



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:36 AM BST

PDB ID : 3KL0
Title : Crystal structure of the glucuronoxylan xylanohydrolase XynC from *Bacillus subtilis*
Authors : St John, F.J.; Hurlbert, J.C.; Pozharski, E.
Deposited on : 2009-11-06
Resolution : 1.64 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

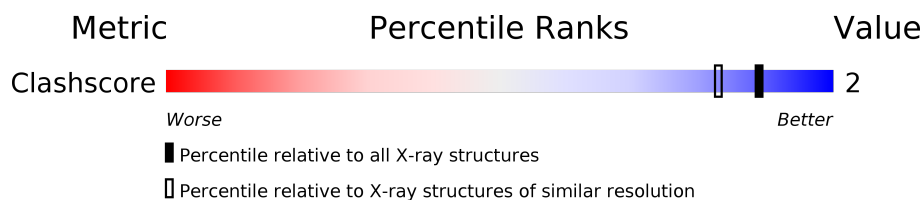
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	3268 (1.66-1.62)

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 ≥ 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	401	96%
1	B	401	94%
1	C	401	93%
1	D	401	93%

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	TAR	A	404	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15095 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 Glucuronoxylanase xynC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	1	15	0
			3244	2057	576	602	9			
1	B	394	Total	C	N	O	S	1	12	0
			3216	2034	570	603	9			
1	C	391	Total	C	N	O	S	0	20	0
			3222	2047	566	600	9			
1	D	389	Total	C	N	O	S	0	7	0
			3149	1996	556	588	9			

There are 44 discrepancies between the modelled and reference sequences:

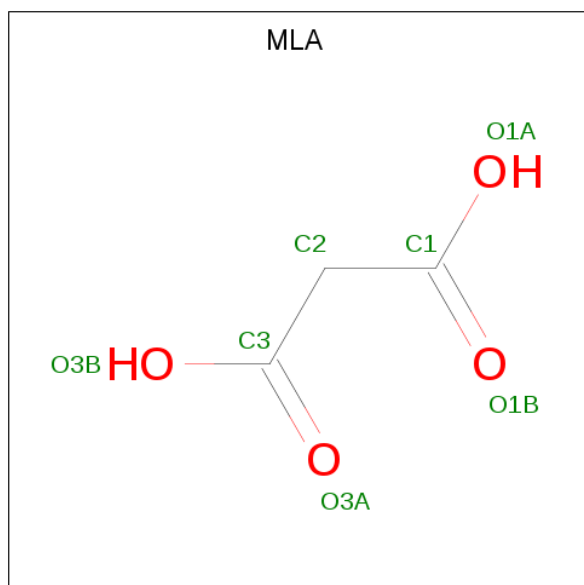
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q45070
A	392	LEU	-	EXPRESSION TAG	UNP Q45070
A	393	GLU	-	EXPRESSION TAG	UNP Q45070
A	394	HIS	-	EXPRESSION TAG	UNP Q45070
A	395	HIS	-	EXPRESSION TAG	UNP Q45070
A	396	HIS	-	EXPRESSION TAG	UNP Q45070
A	397	HIS	-	EXPRESSION TAG	UNP Q45070
A	398	HIS	-	EXPRESSION TAG	UNP Q45070
A	399	HIS	-	EXPRESSION TAG	UNP Q45070
A	400	HIS	-	EXPRESSION TAG	UNP Q45070
A	401	HIS	-	EXPRESSION TAG	UNP Q45070
B	1	MET	-	EXPRESSION TAG	UNP Q45070
B	392	LEU	-	EXPRESSION TAG	UNP Q45070
B	393	GLU	-	EXPRESSION TAG	UNP Q45070
B	394	HIS	-	EXPRESSION TAG	UNP Q45070
B	395	HIS	-	EXPRESSION TAG	UNP Q45070
B	396	HIS	-	EXPRESSION TAG	UNP Q45070
B	397	HIS	-	EXPRESSION TAG	UNP Q45070
B	398	HIS	-	EXPRESSION TAG	UNP Q45070
B	399	HIS	-	EXPRESSION TAG	UNP Q45070
B	400	HIS	-	EXPRESSION TAG	UNP Q45070

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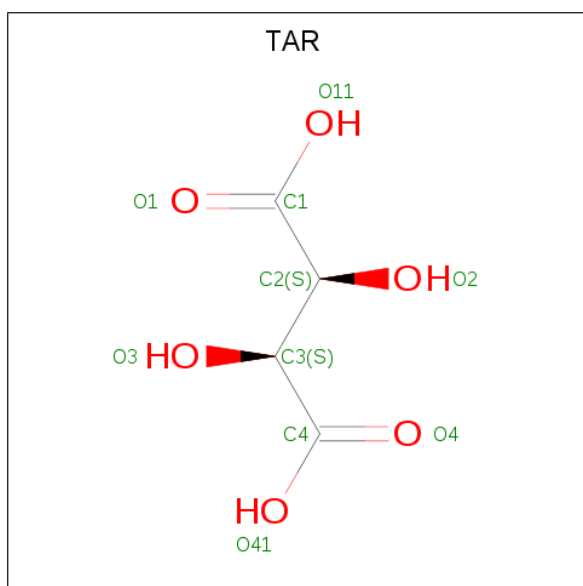
Chain	Residue	Modelled	Actual	Comment	Reference
B	401	HIS	-	EXPRESSION TAG	UNP Q45070
C	1	MET	-	EXPRESSION TAG	UNP Q45070
C	392	LEU	-	EXPRESSION TAG	UNP Q45070
C	393	GLU	-	EXPRESSION TAG	UNP Q45070
C	394	HIS	-	EXPRESSION TAG	UNP Q45070
C	395	HIS	-	EXPRESSION TAG	UNP Q45070
C	396	HIS	-	EXPRESSION TAG	UNP Q45070
C	397	HIS	-	EXPRESSION TAG	UNP Q45070
C	398	HIS	-	EXPRESSION TAG	UNP Q45070
C	399	HIS	-	EXPRESSION TAG	UNP Q45070
C	400	HIS	-	EXPRESSION TAG	UNP Q45070
C	401	HIS	-	EXPRESSION TAG	UNP Q45070
D	1	MET	-	EXPRESSION TAG	UNP Q45070
D	392	LEU	-	EXPRESSION TAG	UNP Q45070
D	393	GLU	-	EXPRESSION TAG	UNP Q45070
D	394	HIS	-	EXPRESSION TAG	UNP Q45070
D	395	HIS	-	EXPRESSION TAG	UNP Q45070
D	396	HIS	-	EXPRESSION TAG	UNP Q45070
D	397	HIS	-	EXPRESSION TAG	UNP Q45070
D	398	HIS	-	EXPRESSION TAG	UNP Q45070
D	399	HIS	-	EXPRESSION TAG	UNP Q45070
D	400	HIS	-	EXPRESSION TAG	UNP Q45070
D	401	HIS	-	EXPRESSION TAG	UNP Q45070

- Molecule 2 is MALONIC ACID (three-letter code: MLA) (formula: C₃H₄O₄).



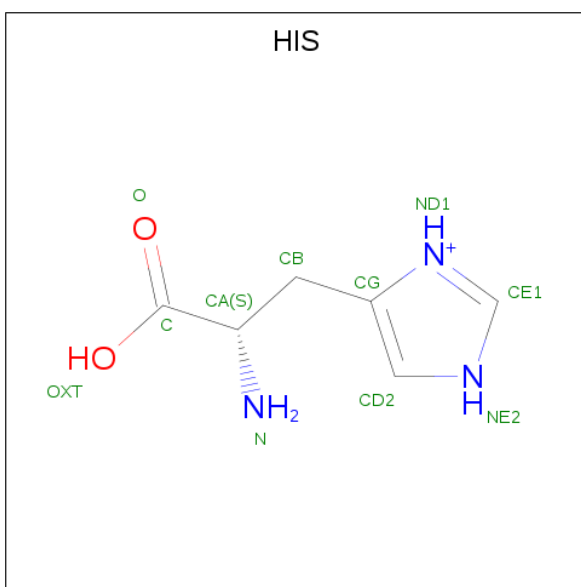
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	A	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		
2	C	1	Total	C	O	0	0
			7	3	4		
2	D	1	Total	C	O	0	0
			7	3	4		

- Molecule 3 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



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

- Molecule 4 is HISTIDINE (three-letter code: HIS) (formula: $C_6H_{10}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 10	C 6	N 3	O 1	0	0
4	A	1	Total 17	C 11	N 5	O 1	0	1

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na 1 1	0	0
5	A	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	629	Total O 629 629	0	0
6	B	582	Total O 582 582	0	0
6	C	561	Total O 561 561	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	416	Total	O	0	0
			416	416		

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Glucuronoxylanase xynC

Chain A:  96%



- Molecule 1: Glucuronoxylanase xynC

Chain B:  94%



- Molecule 1: Glucuronoxylanase xynC

Chain C:  93%



- Molecule 1: Glucuronoxylanase xynC

Chain D:  93%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	138.49 Å 195.80 Å 66.25 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.64	Depositor
% Data completeness (in resolution range)	99.6 (50.00-1.64)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.64 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.167 , 0.201	Depositor
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.014	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15095	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NA, MLA, TAR

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	0.74	2/3376 (0.1%)	0.78	4/4597 (0.1%)
1	B	0.80	3/3330 (0.1%)	0.75	7/4536 (0.2%)
1	C	0.76	0/3357	0.73	0/4573
1	D	0.62	0/3256	0.62	1/4434 (0.0%)
All	All	0.74	5/13319 (0.0%)	0.72	12/18140 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45[A]	ASN	CG-ND2	7.43	1.51	1.32
1	B	45[B]	ASN	CG-ND2	7.43	1.51	1.32
1	A	350[A]	ASN	CG-ND2	-5.50	1.19	1.32
1	A	350[B]	ASN	CG-ND2	-5.50	1.19	1.32
1	B	354	TRP	CB-CG	-5.03	1.41	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350[A]	ASN	CB-CG-ND2	11.26	143.73	116.70
1	A	350[B]	ASN	CB-CG-ND2	11.26	143.73	116.70
1	A	350[A]	ASN	OD1-CG-ND2	-11.22	96.08	121.90
1	A	350[B]	ASN	OD1-CG-ND2	-11.22	96.08	121.90
1	B	242	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	B	45[A]	ASN	OD1-CG-ND2	6.10	135.93	121.90
1	B	45[B]	ASN	OD1-CG-ND2	6.10	135.93	121.90
1	D	242	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	45[A]	ASN	CB-CG-ND2	-5.58	103.31	116.70
1	B	45[B]	ASN	CB-CG-ND2	-5.58	103.31	116.70
1	B	60	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	242	ARG	NE-CZ-NH1	5.13	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3244	0	3121	9	0
1	B	3216	0	3071	10	0
1	C	3222	0	3127	14	0
1	D	3149	0	3012	12	0
2	A	14	0	4	0	0
2	B	7	0	2	0	0
2	C	7	0	2	0	0
2	D	7	0	2	0	0
3	A	10	0	4	0	0
4	A	27	0	20	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	629	0	0	6	1
6	B	582	0	0	5	1
6	C	561	0	0	3	0
6	D	416	0	0	4	0
All	All	15095	0	12365	47	1

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 2.

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:B:366:THR:HB	6:B:1640:HOH:O	1.71	0.89
6:B:1036:HOH:O	1:C:218:GLN:HG3	1.79	0.81
1:C:391:ARG:O	1:C:392:LEU:HB2	1.90	0.71
1:D:68[B]:GLU:OE1	6:D:2053:HOH:O	2.09	0.70
1:C:353[B]:ARG:HD2	1:C:365:GLY:HA3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153[A]:GLN:NE2	6:D:1260:HOH:O	2.25	0.68
1:C:360:SER:HB2	1:C:363[B]:GLN:HG3	1.74	0.67
1:C:141:PRO:HG2	1:C:182:LEU:HD21	1.76	0.66
1:C:344:GLN:HG3	6:C:1678:HOH:O	1.95	0.65
1:D:72:SER:HA	1:D:75[A]:LYS:HE3	1.78	0.65
4:A:405:HIS:N	6:A:1544:HOH:O	2.31	0.63
1:C:346[B]:GLY:O	1:C:347[B]:SER:O	2.19	0.61
1:C:363[A]:GLN:HG3	6:C:1707:HOH:O	2.00	0.60
1:B:332:LYS:HE2	6:C:723:HOH:O	2.02	0.59
1:C:346[B]:GLY:O	1:C:347[B]:SER:C	2.41	0.59
1:A:393:GLU:HG2	1:A:393:GLU:O	2.04	0.56
1:C:353[B]:ARG:NH1	1:C:366:THR:HB	2.20	0.56
1:D:3:SER:N	6:D:2036:HOH:O	2.38	0.55
1:B:15:VAL:HG22	1:B:302[B]:VAL:HG22	1.90	0.54
1:D:92:VAL:HG11	1:D:104:LYS:HE2	1.89	0.54
1:A:396:HIS:HB3	1:B:143:TYR:OH	2.07	0.54
1:B:302[B]:VAL:HG21	6:B:1882:HOH:O	2.09	0.53
1:B:325:VAL:HG23	1:B:392:LEU:HD13	1.90	0.52
1:B:348:ALA:HB1	1:B:389:VAL:HG12	1.91	0.52
4:A:406[B]:HIS:HD2	6:A:1527:HOH:O	1.92	0.52
1:A:278:LYS:NZ	6:A:1714:HOH:O	2.44	0.50
1:C:360:SER:HB2	1:C:363[B]:GLN:CG	2.40	0.50
4:A:406[B]:HIS:CD2	6:A:1527:HOH:O	2.65	0.49
1:D:3:SER:HB3	6:D:1978:HOH:O	2.12	0.48
1:A:191[A]:GLN:NE2	6:A:1921:HOH:O	2.46	0.48
1:D:184:ASP:HB2	1:D:185:PRO:HD3	1.95	0.48
1:A:104:LYS:HE2	6:A:1677:HOH:O	2.17	0.45
1:C:372:GLY:O	1:C:373[B]:ASN:OD1	2.35	0.43
1:A:354:TRP:HB3	1:A:362[A]:LEU:HD22	2.00	0.43
1:D:324:LYS:HB2	1:D:324:LYS:HE2	1.83	0.43
1:B:3:SER:N	6:B:1180:HOH:O	2.51	0.42
1:D:86:ASN:HD21	1:D:147[B]:TRP:HE3	1.66	0.42
1:D:20:GLY:HA3	1:D:51:ILE:O	2.20	0.42
1:C:353[A]:ARG:NH2	1:C:368:LEU:HD11	2.35	0.42
1:A:202:HIS:N	1:A:202:HIS:CD2	2.88	0.42
1:C:6:THR:O	1:C:306:ALA:HA	2.20	0.41
1:D:86:ASN:ND2	1:D:147[B]:TRP:HE3	2.18	0.41
1:D:139:ASN:OD1	1:D:202:HIS:HE1	2.03	0.41
1:A:107:LYS:HB2	1:A:110[A]:LYS:HG2	2.03	0.41
1:A:395:HIS:HB2	1:A:396:HIS:H	1.49	0.40
1:B:367[B]:ASN:ND2	6:B:1766:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:VAL:HA	1:B:330:ILE:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:578:HOH:O	6:B:1682:HOH:O[1_556]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	HIS	A	406[A]	-	5,10,11	0.53	0	3,12,14	1.25	0
3	TAR	A	404	-	3,9,9	0.31	0	6,12,12	1.62	2 (33%)
2	MLA	A	402	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	C	402	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	A	403	-	0,6,6	0.00	-	0,7,7	0.00	-
4	HIS	A	406[B]	-	5,10,11	0.53	0	3,12,14	1.28	0
2	MLA	B	402	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	D	402	-	0,6,6	0.00	-	0,7,7	0.00	-
4	HIS	A	405	4	5,10,11	0.76	0	3,12,14	1.27	1 (33%)

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	HIS	A	406[A]	-	-	0/5/6/8	0/1/1/1
3	TAR	A	404	-	2/2/4/4	0/4/12/12	-
2	MLA	A	402	-	-	0/0/4/4	-
2	MLA	C	402	-	-	0/0/4/4	-
2	MLA	A	403	-	-	0/0/4/4	-
4	HIS	A	406[B]	-	-	2/5/6/8	0/1/1/1
2	MLA	B	402	-	-	0/0/4/4	-
2	MLA	D	402	-	-	0/0/4/4	-
4	HIS	A	405	4	-	1/5/6/8	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	TAR	C1-C2-C3	-2.83	107.01	113.11
3	A	404	TAR	O3-C3-C4	-2.35	105.45	111.10
4	A	405	HIS	CD2-NE2-CE1	2.01	108.91	105.78

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	404	TAR	C2
3	A	404	TAR	C3

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	406[B]	HIS	CA-CB-CG-ND1
4	A	406[B]	HIS	CA-CB-CG-CD2
4	A	405	HIS	CA-CB-CG-ND1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	406[B]	HIS	2	0
4	A	405	HIS	1	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

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.