



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7SFA / pdb_00007sfa
Title : Branchiostoma floridae fluorescent protein LanFP10A2
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Deposited on : 2021-10-03
Resolution : 1.65 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

A user guide is available at

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

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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

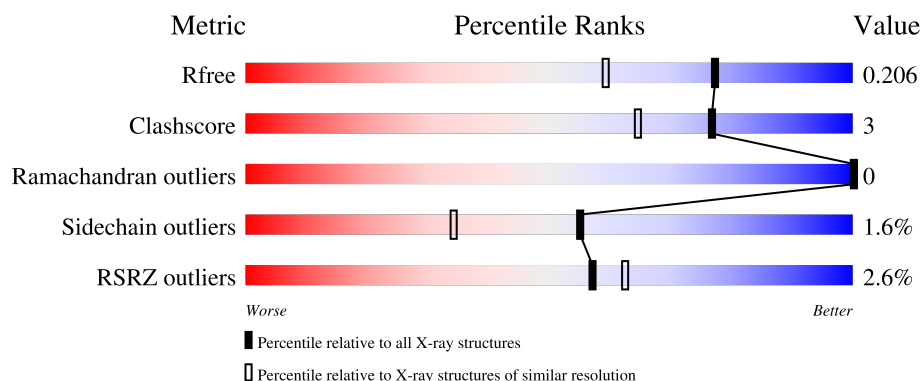
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	236	2% 84% 7% 8%
1	B	236	4% 85% 8% 6%
1	C	236	2% 85% 7% 8%
1	D	236	2% 84% 7% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7834 atoms, of which 0 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 Fluorescent protein lanFP10A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	6	0
			1785	1140	297	337	11			
1	B	222	Total	C	N	O	S	0	6	0
			1825	1163	308	343	11			
1	C	217	Total	C	N	O	S	0	4	0
			1772	1132	295	334	11			
1	D	218	Total	C	N	O	S	0	6	0
			1792	1142	299	340	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	163	Total	O	0	0
			163	163		
2	B	178	Total	O	0	0
			178	178		
2	C	175	Total	O	0	0
			175	175		
2	D	144	Total	O	0	0
			144	144		

- Molecule 1: Fluorescent protein lanFP10A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.24Å 96.22Å 158.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.79 – 1.65 27.79 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.9 (27.79-1.65) 97.9 (27.79-1.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.165 , 0.197 0.177 , 0.206	Depositor DCC
R_{free} test set	1096 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7834	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: JBY

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	1.01	3/1814 (0.2%)	1.02	2/2449 (0.1%)
1	B	1.03	3/1856 (0.2%)	1.04	1/2504 (0.0%)
1	C	1.03	1/1801 (0.1%)	1.03	1/2433 (0.0%)
1	D	1.01	2/1821 (0.1%)	1.04	1/2460 (0.0%)
All	All	1.02	9/7292 (0.1%)	1.03	5/9846 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	HIS	CE1-NE2	8.02	1.40	1.32
1	D	110	HIS	CE1-NE2	5.96	1.38	1.32
1	D	110	HIS	CG-ND1	5.44	1.44	1.38
1	A	145	MET	C-O	-5.32	1.17	1.24
1	C	96	HIS	CE1-NE2	5.28	1.37	1.32
1	B	65	HIS	CE1-NE2	5.25	1.37	1.32
1	B	175	ARG	C-O	-5.21	1.17	1.23
1	B	139	THR	N-CA	5.13	1.52	1.46
1	A	52	ASN	N-CA	5.02	1.55	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	VAL	O-C-N	-7.22	115.80	120.42
1	A	157	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	34	GLU	CB-CG-CD	5.88	122.59	112.60
1	A	52	ASN	CA-CB-CG	5.50	118.10	112.60
1	C	189	PRO	CB-CA-C	5.13	118.08	111.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	232	SER	Mainchain

5.2 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 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	1785	0	1698	8	0
1	B	1825	0	1735	12	0
1	C	1772	0	1686	6	0
1	D	1792	0	1700	15	0
2	A	163	0	0	2	0
2	B	178	0	0	3	0
2	C	175	0	0	4	0
2	D	144	0	0	2	0
All	All	7834	0	6819	41	0

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 3.

All (41) 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:B:48:LEU:HD13	1:B:215:LEU:HD11	1.53	0.91
1:B:233:HIS:O	1:B:234:HIS:HB2	1.71	0.87
1:A:98:THR:HG21	2:C:439:HOH:O	1.86	0.75
1:A:33:GLY:HA3	1:A:48:LEU:HD23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181[B]:ARG:NH2	2:C:301:HOH:O	2.27	0.67
1:B:48:LEU:CD1	1:B:215:LEU:HD11	2.26	0.64
1:B:48:LEU:HD13	1:B:215:LEU:CD1	2.30	0.58
1:A:45[A]:GLU:HG3	2:A:338:HOH:O	2.04	0.57
1:B:215:LEU:HD12	1:B:215:LEU:C	2.31	0.55
1:A:16:HIS:HE1	2:A:324:HOH:O	1.93	0.52
1:B:174:LYS:HE2	2:B:377:HOH:O	2.12	0.50
1:D:215:LEU:C	1:D:215:LEU:HD12	2.38	0.49
1:D:54:PRO:HB3	1:D:212:LYS:HB3	1.96	0.47
1:C:16:HIS:HE1	2:C:342:HOH:O	1.97	0.47
1:B:54:PRO:HB3	1:B:212:LYS:HB3	1.97	0.46
1:A:18:LEU:HD11	1:A:124:PHE:CD2	2.51	0.46
1:D:16:HIS:HE1	2:D:308:HOH:O	1.98	0.46
1:C:54:PRO:HB3	1:C:212:LYS:HB3	1.97	0.45
1:B:45[B]:GLU:HG2	1:B:218:LYS:HG2	1.99	0.45
1:B:52:ASN:ND2	2:B:305:HOH:O	2.50	0.45
1:D:181[A]:ARG:NH2	1:D:181[A]:ARG:HG2	2.32	0.45
1:A:207[B]:GLU:OE2	1:A:209:GLN:NE2	2.50	0.44
1:A:181[B]:ARG:HG2	1:A:181[B]:ARG:HH21	1.84	0.43
1:D:181[A]:ARG:HG2	1:D:181[A]:ARG:HH21	1.83	0.43
1:B:16:HIS:HE1	2:B:320:HOH:O	2.01	0.43
1:D:42:GLY:HA2	1:D:73:TYR:O	2.18	0.43
1:C:56:LYS:HD3	2:C:473:HOH:O	2.18	0.42
1:B:67:JBY:N2	1:B:219:GLU:OE2	2.53	0.42
1:D:81:SER:HB2	1:D:82:PRO:HD2	2.02	0.42
1:D:110:HIS:HE1	2:D:339:HOH:O	2.03	0.41
1:D:16:HIS:CD2	1:D:73:TYR:OH	2.73	0.41
1:D:209:GLN:HE21	1:D:209:GLN:HB2	1.51	0.41
1:C:35:GLY:HA3	1:C:45:GLU:O	2.21	0.41
1:D:67:JBY:N2	1:D:219:GLU:OE2	2.54	0.41
1:B:46:LEU:HD23	1:B:48:LEU:HD11	2.03	0.41
1:C:33:GLY:HA3	1:C:48:LEU:HD23	2.02	0.41
1:D:61:ILE:HD12	1:D:61:ILE:HA	1.87	0.41
1:A:16:HIS:CD2	1:A:73:TYR:OH	2.73	0.41
1:D:12:LEU:HB3	1:D:13:PRO:HD2	2.04	0.40
1:D:62:LEU:O	1:D:63:VAL:C	2.64	0.40
1:D:13:PRO:HB3	1:D:120:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

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	217/236 (92%)	215 (99%)	2 (1%)	0	100	100
1	B	223/236 (94%)	222 (100%)	1 (0%)	0	100	100
1	C	216/236 (92%)	214 (99%)	2 (1%)	0	100	100
1	D	219/236 (93%)	218 (100%)	1 (0%)	0	100	100
All	All	875/944 (93%)	869 (99%)	6 (1%)	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	193/203 (95%)	190 (98%)	3 (2%)	55	34
1	B	197/203 (97%)	194 (98%)	3 (2%)	57	37
1	C	191/203 (94%)	187 (98%)	4 (2%)	47	24
1	D	194/203 (96%)	192 (99%)	2 (1%)	68	52
All	All	775/812 (95%)	763 (98%)	12 (2%)	55	37

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	145	MET

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Mol	Chain	Res	Type
1	A	196	GLN
1	B	145	MET
1	B	182	GLU
1	B	234	HIS
1	C	34	GLU
1	C	145	MET
1	C	196	GLN
1	C	197	LYS
1	D	145	MET
1	D	209	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	94	GLN
1	A	110	HIS
1	A	125	GLN
1	A	140	ASN
1	B	16	HIS
1	B	52	ASN
1	B	110	HIS
1	B	125	GLN
1	B	210	HIS
1	C	16	HIS
1	C	94	GLN
1	C	125	GLN
1	C	177	GLN
1	C	196	GLN
1	C	209	GLN
1	D	16	HIS
1	D	110	HIS
1	D	125	GLN
1	D	209	GLN
1	D	210	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	JBV	A	67	1	20,21,22	3.26	3 (15%)	26,29,31	2.86	12 (46%)
1	JBV	C	67	1	20,21,22	3.60	7 (35%)	26,29,31	3.33	12 (46%)
1	JBV	D	67	1	20,21,22	3.73	3 (15%)	26,29,31	2.97	13 (50%)
1	JBV	B	67	1	20,21,22	3.30	7 (35%)	26,29,31	3.47	11 (42%)

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	JBV	A	67	1	-	1/9/28/30	0/2/2/2
1	JBV	C	67	1	-	1/9/28/30	0/2/2/2
1	JBV	D	67	1	-	1/9/28/30	0/2/2/2
1	JBV	B	67	1	-	1/9/28/30	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	67	JBV	CB2-CA2	13.84	1.48	1.35
1	A	67	JBV	CB2-CA2	12.76	1.47	1.35
1	C	67	JBV	CB2-CA2	12.62	1.47	1.35
1	B	67	JBV	CB2-CA2	11.08	1.45	1.35
1	D	67	JBV	CA2-C2	-7.64	1.40	1.48
1	C	67	JBV	CA2-C2	-6.73	1.41	1.48
1	B	67	JBV	CA2-C2	-6.56	1.41	1.48
1	C	67	JBV	C1-N2	4.68	1.40	1.32
1	A	67	JBV	O2-C2	4.27	1.31	1.23
1	B	67	JBV	CA1-C1	3.60	1.53	1.49
1	D	67	JBV	OH-CZ	-3.43	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	JBV	OH-CZ	-3.33	1.29	1.37
1	B	67	JBV	O2-C2	2.82	1.28	1.23
1	C	67	JBV	CD1-CE1	2.70	1.43	1.38
1	C	67	JBV	O2-C2	2.64	1.28	1.23
1	B	67	JBV	C1-N2	2.61	1.37	1.32
1	C	67	JBV	OH-CZ	-2.44	1.31	1.37
1	C	67	JBV	CA2-N2	-2.39	1.33	1.38
1	B	67	JBV	OH-CZ	-2.30	1.31	1.37
1	B	67	JBV	C1-N3	2.10	1.41	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	JBV	CA2-C2-N3	12.80	109.34	103.36
1	B	67	JBV	CA2-C2-N3	11.90	108.92	103.36
1	D	67	JBV	CA2-C2-N3	8.38	107.27	103.36
1	A	67	JBV	O2-C2-CA2	-7.08	126.50	131.02
1	A	67	JBV	CA2-C2-N3	7.04	106.65	103.36
1	B	67	JBV	O2-C2-CA2	-5.26	127.66	131.02
1	B	67	JBV	CB2-CA2-C2	-5.05	116.24	122.36
1	D	67	JBV	CB3-CA3-N3	-4.60	104.77	111.16
1	D	67	JBV	C1-CA1-N1	-4.47	102.95	112.85
1	D	67	JBV	CB2-CA2-C2	-4.44	116.97	122.36
1	B	67	JBV	CB3-CA3-N3	-4.43	105.01	111.16
1	D	67	JBV	O2-C2-CA2	-4.43	128.19	131.02
1	B	67	JBV	CB2-CA2-N2	4.31	134.61	128.76
1	C	67	JBV	N3-C1-N2	-4.30	110.79	113.64
1	C	67	JBV	CA3-N3-C1	4.09	134.03	124.29
1	A	67	JBV	C1-CA1-N1	-4.05	103.89	112.85
1	A	67	JBV	CB3-CA3-N3	-3.99	105.62	111.16
1	B	67	JBV	C1-CA1-N1	-3.97	104.07	112.85
1	D	67	JBV	CB2-CA2-N2	3.64	133.70	128.76
1	D	67	JBV	CA3-N3-C1	3.62	132.89	124.29
1	B	67	JBV	CD1-CG2-CD2	3.58	122.96	117.65
1	B	67	JBV	CA3-N3-C1	3.55	132.73	124.29
1	A	67	JBV	CA3-N3-C1	3.49	132.59	124.29
1	C	67	JBV	CB2-CA2-C2	-3.45	118.18	122.36
1	C	67	JBV	C1-CA1-N1	-3.26	105.64	112.85
1	C	67	JBV	CB2-CA2-N2	3.25	133.18	128.76
1	A	67	JBV	CE1-CD1-CG2	-3.16	117.14	121.22
1	B	67	JBV	CE2-CD2-CG2	-3.12	117.20	121.22
1	D	67	JBV	CE1-CD1-CG2	-3.06	117.27	121.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	JBV	CD1-CG2-CD2	3.05	122.18	117.65
1	C	67	JBV	O2-C2-CA2	-3.00	129.11	131.02
1	A	67	JBV	CB2-CA2-N2	2.98	132.81	128.76
1	B	67	JBV	N3-C1-N2	-2.68	111.86	113.64
1	B	67	JBV	C2-N3-C1	-2.63	105.15	108.31
1	C	67	JBV	CE2-CD2-CG2	-2.55	117.93	121.22
1	A	67	JBV	CB2-CA2-C2	-2.54	119.27	122.36
1	A	67	JBV	N3-C1-N2	-2.53	111.96	113.64
1	D	67	JBV	N3-C1-N2	-2.52	111.97	113.64
1	C	67	JBV	C2-N3-C1	-2.51	105.29	108.31
1	A	67	JBV	CD1-CG2-CD2	2.49	121.34	117.65
1	A	67	JBV	CD2-CE2-CZ	-2.46	117.27	119.88
1	C	67	JBV	CD1-CG2-CD2	2.46	121.30	117.65
1	C	67	JBV	CD2-CE2-CZ	2.44	122.46	119.88
1	A	67	JBV	CA3-N3-C2	-2.43	118.91	123.90
1	D	67	JBV	CA3-N3-C2	-2.11	119.55	123.90
1	D	67	JBV	CA1-C1-N2	-2.11	121.45	124.28
1	D	67	JBV	CA1-C1-N3	2.11	126.28	122.98
1	C	67	JBV	CG2-CB2-CA2	-2.06	127.42	129.87

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	67	JBV	O3-C3-CA3-CB3
1	B	67	JBV	O3-C3-CA3-CB3
1	C	67	JBV	O3-C3-CA3-CB3
1	D	67	JBV	O3-C3-CA3-CB3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	67	JBV	1	0
1	B	67	JBV	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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, 95th 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 ²)	Q<0.9
1	A	215/236 (91%)	-0.24	5 (2%) 61 66	6, 15, 31, 69	6 (2%)
1	B	221/236 (93%)	-0.12	9 (4%) 41 45	7, 15, 32, 55	6 (2%)
1	C	216/236 (91%)	-0.22	5 (2%) 61 66	6, 16, 32, 48	4 (1%)
1	D	217/236 (91%)	-0.07	4 (1%) 67 73	6, 18, 33, 46	6 (2%)
All	All	869/944 (92%)	-0.17	23 (2%) 57 62	6, 16, 32, 69	22 (2%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	HIS	6.7
1	B	230	GLY	5.3
1	B	233	HIS	4.9
1	B	231	GLY	4.0
1	B	229	SER	3.8
1	C	10	ALA	3.8
1	A	213	THR	3.8
1	B	232	SER	3.6
1	C	192	ALA	3.5
1	A	212	LYS	3.1
1	D	78[A]	ASP	2.9
1	A	211	SER	2.8
1	C	196	GLN	2.7
1	B	12	LEU	2.7
1	A	11	SER	2.7
1	D	10	ALA	2.6
1	B	11	SER	2.5
1	A	52	ASN	2.3
1	D	173	GLY	2.3
1	C	173	GLY	2.2
1	C	193	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	171	THR	2.1
1	B	213	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	JBV	C	67	20/21	0.96	0.06	11,13,20,22	0
1	JBV	D	67	20/21	0.96	0.06	13,15,18,19	0
1	JBV	A	67	20/21	0.97	0.05	11,12,19,20	0
1	JBV	B	67	20/21	0.97	0.05	11,12,18,19	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.