



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2023 – 07:59 PM EST

PDB ID : 3FSE
Title : Crystal structure of a two-domain protein containing dj-1/thij/pfpi-like and ferritin-like domains (ava_4496) from anabaena variabilis atcc 29413 at 1.90 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2009-01-09
Resolution : 1.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

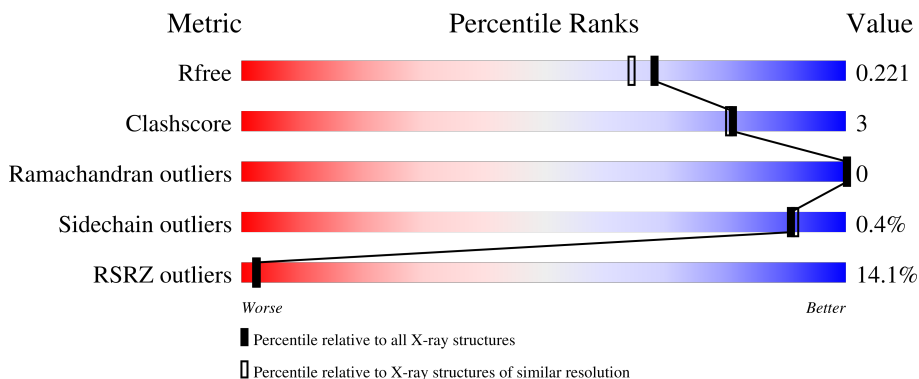
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	365	
1	B	365	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5755 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 two-domain protein containing DJ-1/ThiJ/PfpI-like and ferritin-like domains.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	337	2595	1637	444	502	3	9	0	10	0
1	B	349	2695	1701	456	525	4	9	0	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q3M4J2
B	0	GLY	-	expression tag	UNP Q3M4J2

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	4	2	2	0	0

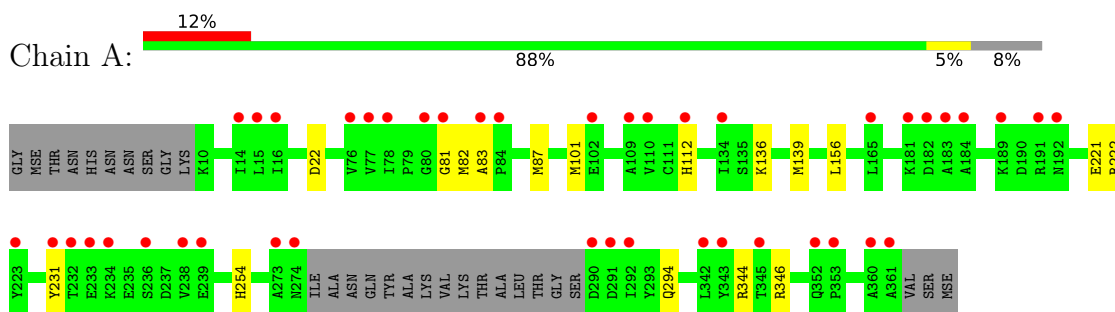
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	213	Total 215	O 215	0	2
3	B	243	Total 246	O 246	0	3

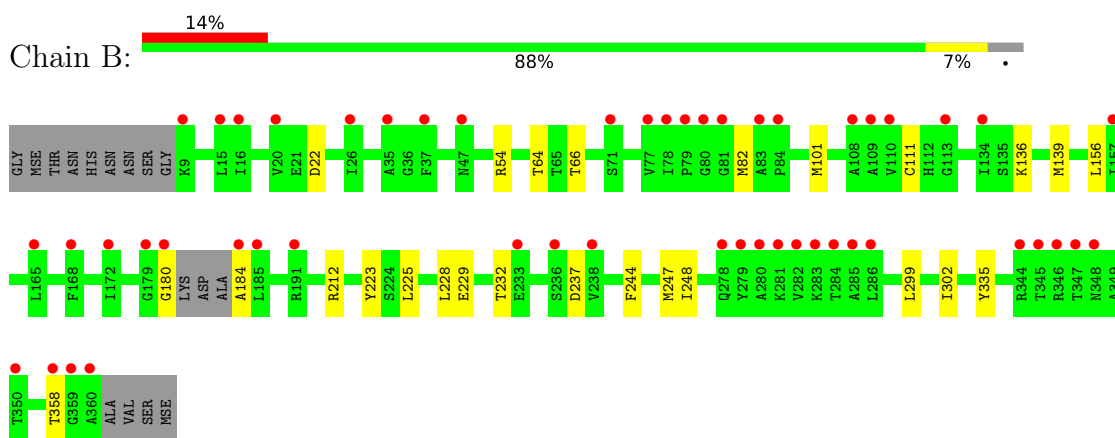
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: two-domain protein containing DJ-1/ThiJ/PfpI-like and ferritin-like domains



- Molecule 1: two-domain protein containing DJ-1/ThiJ/PfpI-like and ferritin-like domains



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.36Å 39.69Å 123.06Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	29.98 – 1.90 29.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.98-1.90) 99.5 (29.97-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.176 , 0.219 0.184 , 0.221	Depositor DCC
R_{free} test set	2676 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtrriage
Anisotropy	0.169	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5755	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSX, EDO

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	0.70	0/2645	0.81	4/3560 (0.1%)
1	B	0.69	0/2737	0.84	3/3684 (0.1%)
All	All	0.70	0/5382	0.83	7/7244 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	346	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	54	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	344	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	237	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	222[A]	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	222[B]	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2595	0	2593	11	0
1	B	2695	0	2695	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	6	0	0
3	A	215	0	0	0	0
3	B	246	0	0	0	0
All	All	5755	0	5294	27	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 (27) 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:A:82[B]:MSE:SE	1:B:82[B]:MSE:SE	2.77	1.02
1:A:136:LYS:HA	1:A:139:MSE:HE3	1.66	0.77
1:A:82[B]:MSE:SE	1:B:82[B]:MSE:CE	2.93	0.66
1:B:136:LYS:HA	1:B:139:MSE:HE3	1.80	0.64
1:B:228:LEU:O	1:B:232[B]:THR:HG23	2.05	0.57
1:A:101:MSE:HE1	1:A:156:LEU:HD13	1.89	0.55
1:B:232[B]:THR:HG22	1:B:244:PHE:HB2	1.88	0.55
1:B:64:THR:HG22	1:B:66:THR:H	1.74	0.53
1:B:180:GLY:C	1:B:184:ALA:HB3	2.31	0.51
1:A:82[B]:MSE:SE	1:B:82[B]:MSE:HE3	2.60	0.50
1:A:82[A]:MSE:SE	1:B:82[A]:MSE:SE	3.31	0.49
1:B:101:MSE:HE1	1:B:156:LEU:HD13	1.94	0.48
1:A:83:ALA:HB1	1:A:87:MSE:HE3	1.97	0.46
1:B:299:LEU:O	1:B:302:ILE:HG22	2.16	0.45
1:A:81:GLY:C	1:A:82[A]:MSE:HE2	2.36	0.45
1:B:223:TYR:CZ	1:B:358:THR:HG23	2.51	0.45
1:A:221:GLU:OE1	1:A:254:HIS:ND1	2.42	0.44
1:B:232[B]:THR:HG22	1:B:244:PHE:CB	2.47	0.43
1:B:64:THR:CG2	1:B:66:THR:H	2.31	0.43
1:A:82[A]:MSE:HE1	1:A:112:HIS:CE1	2.55	0.42
1:B:229:GLU:HA	1:B:232[A]:THR:HG22	2.02	0.42
1:B:247:MSE:HE3	1:B:302:ILE:HD12	2.01	0.42
1:A:231:TYR:HA	1:A:294:GLN:NE2	2.35	0.41
1:B:225:LEU:HD11	1:B:248:ILE:HG23	2.02	0.41
1:B:302:ILE:HD11	1:B:335:TYR:HB2	2.03	0.41
1:B:223:TYR:CZ	1:B:358:THR:CG2	3.04	0.41
1:B:225:LEU:CD1	1:B:248:ILE:HG23	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 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	342/365 (94%)	339 (99%)	3 (1%)	0	100	100
1	B	352/365 (96%)	348 (99%)	4 (1%)	0	100	100
All	All	694/730 (95%)	687 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 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 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	264/282 (94%)	263 (100%)	1 (0%)	91	91
1	B	275/282 (98%)	274 (100%)	1 (0%)	91	91
All	All	539/564 (96%)	537 (100%)	2 (0%)	91	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	B	22	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN

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Mol	Chain	Res	Type
1	B	303	GLN
1	B	337	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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	CSX	B	111[B]	-	3,6,7	0.50	0	1,6,8	1.07	0
1	CSX	A	111	1	3,6,7	0.64	0	1,6,8	0.57	0
1	CSX	B	111[A]	-	3,6,7	0.69	0	1,6,8	2.60	1 (100%)

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	CSX	B	111[B]	-	-	0/1/5/7	-
1	CSX	A	111	1	-	0/1/5/7	-
1	CSX	B	111[A]	-	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	111[A]	CSX	CA-CB-SG	2.60	119.03	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
2	EDO	B	365	-	3,3,3	0.58	0	2,2,2	0.24	0

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
2	EDO	B	365	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	365	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	328/365 (89%)	0.88	43 (13%) 3 3	25, 41, 58, 70	0
1	B	340/365 (93%)	0.99	51 (15%) 2 2	34, 41, 57, 68	0
All	All	668/730 (91%)	0.94	94 (14%) 2 2	25, 41, 58, 70	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	ASN	8.9
1	A	290	ASP	8.8
1	B	285	ALA	7.7
1	B	238	VAL	6.2
1	B	184	ALA	6.1
1	B	286	LEU	6.1
1	A	238	VAL	6.0
1	A	273	ALA	5.5
1	B	236	SER	5.4
1	B	280	ALA	5.3
1	B	9	LYS	5.3
1	A	361	ALA	5.2
1	B	284	THR	5.0
1	A	183	ALA	4.9
1	A	236	SER	4.8
1	B	110	VAL	4.8
1	A	77	VAL	4.3
1	B	78	ILE	4.3
1	A	184	ALA	4.2
1	B	77	VAL	4.2
1	A	291	ASP	4.1
1	A	181	LYS	4.0
1	B	360	ALA	3.9
1	A	182	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	347	THR	3.8
1	B	185	LEU	3.8
1	A	233	GLU	3.8
1	B	113	GLY	3.5
1	A	15	LEU	3.5
1	B	83	ALA	3.5
1	A	110	VAL	3.5
1	B	20	VAL	3.5
1	B	283	LYS	3.4
1	B	282	VAL	3.4
1	A	80	GLY	3.3
1	B	80	GLY	3.3
1	A	292	ILE	3.3
1	B	281	LYS	3.3
1	A	232	THR	3.2
1	B	79	PRO	3.2
1	B	179	GLY	3.2
1	A	239	GLU	3.2
1	B	165	LEU	3.1
1	A	353	PRO	3.1
1	A	191	ARG	3.1
1	A	274	ASN	3.1
1	A	189	LYS	3.1
1	A	352	GLN	3.1
1	B	15	LEU	3.0
1	B	350	THR	3.0
1	A	109	ALA	3.0
1	B	108	ALA	3.0
1	B	358	THR	2.9
1	A	78	ILE	2.9
1	A	223	TYR	2.9
1	A	234	LYS	2.9
1	B	233	GLU	2.9
1	A	342	LEU	2.9
1	B	109	ALA	2.8
1	B	345	THR	2.7
1	B	47	ASN	2.7
1	B	37	PHE	2.6
1	B	279	TYR	2.6
1	B	278	GLN	2.6
1	A	360	ALA	2.6
1	B	168	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	14	ILE	2.4
1	A	134	ILE	2.4
1	B	16	ILE	2.4
1	A	81	GLY	2.4
1	A	343	TYR	2.4
1	A	83	ALA	2.4
1	B	157	ILE	2.4
1	A	231	TYR	2.3
1	B	180	GLY	2.3
1	B	84	PRO	2.3
1	B	71	SER	2.3
1	A	102	GLU	2.3
1	B	346	ARG	2.2
1	B	81	GLY	2.2
1	B	134	ILE	2.2
1	B	359	GLY	2.2
1	B	191	ARG	2.2
1	A	16	ILE	2.2
1	B	26	ILE	2.2
1	A	76	VAL	2.2
1	B	172	ILE	2.1
1	A	192	ASN	2.1
1	B	35	ALA	2.1
1	A	112	HIS	2.1
1	B	344[A]	ARG	2.1
1	A	84	PRO	2.1
1	A	165	LEU	2.0
1	A	345	THR	2.0

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	CSX	A	111	7/8	0.93	0.18	39,40,53,56	0
1	CSX	B	111[A]	7/8	0.94	0.25	37,39,45,49	4
1	CSX	B	111[B]	7/8	0.94	0.25	37,39,42,50	4

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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
2	EDO	B	365	4/4	0.80	0.23	64,66,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.