



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2024 – 12:42 PM EDT

PDB ID : 7H51
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 Z1198183601 (A71EV2A-x1180)
Authors : Lithgo, R.M.; Fairhead, M.; Koekemoer, L.; Balcomb, B.H.; Capkin, E.; Chandran, A.V.; Golding, M.; Godoy, A.S.; Aschenbrenner, J.C.; Marples, P.G.; Ni, X.; Thompson, W.; Tomlinson, C.W.E.; Wild, C.; Winokan, M.; Xavier, M.-A.E.; Fearon, D.; von Delft, F.
Deposited on : 2024-04-04
Resolution : 1.05 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)
Xtriage (Phenix) : 1.13
EDS : 2.36.1
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)

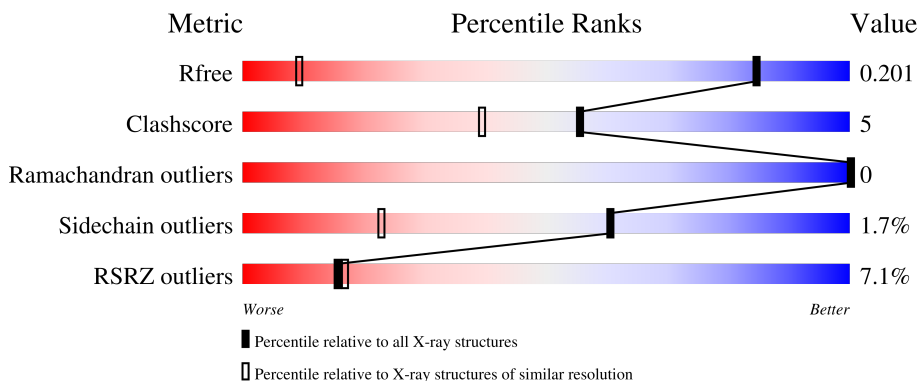
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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	1202 (1.10-1.02)
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

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	
1	B	150	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36.1

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
5	DMS	A	206	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2644 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
			Total	C	N	O	S			
1	A	140	1101	685	196	213	7	0	3	0
1	B	140	1103	688	196	212	7	0	3	0

There are 12 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
B	1	GLN	-	expression tag	UNP Q65900
B	2	GLU	-	expression tag	UNP Q65900
B	3	GLN	-	expression tag	UNP Q65900
B	4	THR	-	expression tag	UNP Q65900
B	5	GLY	-	expression tag	UNP Q65900
B	6	GLY	-	expression tag	UNP Q65900

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

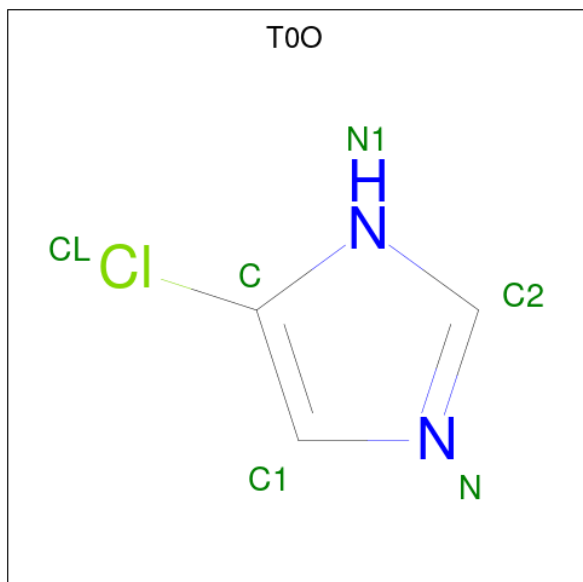


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

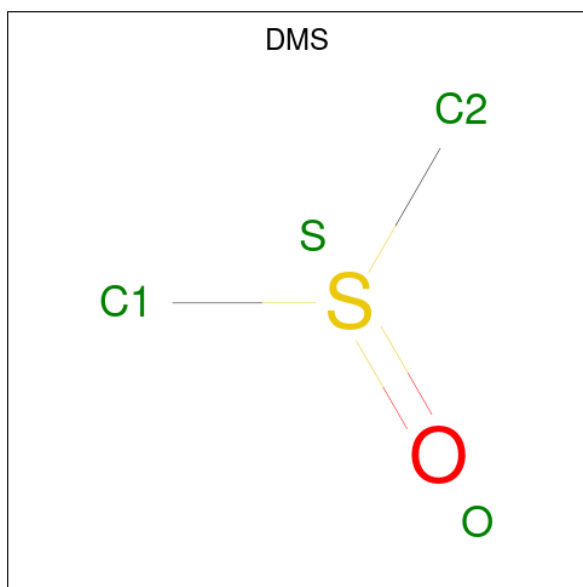
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is 5-chloro-1H-imidazole (three-letter code: T0O) (formula: C₃H₃ClN₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			6	3	1	2		
4	B	1	Total	C	Cl	N	0	0
			6	3	1	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

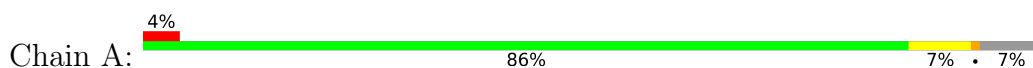
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	203	Total	O	0	0
			203	203		
6	B	205	Total	O	0	0
			205	205		

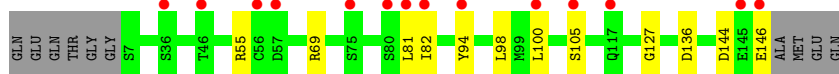
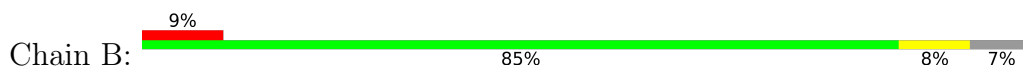
3 Residue-property plots [i](#)

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



- 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	86.21Å 56.74Å 64.51Å 90.00° 94.68° 90.00°	Depositor
Resolution (Å)	43.00 – 1.05 42.96 – 1.05	Depositor EDS
% Data completeness (in resolution range)	89.2 (43.00-1.05) 89.2 (42.96-1.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.05Å)	Xtrriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.175 , 0.192 0.185 , 0.201	Depositor DCC
R_{free} test set	5304 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtrriage
Anisotropy	0.031	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2644	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0951e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, T0O, ZN, DMS

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	0.78	0/1127	0.86	0/1532
1	B	0.79	0/1129	0.90	2/1535 (0.1%)
All	All	0.78	0/2256	0.88	2/3067 (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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	136	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	B	69	ARG	NE-CZ-NH2	-5.52	117.54	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	GLU	Peptide

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	1101	0	1035	8	0
1	B	1103	0	1041	8	0
2	A	6	0	8	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
5	A	12	0	18	5	0
6	A	203	0	0	10	2
6	B	205	0	0	1	2
All	All	2644	0	2102	22	2

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 5.

All (22) 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:82:ILE:HD13	1:B:100[A]:LEU:HG	1.41	1.01
5:A:206:DMS:H13	6:A:396:HOH:O	1.68	0.94
1:B:82:ILE:CD1	1:B:100[A]:LEU:HG	2.07	0.85
1:A:85:GLU:OE1	6:A:301:HOH:O	2.00	0.79
1:A:146:GLU:HG3	1:A:146:GLU:O	1.95	0.66
2:A:201:GOL:O2	6:A:301:HOH:O	2.12	0.65
1:B:82:ILE:HD13	1:B:100[A]:LEU:CG	2.23	0.61
5:A:206:DMS:H22	6:A:447:HOH:O	1.99	0.61
5:A:206:DMS:O	6:A:302:HOH:O	2.16	0.56
5:A:206:DMS:C1	6:A:396:HOH:O	2.40	0.52
1:A:146:GLU:O	1:A:146:GLU:CG	2.57	0.52
2:A:201:GOL:O3	5:A:206:DMS:H13	2.11	0.51
1:A:71:HIS:HD2	6:A:464:HOH:O	1.96	0.47
1:B:105:SER:HB3	1:B:127:GLY:HA3	1.97	0.47
1:A:117:GLN:HG2	6:A:357:HOH:O	2.14	0.46
1:B:82:ILE:HD11	6:B:325:HOH:O	2.16	0.45
1:A:115:ARG:NH1	6:A:306:HOH:O	2.50	0.45
1:B:81:LEU:HG	1:B:94:TYR:HB3	2.01	0.41
1:B:82:ILE:HB	1:B:98:LEU:HD23	2.02	0.41
1:B:55:ARG:HH21	1:B:144:ASP:CG	2.24	0.41
1:A:78:LYS:HD3	6:A:460:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:O	1:A:95:GLN:HG3	2.21	0.40

All (2) 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)
6:A:395:HOH:O	6:B:461:HOH:O[1_545]	2.15	0.05
6:A:473:HOH:O	6:B:303:HOH:O[4_545]	2.18	0.02

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	141/150 (94%)	139 (99%)	2 (1%)	0	100	100
1	B	141/150 (94%)	138 (98%)	3 (2%)	0	100	100
All	All	282/300 (94%)	277 (98%)	5 (2%)	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	120/124 (97%)	117 (98%)	3 (2%)	47	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	120/124 (97%)	119 (99%)	1 (1%)	81	52
All	All	240/248 (97%)	236 (98%)	4 (2%)	60	23

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	129	ASN
1	A	146	GLU
1	B	146	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	48	GLN
1	A	71	HIS
1	A	129	ASN
1	B	14	ASN
1	B	71	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	DMS	A	206	-	3,3,3	0.19	0	3,3,3	0.09	0
5	DMS	A	204	-	3,3,3	0.36	0	3,3,3	0.18	0
4	T0O	A	203	-	3,6,6	2.02	1 (33%)	1,7,7	1.10	0
5	DMS	A	205	-	3,3,3	0.22	0	3,3,3	0.12	0
4	T0O	B	202	-	3,6,6	1.47	1 (33%)	1,7,7	0.99	0
2	GOL	A	201	-	5,5,5	0.12	0	5,5,5	0.40	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
4	T0O	B	202	-	-	-	0/1/1/1
4	T0O	A	203	-	-	-	0/1/1/1
2	GOL	A	201	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	T0O	C1-C	3.45	1.41	1.36
4	B	202	T0O	C1-C	2.47	1.40	1.36

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	206	DMS	5	0
2	A	201	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.30	6 (4%) 35 30	8, 12, 21, 55	5 (3%)
1	B	140/150 (93%)	0.72	14 (10%) 7 10	8, 12, 25, 57	7 (5%)
All	All	280/300 (93%)	0.51	20 (7%) 16 17	8, 12, 23, 57	12 (4%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100[A]	LEU	18.2
1	B	82	ILE	16.2
1	B	81	LEU	12.8
1	B	75[A]	SER	9.1
1	B	80	SER	9.0
1	A	75[A]	SER	8.8
1	B	36[A]	SER	7.7
1	A	66[A]	SER	7.2
1	A	36[A]	SER	6.9
1	B	105	SER	6.4
1	A	69	ARG	5.4
1	B	146	GLU	3.5
1	A	146	GLU	3.0
1	B	94	TYR	2.8
1	B	57	ASP	2.6
1	B	117	GLN	2.5
1	B	145	GLU	2.5
1	B	46	THR	2.5
1	A	50	CYS	2.3
1	B	56	CYS	2.2

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 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
5	DMS	A	206	4/4	0.76	0.23	35,37,37,37	4
5	DMS	A	205	4/4	0.79	0.17	66,71,72,74	0
4	T0O	A	203	6/6	0.79	0.20	16,17,19,31	6
2	GOL	A	201	6/6	0.83	0.14	15,16,16,17	6
5	DMS	A	204	4/4	0.88	0.26	33,58,62,66	0
3	ZN	B	201	1/1	0.89	0.10	15,15,15,15	0
4	T0O	B	202	6/6	0.90	0.17	21,23,24,24	6
3	ZN	A	202	1/1	0.99	0.05	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.