



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:21 PM UTC

PDB ID : 7H39 / pdb_00007h39
Title : Group deposition for crystallographic fragment screening of Coxsackievirus A16 (G-10) 2A protease – Crystal structure of Coxsackievirus A16 (G-10) 2A protease in complex with Z50145861 (A71EV2A-x0341)
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Deposited on : 2024-04-04
Resolution : 1.25 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)

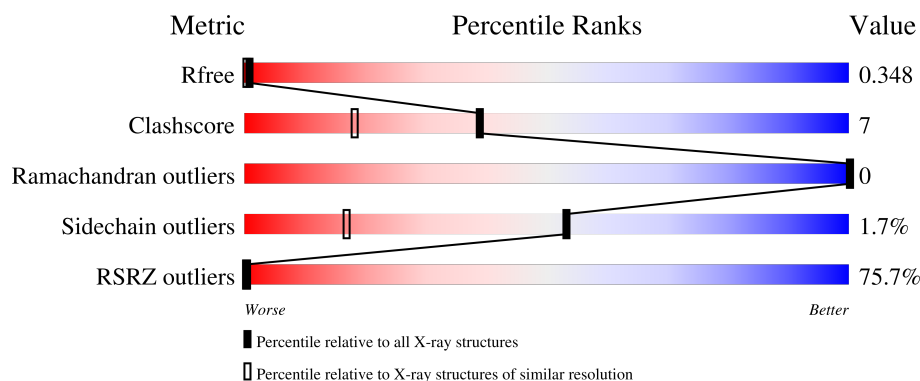
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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	150	71% 77% 15% 7%

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:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	A	203	-	-	-	X
4	DMS	A	205	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 1365 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.

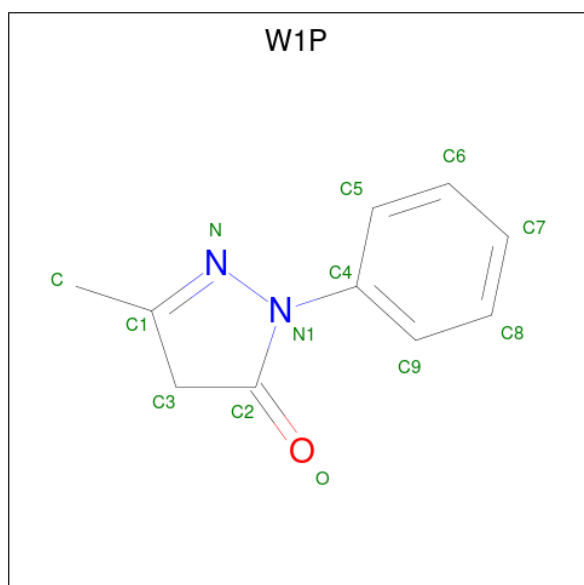
- Molecule 1 is a protein called Protease 2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	3	0
			1103	686	196	214	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLN	-	expression tag	UNP Q65900
A	2	GLU	-	expression tag	UNP Q65900
A	3	GLN	-	expression tag	UNP Q65900
A	4	THR	-	expression tag	UNP Q65900
A	5	GLY	-	expression tag	UNP Q65900
A	6	GLY	-	expression tag	UNP Q65900

- Molecule 2 is 5-methyl-2-phenyl-2,4-dihydro-3H-pyrazol-3-one (CCD ID: W1P) (formula: $C_{10}H_{10}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	10	2	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

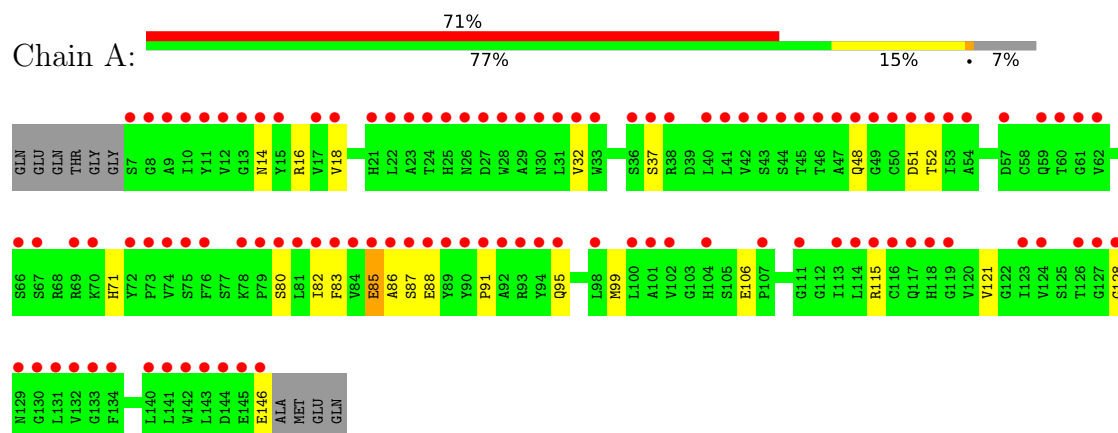
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	231	Total	O	0	0
			231	231		

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: Protease 2A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.64Å 57.71Å 32.63Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	48.02 – 1.25 48.02 – 1.25	Depositor EDS
% Data completeness (in resolution range)	89.3 (48.02-1.25) 89.4 (48.02-1.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.300 , 0.339 0.323 , 0.348	Depositor DCC
R_{free} test set	2198 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	1.2	Xtriage
Anisotropy	2.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	1365	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.64% 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: ZN, DMS, SO4, W1P

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	1.09	1/1129 (0.1%)	1.33	8/1535 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	ASP	C-O	-5.24	1.17	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLU	CB-CA-C	-7.51	94.11	109.65
1	A	115	ARG	CB-CG-CD	-6.02	97.45	111.30
1	A	82	ILE	CA-C-N	-5.85	113.05	121.42
1	A	82	ILE	C-N-CA	-5.85	113.05	121.42
1	A	128	GLY	CA-C-O	-5.80	118.45	122.22
1	A	32	VAL	N-CA-C	-5.17	107.11	111.56
1	A	83	PHE	CA-C-N	-5.03	115.84	122.98
1	A	83	PHE	C-N-CA	-5.03	115.84	122.98

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	1103	0	1034	15	0
2	A	13	0	0	2	0
3	A	1	0	0	0	0
4	A	12	0	18	0	0
5	A	5	0	0	0	1
6	A	231	0	0	8	3
All	All	1365	0	1052	15	4

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 7.

All (15) 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:88:GLU:HG3	6:A:499:HOH:O	1.79	0.81
1:A:87:SER:O	6:A:302:HOH:O	1.99	0.80
1:A:71:HIS:HE1	2:A:201:W1P:O	1.65	0.78
1:A:71:HIS:CE1	2:A:201:W1P:O	2.38	0.77
1:A:91:PRO:HG2	6:A:329:HOH:O	1.89	0.71
1:A:14:ASN:HD21	1:A:48:GLN:HG3	1.68	0.58
1:A:106:GLU:OE1	6:A:304:HOH:O	2.17	0.57
1:A:16:ARG:CZ	1:A:18:VAL:HG11	2.40	0.52
1:A:14:ASN:ND2	1:A:48:GLN:HG3	2.25	0.51
1:A:85:GLU:OE1	6:A:305:HOH:O	2.19	0.48
1:A:86:ALA:HB1	6:A:302:HOH:O	2.18	0.44
1:A:52:THR:HG21	6:A:318:HOH:O	2.18	0.43
1:A:99:MET:HE1	1:A:121:VAL:HG12	2.00	0.43
1:A:37:SER:O	1:A:95:GLN:HG3	2.19	0.42
1:A:91:PRO:CG	6:A:329:HOH:O	2.60	0.41

All (4) 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)
5:A:206:SO4:O2	5:A:206:SO4:O4[2_556]	1.72	0.48
6:A:426:HOH:O	6:A:426:HOH:O[2_556]	2.12	0.08
6:A:482:HOH:O	6:A:491:HOH:O[4_546]	2.12	0.08
6:A:512:HOH:O	6:A:512:HOH:O[2_556]	2.14	0.06

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	141/150 (94%)	139 (99%)	2 (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	120/124 (97%)	117 (98%)	3 (2%)	42	8

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80[A]	SER
1	A	80[B]	SER
1	A	146	GLU

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	14	ASN
1	A	71	HIS
1	A	117	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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$
5	SO4	A	206	-	4,4,4	0.34	0	6,6,6	0.08	0
2	W1P	A	201	-	12,14,14	0.85	1 (8%)	15,19,19	3.00	6 (40%)
4	DMS	A	205	-	3,3,3	0.26	0	3,3,3	0.05	0
4	DMS	A	204	-	3,3,3	0.29	0	3,3,3	0.16	0
4	DMS	A	203	-	3,3,3	0.23	0	3,3,3	0.10	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	W1P	A	201	-	-	4/4/16/16	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	W1P	C1-N	2.03	1.29	1.28

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	W1P	C4-N1-N	5.72	126.97	118.67
2	A	201	W1P	C1-N-N1	5.58	111.32	107.94
2	A	201	W1P	C3-C1-N	-5.07	111.35	114.59
2	A	201	W1P	C-C1-N	4.56	125.48	121.70
2	A	201	W1P	C4-N1-C2	-3.24	125.24	128.64
2	A	201	W1P	C8-C9-C4	2.61	122.78	119.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	W1P	C9-C4-N1-C2
2	A	201	W1P	C5-C4-N1-C2
2	A	201	W1P	C9-C4-N1-N
2	A	201	W1P	C5-C4-N1-N

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	206	SO4	0	1
2	A	201	W1P	2	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	140/150 (93%)	4.84	106 (75%) 0 0	4, 22, 36, 79	24 (17%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	CYS	24.2
1	A	113	ILE	21.5
1	A	53	ILE	21.2
1	A	116	CYS	20.3
1	A	114	LEU	19.7
1	A	89	TYR	19.2
1	A	52	THR	18.7
1	A	49	GLY	18.3
1	A	48	GLN	16.5
1	A	115	ARG	14.3
1	A	117	GLN	13.8
1	A	51	ASP	13.6
1	A	83	PHE	12.9
1	A	90	TYR	12.7
1	A	86	ALA	11.5
1	A	88	GLU	11.5
1	A	91	PRO	11.4
1	A	146	GLU	10.6
1	A	84	VAL	10.4
1	A	87	SER	10.1
1	A	92	ALA	9.6
1	A	57[A]	ASP	8.9
1	A	36[A]	SER	8.3
1	A	80[A]	SER	8.2
1	A	85	GLU	6.5
1	A	46	THR	6.3
1	A	145	GLU	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	47	ALA	5.6
1	A	29	ALA	5.2
1	A	14	ASN	5.2
1	A	32	VAL	5.1
1	A	143	LEU	4.9
1	A	7	SER	4.9
1	A	33	TRP	4.9
1	A	62	VAL	4.9
1	A	76	PHE	4.6
1	A	144	ASP	4.6
1	A	15	TYR	4.5
1	A	141	LEU	4.5
1	A	82	ILE	4.5
1	A	24	THR	4.5
1	A	129	ASN	4.3
1	A	40	LEU	4.3
1	A	94	TYR	4.3
1	A	142	TRP	4.2
1	A	128	GLY	4.2
1	A	12	VAL	4.2
1	A	31	LEU	4.0
1	A	81	LEU	4.0
1	A	17	VAL	4.0
1	A	131	LEU	4.0
1	A	130	GLY	3.9
1	A	70	LYS	3.9
1	A	67	SER	3.8
1	A	18	VAL	3.8
1	A	100	LEU	3.5
1	A	102	VAL	3.5
1	A	124	VAL	3.4
1	A	93	ARG	3.4
1	A	11	TYR	3.3
1	A	66	SER	3.3
1	A	74	VAL	3.2
1	A	28	TRP	3.2
1	A	54	ALA	3.1
1	A	27	ASP	3.1
1	A	78	LYS	3.1
1	A	23	ALA	3.0
1	A	26	ASN	3.0
1	A	45	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	140	LEU	3.0
1	A	41	LEU	2.9
1	A	30	ASN	2.9
1	A	22	LEU	2.9
1	A	75	SER	2.8
1	A	9	ALA	2.8
1	A	101	ALA	2.8
1	A	119	GLY	2.8
1	A	132	VAL	2.8
1	A	104	HIS	2.8
1	A	42	VAL	2.7
1	A	133	GLY	2.7
1	A	25	HIS	2.6
1	A	79	PRO	2.6
1	A	107	PRO	2.6
1	A	72	TYR	2.6
1	A	98	LEU	2.6
1	A	60	THR	2.6
1	A	127	GLY	2.6
1	A	10	ILE	2.5
1	A	118	HIS	2.5
1	A	13	GLY	2.4
1	A	123	ILE	2.4
1	A	8	GLY	2.4
1	A	111	GLY	2.3
1	A	126	THR	2.2
1	A	43	SER	2.2
1	A	21	HIS	2.2
1	A	38	ARG	2.2
1	A	73	PRO	2.2
1	A	61	GLY	2.1
1	A	44	SER	2.1
1	A	95	GLN	2.1
1	A	37	SER	2.0
1	A	69	ARG	2.0
1	A	134	PHE	2.0
1	A	59	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

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
4	DMS	A	205	4/4	0.48	0.42	82,85,89,90	0
4	DMS	A	203	4/4	0.49	0.41	114,115,116,121	0
5	SO4	A	206	5/5	0.53	0.21	62,65,66,67	0
2	W1P	A	201	13/13	0.61	0.33	20,20,20,20	13
4	DMS	A	204	4/4	0.68	0.29	52,57,61,64	0
3	ZN	A	202	1/1	0.98	0.04	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.