Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 07:13 PM EST

PDB ID	:	2EDO
Title	:	Solution structure of the first ig-like domain from human CD48 antigen
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Deposited on	:	2007-02-14

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 (i) symbol.

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

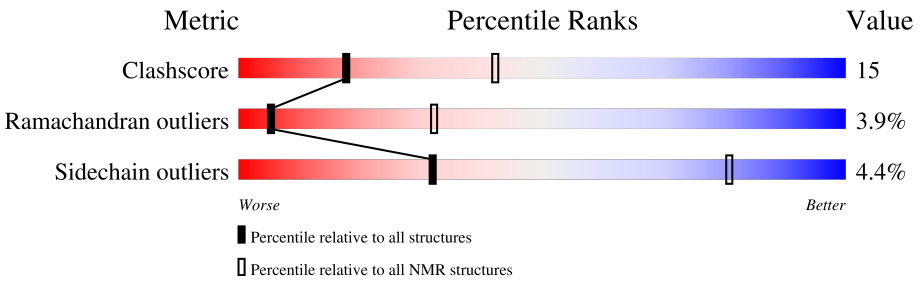
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	121	57% 25% • 17%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 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:11-A:111 (101)	0.34	7

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 and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1976 atoms, of which 997 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CD48 antigen.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	121	1976	626	997	167	184	2	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P09326
A	2	SER	-	cloning artifact	UNP P09326
A	3	SER	-	cloning artifact	UNP P09326
A	4	GLY	-	cloning artifact	UNP P09326
A	5	SER	-	cloning artifact	UNP P09326
A	6	SER	-	cloning artifact	UNP P09326
A	7	GLY	-	cloning artifact	UNP P09326

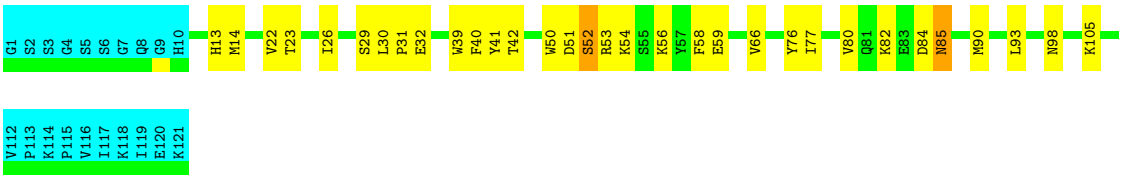
4 Residue-property plots (i)

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: CD48 antigen

Chain A:



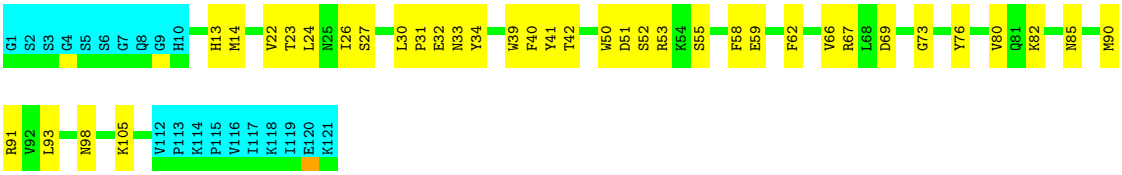
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CD48 antigen

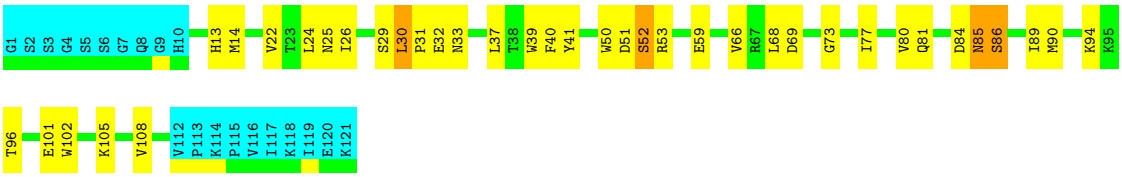
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: CD48 antigen

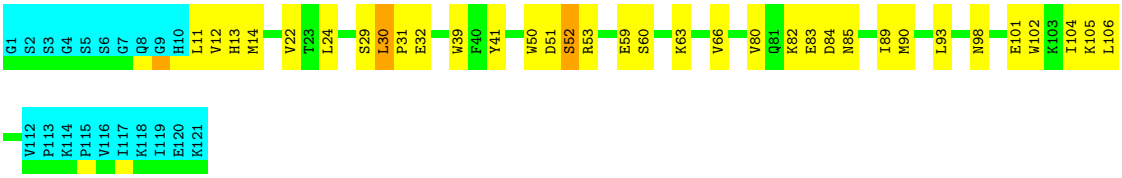
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: CD48 antigen

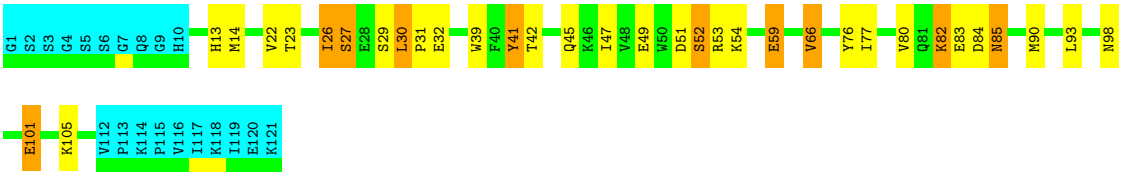
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: CD48 antigen

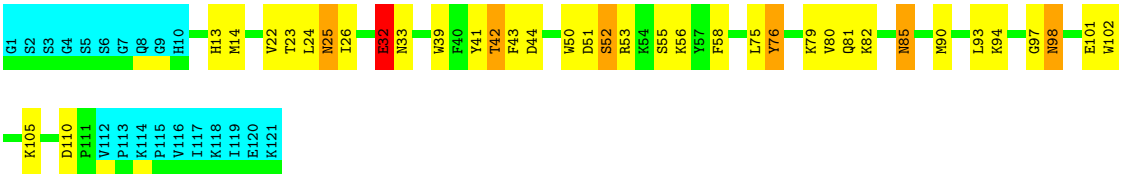
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: CD48 antigen

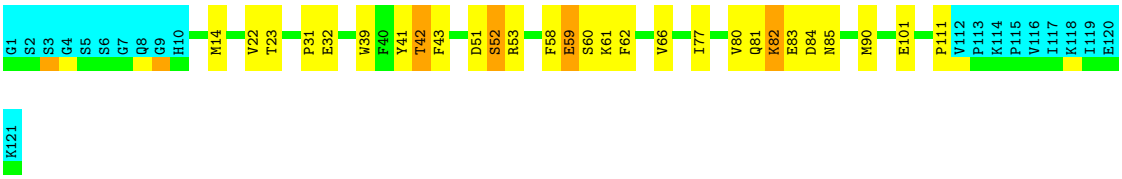
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: CD48 antigen

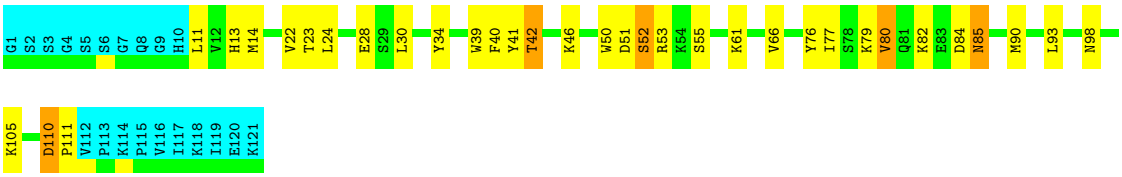
Chain A: 60% 20% • 17%



4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: CD48 antigen

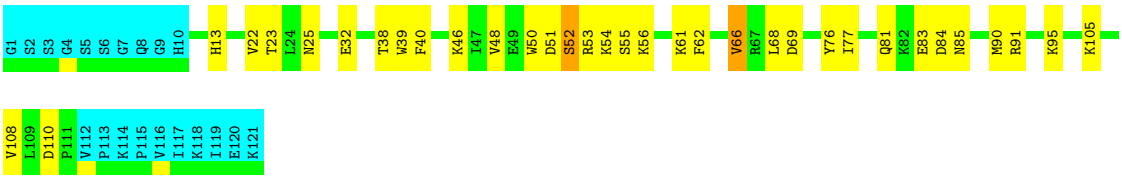
Chain A: 55% 24% • 17%



4.2.8 Score per residue for model 8

- Molecule 1: CD48 antigen

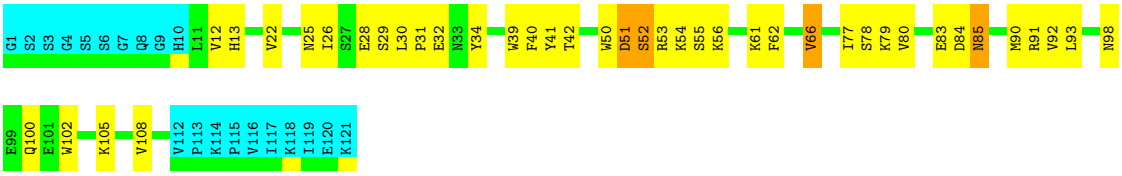
Chain A: 55% 26% • 17%



4.2.9 Score per residue for model 9

- Molecule 1: CD48 antigen

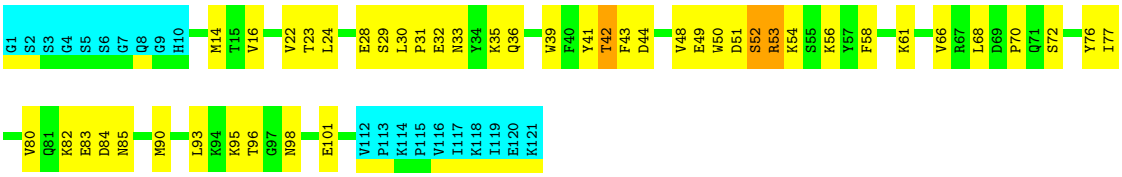
Chain A: 50% 31% • 17%



4.2.10 Score per residue for model 10

- Molecule 1: CD48 antigen

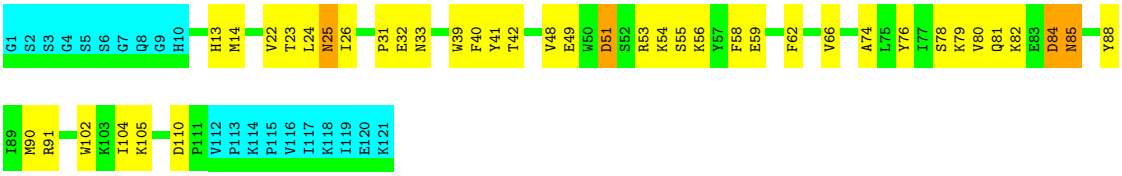
Chain A: 46% 35% • 17%



4.2.11 Score per residue for model 11

- Molecule 1: CD48 antigen

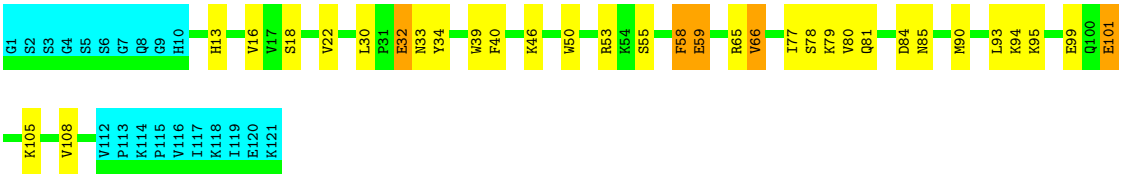
Chain A: 50% 31% • 17%



4.2.12 Score per residue for model 12

- Molecule 1: CD48 antigen

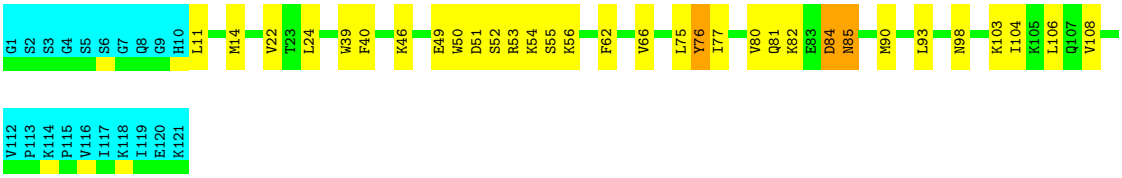
Chain A: 56% 23% • 17%



4.2.13 Score per residue for model 13

- Molecule 1: CD48 antigen

Chain A: 57% 24% • 17%



4.2.14 Score per residue for model 14

- Molecule 1: CD48 antigen

Chain A: 55% 27% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 G9 H10 H13 T23 E28 S29 L30 P31 E32 K35 W39 F40 Y41 T42 W50 D51 S52 R53 K54 S55 K56 F62 V66 S72 Y76 V80 Q81 K82 E83 D84 N85 S86 M90 L93 K94 K95 N98

K105 V108 V112 P113 K114 P115 V116 I117 K118 I119 E120 K121

4.2.15 Score per residue for model 15

- Molecule 1: CD48 antigen

Chain A: 54% 26% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 G9 H10 V22 T23 L24 N25 S29 L30 P31 E32 N33 Y34 K35 W39 F40 Y41 T42 F43 D44 Q45 E49 W50 D51 S52 R53 K54 F58 E59 F62 V66 P70 Y76 V80 Q81 K82 N85 M90 R91 V92 L93

K94 N98 E99 Q100 E101 V112 P113 K114 P115 V116 I117 K118 I119 E120 K121

4.2.16 Score per residue for model 16

- Molecule 1: CD48 antigen

Chain A: 54% 26% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 G9 H10 M14 V22 T23 L24 N25 E28 S29 Y34 K35 Q36 W39 F40 Y41 T42 F43 D44 Q45 D51 S52 R53 K54 F58 E59 D69 G73 Y76 I77 V80 Q81 K82 E83 D84 N85 M90 L93 K94

N98 I104 D110 P111 V112 P113 K114 P115 V116 I117 K118 I119 E120 K121

4.2.17 Score per residue for model 17

- Molecule 1: CD48 antigen

Chain A: 50% 31% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 G9 H10 L11 V12 H13 V16 V22 T23 L30 P31 E32 N33 Y34 W39 F40 Y41 T42 F43 D44 E49 W50 D51 S52 R53 K54 S55 K56 Y57 F58 E59 S60 K63 L68 D69 P70 A74 I77 S78 K79 V80 E83 D84

N85 M90 L93 K94 N98 W102 K105 V112 P113 K114 P115 V116 I117 K118 I119 E120 K121

4.2.18 Score per residue for model 18

- Molecule 1: CD48 antigen

Chain A: 56% 24% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 G9 H10 L11 V12 H13 M14 V22 T23 I26 S27 P31 E32 N33 W39 F40 K46 D51 S52 R53 K54 S55 K56 Y57 F58 F62 V66 Y76 V80 Q81 K82 E83 D84 N85 S86 M90 K95 K105 V112

P113 K114 P115 V116 I117 K118 I119 E120 K121

4.2.19 Score per residue for model 19

- Molecule 1: CD48 antigen

Chain A: 54% 26% • 17%

G1 S2 S3 G4 S5 S6 G7 Q8 G9 H10 H13 M14 T15 V16 V22 T23 I26 S27 E28 S29 L30 P31 E32 N33 Y34 K35 W39 F40 Y41 T42 I47 W50 D51 S52 R53 K54 S55 K56 F62 V66 S72 Y76 K82 N85 M90 L93

N98 K105 L106 Q107 V108 P111 V112 P113 K114 P115 V116 I117 K118 I119 E120 K121

4.2.20 Score per residue for model 20

- Molecule 1: CD48 antigen

Chain A: 55% 24% 5% 17%

G1 S2 S3 G4 S5 S6 G7 Q8 G9 H10 H13 M14 V22 I26 S27 E28 S29 L30 P31 E32 K35 Q36 L37 T38 W39 F40 Y41 T42 F43 D51 S52 R53 V66 I77 V80 Q81 K82 E83 D84 N85 S86 M90 L93 K94 N98 E99 K105 L106

Q107 D110 P111 V112 P113 K114 P115 V116 I117 K118 I119 E120 K121

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	840	850	849	25±3
All	All	16800	17000	16980	507

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:LEU:HD12	1:A:98:ASN:O	0.87	1.68	13	11
1:A:16:VAL:HG11	1:A:22:VAL:HG23	0.79	1.52	19	2
1:A:84:ASP:OD1	1:A:106:LEU:HD23	0.75	1.80	13	1
1:A:16:VAL:HG11	1:A:22:VAL:HG22	0.72	1.58	17	1
1:A:16:VAL:HG21	1:A:22:VAL:HG21	0.71	1.60	17	1
1:A:30:LEU:HD12	1:A:72:SER:O	0.69	1.88	10	2
1:A:11:LEU:HD11	1:A:13:HIS:CD2	0.68	2.23	3	3
1:A:16:VAL:HG21	1:A:22:VAL:HG12	0.68	1.63	12	1
1:A:23:THR:HG23	1:A:76:TYR:CE1	0.67	2.25	18	8
1:A:62:PHE:O	1:A:66:VAL:HG22	0.67	1.89	19	6
1:A:30:LEU:HD21	1:A:92:VAL:HG21	0.67	1.67	9	1
1:A:11:LEU:HD13	1:A:12:VAL:N	0.65	2.05	17	3
1:A:16:VAL:HG21	1:A:22:VAL:CG2	0.64	2.21	17	1
1:A:23:THR:HG23	1:A:76:TYR:CD1	0.63	2.27	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:HD11	1:A:30:LEU:HG	0.61	1.72	9	1
1:A:30:LEU:CD2	1:A:92:VAL:HG21	0.61	2.24	9	1
1:A:39:TRP:CZ2	1:A:90:MET:SD	0.60	2.95	3	20
1:A:85:ASN:OD1	1:A:108:VAL:HG23	0.60	1.97	9	1
1:A:43:PHE:CE2	1:A:44:ASP:OD1	0.60	2.55	17	1
1:A:14:MET:HB3	1:A:106:LEU:HD12	0.58	1.74	19	1
1:A:41:TYR:CD1	1:A:41:TYR:O	0.58	2.56	16	7
1:A:22:VAL:HG12	1:A:77:ILE:HB	0.58	1.75	2	6
1:A:93:LEU:HD13	1:A:99:GLU:HG3	0.58	1.74	20	3
1:A:66:VAL:HG12	1:A:77:ILE:HG12	0.57	1.75	8	1
1:A:11:LEU:HD13	1:A:11:LEU:C	0.57	2.20	17	2
1:A:30:LEU:HD13	1:A:34:TYR:CD2	0.56	2.36	12	1
1:A:50:TRP:CE2	1:A:51:ASP:O	0.56	2.59	3	2
1:A:40:PHE:CE2	1:A:46:LYS:CG	0.55	2.88	7	1
1:A:39:TRP:C	1:A:40:PHE:CD1	0.55	2.80	14	1
1:A:56:LYS:HG2	1:A:58:PHE:CE1	0.55	2.37	18	1
1:A:30:LEU:HD13	1:A:34:TYR:CE1	0.54	2.38	1	2
1:A:25:ASN:ND2	1:A:25:ASN:H	0.54	2.00	11	2
1:A:30:LEU:HD13	1:A:34:TYR:CE2	0.54	2.37	7	1
1:A:16:VAL:HG11	1:A:22:VAL:CG2	0.53	2.31	19	1
1:A:22:VAL:HG22	1:A:23:THR:H	0.53	1.63	7	6
1:A:41:TYR:CD2	1:A:42:THR:CG2	0.52	2.92	6	9
1:A:22:VAL:HG22	1:A:23:THR:N	0.52	2.20	8	8
1:A:23:THR:HG23	1:A:74:ALA:HB1	0.52	1.80	17	1
1:A:16:VAL:CG1	1:A:22:VAL:HG23	0.51	2.32	19	1
1:A:51:ASP:O	1:A:53:ARG:N	0.51	2.44	3	18
1:A:77:ILE:CG2	1:A:80:VAL:HG12	0.51	2.36	12	4
1:A:41:TYR:HB2	1:A:47:ILE:HD11	0.51	1.82	4	1
1:A:14:MET:HE1	1:A:22:VAL:CG2	0.51	2.36	6	10
1:A:84:ASP:OD1	1:A:108:VAL:HG21	0.51	2.04	2	1
1:A:24:LEU:HD12	1:A:75:LEU:HD23	0.51	1.83	5	2
1:A:11:LEU:C	1:A:11:LEU:CD1	0.51	2.79	17	1
1:A:84:ASP:OD1	1:A:85:ASN:N	0.51	2.44	12	4
1:A:84:ASP:OD2	1:A:108:VAL:CG2	0.50	2.59	2	2
1:A:56:LYS:CG	1:A:58:PHE:CE1	0.50	2.94	18	1
1:A:50:TRP:CZ3	1:A:54:LYS:HA	0.50	2.41	19	2
1:A:82:LYS:HA	1:A:108:VAL:HG11	0.50	1.84	19	2
1:A:89:ILE:HG23	1:A:101:GLU:OE1	0.50	2.06	2	1
1:A:101:GLU:CD	1:A:101:GLU:C	0.50	2.70	12	2
1:A:62:PHE:HB3	1:A:66:VAL:HG11	0.50	1.83	9	5
1:A:50:TRP:HB2	1:A:68:LEU:HD23	0.50	1.83	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:PHE:CE2	1:A:46:LYS:HG2	0.49	2.41	7	1
1:A:34:TYR:CD1	1:A:34:TYR:C	0.49	2.85	15	2
1:A:13:HIS:CD2	1:A:105:LYS:HB3	0.49	2.43	20	14
1:A:14:MET:SD	1:A:24:LEU:CD2	0.49	3.00	7	7
1:A:48:VAL:HG23	1:A:56:LYS:O	0.49	2.07	11	2
1:A:30:LEU:HD13	1:A:34:TYR:CD1	0.49	2.43	1	1
1:A:13:HIS:CE1	1:A:105:LYS:HD3	0.49	2.43	20	5
1:A:22:VAL:HG11	1:A:77:ILE:HD12	0.49	1.85	2	2
1:A:41:TYR:CD2	1:A:42:THR:HG23	0.48	2.43	9	5
1:A:50:TRP:CZ3	1:A:55:SER:N	0.48	2.81	8	3
1:A:49:GLU:HB3	1:A:58:PHE:CZ	0.48	2.43	10	3
1:A:26:ILE:O	1:A:28:GLU:N	0.48	2.46	20	1
1:A:26:ILE:HD12	1:A:28:GLU:O	0.48	2.07	19	1
1:A:84:ASP:OD2	1:A:106:LEU:CD2	0.48	2.60	3	1
1:A:56:LYS:HD2	1:A:58:PHE:CE1	0.48	2.43	5	1
1:A:51:ASP:N	1:A:54:LYS:O	0.48	2.46	10	1
1:A:43:PHE:CD2	1:A:44:ASP:OD1	0.48	2.66	17	1
1:A:39:TRP:CE2	1:A:90:MET:SD	0.48	3.06	19	10
1:A:14:MET:SD	1:A:104:ILE:CG2	0.48	3.01	16	4
1:A:84:ASP:OD2	1:A:108:VAL:HG21	0.48	2.09	8	3
1:A:32:GLU:O	1:A:33:ASN:ND2	0.48	2.47	12	3
1:A:30:LEU:CD1	1:A:72:SER:O	0.48	2.62	14	1
1:A:35:LYS:HB3	1:A:93:LEU:HD23	0.48	1.85	14	1
1:A:40:PHE:CZ	1:A:46:LYS:HE2	0.48	2.44	13	1
1:A:36:GLN:NE2	1:A:51:ASP:OD1	0.47	2.47	16	1
1:A:25:ASN:ND2	1:A:25:ASN:N	0.47	2.62	5	2
1:A:40:PHE:CE1	1:A:91:ARG:HD3	0.47	2.43	9	1
1:A:11:LEU:HD12	1:A:103:LYS:O	0.47	2.09	13	1
1:A:50:TRP:CZ3	1:A:70:PRO:HG3	0.47	2.44	15	1
1:A:85:ASN:O	1:A:85:ASN:CG	0.47	2.52	17	2
1:A:40:PHE:CZ	1:A:91:ARG:HD2	0.47	2.44	1	3
1:A:66:VAL:HG12	1:A:77:ILE:HG23	0.47	1.87	4	3
1:A:50:TRP:CE3	1:A:54:LYS:C	0.47	2.89	13	2
1:A:35:LYS:CB	1:A:93:LEU:HD23	0.47	2.39	10	1
1:A:40:PHE:CE1	1:A:91:ARG:HD2	0.47	2.45	11	1
1:A:45:GLN:OE1	1:A:45:GLN:C	0.46	2.54	4	1
1:A:50:TRP:NE1	1:A:51:ASP:O	0.46	2.48	2	1
1:A:42:THR:O	1:A:43:PHE:C	0.46	2.54	10	6
1:A:23:THR:HG23	1:A:76:TYR:CD2	0.46	2.45	8	1
1:A:54:LYS:CG	1:A:55:SER:N	0.46	2.79	13	3
1:A:40:PHE:CZ	1:A:46:LYS:HE3	0.46	2.44	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:O	1:A:27:SER:C	0.46	2.53	20	4
1:A:79:LYS:O	1:A:81:GLN:NE2	0.46	2.49	5	3
1:A:40:PHE:CD1	1:A:40:PHE:N	0.46	2.84	14	2
1:A:98:ASN:O	1:A:99:GLU:C	0.45	2.55	15	1
1:A:31:PRO:O	1:A:32:GLU:C	0.45	2.54	9	14
1:A:50:TRP:CE3	1:A:55:SER:N	0.45	2.85	5	4
1:A:58:PHE:O	1:A:59:GLU:C	0.45	2.54	12	5
1:A:78:SER:O	1:A:79:LYS:C	0.45	2.54	12	3
1:A:22:VAL:CG1	1:A:23:THR:N	0.45	2.79	17	1
1:A:40:PHE:CE2	1:A:46:LYS:HE3	0.45	2.46	18	1
1:A:23:THR:HG22	1:A:25:ASN:OD1	0.45	2.11	5	1
1:A:81:GLN:O	1:A:84:ASP:CG	0.45	2.54	12	2
1:A:29:SER:O	1:A:30:LEU:C	0.45	2.54	2	5
1:A:61:LYS:O	1:A:62:PHE:C	0.45	2.55	6	1
1:A:81:GLN:O	1:A:84:ASP:N	0.45	2.50	18	4
1:A:96:THR:HG21	1:A:98:ASN:ND2	0.45	2.27	10	1
1:A:22:VAL:CG2	1:A:80:VAL:HG11	0.45	2.42	12	1
1:A:84:ASP:OD1	1:A:84:ASP:C	0.45	2.55	13	1
1:A:82:LYS:O	1:A:85:ASN:CG	0.45	2.55	7	10
1:A:89:ILE:HG23	1:A:102:TRP:O	0.45	2.12	3	1
1:A:32:GLU:O	1:A:33:ASN:CG	0.44	2.55	1	1
1:A:42:THR:HG21	1:A:45:GLN:OE1	0.44	2.12	15	1
1:A:41:TYR:CA	1:A:47:ILE:HD11	0.44	2.42	19	1
1:A:51:ASP:C	1:A:53:ARG:N	0.44	2.71	19	17
1:A:24:LEU:HB3	1:A:39:TRP:CH2	0.44	2.47	2	1
1:A:26:ILE:HG22	1:A:102:TRP:CD1	0.44	2.48	11	1
1:A:67:ARG:NH1	1:A:69:ASP:OD1	0.44	2.51	1	1
1:A:48:VAL:CG1	1:A:68:LEU:HD22	0.44	2.42	8	1
1:A:32:GLU:O	1:A:33:ASN:C	0.44	2.55	5	1
1:A:40:PHE:CD1	1:A:89:ILE:O	0.44	2.70	2	1
1:A:50:TRP:CH2	1:A:53:ARG:O	0.44	2.71	2	2
1:A:51:ASP:O	1:A:52:SER:C	0.43	2.55	4	12
1:A:83:GLU:O	1:A:84:ASP:C	0.43	2.56	9	6
1:A:60:SER:O	1:A:63:LYS:N	0.43	2.51	3	2
1:A:76:TYR:CD1	1:A:76:TYR:N	0.43	2.86	5	2
1:A:94:LYS:O	1:A:97:GLY:N	0.43	2.51	5	1
1:A:35:LYS:HE2	1:A:93:LEU:HD21	0.43	1.90	15	1
1:A:91:ARG:CZ	1:A:101:GLU:OE1	0.43	2.65	15	1
1:A:26:ILE:HD13	1:A:102:TRP:CE3	0.43	2.48	2	1
1:A:101:GLU:OE1	1:A:101:GLU:C	0.43	2.56	4	1
1:A:23:THR:HG23	1:A:76:TYR:CE2	0.43	2.48	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:GLU:CB	1:A:58:PHE:CZ	0.43	3.01	11	3
1:A:51:ASP:CB	1:A:54:LYS:O	0.43	2.67	10	3
1:A:50:TRP:CE3	1:A:55:SER:HB2	0.43	2.48	12	1
1:A:32:GLU:C	1:A:33:ASN:ND2	0.43	2.72	1	2
1:A:26:ILE:HD13	1:A:102:TRP:CZ3	0.43	2.49	2	1
1:A:28:GLU:O	1:A:29:SER:C	0.43	2.57	14	5
1:A:18:SER:N	1:A:108:VAL:HG13	0.43	2.29	12	1
1:A:14:MET:CE	1:A:22:VAL:CG2	0.42	2.97	20	2
1:A:94:LYS:CG	1:A:98:ASN:HB3	0.42	2.44	20	1
1:A:84:ASP:O	1:A:86:SER:N	0.42	2.52	2	3
1:A:60:SER:O	1:A:61:LYS:C	0.42	2.57	6	1
1:A:81:GLN:O	1:A:82:LYS:C	0.42	2.57	18	1
1:A:69:ASP:O	1:A:73:GLY:N	0.42	2.52	2	3
1:A:83:GLU:O	1:A:85:ASN:N	0.42	2.52	10	1
1:A:50:TRP:CE2	1:A:70:PRO:HB3	0.42	2.49	17	1
1:A:38:THR:HG21	1:A:46:LYS:CE	0.42	2.45	8	1
1:A:94:LYS:HB3	1:A:96:THR:HG22	0.42	1.90	2	1
1:A:50:TRP:CZ3	1:A:54:LYS:C	0.42	2.93	13	2
1:A:41:TYR:CD1	1:A:41:TYR:C	0.42	2.91	19	4
1:A:41:TYR:HB2	1:A:47:ILE:CG1	0.42	2.45	4	1
1:A:11:LEU:CD1	1:A:13:HIS:CD2	0.42	3.03	18	1
1:A:84:ASP:O	1:A:85:ASN:C	0.42	2.58	8	3
1:A:84:ASP:OD1	1:A:108:VAL:CG2	0.42	2.67	2	1
1:A:14:MET:SD	1:A:104:ILE:HG21	0.42	2.55	16	2
1:A:44:ASP:O	1:A:45:GLN:OE1	0.42	2.37	16	1
1:A:96:THR:CG2	1:A:98:ASN:ND2	0.42	2.82	10	1
1:A:81:GLN:O	1:A:84:ASP:OD2	0.41	2.38	13	1
1:A:49:GLU:HB2	1:A:58:PHE:CZ	0.41	2.50	17	1
1:A:49:GLU:HB2	1:A:58:PHE:CE2	0.41	2.50	17	1
1:A:33:ASN:OD1	1:A:95:LYS:CD	0.41	2.68	18	1
1:A:14:MET:O	1:A:107:GLN:N	0.41	2.53	20	1
1:A:25:ASN:O	1:A:26:ILE:C	0.41	2.58	9	1
1:A:50:TRP:NE1	1:A:52:SER:O	0.41	2.54	17	1
1:A:85:ASN:OD1	1:A:108:VAL:N	0.41	2.54	2	1
1:A:100:GLN:HG2	1:A:102:TRP:CZ2	0.41	2.49	9	1
1:A:101:GLU:CD	1:A:101:GLU:O	0.41	2.59	2	1
1:A:50:TRP:HB2	1:A:68:LEU:HD21	0.41	1.92	10	1
1:A:50:TRP:CZ3	1:A:55:SER:HB2	0.41	2.50	12	1
1:A:11:LEU:HD13	1:A:103:LYS:CB	0.41	2.46	13	1
1:A:94:LYS:HE2	1:A:98:ASN:CB	0.41	2.46	15	1
1:A:14:MET:HE1	1:A:22:VAL:HG21	0.41	1.92	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:CG2	1:A:102:TRP:CD1	0.41	3.03	11	1
1:A:85:ASN:O	1:A:85:ASN:OD1	0.41	2.38	17	2
1:A:22:VAL:CG1	1:A:77:ILE:HD12	0.41	2.45	2	1
1:A:50:TRP:CZ2	1:A:70:PRO:HB3	0.41	2.50	17	1
1:A:110:ASP:C	1:A:110:ASP:OD1	0.41	2.58	7	1
1:A:50:TRP:CZ3	1:A:70:PRO:HB3	0.41	2.51	10	1
1:A:40:PHE:CE2	1:A:46:LYS:HE2	0.41	2.51	12	2
1:A:25:ASN:O	1:A:25:ASN:CG	0.41	2.59	15	1
1:A:25:ASN:HB3	1:A:74:ALA:HB2	0.41	1.92	11	1
1:A:50:TRP:CG	1:A:51:ASP:N	0.40	2.90	3	1
1:A:26:ILE:HG21	1:A:102:TRP:CE3	0.40	2.51	5	1
1:A:14:MET:HE2	1:A:22:VAL:CG2	0.40	2.46	19	1
1:A:94:LYS:HG3	1:A:98:ASN:CB	0.40	2.46	20	1
1:A:37:LEU:HD22	1:A:68:LEU:HD11	0.40	1.93	2	1
1:A:11:LEU:HD21	1:A:13:HIS:NE2	0.40	2.32	7	1
1:A:30:LEU:HD11	1:A:37:LEU:HD11	0.40	1.91	20	1
1:A:79:LYS:O	1:A:80:VAL:O	0.40	2.40	7	1
1:A:81:GLN:O	1:A:84:ASP:OD1	0.40	2.40	12	2
1:A:65:ARG:HG3	1:A:66:VAL:N	0.40	2.31	12	1
1:A:18:SER:HB2	1:A:108:VAL:CG1	0.40	2.47	12	1
1:A:34:TYR:CD1	1:A:34:TYR:O	0.40	2.74	12	1
1:A:35:LYS:HD3	1:A:93:LEU:CD2	0.40	2.47	19	1
1:A:85:ASN:OD1	1:A:85:ASN:O	0.40	2.40	1	2
1:A:25:ASN:OD1	1:A:25:ASN:O	0.40	2.40	8	1
1:A:62:PHE:O	1:A:66:VAL:CG2	0.40	2.69	9	1
1:A:50:TRP:CH2	1:A:70:PRO:CB	0.40	3.04	10	1
1:A:24:LEU:CD1	1:A:88:TYR:CD2	0.40	3.05	11	1
1:A:50:TRP:CZ2	1:A:70:PRO:HG3	0.40	2.52	17	1
1:A:41:TYR:HA	1:A:47:ILE:HD11	0.40	1.93	19	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	101/121 (83%)	83±3 (82±3%)	14±3 (14±3%)	4±2 (4±2%)	5 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2020/2420 (83%)	1662 (82%)	279 (14%)	79 (4%)	5 32

All 16 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	52	SER	17
1	A	80	VAL	15
1	A	85	ASN	13
1	A	66	VAL	7
1	A	59	GLU	6
1	A	30	LEU	5
1	A	26	ILE	3
1	A	27	SER	2
1	A	32	GLU	2
1	A	34	TYR	2
1	A	58	PHE	2
1	A	98	ASN	1
1	A	28	GLU	1
1	A	61	LYS	1
1	A	84	ASP	1
1	A	29	SER	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	96/112 (86%)	92±2 (96±2%)	4±2 (4±2%)	32 81
All	All	1920/2240 (86%)	1836 (96%)	84 (4%)	32 81

All 27 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	42	THR	9
1	A	56	LYS	7
1	A	82	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	101	GLU	6
1	A	84	ASP	6
1	A	25	ASN	4
1	A	76	TYR	4
1	A	95	LYS	4
1	A	94	LYS	4
1	A	54	LYS	4
1	A	61	LYS	3
1	A	51	ASP	3
1	A	33	ASN	3
1	A	86	SER	2
1	A	49	GLU	2
1	A	59	GLU	2
1	A	32	GLU	2
1	A	44	ASP	2
1	A	110	ASP	2
1	A	69	ASP	2
1	A	83	GLU	1
1	A	41	TYR	1
1	A	36	GLN	1
1	A	53	ARG	1
1	A	78	SER	1
1	A	72	SER	1
1	A	35	LYS	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 monosaccharides 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 (i)

No chemical shift data were provided