



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:15 am GMT

PDB ID : 1A0E  
Title : XYLOSE ISOMERASE FROM THERMOTOGA NEAPOLITANA  
Authors : Gallay, O.; Chopra, R.; Conti, E.; Brick, P.; Blow, D.  
Deposited on : 1997-11-28  
Resolution : 2.70 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

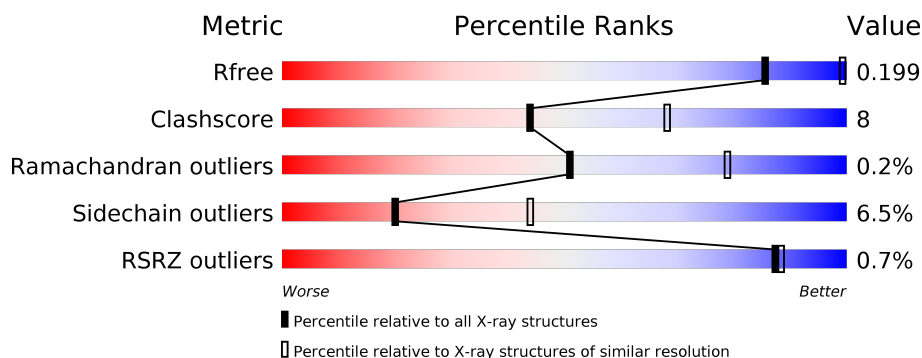
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	443	<div> <div>80%</div> <div>18%</div> <div>•</div> </div>
1	D	443	<div> <div>%</div> <div>80%</div> <div>17%</div> <div>•</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7274 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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3506	2272	572	652	10			
1	D	443	Total	C	N	O	S	0	0	0
			3506	2272	572	652	10			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Co	0	0
			3	3		
2	D	3	Total	Co	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	D	128	Total	O	0	0
			128	128		



● Molecule 1: XYLOSE ISOMERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.79Å 121.87Å 98.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.50 – 2.70 12.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (12.50-2.70) 97.1 (12.49-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 2.71Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.180 , 0.203 0.178 , 0.199	Depositor DCC
$R_{free}$ test set	1265 reflections (4.84%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.98% 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: CO

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	0.43	1/3596 (0.0%)	0.63	2/4865 (0.0%)
1	D	0.43	1/3596 (0.0%)	0.62	2/4865 (0.0%)
All	All	0.43	2/7192 (0.0%)	0.63	4/9730 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	GLU	CG-CD	5.56	1.60	1.51
1	D	349	GLU	CG-CD	5.55	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	D	306	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	D	306	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	306	ASP	CB-CG-OD1	5.82	123.53	118.30

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	3506	0	3359	57	0
1	D	3506	0	3359	51	2
2	A	3	0	0	0	1
2	D	3	0	0	0	1
3	A	128	0	0	2	0
3	D	128	0	0	3	0
All	All	7274	0	6718	104	3

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 8.

All (104) 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:D:306:ASP:HB3	3:D:621:HOH:O	1.71	0.90
1:A:306:ASP:HB3	3:A:616:HOH:O	1.71	0.89
1:D:402:VAL:CG1	1:D:407:LEU:HG	2.08	0.84
1:A:402:VAL:CG1	1:A:407:LEU:HG	2.08	0.83
1:A:402:VAL:HG11	1:A:407:LEU:HG	1.67	0.77
1:D:402:VAL:HG11	1:D:407:LEU:HG	1.67	0.76
1:D:79:PHE:CD1	1:D:124:ARG:HD2	2.21	0.76
1:A:79:PHE:CD1	1:A:124:ARG:HD2	2.21	0.75
1:D:213:ARG:HB3	1:D:213:ARG:NH1	2.06	0.70
1:A:213:ARG:NH1	1:A:213:ARG:HB3	2.06	0.70
1:A:396:ASP:HB3	1:A:402:VAL:HG23	1.77	0.65
1:D:396:ASP:HB3	1:D:402:VAL:HG23	1.77	0.65
1:D:439:ILE:HA	1:D:442:LEU:HD22	1.80	0.63
1:A:245:ASP:HB2	1:A:281:GLU:OE2	1.99	0.63
1:D:198:ASN:C	1:D:198:ASN:HD22	2.02	0.63
1:A:439:ILE:HA	1:A:442:LEU:HD22	1.80	0.62
1:A:198:ASN:HD22	1:A:198:ASN:C	2.01	0.62
1:D:245:ASP:HB2	1:D:281:GLU:OE2	1.99	0.61
1:A:317:THR:HG21	1:A:361:THR:HG22	1.83	0.60
1:A:190:ARG:HD3	3:A:604:HOH:O	2.01	0.60
1:D:317:THR:HG21	1:D:361:THR:HG22	1.83	0.60
1:D:6:GLU:HG2	1:D:7:ILE:HD12	1.85	0.59
1:D:190:ARG:HD3	3:D:609:HOH:O	2.01	0.59
1:A:57:ASP:HB2	1:A:58:PRO:HD2	1.84	0.58
1:D:272:THR:HA	1:D:276:HIS:O	2.04	0.58
1:D:57:ASP:HB2	1:D:58:PRO:HD2	1.84	0.58
1:A:6:GLU:HG2	1:A:7:ILE:HD12	1.84	0.57
1:A:272:THR:HA	1:A:276:HIS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:PHE:CZ	1:D:85:LEU:HA	2.41	0.56
1:A:51:PHE:CZ	1:A:85:LEU:HA	2.41	0.56
1:D:100:HIS:CD2	1:D:140:THR:HG23	2.41	0.56
1:A:233:LYS:HE2	1:A:235:LYS:O	2.06	0.56
1:A:100:HIS:CD2	1:A:140:THR:HG23	2.41	0.55
1:A:402:VAL:HG11	1:A:407:LEU:CG	2.37	0.55
1:D:402:VAL:HG11	1:D:407:LEU:CG	2.37	0.55
1:D:233:LYS:HE2	1:D:235:LYS:O	2.06	0.54
1:A:288:LEU:HB3	1:A:290:LYS:HG3	1.94	0.49
1:D:288:LEU:HB3	1:D:290:LYS:HG3	1.94	0.49
1:A:402:VAL:HG12	1:A:403:ASP:N	2.28	0.49
1:D:49:HIS:O	1:D:53:ASN:HB3	2.13	0.49
1:A:49:HIS:O	1:A:53:ASN:HB3	2.13	0.49
1:D:402:VAL:HG12	1:D:403:ASP:N	2.28	0.48
1:A:439:ILE:HG23	1:D:436:VAL:HG13	1.94	0.48
1:D:263:LYS:HA	1:D:290:LYS:HB3	1.94	0.48
1:A:436:VAL:HG13	1:D:439:ILE:HG23	1.95	0.48
1:D:67:PRO:HG2	1:D:68:TRP:CE3	2.49	0.48
1:A:263:LYS:HA	1:A:290:LYS:HB3	1.94	0.48
1:A:213:ARG:HH11	1:A:213:ARG:CG	2.27	0.47
1:A:314:VAL:HG22	1:D:315:TYR:OH	2.14	0.47
1:D:213:ARG:HH11	1:D:213:ARG:CG	2.27	0.47
1:A:67:PRO:HG2	1:A:68:TRP:CE3	2.49	0.47
1:A:170:LYS:HG3	1:A:218:TYR:CE2	2.50	0.47
1:A:92:LEU:HD13	1:A:352:PHE:HD1	1.80	0.46
1:D:170:LYS:HG3	1:D:218:TYR:CE2	2.50	0.46
1:D:92:LEU:HD13	1:D:352:PHE:HD1	1.80	0.46
1:A:4:PHE:O	1:A:91:LYS:NZ	2.50	0.44
1:A:146:HIS:ND1	1:A:148:ARG:HB3	2.33	0.44
1:D:306:ASP:CB	3:D:621:HOH:O	2.48	0.44
1:D:4:PHE:O	1:D:91:LYS:NZ	2.50	0.44
1:A:213:ARG:CZ	1:A:213:ARG:HB3	2.48	0.44
1:D:146:HIS:ND1	1:D:148:ARG:HB3	2.33	0.44
1:D:213:ARG:HB3	1:D:213:ARG:CZ	2.48	0.44
1:A:50:THR:HG23	1:A:351:LEU:HD22	1.99	0.44
1:A:107:GLU:HG2	1:A:114:THR:OG1	2.18	0.43
1:D:50:THR:HG23	1:D:351:LEU:HD22	1.99	0.43
1:A:207:ASN:OD1	1:A:210:ARG:NH1	2.51	0.43
1:D:107:GLU:HG2	1:D:114:THR:OG1	2.18	0.43
1:A:100:HIS:HB2	1:A:103:ASP:CG	2.39	0.43
1:D:286:ARG:NH1	1:D:323:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:HD12	1:A:307:THR:HG21	2.00	0.43
1:D:100:HIS:HB2	1:D:103:ASP:CG	2.39	0.43
1:D:207:ASN:OD1	1:D:210:ARG:NH1	2.51	0.42
1:D:303:LEU:HD12	1:D:307:THR:HG21	2.01	0.42
1:A:439:ILE:O	1:A:442:LEU:HB2	2.19	0.42
1:D:439:ILE:O	1:D:442:LEU:HB2	2.19	0.42
1:A:213:ARG:NH1	1:A:213:ARG:CB	2.81	0.42
1:A:286:ARG:NH1	1:A:323:GLU:OE1	2.51	0.42
1:D:421:SER:HB3	1:D:423:LYS:HE2	2.01	0.42
1:D:69:ASN:HD22	1:D:77:LYS:HE3	1.85	0.42
1:A:421:SER:HB3	1:A:423:LYS:HE2	2.01	0.42
1:A:315:TYR:OH	1:D:314:VAL:HG22	2.20	0.41
1:A:173:LEU:HA	1:A:173:LEU:HD23	1.92	0.41
1:A:286:ARG:HG3	1:A:327:ALA:HB2	2.02	0.41
1:A:69:ASN:HD22	1:A:77:LYS:HE3	1.85	0.41
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.85	0.41
1:D:385:LYS:HD3	1:D:386:TYR:CE1	2.56	0.41
1:A:385:LYS:HD3	1:A:386:TYR:CE1	2.56	0.41
1:D:286:ARG:HG3	1:D:327:ALA:HB2	2.02	0.41
1:A:31:ILE:HA	1:A:35:LYS:O	2.21	0.41
1:D:213:ARG:O	1:D:216:VAL:HG22	2.21	0.41
1:A:213:ARG:O	1:A:216:VAL:HG22	2.21	0.40
1:D:31:ILE:HA	1:D:35:LYS:O	2.22	0.40
1:D:427:LEU:O	1:D:430:LEU:HB2	2.21	0.40
1:A:384:GLU:O	1:A:387:ARG:HB2	2.22	0.40
1:D:233:LYS:O	1:D:241:GLN:HB3	2.21	0.40
1:A:283:ARG:HD3	1:A:323:GLU:OE1	2.22	0.40
1:A:419:LEU:HA	1:A:420:PRO:HD3	1.91	0.40
1:A:430:LEU:HA	1:A:430:LEU:HD23	1.93	0.40
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.77	0.40
1:D:402:VAL:CG1	1:D:403:ASP:N	2.84	0.40
1:D:431:ILE:O	1:D:435:ILE:HG13	2.21	0.40
1:A:402:VAL:CG1	1:A:403:ASP:N	2.84	0.40
1:A:431:ILE:O	1:A:435:ILE:HG13	2.21	0.40
1:A:69:ASN:HA	1:A:69:ASN:HD22	1.61	0.40

All (3) 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)
2:A:493:CO:CO	2:A:493:CO:CO[3_655]	0.32	1.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:GLU:CG	2:D:493:CO:CO[3_555]	1.42	0.78
1:D:2:GLU:CB	1:D:2:GLU:OE2[3_555]	2.14	0.06

## 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	441/443 (100%)	424 (96%)	16 (4%)	1 (0%)	51	79
1	D	441/443 (100%)	424 (96%)	16 (4%)	1 (0%)	51	79
All	All	882/886 (100%)	848 (96%)	32 (4%)	2 (0%)	51	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	GLU
1	D	236	GLU

### 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	354/374 (95%)	331 (94%)	23 (6%)	20	44
1	D	354/374 (95%)	331 (94%)	23 (6%)	20	44
All	All	708/748 (95%)	662 (94%)	46 (6%)	20	44

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	18	THR
1	A	29	GLU
1	A	31	ILE
1	A	69	ASN
1	A	85	LEU
1	A	113	GLU
1	A	134	VAL
1	A	198	ASN
1	A	212	LEU
1	A	213	ARG
1	A	258	LEU
1	A	269	ASN
1	A	282	LEU
1	A	283	ARG
1	A	288	LEU
1	A	290	LYS
1	A	306	ASP
1	A	319	LEU
1	A	371	LYS
1	A	411	ILE
1	A	427	LEU
1	A	442	LEU
1	D	6	GLU
1	D	18	THR
1	D	29	GLU
1	D	31	ILE
1	D	69	ASN
1	D	85	LEU
1	D	113	GLU
1	D	134	VAL
1	D	198	ASN
1	D	212	LEU
1	D	213	ARG
1	D	258	LEU
1	D	269	ASN
1	D	282	LEU
1	D	283	ARG
1	D	288	LEU
1	D	290	LYS
1	D	306	ASP
1	D	319	LEU

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Mol	Chain	Res	Type
1	D	371	LYS
1	D	411	ILE
1	D	427	LEU
1	D	442	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	100	HIS
1	A	115	ASN
1	A	198	ASN
1	A	241	GLN
1	A	424	GLN
1	A	432	ASN
1	D	69	ASN
1	D	115	ASN
1	D	198	ASN
1	D	241	GLN
1	D	424	GLN
1	D	432	ASN

### 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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

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	443/443 (100%)	-0.72	2 (0%) 90 92	18, 36, 63, 84	0
1	D	443/443 (100%)	-0.60	4 (0%) 84 85	18, 36, 63, 84	0
All	All	886/886 (100%)	-0.66	6 (0%) 87 88	18, 36, 64, 84	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	3.0
1	D	127	GLU	2.5
1	D	391	GLU	2.4
1	D	383	GLU	2.3
1	A	70	ARG	2.2
1	A	1	ALA	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 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( $\text{\AA}^2$ )	Q<0.9
2	CO	A	492	1/1	0.97	0.07	-1.69	44,44,44,44	0
2	CO	A	491	1/1	0.97	0.04	-2.97	48,48,48,48	0
2	CO	D	492	1/1	0.99	0.05	-4.41	44,44,44,44	0
2	CO	D	491	1/1	0.98	0.03	-10.75	48,48,48,48	0
2	CO	A	493	1/1	0.94	0.36	-	56,56,56,56	0
2	CO	D	493	1/1	0.94	0.28	-	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.