



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:57 AM UTC

PDB ID : 1VSJ / pdb_00001vsj
Title : ASV INTEGRASE CORE DOMAIN WITH CD(II) COFACTORS
Authors : Bujacz, G.; Alexandratos, J.; Wlodawer, A.
Deposited on : 1997-03-04
Resolution : 2.10 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

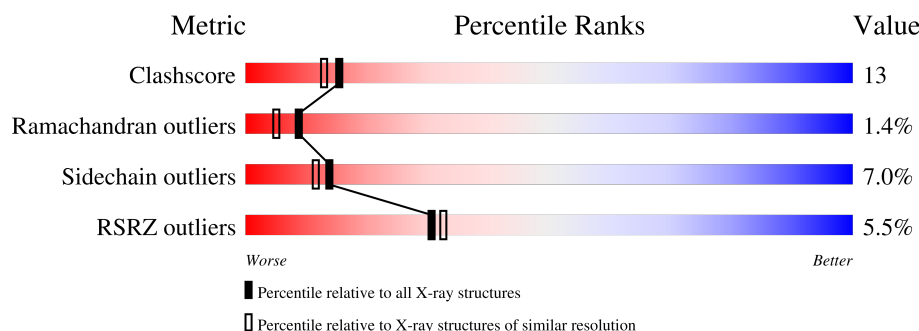
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	152	5% 56% 32% 7% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1261 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 INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1127	711	210	201	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ALA	VAL	variant	UNP P03354
A	125	OCY	CYS	modified residue	UNP P03354
A	166	LYS	ARG	variant	UNP P03354

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cd	0	0
			2	2		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

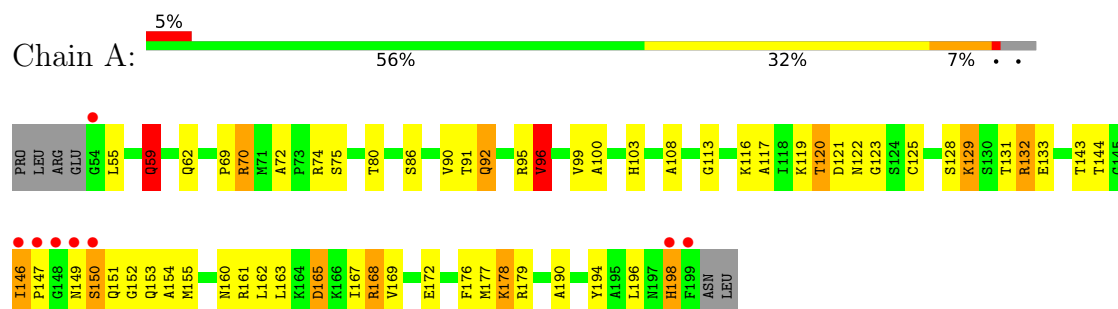
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		

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: INTEGRASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	66.33Å 66.33Å 80.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.1 (10.00-2.10) 87.9 (10.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.175 , (Not available) 0.169 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 116.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1261	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: OCY, CD, EPE

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	0.95	0/1142	2.19	51/1547 (3.3%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	HIS	CA-C-O	11.84	132.97	120.30
1	A	132	ARG	CB-CG-CD	8.83	131.61	111.30
1	A	160	ASN	OD1-CG-ND2	-8.05	114.55	122.60
1	A	179	ARG	NE-CZ-NH2	-7.99	112.00	119.20
1	A	153	GLN	N-CA-C	-7.29	101.66	113.19
1	A	168	ARG	CA-C-O	-7.04	113.43	120.82
1	A	179	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	A	151	GLN	CB-CG-CD	6.69	123.97	112.60
1	A	108	ALA	CA-C-O	6.58	127.53	120.55
1	A	92	GLN	CB-CA-C	-6.51	97.45	109.37
1	A	198	HIS	N-CA-C	6.47	118.96	108.41
1	A	154	ALA	CA-C-O	-6.43	113.74	120.55
1	A	161	ARG	CA-CB-CG	6.36	126.83	114.10
1	A	162	LEU	CA-C-O	6.10	127.01	120.55
1	A	100	ALA	CA-C-N	5.97	128.56	120.44
1	A	100	ALA	C-N-CA	5.97	128.56	120.44
1	A	72	ALA	O-C-N	5.93	128.08	121.43
1	A	113	GLY	N-CA-C	-5.92	104.04	112.81
1	A	161	ARG	CA-C-O	-5.92	114.61	120.70
1	A	113	GLY	CA-C-O	-5.88	117.16	122.57
1	A	120	THR	CA-C-O	5.88	128.31	121.49
1	A	70	ARG	CD-NE-CZ	-5.85	116.22	124.40
1	A	165	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	96	VAL	CA-C-O	-5.72	113.77	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	HIS	CA-C-N	5.72	131.99	121.70
1	A	198	HIS	C-N-CA	5.72	131.99	121.70
1	A	194	TYR	N-CA-C	-5.69	104.98	111.07
1	A	176	PHE	CA-CB-CG	5.66	119.45	113.80
1	A	129	LYS	CB-CA-C	-5.64	101.42	110.79
1	A	75	SER	N-CA-C	5.62	119.98	113.18
1	A	133	GLU	CB-CG-CD	5.59	122.10	112.60
1	A	90	VAL	CB-CA-C	-5.50	102.03	110.50
1	A	117	ALA	CA-C-N	-5.44	115.55	123.06
1	A	117	ALA	C-N-CA	-5.44	115.55	123.06
1	A	59	GLN	CB-CG-CD	5.44	121.84	112.60
1	A	91	THR	CA-CB-OG1	5.39	117.69	109.60
1	A	69	PRO	CB-CA-C	5.38	119.49	111.85
1	A	131	THR	CA-CB-CG2	5.36	119.60	110.50
1	A	167	ILE	N-CA-CB	5.35	116.81	110.55
1	A	72	ALA	CA-C-O	-5.34	114.66	120.69
1	A	153	GLN	CA-C-O	5.31	124.55	119.08
1	A	121	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	162	LEU	CB-CA-C	-5.29	102.01	110.79
1	A	190	ALA	N-CA-CB	5.22	117.80	110.12
1	A	152	GLY	N-CA-C	5.17	122.87	114.90
1	A	90	VAL	N-CA-C	5.09	116.05	108.46
1	A	62	GLN	CA-C-O	-5.07	114.88	120.30
1	A	128	SER	CA-C-N	5.03	127.03	120.28
1	A	128	SER	C-N-CA	5.03	127.03	120.28
1	A	190	ALA	CA-C-N	5.01	126.96	120.44
1	A	190	ALA	C-N-CA	5.01	126.96	120.44

There are no chirality outliers.

There are no planarity outliers.

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	1127	0	1143	31	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	18	3	0
4	A	117	0	0	7	1
All	All	1261	0	1161	31	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 13.

All (31) 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:165:ASP:HB2	4:A:373:HOH:O	1.72	0.88
1:A:129:LYS:HE2	1:A:132:ARG:HH22	1.49	0.78
1:A:198:HIS:HD2	4:A:428:HOH:O	1.75	0.69
1:A:95:ARG:NH1	1:A:96:VAL:HG23	2.10	0.67
1:A:146:ILE:HD12	1:A:146:ILE:H	1.60	0.65
1:A:146:ILE:HD12	1:A:146:ILE:N	2.13	0.64
1:A:59:GLN:NE2	1:A:116:LYS:HD3	2.12	0.64
1:A:95:ARG:HD3	3:A:261:EPE:O3S	2.00	0.62
1:A:178:LYS:HZ2	1:A:178:LYS:HB3	1.65	0.62
1:A:178:LYS:HB3	1:A:178:LYS:NZ	2.18	0.59
1:A:178:LYS:HA	1:A:178:LYS:HZ3	1.69	0.57
1:A:177:MET:O	1:A:178:LYS:HD2	2.04	0.57
1:A:95:ARG:HH11	1:A:96:VAL:HG23	1.70	0.55
1:A:74:ARG:O	1:A:92:GLN:HG2	2.07	0.54
1:A:70:ARG:HD2	4:A:419:HOH:O	2.07	0.54
1:A:59:GLN:HB2	1:A:116:LYS:HG2	1.90	0.53
1:A:95:ARG:CZ	3:A:261:EPE:O1S	2.57	0.52
1:A:122:ASN:O	1:A:123:GLY:C	2.53	0.51
1:A:86:SER:OG	1:A:155:MET:HE1	2.11	0.50
1:A:178:LYS:NZ	1:A:178:LYS:CB	2.74	0.50
1:A:198:HIS:CD2	4:A:428:HOH:O	2.58	0.49
1:A:149:ASN:O	1:A:150:SER:CB	2.60	0.48
1:A:99:VAL:HG12	1:A:103:HIS:CE1	2.48	0.48
1:A:163:LEU:HA	1:A:196:LEU:HD11	1.95	0.48
1:A:99:VAL:HG23	4:A:328:HOH:O	2.14	0.47
1:A:120:THR:O	1:A:144:THR:HA	2.15	0.47
1:A:119:LYS:HG2	4:A:343:HOH:O	2.16	0.46
1:A:74:ARG:HD3	4:A:331:HOH:O	2.19	0.43
1:A:70:ARG:NH2	1:A:177:MET:C	2.77	0.42
1:A:168:ARG:O	1:A:172:GLU:HG3	2.20	0.42
1:A:95:ARG:CD	3:A:261:EPE:O3S	2.67	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)
4:A:301:HOH:O	4:A:413:HOH:O[6_566]	2.17	0.03

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	143/152 (94%)	134 (94%)	7 (5%)	2 (1%)	9 5

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	SER
1	A	147	PRO

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	115/121 (95%)	107 (93%)	8 (7%)	14 11

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU

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Mol	Chain	Res	Type
1	A	59	GLN
1	A	80	THR
1	A	96	VAL
1	A	143	THR
1	A	146	ILE
1	A	169	VAL
1	A	178	LYS

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	62	GLN
1	A	153	GLN
1	A	198	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	OCY	A	125	1	7,8,9	0.57	0	4,8,10	2.21	2 (50%)

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	OCY	A	125	1	-	1/5/7/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	OCY	CB-SG-CD	3.57	112.85	102.26
1	A	125	OCY	OZ-CE-CD	-2.37	101.57	110.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	125	OCY	CA-CB-SG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
3	EPE	A	261	-	15,15,15	1.86	2 (13%)	19,20,20	1.60	4 (21%)

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
3	EPE	A	261	-	-	5/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	261	EPE	O3S-S	4.98	1.66	1.47
3	A	261	EPE	C10-S	3.51	1.82	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	261	EPE	O1S-S-C10	3.31	111.73	106.73
3	A	261	EPE	O3S-S-C10	-3.16	99.83	106.00
3	A	261	EPE	O2S-S-C10	2.23	110.10	106.73
3	A	261	EPE	C7-N4-C3	2.21	117.12	111.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	261	EPE	C9-C10-S-O2S
3	A	261	EPE	C9-C10-S-O3S
3	A	261	EPE	C10-C9-N1-C6
3	A	261	EPE	C9-C10-S-O1S
3	A	261	EPE	C10-C9-N1-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	261	EPE	3	0

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	145/152 (95%)	-0.53	8 (5%) 30 32	4, 13, 67, 103	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	HIS	4.4
1	A	199	PHE	3.4
1	A	149	ASN	2.9
1	A	54	GLY	2.7
1	A	148	GLY	2.5
1	A	146	ILE	2.4
1	A	150	SER	2.3
1	A	147	PRO	2.2

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, 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	OCY	A	125	9/10	0.95	0.06	11,19,28,30	0

6.3 Carbohydrates

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	CD	A	290	1/1	0.97	0.04	34,34,34,34	1
3	EPE	A	261	15/15	0.97	0.05	11,18,27,27	0
2	CD	A	280	1/1	1.00	0.01	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.