Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 11:25 AM EDT

PDB ID	:	2B5E
Title	:	Crystal Structure of Yeast Protein Disulfide Isomerase
Authors	:	Schindelin, H.; Tian, G.
Deposited on	:	2005-09-28
Resolution	:	2.40 Å(reported)

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

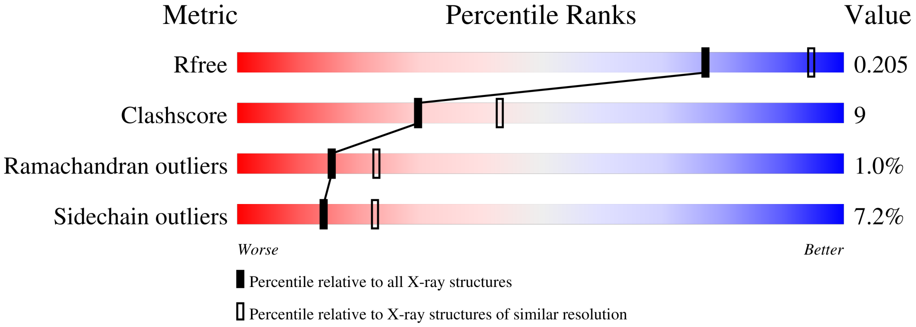
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Mol	Chain	Length	Quality of chain
1	A	504	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3975 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 Protein disulfide-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	483	3824	2441	605	761	17	0	2	0

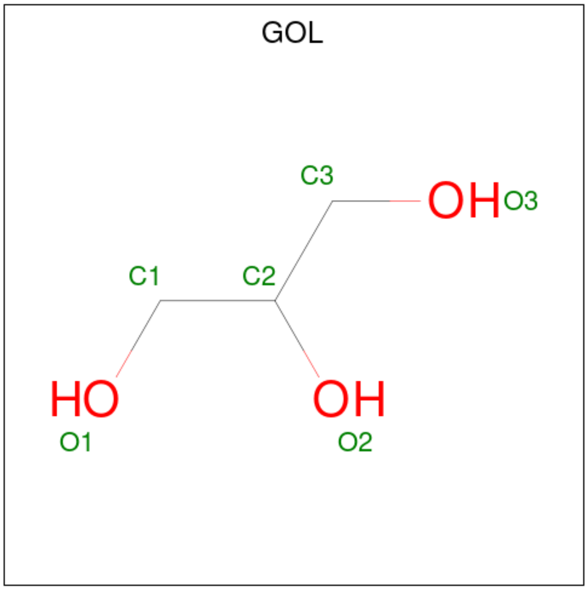
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	-	CLONING ARTIFACT	UNP P17967
A	20	GLY	-	CLONING ARTIFACT	UNP P17967
A	21	HIS	-	CLONING ARTIFACT	UNP P17967
A	22	MET	-	INITIATING METHIONINE	UNP P17967

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ba		
2	A	1	1	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

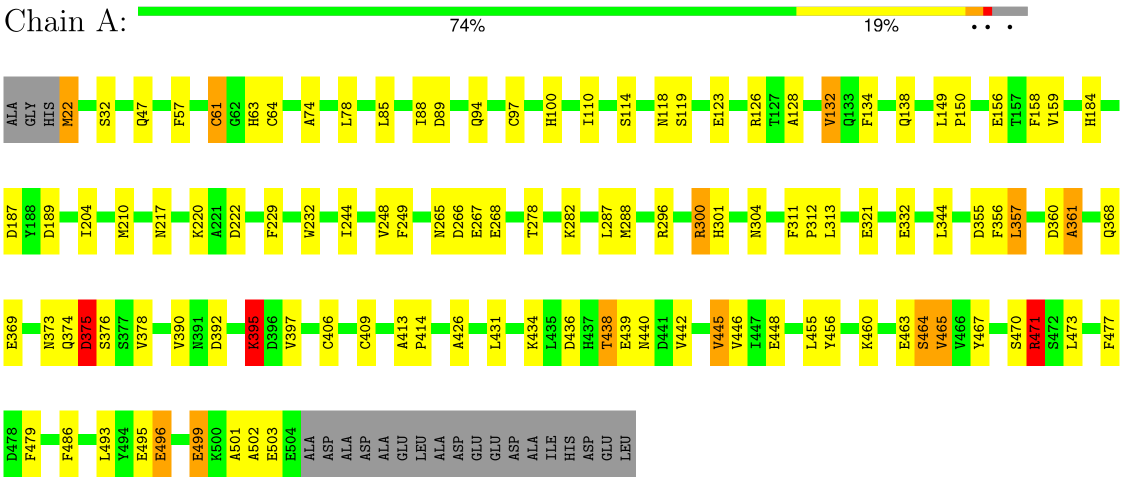
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	138	Total O 138 138	0	0

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. 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.

- Molecule 1: Protein disulfide-isomerase



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	136.56Å 136.56Å 69.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 48.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.40) 98.4 (48.28-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.191 , 0.246 0.210 , 0.205	Depositor DCC
R_{free} test set	1234 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 73.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3975	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, BA

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	0.83	2/3919 (0.1%)	0.82	4/5317 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	CYS	CB-SG	8.61	1.96	1.82
1	A	32	SER	CB-OG	7.45	1.51	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	471	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	A	189	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	A	89	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	126	ARG	NE-CZ-NH2	-5.32	117.64	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	395	LYS	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	3824	0	3661	71	0
2	A	1	0	0	0	0
3	A	12	0	16	1	0
4	A	138	0	0	4	0
All	All	3975	0	3677	71	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 9.

All (71) 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:61[B]:CYS:SG	4:A:558:HOH:O	2.11	1.08
1:A:373:ASN:ND2	4:A:644:HOH:O	1.67	0.98
1:A:467:TYR:OH	1:A:470:SER:O	1.81	0.97
1:A:463:GLU:O	1:A:465:VAL:N	2.02	0.93
1:A:300:ARG:HD2	1:A:300:ARG:H	1.49	0.77
1:A:395:LYS:HB2	1:A:397:VAL:HG23	1.70	0.73
1:A:128:ALA:O	1:A:132:VAL:HG13	1.91	0.71
1:A:436:ASP:OD2	1:A:438:THR:HB	1.93	0.69
1:A:496:GLU:O	1:A:499:GLU:HG3	1.93	0.68
1:A:438:THR:HG22	1:A:439:GLU:HG2	1.75	0.67
1:A:426:ALA:CB	1:A:493:LEU:HD11	2.25	0.66
1:A:368:GLN:NE2	1:A:440:ASN:HD21	1.95	0.64
1:A:413:ALA:HB3	1:A:414:PRO:HD3	1.80	0.63
1:A:368:GLN:HE21	1:A:440:ASN:HD21	1.46	0.61
1:A:395:LYS:HD2	1:A:456:TYR:O	2.00	0.61
1:A:288:MET:CE	1:A:356:PHE:CD2	2.84	0.60
1:A:471:ARG:HG3	1:A:471:ARG:HH11	1.68	0.59
1:A:374:GLN:O	1:A:376:SER:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ASP:O	1:A:361:ALA:HB2	2.05	0.57
1:A:158:PHE:HB2	1:A:210:MET:HE3	1.87	0.57
1:A:288:MET:HE3	1:A:356:PHE:HD2	1.70	0.56
1:A:118:ASN:O	1:A:118:ASN:OD1	2.24	0.55
1:A:446:VAL:O	1:A:446:VAL:HG13	2.07	0.55
1:A:158:PHE:HB2	1:A:210:MET:CE	2.37	0.55
1:A:378:VAL:HG11	1:A:434:LYS:HD2	1.89	0.54
1:A:471:ARG:HH11	1:A:471:ARG:CG	2.19	0.54
1:A:332:GLU:HB2	4:A:649:HOH:O	2.07	0.54
1:A:390:VAL:HG13	1:A:456:TYR:CG	2.44	0.53
1:A:355:ASP:HB3	1:A:360:ASP:O	2.09	0.53
1:A:397:VAL:HG22	1:A:431:LEU:HB3	1.91	0.52
1:A:426:ALA:HB1	1:A:493:LEU:HD11	1.91	0.52
1:A:74:ALA:O	1:A:78:LEU:HB2	2.11	0.51
1:A:63:HIS:HD2	4:A:526:HOH:O	1.93	0.51
1:A:300:ARG:H	1:A:300:ARG:CD	2.14	0.51
1:A:184:HIS:HD2	1:A:187:ASP:OD2	1.93	0.51
1:A:465:VAL:HG12	1:A:479:PHE:CE1	2.46	0.50
1:A:375:ASP:OD1	1:A:375:ASP:N	2.40	0.49
1:A:57:PHE:HB2	1:A:64[B]:CYS:SG	2.53	0.49
1:A:471:ARG:CG	1:A:471:ARG:NH1	2.76	0.49
1:A:501:ALA:C	1:A:503:GLU:H	2.16	0.48
1:A:110:ILE:O	1:A:119:SER:HA	2.14	0.47
1:A:288:MET:HE3	1:A:356:PHE:CD2	2.48	0.47
1:A:149:LEU:N	1:A:150:PRO:HD2	2.30	0.47
1:A:356:PHE:CD2	1:A:357:LEU:HD13	2.50	0.47
1:A:397:VAL:O	1:A:455:LEU:HD12	2.15	0.47
1:A:406:CYS:HG	1:A:409:CYS:HG	1.62	0.47
1:A:288:MET:HE1	1:A:356:PHE:CD2	2.51	0.46
1:A:313:LEU:C	1:A:313:LEU:HD12	2.36	0.46
1:A:464:SER:O	1:A:464:SER:OG	2.29	0.46
1:A:288:MET:CE	1:A:356:PHE:CE2	2.99	0.45
1:A:265:ASN:O	1:A:296:ARG:HD2	2.16	0.45
1:A:134:PHE:O	1:A:138:GLN:HG2	2.17	0.45
1:A:288:MET:HE1	1:A:356:PHE:CE2	2.52	0.45
1:A:100:HIS:HA	3:A:524:GOL:H2	1.99	0.45
1:A:360:ASP:O	1:A:361:ALA:CB	2.65	0.45
1:A:61[B]:CYS:HB3	1:A:64[B]:CYS:HB2	1.99	0.44
1:A:395:LYS:CB	1:A:397:VAL:HG23	2.43	0.44
1:A:159:VAL:O	1:A:159:VAL:HG12	2.18	0.44
1:A:278:THR:O	1:A:282:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASP:OD1	1:A:268:GLU:HG3	2.17	0.43
1:A:311:PHE:HA	1:A:312:PRO:C	2.37	0.43
1:A:78:LEU:HD23	1:A:85:LEU:CD1	2.48	0.43
1:A:47:GLN:HA	1:A:114:SER:HB3	2.01	0.43
1:A:22:MET:N	1:A:22:MET:SD	2.92	0.42
1:A:395:LYS:O	1:A:486:PHE:HE1	2.02	0.42
1:A:244:ILE:HD11	1:A:249:PHE:HD1	1.85	0.42
1:A:473:LEU:HG	1:A:477:PHE:CE1	2.55	0.42
1:A:88:ILE:HD12	1:A:88:ILE:N	2.35	0.42
1:A:204:ILE:HG13	1:A:232:TRP:CH2	2.56	0.41
1:A:465:VAL:HG12	1:A:479:PHE:CZ	2.55	0.41
1:A:301:HIS:O	1:A:304:ASN:HB2	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	483/504 (96%)	456 (94%)	22 (5%)	5 (1%)	15 23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	ALA
1	A	464	SER
1	A	375	ASP
1	A	502	ALA
1	A	445	VAL

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	417/429 (97%)	386 (93%)	31 (7%)	13 22

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	61[A]	CYS
1	A	61[B]	CYS
1	A	94	GLN
1	A	123	GLU
1	A	132	VAL
1	A	156	GLU
1	A	220	LYS
1	A	222	ASP
1	A	229	PHE
1	A	248	VAL
1	A	267	GLU
1	A	287	LEU
1	A	300	ARG
1	A	321	GLU
1	A	344	LEU
1	A	357	LEU
1	A	369	GLU
1	A	375	ASP
1	A	392	ASP
1	A	395	LYS
1	A	438	THR
1	A	442	VAL
1	A	445	VAL
1	A	448	GLU
1	A	460	LYS
1	A	465	VAL
1	A	471	ARG
1	A	495	GLU
1	A	496	GLU

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Mol	Chain	Res	Type
1	A	499	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	118	ASN
1	A	184	HIS
1	A	317	HIS
1	A	368	GLN
1	A	386	HIS
1	A	417	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	A	524	-	5,5,5	0.58	0	5,5,5	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	523	-	5,5,5	0.37	0	5,5,5	0.27	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	A	524	-	-	3/4/4/4	-
3	GOL	A	523	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	523	GOL	O1-C1-C2-O2
3	A	523	GOL	O1-C1-C2-C3
3	A	524	GOL	O1-C1-C2-C3
3	A	524	GOL	O1-C1-C2-O2
3	A	524	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	524	GOL	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.