



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 04:16 PM UTC

PDB ID : 1JBj / pdb_00001jbj
Title : CD3 Epsilon and gamma Ectodomain Fragment Complex in Single-Chain Construct
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Deposited on : 2001-06-05

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

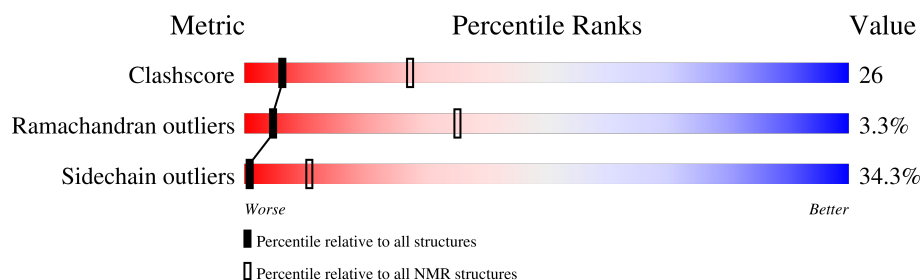
1 Overall quality at a glance

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	186	34% 37% 9% 20%

2 Ensemble composition and analysis

This entry contains 18 models. Model 12 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:6-A:80, A:113-A:185 (148)	1.21	12

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 2 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2858 atoms, of which 1411 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CD3 Epsilon and gamma Ectodomain Fragment Complex.

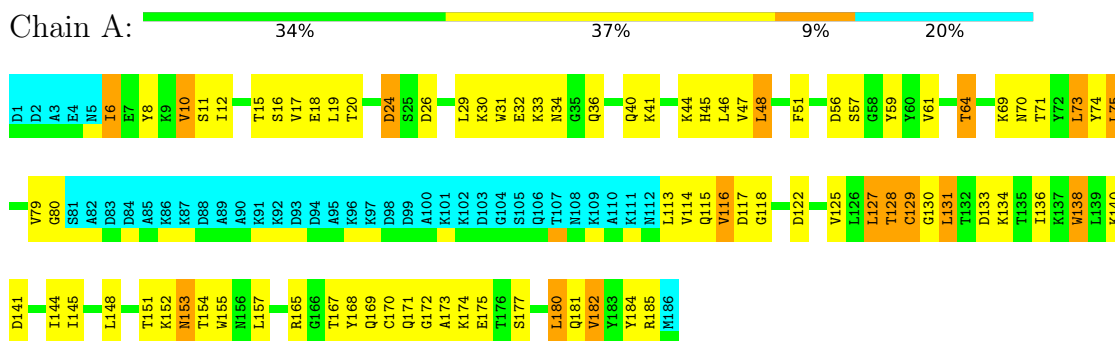
Mol	Chain	Residues	Atoms						Trace
1	A	186	Total	C	H	N	O	S	0
			2858	892	1411	249	301	5	

4 Residue-property plots [i](#)

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: CD3 Epsilon and gamma Ectodomain Fragment Complex



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

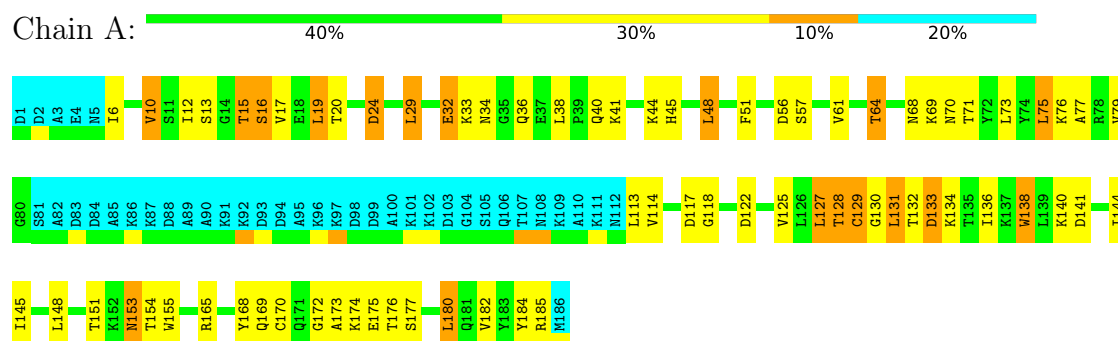
4.2.1 Score per residue for model 1

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



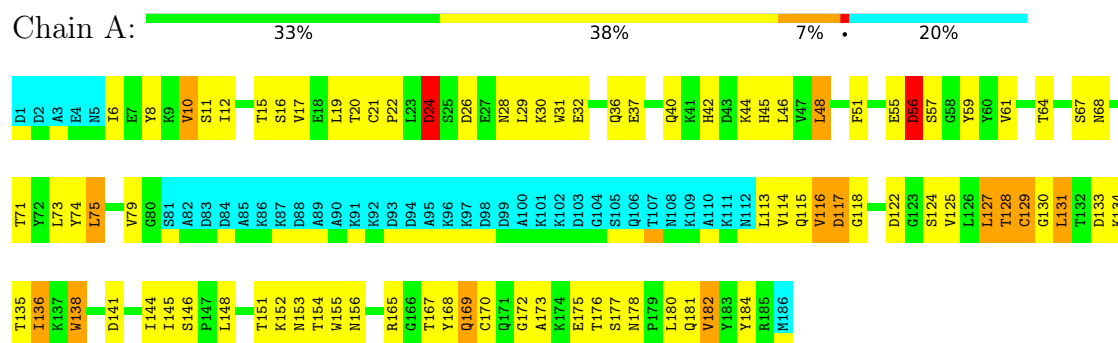
4.2.2 Score per residue for model 2

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



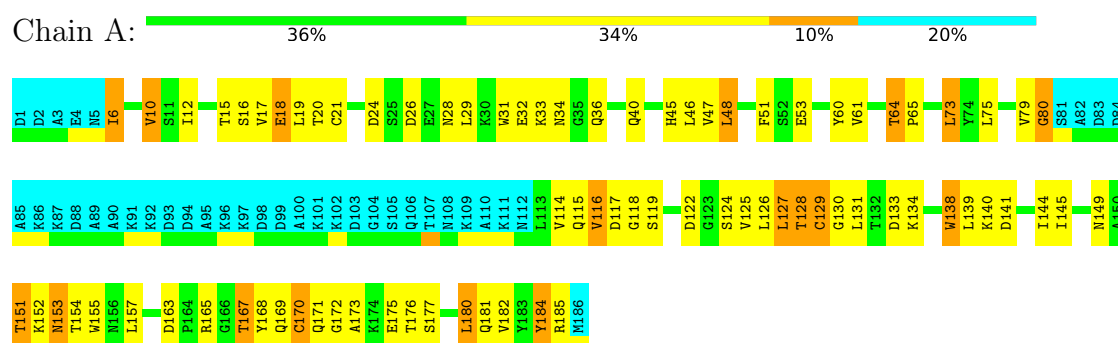
4.2.3 Score per residue for model 3

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



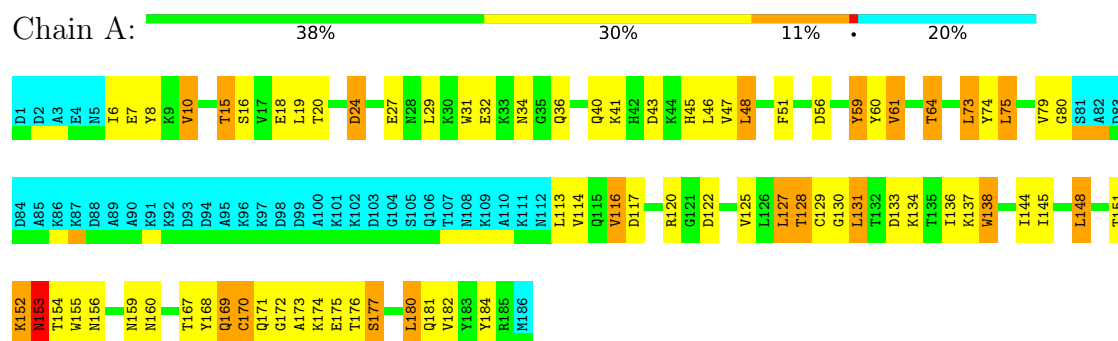
4.2.4 Score per residue for model 4

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



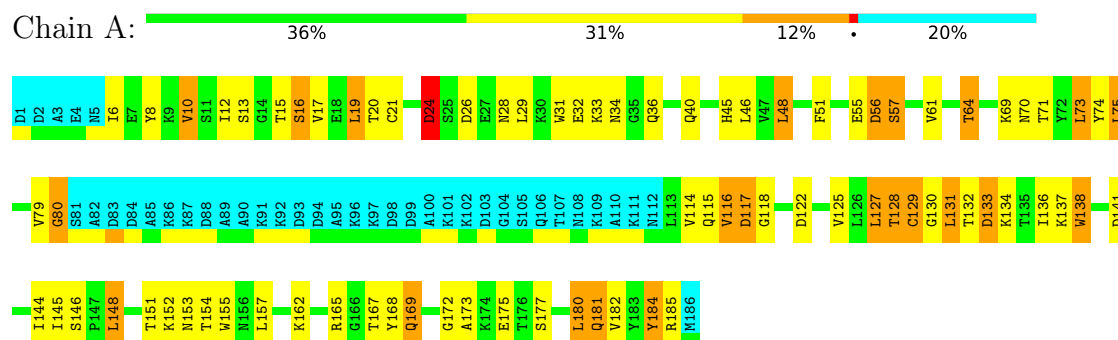
4.2.5 Score per residue for model 5

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



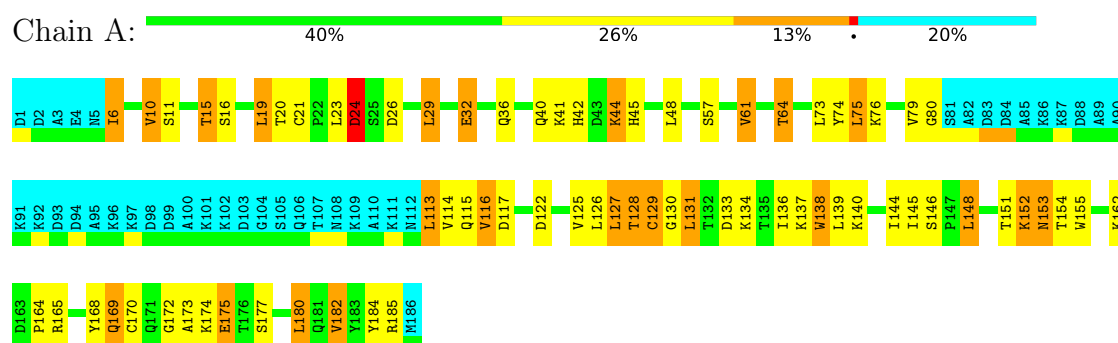
4.2.6 Score per residue for model 6

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



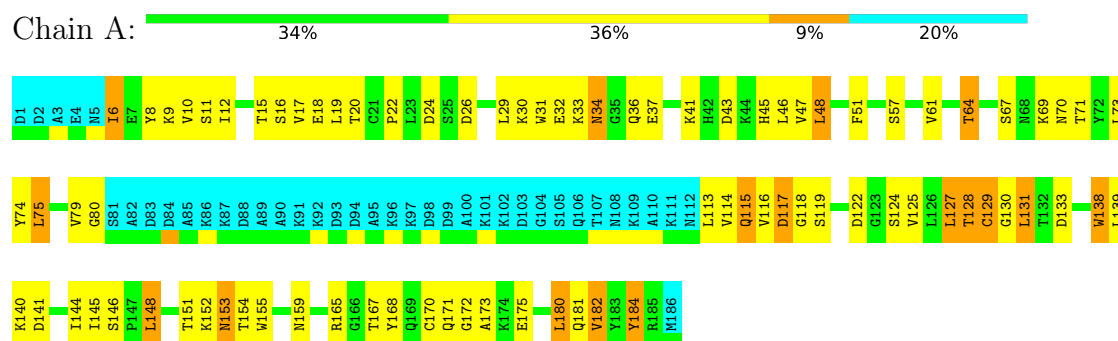
4.2.7 Score per residue for model 7

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



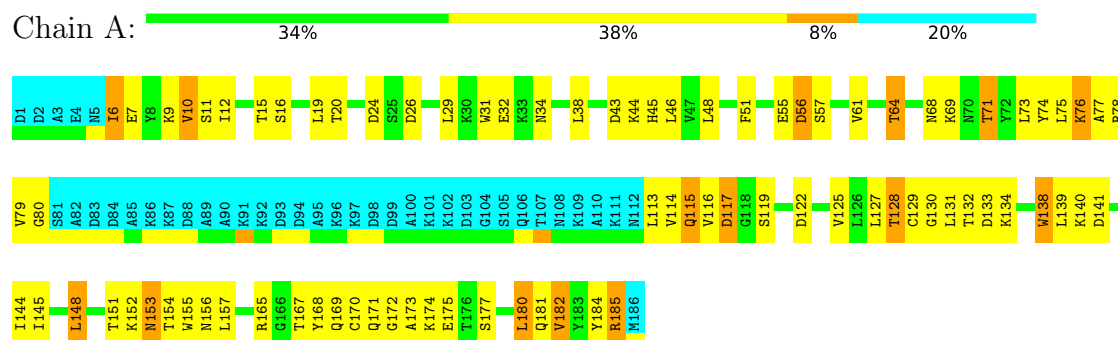
4.2.8 Score per residue for model 8

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



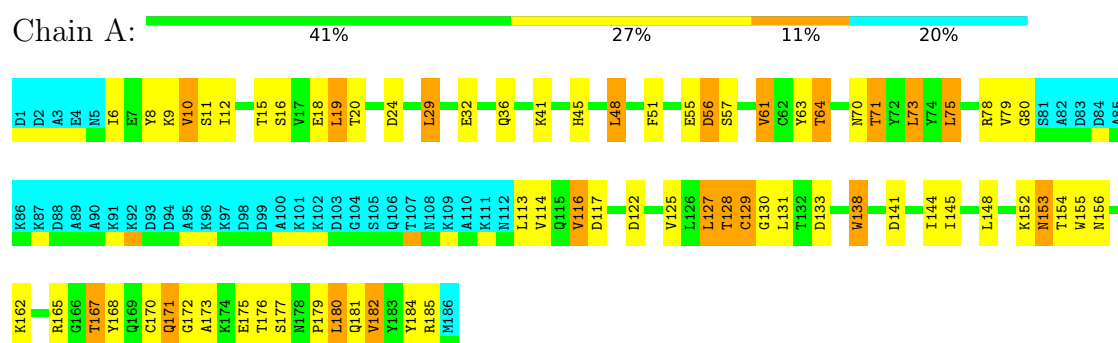
4.2.9 Score per residue for model 9

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



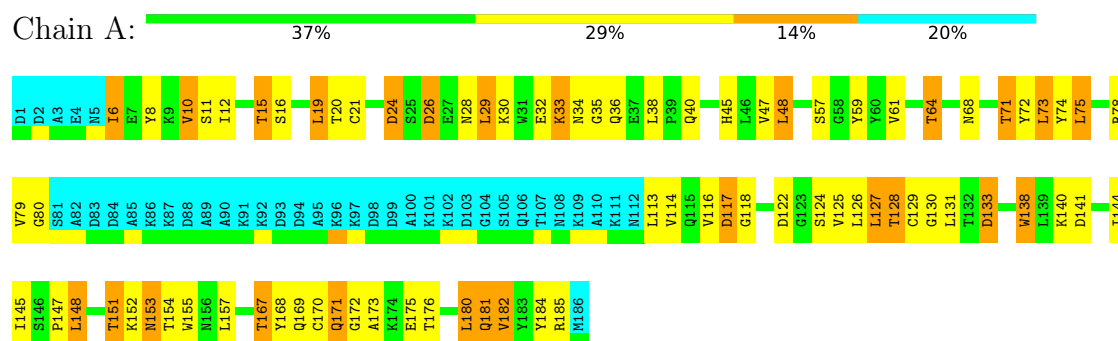
4.2.10 Score per residue for model 10

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



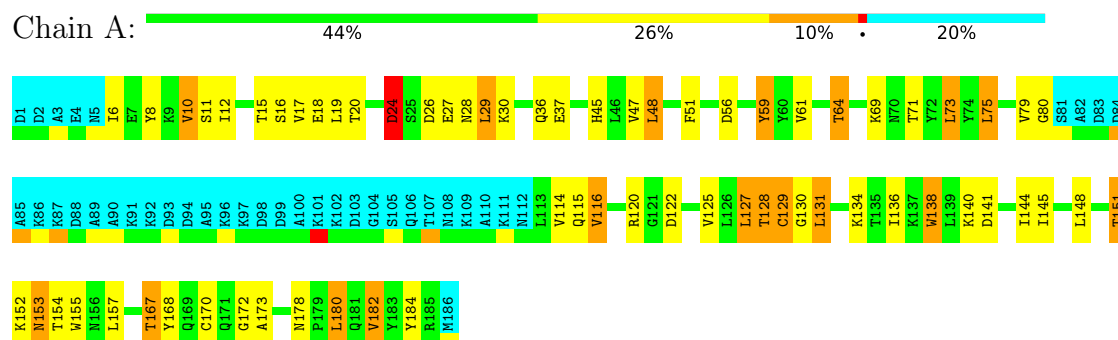
4.2.11 Score per residue for model 11

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



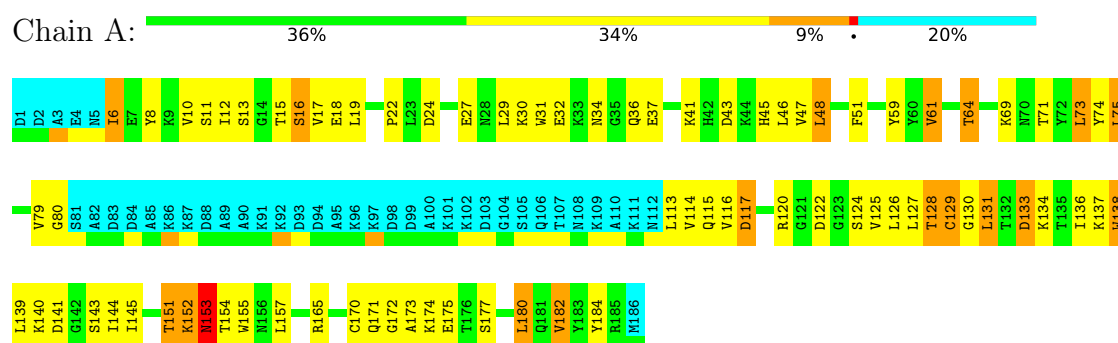
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



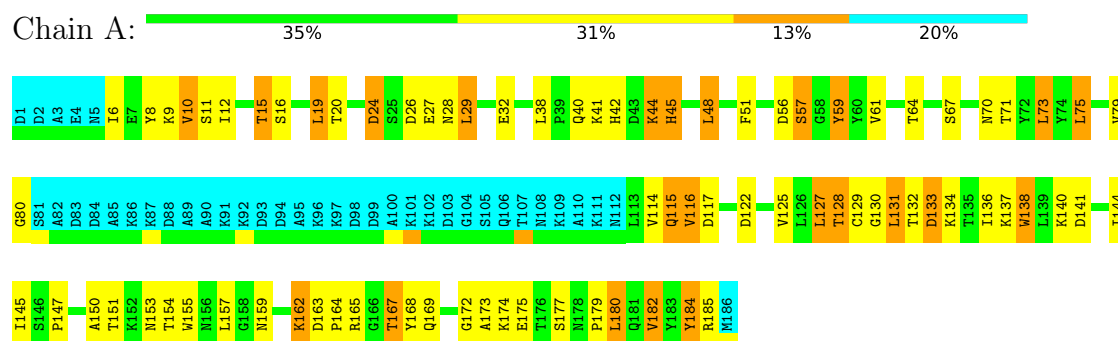
4.2.13 Score per residue for model 13

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



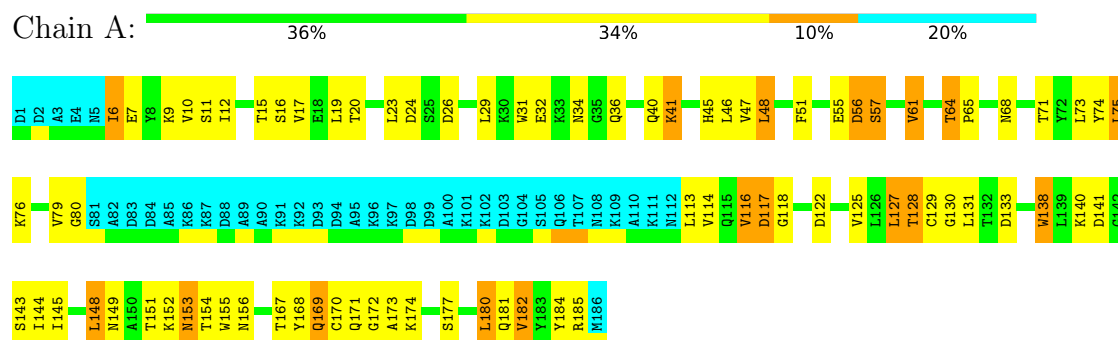
4.2.14 Score per residue for model 14

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



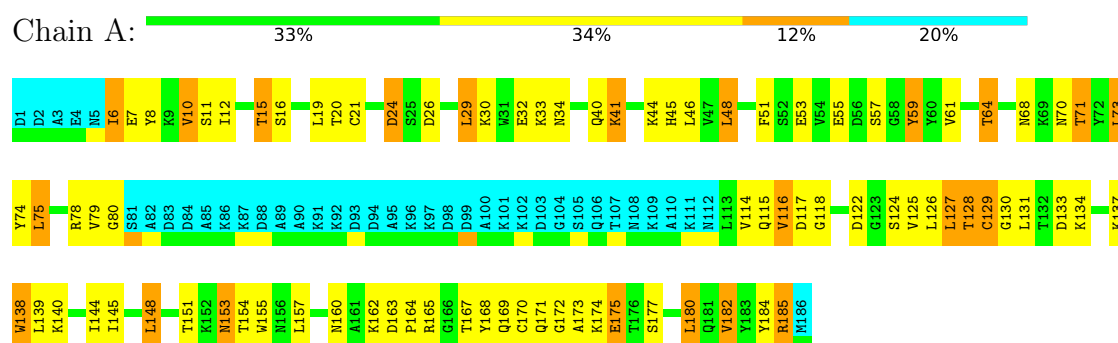
4.2.15 Score per residue for model 15

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



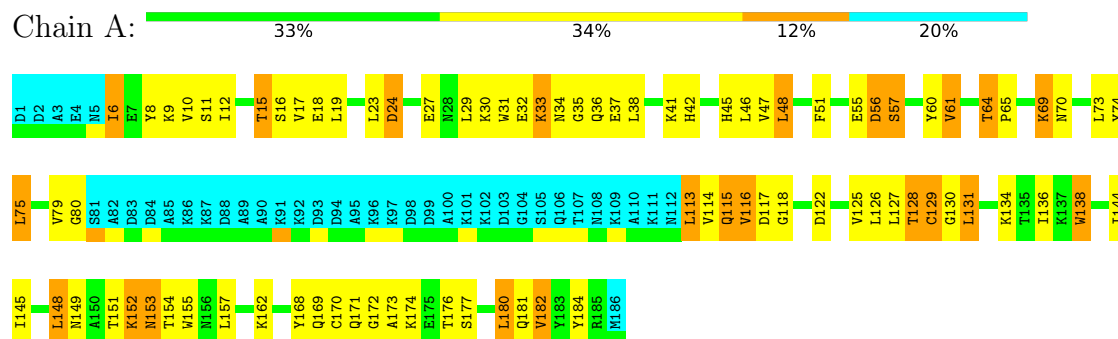
4.2.16 Score per residue for model 16

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



4.2.17 Score per residue for model 17

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



4.2.18 Score per residue for model 18

- Molecule 1: CD3 Epsilon and gamma Ectodomain Fragment Complex



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 18 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
DYANA	structure solution	1.4
X-PLOR	structure solution	3.1
X-PLOR	refinement	3.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1163	1138	1136	59±5
All	All	20934	20484	20448	1067

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:29:LEU:HD12	1:A:64:THR:HG23	1.00	1.27	4	14
1:A:128:THR:HG23	1:A:154:THR:HG22	0.99	1.34	4	18
1:A:114:VAL:HG11	1:A:180:LEU:HD11	0.98	1.26	5	9
1:A:128:THR:CG2	1:A:154:THR:HG22	0.93	1.93	7	7
1:A:127:LEU:HD21	1:A:180:LEU:HD22	0.88	1.45	2	9
1:A:10:VAL:HG22	1:A:19:LEU:HD22	0.86	1.47	13	4
1:A:10:VAL:HG13	1:A:19:LEU:CD2	0.86	2.01	15	18
1:A:19:LEU:HD11	1:A:48:LEU:HD11	0.86	1.45	6	9
1:A:114:VAL:HG11	1:A:180:LEU:CD1	0.83	2.03	5	7
1:A:10:VAL:HG13	1:A:19:LEU:HD23	0.82	1.49	7	14
1:A:116:VAL:HG12	1:A:127:LEU:CD2	0.82	2.05	7	9
1:A:29:LEU:CD1	1:A:64:THR:HG23	0.82	2.05	4	3
1:A:61:VAL:HG23	1:A:71:THR:O	0.81	1.76	3	10
1:A:180:LEU:HD11	1:A:182:VAL:HG22	0.80	1.52	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:GLU:CB	1:A:61:VAL:HG12	0.80	2.06	5	13
1:A:135:THR:C	1:A:136:ILE:HD13	0.79	2.02	3	1
1:A:18:GLU:CG	1:A:47:VAL:HG22	0.79	2.07	17	4
1:A:128:THR:HG23	1:A:154:THR:CG2	0.78	2.09	18	12
1:A:114:VAL:HG11	1:A:180:LEU:CD2	0.77	2.09	8	3
1:A:152:LYS:O	1:A:154:THR:HG23	0.77	1.80	11	6
1:A:116:VAL:HG12	1:A:127:LEU:HD23	0.77	1.56	12	9
1:A:131:LEU:HD12	1:A:133:ASP:HB2	0.77	1.56	11	1
1:A:180:LEU:C	1:A:180:LEU:HD12	0.76	2.04	8	1
1:A:147:PRO:HG3	1:A:151:THR:HG23	0.76	1.58	1	1
1:A:167:THR:HG23	1:A:181:GLN:HG2	0.75	1.57	11	1
1:A:32:GLU:HB3	1:A:61:VAL:HG12	0.75	1.59	17	12
1:A:31:TRP:CE3	1:A:46:LEU:HD22	0.74	2.18	17	9
1:A:130:GLY:C	1:A:131:LEU:HD23	0.73	2.08	18	6
1:A:17:VAL:HG11	1:A:75:LEU:HD11	0.73	1.59	15	3
1:A:136:ILE:HD11	1:A:153:ASN:OD1	0.73	1.82	14	2
1:A:10:VAL:HG13	1:A:19:LEU:HD21	0.72	1.59	8	4
1:A:148:LEU:HD13	1:A:148:LEU:O	0.72	1.84	6	8
1:A:114:VAL:HG21	1:A:180:LEU:HD13	0.71	1.61	18	7
1:A:129:CYS:O	1:A:136:ILE:HD13	0.71	1.86	1	4
1:A:125:VAL:HG11	1:A:184:TYR:OH	0.71	1.84	3	2
1:A:6:ILE:N	1:A:6:ILE:HD12	0.71	1.99	15	1
1:A:117:ASP:O	1:A:125:VAL:HG13	0.71	1.86	3	17
1:A:125:VAL:HG11	1:A:184:TYR:CE2	0.71	2.20	17	7
1:A:116:VAL:HB	1:A:127:LEU:HD23	0.71	1.61	14	1
1:A:133:ASP:OD1	1:A:173:ALA:HB3	0.70	1.87	10	5
1:A:127:LEU:HD21	1:A:182:VAL:HG11	0.69	1.63	11	5
1:A:32:GLU:HB2	1:A:61:VAL:HG12	0.69	1.63	1	5
1:A:128:THR:HG22	1:A:153:ASN:O	0.69	1.86	1	18
1:A:130:GLY:O	1:A:133:ASP:HB2	0.69	1.88	14	9
1:A:136:ILE:HD12	1:A:153:ASN:HA	0.69	1.61	1	3
1:A:125:VAL:HG21	1:A:164:PRO:HG3	0.69	1.63	1	1
1:A:138:TRP:C	1:A:139:LEU:HD12	0.69	2.12	18	4
1:A:114:VAL:HG21	1:A:180:LEU:CD1	0.68	2.18	18	5
1:A:130:GLY:C	1:A:131:LEU:HD22	0.68	2.13	12	7
1:A:12:ILE:HD13	1:A:79:VAL:HG12	0.68	1.64	11	2
1:A:131:LEU:HD11	1:A:175:GLU:CB	0.68	2.18	10	4
1:A:64:THR:HG22	1:A:65:PRO:HD2	0.68	1.66	17	4
1:A:157:LEU:HD22	1:A:168:TYR:CZ	0.67	2.25	14	2
1:A:131:LEU:HD11	1:A:175:GLU:CG	0.67	2.20	4	2
1:A:168:TYR:CD1	1:A:182:VAL:HG23	0.67	2.25	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:VAL:HG12	1:A:184:TYR:CE1	0.67	2.25	1	3
1:A:167:THR:HG23	1:A:181:GLN:CG	0.66	2.20	11	1
1:A:131:LEU:HD13	1:A:175:GLU:HB3	0.66	1.67	5	1
1:A:74:TYR:CZ	1:A:116:VAL:HG22	0.66	2.26	16	2
1:A:41:LYS:HE3	1:A:46:LEU:HD12	0.66	1.66	5	2
1:A:41:LYS:HE2	1:A:46:LEU:HD12	0.66	1.65	15	1
1:A:170:CYS:O	1:A:176:THR:HG23	0.66	1.91	2	6
1:A:41:LYS:CE	1:A:46:LEU:HD12	0.65	2.22	16	2
1:A:74:TYR:CE2	1:A:116:VAL:HG22	0.65	2.27	3	1
1:A:127:LEU:HD21	1:A:182:VAL:CG1	0.65	2.21	14	1
1:A:8:TYR:CD2	1:A:73:LEU:HD13	0.65	2.26	6	3
1:A:129:CYS:HB2	1:A:138:TRP:CH2	0.65	2.27	15	11
1:A:10:VAL:CG1	1:A:19:LEU:HD23	0.65	2.22	7	13
1:A:135:THR:O	1:A:136:ILE:HD13	0.65	1.92	3	1
1:A:130:GLY:HA3	1:A:136:ILE:HD12	0.64	1.68	3	1
1:A:131:LEU:HD11	1:A:175:GLU:HB2	0.63	1.68	9	4
1:A:157:LEU:HD13	1:A:184:TYR:OH	0.63	1.93	4	3
1:A:114:VAL:HG11	1:A:180:LEU:HD23	0.63	1.69	8	1
1:A:29:LEU:HD12	1:A:64:THR:HG22	0.62	1.71	2	2
1:A:18:GLU:HG3	1:A:47:VAL:HG22	0.62	1.69	17	2
1:A:47:VAL:C	1:A:48:LEU:HD23	0.62	2.20	17	6
1:A:131:LEU:HD11	1:A:175:GLU:HB3	0.61	1.71	18	1
1:A:114:VAL:HG23	1:A:128:THR:O	0.61	1.94	2	4
1:A:131:LEU:HD13	1:A:175:GLU:HB2	0.61	1.70	11	1
1:A:12:ILE:HG21	1:A:79:VAL:CG1	0.61	2.25	13	3
1:A:15:THR:HG23	1:A:80:GLY:O	0.61	1.96	7	4
1:A:18:GLU:HG2	1:A:47:VAL:HG22	0.60	1.73	17	3
1:A:130:GLY:HA2	1:A:136:ILE:HD11	0.60	1.72	2	2
1:A:51:PHE:HB3	1:A:79:VAL:HG22	0.60	1.71	2	8
1:A:145:ILE:O	1:A:145:ILE:HG23	0.60	1.96	9	18
1:A:24:ASP:O	1:A:29:LEU:HD13	0.59	1.96	11	8
1:A:128:THR:HG22	1:A:154:THR:HG22	0.59	1.74	7	3
1:A:144:ILE:HD12	1:A:144:ILE:N	0.59	2.12	5	11
1:A:12:ILE:HG21	1:A:79:VAL:HG12	0.59	1.74	10	10
1:A:26:ASP:OD2	1:A:64:THR:HG21	0.59	1.98	14	1
1:A:17:VAL:HG21	1:A:51:PHE:CD2	0.59	2.33	18	2
1:A:127:LEU:HD13	1:A:138:TRP:CZ2	0.58	2.32	7	4
1:A:6:ILE:HD12	1:A:6:ILE:H	0.58	1.58	15	1
1:A:8:TYR:CD2	1:A:73:LEU:HD22	0.58	2.33	16	1
1:A:114:VAL:CG1	1:A:180:LEU:HD11	0.58	2.28	16	4
1:A:125:VAL:HG21	1:A:163:ASP:OD2	0.58	1.98	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:GLY:O	1:A:132:THR:N	0.58	2.34	6	2
1:A:127:LEU:HD21	1:A:157:LEU:HD11	0.58	1.75	11	4
1:A:17:VAL:HB	1:A:48:LEU:HD12	0.57	1.76	1	2
1:A:114:VAL:HG13	1:A:128:THR:O	0.57	1.99	14	2
1:A:51:PHE:O	1:A:79:VAL:HG22	0.57	2.00	14	2
1:A:125:VAL:HG22	1:A:160:ASN:OD1	0.57	2.00	16	2
1:A:131:LEU:HD13	1:A:175:GLU:CB	0.57	2.28	5	1
1:A:182:VAL:HG12	1:A:184:TYR:CE2	0.57	2.35	16	6
1:A:48:LEU:HD11	1:A:75:LEU:HD11	0.56	1.77	14	3
1:A:131:LEU:HD21	1:A:175:GLU:HB2	0.56	1.76	4	2
1:A:12:ILE:N	1:A:12:ILE:HD12	0.56	2.15	10	5
1:A:29:LEU:HD12	1:A:64:THR:CG2	0.56	2.28	9	5
1:A:51:PHE:CE2	1:A:75:LEU:HD22	0.56	2.35	17	4
1:A:74:TYR:CZ	1:A:116:VAL:HG13	0.56	2.36	8	1
1:A:151:THR:HG23	1:A:151:THR:O	0.56	2.01	3	8
1:A:167:THR:HG22	1:A:179:PRO:CB	0.56	2.30	10	1
1:A:127:LEU:CD2	1:A:182:VAL:HG11	0.56	2.31	11	1
1:A:127:LEU:CD1	1:A:157:LEU:HD21	0.56	2.30	14	1
1:A:157:LEU:HD22	1:A:168:TYR:CE2	0.56	2.36	18	1
1:A:8:TYR:CG	1:A:73:LEU:HD13	0.55	2.35	6	4
1:A:75:LEU:HD22	1:A:76:LYS:N	0.55	2.16	2	2
1:A:10:VAL:HG22	1:A:19:LEU:HD23	0.55	1.77	6	12
1:A:75:LEU:HD22	1:A:75:LEU:C	0.55	2.27	2	1
1:A:114:VAL:HG22	1:A:129:CYS:SG	0.55	2.42	7	2
1:A:73:LEU:C	1:A:73:LEU:HD12	0.55	2.27	9	3
1:A:139:LEU:HD12	1:A:139:LEU:N	0.55	2.16	9	2
1:A:157:LEU:HD21	1:A:168:TYR:CE2	0.54	2.37	1	1
1:A:61:VAL:HG21	1:A:70:ASN:ND2	0.54	2.17	1	2
1:A:12:ILE:HG21	1:A:79:VAL:HG11	0.54	1.79	13	1
1:A:131:LEU:HD23	1:A:131:LEU:N	0.54	2.17	6	2
1:A:125:VAL:HG11	1:A:184:TYR:CZ	0.54	2.38	13	6
1:A:130:GLY:O	1:A:131:LEU:HG	0.54	2.03	16	6
1:A:114:VAL:HG11	1:A:180:LEU:HD22	0.54	1.80	18	1
1:A:26:ASP:HB2	1:A:64:THR:HG21	0.54	1.80	8	2
1:A:131:LEU:HD11	1:A:175:GLU:HG3	0.54	1.80	10	1
1:A:116:VAL:HG21	1:A:184:TYR:OH	0.53	2.03	12	1
1:A:153:ASN:O	1:A:153:ASN:ND2	0.53	2.41	14	1
1:A:182:VAL:HG12	1:A:184:TYR:HE1	0.53	1.63	1	1
1:A:138:TRP:CE3	1:A:155:TRP:HB2	0.53	2.38	13	17
1:A:131:LEU:HD23	1:A:175:GLU:HB3	0.53	1.81	8	2
1:A:116:VAL:HG12	1:A:127:LEU:HD21	0.53	1.78	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LEU:C	1:A:75:LEU:HD22	0.53	2.28	7	1
1:A:12:ILE:HG13	1:A:17:VAL:HG22	0.53	1.80	18	6
1:A:127:LEU:HD11	1:A:157:LEU:HD21	0.52	1.81	14	1
1:A:115:GLN:O	1:A:128:THR:OG1	0.52	2.24	18	5
1:A:19:LEU:HD21	1:A:75:LEU:HD11	0.52	1.80	13	2
1:A:140:LYS:HD3	1:A:145:ILE:HD12	0.52	1.80	13	1
1:A:138:TRP:CZ3	1:A:155:TRP:HB2	0.52	2.39	10	10
1:A:131:LEU:HD23	1:A:175:GLU:CB	0.52	2.35	8	2
1:A:51:PHE:CZ	1:A:75:LEU:HD22	0.52	2.39	13	5
1:A:12:ILE:HD13	1:A:79:VAL:CG1	0.52	2.34	9	3
1:A:10:VAL:HG22	1:A:19:LEU:CD2	0.51	2.34	1	1
1:A:8:TYR:CE2	1:A:71:THR:HG21	0.51	2.40	8	1
1:A:6:ILE:HD13	1:A:6:ILE:N	0.51	2.21	11	6
1:A:59:TYR:CE2	1:A:74:TYR:CE2	0.51	2.99	1	2
1:A:59:TYR:N	1:A:59:TYR:CD1	0.51	2.77	14	4
1:A:12:ILE:CG1	1:A:17:VAL:HG22	0.51	2.35	13	1
1:A:15:THR:HG22	1:A:79:VAL:CG2	0.51	2.36	17	2
1:A:125:VAL:HG21	1:A:184:TYR:CD2	0.51	2.41	11	1
1:A:74:TYR:CZ	1:A:116:VAL:CG2	0.51	2.94	9	5
1:A:19:LEU:HD21	1:A:75:LEU:CD1	0.51	2.35	10	5
1:A:6:ILE:HG22	1:A:7:GLU:H	0.51	1.65	15	1
1:A:172:GLY:N	1:A:175:GLU:O	0.51	2.44	18	5
1:A:180:LEU:CD1	1:A:182:VAL:HG22	0.51	2.30	8	1
1:A:75:LEU:HD23	1:A:76:LYS:N	0.51	2.21	9	1
1:A:131:LEU:O	1:A:131:LEU:HG	0.50	2.05	2	2
1:A:163:ASP:N	1:A:164:PRO:CD	0.50	2.74	14	2
1:A:23:LEU:HD11	1:A:69:LYS:HB2	0.50	1.83	17	1
1:A:19:LEU:HD11	1:A:75:LEU:CD1	0.50	2.36	11	2
1:A:15:THR:HG22	1:A:79:VAL:HG23	0.50	1.83	17	3
1:A:172:GLY:O	1:A:173:ALA:C	0.50	2.55	15	15
1:A:125:VAL:CG1	1:A:157:LEU:HD12	0.49	2.37	12	2
1:A:125:VAL:HG11	1:A:184:TYR:HH	0.49	1.67	3	1
1:A:48:LEU:HD11	1:A:75:LEU:CD1	0.49	2.37	5	5
1:A:131:LEU:C	1:A:132:THR:HG23	0.49	2.32	14	3
1:A:48:LEU:HD13	1:A:51:PHE:CE1	0.49	2.42	1	2
1:A:64:THR:HG22	1:A:65:PRO:CD	0.49	2.37	1	2
1:A:115:GLN:C	1:A:128:THR:HG1	0.49	2.15	9	3
1:A:8:TYR:OH	1:A:71:THR:HG21	0.49	2.08	8	1
1:A:113:LEU:CB	1:A:131:LEU:HD12	0.49	2.37	1	1
1:A:127:LEU:O	1:A:155:TRP:N	0.49	2.46	8	17
1:A:61:VAL:O	1:A:61:VAL:HG13	0.49	2.08	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:ILE:N	1:A:6:ILE:CD1	0.49	2.71	15	2
1:A:149:ASN:O	1:A:150:ALA:HB3	0.48	2.09	1	1
1:A:129:CYS:CB	1:A:138:TRP:CH2	0.48	2.96	5	1
1:A:182:VAL:HG12	1:A:184:TYR:CZ	0.48	2.42	13	4
1:A:127:LEU:HB2	1:A:138:TRP:CH2	0.48	2.43	13	3
1:A:157:LEU:HD22	1:A:184:TYR:OH	0.48	2.08	6	1
1:A:180:LEU:C	1:A:180:LEU:CD1	0.48	2.77	8	1
1:A:128:THR:CG2	1:A:154:THR:CG2	0.48	2.91	8	12
1:A:74:TYR:CE1	1:A:116:VAL:HG22	0.48	2.43	7	1
1:A:145:ILE:O	1:A:155:TRP:CH2	0.48	2.66	1	2
1:A:168:TYR:CD1	1:A:168:TYR:N	0.48	2.81	10	11
1:A:55:GLU:O	1:A:56:ASP:CB	0.48	2.62	17	6
1:A:167:THR:HG22	1:A:181:GLN:OE1	0.48	2.09	6	1
1:A:74:TYR:CE2	1:A:116:VAL:CG2	0.47	2.97	3	1
1:A:74:TYR:CZ	1:A:116:VAL:CG1	0.47	2.98	8	1
1:A:10:VAL:CG2	1:A:19:LEU:HD22	0.47	2.32	17	2
1:A:163:ASP:CB	1:A:164:PRO:CD	0.47	2.92	1	1
1:A:17:VAL:O	1:A:48:LEU:N	0.47	2.46	1	2
1:A:125:VAL:CG1	1:A:184:TYR:CE2	0.47	2.97	2	2
1:A:74:TYR:CE2	1:A:116:VAL:CG1	0.47	2.98	18	3
1:A:57:SER:CB	1:A:74:TYR:CZ	0.47	2.98	3	2
1:A:32:GLU:OE2	1:A:61:VAL:HG11	0.47	2.09	8	1
1:A:8:TYR:CB	1:A:73:LEU:HD21	0.47	2.40	13	1
1:A:159:ASN:O	1:A:163:ASP:N	0.47	2.40	14	1
1:A:51:PHE:HE2	1:A:75:LEU:HD22	0.47	1.70	17	1
1:A:116:VAL:CG1	1:A:180:LEU:HD21	0.47	2.40	9	1
1:A:145:ILE:O	1:A:145:ILE:CG2	0.46	2.63	11	14
1:A:74:TYR:OH	1:A:116:VAL:HG22	0.46	2.10	15	1
1:A:148:LEU:O	1:A:148:LEU:CD1	0.46	2.63	16	3
1:A:12:ILE:HG23	1:A:16:SER:O	0.46	2.10	2	1
1:A:15:THR:O	1:A:79:VAL:HG21	0.46	2.09	2	1
1:A:131:LEU:N	1:A:131:LEU:HD13	0.46	2.25	1	6
1:A:125:VAL:HG12	1:A:157:LEU:HD12	0.46	1.87	16	3
1:A:168:TYR:CE2	1:A:182:VAL:CG2	0.46	2.99	1	3
1:A:79:VAL:O	1:A:80:GLY:C	0.46	2.59	6	7
1:A:19:LEU:CD1	1:A:48:LEU:HD11	0.46	2.32	6	1
1:A:116:VAL:CB	1:A:127:LEU:HD23	0.46	2.37	14	1
1:A:128:THR:HA	1:A:153:ASN:O	0.46	2.10	14	8
1:A:131:LEU:N	1:A:131:LEU:CD2	0.46	2.79	2	2
1:A:130:GLY:HA3	1:A:136:ILE:CD1	0.46	2.40	18	2
1:A:171:GLN:CG	1:A:176:THR:HG23	0.45	2.41	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:H	1:A:131:LEU:CD2	0.45	2.23	6	1
1:A:182:VAL:CG1	1:A:184:TYR:CE2	0.45	2.98	16	3
1:A:127:LEU:HD11	1:A:182:VAL:HG21	0.45	1.87	17	2
1:A:59:TYR:CE2	1:A:74:TYR:CD2	0.45	3.05	1	1
1:A:19:LEU:HD11	1:A:75:LEU:HD12	0.45	1.88	11	4
1:A:168:TYR:CD2	1:A:182:VAL:HG21	0.45	2.46	7	2
1:A:168:TYR:CD2	1:A:182:VAL:CG2	0.45	3.00	3	3
1:A:127:LEU:HD21	1:A:157:LEU:CD1	0.45	2.42	11	4
1:A:8:TYR:CD1	1:A:73:LEU:CD2	0.45	3.00	18	1
1:A:114:VAL:CG1	1:A:180:LEU:CD1	0.45	2.95	2	1
1:A:138:TRP:CZ2	1:A:170:CYS:SG	0.45	3.10	3	1
1:A:171:GLN:HG3	1:A:176:THR:HG23	0.45	1.89	11	1
1:A:127:LEU:CB	1:A:138:TRP:CH2	0.45	3.00	9	2
1:A:127:LEU:O	1:A:138:TRP:CZ3	0.45	2.70	15	8
1:A:131:LEU:CD2	1:A:131:LEU:H	0.45	2.24	2	1
1:A:61:VAL:HG22	1:A:70:ASN:HB2	0.44	1.90	1	1
1:A:12:ILE:HD11	1:A:77:ALA:HB1	0.44	1.88	9	1
1:A:12:ILE:CG2	1:A:79:VAL:HG12	0.44	2.42	11	1
1:A:33:LYS:O	1:A:35:GLY:N	0.44	2.51	18	3
1:A:114:VAL:HG11	1:A:180:LEU:HD21	0.44	1.90	14	1
1:A:157:LEU:CD2	1:A:168:TYR:CZ	0.44	2.99	14	1
1:A:130:GLY:O	1:A:131:LEU:C	0.44	2.61	5	2
1:A:148:LEU:HD13	1:A:149:ASN:CG	0.44	2.37	15	1
1:A:33:LYS:CB	1:A:60:TYR:CE2	0.44	3.01	17	1
1:A:148:LEU:O	1:A:149:ASN:CG	0.44	2.61	18	1
1:A:144:ILE:N	1:A:144:ILE:CD1	0.44	2.81	5	4
1:A:21:CYS:CB	1:A:44:LYS:O	0.43	2.66	7	2
1:A:138:TRP:O	1:A:139:LEU:HD12	0.43	2.13	4	1
1:A:125:VAL:HG22	1:A:160:ASN:CG	0.43	2.38	5	2
1:A:153:ASN:O	1:A:153:ASN:CG	0.43	2.61	7	6
1:A:167:THR:HG22	1:A:179:PRO:HB3	0.43	1.89	10	2
1:A:167:THR:C	1:A:168:TYR:CD1	0.43	2.96	8	7
1:A:19:LEU:HD12	1:A:46:LEU:HD23	0.43	1.89	5	1
1:A:131:LEU:HD21	1:A:175:GLU:CB	0.43	2.43	10	1
1:A:136:ILE:HD11	1:A:153:ASN:CG	0.43	2.38	14	1
1:A:126:LEU:HD22	1:A:154:THR:OG1	0.43	2.13	1	1
1:A:139:LEU:HD11	1:A:144:ILE:HG13	0.43	1.90	4	1
1:A:126:LEU:HD22	1:A:154:THR:CB	0.43	2.43	1	1
1:A:127:LEU:HD11	1:A:157:LEU:HD11	0.43	1.89	9	2
1:A:21:CYS:HB2	1:A:31:TRP:CZ2	0.43	2.48	4	2
1:A:182:VAL:HG12	1:A:184:TYR:OH	0.43	2.13	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:VAL:CG2	1:A:125:VAL:CG1	0.43	2.97	18	1
1:A:131:LEU:HD23	1:A:131:LEU:H	0.43	1.72	6	1
1:A:139:LEU:HG	1:A:144:ILE:HD13	0.43	1.90	18	2
1:A:147:PRO:HG2	1:A:150:ALA:O	0.43	2.14	14	1
1:A:144:ILE:H	1:A:144:ILE:HD12	0.43	1.74	8	4
1:A:127:LEU:HD21	1:A:180:LEU:CD2	0.43	2.42	18	3
1:A:29:LEU:HA	1:A:64:THR:HG23	0.43	1.91	16	1
1:A:26:ASP:C	1:A:28:ASN:H	0.43	2.22	3	7
1:A:147:PRO:CG	1:A:150:ALA:O	0.43	2.67	18	1
1:A:52:SER:O	1:A:56:ASP:N	0.43	2.52	1	1
1:A:130:GLY:C	1:A:131:LEU:CD2	0.43	2.87	18	1
1:A:152:LYS:O	1:A:153:ASN:HB3	0.42	2.13	1	1
1:A:138:TRP:CD1	1:A:169:GLN:O	0.42	2.72	18	7
1:A:48:LEU:CD1	1:A:75:LEU:CD1	0.42	2.97	3	3
1:A:127:LEU:HD22	1:A:138:TRP:CZ2	0.42	2.49	3	1
1:A:168:TYR:CD1	1:A:182:VAL:CG2	0.42	3.00	8	1
1:A:8:TYR:CG	1:A:73:LEU:HD22	0.42	2.49	5	1
1:A:13:SER:N	1:A:16:SER:O	0.42	2.50	2	4
1:A:131:LEU:CD1	1:A:175:GLU:CB	0.42	2.97	5	1
1:A:61:VAL:HG21	1:A:70:ASN:HB2	0.42	1.90	16	1
1:A:152:LYS:C	1:A:154:THR:N	0.42	2.76	5	2
1:A:168:TYR:CE2	1:A:182:VAL:HG21	0.42	2.49	12	2
1:A:125:VAL:O	1:A:126:LEU:HD12	0.42	2.14	17	1
1:A:147:PRO:HD3	1:A:155:TRP:CZ3	0.42	2.50	11	1
1:A:8:TYR:CG	1:A:73:LEU:HD21	0.42	2.50	13	1
1:A:130:GLY:CA	1:A:136:ILE:HD13	0.42	2.44	5	1
1:A:113:LEU:O	1:A:131:LEU:HD12	0.42	2.15	17	1
1:A:171:GLN:HG2	1:A:176:THR:HG23	0.42	1.90	17	1
1:A:32:GLU:CB	1:A:61:VAL:CG1	0.42	2.98	3	1
1:A:148:LEU:C	1:A:148:LEU:HD13	0.42	2.39	5	1
1:A:9:LYS:O	1:A:19:LEU:HA	0.42	2.15	17	1
1:A:48:LEU:CD1	1:A:75:LEU:HD11	0.42	2.45	12	1
1:A:32:GLU:O	1:A:61:VAL:HG12	0.42	2.14	14	1
1:A:44:LYS:CG	1:A:45:HIS:CD2	0.42	3.03	14	1
1:A:12:ILE:N	1:A:12:ILE:CD1	0.41	2.83	6	3
1:A:78:ARG:CG	1:A:79:VAL:N	0.41	2.83	9	2
1:A:138:TRP:CE2	1:A:170:CYS:SG	0.41	3.14	18	1
1:A:138:TRP:CD1	1:A:168:TYR:HB3	0.41	2.50	3	1
1:A:10:VAL:CG2	1:A:19:LEU:HD23	0.41	2.46	6	1
1:A:129:CYS:O	1:A:136:ILE:HD12	0.41	2.14	6	1
1:A:33:LYS:HB3	1:A:60:TYR:CE2	0.41	2.50	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:TYR:CD1	1:A:184:TYR:N	0.41	2.88	18	1
1:A:8:TYR:CZ	1:A:22:PRO:HD3	0.41	2.51	8	2
1:A:15:THR:CG2	1:A:80:GLY:O	0.41	2.69	14	1
1:A:159:ASN:O	1:A:162:LYS:N	0.41	2.52	18	2
1:A:51:PHE:CZ	1:A:75:LEU:HD13	0.41	2.50	6	1
1:A:18:GLU:CD	1:A:47:VAL:HG22	0.41	2.41	13	1
1:A:163:ASP:N	1:A:164:PRO:HD3	0.41	2.30	14	1
1:A:157:LEU:CD2	1:A:168:TYR:CE2	0.41	3.04	1	1
1:A:8:TYR:CE2	1:A:22:PRO:CD	0.41	3.04	3	1
1:A:163:ASP:OD1	1:A:184:TYR:CD1	0.41	2.74	4	1
1:A:10:VAL:CG1	1:A:19:LEU:CD2	0.41	2.95	7	2
1:A:151:THR:O	1:A:152:LYS:C	0.41	2.63	13	1
1:A:136:ILE:CD1	1:A:153:ASN:OD1	0.41	2.69	1	1
1:A:59:TYR:C	1:A:60:TYR:CD1	0.41	2.99	5	1
1:A:152:LYS:O	1:A:153:ASN:ND2	0.41	2.54	7	1
1:A:129:CYS:O	1:A:136:ILE:CD1	0.41	2.69	18	1
1:A:12:ILE:HA	1:A:16:SER:O	0.41	2.16	2	1
1:A:171:GLN:HA	1:A:176:THR:HG23	0.41	1.92	10	1
1:A:144:ILE:HD12	1:A:144:ILE:H	0.41	1.76	16	1
1:A:167:THR:O	1:A:168:TYR:CD1	0.40	2.74	12	1
1:A:130:GLY:CA	1:A:136:ILE:CD1	0.40	2.99	5	1
1:A:74:TYR:CE2	1:A:116:VAL:HG11	0.40	2.51	18	1
1:A:127:LEU:CG	1:A:157:LEU:HD11	0.40	2.46	9	1
1:A:51:PHE:CE2	1:A:77:ALA:O	0.40	2.74	2	1
1:A:130:GLY:HA3	1:A:136:ILE:HD13	0.40	1.92	5	1
1:A:17:VAL:CB	1:A:48:LEU:HD12	0.40	2.45	6	1
1:A:130:GLY:O	1:A:133:ASP:CB	0.40	2.70	10	1
1:A:151:THR:O	1:A:153:ASN:N	0.40	2.51	1	1
1:A:61:VAL:HG23	1:A:71:THR:C	0.40	2.39	3	2
1:A:33:LYS:CG	1:A:60:TYR:CE1	0.40	3.04	4	1
1:A:8:TYR:CD2	1:A:73:LEU:CD2	0.40	3.04	10	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	148/186 (80%)	122±3 (83±2%)	21±4 (14±2%)	5±1 (3±1%)	5	35
All	All	2664/3348 (80%)	2203 (83%)	374 (14%)	87 (3%)	5	35

All 17 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	34	ASN	12
1	A	118	GLY	11
1	A	24	ASP	11
1	A	56	ASP	10
1	A	151	THR	9
1	A	57	SER	9
1	A	80	GLY	5
1	A	185	ARG	4
1	A	165	ARG	3
1	A	113	LEU	3
1	A	131	LEU	2
1	A	153	ASN	2
1	A	164	PRO	2
1	A	163	ASP	1
1	A	68	ASN	1
1	A	129	CYS	1
1	A	59	TYR	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/160 (82%)	86±3 (66±2%)	45±3 (34±2%)	1	11
All	All	2358/2880 (82%)	1549 (66%)	809 (34%)	1	11

All 94 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	6	ILE	18

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Mol	Chain	Res	Type	Models (Total)
1	A	15	THR	18
1	A	16	SER	18
1	A	45	HIS	18
1	A	48	LEU	18
1	A	122	ASP	18
1	A	128	THR	18
1	A	138	TRP	18
1	A	180	LEU	18
1	A	182	VAL	18
1	A	64	THR	17
1	A	73	LEU	17
1	A	75	LEU	17
1	A	20	THR	16
1	A	36	GLN	15
1	A	127	LEU	15
1	A	129	CYS	15
1	A	148	LEU	15
1	A	177	SER	15
1	A	10	VAL	14
1	A	11	SER	14
1	A	24	ASP	14
1	A	141	ASP	14
1	A	134	LYS	13
1	A	153	ASN	13
1	A	116	VAL	12
1	A	140	LYS	12
1	A	169	GLN	12
1	A	40	GLN	11
1	A	152	LYS	11
1	A	174	LYS	11
1	A	170	CYS	11
1	A	41	LYS	10
1	A	131	LEU	10
1	A	165	ARG	10
1	A	181	GLN	10
1	A	30	LYS	9
1	A	69	LYS	9
1	A	133	ASP	9
1	A	113	LEU	9
1	A	171	GLN	9
1	A	33	LYS	8
1	A	185	ARG	8

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Mol	Chain	Res	Type	Models (Total)
1	A	117	ASP	8
1	A	115	GLN	8
1	A	44	LYS	7
1	A	57	SER	7
1	A	70	ASN	7
1	A	137	LYS	7
1	A	29	LEU	7
1	A	71	THR	7
1	A	167	THR	7
1	A	26	ASP	6
1	A	68	ASN	6
1	A	146	SER	6
1	A	19	LEU	6
1	A	38	LEU	6
1	A	37	GLU	6
1	A	59	TYR	6
1	A	124	SER	6
1	A	27	GLU	6
1	A	61	VAL	6
1	A	162	LYS	6
1	A	9	LYS	6
1	A	42	HIS	5
1	A	156	ASN	5
1	A	126	LEU	5
1	A	184	TYR	5
1	A	18	GLU	4
1	A	21	CYS	4
1	A	175	GLU	4
1	A	67	SER	4
1	A	119	SER	4
1	A	43	ASP	4
1	A	53	GLU	3
1	A	136	ILE	3
1	A	151	THR	3
1	A	178	ASN	3
1	A	7	GLU	3
1	A	120	ARG	3
1	A	139	LEU	3
1	A	78	ARG	3
1	A	32	GLU	2
1	A	149	ASN	2
1	A	159	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	34	ASN	2
1	A	23	LEU	2
1	A	76	LYS	2
1	A	143	SER	2
1	A	56	ASP	1
1	A	63	TYR	1
1	A	72	TYR	1
1	A	55	GLU	1
1	A	8	TYR	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