



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:16 pm BST

PDB ID : 2WW7  
Title : foldon containing beta-turn mimic  
Authors : Eckhardt, B.; Grosse, W.; Essen, L.-O.; Geyer, A.  
Deposited on : 2009-10-22  
Resolution : 1.06 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

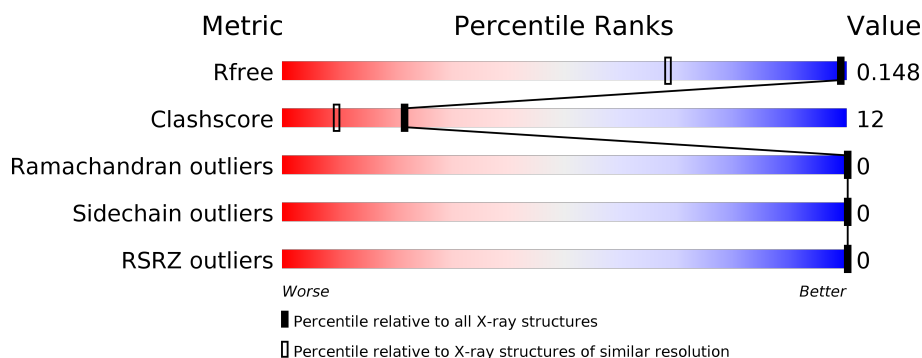
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.06 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1202 (1.10-1.02)
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	26	 77% 23%
1	B	26	 88% 12%
1	C	26	 81% 15% •
1	D	26	 88% 8% •
1	E	26	 77% 23%
1	F	26	 81% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PRS	C	18[A]	-	-	X	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3620 atoms, of which 1590 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FIBRITIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	26	Total	C	H	N	O	S	0	8	0
			559	189	281	42	46	1			
1	B	26	Total	C	H	N	O	S	0	5	0
			514	170	261	39	43	1			
1	C	26	Total	C	H	N	O	S	0	5	0
			512	170	255	39	46	2			
1	D	26	Total	C	H	N	O	S	0	3	0
			490	161	246	41	41	1			
1	E	26	Total	C	H	N	O	S	0	6	0
			536	179	267	42	47	1			
1	F	26	Total	C	H	N	O	S	0	7	0
			562	191	280	43	47	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	NA8	TYR	SEE REMARK 999	UNP Q76VI8
A	10	DAL	GLY	SEE REMARK 999	UNP Q76VI8
A	17	TH6	ASP	SEE REMARK 999	UNP Q76VI8
A	18	PRS	GLY	SEE REMARK 999	UNP Q76VI8
B	2	NA8	TYR	SEE REMARK 999	UNP Q76VI8
B	10	DAL	GLY	SEE REMARK 999	UNP Q76VI8
B	17	TH6	ASP	SEE REMARK 999	UNP Q76VI8
B	18	PRS	GLY	SEE REMARK 999	UNP Q76VI8
C	2	NA8	TYR	SEE REMARK 999	UNP Q76VI8
C	10	DAL	GLY	SEE REMARK 999	UNP Q76VI8
C	17	TH6	ASP	SEE REMARK 999	UNP Q76VI8
C	18	PRS	GLY	SEE REMARK 999	UNP Q76VI8
D	2	NA8	TYR	SEE REMARK 999	UNP Q76VI8
D	10	DAL	GLY	SEE REMARK 999	UNP Q76VI8
D	17	TH6	ASP	SEE REMARK 999	UNP Q76VI8
D	18	PRS	GLY	SEE REMARK 999	UNP Q76VI8
E	2	NA8	TYR	SEE REMARK 999	UNP Q76VI8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	DAL	GLY	SEE REMARK 999	UNP Q76VI8
E	17	TH6	ASP	SEE REMARK 999	UNP Q76VI8
E	18	PRS	GLY	SEE REMARK 999	UNP Q76VI8
F	2	NA8	TYR	SEE REMARK 999	UNP Q76VI8
F	10	DAL	GLY	SEE REMARK 999	UNP Q76VI8
F	17	TH6	ASP	SEE REMARK 999	UNP Q76VI8
F	18	PRS	GLY	SEE REMARK 999	UNP Q76VI8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	76	Total O 76 76	0	0
2	B	91	Total O 91 91	0	0
2	C	76	Total O 76 76	0	0
2	D	62	Total O 62 62	0	0
2	E	72	Total O 72 72	0	0
2	F	70	Total O 70 70	0	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

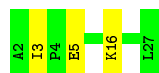
#### • Molecule 1: FIBRITIN

Chain A:  77% 23%




#### • Molecule 1: FIBRITIN

Chain B:  88% 12%




#### • Molecule 1: FIBRITIN

Chain C:  81% 15% •



#### • Molecule 1: FIBRITIN

Chain D:  88% 8% •




#### • Molecule 1: FIBRITIN

Chain E:  77% 23%



#### • Molecule 1: FIBRITIN

Chain F:  81% 19%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	27.73 Å 28.50 Å 48.76 Å 77.25° 88.00° 69.45°	Depositor
Resolution (Å)	26.02 – 1.06 26.02 – 1.06	Depositor EDS
% Data completeness (in resolution range)	94.2 (26.02-1.06) 85.9 (26.02-1.06)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.23 (at 1.06 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.108 , 0.140 0.119 , 0.148	Depositor DCC
$R_{free}$ test set	1065 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	5.8	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, TH6, NA8, PRS

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 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	0.45	0/242	1.15	0/320
1	B	0.44	0/235	1.02	0/312
1	C	0.53	0/215	1.16	2/286 (0.7%)
1	D	0.49	0/221	2.01	8/294 (2.7%)
1	E	0.49	0/246	1.17	0/326
1	F	0.46	0/241	1.09	0/320
All	All	0.48	0/1400	1.30	10/1858 (0.5%)

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 outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8[A]	ARG	NE-CZ-NH1	15.45	128.02	120.30
1	D	8[B]	ARG	NE-CZ-NH1	15.45	128.02	120.30
1	D	8[A]	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	D	8[B]	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	C	16[A]	LYS	CD-CE-NZ	6.95	127.69	111.70
1	C	16[B]	LYS	CD-CE-NZ	6.95	127.69	111.70
1	D	15[A]	ARG	N-CA-CB	5.89	121.19	110.60
1	D	15[B]	ARG	N-CA-CB	5.89	121.19	110.60
1	D	8[A]	ARG	CG-CD-NE	5.63	123.62	111.80
1	D	8[B]	ARG	CG-CD-NE	5.63	123.62	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	19[A]	GLU	Peptide

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	278	281	287	9	0
1	B	253	261	263	4	0
1	C	257	255	252	8	0
1	D	244	246	247	2	0
1	E	269	267	268	12	0
1	F	282	280	281	7	0
2	A	76	0	0	5	0
2	B	91	0	0	2	1
2	C	76	0	0	2	0
2	D	62	0	0	1	1
2	E	72	0	0	0	0
2	F	70	0	0	5	0
All	All	2030	1590	1598	38	1

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 12.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26[B]:PHE:O	1:E:27[B]:LEU:C	1.72	1.16
1:E:26[B]:PHE:O	1:E:27[B]:LEU:O	1.65	1.14
1:D:8[A]:ARG:NH1	2:D:2020:HOH:O	1.80	1.12
1:E:8[B]:ARG:HG3	1:E:8[B]:ARG:HH11	1.27	0.98
1:E:8[B]:ARG:CG	1:E:8[B]:ARG:HH11	1.80	0.95
1:B:5[B]:GLU:OE2	2:B:2015:HOH:O	1.91	0.87
1:E:25[B]:THR:OG1	1:E:26[B]:PHE:CD1	2.33	0.82
1:E:8[B]:ARG:NH1	1:E:8[B]:ARG:HG3	1.89	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25[B]:THR:OG1	1:E:26[B]:PHE:CE1	2.48	0.67
2:A:2029:HOH:O	1:C:18[A]:PRS:HB3	1.94	0.65
1:A:11[B]:GLN:OE1	2:A:2052:HOH:O	2.14	0.65
1:B:5[A]:GLU:OE2	2:B:2015:HOH:O	2.16	0.60
1:C:19[A]:GLU:OE2	2:C:2061:HOH:O	2.17	0.59
1:C:25:THR:HG21	2:C:2039:HOH:O	2.03	0.58
1:A:8:ARG:NH1	1:C:18[A]:PRS:HB2	2.19	0.57
1:A:8:ARG:HH12	1:C:18[A]:PRS:HB2	1.71	0.56
1:C:18[A]:PRS:HD3	1:C:19[A]:GLU:HG3	1.90	0.54
1:F:8[B]:ARG:NH1	2:F:2030:HOH:O	2.40	0.53
1:C:18[B]:PRS:HB3	1:C:19[B]:GLU:HG3	1.93	0.51
1:E:8[B]:ARG:HG2	1:E:8[B]:ARG:HH11	1.71	0.50
1:F:8[B]:ARG:NH2	2:F:2030:HOH:O	2.44	0.50
1:A:16[B]:LYS:HD3	1:A:21:VAL:HG21	1.95	0.49
1:E:26[B]:PHE:O	1:E:27[B]:LEU:OXT	2.23	0.49
1:F:2[B]:NA8:C6	2:F:2006:HOH:O	2.62	0.48
1:A:16[B]:LYS:HE2	2:F:2064:HOH:O	2.14	0.47
1:F:23:LEU:O	1:F:24[B]:SER:C	2.54	0.46
1:A:16[B]:LYS:NZ	2:A:2060:HOH:O	1.92	0.45
1:E:22:LEU:HB2	1:E:25[A]:THR:HG23	1.98	0.45
1:E:22:LEU:HB2	1:E:25[B]:THR:HG23	2.00	0.44
1:A:9[B]:ASP:CB	2:A:2042:HOH:O	2.65	0.44
1:A:9[B]:ASP:OD2	1:A:13:TYR:OH	2.30	0.43
1:A:9[B]:ASP:HB3	2:A:2042:HOH:O	2.19	0.42
1:E:24:SER:O	1:E:25[B]:THR:C	2.58	0.41
1:B:3[B]:ILE:HG21	1:B:3[B]:ILE:HD13	1.72	0.41
1:B:16[A]:LYS:HE3	1:C:10:DAL:O	2.21	0.40
1:D:3:ILE:HD12	1:F:3:ILE:HG13	2.02	0.40
1:F:8[B]:ARG:CZ	2:F:2030:HOH:O	2.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2007:HOH:O	2:D:2060:HOH:O[1_645]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	25/26 (96%)	25 (100%)	0	0	100	100
1	B	24/26 (92%)	24 (100%)	0	0	100	100
1	C	22/26 (85%)	22 (100%)	0	0	100	100
1	D	23/26 (88%)	22 (96%)	1 (4%)	0	100	100
1	E	25/26 (96%)	23 (92%)	2 (8%)	0	100	100
1	F	25/26 (96%)	25 (100%)	0	0	100	100
All	All	144/156 (92%)	141 (98%)	3 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	26/20 (130%)	26 (100%)	0	100	100
1	B	25/20 (125%)	25 (100%)	0	100	100
1	C	23/20 (115%)	23 (100%)	0	100	100
1	D	23/20 (115%)	23 (100%)	0	100	100
1	E	26/20 (130%)	26 (100%)	0	100	100
1	F	26/20 (130%)	26 (100%)	0	100	100
All	All	149/120 (124%)	149 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

29 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	NA8	C	2	1	15,16,17	0.74	0	18,21,23	0.89	0
1	NA8	D	2	1	15,16,17	0.59	0	18,21,23	0.51	0
1	TH6	D	17	1	5,7,8	0.54	0	5,8,10	1.86	2 (40%)
1	NA8	E	2	1	15,16,17	0.89	0	18,21,23	0.85	1 (5%)
1	NA8	B	2	1	15,16,17	0.82	0	18,21,23	1.14	1 (5%)
1	TH6	C	17[A]	1	5,7,8	0.49	0	5,8,10	2.04	2 (40%)
1	NA8	F	2[A]	-	15,16,17	0.96	0	18,21,23	1.07	1 (5%)
1	TH6	B	17	1	5,7,8	0.52	0	5,8,10	1.72	1 (20%)
1	TH6	C	17[B]	1	5,7,8	0.39	0	5,8,10	1.50	1 (20%)
1	NA8	F	2[B]	-	15,16,17	1.03	0	18,21,23	1.70	7 (38%)
1	TH6	F	17	1	5,7,8	0.49	0	5,8,10	2.25	2 (40%)
1	PRS	F	18	1	5,7,8	2.23	1 (20%)	3,8,10	2.74	1 (33%)
1	PRS	B	18	1	5,7,8	0.75	0	3,8,10	1.20	0
1	PRS	C	18[B]	1	5,7,8	1.42	1 (20%)	3,8,10	1.59	1 (33%)
1	PRS	A	18	1	5,7,8	0.78	0	3,8,10	1.29	0
1	NA8	A	2[B]	-	15,16,17	0.92	0	18,21,23	1.11	2 (11%)
1	PRS	C	18[A]	1	5,7,8	1.66	1 (20%)	3,8,10	6.94	2 (66%)
1	NA8	A	2[A]	-	15,16,17	1.04	0	18,21,23	1.21	1 (5%)
1	PRS	E	18	1	5,7,8	0.82	0	3,8,10	1.57	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TH6	E	17	1	5,7,8	0.64	0	5,8,10	2.17	2 (40%)
1	PRS	D	18	1	5,7,8	0.59	0	3,8,10	1.21	0
1	TH6	A	17	1	5,7,8	0.52	0	5,8,10	2.27	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NA8	C	2	1	-	0/5/6/8	0/2/2/2
1	NA8	D	2	1	-	0/5/6/8	0/2/2/2
1	TH6	D	17	1	-	4/7/8/10	-
1	NA8	E	2	1	-	0/5/6/8	0/2/2/2
1	NA8	B	2	1	-	0/5/6/8	0/2/2/2
1	TH6	C	17[A]	1	-	4/7/8/10	-
1	NA8	F	2[A]	-	-	0/5/6/8	0/2/2/2
1	TH6	B	17	1	-	4/7/8/10	-
1	TH6	C	17[B]	1	-	4/7/8/10	-
1	NA8	F	2[B]	-	-	0/5/6/8	0/2/2/2
1	TH6	F	17	1	-	3/7/8/10	-
1	PRS	F	18	1	-	0/0/9/11	0/1/1/1
1	PRS	B	18	1	-	0/0/9/11	0/1/1/1
1	PRS	C	18[B]	1	-	0/0/9/11	0/1/1/1
1	PRS	A	18	1	-	0/0/9/11	0/1/1/1
1	NA8	A	2[B]	-	-	0/5/6/8	0/2/2/2
1	PRS	C	18[A]	1	-	0/0/9/11	0/1/1/1
1	NA8	A	2[A]	-	-	0/5/6/8	0/2/2/2
1	PRS	E	18	1	-	0/0/9/11	0/1/1/1
1	TH6	E	17	1	-	4/7/8/10	-
1	PRS	D	18	1	-	0/0/9/11	0/1/1/1
1	TH6	A	17	1	-	4/7/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	18	PRS	CD-SG	-4.41	1.74	1.81
1	C	18[A]	PRS	CB-SG	-3.05	1.70	1.81
1	C	18[B]	PRS	CB-SG	-2.53	1.72	1.81

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18[A]	PRS	SG-CD-N	-10.40	94.98	105.72
1	C	18[A]	PRS	O-C-CA	-5.80	109.57	124.78
1	F	18	PRS	SG-CD-N	4.53	110.40	105.72
1	E	17	TH6	CB-CA-C	3.93	118.05	111.77
1	A	17	TH6	CB-CA-C	3.88	117.97	111.77
1	F	17	TH6	OG1-CG-CB	-3.80	102.80	111.07
1	C	17[A]	TH6	O-C-CA	-3.37	115.96	124.78
1	B	17	TH6	CB-CA-C	3.07	116.68	111.77
1	C	17[B]	TH6	CB-CA-C	3.06	116.66	111.77
1	D	17	TH6	CB-CA-C	3.02	116.59	111.77
1	A	2[A]	NA8	C3-C4-C4A	2.93	125.36	120.82
1	F	2[B]	NA8	C9-C10-C11	-2.89	106.06	111.47
1	C	17[A]	TH6	CB-CA-C	2.86	116.33	111.77
1	B	2	NA8	C1-C8A-C4A	2.68	122.78	118.96
1	F	2[B]	NA8	C3-C4-C4A	2.67	124.95	120.82
1	F	2[B]	NA8	C2-C9-C10	-2.57	108.90	114.10
1	F	2[B]	NA8	C5-C4A-C8A	2.47	123.35	118.92
1	A	17	TH6	OB1-CB-CG	2.45	114.89	109.14
1	F	2[B]	NA8	C4-C3-C2	-2.44	116.11	121.14
1	C	18[B]	PRS	SG-CD-N	2.44	108.24	105.72
1	D	17	TH6	O-C-CA	-2.39	118.50	124.78
1	E	18	PRS	SG-CD-N	-2.16	103.49	105.72
1	F	17	TH6	OB1-CB-CG	2.14	114.17	109.14
1	A	2[B]	NA8	C9-C2-C3	2.14	125.14	120.91
1	F	2[B]	NA8	C6-C7-C8	2.12	123.42	120.44
1	E	2	NA8	C1-C8A-C4A	2.11	121.97	118.96
1	A	2[B]	NA8	C9-C10-C11	-2.11	107.51	111.47
1	E	17	TH6	O-C-CA	-2.10	119.26	124.78
1	F	2[B]	NA8	C7-C6-C5	-2.07	117.54	120.44
1	F	2[A]	NA8	C3-C4-C4A	-2.04	117.66	120.82

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	17	TH6	N-CA-CB-CG
1	C	17[A]	TH6	N-CA-CB-CG
1	B	17	TH6	N-CA-CB-CG
1	C	17[B]	TH6	N-CA-CB-CG
1	F	17	TH6	N-CA-CB-CG
1	E	17	TH6	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	17	TH6	N-CA-CB-CG
1	D	17	TH6	C-CA-CB-OB1
1	C	17[A]	TH6	C-CA-CB-OB1
1	B	17	TH6	C-CA-CB-OB1
1	C	17[B]	TH6	C-CA-CB-OB1
1	E	17	TH6	C-CA-CB-OB1
1	A	17	TH6	C-CA-CB-OB1
1	F	17	TH6	C-CA-CB-OB1
1	D	17	TH6	C-CA-CB-CG
1	C	17[A]	TH6	C-CA-CB-CG
1	B	17	TH6	C-CA-CB-CG
1	C	17[B]	TH6	C-CA-CB-CG
1	E	17	TH6	C-CA-CB-CG
1	A	17	TH6	C-CA-CB-CG
1	D	17	TH6	O-C-CA-CB
1	C	17[A]	TH6	O-C-CA-CB
1	B	17	TH6	O-C-CA-CB
1	C	17[B]	TH6	O-C-CA-CB
1	F	17	TH6	O-C-CA-CB
1	E	17	TH6	O-C-CA-CB
1	A	17	TH6	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	2[B]	NA8	2	0
1	C	18[B]	PRS	1	0
1	C	18[A]	PRS	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	22/26 (84%)	-0.74	0 100 100	4, 5, 7, 8	1 (4%)
1	B	22/26 (84%)	-0.81	0 100 100	4, 5, 8, 9	0
1	C	22/26 (84%)	-0.83	0 100 100	3, 5, 9, 12	0
1	D	22/26 (84%)	-0.87	0 100 100	4, 6, 10, 15	0
1	E	22/26 (84%)	-0.30	0 100 100	5, 8, 11, 14	0
1	F	22/26 (84%)	-0.72	0 100 100	5, 6, 11, 13	0
All	All	132/156 (84%)	-0.71	0 100 100	3, 6, 11, 15	1 (0%)

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	NA8	C	2	15/16	0.97	0.09	7,9,12,13	0
1	NA8	E	2	15/16	0.97	0.06	6,8,8,8	0
1	NA8	B	2	15/16	0.97	0.07	7,11,18,19	0
1	DAL	E	10	5/6	0.97	0.07	7,7,8,8	0
1	TH6	C	17[A]	8/9	0.98	0.08	6,6,8,12	14
1	NA8	F	2[A]	15/16	0.98	0.06	8,10,14,15	22
1	TH6	C	17[B]	8/9	0.98	0.08	4,5,6,7	14
1	NA8	F	2[B]	15/16	0.98	0.06	4,7,9,12	22
1	TH6	F	17	8/9	0.98	0.06	7,10,19,20	0
1	NA8	A	2[B]	15/16	0.98	0.07	5,6,9,10	25
1	DAL	A	10[A]	5/6	0.98	0.07	5,8,10,14	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	DAL	A	10[B]	5/6	0.98	0.07	9,10,13,15	10
1	NA8	A	2[A]	15/16	0.98	0.07	6,7,9,9	25
1	DAL	F	10	5/6	0.99	0.04	5,6,6,6	0
1	PRS	C	18[A]	7/8	0.99	0.06	3,8,9,10	11
1	PRS	E	18	7/8	0.99	0.04	6,8,10,13	0
1	DAL	B	10	5/6	0.99	0.05	3,4,5,5	0
1	PRS	C	18[B]	7/8	0.99	0.06	3,5,8,9	11
1	PRS	F	18	7/8	0.99	0.04	7,8,10,12	0
1	DAL	D	10	5/6	0.99	0.05	6,6,7,7	0
1	NA8	D	2	15/16	1.00	0.04	3,4,4,4	0
1	TH6	B	17	8/9	1.00	0.03	3,4,4,5	0
1	PRS	D	18	7/8	1.00	0.02	4,5,6,8	0
1	TH6	E	17	8/9	1.00	0.04	5,5,7,8	0
1	PRS	B	18	7/8	1.00	0.04	4,5,7,8	0
1	TH6	A	17	8/9	1.00	0.04	3,4,5,5	0
1	TH6	D	17	8/9	1.00	0.03	4,5,5,6	0
1	DAL	C	10	5/6	1.00	0.03	3,3,4,5	0
1	PRS	A	18	7/8	1.00	0.03	4,5,6,7	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.