



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 06:00 PM UTC

PDB ID : 1EMO / pdb_00001emo
Title : NMR STUDY OF A PAIR OF FIBRILLIN CA2+ BINDING EPIDERMAL GROWTH FACTOR-LIKE DOMAINS, 22 STRUCTURES
Authors : Downing, A.K.; Campbell, I.D.; Handford, P.A.
Deposited on : 1996-08-05

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

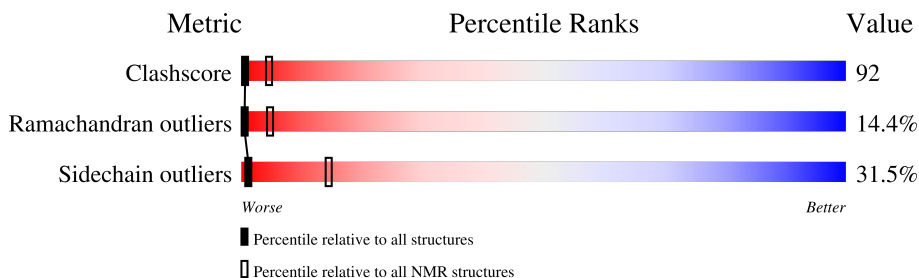
1 Overall quality at a glance

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	82	

2 Ensemble composition and analysis i

This entry contains 22 models. Model 3 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:2129-A:2205 (77)	0.88	3

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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 4, 6, 10, 11, 17, 22
2	1, 3, 5, 8, 9, 13
3	7, 19, 20
4	15, 16, 21
5	14, 18
Single-model clusters	12

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1120 atoms, of which 520 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FIBRILLIN.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	82	1118	356	520	96	131	15	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2158	ILE	THR	conflict	UNP P35555

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

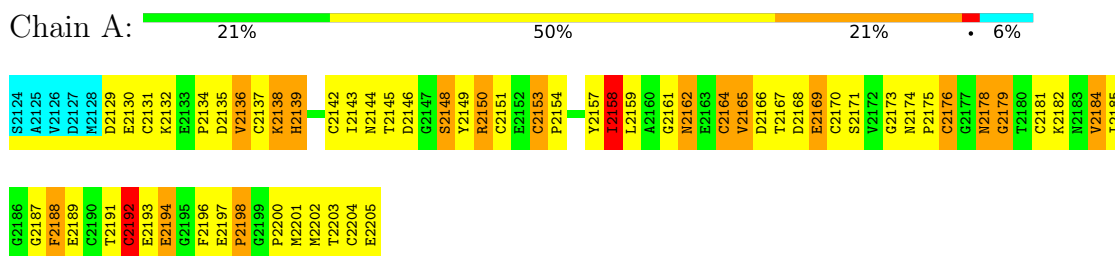
Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	2	2	2

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: FIBRILLIN

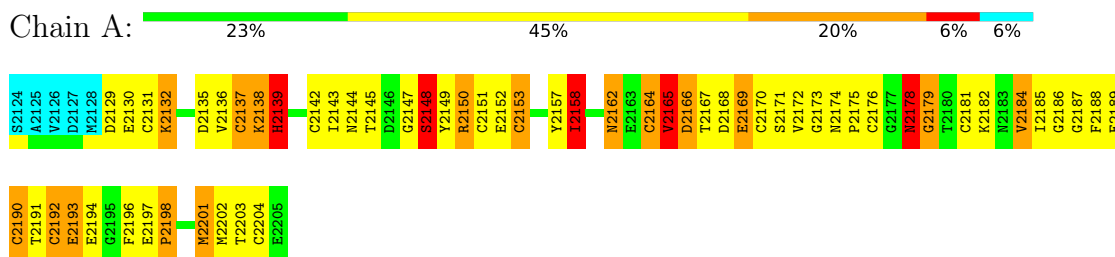


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

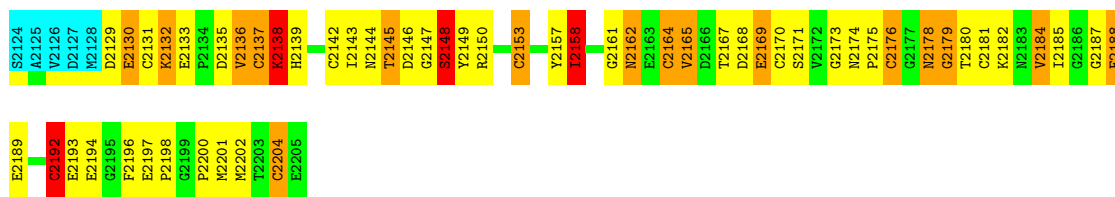
- Molecule 1: FIBRILLIN



4.2.2 Score per residue for model 2

- Molecule 1: FIBRILLIN

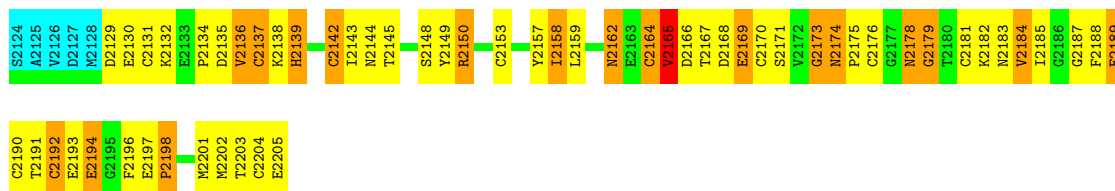




4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: FIBRILLIN

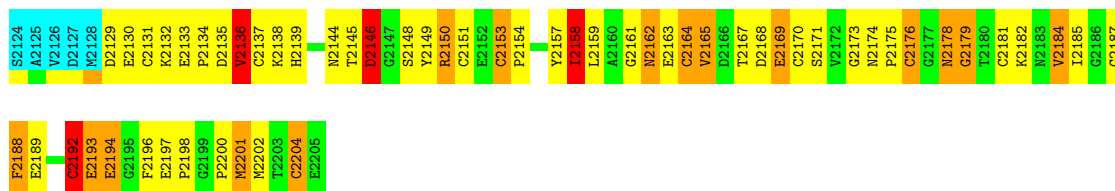
Chain A: 24% 46% 22% 6%



4.2.4 Score per residue for model 4

- Molecule 1: FIBRILLIN

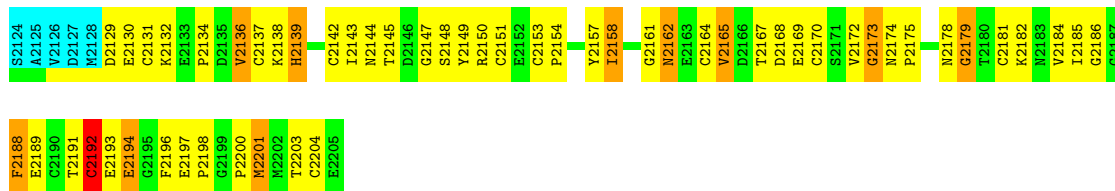
Chain A: 26% 45% 18% 5% 6%



4.2.5 Score per residue for model 5

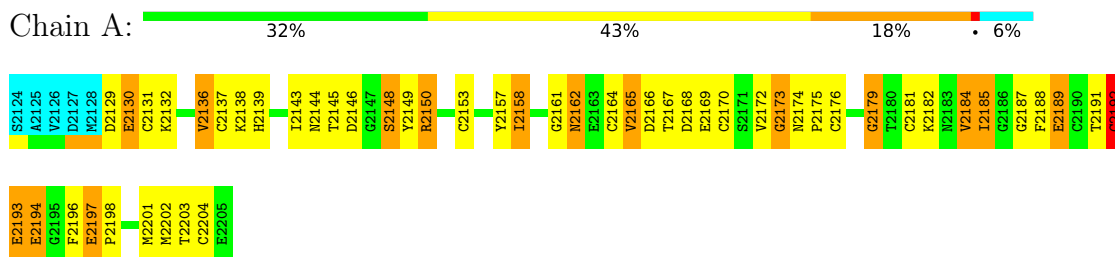
- Molecule 1: FIBRILLIN

Chain A: 28% 52% 12% 6%



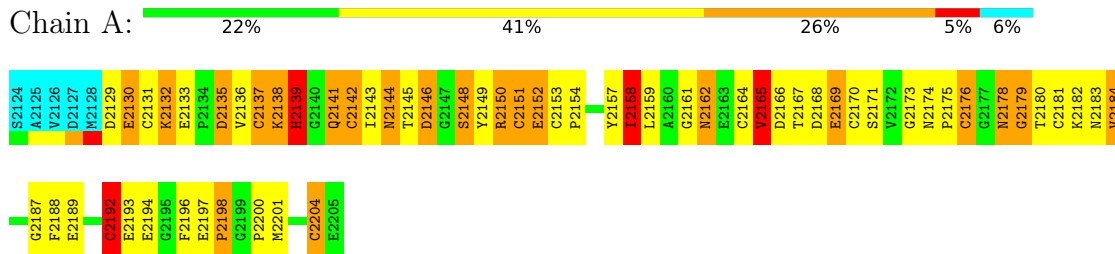
4.2.6 Score per residue for model 6

- Molecule 1: FIBRILLIN



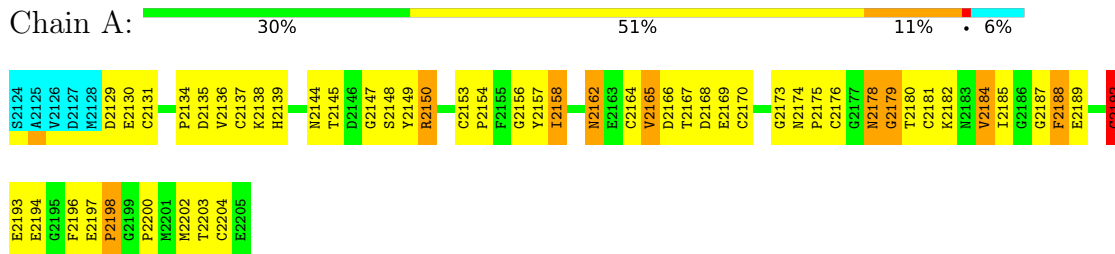
4.2.7 Score per residue for model 7

- Molecule 1: FIBRILLIN



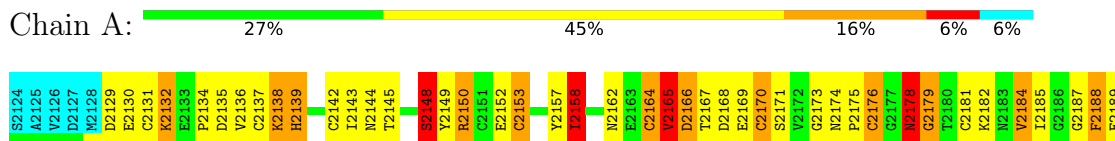
4.2.8 Score per residue for model 8

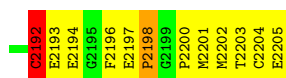
- Molecule 1: FIBRILLIN



4.2.9 Score per residue for model 9

- Molecule 1: FIBRILLIN

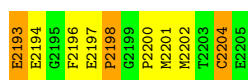




4.2.10 Score per residue for model 10

- Molecule 1: FIBRILLIN

Chain A: 32% 48% 13% 6%



4.2.11 Score per residue for model 11

- Molecule 1: FIBRILLIN

Chain A: 32% 45% 16% 6%



4.2.12 Score per residue for model 12

- Molecule 1: FIBRILLIN

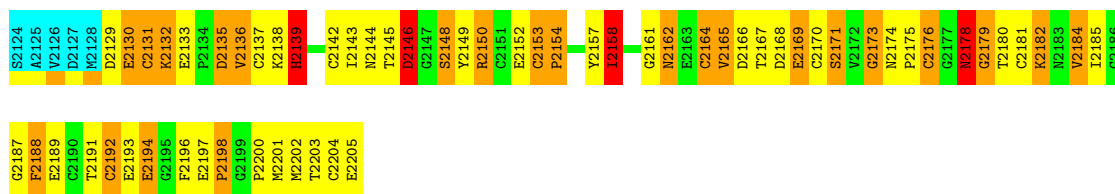
Chain A: 27% 41% 20% 6% 6%



4.2.13 Score per residue for model 13

- Molecule 1: FIBRILLIN

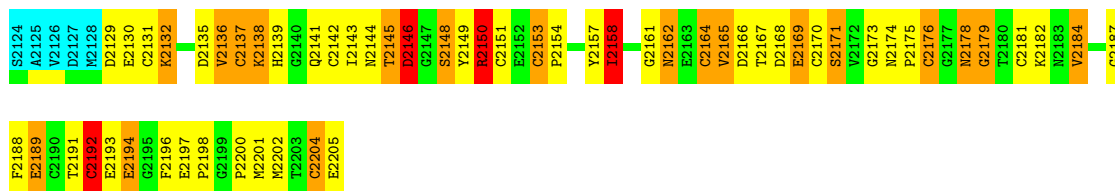
Chain A: 21% 40% 28% 5% 6%



4.2.14 Score per residue for model 14

- Molecule 1: FIBRILLIN

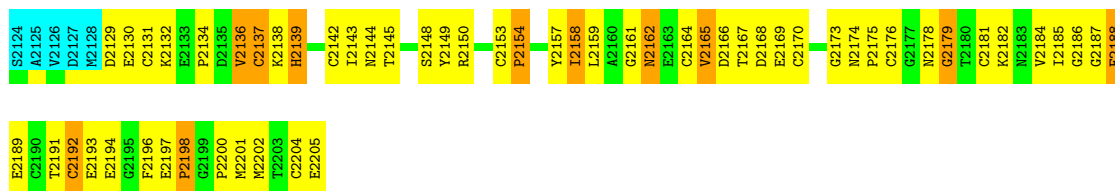
Chain A: 24% 41% 23% 5% 6%



4.2.15 Score per residue for model 15

- Molecule 1: FIBRILLIN

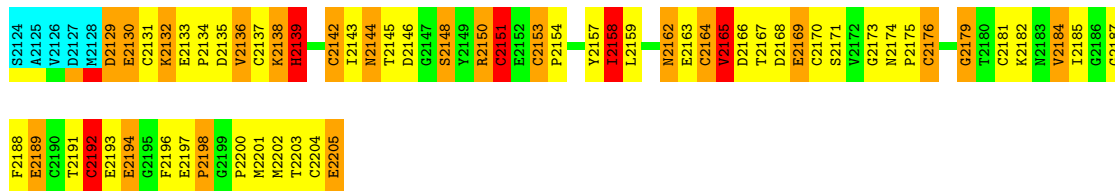
Chain A: 26% 55% 13% 6%



4.2.16 Score per residue for model 16

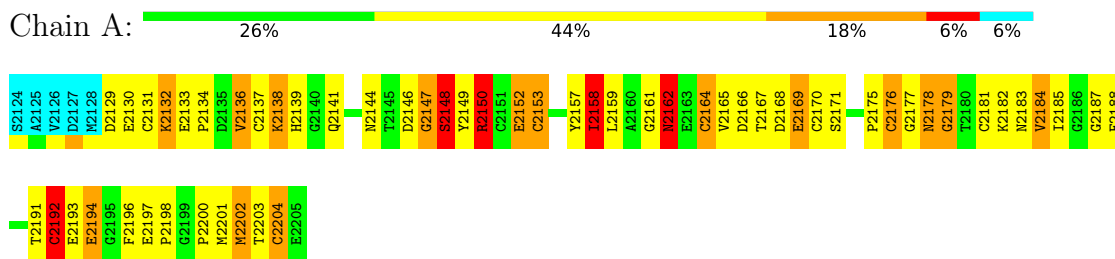
- Molecule 1: FIBRILLIN

Chain A: 22% 41% 24% 6% 6%



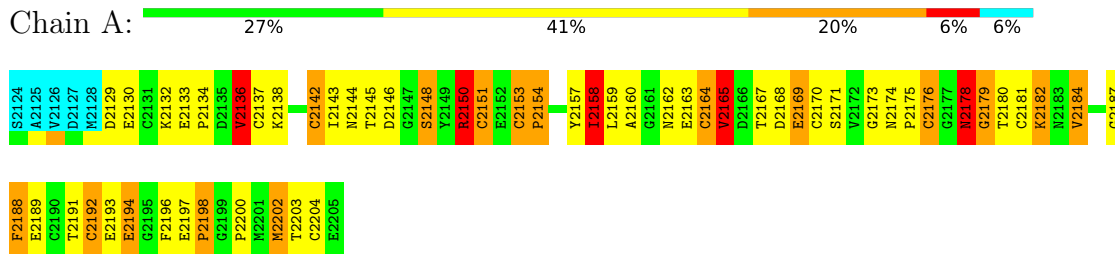
4.2.17 Score per residue for model 17

- Molecule 1: FIBRILLIN



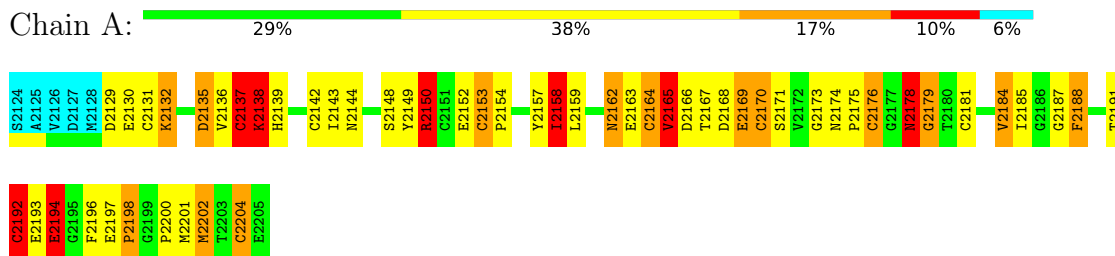
4.2.18 Score per residue for model 18

- Molecule 1: FIBRILLIN



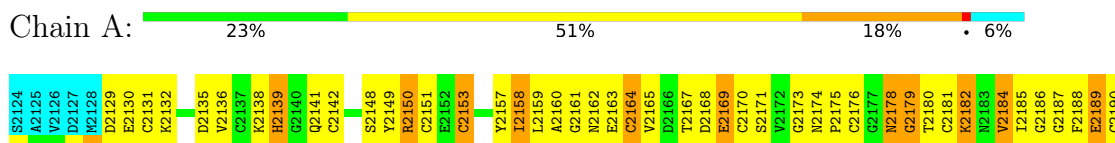
4.2.19 Score per residue for model 19

- Molecule 1: FIBRILLIN



4.2.20 Score per residue for model 20

- Molecule 1: FIBRILLIN





4.2.21 Score per residue for model 21

- Molecule 1: FIBRILLIN

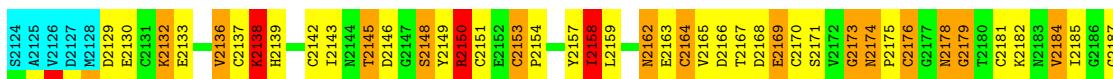
Chain A: 26% 38% 24% 6% 6%



4.2.22 Score per residue for model 22

- Molecule 1: FIBRILLIN

Chain A: 26% 43% 21% 5% 6%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 22 were deposited, based on the following criterion: $F(NOE) < 165 \text{ KJ MOL}^{-1}$ TORSION ANGLE CONSTRAINTS VIOLATED BY $> 3 \text{ DEGREES}$.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure calculation	3.1

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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

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	1.41±0.01	0±0/574 (0.0± 0.0%)	1.29±0.01	1±0/773 (0.1± 0.1%)
All	All	1.41	0/12628 (0.0%)	1.29	13/17006 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.0±0.0
All	All	0	22

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	2188	PHE	CA-CB-CG	-5.55	108.25	113.80	5	12
1	A	2177	GLY	N-CA-C	-5.26	108.22	114.48	17	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	2150	ARG	Sidechain	22

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	564	486	486	97±7
All	All	12452	10692	10692	2126

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 92.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2158:ILE:HD11	1:A:2165:VAL:HG23	0.91	1.40	11	9
1:A:2142:CYS:C	1:A:2143:ILE:HD13	0.91	1.90	19	2
1:A:2136:VAL:HG23	1:A:2149:TYR:CE1	0.89	2.02	4	1
1:A:2136:VAL:HG12	1:A:2151:CYS:SG	0.84	2.12	16	1
1:A:2136:VAL:HG11	1:A:2149:TYR:CE1	0.84	2.07	3	2
1:A:2142:CYS:C	1:A:2143:ILE:HD12	0.84	1.98	15	11
1:A:2142:CYS:O	1:A:2143:ILE:HD13	0.83	1.72	19	2
1:A:2167:THR:HG23	1:A:2169:GLU:OE1	0.82	1.73	20	15
1:A:2164:CYS:O	1:A:2165:VAL:HG13	0.82	1.75	18	21
1:A:2184:VAL:HG12	1:A:2188:PHE:N	0.82	1.88	22	22
1:A:2184:VAL:HG12	1:A:2188:PHE:CA	0.77	2.09	15	22
1:A:2135:ASP:OD1	1:A:2136:VAL:HG23	0.74	1.82	14	2
1:A:2133:GLU:HB2	1:A:2136:VAL:HG23	0.74	1.60	13	3
1:A:2130:GLU:O	1:A:2136:VAL:HG21	0.72	1.84	15	16
1:A:2158:ILE:HD13	1:A:2158:ILE:N	0.71	2.01	16	22
1:A:2184:VAL:HG13	1:A:2185:ILE:N	0.70	2.00	1	13
1:A:2136:VAL:HG22	1:A:2137:CYS:N	0.70	2.01	4	1
1:A:2158:ILE:HD13	1:A:2158:ILE:H	0.69	1.46	16	22
1:A:2186:GLY:O	1:A:2201:MET:HE2	0.69	1.87	20	1
1:A:2136:VAL:HG12	1:A:2137:CYS:N	0.69	2.02	22	10
1:A:2196:PHE:CZ	1:A:2198:PRO:CG	0.69	2.76	12	22
1:A:2157:TYR:OH	1:A:2185:ILE:HG23	0.67	1.89	6	10
1:A:2175:PRO:CB	1:A:2188:PHE:CD1	0.66	2.78	5	2
1:A:2192:CYS:N	1:A:2196:PHE:CZ	0.65	2.64	20	1
1:A:2175:PRO:CB	1:A:2188:PHE:CE2	0.65	2.80	19	7
1:A:2159:LEU:HD12	1:A:2163:GLU:O	0.64	1.92	16	4
1:A:2136:VAL:CG1	1:A:2149:TYR:CE1	0.64	2.81	9	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2184:VAL:HG12	1:A:2188:PHE:HA	0.64	1.69	15	19
1:A:2196:PHE:CZ	1:A:2198:PRO:CD	0.64	2.81	14	22
1:A:2136:VAL:HG13	1:A:2149:TYR:CE2	0.64	2.27	10	2
1:A:2136:VAL:CG1	1:A:2149:TYR:CE2	0.64	2.80	19	7
1:A:2130:GLU:CB	1:A:2149:TYR:CD2	0.64	2.80	15	2
1:A:2175:PRO:CB	1:A:2188:PHE:CE1	0.64	2.81	21	5
1:A:2130:GLU:CB	1:A:2149:TYR:CD1	0.63	2.81	14	5
1:A:2196:PHE:CE2	1:A:2198:PRO:CD	0.63	2.81	20	1
1:A:2135:ASP:O	1:A:2136:VAL:C	0.63	2.41	4	1
1:A:2136:VAL:CG2	1:A:2149:TYR:CE1	0.63	2.82	4	1
1:A:2184:VAL:HG12	1:A:2187:GLY:C	0.62	2.19	8	19
1:A:2158:ILE:HD12	1:A:2167:THR:HB	0.62	1.70	18	2
1:A:2130:GLU:O	1:A:2136:VAL:HG11	0.62	1.94	4	4
1:A:2136:VAL:HG12	1:A:2137:CYS:SG	0.61	2.35	10	1
1:A:2136:VAL:HG22	1:A:2137:CYS:SG	0.61	2.36	4	1
1:A:2158:ILE:N	1:A:2158:ILE:CD1	0.61	2.64	14	21
1:A:2143:ILE:O	1:A:2145:THR:HG23	0.60	1.95	5	3
1:A:2187:GLY:C	1:A:2188:PHE:CD1	0.60	2.80	17	15
1:A:2169:GLU:O	1:A:2172:VAL:HG23	0.60	1.96	1	5
1:A:2193:GLU:O	1:A:2194:GLU:C	0.59	2.45	19	22
1:A:2157:TYR:CD2	1:A:2165:VAL:C	0.59	2.80	19	13
1:A:2150:ARG:O	1:A:2151:CYS:C	0.59	2.45	18	2
1:A:2188:PHE:CD1	1:A:2188:PHE:N	0.59	2.69	11	1
1:A:2131:CYS:HA	1:A:2136:VAL:HG11	0.59	1.73	12	2
1:A:2184:VAL:CG1	1:A:2188:PHE:CA	0.59	2.81	12	15
1:A:2130:GLU:HB3	1:A:2149:TYR:CD1	0.58	2.33	14	10
1:A:2196:PHE:CG	1:A:2197:GLU:N	0.58	2.71	14	22
1:A:2196:PHE:CD2	1:A:2204:CYS:SG	0.58	2.97	17	20
1:A:2184:VAL:CG1	1:A:2188:PHE:N	0.58	2.66	16	11
1:A:2175:PRO:HB3	1:A:2188:PHE:CE1	0.58	2.32	21	2
1:A:2138:LYS:O	1:A:2139:HIS:CG	0.58	2.56	15	4
1:A:2196:PHE:CE2	1:A:2198:PRO:HD3	0.58	2.34	20	1
1:A:2196:PHE:CD2	1:A:2204:CYS:HB2	0.58	2.34	20	1
1:A:2196:PHE:CZ	1:A:2198:PRO:HD3	0.58	2.34	7	22
1:A:2143:ILE:HD12	1:A:2143:ILE:N	0.58	2.13	7	5
1:A:2136:VAL:HG11	1:A:2149:TYR:CE2	0.58	2.34	14	3
1:A:2145:THR:HG1	1:A:2148:SER:C	0.57	2.07	2	5
1:A:2196:PHE:CZ	1:A:2198:PRO:HG3	0.57	2.34	12	22
1:A:2129:ASP:O	1:A:2130:GLU:HB2	0.57	1.97	16	19
1:A:2169:GLU:CB	1:A:2188:PHE:CD1	0.57	2.88	15	17
1:A:2175:PRO:HB3	1:A:2188:PHE:CE2	0.57	2.34	12	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2196:PHE:CE2	1:A:2204:CYS:SG	0.56	2.98	2	15
1:A:2192:CYS:HB2	1:A:2196:PHE:CD2	0.56	2.34	20	22
1:A:2130:GLU:HB3	1:A:2149:TYR:CD2	0.56	2.36	15	6
1:A:2182:LYS:CB	1:A:2189:GLU:O	0.56	2.54	22	7
1:A:2156:GLY:O	1:A:2167:THR:HG22	0.56	2.00	11	1
1:A:2188:PHE:N	1:A:2188:PHE:CD1	0.56	2.74	6	12
1:A:2196:PHE:CD2	1:A:2197:GLU:N	0.56	2.74	20	19
1:A:2158:ILE:HD13	1:A:2165:VAL:O	0.56	2.01	18	13
1:A:2136:VAL:HG13	1:A:2149:TYR:CE1	0.56	2.36	9	1
1:A:2149:TYR:CD1	1:A:2149:TYR:N	0.55	2.73	1	5
1:A:2159:LEU:HD11	1:A:2162:ASN:O	0.55	2.00	15	2
1:A:2158:ILE:CG2	1:A:2167:THR:HB	0.55	2.32	14	21
1:A:2192:CYS:HB2	1:A:2196:PHE:CE1	0.55	2.37	1	21
1:A:2129:ASP:O	1:A:2144:ASN:ND2	0.55	2.40	19	7
1:A:2167:THR:CG2	1:A:2169:GLU:OE1	0.55	2.55	6	17
1:A:2175:PRO:HG2	1:A:2188:PHE:CD2	0.55	2.37	13	14
1:A:2136:VAL:CG2	1:A:2149:TYR:CZ	0.55	2.90	4	1
1:A:2158:ILE:CD1	1:A:2165:VAL:HG23	0.55	2.25	7	2
1:A:2175:PRO:HG2	1:A:2188:PHE:CE2	0.55	2.37	3	3
1:A:2192:CYS:HB2	1:A:2196:PHE:CD1	0.55	2.37	1	21
1:A:2130:GLU:O	1:A:2136:VAL:CG2	0.55	2.55	21	9
1:A:2137:CYS:CA	1:A:2162:ASN:O	0.54	2.55	7	2
1:A:2138:LYS:O	1:A:2139:HIS:CB	0.54	2.56	11	13
1:A:2157:TYR:OH	1:A:2185:ILE:CG2	0.54	2.56	10	17
1:A:2132:LYS:O	1:A:2132:LYS:CG	0.54	2.56	12	2
1:A:2162:ASN:CG	1:A:2163:GLU:N	0.54	2.66	22	4
1:A:2182:LYS:N	1:A:2189:GLU:O	0.54	2.40	18	7
1:A:2175:PRO:CG	1:A:2188:PHE:CE2	0.54	2.91	15	6
1:A:2129:ASP:O	1:A:2130:GLU:CB	0.53	2.55	12	17
1:A:2130:GLU:O	1:A:2136:VAL:CB	0.53	2.56	1	8
1:A:2192:CYS:HB2	1:A:2196:PHE:CZ	0.53	2.38	3	21
1:A:2130:GLU:O	1:A:2136:VAL:CG1	0.53	2.56	4	1
1:A:2149:TYR:O	1:A:2150:ARG:CG	0.53	2.57	13	4
1:A:2196:PHE:CE1	1:A:2198:PRO:HD3	0.53	2.39	13	21
1:A:2136:VAL:CG1	1:A:2149:TYR:CZ	0.53	2.92	9	1
1:A:2169:GLU:HB3	1:A:2188:PHE:CD1	0.53	2.38	15	15
1:A:2130:GLU:HB2	1:A:2149:TYR:CD2	0.53	2.38	15	2
1:A:2134:PRO:O	1:A:2138:LYS:CE	0.53	2.57	21	2
1:A:2158:ILE:HG21	1:A:2167:THR:HB	0.53	1.80	9	5
1:A:2129:ASP:OD1	1:A:2132:LYS:N	0.53	2.41	15	1
1:A:2157:TYR:C	1:A:2158:ILE:CG2	0.52	2.82	19	21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2188:PHE:CE2	1:A:2202:MET:O	0.52	2.61	1	5
1:A:2192:CYS:HB2	1:A:2196:PHE:CE2	0.52	2.40	3	22
1:A:2178:ASN:CG	1:A:2179:GLY:N	0.52	2.67	2	1
1:A:2187:GLY:C	1:A:2188:PHE:CD2	0.52	2.87	2	1
1:A:2164:CYS:O	1:A:2165:VAL:CG1	0.52	2.57	21	10
1:A:2136:VAL:O	1:A:2162:ASN:CB	0.52	2.58	8	3
1:A:2136:VAL:CG2	1:A:2137:CYS:SG	0.52	2.97	4	1
1:A:2192:CYS:N	1:A:2196:PHE:CE1	0.52	2.77	16	21
1:A:2141:GLN:O	1:A:2152:GLU:CG	0.52	2.58	12	1
1:A:2134:PRO:O	1:A:2138:LYS:CD	0.52	2.58	16	3
1:A:2157:TYR:CD2	1:A:2165:VAL:O	0.52	2.62	6	7
1:A:2149:TYR:C	1:A:2150:ARG:CG	0.52	2.83	7	4
1:A:2192:CYS:HB2	1:A:2196:PHE:CG	0.52	2.39	3	21
1:A:2135:ASP:O	1:A:2162:ASN:ND2	0.52	2.43	1	5
1:A:2149:TYR:C	1:A:2149:TYR:CD1	0.52	2.88	4	3
1:A:2136:VAL:O	1:A:2138:LYS:N	0.52	2.43	3	2
1:A:2196:PHE:CE2	1:A:2204:CYS:HB2	0.52	2.40	20	2
1:A:2138:LYS:C	1:A:2139:HIS:CG	0.52	2.87	8	3
1:A:2190:CYS:SG	1:A:2191:THR:N	0.51	2.83	3	2
1:A:2136:VAL:CG2	1:A:2137:CYS:N	0.51	2.72	4	1
1:A:2169:GLU:OE1	1:A:2169:GLU:N	0.51	2.43	16	4
1:A:2175:PRO:CD	1:A:2181:CYS:HB3	0.51	2.35	6	18
1:A:2137:CYS:O	1:A:2164:CYS:N	0.51	2.43	19	1
1:A:2158:ILE:HD12	1:A:2167:THR:N	0.51	2.20	18	1
1:A:2157:TYR:C	1:A:2158:ILE:HG23	0.51	2.29	14	20
1:A:2174:ASN:ND2	1:A:2179:GLY:C	0.51	2.68	6	2
1:A:2174:ASN:O	1:A:2174:ASN:CG	0.51	2.54	9	15
1:A:2175:PRO:HB2	1:A:2188:PHE:CE1	0.51	2.41	5	2
1:A:2173:GLY:O	1:A:2174:ASN:C	0.51	2.54	8	15
1:A:2136:VAL:O	1:A:2162:ASN:CA	0.51	2.59	4	1
1:A:2176:CYS:O	1:A:2204:CYS:CB	0.51	2.59	18	4
1:A:2176:CYS:SG	1:A:2204:CYS:CB	0.51	2.99	14	7
1:A:2158:ILE:HG23	1:A:2167:THR:HB	0.51	1.81	16	6
1:A:2157:TYR:O	1:A:2158:ILE:CG2	0.51	2.59	14	18
1:A:2196:PHE:CE2	1:A:2198:PRO:N	0.51	2.79	7	22
1:A:2161:GLY:O	1:A:2162:ASN:CB	0.51	2.59	15	8
1:A:2134:PRO:HA	1:A:2138:LYS:CG	0.51	2.36	8	4
1:A:2131:CYS:SG	1:A:2132:LYS:N	0.50	2.84	14	4
1:A:2178:ASN:O	1:A:2179:GLY:O	0.50	2.29	2	10
1:A:2174:ASN:OD1	1:A:2178:ASN:N	0.50	2.43	20	1
1:A:2191:THR:HG22	1:A:2191:THR:O	0.50	2.04	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2136:VAL:O	1:A:2137:CYS:C	0.50	2.54	9	5
1:A:2133:GLU:CB	1:A:2134:PRO:HD2	0.50	2.36	4	2
1:A:2129:ASP:O	1:A:2130:GLU:OE1	0.50	2.30	9	15
1:A:2182:LYS:HB3	1:A:2189:GLU:HB3	0.50	1.83	9	13
1:A:2137:CYS:N	1:A:2151:CYS:SG	0.50	2.84	16	1
1:A:2145:THR:OG1	1:A:2148:SER:C	0.50	2.55	22	15
1:A:2175:PRO:HG2	1:A:2188:PHE:CD1	0.50	2.42	8	2
1:A:2169:GLU:HB2	1:A:2188:PHE:HB3	0.50	1.83	8	17
1:A:2176:CYS:O	1:A:2204:CYS:HB2	0.50	2.06	15	8
1:A:2169:GLU:OE2	1:A:2187:GLY:CA	0.50	2.60	11	1
1:A:2149:TYR:O	1:A:2150:ARG:CD	0.50	2.59	19	2
1:A:2168:ASP:C	1:A:2168:ASP:OD1	0.49	2.55	22	17
1:A:2184:VAL:HG21	1:A:2189:GLU:OE1	0.49	2.06	20	2
1:A:2142:CYS:SG	1:A:2143:ILE:N	0.49	2.85	14	1
1:A:2130:GLU:OE2	1:A:2148:SER:N	0.49	2.45	11	2
1:A:2130:GLU:HB2	1:A:2149:TYR:CD1	0.49	2.42	14	1
1:A:2148:SER:C	1:A:2149:TYR:CD2	0.49	2.89	20	1
1:A:2137:CYS:CB	1:A:2142:CYS:SG	0.49	3.00	7	2
1:A:2137:CYS:N	1:A:2162:ASN:O	0.49	2.45	7	2
1:A:2170:CYS:O	1:A:2181:CYS:SG	0.49	2.71	13	16
1:A:2184:VAL:CG1	1:A:2185:ILE:N	0.49	2.71	1	4
1:A:2133:GLU:OE1	1:A:2136:VAL:HG21	0.49	2.07	2	1
1:A:2176:CYS:SG	1:A:2192:CYS:N	0.49	2.86	19	7
1:A:2157:TYR:CE1	1:A:2166:ASP:OD1	0.49	2.66	15	2
1:A:2150:ARG:CZ	1:A:2150:ARG:CB	0.49	2.88	3	2
1:A:2130:GLU:OE1	1:A:2148:SER:O	0.49	2.31	15	10
1:A:2182:LYS:HB3	1:A:2189:GLU:O	0.49	2.07	6	7
1:A:2143:ILE:HG22	1:A:2143:ILE:O	0.49	2.07	11	1
1:A:2175:PRO:O	1:A:2203:THR:OG1	0.49	2.31	16	11
1:A:2169:GLU:HB3	1:A:2188:PHE:CD2	0.49	2.43	5	5
1:A:2129:ASP:HA	1:A:2144:ASN:ND2	0.49	2.23	15	12
1:A:2129:ASP:C	1:A:2129:ASP:OD1	0.49	2.55	7	6
1:A:2131:CYS:O	1:A:2136:VAL:O	0.49	2.30	9	1
1:A:2143:ILE:HD13	1:A:2143:ILE:N	0.49	2.22	19	1
1:A:2151:CYS:HB2	1:A:2159:LEU:HD22	0.48	1.84	7	1
1:A:2176:CYS:SG	1:A:2190:CYS:O	0.48	2.71	20	1
1:A:2153:CYS:SG	1:A:2157:TYR:HB3	0.48	2.48	8	21
1:A:2191:THR:O	1:A:2192:CYS:O	0.48	2.30	16	14
1:A:2147:GLY:O	1:A:2148:SER:CB	0.48	2.62	2	2
1:A:2136:VAL:HG23	1:A:2149:TYR:CZ	0.48	2.41	4	1
1:A:2175:PRO:HB2	1:A:2188:PHE:CE2	0.48	2.43	19	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2179:GLY:HA3	1:A:2192:CYS:HA	0.48	1.85	6	22
1:A:2196:PHE:CZ	1:A:2198:PRO:CB	0.48	2.97	19	21
1:A:2136:VAL:O	1:A:2162:ASN:C	0.48	2.57	12	3
1:A:2138:LYS:O	1:A:2139:HIS:CD2	0.48	2.67	11	3
1:A:2142:CYS:C	1:A:2143:ILE:CD1	0.48	2.83	15	1
1:A:2142:CYS:SG	1:A:2150:ARG:C	0.48	2.96	20	1
1:A:2136:VAL:O	1:A:2162:ASN:O	0.48	2.32	15	9
1:A:2169:GLU:OE1	1:A:2187:GLY:O	0.48	2.32	9	2
1:A:2143:ILE:O	1:A:2144:ASN:C	0.48	2.57	14	1
1:A:2185:ILE:O	1:A:2201:MET:SD	0.48	2.72	4	2
1:A:2139:HIS:CB	1:A:2164:CYS:O	0.48	2.62	16	3
1:A:2129:ASP:OD1	1:A:2131:CYS:SG	0.48	2.71	3	13
1:A:2129:ASP:C	1:A:2144:ASN:OD1	0.47	2.57	7	2
1:A:2145:THR:HG23	1:A:2149:TYR:HA	0.47	1.85	7	1
1:A:2144:ASN:OD1	1:A:2144:ASN:C	0.47	2.57	12	1
1:A:2157:TYR:CB	1:A:2165:VAL:O	0.47	2.63	7	7
1:A:2169:GLU:OE2	1:A:2187:GLY:O	0.47	2.32	11	7
1:A:2175:PRO:CD	1:A:2181:CYS:CB	0.47	2.92	21	2
1:A:2129:ASP:O	1:A:2129:ASP:OD1	0.47	2.32	16	4
1:A:2158:ILE:HD12	1:A:2167:THR:CB	0.47	2.38	18	1
1:A:2135:ASP:OD1	1:A:2135:ASP:C	0.47	2.57	2	2
1:A:2152:GLU:O	1:A:2153:CYS:C	0.47	2.58	17	1
1:A:2158:ILE:O	1:A:2164:CYS:SG	0.47	2.72	7	18
1:A:2170:CYS:O	1:A:2170:CYS:SG	0.47	2.73	13	12
1:A:2153:CYS:SG	1:A:2158:ILE:O	0.47	2.73	7	11
1:A:2176:CYS:SG	1:A:2204:CYS:HB2	0.47	2.49	14	9
1:A:2175:PRO:HB2	1:A:2188:PHE:CD1	0.47	2.44	5	2
1:A:2167:THR:O	1:A:2183:ASN:OD1	0.47	2.32	11	1
1:A:2135:ASP:OD1	1:A:2136:VAL:CG2	0.47	2.62	3	1
1:A:2166:ASP:OD2	1:A:2184:VAL:O	0.47	2.33	3	8
1:A:2145:THR:OG1	1:A:2148:SER:O	0.47	2.31	16	3
1:A:2136:VAL:HG13	1:A:2149:TYR:CZ	0.47	2.44	9	1
1:A:2137:CYS:O	1:A:2138:LYS:HB2	0.47	2.09	1	11
1:A:2196:PHE:CE2	1:A:2198:PRO:CA	0.47	2.98	7	21
1:A:2131:CYS:O	1:A:2137:CYS:O	0.47	2.33	4	2
1:A:2158:ILE:CD1	1:A:2165:VAL:O	0.47	2.62	10	3
1:A:2173:GLY:O	1:A:2181:CYS:SG	0.47	2.73	10	3
1:A:2160:ALA:O	1:A:2161:GLY:C	0.47	2.56	20	1
1:A:2135:ASP:O	1:A:2162:ASN:CG	0.46	2.58	20	2
1:A:2188:PHE:CE1	1:A:2202:MET:O	0.46	2.68	21	2
1:A:2173:GLY:O	1:A:2174:ASN:OD1	0.46	2.34	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2133:GLU:HB2	1:A:2136:VAL:CG2	0.46	2.40	10	1
1:A:2174:ASN:HA	1:A:2181:CYS:HB3	0.46	1.86	3	9
1:A:2176:CYS:HA	1:A:2204:CYS:HB3	0.46	1.88	2	9
1:A:2145:THR:OG1	1:A:2149:TYR:HA	0.46	2.11	22	3
1:A:2156:GLY:O	1:A:2166:ASP:OD1	0.46	2.34	8	1
1:A:2170:CYS:SG	1:A:2170:CYS:O	0.46	2.73	22	5
1:A:2174:ASN:OD1	1:A:2174:ASN:O	0.46	2.34	1	1
1:A:2175:PRO:HD2	1:A:2181:CYS:HB3	0.46	1.86	12	6
1:A:2137:CYS:SG	1:A:2142:CYS:SG	0.46	3.14	16	3
1:A:2139:HIS:O	1:A:2164:CYS:SG	0.46	2.74	7	1
1:A:2129:ASP:O	1:A:2144:ASN:OD1	0.46	2.34	16	1
1:A:2136:VAL:O	1:A:2151:CYS:SG	0.46	2.73	4	1
1:A:2175:PRO:HB3	1:A:2188:PHE:CD1	0.46	2.46	21	2
1:A:2146:ASP:O	1:A:2146:ASP:OD1	0.46	2.33	17	2
1:A:2168:ASP:OD1	1:A:2168:ASP:C	0.46	2.58	20	1
1:A:2175:PRO:CG	1:A:2188:PHE:CD1	0.46	2.98	9	3
1:A:2131:CYS:SG	1:A:2131:CYS:O	0.46	2.73	16	1
1:A:2133:GLU:CB	1:A:2134:PRO:CD	0.46	2.94	4	2
1:A:2197:GLU:O	1:A:2197:GLU:CG	0.46	2.62	6	1
1:A:2173:GLY:O	1:A:2174:ASN:O	0.46	2.34	11	2
1:A:2204:CYS:SG	1:A:2204:CYS:O	0.46	2.73	20	1
1:A:2130:GLU:O	1:A:2136:VAL:HB	0.46	2.11	9	3
1:A:2145:THR:O	1:A:2146:ASP:O	0.46	2.33	13	2
1:A:2131:CYS:HB2	1:A:2137:CYS:CB	0.46	2.41	13	1
1:A:2167:THR:HG23	1:A:2168:ASP:N	0.46	2.25	19	3
1:A:2176:CYS:CA	1:A:2204:CYS:HB2	0.46	2.40	18	5
1:A:2189:GLU:OE1	1:A:2200:PRO:O	0.46	2.34	12	1
1:A:2134:PRO:CA	1:A:2138:LYS:HD3	0.46	2.41	18	1
1:A:2131:CYS:O	1:A:2131:CYS:SG	0.45	2.73	7	1
1:A:2137:CYS:O	1:A:2162:ASN:O	0.45	2.34	22	3
1:A:2150:ARG:O	1:A:2151:CYS:SG	0.45	2.74	14	1
1:A:2142:CYS:SG	1:A:2151:CYS:N	0.45	2.89	20	1
1:A:2175:PRO:HD3	1:A:2181:CYS:HB3	0.45	1.87	9	9
1:A:2131:CYS:O	1:A:2137:CYS:HB2	0.45	2.11	14	4
1:A:2144:ASN:C	1:A:2144:ASN:OD1	0.45	2.58	11	1
1:A:2130:GLU:OE1	1:A:2144:ASN:CG	0.45	2.59	16	1
1:A:2138:LYS:O	1:A:2139:HIS:C	0.45	2.59	17	1
1:A:2145:THR:O	1:A:2146:ASP:C	0.45	2.58	4	4
1:A:2132:LYS:O	1:A:2132:LYS:HG3	0.45	2.10	12	2
1:A:2184:VAL:HG11	1:A:2201:MET:HG2	0.45	1.86	14	1
1:A:2160:ALA:O	1:A:2162:ASN:N	0.45	2.49	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2178:ASN:OD1	1:A:2192:CYS:SG	0.45	2.74	2	1
1:A:2158:ILE:HG12	1:A:2159:LEU:N	0.45	2.26	12	7
1:A:2173:GLY:C	1:A:2174:ASN:OD1	0.45	2.59	3	1
1:A:2130:GLU:OE1	1:A:2144:ASN:ND2	0.45	2.49	4	2
1:A:2133:GLU:HB2	1:A:2136:VAL:CG1	0.45	2.41	4	1
1:A:2167:THR:HG22	1:A:2169:GLU:OE1	0.45	2.11	4	3
1:A:2131:CYS:HA	1:A:2136:VAL:CG1	0.45	2.42	19	4
1:A:2158:ILE:CD1	1:A:2167:THR:HB	0.45	2.41	14	2
1:A:2176:CYS:SG	1:A:2192:CYS:SG	0.45	3.15	15	3
1:A:2173:GLY:O	1:A:2175:PRO:N	0.45	2.50	16	5
1:A:2170:CYS:HB2	1:A:2182:LYS:N	0.45	2.27	12	3
1:A:2193:GLU:O	1:A:2193:GLU:OE1	0.45	2.35	4	2
1:A:2149:TYR:O	1:A:2150:ARG:HG2	0.45	2.12	8	2
1:A:2182:LYS:HG3	1:A:2183:ASN:N	0.45	2.27	17	2
1:A:2144:ASN:ND2	1:A:2144:ASN:C	0.45	2.75	16	2
1:A:2176:CYS:C	1:A:2204:CYS:HB2	0.45	2.37	18	5
1:A:2135:ASP:O	1:A:2162:ASN:HB3	0.45	2.12	20	3
1:A:2137:CYS:CB	1:A:2142:CYS:HB3	0.45	2.42	18	1
1:A:2176:CYS:SG	1:A:2204:CYS:HB3	0.45	2.52	20	1
1:A:2129:ASP:HB3	1:A:2132:LYS:CG	0.45	2.42	22	1
1:A:2176:CYS:CA	1:A:2204:CYS:HB3	0.44	2.42	2	7
1:A:2166:ASP:OD2	1:A:2167:THR:O	0.44	2.35	17	1
1:A:2138:LYS:CE	1:A:2163:GLU:OE2	0.44	2.65	18	1
1:A:2169:GLU:CB	1:A:2188:PHE:HB3	0.44	2.42	21	1
1:A:2136:VAL:CG1	1:A:2137:CYS:N	0.44	2.71	10	1
1:A:2158:ILE:HD11	1:A:2165:VAL:CG2	0.44	2.30	11	1
1:A:2129:ASP:CG	1:A:2132:LYS:HB2	0.44	2.36	19	3
1:A:2176:CYS:O	1:A:2204:CYS:HB3	0.44	2.12	17	5
1:A:2193:GLU:OE2	1:A:2194:GLU:O	0.44	2.35	9	1
1:A:2131:CYS:HB3	1:A:2149:TYR:CD2	0.44	2.46	12	1
1:A:2136:VAL:O	1:A:2162:ASN:HA	0.44	2.12	4	1
1:A:2141:GLN:O	1:A:2152:GLU:HB2	0.44	2.12	7	1
1:A:2139:HIS:C	1:A:2164:CYS:HB3	0.44	2.37	5	5
1:A:2175:PRO:O	1:A:2176:CYS:C	0.44	2.57	18	4
1:A:2169:GLU:CB	1:A:2188:PHE:CD2	0.44	3.00	2	1
1:A:2138:LYS:CE	1:A:2163:GLU:CD	0.44	2.91	18	1
1:A:2137:CYS:O	1:A:2138:LYS:CB	0.44	2.64	14	3
1:A:2129:ASP:C	1:A:2130:GLU:HG3	0.44	2.38	12	6
1:A:2134:PRO:O	1:A:2138:LYS:HD2	0.44	2.11	21	2
1:A:2158:ILE:CD1	1:A:2158:ILE:N	0.44	2.81	7	1
1:A:2186:GLY:O	1:A:2201:MET:SD	0.44	2.76	11	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2149:TYR:C	1:A:2150:ARG:HG3	0.44	2.38	4	2
1:A:2170:CYS:SG	1:A:2181:CYS:C	0.44	3.00	17	1
1:A:2201:MET:O	1:A:2201:MET:SD	0.44	2.76	22	2
1:A:2129:ASP:OD2	1:A:2132:LYS:HB3	0.43	2.12	15	1
1:A:2173:GLY:O	1:A:2175:PRO:HD3	0.43	2.13	8	9
1:A:2142:CYS:HA	1:A:2150:ARG:O	0.43	2.13	21	2
1:A:2129:ASP:CG	1:A:2132:LYS:CB	0.43	2.91	12	2
1:A:2129:ASP:O	1:A:2144:ASN:HB2	0.43	2.13	16	1
1:A:2197:GLU:O	1:A:2205:GLU:HG3	0.43	2.13	21	1
1:A:2139:HIS:HB2	1:A:2164:CYS:O	0.43	2.13	11	3
1:A:2166:ASP:CG	1:A:2167:THR:N	0.43	2.77	22	1
1:A:2129:ASP:C	1:A:2130:GLU:CG	0.43	2.89	15	6
1:A:2192:CYS:O	1:A:2193:GLU:C	0.43	2.60	3	2
1:A:2184:VAL:HG22	1:A:2185:ILE:H	0.43	1.74	15	1
1:A:2197:GLU:O	1:A:2205:GLU:O	0.43	2.36	16	1
1:A:2136:VAL:O	1:A:2137:CYS:HB2	0.43	2.14	19	1
1:A:2149:TYR:C	1:A:2150:ARG:HD3	0.43	2.39	19	1
1:A:2170:CYS:HA	1:A:2181:CYS:HB2	0.43	1.91	20	4
1:A:2134:PRO:HA	1:A:2138:LYS:CD	0.43	2.44	9	1
1:A:2146:ASP:OD1	1:A:2146:ASP:N	0.43	2.51	12	1
1:A:2151:CYS:SG	1:A:2159:LEU:HD13	0.43	2.54	22	1
1:A:2175:PRO:CG	1:A:2188:PHE:CD2	0.43	3.01	15	3
1:A:2129:ASP:OD2	1:A:2132:LYS:HB2	0.43	2.13	19	3
1:A:2157:TYR:O	1:A:2158:ILE:HG22	0.43	2.14	12	5
1:A:2130:GLU:HG2	1:A:2148:SER:O	0.43	2.14	16	2
1:A:2162:ASN:ND2	1:A:2163:GLU:N	0.43	2.67	12	1
1:A:2138:LYS:O	1:A:2139:HIS:HB2	0.43	2.14	5	9
1:A:2153:CYS:SG	1:A:2154:PRO:HD2	0.43	2.54	21	8
1:A:2158:ILE:HG21	1:A:2167:THR:CB	0.43	2.44	9	1
1:A:2135:ASP:OD1	1:A:2135:ASP:N	0.43	2.52	13	1
1:A:2132:LYS:CD	1:A:2132:LYS:C	0.43	2.91	22	1
1:A:2136:VAL:O	1:A:2162:ASN:HB2	0.42	2.14	4	3
1:A:2136:VAL:O	1:A:2162:ASN:CG	0.42	2.62	8	1
1:A:2130:GLU:CD	1:A:2148:SER:O	0.42	2.61	16	2
1:A:2139:HIS:ND1	1:A:2139:HIS:N	0.42	2.66	6	1
1:A:2129:ASP:HB3	1:A:2132:LYS:CB	0.42	2.44	7	1
1:A:2142:CYS:HB2	1:A:2150:ARG:C	0.42	2.39	14	1
1:A:2139:HIS:O	1:A:2164:CYS:HB3	0.42	2.13	8	6
1:A:2161:GLY:O	1:A:2162:ASN:CG	0.42	2.61	5	2
1:A:2205:GLU:O	1:A:2205:GLU:CG	0.42	2.67	20	1
1:A:2149:TYR:O	1:A:2150:ARG:HG3	0.42	2.14	9	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2179:GLY:HA3	1:A:2191:THR:O	0.42	2.15	20	2
1:A:2159:LEU:HD11	1:A:2162:ASN:C	0.42	2.39	15	1
1:A:2135:ASP:O	1:A:2162:ASN:CB	0.42	2.68	20	1
1:A:2137:CYS:O	1:A:2138:LYS:O	0.42	2.38	10	1
1:A:2131:CYS:SG	1:A:2137:CYS:HB3	0.42	2.54	21	1
1:A:2157:TYR:HB3	1:A:2165:VAL:O	0.42	2.14	6	3
1:A:2139:HIS:CB	1:A:2164:CYS:HB3	0.42	2.44	7	1
1:A:2175:PRO:CG	1:A:2188:PHE:CE1	0.42	3.02	9	1
1:A:2136:VAL:HG13	1:A:2162:ASN:OD1	0.42	2.14	21	1
1:A:2130:GLU:HB3	1:A:2149:TYR:CE2	0.42	2.49	3	1
1:A:2136:VAL:HG23	1:A:2149:TYR:CD1	0.42	2.49	4	1
1:A:2169:GLU:OE2	1:A:2187:GLY:HA2	0.42	2.15	11	1
1:A:2134:PRO:C	1:A:2138:LYS:HG3	0.42	2.40	12	1
1:A:2182:LYS:CG	1:A:2183:ASN:N	0.42	2.82	3	2
1:A:2131:CYS:HB2	1:A:2137:CYS:SG	0.42	2.55	6	1
1:A:2159:LEU:HG	1:A:2160:ALA:N	0.42	2.29	18	1
1:A:2134:PRO:O	1:A:2138:LYS:HG3	0.42	2.15	16	1
1:A:2188:PHE:CZ	1:A:2202:MET:O	0.42	2.73	21	2
1:A:2136:VAL:HA	1:A:2162:ASN:ND2	0.41	2.30	14	4
1:A:2157:TYR:CD1	1:A:2166:ASP:OD1	0.41	2.73	15	1
1:A:2135:ASP:N	1:A:2135:ASP:OD1	0.41	2.53	8	1
1:A:2175:PRO:CB	1:A:2188:PHE:CD2	0.41	3.02	11	1
1:A:2169:GLU:OE2	1:A:2187:GLY:C	0.41	2.63	11	1
1:A:2186:GLY:C	1:A:2201:MET:SD	0.41	3.04	15	1
1:A:2197:GLU:O	1:A:2205:GLU:CG	0.41	2.67	21	1
1:A:2147:GLY:O	1:A:2148:SER:HB2	0.41	2.16	2	2
1:A:2129:ASP:CB	1:A:2132:LYS:HB2	0.41	2.46	9	1
1:A:2158:ILE:CG1	1:A:2167:THR:HB	0.41	2.46	14	1
1:A:2188:PHE:O	1:A:2201:MET:HA	0.41	2.15	22	1
1:A:2157:TYR:N	1:A:2157:TYR:CD1	0.41	2.89	12	3
1:A:2130:GLU:OE2	1:A:2147:GLY:C	0.41	2.63	11	1
1:A:2184:VAL:CG1	1:A:2188:PHE:HA	0.41	2.45	16	1
1:A:2134:PRO:O	1:A:2138:LYS:HE3	0.41	2.16	5	1
1:A:2182:LYS:HB3	1:A:2189:GLU:CB	0.41	2.45	9	2
1:A:2169:GLU:HG2	1:A:2188:PHE:CD1	0.41	2.51	11	1
1:A:2130:GLU:HB3	1:A:2149:TYR:CE1	0.41	2.49	12	1
1:A:2150:ARG:CZ	1:A:2150:ARG:HB3	0.41	2.45	3	1
1:A:2151:CYS:HB2	1:A:2159:LEU:HD13	0.41	1.92	4	1
1:A:2161:GLY:O	1:A:2162:ASN:HB3	0.41	2.16	4	1
1:A:2131:CYS:SG	1:A:2137:CYS:HB2	0.41	2.56	7	1
1:A:2129:ASP:OD1	1:A:2129:ASP:C	0.41	2.64	19	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2142:CYS:SG	1:A:2151:CYS:HA	0.41	2.56	20	1
1:A:2157:TYR:CD1	1:A:2157:TYR:N	0.41	2.88	17	2
1:A:2191:THR:C	1:A:2192:CYS:O	0.41	2.64	10	4
1:A:2149:TYR:C	1:A:2150:ARG:CD	0.41	2.94	17	1
1:A:2160:ALA:C	1:A:2162:ASN:N	0.41	2.75	20	1
1:A:2191:THR:O	1:A:2192:CYS:C	0.41	2.63	1	3
1:A:2173:GLY:O	1:A:2175:PRO:CD	0.41	2.69	16	2
1:A:2166:ASP:CG	1:A:2185:ILE:HA	0.41	2.41	12	1
1:A:2203:THR:HG23	1:A:2204:CYS:N	0.41	2.31	17	3
1:A:2138:LYS:HE2	1:A:2163:GLU:OE1	0.41	2.16	18	1
1:A:2148:SER:O	1:A:2149:TYR:HB3	0.41	2.16	20	1
1:A:2138:LYS:O	1:A:2164:CYS:HB2	0.41	2.16	22	1
1:A:2138:LYS:O	1:A:2164:CYS:CB	0.40	2.69	9	1
1:A:2168:ASP:O	1:A:2171:SER:HB2	0.40	2.17	14	2
1:A:2176:CYS:HA	1:A:2203:THR:OG1	0.40	2.16	20	1
1:A:2142:CYS:O	1:A:2143:ILE:HD12	0.40	2.14	14	1
1:A:2147:GLY:C	1:A:2148:SER:OG	0.40	2.64	5	2
1:A:2142:CYS:HB2	1:A:2150:ARG:O	0.40	2.16	14	1
1:A:2201:MET:SD	1:A:2201:MET:C	0.40	3.04	20	1
1:A:2136:VAL:HA	1:A:2162:ASN:CG	0.40	2.42	2	1
1:A:2191:THR:O	1:A:2191:THR:HG22	0.40	2.16	13	1
1:A:2166:ASP:OD2	1:A:2185:ILE:HA	0.40	2.17	9	1
1:A:2136:VAL:HG12	1:A:2137:CYS:H	0.40	1.76	13	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	76/82 (93%)	45±7 (59±9%)	18±4 (24±5%)	11±2 (14±2%)	0	5
All	All	1615/1804 (90%)	983 (61%)	399 (25%)	233 (14%)	0	5

All 22 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	2179	GLY	22
1	A	2192	CYS	22
1	A	2158	ILE	21
1	A	2162	ASN	20
1	A	2165	VAL	19
1	A	2178	ASN	18
1	A	2200	PRO	17
1	A	2136	VAL	16
1	A	2198	PRO	14
1	A	2154	PRO	10
1	A	2139	HIS	9
1	A	2173	GLY	8
1	A	2138	LYS	7
1	A	2146	ASP	7
1	A	2148	SER	6
1	A	2137	CYS	5
1	A	2151	CYS	4
1	A	2174	ASN	3
1	A	2143	ILE	2
1	A	2142	CYS	1
1	A	2147	GLY	1
1	A	2194	GLU	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	65/69 (94%)	35±15 (54±23%)	16±7 (25±11%)	2	25
All	All	1123/1518 (74%)	769 (68%)	354 (32%)	1	14

All 45 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	2184	VAL	18
1	A	2201	MET	17
1	A	2192	CYS	17
1	A	2171	SER	16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	2202	MET	16
1	A	2132	LYS	15
1	A	2158	ILE	15
1	A	2164	CYS	15
1	A	2169	GLU	15
1	A	2176	CYS	15
1	A	2148	SER	14
1	A	2153	CYS	14
1	A	2194	GLU	14
1	A	2178	ASN	13
1	A	2146	ASP	10
1	A	2189	GLU	9
1	A	2204	CYS	9
1	A	2205	GLU	9
1	A	2138	LYS	8
1	A	2165	VAL	8
1	A	2139	HIS	7
1	A	2193	GLU	7
1	A	2180	THR	7
1	A	2152	GLU	6
1	A	2150	ARG	6
1	A	2182	LYS	5
1	A	2130	GLU	5
1	A	2137	CYS	4
1	A	2135	ASP	4
1	A	2141	GLN	4
1	A	2142	CYS	4
1	A	2151	CYS	3
1	A	2166	ASP	3
1	A	2145	THR	3
1	A	2131	CYS	3
1	A	2136	VAL	2
1	A	2185	ILE	2
1	A	2144	ASN	2
1	A	2170	CYS	2
1	A	2162	ASN	2
1	A	2133	GLU	2
1	A	2190	CYS	1
1	A	2197	GLU	1
1	A	2129	ASP	1
1	A	2174	ASN	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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