



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:25 PM BST

PDB ID : 5YN3  
Title : Crystal structure of xylose isomerase from *Piromyces* sp. E2  
Authors : Son, H.-F.; Kim, K.-J.  
Deposited on : 2017-10-24  
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

<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 : 2.14.2  
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) : 2.14.2

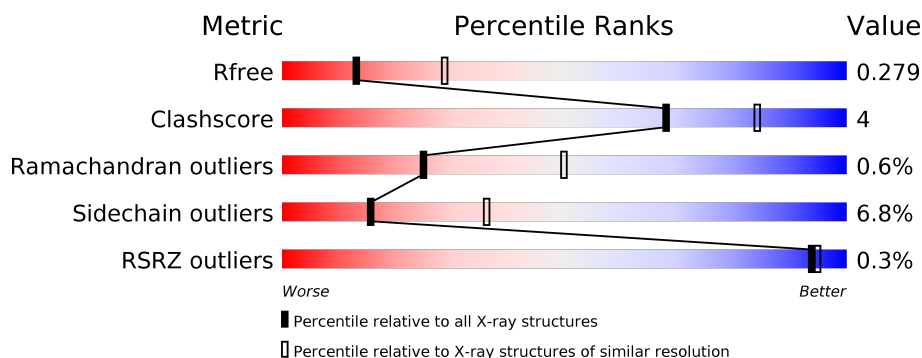
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	449	<div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
1	B	449	<div> <div>82%</div> <div>13%</div> <div>• •</div> </div>
1	C	449	<div> <div>83%</div> <div>13%</div> <div>• •</div> </div>
1	D	449	<div> <div>82%</div> <div>14%</div> <div>• •</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14080 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 Xylose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3463	2198	581	665	19			
1	B	435	Total	C	N	O	S	0	0	0
			3463	2198	581	665	19			
1	C	435	Total	C	N	O	S	0	0	0
			3463	2198	581	665	19			
1	D	435	Total	C	N	O	S	0	0	0
			3463	2198	581	665	19			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9P8C9
A	-10	ARG	-	expression tag	UNP Q9P8C9
A	-9	GLY	-	expression tag	UNP Q9P8C9
A	-8	SER	-	expression tag	UNP Q9P8C9
A	-7	HIS	-	expression tag	UNP Q9P8C9
A	-6	HIS	-	expression tag	UNP Q9P8C9
A	-5	HIS	-	expression tag	UNP Q9P8C9
A	-4	HIS	-	expression tag	UNP Q9P8C9
A	-3	HIS	-	expression tag	UNP Q9P8C9
A	-2	HIS	-	expression tag	UNP Q9P8C9
A	-1	GLY	-	expression tag	UNP Q9P8C9
A	0	SER	-	expression tag	UNP Q9P8C9
B	-11	MET	-	expression tag	UNP Q9P8C9
B	-10	ARG	-	expression tag	UNP Q9P8C9
B	-9	GLY	-	expression tag	UNP Q9P8C9
B	-8	SER	-	expression tag	UNP Q9P8C9
B	-7	HIS	-	expression tag	UNP Q9P8C9
B	-6	HIS	-	expression tag	UNP Q9P8C9
B	-5	HIS	-	expression tag	UNP Q9P8C9
B	-4	HIS	-	expression tag	UNP Q9P8C9
B	-3	HIS	-	expression tag	UNP Q9P8C9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q9P8C9
B	-1	GLY	-	expression tag	UNP Q9P8C9
B	0	SER	-	expression tag	UNP Q9P8C9
C	-11	MET	-	expression tag	UNP Q9P8C9
C	-10	ARG	-	expression tag	UNP Q9P8C9
C	-9	GLY	-	expression tag	UNP Q9P8C9
C	-8	SER	-	expression tag	UNP Q9P8C9
C	-7	HIS	-	expression tag	UNP Q9P8C9
C	-6	HIS	-	expression tag	UNP Q9P8C9
C	-5	HIS	-	expression tag	UNP Q9P8C9
C	-4	HIS	-	expression tag	UNP Q9P8C9
C	-3	HIS	-	expression tag	UNP Q9P8C9
C	-2	HIS	-	expression tag	UNP Q9P8C9
C	-1	GLY	-	expression tag	UNP Q9P8C9
C	0	SER	-	expression tag	UNP Q9P8C9
D	-11	MET	-	expression tag	UNP Q9P8C9
D	-10	ARG	-	expression tag	UNP Q9P8C9
D	-9	GLY	-	expression tag	UNP Q9P8C9
D	-8	SER	-	expression tag	UNP Q9P8C9
D	-7	HIS	-	expression tag	UNP Q9P8C9
D	-6	HIS	-	expression tag	UNP Q9P8C9
D	-5	HIS	-	expression tag	UNP Q9P8C9
D	-4	HIS	-	expression tag	UNP Q9P8C9
D	-3	HIS	-	expression tag	UNP Q9P8C9
D	-2	HIS	-	expression tag	UNP Q9P8C9
D	-1	GLY	-	expression tag	UNP Q9P8C9
D	0	SER	-	expression tag	UNP Q9P8C9

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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

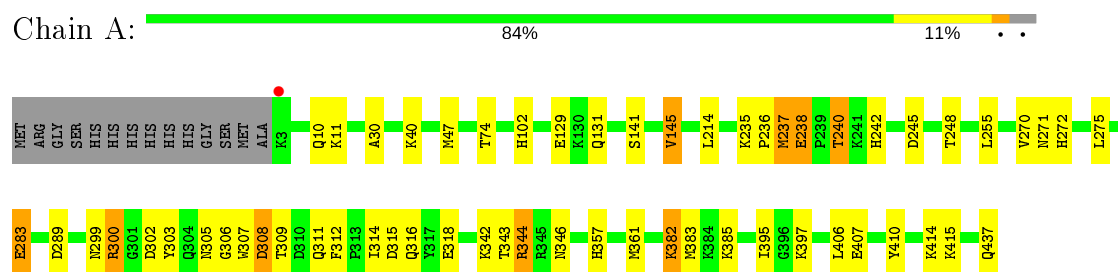
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	42	Total	O	0	0
			42	42		
4	C	41	Total	O	0	0
			41	41		
4	D	54	Total	O	0	0
			54	54		

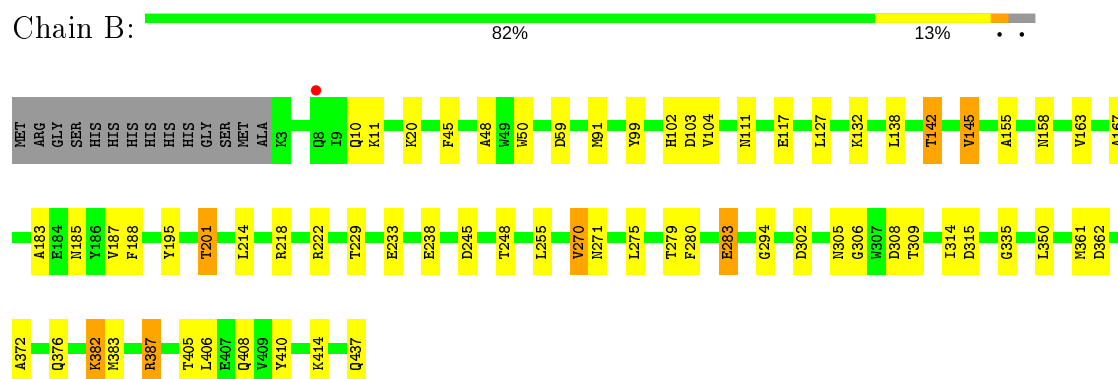
### 3 Residue-property plots [i](#)

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 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.

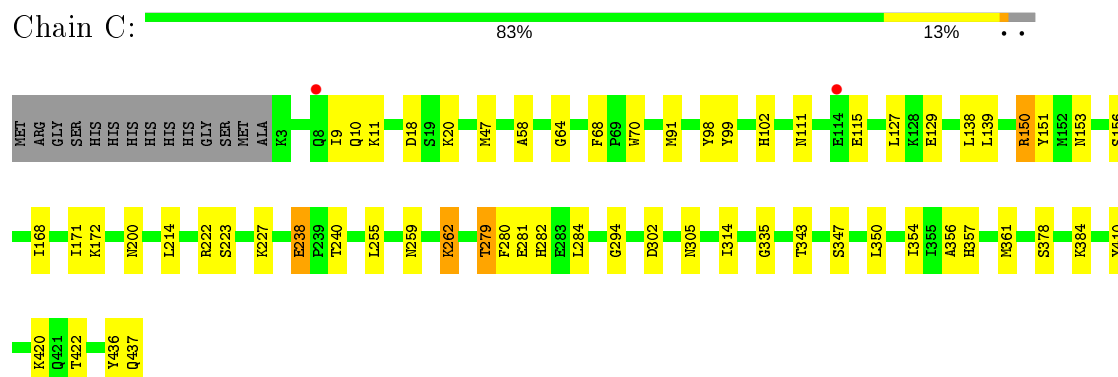
- Molecule 1: Xylose isomerase



- Molecule 1: Xylose isomerase



- Molecule 1: Xylose isomerase



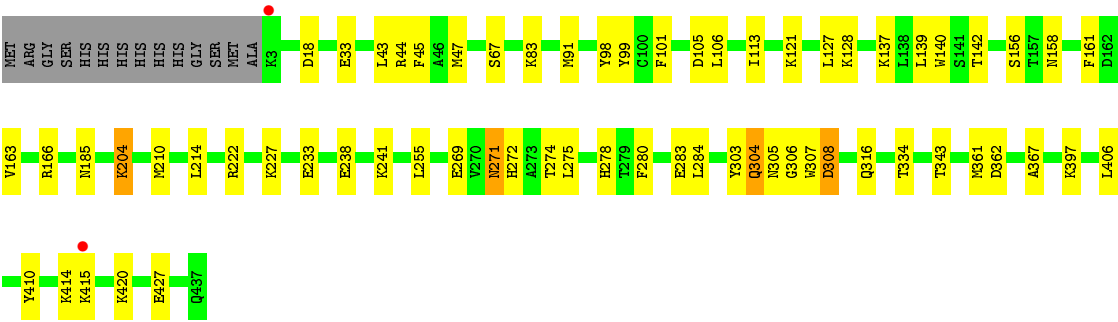
- Molecule 1: Xylose isomerase

Chain D: 

82%

14%

••



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.47Å 126.42Å 171.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.38 – 2.70 37.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.4 (37.38-2.70) 91.5 (37.38-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.86 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, $R_{free}$	0.194 , 0.277 0.201 , 0.279	Depositor DCC
$R_{free}$ test set	2167 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 33.6	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	0.94	EDS
Total number of atoms	14080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1686e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, MN

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	0.53	0/3541	0.71	0/4768
1	B	0.54	0/3541	0.70	1/4768 (0.0%)
1	C	0.53	0/3541	0.71	0/4768
1	D	0.52	0/3541	0.72	0/4768
All	All	0.53	0/14164	0.71	1/19072 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	ARG	NE-CZ-NH1	5.02	122.81	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 the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3463	0	3346	29	0
1	B	3463	0	3346	32	0
1	C	3463	0	3346	24	0
1	D	3463	0	3346	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	12	0	15	3	0
3	B	6	0	7	3	0
3	C	6	0	7	1	0
3	D	6	0	7	2	0
4	A	53	0	0	1	0
4	B	42	0	0	0	0
4	C	41	0	0	0	0
4	D	54	0	0	0	0
All	All	14080	0	13420	104	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 4.

All (104) 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:C:102:HIS:NE2	3:C:503:GOL:O2	2.16	0.77
1:A:102:HIS:NE2	3:A:503:GOL:H31	2.00	0.76
1:D:233:GLU:OE1	3:D:503:GOL:H32	1.95	0.67
1:D:280:PHE:CE2	1:D:284:LEU:HD11	2.33	0.64
1:B:233:GLU:OE1	3:B:503:GOL:C1	2.46	0.62
1:C:357:HIS:O	1:C:361:MET:HG2	2.01	0.61
1:B:271:ASN:ND2	1:B:308:ASP:O	2.33	0.60
1:B:405:THR:H	1:B:408:GLN:HE21	1.49	0.59
1:D:305:ASN:HB3	1:D:307:TRP:CZ3	2.37	0.59
1:A:309:THR:O	1:A:344:ARG:NH2	2.34	0.59
1:C:279:THR:HG22	1:C:282:HIS:H	1.66	0.58
1:B:91:MET:SD	1:B:99:TYR:HB3	2.45	0.57
1:D:271:ASN:OD1	1:D:308:ASP:HA	2.04	0.57
1:A:102:HIS:NE2	3:A:503:GOL:C3	2.69	0.56
1:A:305:ASN:HB3	1:A:307:TRP:CZ3	2.41	0.56
1:C:280:PHE:CE2	1:C:284:LEU:HD11	2.42	0.55
1:A:248:THR:OG1	1:A:283:GLU:HG3	2.07	0.55
1:A:407:GLU:OE1	3:A:504:GOL:O3	2.21	0.54
1:C:91:MET:SD	1:C:99:TYR:HB3	2.49	0.53
1:D:233:GLU:OE1	3:D:503:GOL:C3	2.57	0.52
1:A:240:THR:HB	4:A:609:HOH:O	2.08	0.52
1:B:138:LEU:HD23	1:B:183:ALA:HB2	1.91	0.52
1:B:233:GLU:OE1	3:B:503:GOL:O1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:OD1	1:C:153:ASN:OD1	2.27	0.51
1:D:185:ASN:ND2	1:D:334:THR:OG1	2.43	0.51
1:B:145:VAL:HG21	1:B:167:ALA:HB1	1.93	0.51
1:C:168:ILE:HA	1:C:171:ILE:HD12	1.93	0.50
1:B:142:THR:HG22	1:B:187:VAL:O	2.10	0.50
1:C:9:ILE:HD13	1:C:354:ILE:HG13	1.94	0.50
1:A:315:ASP:OD1	1:A:315:ASP:C	2.50	0.50
1:B:195:TYR:HB2	1:B:201:THR:HG21	1.93	0.50
1:A:410:TYR:CZ	1:A:414:LYS:HD2	2.47	0.50
1:A:342:LYS:O	1:A:344:ARG:NH1	2.45	0.50
1:A:300:ARG:NH1	1:A:312:PHE:O	2.44	0.49
1:C:294:GLY:O	1:C:335:GLY:HA3	2.12	0.49
1:D:101:PHE:CE1	1:D:106:LEU:HD11	2.47	0.49
1:B:410:TYR:CZ	1:B:414:LYS:HD2	2.47	0.49
1:B:117:GLU:OE2	1:C:410:TYR:OH	2.20	0.48
1:C:99:TYR:CE2	1:C:138:LEU:HD13	2.49	0.48
1:D:140:TRP:HB3	1:D:185:ASN:HB2	1.96	0.48
1:B:382:LYS:HG3	1:B:383:MET:N	2.29	0.47
1:C:343:THR:HG22	1:C:347:SER:HB2	1.97	0.47
1:A:30:ALA:HB1	1:A:40:LYS:HG3	1.96	0.47
1:A:395:ILE:HG23	1:D:161:PHE:CE2	2.49	0.47
1:B:248:THR:OG1	1:B:283:GLU:HG3	2.15	0.47
1:B:48:ALA:HB1	1:B:50:TRP:CE2	2.51	0.46
1:C:98:TYR:HB3	1:C:139:LEU:HB2	1.98	0.46
1:D:113:ILE:HD11	1:D:166:ARG:HD3	1.97	0.46
1:D:305:ASN:O	1:D:307:TRP:N	2.49	0.46
1:A:305:ASN:HB3	1:A:307:TRP:CH2	2.52	0.45
1:D:269:GLU:HB3	1:D:272:HIS:CG	2.52	0.45
1:D:158:ASN:ND2	1:D:163:VAL:HG11	2.31	0.45
1:D:98:TYR:HB3	1:D:139:LEU:HB2	1.99	0.45
1:D:156:SER:OG	1:D:210:MET:HA	2.17	0.45
1:B:187:VAL:CG1	1:B:188:PHE:N	2.79	0.44
1:C:68:PHE:HB3	1:C:70:TRP:CE2	2.52	0.44
1:A:240:THR:CG2	1:A:242:HIS:C	2.86	0.44
1:B:294:GLY:O	1:B:335:GLY:HA3	2.17	0.44
1:C:111:ASN:ND2	1:C:115:GLU:OE1	2.51	0.43
1:B:142:THR:HG23	1:B:187:VAL:HB	1.99	0.43
1:C:262:LYS:CE	1:C:262:LYS:HA	2.48	0.43
1:A:316:GLN:H	1:B:437:GLN:HE22	1.65	0.43
1:C:436:TYR:O	1:C:437:GLN:C	2.56	0.43
1:D:83:LYS:NZ	1:D:105:ASP:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:TYR:HA	1:D:137:LYS:O	2.19	0.43
1:D:316:GLN:HE22	1:D:367:ALA:N	2.16	0.43
1:C:356:ALA:HB2	1:D:427:GLU:HG2	2.00	0.43
1:A:236:PRO:O	1:A:237:MET:HB3	2.17	0.43
1:A:357:HIS:O	1:A:361:MET:HG2	2.19	0.43
1:D:275:LEU:HD11	1:D:307:TRP:HA	2.00	0.43
1:B:302:ASP:HB3	1:B:305:ASN:HB2	2.01	0.43
1:A:289:ASP:HB3	1:D:204:LYS:HB3	1.99	0.43
1:A:235:LYS:HG3	1:A:272:HIS:CG	2.54	0.43
1:A:382:LYS:HG3	1:A:383:MET:N	2.34	0.43
1:B:185:ASN:HD22	1:B:229:THR:HB	1.84	0.42
1:D:91:MET:SD	1:D:99:TYR:HB3	2.58	0.42
1:B:10:GLN:O	1:B:11:LYS:C	2.58	0.42
1:B:145:VAL:HG13	1:B:155:ALA:CB	2.49	0.42
1:A:315:ASP:OD2	1:B:315:ASP:OD2	2.37	0.42
1:B:102:HIS:CD2	3:B:503:GOL:HO3	2.34	0.42
1:A:300:ARG:HG2	1:A:311:GLN:HB2	2.01	0.42
1:B:158:ASN:ND2	1:B:163:VAL:HG11	2.34	0.42
1:B:372:ALA:O	1:B:376:GLN:HG3	2.20	0.42
1:A:299:ASN:HB2	1:A:311:GLN:O	2.18	0.42
1:A:238:GLU:OE1	1:A:308:ASP:HB2	2.20	0.42
1:C:58:ALA:N	1:C:64:GLY:HA2	2.35	0.42
1:A:303:TYR:OH	1:A:318:GLU:OE2	2.30	0.41
1:C:150:ARG:O	1:C:151:TYR:CB	2.68	0.41
1:D:45:PHE:O	1:D:98:TYR:HB2	2.21	0.41
1:B:103:ASP:OD1	1:B:104:VAL:N	2.52	0.41
1:B:142:THR:CG2	1:B:187:VAL:O	2.69	0.41
1:B:45:PHE:CZ	1:B:361:MET:HB2	2.56	0.41
1:D:274:THR:HA	1:D:278:HIS:O	2.21	0.41
1:C:10:GLN:O	1:C:11:LYS:C	2.59	0.41
1:C:262:LYS:HE2	1:C:262:LYS:HA	2.03	0.41
1:D:43:LEU:O	1:D:44:ARG:C	2.59	0.41
1:C:302:ASP:HB3	1:C:305:ASN:HB2	2.02	0.41
1:A:302:ASP:HB3	1:A:305:ASN:HB2	2.03	0.41
1:B:59:ASP:C	1:B:59:ASP:OD1	2.59	0.41
1:B:270:VAL:HB	1:B:280:PHE:CG	2.56	0.40
1:D:410:TYR:CZ	1:D:414:LYS:HD2	2.56	0.40
1:D:303:TYR:HB2	1:D:304:GLN:HE21	1.87	0.40
1:A:145:VAL:HG13	1:A:145:VAL:O	2.22	0.40
1:B:387:ARG:NH1	1:C:200:ASN:O	2.54	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	433/449 (96%)	411 (95%)	19 (4%)	3 (1%)	22	46
1	B	433/449 (96%)	410 (95%)	20 (5%)	3 (1%)	22	46
1	C	433/449 (96%)	415 (96%)	16 (4%)	2 (0%)	29	54
1	D	433/449 (96%)	411 (95%)	20 (5%)	2 (0%)	29	54
All	All	1732/1796 (96%)	1647 (95%)	75 (4%)	10 (1%)	25	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	GLY
1	B	306	GLY
1	D	306	GLY
1	A	238	GLU
1	B	314	ILE
1	B	238	GLU
1	C	314	ILE
1	D	238	GLU
1	C	238	GLU
1	A	314	ILE

### 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	357/368 (97%)	330 (92%)	27 (8%)	13	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	357/368 (97%)	336 (94%)	21 (6%)	19	43
1	C	357/368 (97%)	333 (93%)	24 (7%)	16	37
1	D	357/368 (97%)	332 (93%)	25 (7%)	15	35
All	All	1428/1472 (97%)	1331 (93%)	97 (7%)	16	36

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	LYS
1	A	47	MET
1	A	74	THR
1	A	129	GLU
1	A	131	GLN
1	A	141	SER
1	A	145	VAL
1	A	214	LEU
1	A	237	MET
1	A	240	THR
1	A	245	ASP
1	A	255	LEU
1	A	270	VAL
1	A	271	ASN
1	A	275	LEU
1	A	283	GLU
1	A	300	ARG
1	A	308	ASP
1	A	343	THR
1	A	344	ARG
1	A	382	LYS
1	A	385	LYS
1	A	397	LYS
1	A	406	LEU
1	A	415	LYS
1	A	437	GLN
1	B	20	LYS
1	B	111	ASN
1	B	127	LEU
1	B	132	LYS
1	B	142	THR
1	B	145	VAL

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Mol	Chain	Res	Type
1	B	201	THR
1	B	214	LEU
1	B	218	ARG
1	B	222	ARG
1	B	245	ASP
1	B	255	LEU
1	B	270	VAL
1	B	275	LEU
1	B	279	THR
1	B	283	GLU
1	B	309	THR
1	B	350	LEU
1	B	362	ASP
1	B	382	LYS
1	B	406	LEU
1	C	18	ASP
1	C	20	LYS
1	C	47	MET
1	C	127	LEU
1	C	129	GLU
1	C	150	ARG
1	C	156	SER
1	C	172	LYS
1	C	214	LEU
1	C	222	ARG
1	C	223	SER
1	C	227	LYS
1	C	238	GLU
1	C	240	THR
1	C	255	LEU
1	C	259	ASN
1	C	262	LYS
1	C	279	THR
1	C	281	GLU
1	C	350	LEU
1	C	378	SER
1	C	384	LYS
1	C	420	LYS
1	C	422	THR
1	D	18	ASP
1	D	33	GLU
1	D	47	MET

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Mol	Chain	Res	Type
1	D	67	SER
1	D	121	LYS
1	D	127	LEU
1	D	128	LYS
1	D	142	THR
1	D	204	LYS
1	D	214	LEU
1	D	222	ARG
1	D	227	LYS
1	D	241	LYS
1	D	255	LEU
1	D	271	ASN
1	D	283	GLU
1	D	304	GLN
1	D	308	ASP
1	D	343	THR
1	D	361	MET
1	D	362	ASP
1	D	397	LYS
1	D	406	LEU
1	D	415	LYS
1	D	420	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	185	ASN
1	A	271	ASN
1	A	305	ASN
1	A	316	GLN
1	B	8	GLN
1	B	82	GLN
1	B	119	ASN
1	B	185	ASN
1	B	305	ASN
1	B	316	GLN
1	B	321	GLN
1	B	346	ASN
1	B	357	HIS
1	B	408	GLN
1	B	437	GLN

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Mol	Chain	Res	Type
1	C	119	ASN
1	C	185	ASN
1	C	242	HIS
1	C	316	GLN
1	D	60	GLN
1	D	82	GLN
1	D	119	ASN
1	D	185	ASN
1	D	305	ASN
1	D	316	GLN
1	D	321	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 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\# Z  > 2$
3	GOL	C	503	2	5,5,5	0.45	0	5,5,5	0.63	0
3	GOL	A	504	-	5,5,5	0.47	0	5,5,5	0.46	0
3	GOL	A	503	2	5,5,5	0.36	0	5,5,5	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	D	503	2	5,5,5	0.31	0	5,5,5	0.88	0
3	GOL	B	503	2	5,5,5	0.21	0	5,5,5	0.34	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
3	GOL	C	503	2	-	2/4/4/4	-
3	GOL	A	504	-	-	0/4/4/4	-
3	GOL	A	503	2	-	1/4/4/4	-
3	GOL	D	503	2	-	2/4/4/4	-
3	GOL	B	503	2	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GOL	O1-C1-C2-C3
3	C	503	GOL	C1-C2-C3-O3
3	D	503	GOL	O1-C1-C2-C3
3	B	503	GOL	O2-C2-C3-O3
3	C	503	GOL	O2-C2-C3-O3
3	B	503	GOL	C1-C2-C3-O3
3	B	503	GOL	O1-C1-C2-O2
3	D	503	GOL	O1-C1-C2-O2
3	A	503	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	GOL	1	0
3	A	504	GOL	1	0
3	A	503	GOL	2	0
3	D	503	GOL	2	0
3	B	503	GOL	3	0

## 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 [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	435/449 (96%)	-0.44	1 (0%) 95 96	10, 16, 26, 54	0
1	B	435/449 (96%)	-0.36	1 (0%) 95 96	11, 18, 29, 60	0
1	C	435/449 (96%)	-0.34	2 (0%) 91 92	9, 18, 29, 65	0
1	D	435/449 (96%)	-0.36	2 (0%) 91 92	9, 16, 28, 52	0
All	All	1740/1796 (96%)	-0.38	6 (0%) 94 95	9, 17, 28, 65	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	114	GLU	2.8
1	B	8	GLN	2.6
1	A	3	LYS	2.3
1	D	415	LYS	2.3
1	C	8	GLN	2.2
1	D	3	LYS	2.2

### 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 [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. 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
3	GOL	A	504	6/6	0.83	0.19	44,46,47,48	0
3	GOL	C	503	6/6	0.90	0.23	32,33,35,38	0
3	GOL	A	503	6/6	0.93	0.19	30,30,30,31	0
2	MN	B	502	1/1	0.93	0.10	53,53,53,53	0
3	GOL	B	503	6/6	0.94	0.26	35,37,37,41	0
3	GOL	D	503	6/6	0.94	0.20	38,39,39,42	0
2	MN	A	502	1/1	0.96	0.08	36,36,36,36	0
2	MN	D	502	1/1	0.97	0.10	37,37,37,37	0
2	MN	A	501	1/1	0.97	0.08	47,47,47,47	0
2	MN	B	501	1/1	0.97	0.06	34,34,34,34	0
2	MN	C	502	1/1	0.98	0.06	41,41,41,41	0
2	MN	C	501	1/1	0.98	0.07	27,27,27,27	0
2	MN	D	501	1/1	0.99	0.04	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.