Full wwPDB NMR Structure Validation Report (i)

Feb 23, 2022 – 07:07 AM EST

PDB ID	:	1X4A
Title	:	Solution structure of RRM domain in splicing factor SF2
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Deposited on	:	2005-05-14

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:

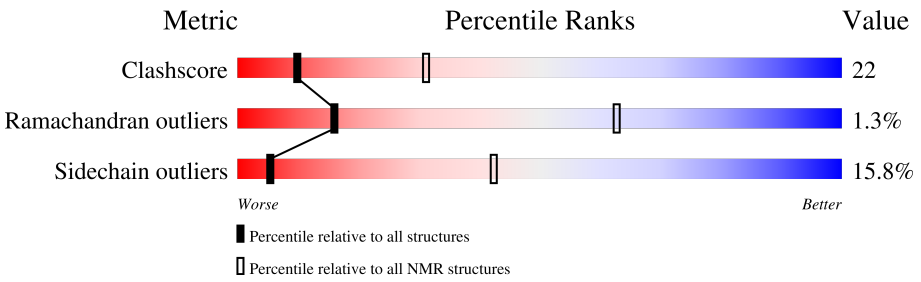
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	109	36% 24% • 38%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:24-A:55, A:61-A:96 (68)	0.20	5

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

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

The models can be grouped into 4 clusters and 7 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1600 atoms, of which 772 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	109	1600	509	772	152	165	2	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q07955
A	2	SER	-	cloning artifact	UNP Q07955
A	3	SER	-	cloning artifact	UNP Q07955
A	4	GLY	-	cloning artifact	UNP Q07955
A	5	SER	-	cloning artifact	UNP Q07955
A	6	SER	-	cloning artifact	UNP Q07955
A	7	GLY	-	cloning artifact	UNP Q07955
A	104	SER	-	cloning artifact	UNP Q07955
A	105	GLY	-	cloning artifact	UNP Q07955
A	106	PRO	-	cloning artifact	UNP Q07955
A	107	SER	-	cloning artifact	UNP Q07955
A	108	SER	-	cloning artifact	UNP Q07955
A	109	GLY	-	cloning artifact	UNP Q07955

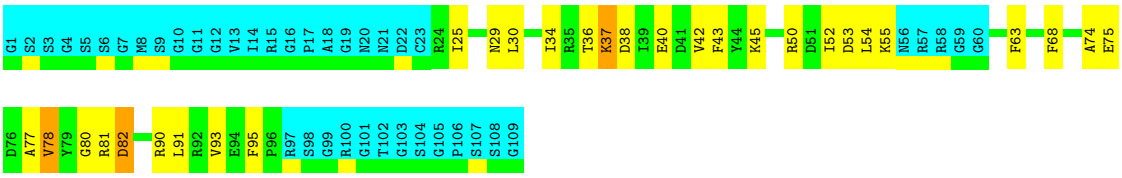
4 Residue-property plots (i)

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: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

Chain A: 36% 24% • 38%



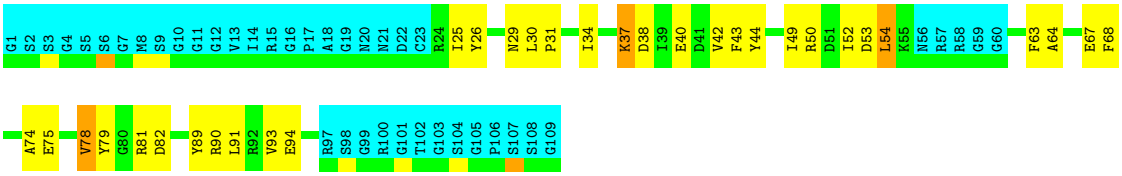
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

Chain A: 33% 27% • 38%



4.2.2 Score per residue for model 2

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

Chain A: 39% 21% • 38%

G1 S2 S3 G4 S5 S6 G7 M8 S9 G10 G11 G12 V13 I14 R15 G16 P17 A18 G19 N20 N21 D22 C23 R24 I25 Y26 L30 I34 K37 D38 I39 E40 D41 V42 F43 R50 D51 I52 D53 L54 K55 N56 R57 R58 G59 G60 F63 F68 E69 D70 A74 A77

V78 R81 D82 Y86 L91 R92 V93 E94 F95 P96 R97 S98 G99 R100 G101 T102 G103 S104 G105 P106 S107 S108 G109

4.2.3 Score per residue for model 3

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

Chain A: 36% 23% • • 38%

G1 S2 S3 G4 S5 S6 G7 M8 S9 G10 G11 G12 V13 I14 R15 G16 P17 A18 G19 N20 N21 D22 C23 R24 I25 N29 L30 I34 R35 T36 K37 D38 I39 E40 D41 V42 K45 R50 D51 I52 D53 L54 K55 N56 R57 R58 G59 G60 F63 F68 E69 D70 A74

V78 Y79 G80 R81 D82 G83 Y84 D85 R90 V93 E94 F95 P96 R97 S98 G99 R100 G101 T102 G103 S104 G105 P106 S107 S108 G109

4.2.4 Score per residue for model 4

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

Chain A: 32% 27% • 38%

G1 S2 S3 G4 S5 S6 G7 M8 S9 G10 G11 G12 V13 I14 R15 G16 P17 A18 G19 N20 N21 D22 C23 R24 I25 N29 L30 D33 K37 D38 I39 E40 D41 V42 F43 Y44 K45 Y46 I49 R50 D51 I52 D53 L54 K55 N56 R57 R58 G59 G60 F63 A64 F65 F68

E69 D70 P71 A74 V78 R81 D82 G83 Y89 R90 L91 R92 V93 E94 F95 P96 R97 S98 G99 R100 G101 T102 G103 S104 G105 P106 S107 S108 G109

4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

Chain A: 32% 27% • • 38%

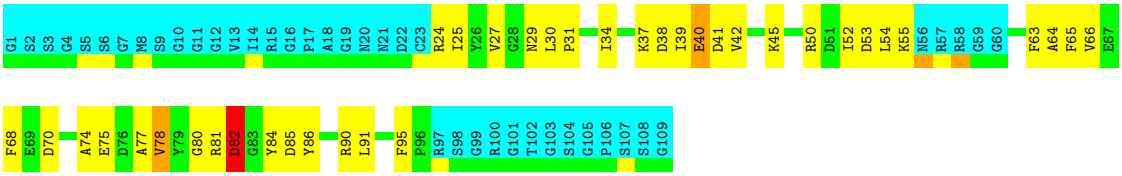
G1 S2 S3 G4 S5 S6 G7 M8 S9 G10 G11 G12 V13 I14 R15 G16 P17 A18 G19 N20 N21 D22 C23 R24 I25 Y26 N29 L30 P31 I34 K37 D38 I39 E40 D41 V42 F43 Y44 K45 I49 R50 D51 I52 D53 L54 K55 N56 R57 R58 G59 G60 F63 A64 F65 V66

E67 D76 A77 V78 Y79 G80 R81 D82 G83 Y84 D85 G88 L91 R92 V93 E94 F95 P96 R97 S98 G99 R100 G101 T102 G103 S104 G105 P106 S107 S108 G109

4.2.6 Score per residue for model 6

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

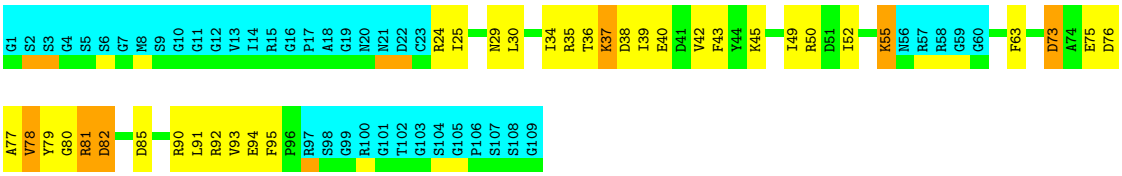
Chain A: 28% 32% • • 38%



4.2.7 Score per residue for model 7

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

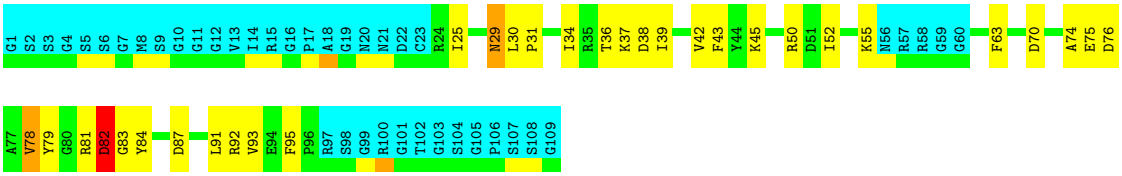
Chain A: 30% 27% 6% 38%



4.2.8 Score per residue for model 8

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

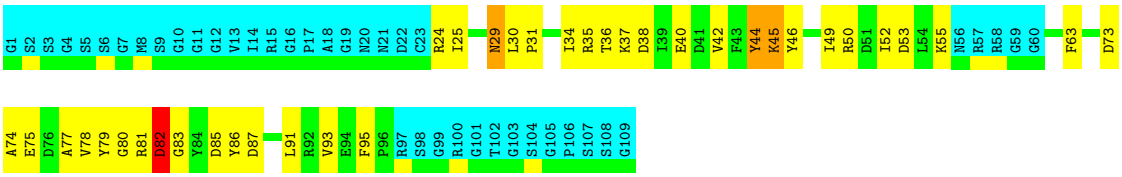
Chain A: 34% 26% • • 38%



4.2.9 Score per residue for model 9

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

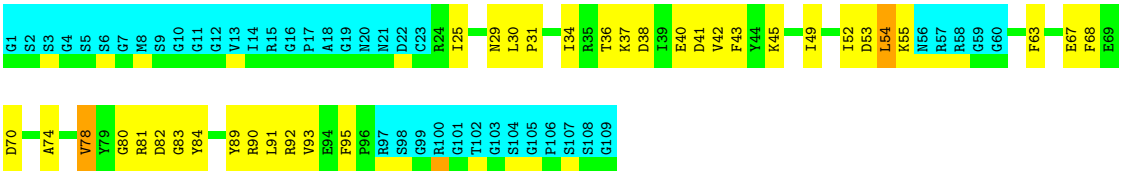
Chain A: 28% 30% • • 38%



4.2.10 Score per residue for model 10

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

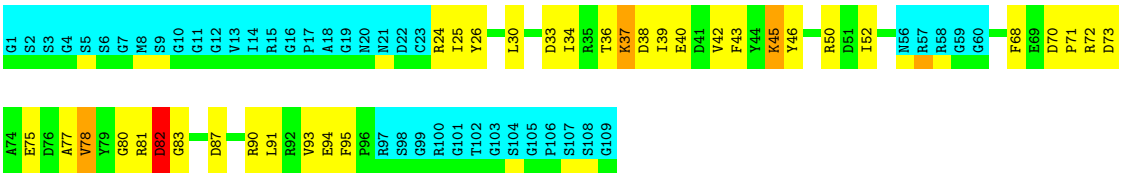
Chain A: 30% 30% • 38%



4.2.11 Score per residue for model 11

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

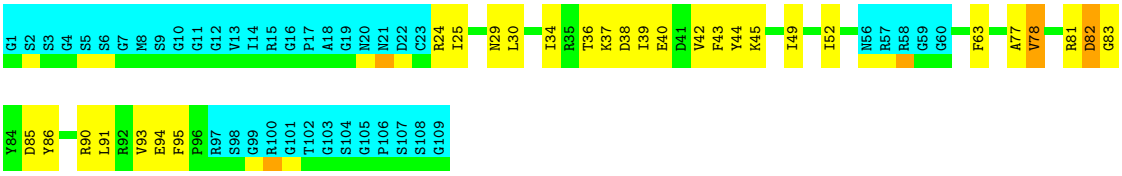
Chain A: 30% 28% • • 38%



4.2.12 Score per residue for model 12

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

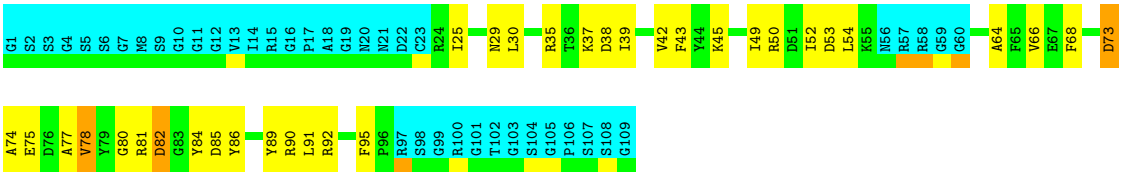
Chain A: 36% 25% • 38%



4.2.13 Score per residue for model 13

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

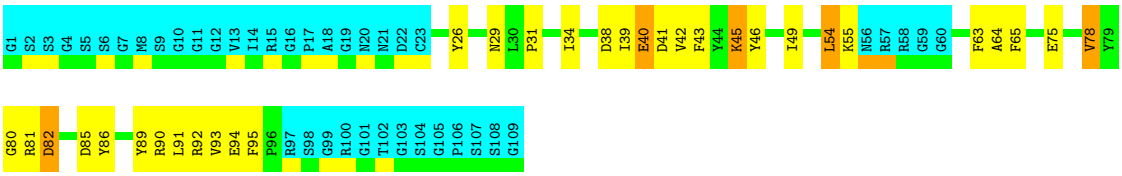
Chain A: 31% 28% • 38%



4.2.14 Score per residue for model 14

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

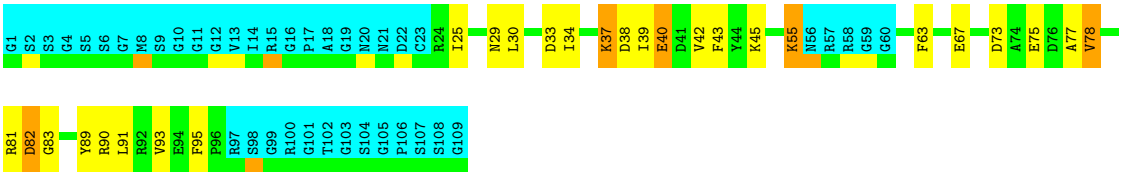
Chain A: 33% 25% 5% 38%



4.2.15 Score per residue for model 15

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

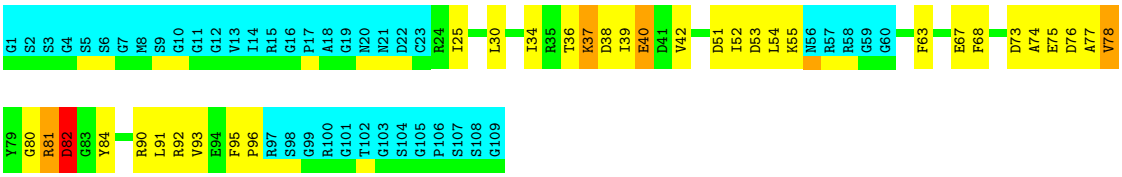
Chain A: 38% 20% 5% 38%



4.2.16 Score per residue for model 16

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

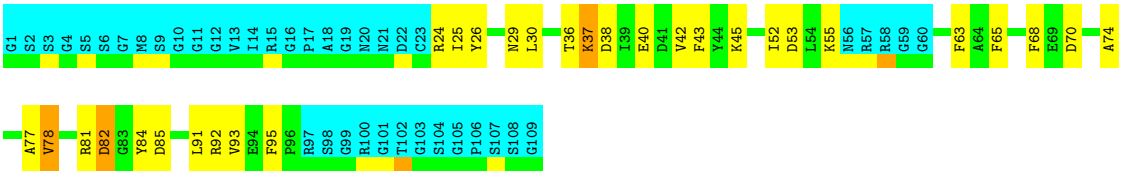
Chain A: 32% 26% • • 38%



4.2.17 Score per residue for model 17

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

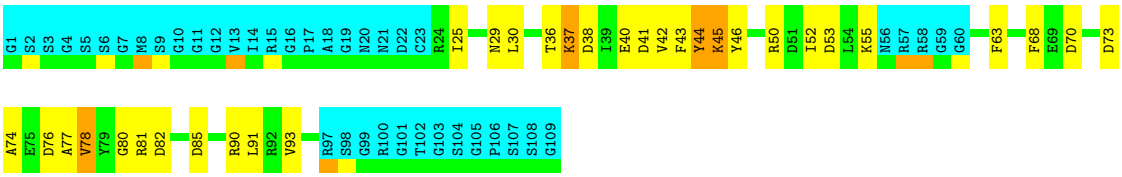
Chain A: 35% 25% • 38%



4.2.18 Score per residue for model 18

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

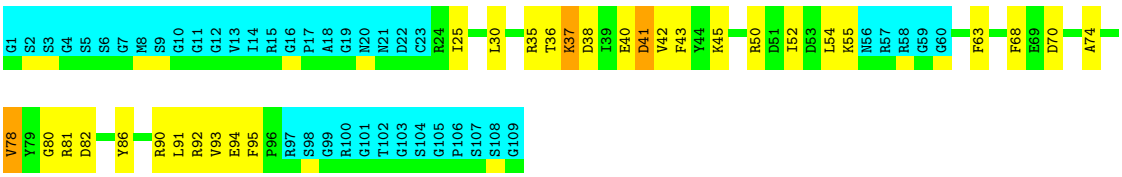
Chain A: 33% 26% • 38%



4.2.19 Score per residue for model 19

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

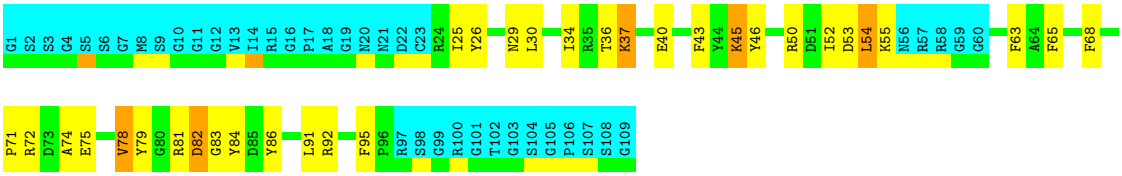
Chain A: 35% 25% • 38%



4.2.20 Score per residue for model 20

• Molecule 1: splicing factor, arginine/serine-rich 1 (splicing factor 2, alternate splicing factor) variant

Chain A: 32% 26% 5% 38%



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: *target function, structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.8
CYANA	refinement	1.0.8

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	572	535	535	24±3
All	All	11440	10700	10700	484

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:VAL:HG23	1:A:93:VAL:HG12	1.13	1.19	1	16
1:A:30:LEU:HD23	1:A:91:LEU:HD22	0.96	1.36	11	18
1:A:38:ASP:O	1:A:42:VAL:HG23	0.86	1.70	15	19
1:A:78:VAL:HG23	1:A:93:VAL:CG1	0.84	2.00	1	8
1:A:29:ASN:O	1:A:91:LEU:HD23	0.75	1.81	4	15
1:A:52:ILE:HG12	1:A:66:VAL:HG13	0.74	1.59	13	2
1:A:81:ARG:HB3	1:A:93:VAL:HG21	0.73	1.59	15	5
1:A:30:LEU:HD23	1:A:91:LEU:CD2	0.73	2.14	17	17
1:A:34:ILE:HG12	1:A:39:ILE:HD11	0.72	1.61	11	5
1:A:25:ILE:HG22	1:A:95:PHE:CE1	0.71	2.21	9	12
1:A:36:THR:HG23	1:A:52:ILE:CG2	0.70	2.15	17	10
1:A:25:ILE:CD1	1:A:43:PHE:CE2	0.69	2.75	13	8
1:A:30:LEU:CD2	1:A:91:LEU:HD22	0.65	2.20	15	13
1:A:78:VAL:CG2	1:A:93:VAL:HG12	0.65	2.17	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ARG:NH1	1:A:84:TYR:CE1	0.65	2.65	16	4
1:A:54:LEU:HD12	1:A:64:ALA:HB2	0.64	1.70	13	3
1:A:34:ILE:CG1	1:A:39:ILE:HD11	0.63	2.22	11	8
1:A:68:PHE:HB2	1:A:74:ALA:HB2	0.61	1.71	3	7
1:A:81:ARG:NH2	1:A:84:TYR:CD2	0.60	2.69	13	1
1:A:25:ILE:HD11	1:A:43:PHE:CE1	0.60	2.32	15	3
1:A:25:ILE:HG22	1:A:95:PHE:CD1	0.59	2.32	12	3
1:A:34:ILE:CD1	1:A:86:TYR:CZ	0.59	2.85	14	4
1:A:81:ARG:NH2	1:A:84:TYR:CE2	0.59	2.71	13	1
1:A:68:PHE:CB	1:A:74:ALA:HB2	0.58	2.28	3	2
1:A:25:ILE:HD11	1:A:43:PHE:CE2	0.58	2.34	8	7
1:A:86:TYR:CB	1:A:91:LEU:HD11	0.57	2.29	9	3
1:A:81:ARG:CB	1:A:93:VAL:HG21	0.56	2.29	10	2
1:A:34:ILE:HG13	1:A:39:ILE:HD11	0.56	1.77	12	4
1:A:36:THR:HG23	1:A:52:ILE:HG21	0.56	1.78	17	5
1:A:55:LYS:CB	1:A:63:PHE:CZ	0.55	2.89	15	4
1:A:25:ILE:CD1	1:A:43:PHE:CE1	0.54	2.90	18	3
1:A:25:ILE:CG2	1:A:95:PHE:CE1	0.54	2.91	4	3
1:A:54:LEU:CD1	1:A:64:ALA:HB2	0.54	2.32	13	1
1:A:78:VAL:HG11	1:A:95:PHE:CE2	0.52	2.39	10	12
1:A:44:TYR:CD1	1:A:44:TYR:C	0.52	2.83	18	3
1:A:55:LYS:CB	1:A:63:PHE:CE2	0.51	2.93	14	3
1:A:35:ARG:O	1:A:39:ILE:HD12	0.51	2.04	13	1
1:A:36:THR:CG2	1:A:52:ILE:CG2	0.51	2.89	3	3
1:A:38:ASP:O	1:A:42:VAL:CG2	0.51	2.59	6	7
1:A:63:PHE:N	1:A:63:PHE:CD1	0.51	2.79	10	4
1:A:55:LYS:HB2	1:A:63:PHE:CE2	0.51	2.41	16	12
1:A:49:ILE:HD13	1:A:52:ILE:HD11	0.50	1.82	13	1
1:A:81:ARG:N	1:A:81:ARG:HE	0.50	2.05	18	2
1:A:78:VAL:HG13	1:A:79:TYR:CD1	0.49	2.42	9	1
1:A:29:ASN:O	1:A:91:LEU:CD2	0.49	2.61	9	5
1:A:35:ARG:O	1:A:39:ILE:CD1	0.49	2.61	13	1
1:A:75:GLU:O	1:A:79:TYR:CD2	0.49	2.66	20	1
1:A:40:GLU:O	1:A:44:TYR:CB	0.48	2.62	1	2
1:A:75:GLU:O	1:A:79:TYR:CG	0.48	2.66	7	2
1:A:49:ILE:HG21	1:A:52:ILE:HG13	0.48	1.84	4	2
1:A:43:PHE:CE1	1:A:81:ARG:HG3	0.48	2.44	7	5
1:A:30:LEU:HD22	1:A:34:ILE:HG12	0.48	1.86	3	2
1:A:43:PHE:CE2	1:A:81:ARG:HG3	0.48	2.44	19	4
1:A:45:LYS:HG3	1:A:46:TYR:CD1	0.47	2.44	4	2
1:A:81:ARG:NH1	1:A:84:TYR:CD1	0.47	2.82	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:PHE:CD2	1:A:74:ALA:HA	0.47	2.45	20	10
1:A:26:TYR:C	1:A:26:TYR:CD1	0.47	2.88	11	1
1:A:81:ARG:NH2	1:A:91:LEU:CD1	0.47	2.78	11	1
1:A:25:ILE:HG22	1:A:95:PHE:HE1	0.46	1.68	9	1
1:A:55:LYS:CG	1:A:63:PHE:CE2	0.46	2.98	7	2
1:A:55:LYS:HB2	1:A:63:PHE:CZ	0.46	2.45	3	4
1:A:85:ASP:OD1	1:A:88:GLY:CA	0.46	2.64	5	1
1:A:43:PHE:CE2	1:A:81:ARG:NH2	0.46	2.84	15	1
1:A:37:LYS:O	1:A:40:GLU:N	0.46	2.49	12	15
1:A:65:PHE:CD1	1:A:65:PHE:N	0.46	2.84	4	2
1:A:40:GLU:HB2	1:A:52:ILE:HD11	0.46	1.88	17	1
1:A:31:PRO:HG2	1:A:34:ILE:HD13	0.46	1.88	10	4
1:A:81:ARG:O	1:A:83:GLY:N	0.46	2.49	9	10
1:A:45:LYS:HG3	1:A:46:TYR:CD2	0.46	2.46	18	3
1:A:78:VAL:O	1:A:82:ASP:CB	0.45	2.64	19	10
1:A:26:TYR:HB2	1:A:65:PHE:CE1	0.45	2.46	5	2
1:A:42:VAL:O	1:A:81:ARG:NH2	0.45	2.49	8	3
1:A:43:PHE:CD2	1:A:77:ALA:HB1	0.45	2.47	13	2
1:A:25:ILE:HG21	1:A:74:ALA:O	0.45	2.11	8	1
1:A:49:ILE:HG21	1:A:52:ILE:CG1	0.45	2.41	4	3
1:A:84:TYR:CE2	1:A:86:TYR:HB2	0.45	2.46	13	1
1:A:75:GLU:O	1:A:79:TYR:CD1	0.45	2.69	7	2
1:A:77:ALA:O	1:A:81:ARG:N	0.45	2.50	7	4
1:A:54:LEU:HA	1:A:64:ALA:HB2	0.45	1.88	14	1
1:A:73:ASP:OD1	1:A:74:ALA:N	0.45	2.50	9	1
1:A:31:PRO:HB3	1:A:89:TYR:CD2	0.45	2.46	14	1
1:A:43:PHE:HD1	1:A:77:ALA:HB1	0.45	1.71	18	1
1:A:81:ARG:O	1:A:82:ASP:O	0.44	2.35	16	1
1:A:76:ASP:O	1:A:80:GLY:N	0.44	2.51	5	2
1:A:80:GLY:O	1:A:82:ASP:N	0.44	2.50	7	5
1:A:73:ASP:O	1:A:76:ASP:N	0.44	2.50	7	2
1:A:43:PHE:CD1	1:A:81:ARG:HG3	0.44	2.47	18	1
1:A:81:ARG:O	1:A:84:TYR:N	0.44	2.51	6	3
1:A:40:GLU:CG	1:A:41:ASP:N	0.44	2.80	10	7
1:A:45:LYS:HD2	1:A:46:TYR:CE2	0.44	2.47	20	1
1:A:31:PRO:O	1:A:34:ILE:HG22	0.44	2.13	6	1
1:A:78:VAL:CG1	1:A:79:TYR:CD1	0.44	3.00	9	1
1:A:26:TYR:CD1	1:A:26:TYR:C	0.44	2.91	2	1
1:A:86:TYR:HB2	1:A:91:LEU:HD11	0.44	1.89	9	1
1:A:86:TYR:HB3	1:A:91:LEU:HD11	0.44	1.89	6	1
1:A:26:TYR:CE2	1:A:63:PHE:HB2	0.43	2.49	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:GLU:HB3	1:A:79:TYR:CE2	0.43	2.48	9	1
1:A:84:TYR:CG	1:A:85:ASP:N	0.43	2.86	3	2
1:A:75:GLU:C	1:A:77:ALA:N	0.43	2.71	15	5
1:A:43:PHE:HB2	1:A:49:ILE:HD11	0.43	1.90	14	2
1:A:34:ILE:CD1	1:A:86:TYR:CE1	0.43	3.01	14	1
1:A:40:GLU:C	1:A:42:VAL:N	0.43	2.70	14	1
1:A:55:LYS:HB3	1:A:63:PHE:CZ	0.43	2.48	14	1
1:A:80:GLY:O	1:A:81:ARG:C	0.43	2.57	11	7
1:A:80:GLY:C	1:A:82:ASP:N	0.43	2.72	19	4
1:A:25:ILE:HD12	1:A:43:PHE:CE2	0.43	2.48	2	2
1:A:43:PHE:CD1	1:A:77:ALA:HB1	0.42	2.49	18	1
1:A:40:GLU:HA	1:A:49:ILE:CD1	0.42	2.44	5	2
1:A:63:PHE:CD1	1:A:63:PHE:N	0.42	2.88	2	3
1:A:54:LEU:C	1:A:54:LEU:CD2	0.42	2.87	20	3
1:A:81:ARG:NE	1:A:81:ARG:CA	0.42	2.82	20	2
1:A:27:VAL:HG12	1:A:30:LEU:HD11	0.42	1.90	6	1
1:A:81:ARG:NH1	1:A:84:TYR:CZ	0.42	2.88	3	1
1:A:55:LYS:HG2	1:A:63:PHE:CE2	0.42	2.50	7	1
1:A:55:LYS:HD2	1:A:63:PHE:CE2	0.42	2.50	10	1
1:A:40:GLU:O	1:A:44:TYR:N	0.42	2.49	12	1
1:A:75:GLU:O	1:A:77:ALA:N	0.41	2.53	16	2
1:A:77:ALA:O	1:A:80:GLY:N	0.41	2.53	13	1
1:A:34:ILE:HD12	1:A:86:TYR:CZ	0.41	2.50	14	1
1:A:73:ASP:O	1:A:77:ALA:N	0.41	2.50	9	1
1:A:68:PHE:CE1	1:A:73:ASP:OD2	0.41	2.74	11	1
1:A:42:VAL:O	1:A:45:LYS:NZ	0.41	2.50	15	1
1:A:49:ILE:HG21	1:A:52:ILE:HD11	0.41	1.92	5	1
1:A:81:ARG:O	1:A:82:ASP:C	0.41	2.59	8	3
1:A:85:ASP:OD1	1:A:88:GLY:N	0.41	2.53	5	1
1:A:81:ARG:NH2	1:A:91:LEU:HD13	0.41	2.30	11	1
1:A:40:GLU:O	1:A:42:VAL:N	0.41	2.54	14	1
1:A:31:PRO:CG	1:A:34:ILE:HD13	0.41	2.46	8	1
1:A:71:PRO:O	1:A:72:ARG:C	0.41	2.59	11	2
1:A:40:GLU:HG3	1:A:49:ILE:HD12	0.41	1.91	12	1
1:A:26:TYR:CD1	1:A:65:PHE:CZ	0.41	3.09	17	1
1:A:75:GLU:O	1:A:76:ASP:C	0.40	2.59	8	2
1:A:78:VAL:HG11	1:A:95:PHE:CZ	0.40	2.50	8	2
1:A:75:GLU:O	1:A:78:VAL:N	0.40	2.54	14	1
1:A:24:ARG:O	1:A:24:ARG:CG	0.40	2.69	3	1
1:A:73:ASP:C	1:A:75:GLU:N	0.40	2.75	13	1
1:A:26:TYR:HB2	1:A:65:PHE:CE2	0.40	2.52	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ASN:CG	1:A:90:ARG:O	0.40	2.60	3	1
1:A:82:ASP:OD1	1:A:93:VAL:O	0.40	2.40	7	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	68/109 (62%)	56±2 (82±3%)	12±2 (17±3%)	1±1 (1±1%)	16	63
All	All	1360/2180 (62%)	1110 (82%)	232 (17%)	18 (1%)	16	63

All 3 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	82	ASP	15
1	A	81	ARG	2
1	A	29	ASN	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	59/84 (70%)	50±1 (84±3%)	9±1 (16±3%)	5	42
All	All	1180/1680 (70%)	993 (84%)	187 (16%)	5	42

All 26 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	78	VAL	19
1	A	45	LYS	16
1	A	37	LYS	15
1	A	50	ARG	14
1	A	90	ARG	14
1	A	53	ASP	12
1	A	82	ASP	12
1	A	70	ASP	10
1	A	92	ARG	10
1	A	54	LEU	7
1	A	85	ASP	7
1	A	94	GLU	6
1	A	24	ARG	6
1	A	67	GLU	5
1	A	89	TYR	5
1	A	40	GLU	5
1	A	73	ASP	4
1	A	33	ASP	3
1	A	44	TYR	3
1	A	55	LYS	3
1	A	35	ARG	3
1	A	87	ASP	3
1	A	51	ASP	2
1	A	29	ASN	1
1	A	79	TYR	1
1	A	41	ASP	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