



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:09 AM GMT

PDB ID : 2FX6
Title : bovine trypsin complexed with 2-aminobenzamidazole
Authors : Katz, B.A.
Deposited on : 2006-02-03
Resolution : 1.57 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

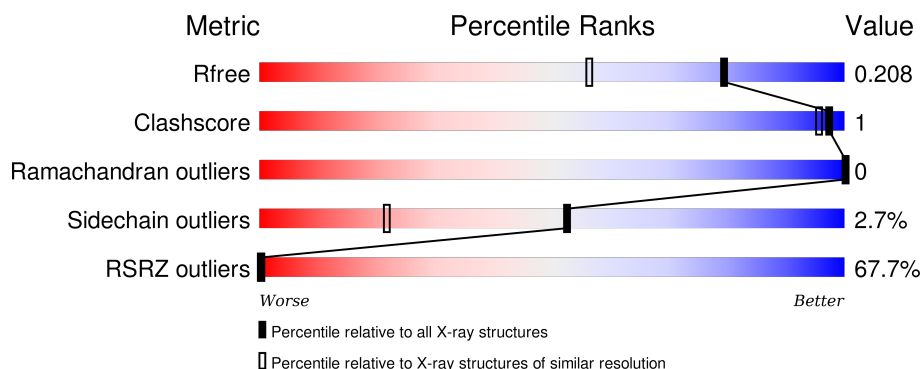
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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}	91344	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	223	

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
2	CA	A	247	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1829 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.

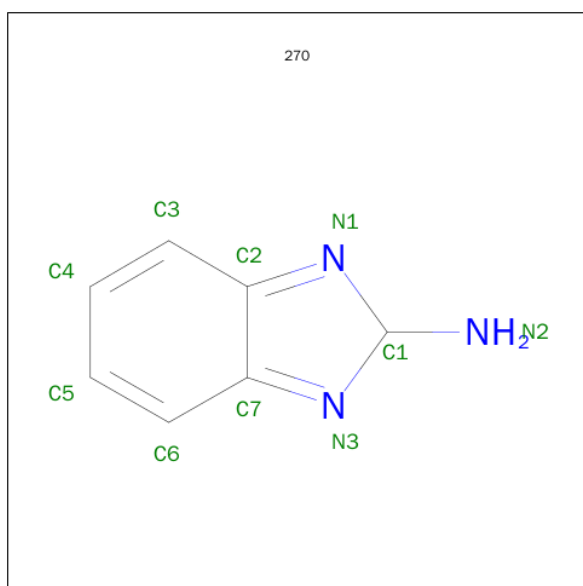
- Molecule 1 is a protein called Trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	13	0
			1672	1042	283	333	14			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2H-BENZOIMIDAZOL-2-YLAMINE (three-letter code: 270) (formula: C₇H₇N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	7	3		

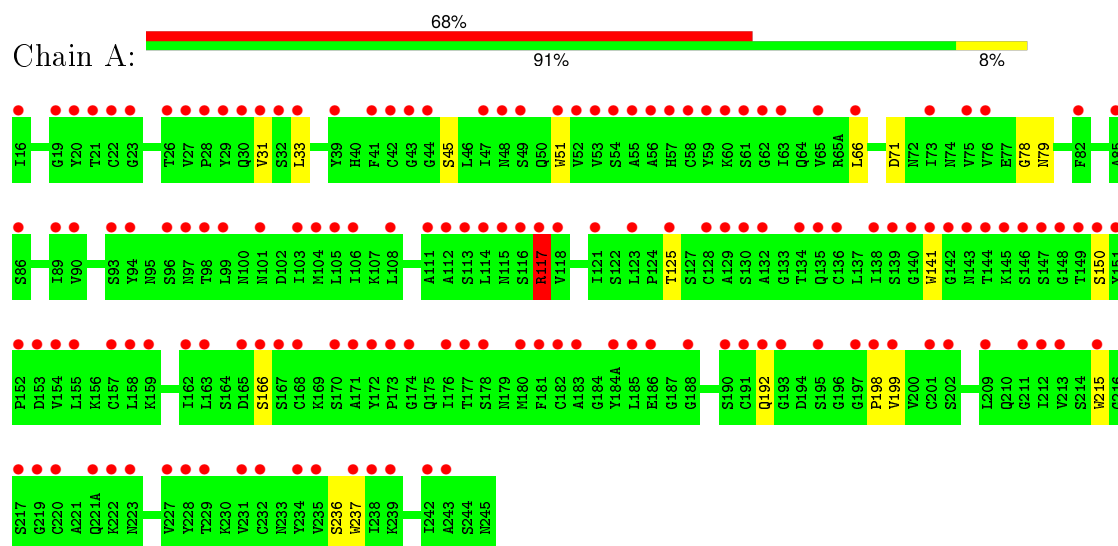
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total 146	O 146	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Trypsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.71Å 63.20Å 69.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.57 28.96 – 1.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-1.57) 99.0 (28.96-1.57)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 1.57Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.202 , 0.215 0.202 , 0.208	Depositor DCC
R_{free} test set	3929 reflections (10.06%)	DCC
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.2	EDS
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 39661 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1829	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 270, CA

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	1.25	0/1755	1.43	21/2375 (0.9%)

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	A	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	TRP	CD1-NE1-CE2	10.03	118.02	109.00
1	A	51	TRP	CD1-NE1-CE2	9.22	117.30	109.00
1	A	141	TRP	CD1-NE1-CE2	9.06	117.16	109.00
1	A	215	TRP	CD1-NE1-CE2	9.02	117.12	109.00
1	A	237	TRP	NE1-CE2-CZ2	8.34	139.57	130.40
1	A	215	TRP	NE1-CE2-CZ2	7.34	138.47	130.40
1	A	237	TRP	NE1-CE2-CD2	-7.23	100.07	107.30
1	A	237	TRP	CG-CD1-NE1	-7.00	103.10	110.10
1	A	141	TRP	CG-CD1-NE1	-6.66	103.44	110.10
1	A	215	TRP	CG-CD1-NE1	-6.46	103.64	110.10
1	A	141	TRP	NE1-CE2-CZ2	6.37	137.40	130.40
1	A	199	VAL	N-CA-C	-6.33	93.90	111.00
1	A	51	TRP	CG-CD1-NE1	-6.29	103.81	110.10
1	A	51	TRP	NE1-CE2-CZ2	6.00	137.00	130.40
1	A	215	TRP	NE1-CE2-CD2	-6.00	101.31	107.30
1	A	51	TRP	NE1-CE2-CD2	-5.71	101.59	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	SER	N-CA-C	-5.52	96.09	111.00
1	A	117	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	71	ASP	N-CA-C	-5.41	96.39	111.00
1	A	141	TRP	NE1-CE2-CD2	-5.30	102.00	107.30
1	A	33	LEU	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain

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	1672	0	1637	3	0
2	A	1	0	0	0	0
3	A	10	0	6	1	0
4	A	146	0	0	1	0
All	All	1829	0	1643	4	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 1.

All (4) 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:31:VAL:HG12	1:A:66[A]:LEU:HD23	1.91	0.52
1:A:45:SER:OG	1:A:198:PRO:HB3	2.14	0.47
1:A:78:GLY:O	1:A:79:ASN:HB2	2.20	0.41
3:A:246:270:C6	4:A:666:HOH:O	2.69	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	234/223 (105%)	227 (97%)	7 (3%)	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	197/184 (107%)	190 (96%)	7 (4%)	42	13

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ARG
1	A	125	THR
1	A	166[A]	SER
1	A	166[B]	SER
1	A	192	GLN
1	A	236[A]	SER
1	A	236[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is 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	270	A	246	-	4,11,11	1.37	0	2,15,15	0.76	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
3	270	A	246	-	-	0/0/8/8	0/1/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	246	270	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	223/223 (100%)	2.74	151 (67%) 0 0	10, 18, 29, 56	16 (7%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	SER	11.5
1	A	148	GLY	10.9
1	A	150	SER	8.3
1	A	151	TYR	7.7
1	A	149	THR	7.1
1	A	52	VAL	6.1
1	A	53[A]	VAL	5.9
1	A	212	ILE	5.7
1	A	125	THR	5.6
1	A	97	ASN	5.5
1	A	16	ILE	5.3
1	A	115	ASN	5.3
1	A	118	VAL	5.1
1	A	162	ILE	4.8
1	A	61	SER	4.7
1	A	114	LEU	4.7
1	A	31	VAL	4.7
1	A	177	THR	4.4
1	A	116	SER	4.3
1	A	33	LEU	4.2
1	A	201	CYS	4.1
1	A	20	TYR	4.1
1	A	174	GLY	4.1
1	A	146	SER	4.1
1	A	106	ILE	4.0
1	A	55	ALA	4.0
1	A	136	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	199	VAL	4.0
1	A	103	ILE	4.0
1	A	202	SER	3.9
1	A	155	LEU	3.9
1	A	191	CYS	3.8
1	A	112	ALA	3.8
1	A	181	PHE	3.8
1	A	215	TRP	3.7
1	A	223	ASN	3.7
1	A	51	TRP	3.6
1	A	154	VAL	3.6
1	A	231	VAL	3.6
1	A	42	CYS	3.6
1	A	111	ALA	3.6
1	A	213	VAL	3.6
1	A	129	ALA	3.5
1	A	144	THR	3.5
1	A	197	GLY	3.5
1	A	238	ILE	3.5
1	A	228	TYR	3.5
1	A	209	LEU	3.5
1	A	76	VAL	3.5
1	A	176	ILE	3.5
1	A	173	PRO	3.5
1	A	59	TYR	3.4
1	A	237	TRP	3.4
1	A	138	ILE	3.4
1	A	86	SER	3.4
1	A	220	CYS	3.4
1	A	141	TRP	3.3
1	A	75	VAL	3.3
1	A	171	ALA	3.2
1	A	172	TYR	3.2
1	A	183	ALA	3.2
1	A	117	ARG	3.2
1	A	134	THR	3.2
1	A	163	LEU	3.2
1	A	235	VAL	3.2
1	A	28	PRO	3.2
1	A	44	GLY	3.2
1	A	105	LEU	3.1
1	A	21	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	60	LYS	3.1
1	A	108	LEU	3.1
1	A	58	CYS	3.1
1	A	73	ILE	3.1
1	A	130[A]	SER	3.0
1	A	158	LEU	3.0
1	A	23	GLY	2.9
1	A	143	ASN	2.9
1	A	27	VAL	2.9
1	A	239	LYS	2.9
1	A	195	SER	2.9
1	A	99	LEU	2.9
1	A	185	LEU	2.9
1	A	167	SER	2.9
1	A	85	ALA	2.9
1	A	89	ILE	2.8
1	A	140	GLY	2.8
1	A	145	LYS	2.8
1	A	152	PRO	2.8
1	A	184(A)	TYR	2.8
1	A	57	HIS	2.8
1	A	132	ALA	2.8
1	A	43	GLY	2.8
1	A	104	MET	2.8
1	A	227	VAL	2.7
1	A	188	GLY	2.7
1	A	165[A]	ASP	2.7
1	A	182	CYS	2.7
1	A	98	THR	2.7
1	A	29	TYR	2.7
1	A	135	GLN	2.7
1	A	96	SER	2.7
1	A	219	GLY	2.7
1	A	178	SER	2.6
1	A	198	PRO	2.6
1	A	62	GLY	2.6
1	A	211	GLY	2.6
1	A	159[A]	LYS	2.6
1	A	66[A]	LEU	2.6
1	A	56	ALA	2.5
1	A	232	CYS	2.5
1	A	186	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	90	VAL	2.5
1	A	26	THR	2.5
1	A	153	ASP	2.5
1	A	142	GLY	2.5
1	A	32	SER	2.5
1	A	170[A]	SER	2.5
1	A	39	TYR	2.5
1	A	229	THR	2.4
1	A	193	GLY	2.4
1	A	180	MET	2.4
1	A	168	CYS	2.4
1	A	139	SER	2.4
1	A	128	CYS	2.4
1	A	121	ILE	2.4
1	A	242	ILE	2.4
1	A	47	ILE	2.4
1	A	49	SER	2.3
1	A	192	GLN	2.3
1	A	217[A]	SER	2.3
1	A	22	CYS	2.3
1	A	243	ALA	2.3
1	A	48	ASN	2.3
1	A	63	ILE	2.3
1	A	93	SER	2.3
1	A	234	TYR	2.2
1	A	221(A)	GLN	2.2
1	A	113[A]	SER	2.2
1	A	157	CYS	2.2
1	A	30	GLN	2.2
1	A	94	TYR	2.1
1	A	19	GLY	2.1
1	A	54	SER	2.1
1	A	222	LYS	2.1
1	A	123	LEU	2.1
1	A	166[A]	SER	2.1
1	A	65	VAL	2.1
1	A	41	PHE	2.0
1	A	82	PHE	2.0
1	A	101	ASN	2.0
1	A	190	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	247	1/1	0.94	0.23	2.93	27,27,27,27	0
3	270	A	246	10/10	0.81	0.14	-1.50	25,27,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.