

Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2021 - 04:03 am BST

PDB ID	:	6T8E
Title	:	Crystal structure of native xylose isomerase from Piromyces E2 grown in yeast,
		in complex with xylose
Authors	:	Rozeboom, H.J.; Janssen, D.B.
Deposited on	:	2019-10-24
Resolution	:	1.86 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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.



Matria	Whole archive	Similar resolution		
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
Clashscore	141614	2625 (1.86-1.86)		
Ramachandran outliers	138981	2592(1.86-1.86)		
Sidechain outliers	138945	2592 (1.86-1.86)		

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 of 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	А	437	95%	5%
1	В	437	93%	6%
1	С	437	94%	5%
1	D	437	95%	

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
6	SO4	А	509	-	-	Х	-



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16096 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	426	Total	С	Ν	0	S	0	1	0
	A	430	3474	2205	582	667	20	0	1	0
1	1 B	3 436	Total	С	Ν	0	S	0	2	0
			3481	2210	583	668	20	0		
1	С	426	Total	С	Ν	0	S	0	2	0
	430	3481	2210	583	668	20	0	2	0	
1 D	426	Total	С	Ν	0	S	0	2	0	
	430	3490	2215	584	669	22	0	5	0	

• Molecule 1 is a protein called Xylose isomerase.

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Ca 2 2	0	0
2	В	2	Total Ca 2 2	0	0
2	С	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0

• Molecule 3 is D-xylose (three-letter code: XLS) (formula: $C_5H_{10}O_5$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 10 5 5 \end{array}$	0	0
3	В	1	Total C O 10 5 5	0	0
3	С	1	Total C O 10 5 5	0	0
3	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 10 5 5 \end{array}$	0	0

• Molecule 4 is beta-D-xylopyranose (three-letter code: XYP) (formula: $C_5H_{10}O_5$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C O 10 5 5	0	0
4	В	1	Total C O 10 5 5	0	0
4	В	1	Total C O 10 5 5	0	0
4	С	1	Total C O 10 5 5	0	0
4	D	1	Total C O 10 5 5	0	0
4	D	1	Total C O 10 5 5	0	0
4	D	1	Total C O 10 5 5	0	0

• Molecule 5 is alpha-D-xylopyranose (three-letter code: XYS) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total C O 10 5 5	0	0
5	А	1	Total C O 10 5 5	0	0
5	А	1	Total C O 10 5 5	0	0
5	В	1	Total C O 10 5 5	0	0
5	В	1	Total C O 10 5 5	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total C O 10 5 5	0	0
5	С	1	Total C O 10 5 5	0	0
5	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 10 5 5 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 10 5 5 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 10 5 5 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 10 5 5 \end{array}$	0	0

• Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	471	Total O 471 471	0	0
7	В	490	Total O 490 490	0	0
7	С	452	Total O 452 452	0	0
7	D	494	Total O 494 494	0	0



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 was not executed.

• Molecule 1: Xylose isomerase





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants	78.45Å 79.27Å 91.88Å	Depositor
a, b, c, α , β , γ	115.46° 89.99° 117.07°	Depositor
Resolution (Å)	46.60 - 1.86	Depositor
% Data completeness	93.6 (46.60-1.86)	Depositor
(in resolution range)	35.0 (10.00 1.00)	Depositor
R_{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.139 , 0.176	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16096	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP



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: XYS, CA, SO4, XYP, XLS

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).

Mal Chair		Bo	nd lengths	Bond angles		
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.70	0/3555	0.80	2/4785~(0.0%)	
1	В	0.70	1/3562~(0.0%)	0.79	0/4795	
1	С	0.70	0/3562	0.81	3/4795~(0.1%)	
1	D	0.72	1/3571~(0.0%)	0.80	0/4805	
All	All	0.71	2/14250~(0.0%)	0.80	5/19180~(0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	D	407	GLU	CD-OE1	5.28	1.31	1.25
1	В	369	GLU	CD-OE1	-5.11	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	222	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	С	300	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	С	196	MET	CG-SD-CE	-5.12	92.01	100.20
1	А	222	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	А	222	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3474	0	3360	10	0
1	В	3481	0	3368	20	0
1	С	3481	0	3368	14	0
1	D	3490	0	3376	12	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
3	А	10	0	8	0	0
3	В	10	0	8	0	0
3	С	10	0	8	1	0
3	D	10	0	8	0	0
4	А	10	0	0	0	0
4	В	20	0	0	0	0
4	С	10	0	0	0	0
4	D	30	0	0	0	0
5	А	30	0	30	0	0
5	В	30	0	30	0	0
5	С	30	0	30	0	0
5	D	20	0	20	0	0
6	А	10	0	0	2	0
6	В	5	0	0	1	0
6	С	10	0	0	0	0
6	D	10	0	0	1	0
7	A	471	0	0	4	0
7	В	490	0	0	4	0
7	С	452	0	0	2	0
7	D	494	0	0	4	0
All	All	16096	0	13614	53	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 (53) 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)	
3:C:503:XLS:H1	7:C:628:HOH:O	1.67	0.94	
1:A:437:GLN:OE1	7:A:601:HOH:O	1.90	0.88	
1:C:60:GLN:HG2	1:D:60:GLN:HG2	1.64	0.78	
1:D:32:LYS:HE2	1:D:369:GLU:OE2	1.83	0.78	



	A h o	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:8:GLN:HE21	1:B:8:GLN:HA	1.51	0.74	
1:B:271:ASN:HD21	1:B:309:THR:H	1.36	0.71	
1:B:256:LYS:NZ	7:B:601:HOH:O	2.26	0.67	
1:C:32:LYS:NZ	1:C:369:GLU:OE1	2.26	0.66	
1:D:376:GLN:HG3	7:D:990:HOH:O	1.96	0.66	
1:D:32:LYS:CE	1:D:369:GLU:OE2	2.46	0.64	
1:B:8:GLN:HG3	7:B:652:HOH:O	1.99	0.63	
6:A:509:SO4:O1	7:A:602:HOH:O	2.17	0.60	
1:B:107:VAL:HB	1:B:123[A]:VAL:HG21	1.84	0.58	
1:A:256:LYS:NZ	7:A:604:HOH:O	2.35	0.58	
1:A:60:GLN:HG2	1:B:60:GLN:HG2	1.85	0.56	
1:A:107:VAL:HB	1:A:123:VAL:HG21	1.88	0.56	
1:D:437:GLN:NE2	7:D:602:HOH:O	2.39	0.55	
1:C:107:VAL:HB	1:C:123[A]:VAL:HG21	1.89	0.55	
1:C:299:ASN:HB2	1:C:311:GLN:O	2.08	0.54	
6:D:510:SO4:O1	7:D:601:HOH:O	2.17	0.54	
1:C:196:MET:SD	1:C:240:THR:HA	2.49	0.53	
1:C:196:MET:SD	7:C:911:HOH:O	2.59	0.52	
1:D:266:VAL:HG22	1:D:292[A]:MET:O	2.11	0.51	
1:B:8:GLN:HE21	1:B:8:GLN:CA	2.17	0.50	
1:A:3:LYS:HE3	1:A:3:LYS:HA	1.92	0.50	
1:B:68:PHE:HB3	1:B:70:TRP:CE2	2.48	0.48	
1:A:351:GLU:N	6:A:509:SO4:O2	2.37	0.48	
1:D:437:GLN:CD	7:D:602:HOH:O	2.52	0.47	
1:A:299:ASN:HB2	1:A:311:GLN:O	2.15	0.46	
1:A:431:ALA:O	1:A:435:MET:HG2	2.16	0.46	
1:B:351:GLU:N	6:B:509:SO4:O1	2.37	0.46	
1:B:196:MET:SD	1:B:240:THR:HA	2.56	0.45	
1:B:397:LYS:HE2	7:B:606:HOH:O	2.18	0.44	
1:B:196:MET:HE1	7:B:808:HOH:O	2.18	0.43	
1:B:270:VAL:HG22	1:B:280:PHE:CD2	2.53	0.43	
1:B:91:MET:SD	1:B:99:TYR:HB3	2.59	0.43	
1:D:299:ASN:HB2	1:D:311:GLN:O	2.18	0.43	
1:B:168:ILE:HD12	1:C:409:VAL:HG11	2.00	0.43	
1:D:374:LEU:C	1:D:374:LEU:HD23	2.39	0.43	
1:B:271:ASN:HD22	1:B:310:ASP:H	1.65	0.42	
1:D:98:TYR:HB3	1:D:139:LEU:HB2	2.02	0.42	
1:A:236:PRO:HA	1:A:246:VAL:HA	2.01	0.42	
1:C:374:LEU:C	1:C:374:LEU:HD23	2.40	0.41	
1:C:98:TYR:HA	1:C:137:LYS:O	2.20	0.41	
1:B:242:HIS:CE1	1:C:282:HIS:CE1	3.09	0.41	



- · · · · · J · · · I	1.5		
Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:282:HIS:CE1	1:C:242:HIS:CE1	3.09	0.41
1:C:144:ASN:C	1:C:144:ASN:OD1	2.59	0.41
1:D:196:MET:SD	1:D:240:THR:HA	2.60	0.41
1:D:46:ALA:HA	1:D:98:TYR:O	2.21	0.41
7:A:772:HOH:O	1:B:196:MET:HG2	2.21	0.40
1:A:196:MET:SD	1:A:240:THR:HA	2.61	0.40
1:C:238:GLU:HA	1:C:239:PRO:HA	1.92	0.40
1:B:400:GLU:HB2	1:C:209:HIS:NE2	2.37	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	Perce	ntiles	s
1	А	435/437~(100%)	426 (98%)	7 (2%)	2(0%)	29	15	
1	В	436/437~(100%)	426 (98%)	8 (2%)	2 (0%)	29	15	
1	С	436/437~(100%)	424 (97%)	10 (2%)	2 (0%)	29	15	
1	D	437/437~(100%)	427~(98%)	8 (2%)	2 (0%)	29	15	
All	All	1744/1748~(100%)	1703 (98%)	33 (2%)	8 (0%)	29	15	

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	238	GLU
1	В	238	GLU
1	С	238	GLU
1	D	238	GLU
1	А	314	ILE
1	В	314	ILE
1	С	314	ILE



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Mol	Chain	Res	Type
1	D	314	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	358/358~(100%)	353~(99%)	5 (1%)	67	55	
1	В	359/358~(100%)	353~(98%)	6(2%)	60	47	
1	С	359/358~(100%)	356~(99%)	3 (1%)	81	76	
1	D	360/358~(101%)	357~(99%)	3(1%)	81	76	
All	All	1436/1432~(100%)	1419 (99%)	17 (1%)	71	62	

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	LYS
1	А	121	LYS
1	А	218	ARG
1	А	241	LYS
1	А	271	ASN
1	В	8	GLN
1	В	72	GLU
1	В	130	LYS
1	В	241	LYS
1	В	400	GLU
1	В	414	LYS
1	С	196	MET
1	С	271	ASN
1	С	414	LYS
1	D	78	GLU
1	D	196	MET
1	D	271	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such side chains are listed below:



Mol	Chain	Res	Type
1	А	437	GLN
1	В	8	GLN
1	В	71	ASN
1	В	271	ASN
1	D	8	GLN
1	D	437	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 8 are monoatomic - leaving 29 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).

Mal	Turne	Chain	Dog	Tink	Bo	ond leng	ths	Bond angles		
INIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	XYS	В	506	-	10,10,10	1.05	0	14,14,14	1.25	2 (14%)
6	SO4	С	508	-	4,4,4	0.31	0	6,6,6	0.15	0
3	XLS	С	503	2	8,9,9	0.62	0	10,11,11	1.85	4 (40%)
6	SO4	А	509	-	4,4,4	0.39	0	6,6,6	0.08	0
4	XYP	D	504	-	10,10,10	0.55	0	14,14,14	1.17	2 (14%)
5	XYS	А	505	-	10,10,10	1.23	2 (20%)	14,14,14	1.32	2 (14%)
5	XYS	А	506	-	10,10,10	1.05	0	14,14,14	1.06	1 (7%)



Mal	Tuno	Chain	Dog	Link	Bond lengths			Bond angles		les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	XYS	А	507	-	10,10,10	0.46	0	14,14,14	1.81	4 (28%)
3	XLS	В	503	2	8,9,9	0.92	1 (12%)	10,11,11	1.97	5 (50%)
5	XYS	D	505	-	10,10,10	0.85	0	14,14,14	1.34	1 (7%)
6	SO4	D	510	-	4,4,4	0.40	0	6,6,6	0.07	0
5	XYS	D	506	-	10,10,10	1.30	2 (20%)	14,14,14	1.24	1 (7%)
4	XYP	В	508	-	10,10,10	0.57	0	14,14,14	2.11	5 (35%)
5	XYS	С	505	-	10,10,10	1.14	1 (10%)	14,14,14	1.58	4 (28%)
6	SO4	С	509	-	4,4,4	0.38	0	6,6,6	0.07	0
5	XYS	С	507	-	10,10,10	0.39	0	14,14,14	1.72	3 (21%)
6	SO4	В	509	-	4,4,4	0.41	0	6,6,6	0.05	0
4	XYP	А	504	-	10,10,10	0.65	0	14,14,14	1.33	2 (14%)
3	XLS	А	503	2	8,9,9	1.03	1 (12%)	10,11,11	1.80	4 (40%)
4	XYP	D	507	-	10,10,10	0.42	0	14,14,14	1.38	2 (14%)
5	XYS	С	506	-	$10,\!10,\!10$	0.90	0	14,14,14	0.92	0
6	SO4	А	508	-	4,4,4	0.36	0	6,6,6	0.05	0
6	SO4	D	509	-	4,4,4	0.32	0	6,6,6	0.15	0
4	XYP	С	504	-	$10,\!10,\!10$	0.66	0	14,14,14	1.12	1 (7%)
4	XYP	В	504	-	10, 10, 10	0.61	0	14,14,14	1.18	1 (7%)
4	XYP	D	508	-	10,10,10	0.44	0	14,14,14	1.42	2(14%)
3	XLS	D	503	2	8,9,9	1.15	1 (12%)	10,11,11	2.70	5 (50%)
5	XYS	В	505	-	10,10,10	0.90	0	14,14,14	1.60	3 (21%)
5	XYS	В	507	-	10,10,10	0.59	0	14,14,14	2.41	6 (42%)

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	XYS	В	506	-	-	-	0/1/1/1
3	XLS	С	503	2	-	1/10/12/12	-
4	XYP	D	504	-	-	-	0/1/1/1
5	XYS	А	505	-	-	-	0/1/1/1
5	XYS	А	506	-	-	-	0/1/1/1
5	XYS	А	507	-	-	-	0/1/1/1
3	XLS	В	503	2	-	2/10/12/12	-
5	XYS	D	505	-	-	-	0/1/1/1
5	XYS	D	506	-	-	-	0/1/1/1
4	XYP	В	508	-	-	-	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	XYS	С	505	-	-	-	0/1/1/1
5	XYS	С	507	-	-	-	0/1/1/1
4	XYP	А	504	-	-	-	0/1/1/1
3	XLS	А	503	2	-	3/10/12/12	-
4	XYP	D	507	-	-	-	0/1/1/1
5	XYS	С	506	-	-	-	0/1/1/1
4	XYP	С	504	-	-	-	0/1/1/1
4	XYP	В	504	-	-	-	0/1/1/1
4	XYP	D	508	-	-	-	0/1/1/1
3	XLS	D	503	2	-	4/10/12/12	-
5	XYS	В	505	-	-	-	0/1/1/1
5	XYS	В	507	-	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	503	XLS	C3-C2	-2.74	1.49	1.53
3	D	503	XLS	C3-C2	-2.74	1.49	1.53
5	А	505	XYS	O4-C4	2.56	1.48	1.43
3	В	503	XLS	C3-C2	-2.38	1.49	1.53
5	D	506	XYS	O5-C1	2.35	1.46	1.43
5	С	505	XYS	O4-C4	2.25	1.48	1.43
5	D	506	XYS	O1-C1	2.13	1.46	1.39
5	А	505	XYS	C4-C3	2.03	1.55	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	В	507	XYS	O5-C5-C4	-6.45	100.81	110.77
4	В	508	XYP	O5-C1-C2	5.37	117.41	109.43
3	D	503	XLS	O2-C2-C1	4.98	121.82	110.08
5	С	507	XYS	C5-C4-C3	-4.12	104.61	109.67
5	А	507	XYS	C5-C4-C3	-3.87	104.91	109.67
5	С	507	XYS	C5-O5-C1	3.65	118.85	112.71
4	D	508	XYP	C5-C4-C3	3.62	114.11	109.67
3	D	503	XLS	C5-C4-C3	-3.58	104.66	112.41
5	А	507	XYS	C5-O5-C1	3.57	118.71	112.71
3	D	503	XLS	O3-C3-C4	3.26	116.69	108.81
3	D	503	XLS	C3-C2-C1	-3.09	101.38	111.10
5	В	507	XYS	C1-C2-C3	3.04	116.63	110.31
4	D	507	XYP	C5-C4-C3	-2.96	106.03	109.67
5	С	505	XYS	O5-C1-C2	2.91	113.75	109.43



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	503	XLS	C5-C4-C3	-2.90	106.12	112.41
3	В	503	XLS	C5-C4-C3	-2.87	106.19	112.41
5	В	505	XYS	C5-O5-C1	2.86	117.53	112.71
5	В	507	XYS	O3-C3-C2	-2.86	103.74	110.35
5	D	506	XYS	C5-C4-C3	2.82	113.13	109.67
4	D	508	XYP	O5-C1-C2	-2.78	105.29	109.43
5	В	507	XYS	C5-C4-C3	-2.74	106.29	109.67
3	А	503	XLS	O5-C5-C4	-2.70	105.20	111.07
4	В	508	XYP	C1-C2-C3	2.61	115.73	110.31
5	В	505	XYS	O5-C5-C4	2.59	114.78	110.77
5	D	505	XYS	O5-C1-C2	2.59	113.28	109.43
3	А	503	XLS	C5-C4-C3	-2.58	106.83	112.41
4	В	508	XYP	C5-O5-C1	2.56	117.01	112.71
3	В	503	XLS	C4-C3-C2	-2.53	106.30	112.97
4	С	504	XYP	O4-C4-C3	-2.50	105.13	110.14
3	С	503	XLS	O4-C4-C3	2.45	115.06	109.10
3	С	503	XLS	O3-C3-C2	2.44	113.63	109.17
4	А	504	XYP	C4-C3-C2	-2.43	106.68	110.89
3	С	503	XLS	O2-C2-C3	2.40	115.15	109.46
3	В	503	XLS	O3-C3-C4	2.35	114.49	108.81
5	А	506	XYS	O4-C4-C3	-2.34	105.45	110.14
5	А	505	XYS	01-C1-C2	-2.33	102.46	109.03
3	В	503	XLS	O2-C2-C1	2.30	115.51	110.08
4	D	504	XYP	C4-C3-C2	-2.30	106.92	110.89
4	В	508	XYP	C5-C4-C3	-2.28	106.86	109.67
5	В	506	XYS	O4-C4-C3	-2.27	105.58	110.14
3	А	503	XLS	C4-C3-C2	-2.27	107.00	112.97
3	D	503	XLS	O4-C4-C3	2.24	114.54	109.10
5	А	507	XYS	O5-C5-C4	-2.23	107.33	110.77
5	В	505	XYS	O3-C3-C4	-2.21	105.76	109.99
5	В	507	XYS	O5-C1-C2	2.20	112.70	109.43
5	С	505	XYS	O2-C2-C1	-2.20	104.06	109.16
5	А	505	XYS	O5-C5-C4	2.13	114.06	110.77
4	В	508	XYP	O4-C4-C5	2.13	113.51	109.15
4	D	507	XYP	C4-C3-C2	-2.10	107.26	110.89
4	В	504	XYP	C5-C4-C3	-2.10	107.08	109.67
4	D	504	XYP	C5-O5-C1	2.10	116.24	112.71
5	C	505	XYS	04-C4-C3	2.09	114.32	110.14
5	С	507	XYS	O5-C5-C4	-2.08	107.56	110.77
5	C	505	XYS	C5-C4-C3	-2.08	107.11	109.67
3	В	503	XLS	O4-C4-C3	2.07	114.13	109.10
4	А	504	XYP	O5-C5-C4	2.05	113.94	110.77



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
5	А	507	XYS	O5-C1-C2	2.04	112.47	109.43
5	В	506	XYS	O4-C4-C5	2.04	113.32	109.15
5	В	507	XYS	C4-C3-C2	2.02	114.38	110.89
3	А	503	XLS	O4-C4-C3	2.01	113.98	109.10

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	503	XLS	C1-C2-C3-C4
3	D	503	XLS	O3-C3-C4-C5
3	D	503	XLS	C2-C3-C4-C5
3	D	503	XLS	O3-C3-C4-O4
3	D	503	XLS	C2-C3-C4-O4
3	В	503	XLS	O3-C3-C4-C5
3	В	503	XLS	C2-C3-C4-C5
3	А	503	XLS	C2-C3-C4-C5
3	А	503	XLS	O3-C3-C4-C5
3	С	503	XLS	C2-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	503	XLS	1	0
6	А	509	SO4	2	0
6	D	510	SO4	1	0
6	В	509	SO4	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

