



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:23 pm GMT

PDB ID : 4C22  
Title : L-Fucose Isomerase In Complex With Fuculose  
Authors : Higgins, M.A.; Suits, M.D.L.; Marsters, C.; Boraston, A.B.  
Deposited on : 2013-08-16  
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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
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

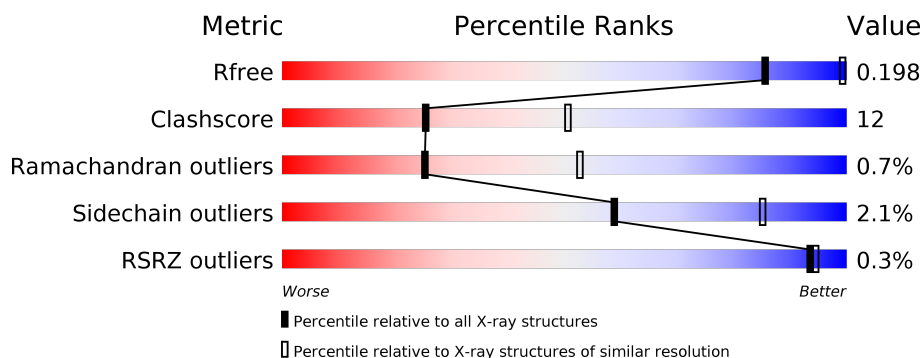
# 1 Overall quality at a glance ⓘ

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	604	
1	B	604	

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
3	FUC	A	603	-	-	-	X
3	FUC	B	603	-	-	-	X
5	EDO	A	1590	-	-	X	X
5	EDO	A	1591	-	-	-	X
5	EDO	A	1592	-	-	X	X
5	EDO	A	1593	-	-	-	X
5	EDO	A	1594	-	-	-	X
5	EDO	A	1595	-	-	-	X
5	EDO	A	1596	-	-	-	X
5	EDO	B	1590	-	-	X	X
5	EDO	B	1591	-	-	-	X
5	EDO	B	1592	-	-	-	X
5	EDO	B	1593	-	-	X	X
5	EDO	B	1594	-	-	-	X
5	EDO	B	1595	-	-	-	X
5	EDO	B	1596	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9901 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 L-FUCOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	1	0
			4612	2916	799	869	28			
1	B	604	Total	C	N	O	S	0	0	0
			4732	2989	826	888	29			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	EXPRESSION TAG	UNP Q97N97
A	-14	HIS	-	EXPRESSION TAG	UNP Q97N97
A	-13	HIS	-	EXPRESSION TAG	UNP Q97N97
A	-12	HIS	-	EXPRESSION TAG	UNP Q97N97
A	-11	SER	-	EXPRESSION TAG	UNP Q97N97
A	-10	SER	-	EXPRESSION TAG	UNP Q97N97
A	-9	GLY	-	EXPRESSION TAG	UNP Q97N97
A	-8	LEU	-	EXPRESSION TAG	UNP Q97N97
A	-7	VAL	-	EXPRESSION TAG	UNP Q97N97
A	-6	PRO	-	EXPRESSION TAG	UNP Q97N97
A	-5	ARG	-	EXPRESSION TAG	UNP Q97N97
A	-4	GLY	-	EXPRESSION TAG	UNP Q97N97
A	-3	SER	-	EXPRESSION TAG	UNP Q97N97
A	-2	HIS	-	EXPRESSION TAG	UNP Q97N97
A	-1	MET	-	EXPRESSION TAG	UNP Q97N97
A	0	ALA	-	EXPRESSION TAG	UNP Q97N97
A	1	SER	-	EXPRESSION TAG	UNP Q97N97
B	-15	HIS	-	EXPRESSION TAG	UNP Q97N97
B	-14	HIS	-	EXPRESSION TAG	UNP Q97N97
B	-13	HIS	-	EXPRESSION TAG	UNP Q97N97
B	-12	HIS	-	EXPRESSION TAG	UNP Q97N97
B	-11	SER	-	EXPRESSION TAG	UNP Q97N97
B	-10	SER	-	EXPRESSION TAG	UNP Q97N97
B	-9	GLY	-	EXPRESSION TAG	UNP Q97N97
B	-8	LEU	-	EXPRESSION TAG	UNP Q97N97

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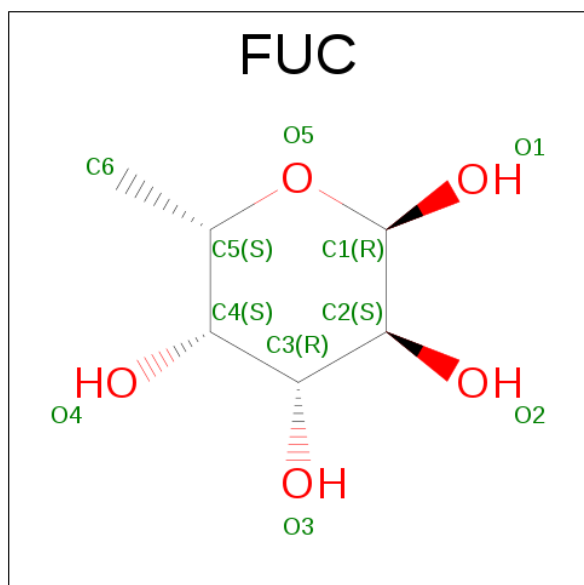
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	VAL	-	EXPRESSION TAG	UNP Q97N97
B	-6	PRO	-	EXPRESSION TAG	UNP Q97N97
B	-5	ARG	-	EXPRESSION TAG	UNP Q97N97
B	-4	GLY	-	EXPRESSION TAG	UNP Q97N97
B	-3	SER	-	EXPRESSION TAG	UNP Q97N97
B	-2	HIS	-	EXPRESSION TAG	UNP Q97N97
B	-1	MET	-	EXPRESSION TAG	UNP Q97N97
B	0	ALA	-	EXPRESSION TAG	UNP Q97N97
B	1	SER	-	EXPRESSION TAG	UNP Q97N97

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

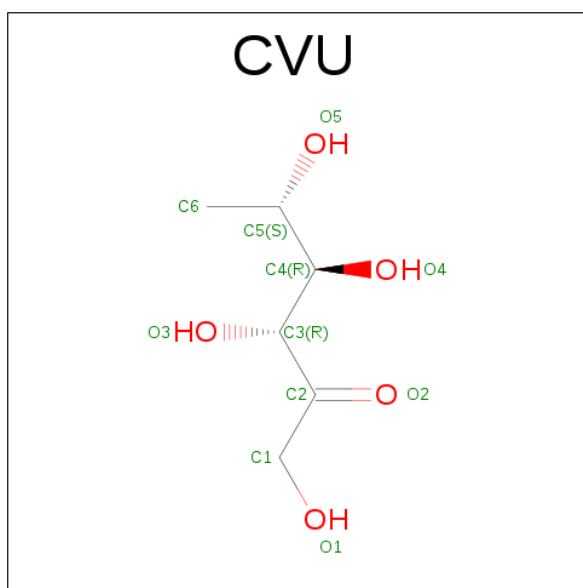
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

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



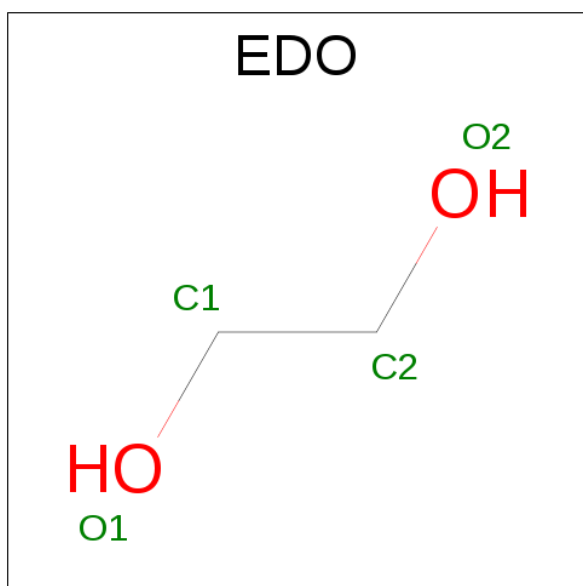
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is L-FUCULOSE OPEN FORM (three-letter code: CVU) (formula:  $C_6H_{12}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	224	Total O 224 224	0	0
6	B	231	Total O 231 231	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.45Å 151.45Å 406.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.26 – 2.70 49.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.26-2.70) 100.0 (49.21-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.144 , 0.198 0.144 , 0.198	Depositor DCC
$R_{free}$ test set	2511 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.2	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9901	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: CVU, EDO, MN, 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	0.59	0/4732	0.75	0/6424
1	B	0.61	0/4854	0.77	4/6587 (0.1%)
All	All	0.60	0/9586	0.76	4/13011 (0.0%)

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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	269	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	16	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	21	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	439	ARG	CB-CG-CD	5.40	125.63	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	326	ILE	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	4612	0	4440	110	0
1	B	4732	0	4560	121	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	11	0	12	0	0
3	B	11	0	12	3	0
4	A	11	0	11	3	0
4	B	11	0	11	0	0
5	A	28	0	42	15	0
5	B	28	0	42	23	0
6	A	224	0	0	16	0
6	B	231	0	0	16	0
All	All	9901	0	9130	222	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 12.

All (222) 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:21:ARG:HH21	1:B:59:THR:HG23	1.07	1.19
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.19	1.07
1:B:21:ARG:NH2	1:B:59:THR:HG23	1.78	0.99
1:A:2:ILE:HB	6:A:2001:HOH:O	1.64	0.97
1:B:21:ARG:HH21	1:B:59:THR:CG2	1.80	0.94
1:B:231:TRP:HE1	3:B:603:FUC:H4	1.34	0.93
1:B:139:ARG:HD2	6:B:2058:HOH:O	1.68	0.92
1:A:471:GLN:HE22	1:A:522:GLY:H	0.92	0.92
1:A:180:SER:H	1:A:298:GLN:HE21	1.15	0.92
1:A:171:ARG:HD2	5:A:1592:EDO:H21	1.52	0.89
1:B:253:GLU:HG3	6:B:2113:HOH:O	1.72	0.89
1:B:542:SER:HB3	5:B:1590:EDO:H11	1.53	0.88
1:B:357:PHE:HB3	5:B:1593:EDO:H12	1.58	0.84
1:B:146:ASP:HB2	6:B:2060:HOH:O	1.78	0.83
1:A:409:ILE:HD11	1:A:411:LYS:HE3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLU:HB3	6:B:2103:HOH:O	1.80	0.82
1:A:471:GLN:NE2	1:A:522:GLY:H	1.77	0.81
1:A:277:ARG:NH1	1:A:277:ARG:HG3	1.82	0.81
1:B:298:GLN:HE22	1:B:302:GLN:NE2	1.80	0.79
1:B:560:ARG:HE	5:B:1590:EDO:C1	1.94	0.78
1:B:116:ALA:HB3	5:B:1596:EDO:H22	1.65	0.78
1:B:151:GLU:HG3	6:B:2063:HOH:O	1.82	0.78
1:A:471:GLN:HE22	1:A:522:GLY:N	1.78	0.76
1:A:571:ASP:HB2	6:A:2216:HOH:O	1.87	0.74
1:A:318:ASN:ND2	5:A:1590:EDO:H12	2.04	0.72
1:A:586:LEU:HD13	5:A:1592:EDO:H11	1.71	0.71
1:A:171:ARG:HD2	5:A:1592:EDO:C2	2.21	0.71
1:A:439:ARG:HE	1:B:217:ARG:HH12	1.38	0.69
1:B:570:GLU:O	6:B:2221:HOH:O	2.09	0.69
1:B:199:LEU:HD13	1:B:201:MET:HE3	1.74	0.69
1:A:439:ARG:CD	6:A:2171:HOH:O	2.41	0.69
1:A:439:ARG:HD2	6:A:2171:HOH:O	1.93	0.69
1:A:446:ARG:HD2	1:A:494:PRO:O	1.93	0.68
1:A:63:VAL:CG1	1:A:64:PRO:HD3	2.23	0.68
1:A:469:VAL:HG12	1:A:547:PRO:HG2	1.76	0.68
1:A:284:GLU:HB2	6:A:2117:HOH:O	1.94	0.67
1:A:217:ARG:HE	1:B:306:HIS:HD2	1.41	0.67
1:B:318:ASN:ND2	5:B:1593:EDO:H21	2.09	0.67
1:B:560:ARG:HE	5:B:1590:EDO:H12	1.59	0.66
1:B:301:ARG:NH1	1:B:305:ASP:OD2	2.28	0.66
1:B:199:LEU:CD1	1:B:201:MET:HE3	2.26	0.66
1:A:586:LEU:HD13	5:A:1592:EDO:C1	2.26	0.65
1:A:357:PHE:HB3	5:A:1590:EDO:H21	1.79	0.65
1:A:217:ARG:HE	1:B:306:HIS:CD2	2.14	0.65
1:A:409:ILE:HG22	1:A:530:TYR:CZ	2.31	0.64
1:B:322:ASP:OD2	1:B:327:ARG:NH1	2.30	0.64
1:A:359:ASP:OD2	4:A:1589:CVU:HC1	1.97	0.64
5:B:1595:EDO:H12	6:B:2117:HOH:O	1.99	0.63
1:B:224:GLU:OE2	1:B:269:ARG:NH2	2.31	0.62
1:B:10:ARG:NH2	1:B:94:THR:O	2.30	0.62
1:B:199:LEU:HB3	1:B:201:MET:HE2	1.81	0.62
1:A:204:GLU:OE1	1:A:290:HIS:HD2	1.83	0.61
1:A:318:ASN:HD22	5:A:1590:EDO:H12	1.63	0.61
1:A:285:GLU:O	1:A:288:VAL:HG22	2.00	0.61
1:A:223:GLU:CB	6:A:2100:HOH:O	2.48	0.60
1:A:320:GLN:HE21	1:A:329:PRO:HD3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:CYS:HB2	1:A:118:TYR:CE1	2.37	0.59
1:A:404:ARG:HH11	1:A:404:ARG:HG3	1.67	0.59
1:A:244:ARG:NH1	1:A:246:ASP:OD2	2.36	0.59
1:A:409:ILE:HG22	1:A:530:TYR:CE1	2.38	0.58
1:B:448:LEU:HD13	1:B:485:HIS:CE1	2.38	0.58
1:A:562:LYS:HZ2	5:A:1596:EDO:H11	1.68	0.58
1:B:25:GLU:OE1	1:B:59:THR:HG21	2.03	0.58
1:B:37:ASP:HB3	6:B:2018:HOH:O	2.03	0.58
1:B:319:THR:O	1:B:327:ARG:NH2	2.37	0.58
1:A:63:VAL:HG13	1:A:64:PRO:HD3	1.86	0.57
1:B:116:ALA:CB	5:B:1596:EDO:H22	2.34	0.57
1:B:45:TYR:CE2	1:B:51:VAL:HA	2.40	0.57
1:B:298:GLN:HE22	1:B:302:GLN:HE22	1.48	0.56
1:B:318:ASN:HD22	5:B:1593:EDO:H21	1.68	0.56
1:A:496:TRP:HB3	1:A:497:PRO:CD	2.36	0.56
1:B:560:ARG:HD3	1:B:564:TRP:CD1	2.40	0.56
1:B:81:THR:HB	1:B:103:HIS:ND1	2.20	0.56
1:B:231:TRP:HE1	3:B:603:FUC:C4	2.12	0.56
1:B:560:ARG:NE	5:B:1590:EDO:H12	2.20	0.56
1:A:45:TYR:CE2	1:A:51:VAL:HA	2.41	0.55
1:B:512:LYS:HE2	6:B:2190:HOH:O	2.06	0.55
1:B:213:ARG:NH2	1:B:286:GLU:OE2	2.40	0.55
1:A:394:CYS:HA	5:A:1590:EDO:H11	1.90	0.54
1:B:199:LEU:C	5:B:1592:EDO:H21	2.27	0.54
1:B:195:PHE:HB2	1:B:203:ASN:HD21	1.70	0.54
1:B:126:HIS:HE1	5:B:1591:EDO:H12	1.72	0.54
1:A:180:SER:H	1:A:298:GLN:NE2	1.97	0.54
1:A:389:ILE:HD11	1:A:496:TRP:HB2	1.88	0.54
1:B:327:ARG:HD3	6:B:2134:HOH:O	2.07	0.54
1:B:542:SER:N	5:B:1590:EDO:H22	2.23	0.54
1:B:199:LEU:HD13	1:B:201:MET:CE	2.36	0.54
1:B:389:ILE:HD11	1:B:496:TRP:HB2	1.90	0.54
1:B:-4:GLY:O	1:B:-3:SER:CB	2.56	0.53
1:A:277:ARG:HH11	1:A:277:ARG:CG	2.07	0.53
1:A:24:LEU:HD11	1:A:113:ARG:HD2	1.91	0.53
1:B:210:GLU:OE1	1:B:213:ARG:NH1	2.42	0.53
1:B:548:VAL:HG23	5:B:1590:EDO:H21	1.90	0.53
1:B:123:LEU:HD13	1:B:562:LYS:HG2	1.91	0.53
1:B:231:TRP:NE1	3:B:603:FUC:H4	2.16	0.53
1:A:63:VAL:HG12	1:A:64:PRO:HD3	1.89	0.53
1:A:85:THR:HG21	1:A:118:TYR:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:HE2	6:B:2019:HOH:O	2.08	0.53
1:B:391:SER:HA	1:B:496:TRP:CE3	2.45	0.52
1:B:143:GLU:HA	6:B:2043:HOH:O	2.09	0.52
1:B:357:PHE:O	1:B:390:ASN:HB2	2.10	0.52
1:B:469:VAL:HG12	1:B:547:PRO:HG2	1.91	0.52
1:A:587:HIS:CE1	5:A:1592:EDO:H22	2.45	0.52
1:B:199:LEU:HB3	1:B:201:MET:CE	2.39	0.51
1:B:265:PHE:HA	1:B:313:MET:HG3	1.92	0.51
1:B:586:LEU:HD12	5:B:1592:EDO:H11	1.91	0.51
1:A:562:LYS:NZ	5:A:1596:EDO:H11	2.25	0.51
1:A:404:ARG:HB2	1:A:409:ILE:HD13	1.91	0.51
1:A:439:ARG:HD3	6:A:2171:HOH:O	2.06	0.51
1:A:251:ARG:NH1	1:A:255:ASP:OD1	2.43	0.51
1:B:320:GLN:HE21	1:B:329:PRO:HD3	1.76	0.51
1:B:199:LEU:O	5:B:1592:EDO:H21	2.11	0.51
1:A:496:TRP:HB3	1:A:497:PRO:HD2	1.92	0.50
1:A:438:PHE:HB3	6:A:2126:HOH:O	2.11	0.50
1:B:89:CYS:HB2	1:B:118:TYR:CE1	2.45	0.50
1:B:285:GLU:O	5:B:1595:EDO:H11	2.11	0.50
1:B:364:TRP:CZ2	1:B:488:LEU:HD22	2.47	0.50
1:B:204:GLU:OE1	1:B:290:HIS:HD2	1.95	0.50
1:B:24:LEU:HD21	1:B:113:ARG:HG3	1.94	0.49
1:A:213:ARG:HG3	1:B:306:HIS:HB2	1.94	0.49
1:A:236:VAL:HG13	1:A:430:PHE:CD1	2.47	0.49
1:B:210:GLU:OE2	1:B:213:ARG:NH1	2.44	0.49
1:B:126:HIS:HE1	5:B:1591:EDO:C1	2.25	0.49
1:B:258:TRP:O	1:B:262:ILE:HG13	2.12	0.49
1:A:4:HIS:O	1:A:6:ARG:HD2	2.12	0.49
1:A:263:LYS:HA	1:A:266:MET:CE	2.43	0.48
1:A:391:SER:HB3	4:A:1589:CVU:O2	2.12	0.48
1:A:290:HIS:HE1	6:A:2120:HOH:O	1.95	0.48
1:A:37:ASP:HB3	6:A:2010:HOH:O	2.11	0.48
1:B:404:ARG:HH11	1:B:404:ARG:HG3	1.77	0.48
1:A:241:ASP:OD1	1:A:243:ASN:HB2	2.13	0.48
1:B:25:GLU:CD	1:B:59:THR:HG21	2.34	0.48
1:B:126:HIS:HD2	1:B:131:ILE:O	1.96	0.48
1:B:541:ALA:C	5:B:1590:EDO:H22	2.35	0.48
1:B:9:ILE:HD12	1:B:36:ALA:HB2	1.96	0.48
1:A:37:ASP:HB3	6:A:2011:HOH:O	2.14	0.47
1:A:302:GLN:HG2	1:B:210:GLU:HB2	1.94	0.47
1:A:7:ILE:HG22	1:A:9:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ALA:O	1:B:145:SER:CB	2.61	0.47
1:A:254:LYS:HE3	6:A:2109:HOH:O	2.14	0.47
1:B:253:GLU:HG2	1:B:256:ARG:NH2	2.29	0.47
1:B:394:CYS:HA	5:B:1593:EDO:H22	1.96	0.47
1:B:486:HIS:O	1:B:490:ASN:ND2	2.39	0.47
1:A:512:LYS:HB2	6:A:2190:HOH:O	2.15	0.47
1:B:86:PRO:HA	1:B:108:PHE:HB3	1.96	0.47
1:B:496:TRP:HB3	1:B:497:PRO:CD	2.44	0.47
1:A:437:TYR:CD2	4:A:1589:CVU:H61	2.51	0.46
1:A:472:ILE:O	1:A:551:HIS:HA	2.16	0.46
1:A:10:ARG:O	1:A:83:THR:HA	2.15	0.46
1:B:126:HIS:CD2	1:B:131:ILE:O	2.68	0.46
1:B:109:ASN:HA	5:B:1596:EDO:H11	1.98	0.46
1:A:217:ARG:NE	1:B:306:HIS:HD2	2.12	0.46
1:A:560:ARG:HD3	1:A:564:TRP:CD1	2.50	0.46
1:B:17:ARG:C	1:B:19:GLY:H	2.19	0.46
1:B:486:HIS:HD2	6:B:2184:HOH:O	1.99	0.46
1:B:70:HIS:HE1	6:B:2027:HOH:O	1.99	0.46
1:B:8:GLY:O	1:B:81:THR:HA	2.16	0.46
1:A:252:GLU:HB3	1:A:256:ARG:HH12	1.81	0.45
1:B:340:ASN:HB2	1:B:459:ARG:HH12	1.82	0.45
1:A:224:GLU:OE2	1:A:269:ARG:NH2	2.50	0.45
1:B:457:MET:HG2	1:B:521:TRP:CZ2	2.51	0.45
1:A:217:ARG:HH12	1:B:439:ARG:HE	1.63	0.45
1:B:210:GLU:CD	1:B:213:ARG:NH1	2.70	0.45
1:B:219:ILE:HG21	1:B:286:GLU:HG2	1.99	0.45
1:B:369:VAL:HG21	1:B:377:LEU:HD11	1.98	0.45
1:B:215:MET:HE2	1:B:263:LYS:HB2	1.99	0.45
1:B:538:ILE:HG23	5:B:1590:EDO:O1	2.16	0.45
1:A:112:GLU:CD	1:A:112:GLU:H	2.20	0.45
1:B:198:TYR:CZ	1:B:468:PRO:HD2	2.52	0.45
1:A:285:GLU:OE2	1:B:301:ARG:NH2	2.50	0.44
1:A:393:SER:OG	5:A:1590:EDO:H22	2.17	0.44
1:B:249:LEU:HD11	1:B:435:ARG:HD3	2.00	0.44
1:B:-4:GLY:O	1:B:-3:SER:HB2	2.17	0.44
1:A:221:ASP:OD2	1:A:277:ARG:HG2	2.17	0.44
1:A:285:GLU:HB3	6:A:2118:HOH:O	2.18	0.44
1:A:10:ARG:HH11	5:A:1595:EDO:H21	1.82	0.44
1:A:269:ARG:NH1	1:A:270:ASP:OD1	2.51	0.44
1:A:478:LEU:HD11	1:A:502:ALA:HB2	1.99	0.44
1:B:351:THR:O	1:B:352:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:THR:O	1:A:491:ARG:HB2	2.17	0.43
1:B:219:ILE:HG12	1:B:283:PHE:CE1	2.53	0.43
1:A:249:LEU:HD11	1:A:435:ARG:HD3	2.00	0.43
1:B:83:THR:HB	1:B:105:ILE:HG13	2.00	0.43
1:A:263:LYS:HA	1:A:266:MET:HE2	2.01	0.43
1:A:114:PRO:HB2	1:A:117:VAL:HB	2.00	0.43
1:A:195:PHE:HB2	1:A:203:ASN:HD21	1.83	0.43
1:B:130:GLY:HA2	6:B:2049:HOH:O	2.19	0.43
1:B:17:ARG:O	1:B:19:GLY:N	2.50	0.43
1:B:496:TRP:HB3	1:B:497:PRO:HD2	2.01	0.43
1:B:85:THR:HG21	1:B:118:TYR:CD2	2.54	0.42
1:A:213:ARG:NH2	1:A:286:GLU:OE2	2.38	0.42
1:B:399:THR:HB	6:B:2159:HOH:O	2.19	0.42
1:A:320:GLN:NE2	6:A:2135:HOH:O	2.53	0.42
1:A:586:LEU:HD13	5:A:1592:EDO:H12	2.02	0.42
1:A:63:VAL:HG13	1:A:64:PRO:CD	2.48	0.42
1:A:489:ASP:OD1	1:A:494:PRO:HA	2.19	0.42
1:A:210:GLU:HB2	1:B:302:GLN:HG3	2.00	0.42
1:B:363:TYR:CD1	1:B:514:VAL:HG12	2.55	0.42
1:B:357:PHE:CB	5:B:1593:EDO:H12	2.39	0.42
1:A:391:SER:HA	1:A:496:TRP:CE3	2.54	0.42
1:B:300:GLN:HA	1:B:301:ARG:HA	1.68	0.42
1:A:309:ASN:HB3	6:A:2126:HOH:O	2.20	0.41
1:A:404:ARG:NH1	1:A:404:ARG:HG3	2.35	0.41
1:A:477:THR:HA	1:A:500:TRP:O	2.20	0.41
1:B:144:ALA:O	1:B:145:SER:OG	2.29	0.41
1:A:342:VAL:HG12	1:A:460:LEU:CD1	2.50	0.41
1:A:542:SER:OG	1:A:561:PRO:HD3	2.20	0.41
1:A:210:GLU:HB2	1:B:302:GLN:CB	2.51	0.41
1:A:425:LEU:HA	1:A:425:LEU:HD23	1.92	0.41
1:A:63:VAL:O	1:A:66:ALA:HB3	2.21	0.41
1:B:236:VAL:HG13	1:B:430:PHE:CD1	2.56	0.41
1:B:344:MET:CE	1:B:357:PHE:HD2	2.33	0.41
1:A:10:ARG:NH1	5:A:1595:EDO:H21	2.36	0.41
1:A:379:GLY:O	1:A:382:ALA:HB2	2.21	0.41
1:A:208:MET:O	1:A:211:PHE:HB2	2.21	0.41
1:A:219:ILE:HG23	1:A:283:PHE:CG	2.56	0.41
1:A:364:TRP:CH2	1:A:488:LEU:HD22	2.56	0.40
1:B:215:MET:CE	1:B:263:LYS:HB2	2.51	0.40
1:A:45:TYR:HB2	1:A:47:ASP:OD1	2.21	0.40
1:A:7:ILE:HG22	1:A:9:ILE:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASN:HB3	1:B:425:LEU:HD13	2.04	0.40
1:A:86:PRO:HA	1:A:108:PHE:HB3	2.02	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	586/604 (97%)	551 (94%)	33 (6%)	2 (0%)	44	73
1	B	602/604 (100%)	566 (94%)	30 (5%)	6 (1%)	18	43
All	All	1188/1208 (98%)	1117 (94%)	63 (5%)	8 (1%)	25	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-3	SER
1	B	91	GLY
1	B	389	ILE
1	A	113	ARG
1	A	391	SER
1	B	-10	SER
1	B	-5	ARG
1	B	-4	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	489/507 (96%)	476 (97%)	13 (3%)	50	80
1	B	502/507 (99%)	494 (98%)	8 (2%)	68	89
All	All	991/1014 (98%)	970 (98%)	21 (2%)	59	85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	34	SER
1	A	54	VAL
1	A	147	THR
1	A	206	VAL
1	A	251	ARG
1	A	277	ARG
1	A	284	GLU
1	A	359	ASP
1	A	426	GLU
1	A	482	GLU
1	A	491	ARG
1	A	518	MET
1	B	-11	SER
1	B	81	THR
1	B	222	PRO
1	B	230	LYS
1	B	245	GLU
1	B	300	GLN
1	B	452	ASP
1	B	563	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	30	ASN
1	A	70	HIS
1	A	203	ASN
1	A	290	HIS
1	A	298	GLN
1	A	320	GLN

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Mol	Chain	Res	Type
1	A	352	ASN
1	A	471	GLN
1	B	-13	HIS
1	B	70	HIS
1	B	126	HIS
1	B	203	ASN
1	B	290	HIS
1	B	302	GLN
1	B	306	HIS
1	B	318	ASN
1	B	320	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\# Z  > 2$
4	CVU	A	1589	2	9,10,10	0.52	0	7,13,13	2.74	3 (42%)
5	EDO	A	1590	-	3,3,3	0.92	0	2,2,2	0.67	0
5	EDO	A	1591	-	3,3,3	0.87	0	2,2,2	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	1592	-	3,3,3	0.59	0	2,2,2	0.09	0
5	EDO	A	1593	-	3,3,3	0.17	0	2,2,2	1.12	0
5	EDO	A	1594	-	3,3,3	0.37	0	2,2,2	1.03	0
5	EDO	A	1595	-	3,3,3	0.60	0	2,2,2	0.28	0
5	EDO	A	1596	-	3,3,3	0.63	0	2,2,2	0.33	0
3	FUC	A	603	-	11,11,11	0.67	0	15,16,16	1.35	2 (13%)
4	CVU	B	1589	2	9,10,10	0.81	0	7,13,13	1.08	1 (14%)
5	EDO	B	1590	-	3,3,3	0.40	0	2,2,2	0.27	0
5	EDO	B	1591	-	3,3,3	0.98	0	2,2,2	0.74	0
5	EDO	B	1592	-	3,3,3	0.49	0	2,2,2	0.05	0
5	EDO	B	1593	-	3,3,3	0.96	0	2,2,2	0.81	0
5	EDO	B	1594	-	3,3,3	0.47	0	2,2,2	0.10	0
5	EDO	B	1595	-	3,3,3	0.66	0	2,2,2	0.16	0
5	EDO	B	1596	-	3,3,3	0.59	0	2,2,2	0.18	0
3	FUC	B	603	-	11,11,11	0.81	0	15,16,16	1.32	2 (13%)

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	CVU	A	1589	2	-	0/14/14/14	0/0/0/0
5	EDO	A	1590	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1591	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1592	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1593	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1594	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1595	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1596	-	-	0/1/1/1	0/0/0/0
3	FUC	A	603	-	-	0/0/20/20	0/1/1/1
4	CVU	B	1589	2	-	0/14/14/14	0/0/0/0
5	EDO	B	1590	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1591	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1592	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1593	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1594	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1595	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1596	-	-	0/1/1/1	0/0/0/0
3	FUC	B	603	-	-	0/0/20/20	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1589	CVU	O3-C3-C2	-6.28	99.99	110.95
3	B	603	FUC	O4-C4-C3	-3.48	102.79	110.36
3	A	603	FUC	C1-C2-C3	-3.02	105.20	110.65
4	A	1589	CVU	C5-C4-C3	-2.09	109.84	113.58
4	B	1589	CVU	O3-C3-C2	-2.08	107.32	110.95
3	A	603	FUC	O5-C1-C2	-2.07	106.61	110.04
3	B	603	FUC	C6-C5-C4	2.21	117.00	113.07
4	A	1589	CVU	O2-C2-C1	2.24	124.01	120.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1589	CVU	3	0
5	A	1590	EDO	5	0
5	A	1592	EDO	6	0
5	A	1595	EDO	2	0
5	A	1596	EDO	2	0
5	B	1590	EDO	8	0
5	B	1591	EDO	2	0
5	B	1592	EDO	3	0
5	B	1593	EDO	5	0
5	B	1595	EDO	2	0
5	B	1596	EDO	3	0
3	B	603	FUC	3	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, 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	587/604 (97%)	-0.70	0	100   100	23, 36, 55, 69	0
1	B	604/604 (100%)	-0.65	3 (0%)	90   92	23, 34, 58, 126	0
All	All	1191/1208 (98%)	-0.67	3 (0%)	93   94	23, 35, 57, 126	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-3	SER	4.4
1	B	-5	ARG	2.7
1	B	-4	GLY	2.1

### 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
5	EDO	B	1591	4/4	0.76	0.41	17.86	53,55,58,60	0
5	EDO	A	1595	4/4	0.91	0.36	15.62	65,72,76,79	0
5	EDO	B	1590	4/4	0.97	0.26	12.03	35,37,38,38	0
5	EDO	A	1592	4/4	0.98	0.23	11.90	49,51,54,56	0
5	EDO	B	1596	4/4	0.82	0.42	10.02	72,90,90,92	0
5	EDO	A	1590	4/4	0.90	0.29	8.02	55,58,58,59	0
5	EDO	B	1593	4/4	0.83	0.28	7.95	49,51,53,56	0
5	EDO	B	1592	4/4	0.98	0.23	7.87	52,56,57,59	0
5	EDO	A	1594	4/4	0.97	0.15	6.08	38,46,47,51	0
5	EDO	A	1593	4/4	0.97	0.17	4.82	36,38,39,49	0
5	EDO	A	1591	4/4	0.83	0.34	4.54	47,55,57,57	0
3	FUC	A	603	11/11	0.94	0.34	4.33	69,81,86,88	0
5	EDO	A	1596	4/4	0.96	0.17	4.33	38,40,46,49	0
3	FUC	B	603	11/11	0.94	0.28	4.06	67,77,81,82	0
5	EDO	B	1595	4/4	0.94	0.18	3.86	45,46,47,47	0
5	EDO	B	1594	4/4	0.97	0.14	2.06	34,34,35,37	0
4	CVU	A	1589	11/11	0.97	0.16	1.38	46,62,65,70	0
4	CVU	B	1589	11/11	0.98	0.15	0.37	45,53,62,72	0
2	MN	A	601	1/1	0.99	0.09	-1.32	66,66,66,66	0
2	MN	B	601	1/1	0.99	0.09	-1.81	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.