY:O	0.53	2.61	3	2
1:A:135:ARG:NH1	1:A:139:GLN:OE1	0.53	2.42	5	1
1:A:116:TYR:CG	1:A:138:PHE:CE2	0.53	2.97	1	2
1:A:167:ALA:O	1:A:174:PHE:CD2	0.53	2.62	8	1
1:A:159:ILE:O	1:A:159:ILE:HG23	0.53	2.03	7	2
1:A:111:LYS:N	1:A:111:LYS:CD	0.53	2.72	6	1
1:A:253:ASP:OD1	1:A:253:ASP:N	0.53	2.42	10	2
1:A:117:ARG:NE	1:A:119:ASN:OD1	0.53	2.42	15	3
1:A:172:HIS:O	1:A:172:HIS:ND1	0.53	2.42	5	1
1:A:218:HIS:CE1	3:A:1:DSV:HN24	0.53	2.21	8	1
1:A:120:ASN:ND2	1:A:163:PHE:O	0.52	2.42	12	1
1:A:118:ILE:O	1:A:121:TYR:CZ	0.52	2.63	8	6
1:A:170:ASP:O	1:A:172:HIS:N	0.52	2.42	13	4
1:A:175:ASP:N	1:A:175:ASP:OD1	0.52	2.42	3	2
1:A:166:GLY:O	1:A:174:PHE:CD2	0.52	2.63	6	1
1:A:167:ALA:O	1:A:174:PHE:CE2	0.52	2.63	8	2
1:A:232:PRO:O	1:A:234:ALA:N	0.52	2.42	16	1
1:A:222:HIS:O	1:A:225:GLY:N	0.52	2.42	8	3
1:A:112:HIS:N	1:A:112:HIS:ND1	0.52	2.57	12	1
1:A:117:ARG:NH1	1:A:119:ASN:OD1	0.52	2.42	10	2
1:A:197:PHE:CZ	1:A:219:GLU:OE1	0.52	2.62	6	5
1:A:152:ILE:O	1:A:152:ILE:HD12	0.52	2.04	8	1
1:A:171:PHE:CE1	1:A:183:HIS:CE1	0.52	2.97	1	1
1:A:197:PHE:CE2	1:A:219:GLU:OE1	0.52	2.63	5	1
1:A:172:HIS:O	1:A:174:PHE:CD2	0.52	2.62	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:HIS:O	1:A:170:ASP:N	0.52	2.42	1	1
1:A:211:ASN:OD1	1:A:211:ASN:N	0.52	2.42	1	1
1:A:130:VAL:CG1	1:A:163:PHE:CZ	0.52	2.92	13	2
1:A:197:PHE:CE1	1:A:219:GLU:OE1	0.52	2.62	8	2
1:A:174:PHE:CG	1:A:198:ASP:OD1	0.52	2.63	12	1
1:A:228:HIS:O	1:A:229:SER:CB	0.52	2.57	11	1
1:A:218:HIS:CE1	3:A:1:DSV:C5	0.52	2.92	6	5
1:A:218:HIS:ND1	3:A:1:DSV:C5	0.52	2.73	4	3
1:A:122:THR:O	1:A:124:ASP:N	0.52	2.42	10	4
1:A:119:ASN:H	1:A:119:ASN:HD22	0.52	1.46	5	2
1:A:199:GLU:OE2	1:A:203:TRP:CD1	0.51	2.63	14	1
1:A:117:ARG:NH1	1:A:155:GLY:O	0.51	2.43	15	1
3:A:1:DSV:HC2B	3:A:1:DSV:O40	0.51	2.05	17	1
1:A:244:ASP:OD1	1:A:245:ILE:N	0.51	2.43	3	1
1:A:117:ARG:NH1	1:A:119:ASN:ND2	0.51	2.59	1	2
1:A:259:GLN:O	1:A:262:TYR:N	0.51	2.40	17	5
1:A:218:HIS:CE1	3:A:1:DSV:C6	0.51	2.93	2	3
1:A:178:GLY:N	1:A:201:GLU:OE2	0.51	2.43	6	2
1:A:124:ASP:OD2	1:A:165:ARG:NH2	0.51	2.43	3	2
1:A:117:ARG:NH1	1:A:153:ASN:O	0.51	2.43	7	2
1:A:224:LEU:O	1:A:226:LEU:N	0.51	2.44	16	3
1:A:174:PHE:CE1	1:A:198:ASP:OD1	0.51	2.63	10	1
1:A:197:PHE:CZ	1:A:219:GLU:OE2	0.51	2.63	13	1
1:A:183:HIS:HD1	1:A:184:ALA:N	0.51	2.03	5	2
1:A:183:HIS:NE2	1:A:196:HIS:O	0.51	2.43	16	3
1:A:171:PHE:O	1:A:171:PHE:CD2	0.51	2.64	2	1
1:A:258:ILE:O	1:A:261:LEU:N	0.51	2.44	14	4
1:A:111:LYS:O	1:A:112:HIS:CG	0.51	2.64	17	1
1:A:170:ASP:N	1:A:170:ASP:OD1	0.51	2.42	14	1
1:A:228:HIS:CD2	1:A:228:HIS:N	0.51	2.78	10	2
1:A:131:ASP:N	1:A:131:ASP:OD1	0.51	2.42	4	4
1:A:218:HIS:HE2	3:A:1:DSV:C37	0.51	2.19	12	1
1:A:218:HIS:CD2	3:A:1:DSV:C5	0.51	2.94	3	3
1:A:230:SER:OG	1:A:231:ASP:N	0.50	2.44	10	2
1:A:201:GLU:N	1:A:201:GLU:OE1	0.50	2.43	2	1
1:A:220:ILE:N	1:A:220:ILE:CD1	0.50	2.74	8	1
1:A:193:GLY:O	1:A:194:ASP:C	0.50	2.50	2	6
1:A:154:THR:HG22	1:A:155:GLY:N	0.50	2.21	17	1
1:A:172:HIS:O	1:A:174:PHE:CE2	0.50	2.64	16	1
1:A:234:ALA:O	1:A:236:MET:N	0.50	2.45	10	15
1:A:156:MET:SD	1:A:157:ALA:O	0.50	2.70	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:HIS:CD2	1:A:183:HIS:O	0.50	2.64	6	3
1:A:206:HIS:CD2	1:A:207:SER:H	0.50	2.24	6	2
1:A:118:ILE:O	1:A:121:TYR:CE2	0.50	2.64	2	3
1:A:211:ASN:O	1:A:215:THR:HG23	0.50	2.06	17	3
1:A:121:TYR:CD2	1:A:131:ASP:OD1	0.50	2.64	3	1
1:A:159:ILE:HG23	1:A:159:ILE:O	0.50	2.06	9	3
1:A:206:HIS:O	1:A:207:SER:CB	0.50	2.58	11	6
1:A:118:ILE:O	1:A:121:TYR:CE1	0.50	2.65	14	2
1:A:234:ALA:C	1:A:236:MET:N	0.50	2.65	14	16
1:A:203:TRP:CZ3	1:A:210:THR:O	0.50	2.65	1	2
1:A:218:HIS:CD2	3:A:1:DSV:C6	0.50	2.94	16	1
1:A:132:TYR:OH	1:A:136:LYS:NZ	0.50	2.44	8	2
1:A:218:HIS:HD1	3:A:1:DSV:C5	0.50	2.19	14	2
1:A:170:ASP:O	1:A:172:HIS:CD2	0.50	2.65	9	1
1:A:185:PHE:CG	1:A:185:PHE:O	0.50	2.65	5	1
1:A:166:GLY:O	1:A:174:PHE:CE2	0.49	2.65	3	2
1:A:222:HIS:CE1	1:A:228:HIS:HE2	0.49	2.17	16	1
1:A:230:SER:O	1:A:231:ASP:CB	0.49	2.61	8	4
1:A:168:HIS:CD2	1:A:169:GLY:H	0.49	2.25	14	2
1:A:120:ASN:OD1	1:A:121:TYR:N	0.49	2.45	4	1
1:A:196:HIS:N	1:A:196:HIS:ND1	0.49	2.60	1	3
1:A:135:ARG:O	1:A:135:ARG:NE	0.49	2.44	11	1
1:A:195:ALA:O	1:A:196:HIS:CD2	0.49	2.65	7	1
1:A:183:HIS:ND1	1:A:183:HIS:C	0.49	2.66	4	2
1:A:168:HIS:CE1	1:A:170:ASP:OD2	0.49	2.65	3	1
1:A:222:HIS:CE1	1:A:228:HIS:CE1	0.49	3.00	2	1
1:A:170:ASP:OD1	1:A:171:PHE:N	0.49	2.45	10	1
1:A:198:ASP:OD1	1:A:198:ASP:N	0.49	2.42	10	3
1:A:171:PHE:CZ	1:A:172:HIS:CD2	0.49	3.01	17	1
1:A:258:ILE:CG2	1:A:259:GLN:N	0.49	2.76	6	10
1:A:126:ASN:ND2	1:A:126:ASN:N	0.49	2.58	6	1
1:A:120:ASN:C	1:A:121:TYR:CG	0.49	2.86	11	1
1:A:191:ILE:HG23	1:A:191:ILE:O	0.49	2.08	15	1
1:A:240:TYR:O	1:A:242:TYR:N	0.49	2.44	14	1
1:A:248:PHE:O	1:A:249:ARG:NE	0.49	2.46	8	2
1:A:258:ILE:C	1:A:260:SER:N	0.49	2.66	10	12
1:A:229:SER:O	1:A:236:MET:SD	0.49	2.71	17	1
1:A:244:ASP:OD1	1:A:244:ASP:N	0.49	2.45	17	1
1:A:171:PHE:O	1:A:172:HIS:CB	0.48	2.61	3	1
1:A:151:LYS:NZ	1:A:151:LYS:CB	0.48	2.76	13	2
1:A:228:HIS:CE1	1:A:236:MET:SD	0.48	3.05	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:TYR:O	1:A:135:ARG:N	0.48	2.44	8	1
1:A:248:PHE:O	1:A:249:ARG:CZ	0.48	2.61	8	1
1:A:116:TYR:CD1	1:A:116:TYR:N	0.48	2.82	1	6
1:A:203:TRP:CE3	1:A:210:THR:O	0.48	2.66	1	2
1:A:211:ASN:CG	1:A:242:TYR:CD1	0.48	2.87	11	1
1:A:115:THR:N	1:A:158:ASP:OD2	0.48	2.43	3	5
1:A:218:HIS:NE2	3:A:1:DSV:C37	0.48	2.77	12	1
1:A:129:ASP:OD1	1:A:129:ASP:N	0.48	2.46	2	1
1:A:174:PHE:CD1	1:A:198:ASP:OD2	0.48	2.66	10	1
1:A:153:ASN:ND2	1:A:153:ASN:N	0.48	2.62	13	1
1:A:197:PHE:CE2	1:A:219:GLU:CD	0.48	2.87	6	4
1:A:238:PRO:O	3:A:1:DSV:CZ2	0.48	2.62	12	11
1:A:197:PHE:CZ	1:A:219:GLU:CD	0.48	2.87	13	2
1:A:191:ILE:HG23	1:A:192:GLY:N	0.48	2.23	17	1
1:A:233:LYS:NZ	1:A:253:ASP:OD1	0.48	2.46	17	1
1:A:168:HIS:NE2	1:A:170:ASP:OD2	0.48	2.47	3	1
1:A:258:ILE:HG23	1:A:259:GLN:H	0.48	1.69	16	1
1:A:224:LEU:C	1:A:226:LEU:N	0.48	2.67	11	3
1:A:183:HIS:O	1:A:183:HIS:CD2	0.47	2.66	17	1
1:A:113:TYR:CD2	1:A:113:TYR:O	0.47	2.67	17	3
1:A:199:GLU:CD	1:A:203:TRP:CD1	0.47	2.88	14	1
1:A:211:ASN:ND2	1:A:211:ASN:N	0.47	2.62	5	1
1:A:201:GLU:CD	1:A:201:GLU:N	0.47	2.67	15	2
3:A:1:DSV:O39	3:A:1:DSV:HC2B	0.47	2.08	13	1
1:A:259:GLN:O	1:A:261:LEU:N	0.47	2.47	17	5
1:A:247:THR:O	1:A:249:ARG:NH1	0.47	2.47	9	1
1:A:156:MET:CE	1:A:157:ALA:O	0.47	2.63	15	2
1:A:259:GLN:C	1:A:261:LEU:N	0.47	2.67	17	6
1:A:128:GLU:CD	1:A:128:GLU:N	0.47	2.68	3	2
1:A:174:PHE:CD1	1:A:198:ASP:CG	0.47	2.88	5	2
1:A:182:ALA:N	3:A:1:DSV:O22	0.47	2.48	14	1
1:A:133:ALA:CB	1:A:213:PHE:CE2	0.47	2.97	8	2
1:A:220:ILE:HD12	1:A:220:ILE:N	0.47	2.23	8	1
1:A:185:PHE:CB	1:A:192:GLY:O	0.47	2.63	5	1
1:A:185:PHE:C	1:A:185:PHE:CD1	0.47	2.88	1	1
1:A:117:ARG:CZ	1:A:155:GLY:O	0.47	2.62	15	1
1:A:117:ARG:NH1	1:A:119:ASN:CG	0.47	2.68	5	2
1:A:119:ASN:OD1	1:A:119:ASN:N	0.47	2.48	1	1
1:A:128:GLU:N	1:A:128:GLU:CD	0.47	2.68	4	2
1:A:201:GLU:N	1:A:201:GLU:CD	0.47	2.68	2	1
1:A:244:ASP:N	1:A:244:ASP:OD1	0.47	2.48	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:TYR:O	1:A:122:THR:C	0.47	2.53	14	3
1:A:113:TYR:O	1:A:113:TYR:CD2	0.47	2.68	2	1
1:A:180:ILE:CD1	1:A:180:ILE:N	0.47	2.78	7	1
1:A:131:ASP:OD1	1:A:131:ASP:N	0.47	2.45	13	4
1:A:261:LEU:O	1:A:262:TYR:CB	0.47	2.62	3	3
1:A:204:THR:O	1:A:206:HIS:O	0.47	2.33	8	1
1:A:120:ASN:C	1:A:121:TYR:CD1	0.47	2.89	11	2
1:A:195:ALA:C	1:A:196:HIS:CG	0.47	2.89	16	1
1:A:239:THR:C	1:A:241:LYS:N	0.47	2.68	11	3
1:A:166:GLY:N	1:A:200:ASP:OD1	0.46	2.41	17	1
1:A:211:ASN:HD21	3:A:1:DSV:CY1	0.46	2.23	4	1
1:A:199:GLU:CG	1:A:199:GLU:O	0.46	2.63	7	2
1:A:120:ASN:ND2	1:A:121:TYR:N	0.46	2.64	1	1
1:A:199:GLU:C	1:A:201:GLU:N	0.46	2.67	2	14
1:A:207:SER:OG	1:A:207:SER:O	0.46	2.32	9	2
1:A:175:ASP:CG	1:A:176:GLY:N	0.46	2.68	17	1
1:A:261:LEU:C	1:A:262:TYR:CG	0.46	2.87	5	1
1:A:171:PHE:CD2	1:A:171:PHE:O	0.46	2.68	14	2
1:A:130:VAL:O	1:A:134:ILE:HD12	0.46	2.11	14	3
1:A:204:THR:C	1:A:206:HIS:N	0.46	2.67	8	3
1:A:229:SER:OG	1:A:234:ALA:CB	0.46	2.63	9	1
1:A:117:ARG:CZ	1:A:119:ASN:OD1	0.46	2.63	15	2
1:A:113:TYR:CG	1:A:113:TYR:O	0.46	2.68	15	1
1:A:113:TYR:CD1	1:A:113:TYR:O	0.46	2.69	9	2
1:A:159:ILE:CG1	1:A:193:GLY:O	0.46	2.64	17	4
1:A:135:ARG:C	1:A:135:ARG:NE	0.46	2.68	11	1
1:A:239:THR:O	1:A:239:THR:OG1	0.46	2.34	17	2
1:A:153:ASN:N	1:A:153:ASN:OD1	0.46	2.45	5	2
1:A:120:ASN:O	1:A:120:ASN:ND2	0.46	2.48	15	1
1:A:242:TYR:O	1:A:243:VAL:HG13	0.46	2.11	6	5
1:A:168:HIS:HD1	1:A:172:HIS:CB	0.46	2.23	7	1
1:A:122:THR:C	1:A:124:ASP:H	0.45	2.14	5	3
1:A:226:LEU:O	1:A:227:GLY:O	0.45	2.34	9	2
1:A:120:ASN:CG	1:A:121:TYR:N	0.45	2.70	4	1
1:A:236:MET:SD	1:A:236:MET:C	0.45	2.95	4	7
1:A:156:MET:SD	1:A:156:MET:C	0.45	2.95	12	2
1:A:120:ASN:OD1	1:A:163:PHE:O	0.45	2.33	17	1
1:A:120:ASN:O	1:A:121:TYR:C	0.45	2.55	14	4
1:A:214:LEU:N	1:A:214:LEU:HD12	0.45	2.27	11	2
1:A:243:VAL:HG22	1:A:244:ASP:H	0.45	1.71	9	1
1:A:218:HIS:CE1	3:A:1:DSV:H6	0.45	2.47	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:HIS:ND1	1:A:172:HIS:C	0.45	2.68	8	1
1:A:206:HIS:CG	1:A:206:HIS:O	0.45	2.69	13	2
1:A:159:ILE:O	1:A:159:ILE:CG2	0.45	2.64	9	2
1:A:115:THR:OG1	1:A:158:ASP:N	0.45	2.42	6	1
1:A:133:ALA:HB2	1:A:213:PHE:CE2	0.45	2.47	8	1
1:A:199:GLU:O	1:A:201:GLU:O	0.45	2.34	4	11
1:A:168:HIS:HE2	1:A:170:ASP:CG	0.45	2.15	12	1
1:A:203:TRP:CH2	1:A:210:THR:CG2	0.45	3.00	14	1
1:A:174:PHE:CD1	1:A:174:PHE:N	0.45	2.84	8	2
1:A:226:LEU:CD2	1:A:226:LEU:N	0.45	2.80	10	1
1:A:181:LEU:CD2	1:A:201:GLU:OE2	0.45	2.64	13	1
1:A:236:MET:C	1:A:236:MET:SD	0.45	2.95	13	4
1:A:172:HIS:O	1:A:172:HIS:CG	0.45	2.68	5	1
1:A:168:HIS:CD2	1:A:196:HIS:CB	0.45	3.00	9	1
1:A:156:MET:CG	1:A:157:ALA:N	0.45	2.80	9	1
1:A:120:ASN:CG	1:A:163:PHE:H	0.45	2.15	17	1
1:A:199:GLU:O	1:A:200:ASP:C	0.45	2.54	9	1
1:A:258:ILE:HD13	1:A:258:ILE:O	0.45	2.12	9	1
1:A:174:PHE:CD2	1:A:198:ASP:OD1	0.45	2.70	6	2
1:A:118:ILE:HG21	1:A:121:TYR:CE2	0.45	2.47	13	2
1:A:168:HIS:CE1	1:A:170:ASP:O	0.45	2.69	4	1
1:A:174:PHE:CZ	1:A:183:HIS:CE1	0.45	3.04	6	1
1:A:127:ARG:CD	1:A:127:ARG:H	0.45	2.24	5	1
1:A:232:PRO:O	1:A:233:LYS:C	0.44	2.55	16	6
1:A:198:ASP:OD1	1:A:200:ASP:N	0.44	2.45	5	1
1:A:117:ARG:NH1	1:A:152:ILE:O	0.44	2.50	11	1
1:A:206:HIS:ND1	1:A:206:HIS:O	0.44	2.50	9	1
1:A:154:THR:OG1	1:A:155:GLY:N	0.44	2.50	9	1
1:A:154:THR:CG2	1:A:155:GLY:N	0.44	2.80	17	1
1:A:168:HIS:CD2	1:A:196:HIS:CG	0.44	3.06	2	1
1:A:141:TRP:O	1:A:145:THR:OG1	0.44	2.33	17	6
1:A:119:ASN:ND2	1:A:160:LEU:HD21	0.44	2.26	6	2
1:A:262:TYR:O	1:A:262:TYR:CD1	0.44	2.71	15	1
1:A:211:ASN:O	1:A:215:THR:OG1	0.44	2.33	14	2
1:A:112:HIS:ND1	1:A:112:HIS:N	0.44	2.66	4	1
1:A:121:TYR:CE2	1:A:131:ASP:CG	0.44	2.91	3	1
1:A:166:GLY:H	1:A:200:ASP:CG	0.44	2.16	15	1
1:A:121:TYR:O	1:A:123:PRO:N	0.44	2.51	12	1
1:A:130:VAL:O	1:A:134:ILE:CG1	0.44	2.66	17	4
1:A:198:ASP:OD1	1:A:198:ASP:O	0.44	2.36	11	3
1:A:124:ASP:OD1	1:A:124:ASP:N	0.44	2.51	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:HIS:NE2	1:A:196:HIS:ND1	0.44	2.66	14	2
1:A:154:THR:C	1:A:156:MET:N	0.44	2.70	17	2
1:A:127:ARG:O	1:A:131:ASP:OD1	0.44	2.35	1	3
1:A:200:ASP:OD1	1:A:200:ASP:N	0.44	2.50	8	2
1:A:242:TYR:C	1:A:242:TYR:CD1	0.44	2.90	10	1
1:A:153:ASN:O	1:A:154:THR:HG23	0.44	2.11	16	1
1:A:206:HIS:O	1:A:207:SER:O	0.44	2.36	8	1
1:A:122:THR:C	1:A:124:ASP:N	0.44	2.71	13	2
1:A:218:HIS:NE2	3:A:1:DSV:O40	0.44	2.51	12	1
1:A:118:ILE:HG22	1:A:121:TYR:H	0.44	1.72	3	1
1:A:185:PHE:O	1:A:185:PHE:CD1	0.44	2.71	5	1
1:A:194:ASP:O	1:A:194:ASP:OD1	0.44	2.35	8	2
1:A:120:ASN:HB3	1:A:162:VAL:HG13	0.44	1.90	8	1
1:A:120:ASN:ND2	1:A:121:TYR:O	0.44	2.51	1	1
1:A:240:TYR:C	1:A:242:TYR:H	0.43	2.15	14	1
1:A:113:TYR:O	1:A:113:TYR:CD1	0.43	2.71	4	1
1:A:248:PHE:CD1	1:A:248:PHE:C	0.43	2.91	7	4
1:A:117:ARG:HH11	1:A:119:ASN:CG	0.43	2.15	5	1
1:A:206:HIS:O	1:A:207:SER:OG	0.43	2.36	17	2
1:A:191:ILE:CG2	1:A:192:GLY:N	0.43	2.80	17	1
1:A:168:HIS:CD2	1:A:168:HIS:C	0.43	2.91	17	1
1:A:115:THR:OG1	1:A:158:ASP:OD2	0.43	2.36	4	1
1:A:118:ILE:CG2	1:A:121:TYR:CE2	0.43	3.01	16	1
1:A:238:PRO:O	1:A:240:TYR:N	0.43	2.49	8	1
1:A:218:HIS:NE2	3:A:1:DSV:O39	0.43	2.51	6	1
1:A:231:ASP:N	1:A:232:PRO:HD2	0.43	2.29	11	2
1:A:234:ALA:C	1:A:236:MET:H	0.43	2.17	10	9
1:A:172:HIS:O	1:A:173:ALA:O	0.43	2.36	17	1
1:A:181:LEU:O	1:A:198:ASP:OD1	0.43	2.36	4	1
1:A:183:HIS:CG	1:A:184:ALA:H	0.43	2.31	2	1
1:A:200:ASP:O	1:A:200:ASP:OD1	0.43	2.36	5	1
1:A:194:ASP:O	1:A:195:ALA:C	0.43	2.56	7	1
1:A:211:ASN:ND2	1:A:242:TYR:CE1	0.43	2.87	15	1
1:A:200:ASP:O	1:A:201:GLU:CG	0.43	2.66	9	1
1:A:174:PHE:CG	1:A:198:ASP:CG	0.43	2.92	12	1
1:A:115:THR:OG1	1:A:158:ASP:OD1	0.43	2.37	15	8
1:A:224:LEU:C	1:A:226:LEU:H	0.43	2.17	11	1
1:A:168:HIS:CG	1:A:168:HIS:O	0.43	2.72	15	1
1:A:243:VAL:O	1:A:244:ASP:C	0.43	2.57	13	1
1:A:207:SER:OG	1:A:242:TYR:OH	0.43	2.36	8	1
1:A:213:PHE:CG	1:A:245:ILE:CG2	0.43	3.02	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:215:THR:OG1	3:A:1:DSV:CY1	0.43	2.67	13	3
1:A:128:GLU:CD	1:A:128:GLU:H	0.43	2.17	3	1
1:A:175:ASP:O	1:A:176:GLY:O	0.43	2.36	16	1
1:A:228:HIS:O	1:A:229:SER:OG	0.43	2.35	11	1
1:A:222:HIS:CE1	1:A:228:HIS:CD2	0.43	3.07	17	1
1:A:165:ARG:O	1:A:166:GLY:O	0.43	2.37	11	3
1:A:174:PHE:CD2	1:A:198:ASP:CG	0.43	2.92	14	1
1:A:204:THR:CG2	1:A:205:THR:N	0.43	2.81	14	1
1:A:156:MET:SD	1:A:160:LEU:HD11	0.43	2.54	6	1
1:A:256:ARG:HH11	1:A:259:GLN:HE22	0.43	1.57	8	1
1:A:239:THR:OG1	1:A:240:TYR:N	0.42	2.49	14	1
1:A:208:GLY:O	1:A:209:GLY:O	0.42	2.37	14	2
1:A:166:GLY:O	1:A:175:ASP:OD1	0.42	2.36	16	1
1:A:135:ARG:C	1:A:135:ARG:HE	0.42	2.16	11	1
1:A:168:HIS:ND1	1:A:168:HIS:N	0.42	2.66	11	2
1:A:218:HIS:ND1	3:A:1:DSV:H5	0.42	2.28	15	1
1:A:122:THR:OG1	1:A:199:GLU:OE2	0.42	2.37	16	2
1:A:166:GLY:O	1:A:167:ALA:O	0.42	2.36	11	3
1:A:170:ASP:O	1:A:171:PHE:O	0.42	2.37	1	1
1:A:160:LEU:O	1:A:195:ALA:O	0.42	2.37	9	1
1:A:116:TYR:N	1:A:116:TYR:CD1	0.42	2.88	2	2
1:A:248:PHE:C	1:A:248:PHE:CD1	0.42	2.93	9	2
1:A:203:TRP:CH2	1:A:210:THR:HG21	0.42	2.49	14	1
1:A:117:ARG:NH2	1:A:119:ASN:OD1	0.42	2.52	8	1
1:A:153:ASN:O	1:A:154:THR:OG1	0.42	2.36	17	1
1:A:215:THR:O	1:A:219:GLU:OE2	0.42	2.37	17	1
1:A:113:TYR:C	1:A:114:ILE:HD12	0.42	2.35	10	1
1:A:120:ASN:O	1:A:121:TYR:O	0.42	2.38	15	1
1:A:129:ASP:OD1	1:A:129:ASP:O	0.42	2.38	6	2
1:A:218:HIS:CE1	1:A:222:HIS:CD2	0.42	3.07	7	1
1:A:171:PHE:C	1:A:173:ALA:H	0.42	2.18	13	2
1:A:213:PHE:CE2	1:A:245:ILE:CD1	0.42	3.03	13	1
1:A:198:ASP:OD1	1:A:200:ASP:OD1	0.42	2.38	12	1
1:A:175:ASP:OD1	1:A:175:ASP:C	0.42	2.58	17	1
1:A:206:HIS:O	1:A:208:GLY:N	0.42	2.53	6	1
1:A:113:TYR:O	1:A:113:TYR:CG	0.42	2.73	17	1
1:A:176:GLY:O	1:A:200:ASP:OD2	0.42	2.37	4	1
1:A:123:PRO:O	1:A:124:ASP:OD2	0.42	2.38	10	1
1:A:259:GLN:C	1:A:261:LEU:H	0.42	2.19	17	3
1:A:172:HIS:ND1	1:A:173:ALA:N	0.42	2.67	2	1
1:A:218:HIS:CE1	3:A:1:DSV:O40	0.42	2.73	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:HIS:N	1:A:222:HIS:CD2	0.42	2.85	1	1
1:A:176:GLY:O	1:A:201:GLU:OE2	0.42	2.38	15	1
1:A:183:HIS:NE2	1:A:196:HIS:N	0.41	2.65	14	1
1:A:211:ASN:HD21	3:A:1:DSV:HY1	0.41	1.75	4	1
1:A:211:ASN:ND2	1:A:211:ASN:O	0.41	2.42	4	1
1:A:111:LYS:CB	1:A:111:LYS:NZ	0.41	2.84	14	1
1:A:118:ILE:CG2	1:A:121:TYR:CE1	0.41	3.02	1	1
1:A:166:GLY:O	1:A:174:PHE:O	0.41	2.38	7	1
1:A:170:ASP:O	1:A:170:ASP:OD1	0.41	2.37	6	1
1:A:138:PHE:CD1	1:A:220:ILE:HD13	0.41	2.50	9	1
1:A:242:TYR:O	1:A:243:VAL:CG1	0.41	2.68	7	4
1:A:237:PHE:CD1	1:A:237:PHE:C	0.41	2.93	3	1
1:A:197:PHE:CD2	1:A:219:GLU:OE2	0.41	2.73	8	1
1:A:207:SER:OG	1:A:242:TYR:CE1	0.41	2.73	13	1
1:A:220:ILE:O	1:A:223:SER:CB	0.41	2.68	5	1
1:A:231:ASP:O	1:A:231:ASP:OD1	0.41	2.37	11	1
1:A:224:LEU:O	1:A:225:GLY:C	0.41	2.59	7	2
1:A:118:ILE:O	1:A:120:ASN:N	0.41	2.54	3	1
1:A:258:ILE:C	1:A:260:SER:H	0.41	2.19	2	1
1:A:183:HIS:ND1	1:A:183:HIS:O	0.41	2.54	11	1
1:A:135:ARG:NH2	1:A:139:GLN:NE2	0.41	2.69	11	1
1:A:194:ASP:OD1	1:A:194:ASP:N	0.41	2.54	12	1
1:A:215:THR:OG1	3:A:1:DSV:C11	0.41	2.68	14	1
1:A:170:ASP:OD1	1:A:170:ASP:O	0.41	2.39	3	1
1:A:118:ILE:O	1:A:119:ASN:C	0.41	2.59	3	1
1:A:238:PRO:O	1:A:239:THR:OG1	0.41	2.36	10	1
1:A:213:PHE:CG	1:A:245:ILE:HG22	0.41	2.51	11	1
1:A:183:HIS:CE1	1:A:196:HIS:ND1	0.41	2.88	13	1
1:A:185:PHE:CD2	1:A:192:GLY:C	0.41	2.94	17	1
1:A:155:GLY:O	1:A:156:MET:C	0.41	2.59	4	2
1:A:123:PRO:O	1:A:124:ASP:CG	0.41	2.59	7	3
1:A:191:ILE:C	1:A:193:GLY:H	0.41	2.19	14	1
1:A:169:GLY:O	1:A:170:ASP:O	0.41	2.39	14	1
1:A:198:ASP:O	1:A:201:GLU:OE1	0.41	2.38	1	1
1:A:243:VAL:HG22	1:A:244:ASP:N	0.40	2.30	9	1
1:A:176:GLY:O	1:A:177:LYS:C	0.40	2.60	9	1
1:A:124:ASP:N	1:A:124:ASP:OD1	0.40	2.54	5	1
1:A:239:THR:C	1:A:241:LYS:H	0.40	2.19	13	1
1:A:230:SER:O	1:A:231:ASP:CG	0.40	2.60	17	2
1:A:249:ARG:O	1:A:250:LEU:O	0.40	2.39	13	1
1:A:119:ASN:O	1:A:120:ASN:CB	0.40	2.69	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:TYR:CD1	1:A:113:TYR:N	0.40	2.89	6	1
1:A:237:PHE:C	1:A:237:PHE:CD1	0.40	2.95	9	1
1:A:147:LEU:O	1:A:148:LYS:CG	0.40	2.69	16	1
1:A:165:ARG:CG	1:A:166:GLY:N	0.40	2.84	5	1
1:A:211:ASN:ND2	1:A:242:TYR:CD1	0.40	2.89	16	1
1:A:239:THR:O	1:A:240:TYR:C	0.40	2.60	15	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	147/165 (89%)	108±3 (73±2%)	24±3 (16±2%)	16±3 (11±2%)	1 9
All	All	2499/2805 (89%)	1832 (73%)	401 (16%)	266 (11%)	1 9

All 50 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	194	ASP	15
1	A	200	ASP	15
1	A	259	GLN	14
1	A	238	PRO	13
1	A	231	ASP	11
1	A	207	SER	11
1	A	225	GLY	11
1	A	124	ASP	10
1	A	262	TYR	10
1	A	209	GLY	10
1	A	244	ASP	8
1	A	168	HIS	8
1	A	208	GLY	8
1	A	169	GLY	7
1	A	191	ILE	7
1	A	172	HIS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	171	PHE	6
1	A	179	GLY	6
1	A	175	ASP	6
1	A	193	GLY	6
1	A	227	GLY	6
1	A	121	TYR	5
1	A	167	ALA	5
1	A	111	LYS	5
1	A	155	GLY	5
1	A	123	PRO	5
1	A	205	THR	4
1	A	235	VAL	4
1	A	166	GLY	4
1	A	260	SER	3
1	A	173	ALA	3
1	A	242	TYR	3
1	A	170	ASP	2
1	A	195	ALA	2
1	A	176	GLY	2
1	A	232	PRO	2
1	A	240	TYR	2
1	A	174	PHE	2
1	A	229	SER	2
1	A	122	THR	1
1	A	120	ASN	1
1	A	156	MET	1
1	A	119	ASN	1
1	A	243	VAL	1
1	A	233	LYS	1
1	A	241	LYS	1
1	A	226	LEU	1
1	A	206	HIS	1
1	A	250	LEU	1
1	A	192	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	121/133 (91%)	113±2 (94±2%)	8±2 (6±2%)	27	72
All	All	2057/2261 (91%)	1927 (94%)	130 (6%)	27	72

All 44 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	160	LEU	16
1	A	122	THR	16
1	A	149	PHE	7
1	A	239	THR	7
1	A	231	ASP	6
1	A	156	MET	5
1	A	175	ASP	5
1	A	121	TYR	4
1	A	240	TYR	4
1	A	196	HIS	4
1	A	120	ASN	3
1	A	172	HIS	3
1	A	253	ASP	3
1	A	200	ASP	3
1	A	135	ARG	3
1	A	211	ASN	3
1	A	219	GLU	2
1	A	119	ASN	2
1	A	154	THR	2
1	A	207	SER	2
1	A	194	ASP	2
1	A	124	ASP	2
1	A	174	PHE	2
1	A	183	HIS	2
1	A	153	ASN	2
1	A	131	ASP	2
1	A	152	ILE	1
1	A	115	THR	1
1	A	143	ASN	1
1	A	229	SER	1
1	A	241	LYS	1
1	A	226	LEU	1
1	A	244	ASP	1
1	A	163	PHE	1
1	A	242	TYR	1
1	A	111	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	127	ARG	1
1	A	198	ASP	1
1	A	256	ARG	1
1	A	236	MET	1
1	A	144	VAL	1
1	A	126	ASN	1
1	A	258	ILE	1
1	A	112	HIS	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	DSV	A	1	2	23,26,26	2.78±0.02	3±0 (13±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard

deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	DSV	A	1	2	25,39,39	1.13±0.01	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DSV	A	1	2	-	0±0,15,19,19	0±0,3,3,3

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	1	DSV	S21-N24	8.19	1.74	1.61	13	17
3	A	1	DSV	C11-S10	6.00	1.78	1.74	4	17
3	A	1	DSV	C3-S10	5.67	1.78	1.74	6	17

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided