



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:23 PM BST

PDB ID : 4Z80  
Title : Crystal structure of Toxoplasma gondii AMA4 DI-DII-EGF1 in complex with a 33 aa TgRON2L1 peptide  
Authors : Parker, M.L.; Boulanger, M.J.  
Deposited on : 2015-04-08  
Resolution : 1.53 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

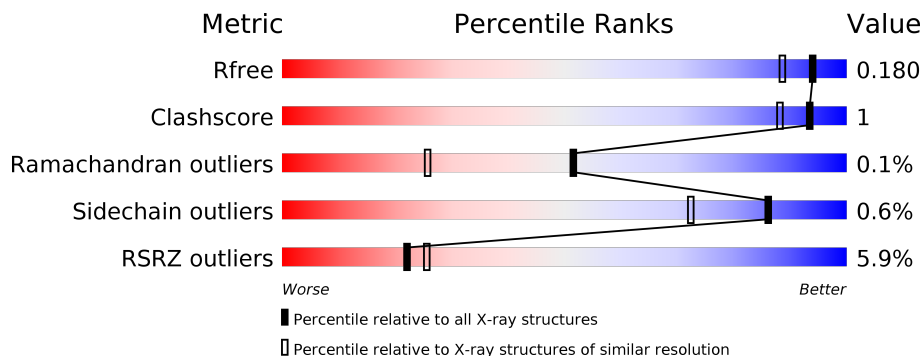
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.53 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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 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	508	<p>4% 89% 5% 2% 8%</p>
1	B	508	<p>5% 89% 5% 2% 8%</p>
2	C	37	<p>22% 78% 5% 2% 14%</p>
2	D	37	<p>19% 76% 8% 2% 16%</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9077 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 EGF family domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	466	3608	2238	630	702	38	0	2	0
1	B	466	3613	2241	631	703	38	0	3	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	GLY	-	expression tag	UNP V4YLU4
A	54	SER	-	expression tag	UNP V4YLU4
A	55	ALA	-	expression tag	UNP V4YLU4
A	56	MET	-	expression tag	UNP V4YLU4
A	57	GLY	-	expression tag	UNP V4YLU4
A	554	ALA	-	expression tag	UNP V4YLU4
A	555	ALA	-	expression tag	UNP V4YLU4
A	556	ALA	-	expression tag	UNP V4YLU4
A	557	LEU	-	expression tag	UNP V4YLU4
A	558	VAL	-	expression tag	UNP V4YLU4
A	559	PRO	-	expression tag	UNP V4YLU4
A	560	ARG	-	expression tag	UNP V4YLU4
B	53	GLY	-	expression tag	UNP V4YLU4
B	54	SER	-	expression tag	UNP V4YLU4
B	55	ALA	-	expression tag	UNP V4YLU4
B	56	MET	-	expression tag	UNP V4YLU4
B	57	GLY	-	expression tag	UNP V4YLU4
B	554	ALA	-	expression tag	UNP V4YLU4
B	555	ALA	-	expression tag	UNP V4YLU4
B	556	ALA	-	expression tag	UNP V4YLU4
B	557	LEU	-	expression tag	UNP V4YLU4
B	558	VAL	-	expression tag	UNP V4YLU4
B	559	PRO	-	expression tag	UNP V4YLU4
B	560	ARG	-	expression tag	UNP V4YLU4

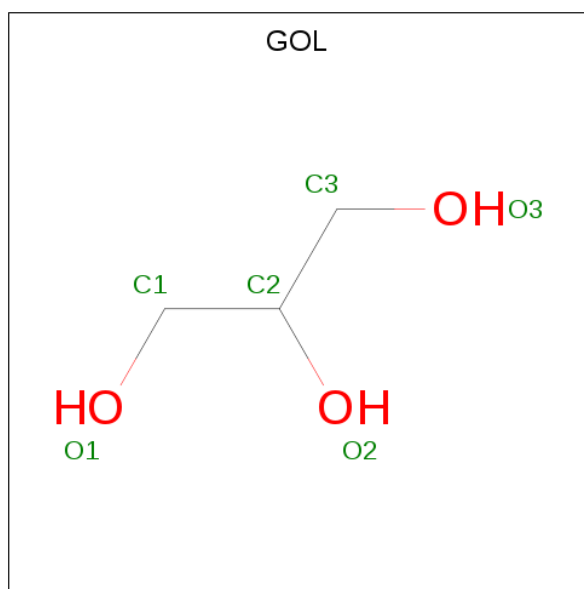
- Molecule 2 is a protein called Cytoadherence-linked asexual protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	32	Total 225	C 138	N 35	O 47	S 5	0	1	0
2	D	31	Total 217	C 132	N 34	O 46	S 5	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1288	GLY	-	expression tag	UNP B6KQU6
C	1289	SER	-	expression tag	UNP B6KQU6
C	1290	ALA	-	expression tag	UNP B6KQU6
C	1291	SER	-	expression tag	UNP B6KQU6
D	1288	GLY	-	expression tag	UNP B6KQU6
D	1289	SER	-	expression tag	UNP B6KQU6
D	1290	ALA	-	expression tag	UNP B6KQU6
D	1291	SER	-	expression tag	UNP B6KQU6

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	682	Total	O	0	0
			682	682		
6	C	30	Total	O	0	0
			30	30		
6	B	627	Total	O	0	0
			627	627		
6	D	22	Total	O	0	0
			22	22		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.56Å 120.56Å 141.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.18 – 1.53 37.18 – 1.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.18-1.53) 98.5 (37.18-1.53)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 1.53Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.153 , 0.172 0.163 , 0.180	Depositor DCC
$R_{free}$ test set	8828 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, SO4

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	0.32	0/3709	0.53	0/5035
1	B	0.31	0/3717	0.51	0/5046
2	C	0.70	0/231	0.71	0/312
2	D	0.26	0/223	0.46	0/301
All	All	0.33	0/7880	0.53	0/10694

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
2	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1319	GLY	Peptide

### 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	3608	0	3413	8	0
1	B	3613	0	3418	7	0
2	C	225	0	222	3	0
2	D	217	0	211	4	0
3	A	18	0	24	0	0
3	B	6	0	8	0	0
4	A	15	0	0	0	0
5	B	14	0	13	0	0
6	A	682	0	0	4	5
6	B	627	0	0	3	5
6	C	30	0	0	3	0
6	D	22	0	0	3	0
All	All	9077	0	7309	21	5

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 (21) 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:163:ARG:NH2	6:B:701:HOH:O	2.12	0.80
2:C:1320:ASP:OD2	6:C:1401:HOH:O	2.10	0.68
1:A:523:CYS:SG	6:A:1327:HOH:O	2.54	0.65
1:B:98:ARG:NH1	6:B:707:HOH:O	2.35	0.59
1:A:321:LYS:HD3	6:A:705:HOH:O	2.10	0.50
1:B:249:THR:HB	2:D:1318:ILE:HD13	1.93	0.50
1:B:283:CYS:HB3	6:B:993:HOH:O	2.12	0.49
1:A:433:CYS:SG	1:A:479[B]:CYS:HB3	2.54	0.47
1:A:129:ALA:O	1:A:134:LYS:NZ	2.38	0.47
1:A:140:PRO:HG2	6:A:871:HOH:O	2.14	0.46
2:D:1317:THR:HB	6:D:1401:HOH:O	2.16	0.46
2:D:1314[A]:MET:HG3	6:D:1416:HOH:O	2.16	0.45
1:B:433:CYS:SG	1:B:479[B]:CYS:HB3	2.57	0.44
1:B:98:ARG:HH11	1:B:98:ARG:HG3	1.83	0.44
2:C:1320:ASP:OD1	6:C:1402:HOH:O	2.21	0.44
2:D:1317:THR:CB	6:D:1401:HOH:O	2.66	0.43
1:A:277:GLN:NE2	6:A:702:HOH:O	2.30	0.42
1:A:221:ARG:HA	1:A:225:VAL:HG22	2.02	0.41
2:C:1314:MET:HG2	6:C:1403:HOH:O	2.20	0.41
1:B:130:LYS:HB3	1:B:325:ASN:HA	2.03	0.41
1:A:89:SER:HB3	1:A:98:ARG:HH21	1.85	0.41

All (5) 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:702:HOH:O	6:B:1094:HOH:O[3_575]	1.90	0.30
6:A:1187:HOH:O	6:B:1147:HOH:O[5_565]	2.03	0.17
6:A:1135:HOH:O	6:B:796:HOH:O[3_575]	2.07	0.13
6:A:798:HOH:O	6:B:1093:HOH:O[5_565]	2.08	0.12
6:A:992:HOH:O	6:B:722:HOH:O[5_565]	2.15	0.05

## 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	466/508 (92%)	447 (96%)	19 (4%)	0	100	100
1	B	467/508 (92%)	449 (96%)	18 (4%)	0	100	100
2	C	31/37 (84%)	30 (97%)	0	1 (3%)	4	0
2	D	30/37 (81%)	30 (100%)	0	0	100	100
All	All	994/1090 (91%)	956 (96%)	37 (4%)	1 (0%)	51	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1319	GLY

### 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	401/428 (94%)	400 (100%)	1 (0%)	93	86
1	B	402/428 (94%)	398 (99%)	4 (1%)	76	55
2	C	27/29 (93%)	27 (100%)	0	100	100
2	D	26/29 (90%)	26 (100%)	0	100	100
All	All	856/914 (94%)	851 (99%)	5 (1%)	86	72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	PHE
1	B	187	SER
1	B	203	PHE
1	B	240	GLU
1	B	256	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 ligands are 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$
3	GOL	A	601	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	A	602	-	5,5,5	0.43	0	5,5,5	0.50	0
4	SO4	A	604	-	4,4,4	0.16	0	6,6,6	0.27	0
4	SO4	A	605	-	4,4,4	0.12	0	6,6,6	0.19	0
3	GOL	A	603	-	5,5,5	0.36	0	5,5,5	0.47	0
4	SO4	A	606	-	4,4,4	0.14	0	6,6,6	0.19	0
5	NAG	B	601	1	14,14,15	0.29	0	17,19,21	0.62	0
3	GOL	B	602	-	5,5,5	0.42	0	5,5,5	0.47	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	GOL	A	602	-	-	2/4/4/4	-
3	GOL	A	601	-	-	0/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
5	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	GOL	B	602	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-C3
3	A	603	GOL	C1-C2-C3-O3
3	B	602	GOL	O1-C1-C2-C3
5	B	601	NAG	C8-C7-N2-C2
5	B	601	NAG	O7-C7-N2-C2
3	A	603	GOL	O2-C2-C3-O3
3	A	602	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-O2

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 [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, 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	466/508 (91%)	0.03	21 (4%) 33 38	10, 16, 32, 63	0
1	B	466/508 (91%)	0.17	23 (4%) 29 33	10, 17, 37, 61	0
2	C	32/37 (86%)	1.16	8 (25%) 0 0	16, 23, 44, 50	0
2	D	31/37 (83%)	1.45	7 (22%) 0 0	22, 31, 40, 48	0
All	All	995/1090 (91%)	0.18	59 (5%) 22 25	10, 17, 37, 63	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1293	ILE	11.0
2	D	1324	SER	7.4
1	B	94	ASN	7.0
1	B	523	CYS	6.9
1	A	523	CYS	6.2
1	A	524	VAL	6.2
1	A	255	THR	6.1
1	A	93	GLY	5.6
1	A	94	ASN	5.5
1	B	524	VAL	5.2
1	B	250	THR	4.8
1	A	254	SER	4.7
2	D	1322	ILE	4.6
1	A	257	PRO	4.6
1	A	252	ARG	4.5
2	C	1317	THR	4.1
1	A	250	THR	4.0
2	D	1316	GLY	4.0
1	B	93	GLY	4.0
1	A	188	ARG	3.9
1	B	252	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	188	ARG	3.8
1	A	253	GLN	3.7
2	C	1316	GLY	3.7
1	A	251	GLN	3.4
2	C	1314	MET	3.2
1	A	415	TYR	3.1
1	B	254	SER	3.0
2	D	1318	ILE	2.9
1	B	318	TRP	2.8
2	D	1323	ALA	2.8
1	B	253	GLN	2.7
1	A	256	GLN	2.7
1	A	522	LYS	2.7
1	B	251	GLN	2.7
1	B	279	SER	2.6
1	B	255	THR	2.6
1	B	257	PRO	2.6
1	B	344	LEU	2.6
2	C	1320	ASP	2.6
2	D	1321	PRO	2.5
1	B	249	THR	2.5
1	B	278	THR	2.5
1	A	59	SER	2.5
1	B	95	THR	2.4
1	B	59	SER	2.4
2	D	1320	ASP	2.4
1	A	344	LEU	2.4
2	C	1313	CYS	2.3
1	A	330	LEU	2.3
1	B	330	LEU	2.3
1	B	415	TYR	2.3
1	A	249	THR	2.2
1	A	95	THR	2.2
1	A	91	THR	2.1
2	C	1319	GLY	2.1
1	B	91	THR	2.1
2	C	1294	VAL	2.0
1	B	241	SER	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 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	601	14/15	0.72	0.20	39,48,52,55	0
3	GOL	A	602	6/6	0.80	0.14	19,25,28,29	0
3	GOL	B	602	6/6	0.84	0.14	22,24,32,34	0
3	GOL	A	601	6/6	0.93	0.12	23,29,33,39	0
3	GOL	A	603	6/6	0.93	0.12	18,33,39,44	0
4	SO4	A	605	5/5	0.96	0.08	24,27,30,33	0
4	SO4	A	604	5/5	0.98	0.09	20,23,28,28	0
4	SO4	A	606	5/5	0.99	0.09	22,24,27,30	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.