



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 04:45 pm GMT

PDB ID : 1C5X
Title : STRUCTURAL BASIS FOR SELECTIVITY OF A SMALL MOLECULE,
S1-BINDING, SUB-MICROMOLAR INHIBITOR OF UROKINASE TYPE
PLASMINOGEN ACTIVATOR
Authors : Katz, B.A.; Mackman, R.; Luong, C.; Radika, K.; Martelli, A.; Sprengeler,
P.A.; Wang, J.; Chan, H.; Wong, L.
Deposited on : 1999-12-22
Resolution : 1.75 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

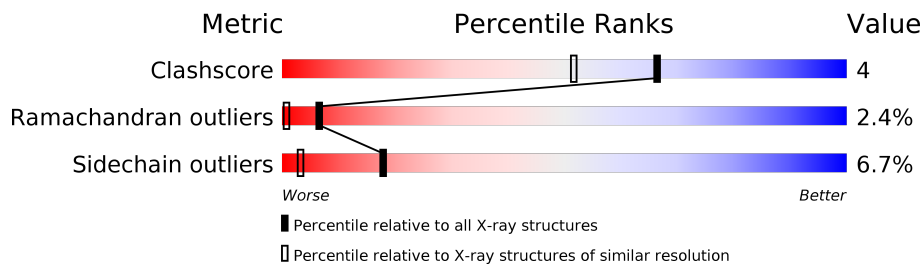
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	122126	2072 (1.76-1.76)
Ramachandran outliers	120053	2050 (1.76-1.76)
Sidechain outliers	120020	2050 (1.76-1.76)

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. 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	23	
2	B	253	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5421 atoms, of which 2887 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 (UROKINASE-TYPE PLASMINOGEN ACTIVATOR).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	9	Total	C	H	N	O	S	0	0	0
			148	46	76	13	12	1			

- Molecule 2 is a protein called PROTEIN (UROKINASE-TYPE PLASMINOGEN ACTIVATOR).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	248	Total	C	H	N	O	S	44	14	0
			4040	1279	2018	349	373	21			

There is a discrepancy between the modelled and reference sequences:

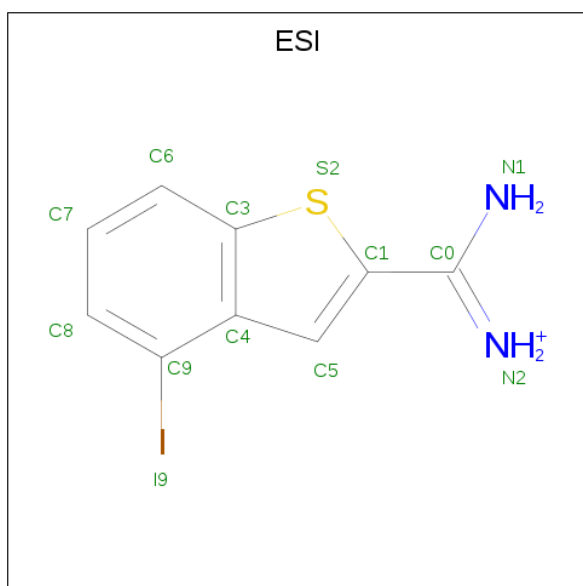
Chain	Residue	Modelled	Actual	Comment	Reference
B	145	ALA	ASN	CONFLICT	UNP P00749

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	1
			18	6	5	7		
3	B	1	Total	C	H	O	0	1
			18	6	5	7		
3	B	1	Total	C	H	O	0	1
			24	8	7	9		

- Molecule 4 is 4-iodobenzo[B]thiophene-2-carboxamidinium (three-letter code: ESI) (formula: C₉H₈IN₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	H	I	N	S	0	0
			21	9	8	1	2	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	15	Total	H	O	0	1
			45	30	15		
5	B	369	Total	H	O	0	11
			1107	738	369		

3 Residue-property plots


These plots are drawn for all protein, RNA and DNA 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.

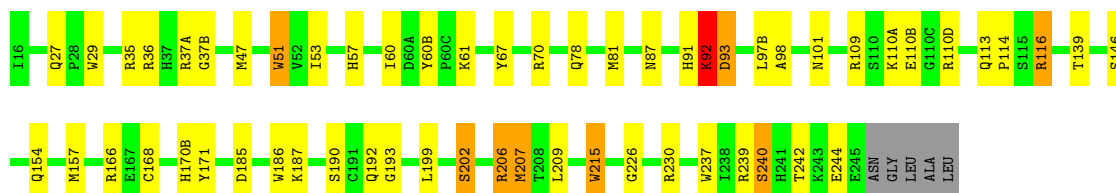
• Molecule 1: PROTEIN (UROKINASE-TYPE PLASMINOGEN ACTIVATOR)

Chain A: 



• Molecule 2: PROTEIN (UROKINASE-TYPE PLASMINOGEN ACTIVATOR)

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.09Å 49.78Å 66.65Å 90.00° 113.29° 90.00°	Depositor
Resolution (Å)	7.50 – 1.75 31.35 – 1.35	Depositor EDS
% Data completeness (in resolution range)	68.0 (7.50-1.75) 43.2 (31.35-1.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.35Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.195 , 0.244 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	4.3	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.047 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.036 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5421	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, ESI

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	1.20	0/72	1.49	1/93 (1.1%)
2	B	1.36	1/2133 (0.0%)	1.59	43/2884 (1.5%)
All	All	1.35	1/2205 (0.0%)	1.59	44/2977 (1.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	51	TRP	CG-CD2	-5.01	1.35	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	35	ARG	NE-CZ-NH2	-10.91	114.85	120.30
2	B	186	TRP	CD1-NE1-CE2	10.31	118.28	109.00
2	B	29	TRP	CD1-NE1-CE2	10.03	118.03	109.00
2	B	237	TRP	CD1-NE1-CE2	9.65	117.68	109.00
2	B	109	ARG	NE-CZ-NH2	-9.35	115.63	120.30
2	B	215	TRP	CD1-NE1-CE2	8.79	116.91	109.00
2	B	51	TRP	CD1-NE1-CE2	8.67	116.80	109.00
2	B	29	TRP	NE1-CE2-CZ2	7.65	138.81	130.40
2	B	36	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	B	186	TRP	CG-CD1-NE1	-7.52	102.58	110.10
2	B	215	TRP	NE1-CE2-CZ2	7.46	138.61	130.40
2	B	51	TRP	NE1-CE2-CZ2	7.46	138.60	130.40
2	B	29	TRP	CG-CD1-NE1	-7.44	102.66	110.10
2	B	186	TRP	NE1-CE2-CZ2	7.38	138.52	130.40
2	B	237	TRP	CG-CD1-NE1	-7.13	102.97	110.10
2	B	237	TRP	NE1-CE2-CZ2	7.13	138.24	130.40
2	B	51	TRP	CG-CD1-NE1	-6.75	103.35	110.10
2	B	215	TRP	CG-CD1-NE1	-6.58	103.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	230	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	B	116[A]	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	B	116[B]	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	B	186	TRP	NE1-CE2-CD2	-6.31	100.99	107.30
2	B	199	LEU	N-CA-C	-6.29	94.02	111.00
2	B	237	TRP	NE1-CE2-CD2	-6.14	101.16	107.30
2	B	215	TRP	NE1-CE2-CD2	-5.98	101.32	107.30
2	B	239	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	B	226	GLY	N-CA-C	-5.81	98.57	113.10
2	B	51	TRP	NE1-CE2-CD2	-5.81	101.49	107.30
2	B	35	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	B	92	LYS	N-CA-C	-5.73	95.52	111.00
2	B	29	TRP	NE1-CE2-CD2	-5.72	101.58	107.30
2	B	166[A]	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	B	166[B]	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	B	70	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	B	67	TYR	CB-CG-CD1	5.39	124.23	121.00
2	B	206	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	12	GLN	N-CA-C	-5.29	96.72	111.00
2	B	110(D)	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	B	70	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	B	37(A)	ARG	NE-CZ-NH2	-5.17	117.72	120.30
2	B	171	TYR	CB-CG-CD2	-5.11	117.93	121.00
2	B	207[A]	MET	N-CA-C	-5.01	97.46	111.00
2	B	207[B]	MET	N-CA-C	-5.01	97.46	111.00
2	B	207[C]	MET	N-CA-C	-5.01	97.46	111.00

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	72	76	75	2	0
2	B	2022	2018	1979	17	2
3	B	43	17	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	13	8	8	1	0
5	A	15	30	0	0	1
5	B	369	738	0	0	1
All	All	2534	2887	2076	18	2

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 (18) 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:27:GLN:HG3	2:B:139[A]:THR:HG21	1.81	0.63
2:B:81[A]:MET:HE1	2:B:113:GLN:H	1.64	0.63
2:B:92:LYS:H	2:B:92:LYS:HD2	1.67	0.59
2:B:91:HIS:CD2	2:B:101:ASN:HB3	2.40	0.57
1:A:10:LYS:HG2	1:A:11:PHE:N	2.21	0.55
2:B:51:TRP:CD1	2:B:242:THR:HG23	2.50	0.47
2:B:57:HIS:NE2	3:B:3[A]:FLC:OG1	2.48	0.46
2:B:98:ALA:HB2	2:B:215:TRP:CZ2	2.50	0.46
1:A:11:PHE:CD1	2:B:114:PRO:HG3	2.51	0.46
2:B:92:LYS:O	2:B:93:ASP:CB	2.65	0.45
2:B:47[B]:MET:SD	2:B:53:ILE:HB	2.57	0.44
2:B:110(A):LYS:HG3	2:B:110(B):GLU:HG3	2.00	0.44
2:B:139[A]:THR:HG22	2:B:157:MET:HB2	2.00	0.43
2:B:27:GLN:CG	2:B:139[A]:THR:HG21	2.47	0.43
2:B:192[A]:GLN:HG2	4:B:251:ESI:C8	2.49	0.42
2:B:60(B):TYR:CE1	2:B:61:LYS:HB2	2.55	0.41
2:B:202:SER:HA	2:B:206:ARG:O	2.20	0.41

All (2) 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)
2:B:154:GLN:OE1	5:B:345:HOH:H2[2_656]	1.55	0.05
2:B:87:ASN:OD1	5:A:467:HOH:H1[4_555]	1.55	0.05

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	7/23 (30%)	7 (100%)	0	0	100	100
2	B	261/253 (103%)	238 (91%)	17 (6%)	6 (2%)	7	1
All	All	268/276 (97%)	245 (91%)	17 (6%)	6 (2%)	6	1

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97(B)	LEU
2	B	244	GLU
2	B	93	ASP
2	B	60	ILE
2	B	240	SER
2	B	37(B)	GLY

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	8/22 (36%)	6 (75%)	2 (25%)	0	0
2	B	231/219 (106%)	215 (93%)	16 (7%)	17	3
All	All	239/241 (99%)	221 (92%)	18 (8%)	18	2

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	17	THR
2	B	78	GLN
2	B	92	LYS
2	B	116[A]	ARG
2	B	116[B]	ARG
2	B	146	SER
2	B	168	CYS
2	B	170(B)	HIS
2	B	185	ASP
2	B	187	LYS
2	B	190	SER
2	B	202	SER
2	B	207[A]	MET
2	B	207[B]	MET
2	B	207[C]	MET
2	B	209	LEU
2	B	240	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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	FLC	B	1[A]	-	3,12,12	2.46	2 (66%)	3,17,17	0.64	0
3	FLC	B	2[B]	-	3,12,12	3.59	2 (66%)	3,17,17	2.61	1 (33%)
4	ESI	B	251	-	10,14,14	3.93	2 (20%)	8,20,20	1.84	3 (37%)
3	FLC	B	3[A]	-	3,12,12	4.59	2 (66%)	3,17,17	2.69	2 (66%)
3	FLC	B	3[B]	-	3,12,12	3.81	2 (66%)	3,17,17	2.34	2 (66%)

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	FLC	B	1[A]	-	-	0/6/16/16	0/0/0/0
3	FLC	B	2[B]	-	-	0/6/16/16	0/0/0/0
4	ESI	B	251	-	-	0/0/4/4	0/2/2/2
3	FLC	B	3[A]	-	-	0/6/16/16	0/0/0/0
3	FLC	B	3[B]	-	-	0/6/16/16	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	251	ESI	C1-C0	-6.40	1.38	1.46
3	B	1[A]	FLC	CA-CB	2.33	1.58	1.54
3	B	2[B]	FLC	CG-CB	3.27	1.59	1.54
3	B	1[A]	FLC	CG-CB	3.51	1.59	1.54
3	B	3[A]	FLC	CA-CB	4.13	1.60	1.54
3	B	3[B]	FLC	CA-CB	4.13	1.60	1.54
3	B	3[B]	FLC	CG-CB	5.12	1.62	1.54
3	B	2[B]	FLC	CA-CB	5.21	1.62	1.54
3	B	3[A]	FLC	CG-CB	6.77	1.64	1.54
4	B	251	ESI	C1-S2	10.27	1.84	1.72

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	251	ESI	C1-C0-N2	-2.97	115.67	119.12
3	B	3[B]	FLC	CB-CG-CGC	2.69	118.98	114.95
4	B	251	ESI	N1-C0-N2	2.93	124.14	120.54
3	B	3[A]	FLC	CB-CG-CGC	2.99	119.43	114.95
3	B	3[A]	FLC	CB-CA-CAC	3.03	119.49	114.95
3	B	3[B]	FLC	CB-CA-CAC	3.03	119.49	114.95
4	B	251	ESI	C4-C9-I9	3.04	125.55	121.19
3	B	2[B]	FLC	CB-CA-CAC	4.22	121.28	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	251	ESI	1	0
3	B	3[A]	FLC	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](#)

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.