



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:06 pm GMT

PDB ID : 1PPO
Title : DETERMINATION OF THE STRUCTURE OF PAPAYA PROTEASE OMEGA
Authors : Pickersgill, R.W.; Rizkallah, P.J.; Harris, G.W.; Goodenough, P.W.
Deposited on : 1991-07-12
Resolution : 1.80 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
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

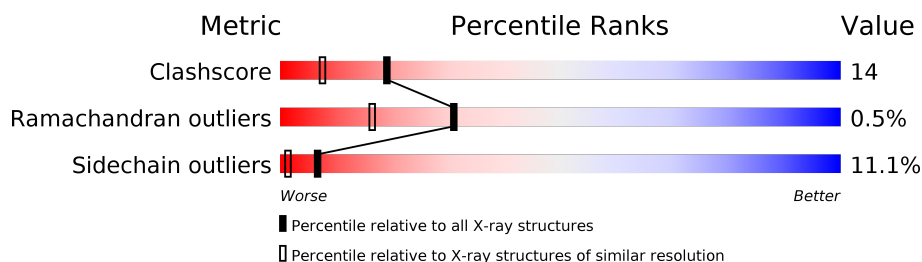
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)

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	216	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1775 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 PROTEASE OMEGA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1641	1037	300	297	7			

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		

3 Residue-property plots [i](#)

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: PROTEASE OMEGA



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	74.11Å 74.11Å 77.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.80 9.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80) 80.4 (9.94-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 1.80Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.155 , (Not available) 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.1	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	1775	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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

5.1 Standard geometry

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

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	1.43	7/1680 (0.4%)	2.37	96/2266 (4.2%)

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	2	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	GLY	N-CA	7.28	1.56	1.46
1	A	114	GLN	CD-OE1	6.17	1.37	1.24
1	A	120	ASN	CG-OD1	5.85	1.36	1.24
1	A	185	TRP	NE1-CE2	-5.81	1.29	1.37
1	A	216	ASN	C-OXT	5.55	1.33	1.23
1	A	92	GLN	CD-OE1	5.40	1.35	1.24
1	A	99	GLN	CD-OE1	5.13	1.35	1.24

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	TYR	CB-CG-CD1	-13.13	113.12	121.00
1	A	102	GLY	C-N-CD	-12.33	93.48	120.60
1	A	139	ARG	CD-NE-CZ	-12.16	106.58	123.60
1	A	211	TYR	CB-CG-CD2	-10.12	114.93	121.00
1	A	88	TYR	CG-CD2-CE2	-9.66	113.57	121.30
1	A	100	VAL	CA-CB-CG2	9.60	125.29	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	VAL	CA-CB-CG2	9.55	125.22	110.90
1	A	59	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	A	96	ARG	CG-CD-NE	9.23	131.18	111.80
1	A	8	ARG	O-C-N	9.19	137.40	122.70
1	A	134	VAL	CG1-CB-CG2	-8.74	96.92	110.90
1	A	96	ARG	NE-CZ-NH2	8.63	124.61	120.30
1	A	216	ASN	CA-CB-CG	8.27	131.60	113.40
1	A	1	LEU	CB-CG-CD2	8.22	124.98	111.00
1	A	134	VAL	CA-CB-CG1	8.10	123.04	110.90
1	A	216	ASN	N-CA-CB	8.07	125.14	110.60
1	A	6	ASP	CB-CG-OD1	8.06	125.55	118.30
1	A	74	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	A	174	TYR	CB-CG-CD2	-7.92	116.25	121.00
1	A	102	GLY	N-CA-C	-7.90	93.36	113.10
1	A	41	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	139	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	A	45	LEU	CB-CA-C	7.66	124.75	110.20
1	A	82	LEU	CB-CG-CD1	7.45	123.66	111.00
1	A	190	TYR	CB-CG-CD1	-7.42	116.55	121.00
1	A	212	TYR	CB-CG-CD2	-7.42	116.55	121.00
1	A	57	GLU	OE1-CD-OE2	-7.39	114.43	123.30
1	A	96	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	A	127	LYS	O-C-N	-7.32	111.00	122.70
1	A	83	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	A	192	ARG	CG-CD-NE	-7.19	96.70	111.80
1	A	67	TYR	CG-CD2-CE2	-7.02	115.69	121.30
1	A	187	GLU	OE1-CD-OE2	-6.94	114.98	123.30
1	A	88	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	A	86	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	A	165	GLY	O-C-N	-6.50	112.31	122.70
1	A	169	SER	O-C-N	6.49	134.23	123.20
1	A	174	TYR	CB-CG-CD1	6.46	124.88	121.00
1	A	58	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	92	GLN	CA-CB-CG	-6.41	99.29	113.40
1	A	158	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	69	PRO	O-C-N	-6.26	112.68	122.70
1	A	208	LYS	CA-CB-CG	-6.21	99.73	113.40
1	A	8	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	188	LYS	N-CA-CB	-6.11	99.59	110.60
1	A	170	GLY	C-N-CA	6.05	135.01	122.30
1	A	123	ASN	O-C-N	-5.92	113.23	122.70
1	A	145	LYS	C-N-CA	-5.92	109.87	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	PRO	CA-N-CD	5.88	119.92	111.70
1	A	12	ALA	N-CA-CB	5.86	118.31	110.10
1	A	169	SER	CA-C-O	-5.86	107.80	120.10
1	A	67	TYR	CD1-CG-CD2	5.83	124.31	117.90
1	A	194	LYS	CA-CB-CG	-5.82	100.60	113.40
1	A	38	ASN	N-CA-CB	5.81	121.06	110.60
1	A	184	ALA	N-CA-CB	5.79	118.21	110.10
1	A	57	GLU	CG-CD-OE2	5.78	129.85	118.30
1	A	143	LEU	CB-CG-CD2	5.77	120.81	111.00
1	A	58	ARG	CD-NE-CZ	5.76	131.67	123.60
1	A	123	ASN	N-CA-CB	-5.72	100.30	110.60
1	A	42	THR	N-CA-C	5.68	126.33	111.00
1	A	211	TYR	CG-CD2-CE2	-5.66	116.78	121.30
1	A	91	LYS	O-C-N	5.64	131.73	122.70
1	A	47	GLU	CA-CB-CG	-5.64	100.99	113.40
1	A	55	ASP	O-C-N	-5.64	113.67	122.70
1	A	24	SER	O-C-N	-5.59	113.76	122.70
1	A	79	GLY	O-C-N	-5.58	113.77	122.70
1	A	88	TYR	CZ-CE2-CD2	5.58	124.82	119.80
1	A	197	PRO	O-C-N	5.56	132.66	123.20
1	A	74	TYR	CG-CD2-CE2	-5.52	116.88	121.30
1	A	8	ARG	CA-C-O	-5.48	108.58	120.10
1	A	70	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	A	135	GLU	CA-CB-CG	-5.48	101.35	113.40
1	A	106	LYS	O-C-N	-5.46	113.95	122.70
1	A	189	GLY	CA-C-N	5.45	129.20	117.20
1	A	165	GLY	CA-C-O	5.45	130.41	120.60
1	A	44	LYS	N-CA-C	-5.42	96.36	111.00
1	A	104	ILE	CB-CA-C	5.39	122.38	111.60
1	A	62	GLY	O-C-N	5.39	131.32	122.70
1	A	20	GLY	CA-C-O	5.36	130.25	120.60
1	A	190	TYR	C-N-CA	5.36	135.09	121.70
1	A	73	GLU	CA-CB-CG	-5.32	101.69	113.40
1	A	88	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
1	A	17	ARG	C-N-CA	5.32	134.99	121.70
1	A	110	VAL	C-N-CA	5.29	133.41	122.30
1	A	164	VAL	CA-C-O	5.28	131.19	120.10
1	A	8	ARG	CG-CD-NE	-5.18	100.92	111.80
1	A	54	VAL	CG1-CB-CG2	5.18	119.19	110.90
1	A	91	LYS	CA-C-N	-5.15	105.86	117.20
1	A	7	TRP	CA-CB-CG	-5.15	103.91	113.70
1	A	133	VAL	CA-CB-CG1	-5.11	103.24	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	LYS	CA-CB-CG	-5.09	102.20	113.40
1	A	108	SER	O-C-N	-5.08	114.56	123.20
1	A	157	VAL	CA-CB-CG2	5.06	118.49	110.90
1	A	179	ASN	OD1-CG-ND2	-5.06	110.27	121.90
1	A	7	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	A	48	LEU	CB-CG-CD1	-5.05	102.41	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	58	ARG	CA
1	A	216	ASN	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Sidechain
1	A	123	ASN	Mainchain
1	A	139	ARG	Sidechain
1	A	169	SER	Peptide
1	A	17	ARG	Sidechain
1	A	195	ARG	Sidechain
1	A	41	ARG	Sidechain
1	A	58	ARG	Sidechain

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	1641	0	1654	46	0
2	A	1	0	0	0	0
3	A	133	0	0	11	1
All	All	1775	0	1654	46	1

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 14.

All (46) 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:89:LYS:HD2	3:A:301:HOH:O	1.45	1.14
1:A:1:LEU:HB2	3:A:283:HOH:O	1.71	0.88
1:A:81:HIS:CD2	1:A:100:VAL:HG23	2.14	0.82
1:A:216:ASN:OXT	3:A:349:HOH:O	2.00	0.78
1:A:168:LYS:HE3	3:A:341:HOH:O	1.86	0.74
1:A:7:TRP:CZ3	1:A:10:LYS:HD2	2.26	0.70
1:A:1:LEU:HD11	1:A:123:ASN:CA	2.27	0.64
1:A:81:HIS:CG	1:A:100:VAL:HG23	2.32	0.64
1:A:89:LYS:HE3	3:A:301:HOH:O	1.98	0.62
1:A:183:THR:O	1:A:188:LYS:HA	2.01	0.61
1:A:12:ALA:HA	1:A:39:LYS:HG2	1.81	0.61
1:A:41:ARG:HD2	1:A:216:ASN:OD1	2.03	0.58
1:A:1:LEU:HD11	1:A:123:ASN:HA	1.84	0.57
1:A:88:TYR:HB2	3:A:271:HOH:O	2.04	0.57
1:A:4:ASN:HD22	1:A:167:GLY:HA3	1.69	0.56
1:A:89:LYS:HE2	1:A:96:ARG:NH2	2.22	0.55
1:A:17:ARG:NH1	1:A:50:GLU:OE2	2.35	0.54
1:A:89:LYS:CE	3:A:301:HOH:O	2.50	0.53
1:A:144:TYR:CD2	1:A:186:GLY:HA2	2.43	0.53
1:A:134:VAL:HG12	1:A:206:LEU:HD13	1.91	0.51
1:A:89:LYS:CD	3:A:301:HOH:O	2.23	0.51
1:A:139:ARG:HB3	1:A:140:PRO:HD3	1.92	0.51
1:A:116:ASN:HA	1:A:200:SER:O	2.10	0.51
1:A:134:VAL:HG12	1:A:206:LEU:CD1	2.41	0.50
1:A:113:VAL:HB	1:A:210:SER:HB2	1.94	0.49
1:A:169:SER:OG	3:A:291:HOH:O	2.19	0.48
1:A:1:LEU:HD11	1:A:123:ASN:N	2.27	0.48
1:A:63:CYS:SG	1:A:91:LYS:HA	2.54	0.47
1:A:81:HIS:CG	1:A:100:VAL:CG2	2.97	0.47
1:A:104:ILE:HG21	1:A:104:ILE:HD12	1.66	0.46
1:A:117:ASN:HB2	1:A:199:ASN:ND2	2.31	0.45
1:A:1:LEU:HD21	1:A:123:ASN:HA	1.99	0.45
1:A:1:LEU:HD12	3:A:283:HOH:O	2.16	0.45
1:A:26:TRP:CG	1:A:66:GLY:HA3	2.53	0.44
1:A:102:GLY:HA2	1:A:103:PRO:HD3	1.49	0.43
1:A:26:TRP:CD2	1:A:66:GLY:HA3	2.55	0.42
1:A:19:GLN:HG3	1:A:180:SER:O	2.20	0.42
1:A:51:GLN:HB2	1:A:88:TYR:HA	2.01	0.42
1:A:118:GLU:OE2	1:A:195:ARG:HD2	2.19	0.42
1:A:215:LYS:HG2	1:A:216:ASN:N	2.35	0.42
1:A:149:PHE:HE1	1:A:204:CYS:SG	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HD12	1:A:172:LYS:HG3	2.02	0.41
1:A:156:LYS:HE2	3:A:288:HOH:O	2.20	0.41
1:A:59:ARG:HB3	1:A:70:TYR:CD2	2.55	0.41
1:A:89:LYS:HE2	1:A:96:ARG:HH21	1.85	0.41
1:A:4:ASN:HD22	1:A:167:GLY:CA	2.32	0.41

All (1) 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)
3:A:329:HOH:O	3:A:329:HOH:O[6_565]	1.58	0.62

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	214/216 (99%)	203 (95%)	10 (5%)	1 (0%)	31 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	GLY

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
1	A	171/171 (100%)	152 (89%)	19 (11%)	7 1

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	58	ARG
1	A	64	LYS
1	A	82	LEU
1	A	86	TYR
1	A	87	PRO
1	A	89	LYS
1	A	96	ARG
1	A	98	LYS
1	A	104	ILE
1	A	112	ARG
1	A	127	LYS
1	A	137	LYS
1	A	139	ARG
1	A	156	LYS
1	A	168	LYS
1	A	169	SER
1	A	194	LYS
1	A	216	ASN

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

Mol	Chain	Res	Type
1	A	4	ASN
1	A	92	GLN
1	A	116	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.