



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:04 PM GMT

PDB ID : 2FGL  
Title : An alkali thermostable F/10 xylanase from alkalophilic Bacillus sp. NG-27  
Authors : Ramakumar, S.; Manikandan, K.; Bhardwaj, A.; Reddy, V.S.; Lokanath, N.K.; Ghosh, A.  
Deposited on : 2005-12-22  
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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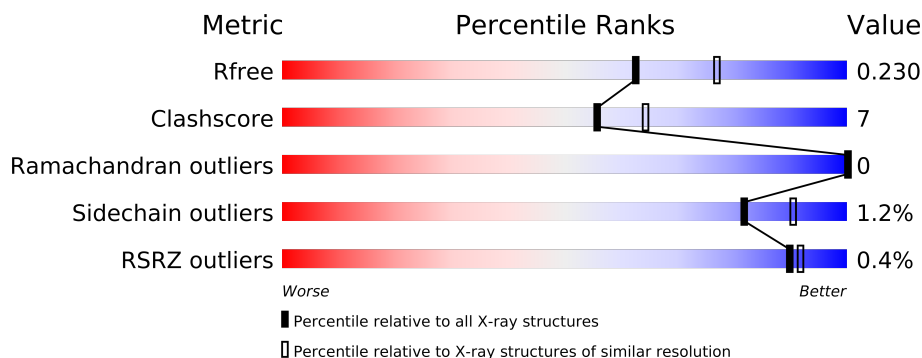
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	354	
1	B	354	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	LXC	B	708	-	X
5	MG	A	601	-	X
5	MG	B	603	-	X
5	MG	B	604	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6378 atoms, of which 0 are hydrogen and 0 are deuterium.

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 alkaline thermostable endoxylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2883	1832	493	553	5			
1	B	354	Total	C	N	O	S	0	0	0
			2883	1832	493	553	5			

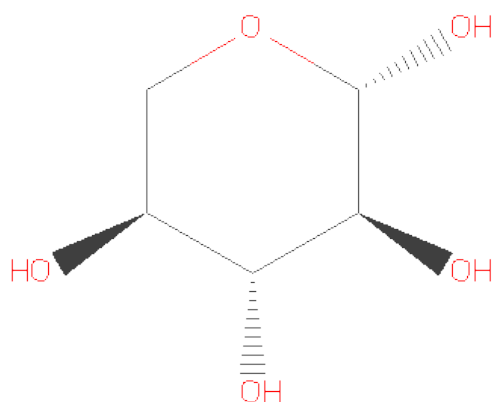
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			28	15	13		
2	B	3	Total	C	O	0	0
			28	15	13		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	C	O	0	0
			19	10	9		

- Molecule 4 is SUGAR (XYLOPYRANOSE) (three-letter code: LXC) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is water.

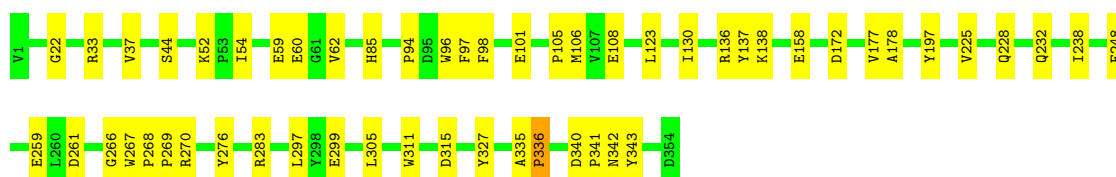
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	285	Total	O	0	0
			285	285		
6	B	238	Total	O	0	0
			238	238		

### 3 Residue-property plots

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.

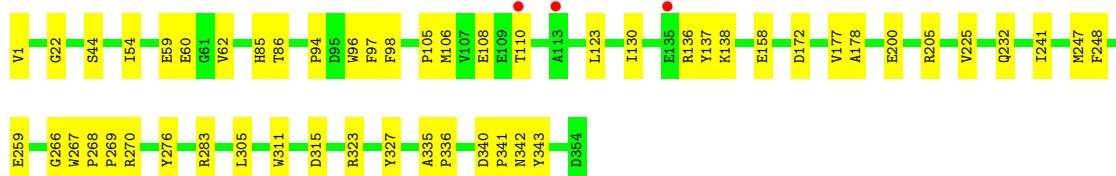
- Molecule 1: alkaline thermostable endoxylanase

Chain A: 



- Molecule 1: alkaline thermostable endoxylanase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.19Å 84.20Å 174.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.20 49.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.00-2.20) 82.5 (49.00-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.26 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.258 0.227 , 0.230	Depositor DCC
$R_{free}$ test set	2018 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	1.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 42617 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, XYS, LXC

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	0.35	0/2963	0.60	0/4041
1	B	0.34	0/2963	0.60	0/4041
All	All	0.35	0/5926	0.60	0/8082

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	A	4	0
2	B	4	0
3	A	3	0
All	All	11	0

There are no bond length outliers.

There are no bond angle outliers.

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	700	XYS	C2
2	A	701	XYS	C2,C3,C4
3	A	703	XYS	C2,C3,C1
2	B	705	XYS	C2
2	B	706	XYS	C2,C3,C4

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2883	0	2697	40	0
1	B	2883	0	2697	37	0
2	A	28	0	23	3	0
2	B	28	0	23	2	0
3	A	19	0	16	1	0
4	B	10	0	10	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	285	0	0	2	0
6	B	238	0	0	2	0
All	All	6378	0	5466	75	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (75) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:GLU:HG2	1:A:311:TRP:CE3	2.26	0.69
1:B:259:GLU:HG2	1:B:311:TRP:CE3	2.28	0.68
1:B:85:HIS:NE2	2:B:705:XYS:H52	2.17	0.59
1:A:94:PRO:HG2	1:A:97:PHE:CD2	2.38	0.59
1:B:323:ARG:HH22	4:B:708:LXC:H5C2	1.67	0.58
1:A:270:ARG:HD3	1:A:327:TYR:O	2.04	0.58
1:B:205:ARG:HD3	1:B:247:MET:SD	2.44	0.57
1:A:60:GLU:HB2	1:A:96:TRP:CE3	2.40	0.57
1:A:85:HIS:NE2	2:A:700:XYS:H52	2.20	0.56
1:B:94:PRO:HG2	1:B:97:PHE:CD2	2.39	0.56
1:A:54:ILE:HA	1:A:94:PRO:HD3	1.88	0.55
1:B:136:ARG:HD3	1:B:137:TYR:CZ	2.41	0.55
1:B:123:LEU:HD22	1:B:177:VAL:HG21	1.87	0.55
1:B:60:GLU:HB2	1:B:96:TRP:CE3	2.42	0.55
1:B:270:ARG:HD3	1:B:327:TYR:O	2.07	0.55
1:B:283:ARG:HA	1:B:283:ARG:HE	1.72	0.55
1:B:105:PRO:HB2	1:B:108:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:259:GLU:OE1	2:B:705:XYX:H3	2.08	0.53
1:B:283:ARG:NE	1:B:283:ARG:HA	2.23	0.53
1:A:259:GLU:HG2	1:A:311:TRP:CZ3	2.43	0.53
1:B:259:GLU:HG2	1:B:311:TRP:CZ3	2.44	0.53
1:B:130:ILE:CD1	1:B:178:ALA:HA	2.39	0.53
1:A:283:ARG:HA	1:A:283:ARG:NE	2.24	0.52
1:A:283:ARG:HA	1:A:283:ARG:HE	1.73	0.52
1:A:340:ASP:HB2	1:A:341:PRO:CD	2.40	0.52
1:A:267:TRP:HA	1:A:268:PRO:C	2.30	0.52
1:A:232:GLN:OE1	1:A:266:GLY:HA2	2.11	0.51
1:B:340:ASP:HB2	1:B:341:PRO:CD	2.41	0.51
1:B:267:TRP:HA	1:B:268:PRO:C	2.31	0.50
1:A:315:ASP:OD2	1:A:335:ALA:HB1	2.11	0.50
1:A:123:LEU:HD22	1:A:177:VAL:HG21	1.94	0.50
1:A:225:VAL:HG21	1:A:248:PHE:CD1	2.47	0.49
1:A:59:GLU:HB2	1:A:62:VAL:HB	1.93	0.49
1:A:94:PRO:HG2	1:A:97:PHE:HD2	1.78	0.49
1:B:342:ASN:O	1:B:343:TYR:HB2	2.13	0.48
1:B:54:ILE:HA	1:B:94:PRO:HD3	1.96	0.48
1:A:98:PHE:O	1:A:106:MET:HG3	2.13	0.48
1:A:136:ARG:HD3	1:A:137:TYR:CZ	2.48	0.48
1:B:225:VAL:HG21	1:B:248:PHE:CD1	2.49	0.48
1:B:59:GLU:HB2	1:B:62:VAL:HB	1.95	0.48
1:A:259:GLU:OE1	2:A:700:XYX:H3	2.14	0.48
1:A:54:ILE:CA	1:A:94:PRO:HD3	2.44	0.48
1:A:105:PRO:HB2	1:A:108:GLU:HG3	1.96	0.47
1:A:342:ASN:O	1:A:343:TYR:HB2	2.14	0.47
1:A:94:PRO:HB2	1:A:96:TRP:CD1	2.50	0.47
1:B:22:GLY:HA2	1:B:44:SER:O	2.15	0.47
1:A:22:GLY:HA2	1:A:44:SER:O	2.14	0.46
1:A:130:ILE:CD1	1:A:178:ALA:HA	2.45	0.46
1:B:94:PRO:HG2	1:B:97:PHE:HD2	1.81	0.46
1:A:340:ASP:HB2	1:A:341:PRO:HD2	1.96	0.46
1:B:172:ASP:OD2	1:B:172:ASP:C	2.54	0.46
1:A:267:TRP:CB	3:A:704:XYX:H51	2.47	0.45
1:A:267:TRP:CE3	1:A:269:PRO:HD3	2.51	0.45
1:A:158:GLU:HG2	6:A:825:HOH:O	2.17	0.45
1:B:315:ASP:OD2	1:B:335:ALA:HB1	2.16	0.45
1:B:94:PRO:HB2	1:B:96:TRP:CD1	2.52	0.45
1:A:172:ASP:C	1:A:172:ASP:OD2	2.55	0.45
1:A:238:ILE:HG23	1:A:297:LEU:HD22	1.99	0.44
1:B:340:ASP:HB2	1:B:341:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:327:TYR:OH	1:B:158:GLU:HB3	2.19	0.43
1:B:267:TRP:CE3	1:B:269:PRO:HD3	2.53	0.43
1:B:232:GLN:OE1	1:B:266:GLY:HA2	2.19	0.42
1:A:197:TYR:HB3	1:A:228:GLN:OE1	2.19	0.42
1:B:110:THR:HG22	6:B:899:HOH:O	2.20	0.42
1:B:1:VAL:N	6:B:860:HOH:O	2.52	0.42
1:A:276:TYR:CE1	1:A:335:ALA:HB2	2.55	0.42
1:A:299:GLU:HB3	6:A:845:HOH:O	2.20	0.42
1:A:108:GLU:O	1:B:270:ARG:NH2	2.54	0.41
1:B:276:TYR:CE1	1:B:335:ALA:HB2	2.55	0.41
1:A:33:ARG:O	1:A:37:VAL:HG23	2.21	0.41
1:B:85:HIS:HA	1:B:86:THR:HA	1.89	0.41
1:A:261:ASP:HB2	1:A:336:PRO:HB2	2.02	0.41
1:A:52:LYS:HZ1	2:A:701:XYS:H51	1.86	0.40
1:B:98:PHE:O	1:B:106:MET:HG3	2.21	0.40
1:B:200:GLU:HG2	1:B:241:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

## 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	352/354 (99%)	340 (97%)	12 (3%)	0	100	100
1	B	352/354 (99%)	340 (97%)	12 (3%)	0	100	100
All	All	704/708 (99%)	680 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	301/306 (98%)	297 (99%)	4 (1%)	80	89
1	B	301/306 (98%)	298 (99%)	3 (1%)	85	93
All	All	602/612 (98%)	595 (99%)	7 (1%)	82	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	GLU
1	A	138	LYS
1	A	305	LEU
1	A	336	PRO
1	B	138	LYS
1	B	305	LEU
1	B	336	PRO

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

8 carbohydrates 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	XYS	A	700	2	10,10,10	1.81	4 (40%)	14,14,14	0.97	0
2	XYS	A	701	2	7,8,10	2.29	5 (71%)	5,10,14	0.81	0
2	XYS	A	702	2	10,10,10	2.30	5 (50%)	14,14,14	1.60	3 (21%)
3	XYS	A	703	3	9,9,10	1.88	3 (33%)	8,12,14	1.25	1 (12%)
3	XYS	A	704	3	10,10,10	1.40	2 (20%)	14,14,14	1.28	2 (14%)
2	XYS	B	705	2	10,10,10	1.70	4 (40%)	14,14,14	0.86	0
2	XYS	B	706	2	7,8,10	2.36	4 (57%)	5,10,14	0.72	0
2	XYS	B	707	2	10,10,10	2.39	4 (40%)	14,14,14	1.56	2 (14%)

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	XYS	A	700	2	1/1/4/4	0/0/17/17	1/1/1/1
2	XYS	A	701	2	3/3/2/4	0/0/11/17	0/1/1/1
2	XYS	A	702	2	-	0/0/17/17	0/1/1/1
3	XYS	A	703	3	3/3/3/4	0/0/14/17	0/1/1/1
3	XYS	A	704	3	-	0/0/17/17	1/1/1/1
2	XYS	B	705	2	1/1/4/4	0/0/17/17	1/1/1/1
2	XYS	B	706	2	3/3/2/4	0/0/11/17	0/1/1/1
2	XYS	B	707	2	-	0/0/17/17	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	707	XYS	C4-C3	4.08	1.58	1.52
2	B	707	XYS	O5-C5	-3.88	1.37	1.43
2	A	702	XYS	O5-C5	-3.78	1.37	1.43
2	B	706	XYS	C1-C2	3.68	1.56	1.38
3	A	703	XYS	O5-C5	-3.66	1.38	1.44
2	A	701	XYS	C1-C2	3.54	1.55	1.38
2	A	702	XYS	C1-C2	3.31	1.59	1.52
3	A	703	XYS	O5-C1	-3.26	1.38	1.43
2	A	702	XYS	C4-C3	3.08	1.56	1.52
2	A	702	XYS	C3-C2	3.06	1.60	1.52
2	B	707	XYS	C1-C2	3.00	1.58	1.52
2	B	707	XYS	C3-C2	2.92	1.60	1.52
3	A	704	XYS	C1-C2	2.81	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	706	XYS	C4-C3	-2.76	1.48	1.53
2	A	700	XYS	C5-C4	2.73	1.58	1.52
3	A	704	XYS	O4-C4	-2.73	1.37	1.43
2	A	701	XYS	C4-C3	-2.69	1.48	1.53
2	B	705	XYS	C1-C2	2.57	1.57	1.52
2	B	705	XYS	C5-C4	2.50	1.58	1.52
2	A	700	XYS	C1-C2	2.46	1.57	1.52
2	B	706	XYS	O5-C5	-2.37	1.38	1.43
2	A	700	XYS	O5-C5	-2.25	1.40	1.43
2	B	706	XYS	O3-C3	-2.16	1.38	1.43
3	A	703	XYS	O2-C2	-2.13	1.37	1.43
2	A	701	XYS	O3-C3	-2.13	1.39	1.43
2	A	701	XYS	C5-C4	2.12	1.57	1.52
2	B	705	XYS	O3-C3	-2.09	1.37	1.43
2	B	705	XYS	O5-C5	-2.02	1.40	1.43
2	A	702	XYS	O3-C3	-2.01	1.38	1.43
2	A	700	XYS	C4-C3	2.01	1.55	1.52
2	A	701	XYS	O4-C4	-2.00	1.38	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	707	XYS	O5-C1-C2	2.86	113.33	109.24
2	A	702	XYS	O5-C1-C2	2.79	113.23	109.24
3	A	704	XYS	O5-C5-C4	2.45	114.73	110.83
3	A	703	XYS	C1-C2-C3	2.35	114.26	110.53
2	A	702	XYS	C1-C2-C3	2.35	114.25	110.53
2	B	707	XYS	C1-C2-C3	2.31	114.20	110.53
2	A	702	XYS	C5-O5-C1	-2.23	108.76	112.86
3	A	704	XYS	O4-C4-C3	2.00	114.11	110.23

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	701	XYS	C2
2	A	701	XYS	C3
2	A	701	XYS	C4
2	B	706	XYS	C2
2	B	706	XYS	C3
2	B	706	XYS	C4
3	A	703	XYS	C2
3	A	703	XYS	C3

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Mol	Chain	Res	Type	Atom
3	A	703	XYS	C1
2	A	700	XYS	C2
2	B	705	XYS	C2

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	XYS	C1-C2-C3-C4-C5-O5
2	A	700	XYS	C1-C2-C3-C4-C5-O5
2	B	705	XYS	C1-C2-C3-C4-C5-O5

## 5.6 Ligand geometry i

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	LXC	B	708	-	10,10,10	1.76	1 (10%)	14,14,14	0.85	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
4	LXC	B	708	-	-	0/0/17/17	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	708	LXC	C4-C3	-4.48	1.46	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

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	354/354 (100%)	-0.49	0 100 100	31, 44, 57, 68	15 (4%)
1	B	354/354 (100%)	-0.40	3 (0%) 83 85	32, 46, 61, 67	14 (3%)
All	All	708/708 (100%)	-0.45	3 (0%) 90 92	31, 45, 59, 68	29 (4%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	GLU	2.4
1	B	110	THR	2.4
1	B	113	ALA	2.2

### 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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	XYS	A	704	10/10	0.26	24.62	65,67,68,68	10
2	XYS	B	705	10/10	0.13	6.60	54,56,58,60	0
2	XYS	B	707	10/10	0.18	5.61	71,75,77,78	6
2	XYS	B	706	8/10	0.13	4.49	63,64,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	XYS	A	702	10/10	0.21	2.72	62,68,69,70	2
2	XYS	A	700	10/10	0.12	1.66	42,46,47,52	0
3	XYS	A	703	9/10	0.11	1.49	67,68,69,70	0
2	XYS	A	701	8/10	0.11	0.88	53,55,57,57	0

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	A	601	1/1	0.20	8.68	37,37,37,37	0
5	MG	B	603	1/1	0.20	8.00	47,47,47,47	0
4	LXC	B	708	10/10	0.19	5.50	61,63,64,65	10
5	MG	B	604	1/1	0.15	3.03	39,39,39,39	1
5	MG	A	602	1/1	0.06	-2.66	46,46,46,46	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.