



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2016 – 01:20 PM EST

PDB ID : 5LKX  
Title : Crystal structure of the p300 acetyltransferase catalytic core with propionyl-coenzyme A.  
Authors : Kaczmarska, Z.; Ortega, E.; Marquez, J.A.; Panne, D.  
Deposited on : 2016-07-25  
Resolution : 2.52 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

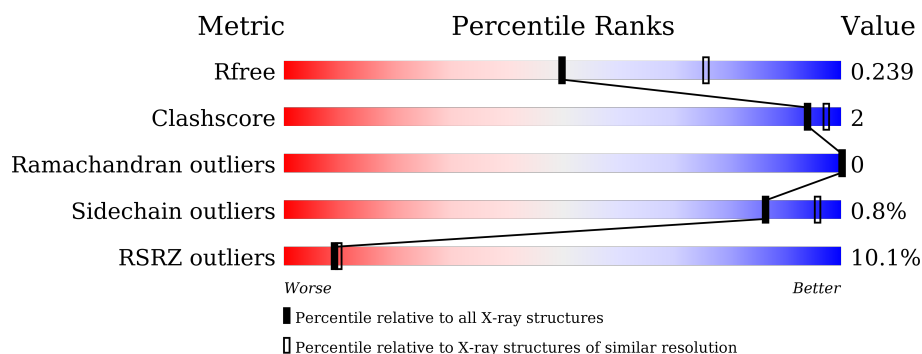
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.52 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	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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  $\geq 3$ , 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	578	<div> <div>10%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>

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
4	DMS	A	1706	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4748 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 Histone acetyltransferase p300,Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	2	0
			4505	2877	768	826	34			

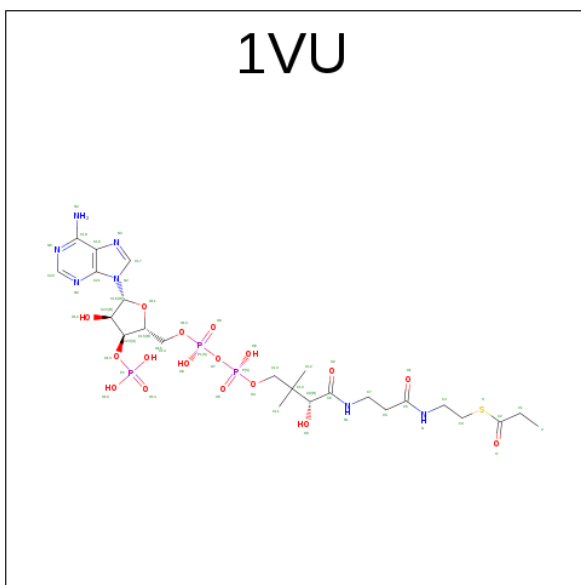
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1033	GLY	-	expression tag	UNP Q09472
A	1034	ALA	-	expression tag	UNP Q09472
A	1035	MET	-	expression tag	UNP Q09472
A	1036	ALA	-	expression tag	UNP Q09472
A	1037	GLY	-	expression tag	UNP Q09472
A	1038	LYS	-	expression tag	UNP Q09472
A	1039	ALA	-	expression tag	UNP Q09472
A	1040	VAL	-	expression tag	UNP Q09472
A	1041	PRO	-	expression tag	UNP Q09472
A	1042	MET	-	expression tag	UNP Q09472
A	1467	PHE	TYR	engineered mutation	UNP Q09472
A	1520	SER	-	linker	UNP Q09472
A	1521	GLY	-	linker	UNP Q09472
A	1522	GLY	-	linker	UNP Q09472
A	1523	SER	-	linker	UNP Q09472
A	1524	GLY	-	linker	UNP Q09472

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

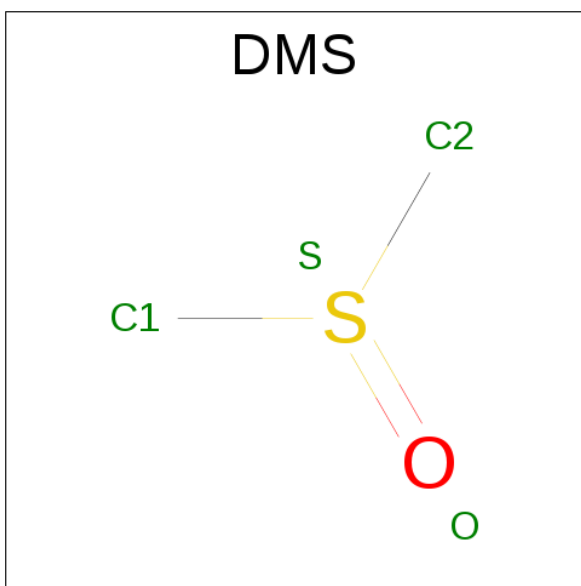
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		

- Molecule 3 is propionyl Coenzyme A (three-letter code: 1VU) (formula: C<sub>24</sub>H<sub>40</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



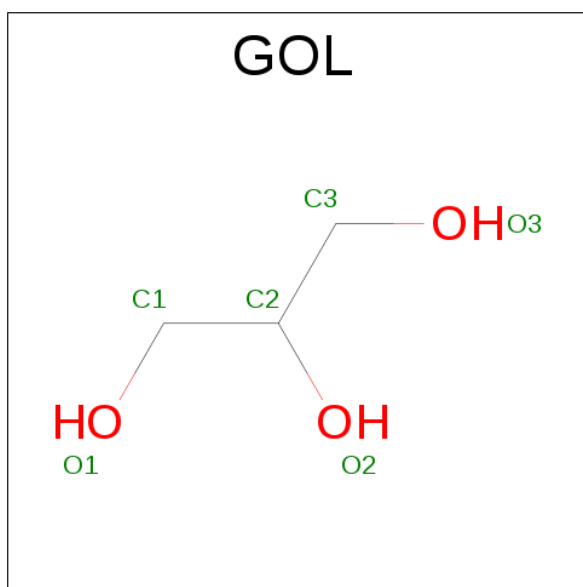
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			52	24	7	17	3	1		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

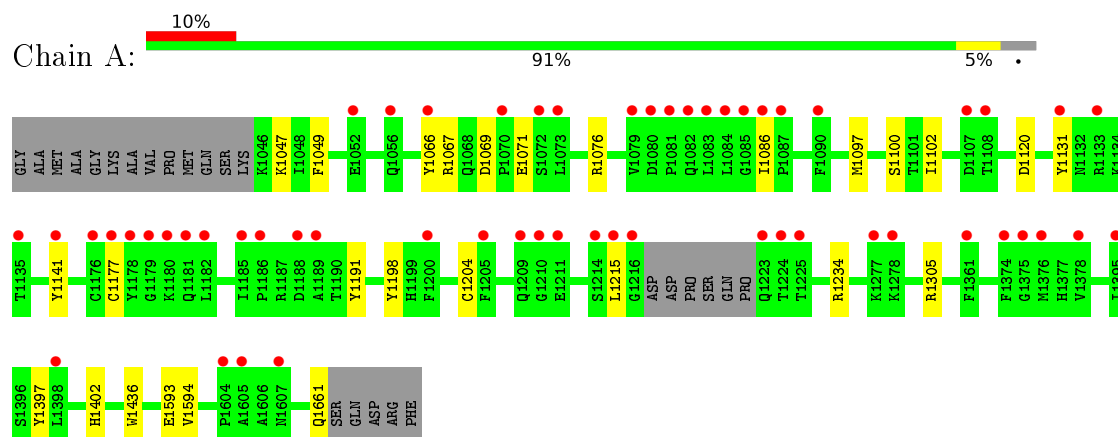
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	171	Total	O	0	0
			171	171		

### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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: Histone acetyltransferase p300, Histone acetyltransferase p300



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.81Å 155.26Å 109.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.52 29.90 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.52) 99.7 (29.90-2.52)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.207 , 0.239 0.210 , 0.239	Depositor DCC
$R_{free}$ test set	1351 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4748	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ZN, DMS, 1VU

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	0.56	0/4633	0.66	1/6267 (0.0%)

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	A	1305	ARG	NE-CZ-NH2	-5.96	117.32	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	4505	0	4367	16	0
2	A	4	0	0	0	0
3	A	52	0	36	0	0
4	A	4	0	6	0	0
5	A	12	0	16	0	0
6	A	171	0	0	2	1
All	All	4748	0	4425	16	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 2.



All (16) 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:1198:TYR:CD2	1:A:1215:LEU:HD13	2.25	0.71
1:A:1066:TYR:HE1	1:A:1076:ARG:NH1	2.00	0.59
1:A:1177:CYS:SG	1:A:1204:CYS:SG	3.02	0.58
1:A:1086:ILE:HG23	1:A:1131:TYR:OH	2.11	0.51
1:A:1066:TYR:CE1	1:A:1076:ARG:NH1	2.79	0.50
1:A:1047:LYS:HG3	1:A:1049:PHE:CE1	2.50	0.47
1:A:1067:ARG:NH2	6:A:1801:HOH:O	2.41	0.47
1:A:1071:GLU:HA	1:A:1141:TYR:CD2	2.50	0.47
1:A:1191:TYR:CE1	1:A:1234:ARG:HG3	2.50	0.46
1:A:1097:MET:HE2	1:A:1120:ASP:HB3	1.96	0.46
1:A:1097:MET:HE2	1:A:1102:ILE:HG12	1.98	0.44
1:A:1436:TRP:HD1	1:A:1594:VAL:HG12	1.83	0.43
1:A:1436:TRP:CD1	1:A:1594:VAL:HG12	2.54	0.43
1:A:1076:ARG:O	1:A:1100:SER:OG	2.26	0.43
1:A:1191:TYR:CZ	1:A:1234:ARG:HG3	2.55	0.41
1:A:1593:GLU:HG2	6:A:1862:HOH:O	2.20	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)
6:A:1957:HOH:O	6:A:1957:HOH:O[3_554]	2.03	0.17

## 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	552/578 (96%)	535 (97%)	17 (3%)	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	495/522 (95%)	491 (99%)	4 (1%)	86	96

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

Mol	Chain	Res	Type
1	A	1069	ASP
1	A	1397	TYR
1	A	1402	HIS
1	A	1661	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	1VU	A	1705	-	44,54,54	1.35	4 (9%)	54,80,80	2.29	10 (18%)
4	DMS	A	1706	-	3,3,3	0.32	0	3,3,3	1.19	0
5	GOL	A	1707	-	5,5,5	0.18	0	5,5,5	0.40	0
5	GOL	A	1708	-	5,5,5	0.28	0	5,5,5	0.62	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	1VU	A	1705	-	-	2/48/69/69	0/3/3/3
4	DMS	A	1706	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1707	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1708	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1705	1VU	P2-O16	-2.39	1.46	1.54
3	A	1705	1VU	P2-O15	-2.16	1.47	1.54
3	A	1705	1VU	C20-N5	3.91	1.41	1.33
3	A	1705	1VU	C20-N6	4.26	1.39	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1705	1VU	N6-C20-N5	-12.24	119.26	128.87
3	A	1705	1VU	C16-N2-C21	-5.30	120.89	126.81
3	A	1705	1VU	C4-C3-S	-2.97	103.58	111.47
3	A	1705	1VU	C6-C5-N	-2.78	111.63	116.46
3	A	1705	1VU	C15-O11-C16	-2.54	106.95	109.64
3	A	1705	1VU	O16-P2-O13	-2.54	99.04	106.62
3	A	1705	1VU	C7-C6-C5	-2.28	108.30	112.22
3	A	1705	1VU	C22-C16-N2	-2.17	107.66	113.47
3	A	1705	1VU	O16-P2-O15	2.37	116.16	107.44
3	A	1705	1VU	C7-N1-C8	3.35	129.34	122.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1705	1VU	C1-C2-S-C3
3	A	1705	1VU	O-C2-S-C3

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	554/578 (95%)	0.45	56 (10%) 9 10	24, 48, 110, 135	1 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1181	GLN	6.7
1	A	1182	LEU	6.5
1	A	1086	ILE	5.5
1	A	1082	GLN	5.2
1	A	1210	GLY	5.2
1	A	1215	LEU	5.0
1	A	1178	TYR	4.7
1	A	1604	PRO	4.7
1	A	1073	LEU	4.1
1	A	1186	PRO	4.0
1	A	1223	GLN	3.9
1	A	1176	CYS	3.8
1	A	1211	GLU	3.7
1	A	1607	ASN	3.6
1	A	1188	ASP	3.6
1	A	1070	PRO	3.5
1	A	1216	GLY	3.5
1	A	1085	GLY	3.3
1	A	1052	GLU	3.3
1	A	1080	ASP	3.2
1	A	1224	THR	3.2
1	A	1200	PHE	3.1
1	A	1225	THR	3.1
1	A	1277	LYS	3.0
1	A	1066	TYR	3.0
1	A	1135	THR	3.0
1	A	1083	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1079	VAL	2.9
1	A	1376	MET	2.8
1	A	1180	LYS	2.7
1	A	1278	LYS	2.7
1	A	1087	PRO	2.7
1	A	1375	GLY	2.7
1	A	1133	ARG	2.6
1	A	1189	ALA	2.6
1	A	1084	LEU	2.6
1	A	1398	LEU	2.6
1	A	1209	GLN	2.6
1	A	1179	GLY	2.5
1	A	1131	TYR	2.5
1	A	1185	ILE	2.4
1	A	1056	GLN	2.4
1	A	1605	ALA	2.4
1	A	1374	PHE	2.3
1	A	1081	PRO	2.3
1	A	1108	THR	2.3
1	A	1141	TYR	2.2
1	A	1090	PHE	2.2
1	A	1072	SER	2.2
1	A	1205	PHE	2.2
1	A	1378	VAL	2.1
1	A	1395	ILE	2.1
1	A	1361	PHE	2.1
1	A	1214	SER	2.1
1	A	1107	ASP	2.0
1	A	1177	CYS	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 ⓘ

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	DMS	A	1706	4/4	0.75	0.40	5.96	64,65,67,82	0
5	GOL	A	1708	6/6	0.92	0.23	0.78	45,53,56,57	0
5	GOL	A	1707	6/6	0.94	0.17	0.10	57,64,69,70	0
3	1VU	A	1705	52/52	0.94	0.15	-0.40	24,36,62,66	0
2	ZN	A	1703	1/1	0.99	0.09	-2.44	42,42,42,42	0
2	ZN	A	1702	1/1	0.99	0.06	-3.32	58,58,58,58	0
2	ZN	A	1704	1/1	0.99	0.07	-8.62	39,39,39,39	1
2	ZN	A	1701	1/1	0.91	0.06	-	115,115,115,115	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.