



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:46 PM BST

PDB ID : 6KJL  
Title : Xylanase J from Bacillus sp. strain 41M-1  
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Deposited on : 2019-07-22  
Resolution : 2.45 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

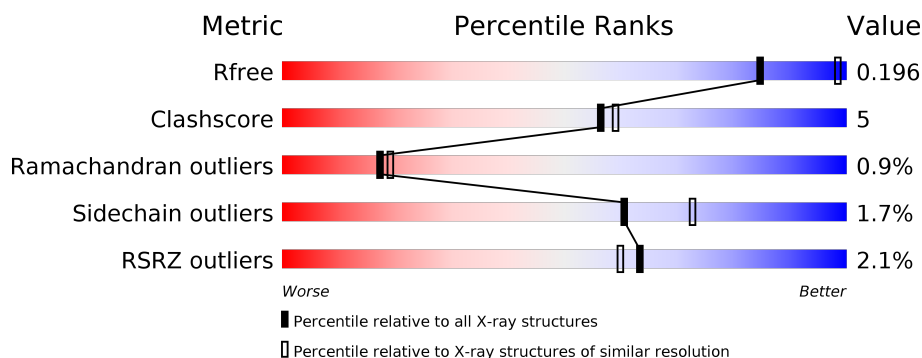
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	328	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	328	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>

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	EPE	A	404	-	-	-	X
4	MPD	B	407	-	-	-	X
5	GOL	A	410	-	-	X	-
5	GOL	B	410	-	-	-	X
5	GOL	B	411	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5577 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 Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	4	0
			2569	1604	441	516	8			
1	B	327	Total	C	N	O	S	0	4	0
			2560	1596	439	518	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q9RC94
B	0	MET	-	initiating methionine	UNP Q9RC94

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

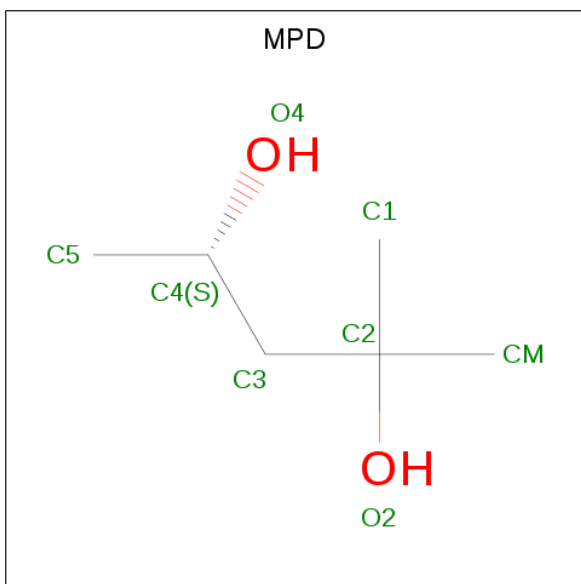
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



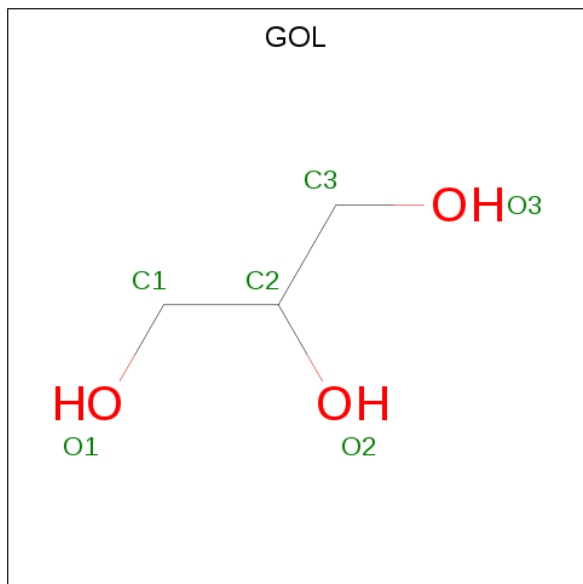
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

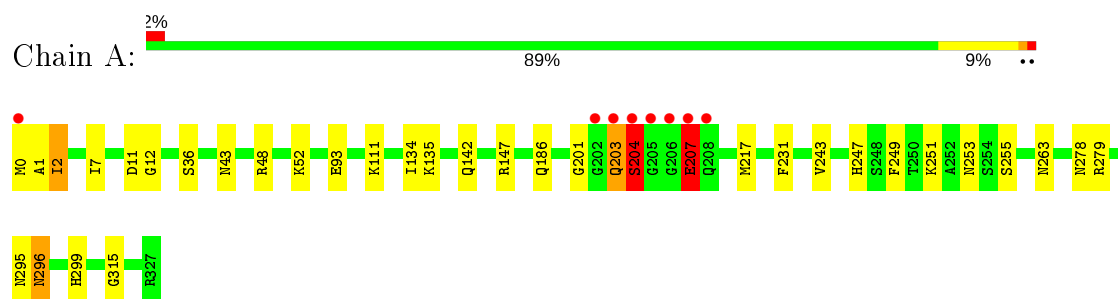
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	145	Total	O	0	0
			145	145		
6	B	146	Total	O	0	0
			146	146		

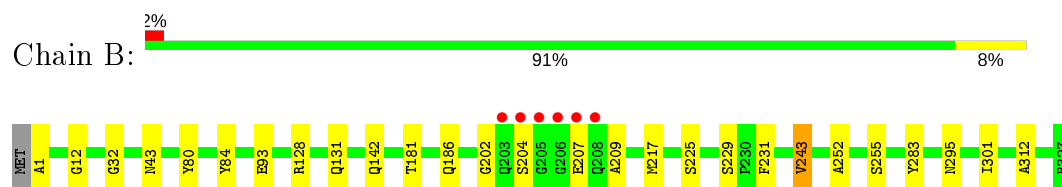
### 3 Residue-property plots

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: Endo-1,4-beta-xylanase



- Molecule 1: Endo-1,4-beta-xylanase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.94Å 125.94Å 318.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.00 – 2.45 49.40 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.00-2.45) 99.8 (49.40-2.45)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, $R_{free}$	0.169 , 0.198 0.169 , 0.196	Depositor DCC
$R_{free}$ test set	2777 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5577	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: GOL, CA, EPE, MPD

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	0.42	0/2641	0.62	0/3590
1	B	0.44	1/2632 (0.0%)	0.62	0/3578
All	All	0.43	1/5273 (0.0%)	0.62	0/7168

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	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	GLU	CG-CD	-6.47	1.42	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	GLN	Peptide
1	A	207	GLU	Peptide
1	B	204	SER	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	2569	0	2399	30	0
1	B	2560	0	2380	13	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	30	0	34	0	0
3	B	15	0	17	1	0
4	A	16	0	28	9	0
4	B	32	0	56	7	0
5	A	30	0	39	7	0
5	B	30	0	40	3	0
6	A	145	0	0	7	0
6	B	146	0	0	2	0
All	All	5577	0	4993	51	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 5.

All (51) 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:263:ASN:HD21	4:A:406:MPD:HM1	1.21	1.00
1:A:253:ASN:HB2	5:A:410:GOL:H32	1.61	0.83
1:A:217:MET:HB2	1:A:243:VAL:HG22	1.60	0.82
1:A:48:ARG:HH12	4:A:405:MPD:H51	1.47	0.79
4:B:406:MPD:HO4	4:B:406:MPD:HO2	1.24	0.78
1:A:251:LYS:HB2	5:A:410:GOL:H2	1.71	0.72
1:B:1:ALA:O	5:B:409:GOL:H2	1.93	0.68
1:A:204:SER:HA	1:A:207:GLU:HB3	1.82	0.62
1:A:12:GLY:H	4:B:406:MPD:HM1	1.65	0.61
1:A:43[B]:ASN:ND2	1:A:186:GLN:OE1	2.27	0.61
4:B:407:MPD:HM3	6:B:508:HOH:O	2.04	0.58
1:A:201:GLY:HA2	5:A:410:GOL:H31	1.84	0.57
1:A:315:GLY:HA2	4:A:406:MPD:H52	1.87	0.57
1:B:217:MET:SD	1:B:243:VAL:HG13	2.46	0.55
1:A:251:LYS:HD2	5:A:410:GOL:H11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ALA:HB2	3:B:403:EPE:H72	1.89	0.54
1:A:255:SER:OG	1:A:295:ASN:OD1	2.26	0.53
1:B:12:GLY:O	4:B:406:MPD:H53	2.09	0.52
1:B:80:TYR:OH	5:B:408:GOL:H32	2.10	0.52
1:A:147[B]:ARG:NH1	6:A:504:HOH:O	2.40	0.51
1:A:48:ARG:HH12	4:A:405:MPD:C5	2.22	0.51
1:B:128:ARG:HB3	1:B:131:GLN:HG3	1.91	0.50
1:A:36:SER:HB2	5:A:411:GOL:H12	1.92	0.50
1:A:201:GLY:HA2	5:A:410:GOL:C3	2.42	0.49
1:A:0:MET:O	1:A:2:ILE:N	2.43	0.48
6:A:501:HOH:O	4:B:407:MPD:HM1	2.13	0.48
1:A:7:ILE:HD11	1:A:52:LYS:HE2	1.94	0.48
4:A:406:MPD:HM3	6:A:560:HOH:O	2.14	0.47
1:A:203:GLN:HG3	1:A:204:SER:N	2.30	0.47
1:B:255:SER:HB3	1:B:295:ASN:OD1	2.14	0.47
1:A:263:ASN:ND2	4:A:406:MPD:HM1	2.06	0.47
1:A:135:LYS:NZ	6:A:509:HOH:O	2.48	0.46
4:B:407:MPD:H53	4:B:407:MPD:H11	1.97	0.46
1:B:43[B]:ASN:OD1	1:B:186:GLN:NE2	2.49	0.46
1:A:134:ILE:HG22	4:A:405:MPD:C1	2.46	0.46
1:A:278:ASN:O	1:A:279:ARG:HD2	2.16	0.46
1:A:249:PHE:CD1	1:A:299:HIS:CE1	3.05	0.44
1:A:93:GLU:O	1:A:142:GLN:HA	2.18	0.44
1:A:12:GLY:N	4:B:406:MPD:HM1	2.31	0.43
5:B:408:GOL:H31	6:B:635:HOH:O	2.18	0.43
1:A:43[A]:ASN:ND2	1:A:186:GLN:OE1	2.45	0.43
1:B:93:GLU:O	1:B:142:GLN:HA	2.18	0.43
1:A:203:GLN:HG3	1:A:204:SER:HA	2.02	0.42
1:A:111:LYS:HE3	1:A:111:LYS:HB3	1.83	0.41
4:A:405:MPD:HM3	1:B:283:TYR:CE2	2.56	0.41
1:B:252:ALA:HB2	1:B:301:ILE:HD11	2.03	0.41
1:A:247:HIS:HD2	6:A:641:HOH:O	2.03	0.41
4:A:405:MPD:H53	4:A:405:MPD:H12	2.02	0.41
6:A:525:HOH:O	1:B:32:GLY:HA2	2.21	0.41
5:A:407:GOL:H2	6:A:521:HOH:O	2.20	0.41
1:B:84:TYR:HB3	1:B:181:THR:OG1	2.21	0.41

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	330/328 (101%)	313 (95%)	12 (4%)	5 (2%)	10	9
1	B	329/328 (100%)	313 (95%)	14 (4%)	2 (1%)	25	29
All	All	659/656 (100%)	626 (95%)	26 (4%)	7 (1%)	17	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	204	SER
1	B	202	GLY
1	A	1	ALA
1	B	209	ALA
1	A	296[A]	ASN
1	A	296[B]	ASN

### 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	275/271 (102%)	269 (98%)	6 (2%)	52	64
1	B	274/271 (101%)	270 (98%)	4 (2%)	65	76
All	All	549/542 (101%)	539 (98%)	10 (2%)	60	71

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	204	SER
1	A	207	GLU
1	A	231	PHE
1	A	296[A]	ASN
1	A	296[B]	ASN
1	B	225	SER
1	B	229	SER
1	B	231	PHE
1	B	243	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	208	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 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
5	GOL	B	408	-	5,5,5	0.95	0	5,5,5	0.94	0
5	GOL	B	412	-	5,5,5	1.05	0	5,5,5	0.87	0
4	MPD	B	406	-	7,7,7	0.63	0	9,10,10	0.73	0
5	GOL	A	409	-	5,5,5	1.17	0	5,5,5	0.62	0
3	EPE	B	403	-	15,15,15	1.06	1 (6%)	18,20,20	1.88	4 (22%)
4	MPD	A	406	-	7,7,7	0.42	0	9,10,10	0.80	0
5	GOL	B	411	-	5,5,5	1.29	1 (20%)	5,5,5	1.04	0
4	MPD	A	405	-	7,7,7	0.40	0	9,10,10	1.05	1 (11%)
5	GOL	A	410	-	5,5,5	1.83	2 (40%)	5,5,5	0.93	0
5	GOL	A	408	-	5,5,5	0.93	0	5,5,5	1.13	1 (20%)
3	EPE	A	404	-	15,15,15	1.06	1 (6%)	18,20,20	1.95	6 (33%)
5	GOL	A	407	-	5,5,5	0.66	0	5,5,5	0.93	0
3	EPE	A	403	-	15,15,15	0.83	1 (6%)	18,20,20	2.01	5 (27%)
4	MPD	B	405	-	7,7,7	0.26	0	9,10,10	0.83	0
5	GOL	B	409	-	5,5,5	1.15	0	5,5,5	1.02	0
5	GOL	B	410	-	5,5,5	1.34	1 (20%)	5,5,5	0.83	0
5	GOL	A	411	-	5,5,5	1.45	2 (40%)	5,5,5	0.85	0
4	MPD	B	407	-	7,7,7	0.57	0	9,10,10	0.93	1 (11%)
4	MPD	B	404	-	7,7,7	0.42	0	9,10,10	0.30	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
5	GOL	B	408	-	-	1/4/4/4	-
5	GOL	B	412	-	-	0/4/4/4	-
4	MPD	B	406	-	-	0/5/5/5	-
5	GOL	A	409	-	-	2/4/4/4	-
3	EPE	B	403	-	-	3/9/19/19	0/1/1/1
4	MPD	A	406	-	-	0/5/5/5	-
5	GOL	B	411	-	-	4/4/4/4	-
4	MPD	A	405	-	-	1/5/5/5	-
5	GOL	A	410	-	-	2/4/4/4	-
5	GOL	A	408	-	-	2/4/4/4	-
3	EPE	A	404	-	-	6/9/19/19	0/1/1/1
5	GOL	A	407	-	-	2/4/4/4	-
3	EPE	A	403	-	-	6/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	B	405	-	-	2/5/5/5	-
5	GOL	B	409	-	-	4/4/4/4	-
5	GOL	B	410	-	-	4/4/4/4	-
5	GOL	A	411	-	-	2/4/4/4	-
4	MPD	B	407	-	-	1/5/5/5	-
4	MPD	B	404	-	-	2/5/5/5	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	EPE	C10-S	3.64	1.82	1.77
3	B	403	EPE	C10-S	3.61	1.82	1.77
5	A	410	GOL	O2-C2	-3.48	1.33	1.43
3	A	403	EPE	C10-S	2.69	1.81	1.77
5	B	410	GOL	C3-C2	2.57	1.62	1.51
5	B	411	GOL	C3-C2	2.26	1.61	1.51
5	A	411	GOL	C1-C2	2.22	1.60	1.51
5	A	410	GOL	C3-C2	2.13	1.60	1.51
5	A	411	GOL	C3-C2	2.00	1.60	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	EPE	C5-N4-C3	5.02	120.13	108.83
3	A	403	EPE	C5-N4-C3	4.88	119.82	108.83
3	A	404	EPE	C5-N4-C3	4.06	117.96	108.83
3	A	404	EPE	C7-N4-C5	3.72	120.75	111.23
3	B	403	EPE	O3S-S-C10	3.46	111.36	105.77
3	A	403	EPE	C7-N4-C3	3.32	119.72	111.23
3	A	404	EPE	C7-N4-C3	3.26	119.57	111.23
3	A	403	EPE	C6-N1-C2	3.07	115.73	108.83
3	A	403	EPE	C7-N4-C5	2.88	118.60	111.23
3	B	403	EPE	C7-N4-C3	2.73	118.22	111.23
3	A	404	EPE	O3S-S-C10	2.69	110.13	105.77
3	A	404	EPE	O2S-S-C10	2.69	110.16	106.92
3	B	403	EPE	C7-N4-C5	2.55	117.76	111.23
4	A	405	MPD	O2-C2-C3	2.51	119.21	109.80
4	B	407	MPD	CM-C2-C1	-2.09	106.23	110.57
5	A	408	GOL	C3-C2-C1	-2.07	103.65	111.70
3	A	403	EPE	C2-C3-N4	2.06	114.88	110.64
3	A	404	EPE	O1S-S-C10	2.06	109.40	106.92



There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	EPE	S-C10-C9-N1
3	A	403	EPE	C8-C7-N4-C5
5	B	410	GOL	O1-C1-C2-C3
5	B	409	GOL	O1-C1-C2-C3
3	B	403	EPE	C9-C10-S-O2S
3	B	403	EPE	C9-C10-S-O3S
5	A	411	GOL	O1-C1-C2-C3
5	B	411	GOL	C1-C2-C3-O3
5	A	407	GOL	C1-C2-C3-O3
3	A	403	EPE	C9-C10-S-O3S
5	A	409	GOL	O1-C1-C2-C3
5	B	410	GOL	C1-C2-C3-O3
5	B	409	GOL	C1-C2-C3-O3
5	A	408	GOL	C1-C2-C3-O3
5	B	411	GOL	O1-C1-C2-C3
5	B	409	GOL	O2-C2-C3-O3
5	A	411	GOL	O1-C1-C2-O2
5	A	407	GOL	O2-C2-C3-O3
3	A	404	EPE	C9-C10-S-O3S
5	B	410	GOL	O1-C1-C2-O2
5	A	408	GOL	O2-C2-C3-O3
5	B	411	GOL	O2-C2-C3-O3
3	A	404	EPE	C10-C9-N1-C2
3	A	404	EPE	C10-C9-N1-C6
3	A	403	EPE	C10-C9-N1-C2
3	A	403	EPE	C10-C9-N1-C6
5	A	409	GOL	O1-C1-C2-O2
5	B	411	GOL	O1-C1-C2-O2
4	B	404	MPD	O2-C2-C3-C4
5	A	410	GOL	O1-C1-C2-O2
5	B	409	GOL	O1-C1-C2-O2
4	A	405	MPD	C2-C3-C4-C5
4	B	405	MPD	C2-C3-C4-C5
3	A	404	EPE	C9-C10-S-O2S
3	A	403	EPE	C9-C10-S-O1S
3	A	403	EPE	C9-C10-S-O2S
3	B	403	EPE	C9-C10-S-O1S
5	A	410	GOL	C1-C2-C3-O3
5	B	410	GOL	O2-C2-C3-O3
5	B	408	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	404	MPD	C2-C3-C4-C5
4	B	407	MPD	C2-C3-C4-C5
3	A	404	EPE	C9-C10-S-O1S
4	B	405	MPD	C2-C3-C4-O4

There are no ring outliers.

10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	408	GOL	2	0
4	B	406	MPD	4	0
3	B	403	EPE	1	0
4	A	406	MPD	4	0
4	A	405	MPD	5	0
5	A	410	GOL	5	0
5	A	407	GOL	1	0
5	B	409	GOL	1	0
5	A	411	GOL	1	0
4	B	407	MPD	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	328/328 (100%)	-0.24	8 (2%) 59 54	33, 43, 57, 135	0
1	B	327/328 (99%)	-0.29	6 (1%) 68 65	33, 44, 60, 128	0
All	All	655/656 (99%)	-0.26	14 (2%) 63 60	33, 44, 60, 135	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	GLY	8.6
1	B	205	GLY	7.4
1	A	204	SER	7.2
1	B	206	GLY	6.3
1	B	204	SER	6.2
1	A	206	GLY	6.1
1	A	208	GLN	5.9
1	A	207	GLU	4.7
1	B	207	GLU	4.1
1	A	0	MET	3.6
1	B	203	GLN	3.3
1	A	203	GLN	2.7
1	A	202	GLY	2.2
1	B	208	GLN	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 monosaccharides in this entry.

## 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. 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	GOL	B	411	6/6	-0.26	0.99	101,119,123,124	0
5	GOL	B	410	6/6	0.56	0.43	67,82,86,89	0
4	MPD	B	407	8/8	0.68	0.41	53,66,74,84	0
5	GOL	B	409	6/6	0.69	0.26	48,72,78,81	0
4	MPD	B	406	8/8	0.74	0.32	56,59,69,82	0
3	EPE	A	404	15/15	0.77	0.51	75,88,143,149	0
4	MPD	A	406	8/8	0.81	0.38	62,65,83,85	0
4	MPD	B	404	8/8	0.81	0.25	73,78,88,91	0
5	GOL	A	411	6/6	0.81	0.31	47,61,68,72	0
5	GOL	B	412	6/6	0.82	0.38	63,69,73,86	0
3	EPE	A	403	15/15	0.83	0.29	48,79,117,128	0
5	GOL	A	407	6/6	0.84	0.25	69,79,83,84	0
5	GOL	A	410	6/6	0.88	0.60	31,73,79,83	0
5	GOL	B	408	6/6	0.90	0.17	63,76,83,91	0
3	EPE	B	403	15/15	0.91	0.23	45,68,100,113	0
5	GOL	A	409	6/6	0.91	0.26	56,66,71,78	0
2	CA	B	401	1/1	0.91	0.08	73,73,73,73	0
4	MPD	B	405	8/8	0.94	0.25	49,53,57,58	0
4	MPD	A	405	8/8	0.94	0.31	51,58,65,67	0
5	GOL	A	408	6/6	0.95	0.16	55,57,62,69	0
2	CA	A	402	1/1	0.98	0.11	70,70,70,70	0
2	CA	B	402	1/1	0.99	0.07	43,43,43,43	0
2	CA	A	401	1/1	0.99	0.07	45,45,45,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.