



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:32 AM BST

PDB ID : 1LSL  
Title : Crystal Structure of the Thrombospondin-1 Type 1 Repeats  
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Deposited on : 2002-05-17  
Resolution : 1.90 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

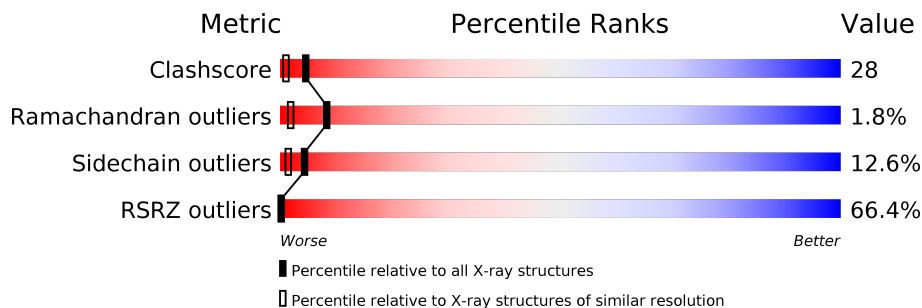
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	113	

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
2	FUL	A	1432	-	-	-	X
3	FUC	A	1489	X	-	-	-

## 2 Entry composition [i](#)

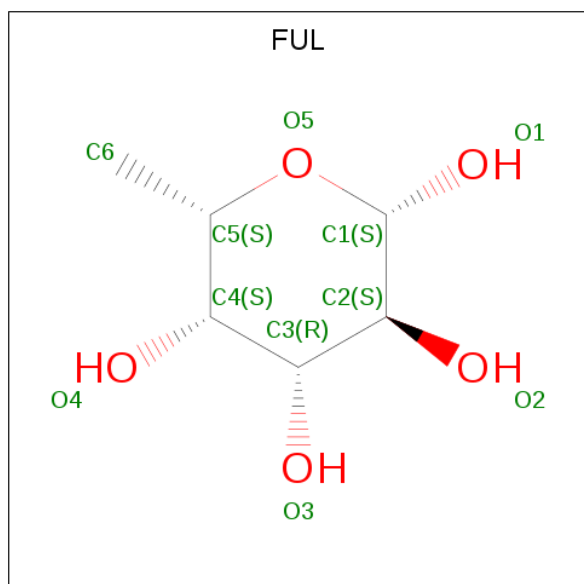
There are 4 unique types of molecules in this entry. The entry contains 1018 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thrombospondin 1.

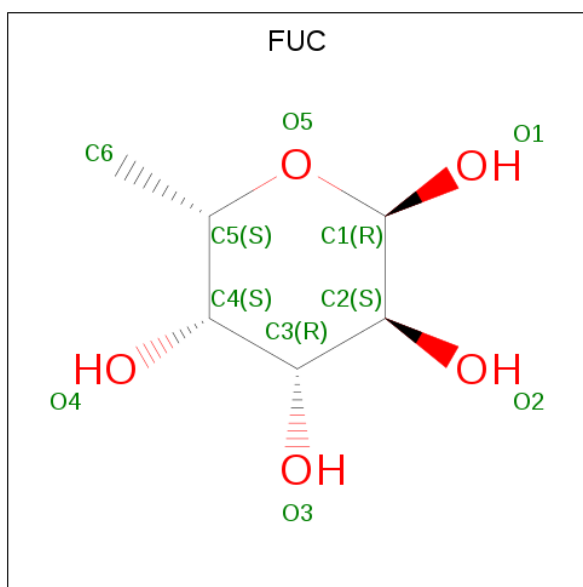
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	113	844	510	156	165	13	0	0	0

- Molecule 2 is beta-L-fucopyranose (three-letter code: FUL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	10	6	4	0	0

- Molecule 3 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

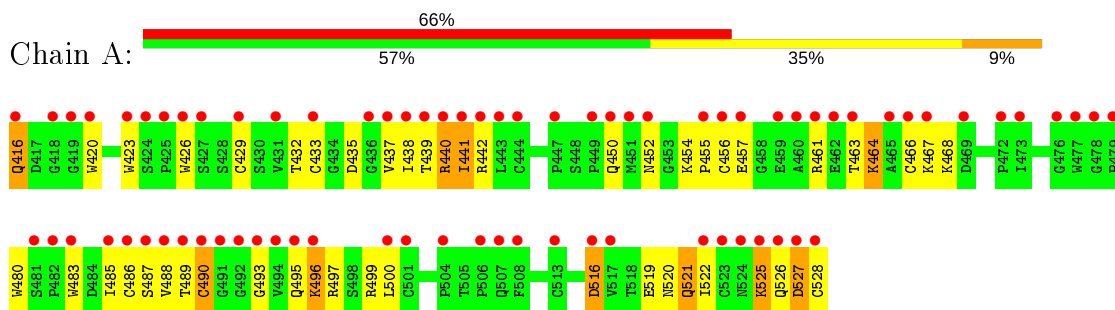
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		

### 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: Thrombospondin 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.63Å 84.41Å 37.17Å 90.00° 108.67° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 18.54 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.90) 97.5 (18.54-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.53 (at 1.90Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.238 , 0.282 0.267 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	7.7	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 68.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.29$ , $\langle L^2 \rangle = 0.13$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	1018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: FUL, FUC

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	0.39	0/866	0.73	0/1174

There are no bond length outliers.

There are no bond angle outliers.

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	844	0	774	46	0
2	A	10	0	10	2	0
3	A	10	0	10	1	0
4	A	154	0	0	5	0
All	All	1018	0	794	47	0

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 28.

All (47) 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:490:CYS:HB2	1:A:528:CYS:HA	1.34	1.07
1:A:441:ILE:HG22	1:A:461:ARG:HG2	1.57	0.86
1:A:516:ASP:HB3	4:A:1148:HOH:O	1.80	0.81
1:A:525:LYS:O	1:A:526:GLN:HG3	1.90	0.70
1:A:488:VAL:HG11	4:A:1153:HOH:O	1.91	0.69
1:A:432:THR:HB	2:A:1432:FUL:O2	1.89	0.68
1:A:488:VAL:HG12	1:A:490:CYS:H	1.65	0.62
3:A:1489:FUC:H2	4:A:1150:HOH:O	2.04	0.57
1:A:483:TRP:CZ3	1:A:497:ARG:HB2	2.40	0.56
1:A:416:GLN:N	1:A:450:GLN:NE2	2.52	0.56
1:A:423:TRP:CH2	1:A:442:ARG:HD2	2.41	0.56
1:A:490:CYS:O	1:A:526:GLN:O	2.24	0.56
1:A:525:LYS:O	1:A:525:LYS:HG2	2.06	0.55
1:A:496:LYS:NZ	1:A:520:ASN:HD21	2.03	0.55
1:A:416:GLN:HB3	1:A:450:GLN:HG2	1.89	0.54
1:A:486:CYS:SG	1:A:493:GLY:HA3	2.47	0.54
1:A:483:TRP:CE3	1:A:497:ARG:HB2	2.43	0.53
1:A:493:GLY:O	1:A:522:ILE:HA	2.08	0.53
1:A:480:TRP:CE3	1:A:499:ARG:HG3	2.44	0.53
1:A:429:CYS:CB	1:A:468:LYS:HE2	2.39	0.53
1:A:416:GLN:HA	1:A:416:GLN:NE2	2.25	0.51
1:A:516:ASP:N	1:A:516:ASP:OD1	2.26	0.51
1:A:525:LYS:C	1:A:526:GLN:HG3	2.31	0.51
1:A:466:CYS:HB2	4:A:1056:HOH:O	2.11	0.50
1:A:437:VAL:HB	1:A:463:THR:HG23	1.94	0.50
1:A:416:GLN:HA	1:A:416:GLN:HE21	1.76	0.50
1:A:433:CYS:HA	1:A:468:LYS:HB2	1.94	0.49
1:A:496:LYS:HG3	1:A:520:ASN:ND2	2.27	0.49
1:A:525:LYS:NZ	4:A:1151:HOH:O	2.45	0.48
1:A:437:VAL:HB	1:A:464:LYS:O	2.16	0.46
1:A:487:SER:O	1:A:488:VAL:HG23	2.15	0.46
1:A:488:VAL:CG1	1:A:489:THR:N	2.79	0.46
1:A:480:TRP:CH2	1:A:499:ARG:HD2	2.51	0.45
1:A:525:LYS:CG	1:A:525:LYS:O	2.64	0.45
1:A:483:TRP:CZ2	1:A:497:ARG:HD2	2.52	0.45
1:A:495:GLN:NE2	1:A:521:GLN:OE1	2.51	0.44
1:A:439:THR:HG22	1:A:440:ARG:N	2.33	0.43
1:A:432:THR:CB	2:A:1432:FUL:O2	2.62	0.43
1:A:435:ASP:OD1	1:A:467:LYS:HG2	2.19	0.42
1:A:497:ARG:NH1	1:A:519:GLU:OE1	2.49	0.42
1:A:420:TRP:CE2	1:A:456:CYS:HB3	2.54	0.42
1:A:438:ILE:HD11	1:A:464:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:HG12	1:A:489:THR:N	2.34	0.42
1:A:416:GLN:CA	1:A:416:GLN:HE21	2.32	0.41
1:A:426:TRP:CZ2	1:A:440:ARG:HD2	2.54	0.41
1:A:527:ASP:OD2	1:A:527:ASP:O	2.39	0.41
1:A:454:LYS:HA	1:A:455:PRO:HD3	1.89	0.40

There are no symmetry-related clashes.

## 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	111/113 (98%)	105 (95%)	4 (4%)	2 (2%)	<b>8</b> <b>2</b>

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	CYS
1	A	527	ASP

### 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	95/95 (100%)	83 (87%)	12 (13%)	<b>4</b> <b>1</b>

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	GLN
1	A	440	ARG
1	A	441	ILE
1	A	452	ASN
1	A	457	GLU
1	A	464	LYS
1	A	485	ILE
1	A	496	LYS
1	A	500	LEU
1	A	516	ASP
1	A	521	GLN
1	A	525	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	GLN
1	A	495	GLN
1	A	520	ASN
1	A	521	GLN
1	A	526	GLN

### 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](#)

2 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
2	FUL	A	1432	1	10,10,11	0.59	0	14,14,16	0.56	0
3	FUC	A	1489	1	10,10,11	0.73	0	14,14,16	0.67	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	FUL	A	1432	1	-	-	0/1/1/1
3	FUC	A	1489	1	1/1/4/5	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1489	FUC	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1432	FUL	2	0
3	A	1489	FUC	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	113/113 (100%)	3.02	75 (66%) <b>0</b> <b>0</b>	17, 35, 89, 100	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	GLY	16.4
1	A	488	VAL	11.4
1	A	490	CYS	9.9
1	A	528	CYS	8.6
1	A	489	THR	8.4
1	A	527	ASP	7.7
1	A	494	VAL	6.9
1	A	451	MET	6.8
1	A	491	GLY	5.7
1	A	438	ILE	5.5
1	A	526	GLN	5.3
1	A	524	ASN	5.3
1	A	485	ILE	4.9
1	A	450	GLN	4.7
1	A	493	GLY	4.6
1	A	525	LYS	4.4
1	A	449	PRO	4.3
1	A	436	GLY	4.3
1	A	437	VAL	4.2
1	A	486	CYS	3.8
1	A	420	TRP	3.7
1	A	516	ASP	3.7
1	A	441	ILE	3.6
1	A	461	ARG	3.6
1	A	523	CYS	3.6
1	A	522	ILE	3.6
1	A	495	GLN	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	444	CYS	3.5
1	A	501	CYS	3.5
1	A	460	ALA	3.5
1	A	452	ASN	3.4
1	A	517	VAL	3.4
1	A	500	LEU	3.4
1	A	508	PHE	3.2
1	A	477	TRP	3.0
1	A	439	THR	3.0
1	A	424	SER	3.0
1	A	426	TRP	2.9
1	A	478	GLY	2.9
1	A	416	GLN	2.9
1	A	423	TRP	2.9
1	A	465	ALA	2.8
1	A	483	TRP	2.7
1	A	463	THR	2.7
1	A	481	SER	2.6
1	A	479	PRO	2.6
1	A	473	ILE	2.6
1	A	466	CYS	2.6
1	A	476	GLY	2.5
1	A	427	SER	2.5
1	A	459	GLU	2.5
1	A	443	LEU	2.5
1	A	442	ARG	2.5
1	A	482	PRO	2.4
1	A	462	GLU	2.4
1	A	487	SER	2.4
1	A	456	CYS	2.4
1	A	447	PRO	2.4
1	A	455	PRO	2.4
1	A	513	CYS	2.3
1	A	506	PRO	2.3
1	A	431	VAL	2.3
1	A	418	GLY	2.2
1	A	504	PRO	2.2
1	A	467	LYS	2.2
1	A	419	GLY	2.2
1	A	507	GLN	2.2
1	A	425	PRO	2.1
1	A	433	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	472	PRO	2.1
1	A	496	LYS	2.1
1	A	457	GLU	2.1
1	A	469	ASP	2.1
1	A	429	CYS	2.1
1	A	440	ARG	2.0

## 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, 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
3	FUC	A	1489	10/11	0.55	0.37	93,95,96,97	0
2	FUL	A	1432	10/11	0.64	0.41	62,69,73,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.