



# Full wwPDB X-ray Structure Validation Report

Oct 18, 2022 – 10:46 am BST

PDB ID : 7QQV  
Title : SpCas9 bound to FANCF off-target3 DNA substrate  
Authors : Pacesa, M.; Jinek, M.  
Deposited on : 2022-01-10  
Resolution : 2.25 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

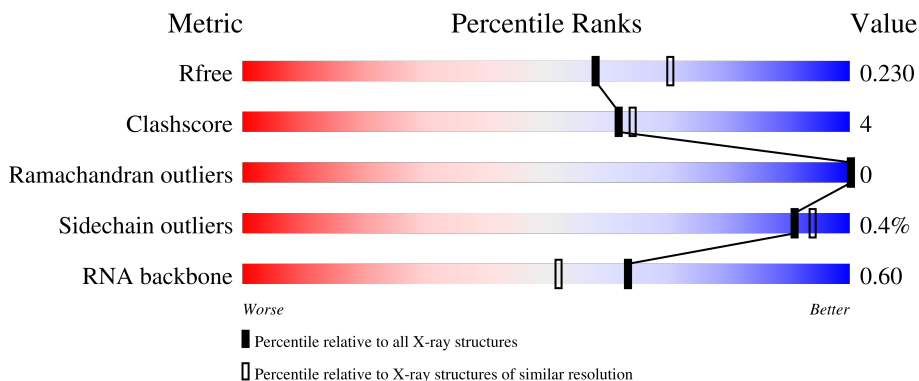
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RNA backbone	3102	1016 (2.66-1.86)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	85	61% (green), 32% (yellow), 7% (orange)
2	B	1368	87% (green), 10% (yellow), 3% (orange), 0% (red), 0% (grey)
3	C	28	71% (green), 29% (yellow)
4	D	12	58% (green), 25% (yellow), 17% (grey)

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14034 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 RNA chain called FANCF sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	85	1778	794	322	578	84	0	0	1

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1331	10878	6931	1887	2038	22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called FANCF off-target3 target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	28	641	302	127	182	30	0	3	0

- Molecule 4 is a DNA chain called FANCF off-target3 non-target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	10	201	97	35	60	9	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total K 2 2	0	0
6	B	7	Total K 7 7	0	0
6	C	1	Total K 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	148	Total O 148 148	0	0
7	B	347	Total O 347 347	0	0
7	C	23	Total O 23 23	0	0
7	D	6	Total O 6 6	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: FANCF sgRNA

Chain A: 



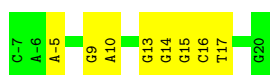
- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

Chain B: 

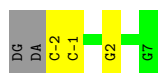


- Molecule 3: FANCF off-target3 target strand

Chain C: 



- Molecule 4: FANCF off-target3 non-target strand



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.02Å 67.14Å 187.77Å 90.00° 111.14° 90.00°	Depositor
Resolution (Å)	47.81 – 2.25 47.81 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.81-2.25) 99.2 (47.81-2.25)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.195 , 0.230 0.195 , 0.230	Depositor DCC
$R_{free}$ test set	4933 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	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	0.95	EDS
Total number of atoms	14034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: MG, K

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	0.31	0/1990	0.82	0/3101
2	B	0.28	0/11070	0.44	0/14873
3	C	0.60	0/721	0.86	0/1113
4	D	0.65	0/224	0.99	0/344
All	All	0.32	0/14005	0.56	0/19431

There are no bond length outliers.

There are no bond angle outliers.

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	1778	0	892	26	0
2	B	10878	0	11053	87	0
3	C	641	0	347	10	0
4	D	201	0	115	3	0
5	A	2	0	0	0	0
6	A	2	0	0	0	0
6	B	7	0	0	0	0
6	C	1	0	0	0	0
7	A	148	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	347	0	0	5	0
7	C	23	0	0	2	0
7	D	6	0	0	0	0
All	All	14034	0	12407	113	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 (113) 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)
2:B:178:ASN:HA	2:B:184:LEU:HD11	1.68	0.75
2:B:80:CYS:SG	7:B:1801:HOH:O	2.44	0.75
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.23	0.71
2:B:895:ARG:NH1	3:C:14[A]:DG:OP1	2.26	0.68
3:C:15[B]:DG:N7	7:C:202:HOH:O	2.28	0.67
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.78	0.66
2:B:898:ASP:O	2:B:905:ARG:NH2	2.29	0.65
2:B:1335:ARG:NH2	4:D:2:DG:O6	2.33	0.61
2:B:974:LYS:NZ	7:B:1505:HOH:O	2.33	0.61
2:B:844:GLN:NE2	2:B:850:ASP:OD1	2.36	0.59
2:B:623:LEU:HD13	2:B:654:ARG:HG3	1.85	0.59
1:A:5:U:H3	3:C:15[A]:DG:H22	1.51	0.59
1:A:69:A:H2'	1:A:70:C:H6	1.68	0.59
1:A:49:A:N3	2:B:1122:ARG:NH2	2.48	0.58
1:A:20:C:OP2	2:B:403:ARG:NH1	2.37	0.57
1:A:46:A:H2'	1:A:47:A:C8	2.40	0.56
2:B:1210:ARG:HA	2:B:1280:VAL:HG22	1.87	0.56
2:B:215:ARG:NH2	2:B:304:ASP:O	2.38	0.56
2:B:790:GLU:HG2	2:B:889:ALA:HA	1.87	0.56
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.87	0.55
2:B:654:ARG:HD2	2:B:656:TYR:CZ	2.40	0.55
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.89	0.55
1:A:22:U:H2'	1:A:23:U:C6	2.42	0.55
2:B:849:ASP:OD2	2:B:895:ARG:NH2	2.40	0.55
2:B:1110:ILE:HG23	2:B:1122:ARG:HD2	1.88	0.54
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.88	0.54
1:A:59:U:OP1	2:B:467:ARG:NH2	2.38	0.54
2:B:1334:LYS:NZ	3:C:-5:DA:OP2	2.31	0.54
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.90	0.53
2:B:846:PHE:O	2:B:920:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:A:H2'	1:A:70:C:C6	2.44	0.53
2:B:391:VAL:HG12	2:B:395:ARG:HD3	1.91	0.52
2:B:788:ILE:HG23	2:B:793:SER:HB3	1.91	0.52
1:A:19:C:H2'	1:A:20:C:O4'	2.10	0.52
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	1.91	0.52
2:B:262:ALA:HB1	2:B:278:LEU:HD12	1.92	0.52
3:C:15[A]:DG:N7	7:C:202:HOH:O	2.41	0.52
2:B:1241:HIS:CD2	2:B:1245:LEU:HD21	2.45	0.51
1:A:0:G:OP1	2:B:918:LYS:NZ	2.43	0.51
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.92	0.50
2:B:1163:LEU:HG	2:B:1343:LEU:HD21	1.94	0.50
2:B:1205:GLU:OE1	2:B:1359:ARG:NH2	2.44	0.50
2:B:814:TYR:CZ	2:B:830:ILE:HG12	2.47	0.49
3:C:13[B]:DG:H8	3:C:13[B]:DG:H5''	1.77	0.49
2:B:308:VAL:HG11	2:B:319:ALA:HB3	1.93	0.49
1:A:77:A:H2'	1:A:78:A:C8	2.48	0.49
2:B:525:THR:HG22	2:B:545:LYS:HZ3	1.77	0.49
2:B:734:LYS:NZ	7:B:1522:HOH:O	2.45	0.49
2:B:525:THR:HG22	2:B:545:LYS:NZ	2.28	0.48
4:D:-2:DC:H2'	4:D:-1:DC:C6	2.48	0.48
1:A:4:A:H2'	1:A:5:U:H6	1.79	0.48
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.42	0.48
2:B:704:PHE:O	2:B:708:ILE:HG12	2.14	0.48
2:B:830:ILE:O	2:B:833:LEU:HG	2.13	0.48
2:B:821:ASP:HB3	2:B:824:VAL:O	2.13	0.48
2:B:323:LYS:HE2	2:B:327:GLU:OE2	2.14	0.47
2:B:982:HIS:HD2	7:B:1505:HOH:O	1.98	0.47
2:B:518:PHE:CD1	2:B:667:ILE:HD12	2.51	0.46
2:B:654:ARG:HD3	2:B:655:ARG:N	2.30	0.46
2:B:633:GLU:HB2	2:B:652:LYS:HD2	1.97	0.46
2:B:15:SER:HA	2:B:51:LEU:O	2.16	0.46
2:B:956:ILE:HG23	2:B:1008:PHE:HB3	1.98	0.46
2:B:985:HIS:CG	2:B:1087:LEU:HD22	2.51	0.46
1:A:28:A:O4'	2:B:122:ILE:HD11	2.16	0.46
2:B:870:VAL:HG13	2:B:871:PRO:HD2	1.97	0.46
1:A:70:C:H2'	1:A:71:U:C6	2.51	0.45
1:A:81:G:N1	2:B:1356:TYR:HB3	2.32	0.45
2:B:841:ILE:HD13	2:B:900:LEU:HG	1.98	0.45
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.98	0.45
2:B:781:MET:HG2	2:B:803:ASN:HA	1.99	0.45
2:B:1306:ALA:O	2:B:1310:ILE:HG12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:GLU:OE2	2:B:356:LYS:HE2	2.17	0.45
2:B:882:TYR:CZ	2:B:886:LEU:HD11	2.52	0.45
2:B:273:ASP:O	2:B:277:ASN:N	2.49	0.45
2:B:278:LEU:O	2:B:282:ILE:HG12	2.17	0.44
2:B:348:LYS:O	2:B:352:PHE:HB2	2.17	0.44
2:B:501:ASN:HB3	2:B:708:ILE:HD12	2.00	0.44
2:B:654:ARG:HD2	2:B:656:TYR:CE2	2.53	0.44
1:A:73:G:H5'	1:A:74:A:OP2	2.17	0.44
2:B:507:VAL:HG11	2:B:660:GLY:O	2.18	0.44
1:A:5:U:H3	3:C:15[B]:DG:H1	1.65	0.43
2:B:680:LEU:HG	2:B:684:LYS:HE3	2.00	0.43
1:A:46:A:H2'	1:A:47:A:H8	1.81	0.43
1:A:70:C:H2'	1:A:71:U:H6	1.83	0.43
2:B:387:GLU:O	2:B:391:VAL:HG23	2.19	0.43
2:B:780:ARG:NH1	2:B:806:LEU:O	2.46	0.43
2:B:1308:ASN:HB3	2:B:1326:TYR:CD1	2.54	0.43
2:B:174:LEU:HA	2:B:174:LEU:HD12	1.77	0.43
2:B:972:PHE:HE1	2:B:1084:ARG:HD3	1.84	0.43
3:C:16:DC:H2'	3:C:17:DT:C6	2.53	0.43
1:A:74:A:OP1	1:A:74:A:H8	2.01	0.43
2:B:784:ILE:HD12	2:B:806:LEU:HD13	2.00	0.43
2:B:258:LEU:HD21	2:B:282:ILE:HD11	2.00	0.43
1:A:54:G:H2'	1:A:55:C:C6	2.54	0.42
2:B:314:LYS:HB3	2:B:314:LYS:HE2	1.80	0.42
2:B:478:PHE:CE1	2:B:482:VAL:HG21	2.53	0.42
2:B:962:LEU:HD23	2:B:962:LEU:HA	1.92	0.42
1:A:18:A:N7	7:A:201:HOH:O	2.37	0.42
2:B:335:LEU:HD21	2:B:376:ILE:HD11	2.02	0.42
2:B:1136:SER:HA	4:D:2:DG:O3'	2.20	0.42
1:A:30:C:H2'	1:A:31:U:C6	2.55	0.42
2:B:185:PHE:HE2	2:B:203:ALA:HB1	1.85	0.41
2:B:901:THR:O	2:B:904:GLU:HG2	2.20	0.41
2:B:733:ILE:HD12	2:B:733:ILE:HA	1.85	0.41
2:B:1122:ARG:HD3	7:B:1569:HOH:O	2.20	0.41
3:C:9:DG:H2'	3:C:10:DA:C8	2.56	0.41
1:A:7:C:H2'	1:A:8:C:O4'	2.21	0.41
3:C:13[B]:DG:H2'	3:C:14[B]:DG:O4'	2.20	0.41
1:A:25:U:H1'	2:B:104:SER:O	2.21	0.40
1:A:70:C:C2	1:A:71:U:C5	3.08	0.40
2:B:526:LYS:HD3	2:B:526:LYS:HA	1.86	0.40
2:B:528:LYS:HE3	2:B:539:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1236:LEU:HD23	2:B:1236:LEU:HA	1.96	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	Percentiles
2	B	1323/1368 (97%)	1283 (97%)	40 (3%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 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
2	B	1194/1225 (98%)	1189 (100%)	5 (0%)	<a href="#">91</a> <a href="#">94</a>

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	174	LEU
2	B	175	ASN
2	B	419	LEU
2	B	1007	GLU
2	B	1280	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	723	HIS
2	B	885	GLN
2	B	1241	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	82/85 (96%)	11 (13%)	0

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	C
1	A	20	C
1	A	28	A
1	A	29	G
1	A	36	A
1	A	51	A
1	A	56	U
1	A	59	U
1	A	68	A
1	A	74	A
1	A	77	A

There are no RNA pucker outliers to report.

## 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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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