STRUCTURAL
BIOLOGY

Volume 75 (2019)

Supporting information for article:

Comparison of automated crystallographic model-building pipelines

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S1. Original Resolutions without the Buccaneer Development Dataset

Table 1. *Structure completeness comparison for the models generated from the original HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	27	28	41	64
ARP(B 5I)	47	0	34	41	75
i1(5I)	64	54	0	50	74
PHENIX/Parrot	48	44	40	0	74
SHELXE/Parrot	30	21	20	20	0

Table 2. *Structure completeness comparison for the models generated from the original HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	100	26	8	11	5
ARP(B 5I)	26	100	12	15	3
i1(5I)	8	12	100	9	6
PHENIX/Parrot	11	15	9	100	5
SHELXE/Parrot	5	3	6	5	100

Table 3. *Structure completeness comparison for the models generated from the original HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	5	13	13	40
ARP(B 5I)	21	0	17	16	47
i1(5I)	28	20	0	21	52
PHENIX/Parrot	27	20	23	0	49
SHELXE/Parrot	18	11	11	8	0

Table 4. *Structure completeness comparison for the models generated from the original HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	21	15	28	24
ARP(B 5I)	26	0	16	25	28
i1(5I)	36	34	0	29	22
PHENIX/Parrot	21	24	17	0	26
SHELXE/Parrot	12	10	9	12	0

Table 5. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the original HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	21	93	32	100
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	43	0	95	42	100
ARP(B 5I) $_{R-free}$	-	0	86	50	-
i1(5I) $_{R-work}$	5	1	0	3	99
i1(5I) $_{R-free}$	-	10	0	3	-
PHENIX/Parrot $_{R-work}$	45	36	95	0	99
PHENIX/Parrot $_{R-free}$	-	44	95	0	-
SHELXE/Parrot $_{R-work}$	0	0	1	1	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 6. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the original HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	100	36	2	23	0
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	36	100	4	22	0
ARP(B 5I) $_{R-free}$	-	100	4	7	-
i1(5I) $_{R-work}$	2	4	100	1	0
i1(5I) $_{R-free}$	-	4	100	3	-
PHENIX/Parrot $_{R-work}$	23	22	1	100	0
PHENIX/Parrot $_{R-free}$	-	7	3	100	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	100
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 7. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the original HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	5	47	4	100
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	4	0	49	6	100
ARP(B 5I) $_{R-free}$	-	0	56	9	-
i1(5I) $_{R-work}$	0	0	0	0	95
i1(5I) $_{R-free}$	-	2	0	0	-
PHENIX/Parrot $_{R-work}$	4	3	50	0	99
PHENIX/Parrot $_{R-free}$	-	13	50	0	-
SHELXE/Parrot $_{R-work}$	0	0	1	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 8. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the original HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	17	46	28	0
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	39	0	46	36	0
ARP(B 5I) $_{R-free}$	-	0	30	40	-
i1(5I) $_{R-work}$	5	1	0	3	4
i1(5I) $_{R-free}$	-	8	0	3	-
PHENIX/Parrot $_{R-work}$	41	33	45	0	0
PHENIX/Parrot $_{R-free}$	-	31	44	0	-
SHELXE/Parrot $_{R-work}$	0	0	0	1	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 9. *Structure completeness comparison for the models generated from the original MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	32	33	40	71
ARP(B 5I)	38	0	33	40	76
i1(5I)	57	53	0	46	78
PHENIX/Parrot	44	43	40	0	75
SHELXE/Parrot	24	17	16	17	0

Table 10. *Structure completeness comparison for the models generated from the original MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	100	31	10	16	5
ARP(B 5I)	31	100	14	17	7
i1(5I)	10	14	100	14	6
PHENIX/Parrot	16	17	14	100	8
SHELXE/Parrot	5	7	6	8	100

Table 11. *Structure completeness comparison for the models generated from the original MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	5	15	16	42
ARP(B 5I)	16	0	15	15	50
i1(5I)	26	19	0	19	54
PHENIX/Parrot	26	19	23	0	52
SHELXE/Parrot	16	8	8	5	0

Table 12. *Structure completeness comparison for the models generated from the original MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	27	17	24	29
ARP(B 5I)	21	0	18	25	26
i1(5I)	32	34	0	26	23
PHENIX/Parrot	17	23	17	0	23
SHELXE/Parrot	8	9	8	11	0

Table 13. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the original MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	16	91	34	100
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	40	0	95	47	100
ARP(B 5I) $_{R-free}$	-	0	88	47	-
i1(5I) $_{R-work}$	6	1	0	3	99
i1(5I) $_{R-free}$	-	10	0	4	-
PHENIX/Parrot $_{R-work}$	46	34	93	0	100
PHENIX/Parrot $_{R-free}$	-	41	93	0	-
SHELXE/Parrot $_{R-work}$	0	0	1	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 14. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the original MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	100	44	3	20	0
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	44	100	3	19	0
ARP(B 5I) $_{R-free}$	-	100	2	12	-
i1(5I) $_{R-work}$	3	3	100	3	0
i1(5I) $_{R-free}$	-	2	100	3	-
PHENIX/Parrot $_{R-work}$	20	19	3	100	0
PHENIX/Parrot $_{R-free}$	-	12	3	100	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	100
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 15. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the original MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	3	47	3	100
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	4	0	54	5	100
ARP(B 5I) $_{R-free}$	-	0	54	11	-
i1(5I) $_{R-work}$	1	0	0	0	97
i1(5I) $_{R-free}$	-	2	0	0	-
PHENIX/Parrot $_{R-work}$	3	3	47	0	100
PHENIX/Parrot $_{R-free}$	-	10	49	0	-
SHELXE/Parrot $_{R-work}$	0	0	1	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 16. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the original MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	13	44	31	0
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	36	0	42	42	0
ARP(B 5I) $_{R-free}$	-	0	34	36	-
i1(5I) $_{R-work}$	5	1	0	3	1
i1(5I) $_{R-free}$	-	8	0	4	-
PHENIX/Parrot $_{R-work}$	42	30	46	0	0
PHENIX/Parrot $_{R-free}$	-	31	44	0	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 17. *Structure completeness comparison for the models generated from the original NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP	100	32	9	12	15	5	7
ARP(B 5I)	32	100	16	13	19	9	5
i1(5I)	9	16	100	9	11	3	4
PHENIX/Parrot	12	13	9	100	22	4	6
PHENIX	15	19	11	22	100	6	7
SHELXE	5	9	3	4	6	100	8
SHELXE/Parrot	7	5	4	6	7	8	100

Table 18. *Structure completeness comparison for the models generated from the original NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP	0	17	18	27	23	24	21
ARP(B 5I)	21	0	20	28	27	22	20
i1(5I)	30	28	0	30	32	21	24
PHENIX/Parrot	21	24	19	0	32	20	22
PHENIX	20	21	18	25	0	21	21
SHELXE	9	7	9	9	9	0	25
SHELXE/Parrot	11	10	7	11	11	26	0

Table 19. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the original NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP $_{R-work}$	100	34	1	20	20	0	0
ARP $_{R-free}$	-	-	-	-	-	-	-
ARP(B 5I) $_{R-work}$	34	100	1	25	23	0	0
ARP(B 5I) $_{R-free}$	-	100	4	5	5	-	-
i1(5I) $_{R-work}$	1	1	100	3	4	0	0
i1(5I) $_{R-free}$	-	4	100	4	3	-	-
PHENIX/Parrot $_{R-work}$	20	25	3	100	51	0	0
PHENIX/Parrot $_{R-free}$	-	5	4	100	38	-	-
PHENIX $_{R-work}$	20	23	4	51	100	0	0
PHENIX $_{R-free}$	-	5	3	38	100	-	-
SHELXE $_{R-work}$	0	0	0	0	0	100	39
SHELXE $_{R-free}$	-	-	-	-	-	-	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0	39	100
SHELXE/Parrot $_{R-free}$	-	-	-	-	-	-	-

Table 20. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the original NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP $_{R-work}$	0	18	42	29	30	0	0
ARP $_{R-free}$	-	-	-	-	-	-	-
ARP(B 5I) $_{R-work}$	39	0	39	38	39	0	0
ARP(B 5I) $_{R-free}$	-	0	25	40	34	-	-
i1(5I) $_{R-work}$	5	0	0	3	2	2	3
i1(5I) $_{R-free}$	-	9	0	3	4	-	-
PHENIX/Parrot $_{R-work}$	42	28	41	0	25	0	0
PHENIX/Parrot $_{R-free}$	-	30	36	0	29	-	-
PHENIX $_{R-work}$	39	30	39	21	0	0	1
PHENIX $_{R-free}$	-	34	35	30	0	-	-
SHELXE $_{R-work}$	0	0	1	0	1	0	19
SHELXE $_{R-free}$	-	-	-	-	-	-	-
SHELXE/Parrot $_{R-work}$	0	0	1	1	1	41	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-	-	-

S2. Synthetic Resolutions without Bucanner Development Dataset

Table 1. *Structure completeness comparison for the models generated from the synthetic HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	21	1	2
ARP(B 5I)	21	0	1	3
i1(5I)	93	94	0	75
PHENIX/Parrot	97	96	23	0

Table 2. *Structure completeness comparison for the models generated from the synthetic HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	100	58	5	1
ARP(B 5I)	58	100	5	1
i1(5I)	5	5	100	2
PHENIX/Parrot	1	1	2	100

Table 3. *Structure completeness comparison for the models generated from the synthetic HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	4	1	2
ARP(B 5I)	7	0	0	3
i1(5I)	84	84	0	70
PHENIX/Parrot	92	91	16	0

Table 4. *Structure completeness comparison for the models generated from the synthetic HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	17	1	0
ARP(B 5I)	14	0	0	0
i1(5I)	9	10	0	5
PHENIX/Parrot	5	5	7	0

Table 5. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	27	93	97
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	60	0	99	100
ARP(B 5I) $_{R-free}$	-	0	48	45
i1(5I) $_{R-work}$	6	1	0	37
i1(5I) $_{R-free}$	-	50	0	38
PHENIX/Parrot $_{R-work}$	2	0	59	0
PHENIX/Parrot $_{R-free}$	-	54	56	0

Table 6. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	100	13	1	0
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	13	100	1	0
ARP(B 5I) $_{R-free}$	-	100	2	2
i1(5I) $_{R-work}$	1	1	100	4
i1(5I) $_{R-free}$	-	2	100	6
PHENIX/Parrot $_{R-work}$	0	0	4	100
PHENIX/Parrot $_{R-free}$	-	2	6	100

Table 7. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	5	86	93
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	20	0	92	99
ARP(B 5I) $_{R-free}$	-	0	43	43
i1(5I) $_{R-work}$	2	0	0	20
i1(5I) $_{R-free}$	-	42	0	19
PHENIX/Parrot $_{R-work}$	0	0	38	0
PHENIX/Parrot $_{R-free}$	-	48	34	0

Table 8. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	22	8	4
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	41	0	7	1
ARP(B 5I) $_{R-free}$	-	0	4	2
i1(5I) $_{R-work}$	4	1	0	18
i1(5I) $_{R-free}$	-	9	0	19
PHENIX/Parrot $_{R-work}$	2	0	21	0
PHENIX/Parrot $_{R-free}$	-	6	22	0

Table 9. *Structure completeness comparison for the models generated from the synthetic MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	21	1	2
ARP(B 5I)	25	0	0	3
i1(5I)	95	95	0	76
PHENIX/Parrot	97	95	22	0

Table 10. *Structure completeness comparison for the models generated from the synthetic MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	100	54	5	1
ARP(B 5I)	54	100	4	1
i1(5I)	5	4	100	2
PHENIX/Parrot	1	1	2	100

Table 11. *Structure completeness comparison for the models generated from the synthetic MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	3	0	2
ARP(B 5I)	9	0	0	3
i1(5I)	86	86	0	72
PHENIX/Parrot	92	91	15	0

Table 12. *Structure completeness comparison for the models generated from the synthetic MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	19	0	0
ARP(B 5I)	16	0	0	0
i1(5I)	9	9	0	4
PHENIX/Parrot	5	5	7	0

Table 13. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	28	93	98
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	59	0	99	100
ARP(B 5I) $_{R-free}$	-	0	48	46
i1(5I) $_{R-work}$	5	1	0	40
i1(5I) $_{R-free}$	-	51	0	41
PHENIX/Parrot $_{R-work}$	2	0	56	0
PHENIX/Parrot $_{R-free}$	-	53	54	0

Table 14. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	100	13	2	0
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	13	100	0	0
ARP(B 5I) $_{R-free}$	-	100	1	1
i1(5I) $_{R-work}$	2	0	100	4
i1(5I) $_{R-free}$	-	1	100	5
PHENIX/Parrot $_{R-work}$	0	0	4	100
PHENIX/Parrot $_{R-free}$	-	1	5	100

Table 15. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	5	86	93
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	19	0	93	99
ARP(B 5I) $_{R-free}$	-	0	43	43
i1(5I) $_{R-work}$	2	0	0	21
i1(5I) $_{R-free}$	-	42	0	21
PHENIX/Parrot $_{R-work}$	0	0	37	0
PHENIX/Parrot $_{R-free}$	-	47	33	0

Table 16. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	23	7	4
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	40	0	6	1
ARP(B 5I) $_{R-free}$	-	0	5	3
i1(5I) $_{R-work}$	4	1	0	18
i1(5I) $_{R-free}$	-	9	0	20
PHENIX/Parrot $_{R-work}$	2	0	19	0
PHENIX/Parrot $_{R-free}$	-	6	21	0

Table 17. *Structure completeness comparison for the models generated from the synthetic NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP	0	20	1	2	2
ARP(B 5I)	20	0	0	3	3
i1(5I)	94	95	0	68	69
PHENIX/Parrot	97	96	29	0	43
PHENIX	97	96	28	45	0

Table 18. *Structure completeness comparison for the models generated from the synthetic NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP	100	60	5	1	1
ARP(B 5I)	60	100	5	1	1
i1(5I)	5	5	100	3	3
PHENIX/Parrot	1	1	3	100	12
PHENIX	1	1	3	12	100

Table 19. *Structure completeness comparison for the models generated from the synthetic NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP	0	4	1	2	2
ARP(B 5I)	8	0	0	3	3
i1(5I)	82	82	0	63	63
PHENIX/Parrot	92	92	21	0	15
PHENIX	92	90	21	16	0

Table 20. *Structure completeness comparison for the models generated from the synthetic NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP	0	16	1	0	0
ARP(B 5I)	12	0	0	0	1
i1(5I)	12	12	0	5	6
PHENIX/Parrot	5	4	8	0	28
PHENIX	5	6	7	29	0

Table 21. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP $_{R-work}$	0	29	95	97	97
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	58	0	99	100	100
ARP(B 5I) $_{R-free}$	-	0	50	45	46
i1(5I) $_{R-work}$	4	1	0	32	31
i1(5I) $_{R-free}$	-	49	0	34	33
PHENIX/Parrot $_{R-work}$	3	0	64	0	33
PHENIX/Parrot $_{R-free}$	-	54	62	0	41
PHENIX $_{R-work}$	2	0	64	36	0
PHENIX $_{R-free}$	-	53	63	43	0

Table 22. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP $_{R-work}$	100	13	1	0	1
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	13	100	0	0	0
ARP(B 5I) $_{R-free}$	-	100	2	1	1
i1(5I) $_{R-work}$	1	0	100	4	5
i1(5I) $_{R-free}$	-	2	100	4	4
PHENIX/Parrot $_{R-work}$	0	0	4	100	31
PHENIX/Parrot $_{R-free}$	-	1	4	100	17
PHENIX $_{R-work}$	1	0	5	31	100
PHENIX $_{R-free}$	-	1	4	17	100

Table 23. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP $_{R-work}$	0	5	88	93	93
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	20	0	94	99	99
ARP(B 5I) $_{R-free}$	-	0	44	43	43
i1(5I) $_{R-work}$	2	0	0	16	16
i1(5I) $_{R-free}$	-	37	0	16	15
PHENIX/Parrot $_{R-work}$	0	0	47	0	1
PHENIX/Parrot $_{R-free}$	-	48	43	0	6
PHENIX $_{R-work}$	1	0	47	1	0
PHENIX $_{R-free}$	-	47	43	7	0

Table 24. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the synthetic NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP $_{R-work}$	0	25	7	4	5
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	38	0	5	1	1
ARP(B 5I) $_{R-free}$	-	0	6	2	3
i1(5I) $_{R-work}$	3	1	0	16	16
i1(5I) $_{R-free}$	-	12	0	18	18
PHENIX/Parrot $_{R-work}$	2	0	17	0	32
PHENIX/Parrot $_{R-free}$	-	6	19	0	34
PHENIX $_{R-work}$	1	0	17	35	0
PHENIX $_{R-free}$	-	6	20	36	0

S3 The Results of the Original Datasets Used in **Buccaneer** Development

Table 1. *Complete and intermediate models produced by the 7 pipeline variants for the 52 original datasets, where (T) and (C) denote intermediate models produced by pipeline executions that timed out and crashed, respectively.*

Pipeline variant	HA-NCS			MR-NCS			NO-NCS		
	Complete	Intermediate	Failed	Complete	Intermediate	Failed	Complete	Intermediate	Failed
ARP	52	0(T) 0(C)	0	52	0(T) 0(C)	0	52	0(T) 0(C)	0
ARP(B 5I)	52	0(T) 0(C)	0	52	0(T) 0(C)	0	52	0(T) 0(C)	0
i1(5I)	52	0(T) 0(C)	0	52	0(T) 0(C)	0	52	0(T) 0(C)	0
PHENIX/Parrot	51	1(T) 0(C)	0	52	0(T) 0(C)	0	52	0(T) 0(C)	0
SHELXE/Parrot	52	0(T) 0(C)	0	52	0(T) 0(C)	0	52	0(T) 0(C)	0
PHENIX	-	-	-	-	-	-	52	0(T) 0(C)	0
SHELXE	-	-	-	-	-	-	52	0(T) 0(C)	0

Models used in the comparison: 52 HA-NCS, 52 MR-NCS and 52 NO-NCS.

Table 2. *Structure completeness comparison for the models generated from the 52 original HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	29	27	29	69
ARP(B 5I)	48	0	29	37	79
i1(5I)	60	52	0	44	90
PHENIX/Parrot	58	50	44	0	83
SHELXE/Parrot	27	19	8	10	0

Table 3. *Structure completeness comparison for the models generated from the 52 original HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	100	23	13	13	4
ARP(B 5I)	23	100	19	13	2
i1(5I)	13	19	100	12	2
PHENIX/Parrot	13	13	12	100	8
SHELXE/Parrot	4	2	2	8	100

Table 4. *Structure completeness comparison for the models generated from the 52 original HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	12	13	13	56
ARP(B 5I)	17	0	15	12	63
i1(5I)	37	29	0	21	73
PHENIX/Parrot	31	31	21	0	67
SHELXE/Parrot	17	15	2	8	0

Table 5. *Structure completeness comparison for the models generated from the 52 original HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	17	13	15	13
ARP(B 5I)	31	0	13	25	15
i1(5I)	23	23	0	23	17
PHENIX/Parrot	27	19	23	0	15
SHELXE/Parrot	10	4	6	2	0

Table 6. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	29	96	52	100
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	42	0	96	62	100
ARP(B 5I) $_{R-free}$	-	0	85	46	-
i1(5I) $_{R-work}$	2	4	0	0	100
i1(5I) $_{R-free}$	-	12	0	6	-
PHENIX/Parrot $_{R-work}$	35	29	98	0	100
PHENIX/Parrot $_{R-free}$	-	44	90	0	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 7. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	100	29	2	13	0
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	29	100	0	10	0
ARP(B 5I) $_{R-free}$	-	100	4	10	-
i1(5I) $_{R-work}$	2	0	100	2	0
i1(5I) $_{R-free}$	-	4	100	4	-
PHENIX/Parrot $_{R-work}$	13	10	2	100	0
PHENIX/Parrot $_{R-free}$	-	10	4	100	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	100
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 8. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	2	60	12	100
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	6	0	71	13	100
ARP(B 5I) $_{R-free}$	-	0	60	21	-
i1(5I) $_{R-work}$	0	0	0	0	96
i1(5I) $_{R-free}$	-	6	0	0	-
PHENIX/Parrot $_{R-work}$	4	0	48	0	100
PHENIX/Parrot $_{R-free}$	-	13	50	0	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 9. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	27	37	40	0
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	37	0	25	48	0
ARP(B 5I) $_{R-free}$	-	0	25	25	-
i1(5I) $_{R-work}$	2	4	0	0	4
i1(5I) $_{R-free}$	-	6	0	6	-
PHENIX/Parrot $_{R-work}$	31	29	50	0	0
PHENIX/Parrot $_{R-free}$	-	31	40	0	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 10. *Structure completeness comparison for the models generated from the 52 original MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	31	25	37	71
ARP(B 5I)	38	0	23	31	77
i1(5I)	60	60	0	50	94
PHENIX/Parrot	50	54	37	0	87
SHELXE/Parrot	23	21	6	8	0

Table 11. *Structure completeness comparison for the models generated from the 52 original MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	100	31	15	13	6
ARP(B 5I)	31	100	17	15	2
i1(5I)	15	17	100	13	0
PHENIX/Parrot	13	15	13	100	6
SHELXE/Parrot	6	2	0	6	100

Table 12. *Structure completeness comparison for the models generated from the 52 original MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	10	10	10	60
ARP(B 5I)	15	0	12	12	62
i1(5I)	37	35	0	21	75
PHENIX/Parrot	33	37	19	0	75
SHELXE/Parrot	12	10	2	4	0

Table 13. *Structure completeness comparison for the models generated from the 52 original MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP	0	21	15	27	12
ARP(B 5I)	23	0	12	19	15
i1(5I)	23	25	0	29	19
PHENIX/Parrot	17	17	17	0	12
SHELXE/Parrot	12	12	4	4	0

Table 14. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	27	92	58	100
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	42	0	94	54	100
ARP(B 5I) $_{R-free}$	-	0	79	44	-
i1(5I) $_{R-work}$	4	2	0	2	100
i1(5I) $_{R-free}$	-	13	0	6	-
PHENIX/Parrot $_{R-work}$	27	31	92	0	100
PHENIX/Parrot $_{R-free}$	-	48	87	0	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 15. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	100	31	4	15	0
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	31	100	4	15	0
ARP(B 5I) $_{R-free}$	-	100	8	8	-
i1(5I) $_{R-work}$	4	4	100	6	0
i1(5I) $_{R-free}$	-	8	100	8	-
PHENIX/Parrot $_{R-work}$	15	15	6	100	0
PHENIX/Parrot $_{R-free}$	-	8	8	100	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	100
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 16. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	2	54	10	100
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	6	0	52	12	100
ARP(B 5I) $_{R-free}$	-	0	52	15	-
i1(5I) $_{R-work}$	0	0	0	0	98
i1(5I) $_{R-free}$	-	8	0	0	-
PHENIX/Parrot $_{R-work}$	2	2	38	0	100
PHENIX/Parrot $_{R-free}$	-	10	40	0	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 17. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	SHELXE/Parrot
ARP $_{R-work}$	0	25	38	48	0
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	37	0	42	42	0
ARP(B 5I) $_{R-free}$	-	0	27	29	-
i1(5I) $_{R-work}$	4	2	0	2	2
i1(5I) $_{R-free}$	-	6	0	6	-
PHENIX/Parrot $_{R-work}$	25	29	54	0	0
PHENIX/Parrot $_{R-free}$	-	38	46	0	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-

Table 18. *Structure completeness comparison for the models generated from the 52 original NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP	0	23	27	35	40	75	73
ARP(B 5I)	50	0	31	33	38	83	81
i1(5I)	62	56	0	40	46	88	90
PHENIX/Parrot	54	46	50	0	38	79	85
PHENIX	50	42	40	29	0	81	85
SHELXE	21	17	6	10	12	0	37
SHELXE/Parrot	23	15	6	8	10	54	0

Table 19. *Structure completeness comparison for the models generated from the 52 original NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP	100	27	12	12	10	4	4
ARP(B 5I)	27	100	13	21	19	0	4
i1(5I)	12	13	100	10	13	6	4
PHENIX/Parrot	12	21	10	100	33	12	8
PHENIX	10	19	13	33	100	8	6
SHELXE	4	0	6	12	8	100	10
SHELXE/Parrot	4	4	4	8	6	10	100

Table 20. *Structure completeness comparison for the models generated from the 52 original NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP	0	2	13	12	13	56	60
ARP(B 5I)	21	0	13	12	19	65	69
i1(5I)	33	27	0	21	27	67	77
PHENIX/Parrot	35	31	27	0	13	67	69
PHENIX	35	27	31	8	0	67	71
SHELXE	13	6	0	6	8	0	10
SHELXE/Parrot	13	8	0	4	8	21	0

Table 21. *Structure completeness comparison for the models generated from the 52 original NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP	0	21	13	23	27	19	13
ARP(B 5I)	29	0	17	21	19	17	12
i1(5I)	29	29	0	19	19	21	13
PHENIX/Parrot	19	15	23	0	25	12	15
PHENIX	15	15	10	21	0	13	13
SHELXE	8	12	6	4	4	0	27
SHELXE/Parrot	10	8	6	4	2	33	0

Table 22. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP $_{R-work}$	0	19	98	56	50	100	100
ARP $_{R-free}$	-	-	-	-	-	-	-
ARP(B 5I) $_{R-work}$	48	0	100	63	62	100	100
ARP(B 5I) $_{R-free}$	-	0	87	42	48	-	-
i1(5I) $_{R-work}$	0	0	0	0	0	100	100
i1(5I) $_{R-free}$	-	8	0	2	4	-	-
PHENIX/Parrot $_{R-work}$	35	23	98	0	33	100	100
PHENIX/Parrot $_{R-free}$	-	46	94	0	40	-	-
PHENIX $_{R-work}$	35	27	100	29	0	100	100
PHENIX $_{R-free}$	-	40	94	25	0	-	-
SHELXE $_{R-work}$	0	0	0	0	0	0	21
SHELXE $_{R-free}$	-	-	-	-	-	-	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0	33	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-	-	-

Table 23. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP $_{R-work}$	100	33	2	10	15	0	0
ARP $_{R-free}$	-	-	-	-	-	-	-
ARP(B 5I) $_{R-work}$	33	100	0	13	12	0	0
ARP(B 5I) $_{R-free}$	-	100	6	12	12	-	-
i1(5I) $_{R-work}$	2	0	100	2	0	0	0
i1(5I) $_{R-free}$	-	6	100	4	2	-	-
PHENIX/Parrot $_{R-work}$	10	13	2	100	38	0	0
PHENIX/Parrot $_{R-free}$	-	12	4	100	35	-	-
PHENIX $_{R-work}$	15	12	0	38	100	0	0
PHENIX $_{R-free}$	-	12	2	35	100	-	-
SHELXE $_{R-work}$	0	0	0	0	0	100	46
SHELXE $_{R-free}$	-	-	-	-	-	-	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0	46	100
SHELXE/Parrot $_{R-free}$	-	-	-	-	-	-	-

Table 24. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP $_{R-work}$	0	4	62	10	12	100	100
ARP $_{R-free}$	-	-	-	-	-	-	-
ARP(B 5I) $_{R-work}$	4	0	67	15	12	100	100
ARP(B 5I) $_{R-free}$	-	0	60	17	27	-	-
i1(5I) $_{R-work}$	0	0	0	0	0	96	96
i1(5I) $_{R-free}$	-	6	0	0	0	-	-
PHENIX/Parrot $_{R-work}$	6	4	56	0	0	100	100
PHENIX/Parrot $_{R-free}$	-	13	62	0	2	-	-
PHENIX $_{R-work}$	6	4	56	0	0	100	100
PHENIX $_{R-free}$	-	12	56	2	0	-	-
SHELXE $_{R-work}$	0	0	0	0	0	0	0
SHELXE $_{R-free}$	-	-	-	-	-	-	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0	0	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-	-	-

Table 25. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 original NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX	SHELXE	SHELXE/Parrot
ARP $_{R-work}$	0	15	37	46	38	0	0
ARP $_{R-free}$	-	-	-	-	-	-	-
ARP(B 5I) $_{R-work}$	44	0	33	48	50	0	0
ARP(B 5I) $_{R-free}$	-	0	27	25	21	-	-
i1(5I) $_{R-work}$	0	0	0	0	0	4	4
i1(5I) $_{R-free}$	-	2	0	2	4	-	-
PHENIX/Parrot $_{R-work}$	29	19	42	0	33	0	0
PHENIX/Parrot $_{R-free}$	-	33	33	0	38	-	-
PHENIX $_{R-work}$	29	23	44	29	0	0	0
PHENIX $_{R-free}$	-	29	38	23	0	-	-
SHELXE $_{R-work}$	0	0	0	0	0	0	21
SHELXE $_{R-free}$	-	-	-	-	-	-	-
SHELXE/Parrot $_{R-work}$	0	0	0	0	0	33	0
SHELXE/Parrot $_{R-free}$	-	-	-	-	-	-	-

S4. **The Results of the Synthetic Datasets for the Original Datasets** Used in Buccaneer Development

Table 1. *Complete and intermediate models produced by the 5 pipeline variants for the 52 synthetic datasets, where (T) and (C) denote intermediate models produced by pipeline executions that timed out and crashed, respectively.*

Pipeline variant	HA-NCS			MR-NCS			NO-NCS		
	Complete	Intermediate	Failed	Complete	Intermediate	Failed	Complete	Intermediate	Failed
ARP	258	1(T) 0(C)	0	258	1(T) 0(C)	0	258	1(T) 0(C)	0
ARP(B 5I)	256	3(T) 0(C)	0	258	1(T) 0(C)	0	257	2(T) 0(C)	0
i1(5I)	259	0(T) 0(C)	0	259	0(T) 0(C)	0	259	0(T) 0(C)	0
PHENIX/Parrot	259	0(T) 0(C)	0	259	0(T) 0(C)	0	257	2(T) 0(C)	0
PHENIX	-	-	-	-	-	-	256	2(T) 0(C)	1

Models used in the comparison: 259 HA-NCS, 259 MR-NCS and 258 NO-NCS.

Table 2. *Structure completeness comparison for the models generated from the 52 synthetic HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	25	1	4
ARP(B 5I)	25	0	0	4
i1(5I)	97	97	0	88
PHENIX/Parrot	95	95	10	0

Table 3. *Structure completeness comparison for the models generated from the 52 synthetic HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	100	50	3	1
ARP(B 5I)	50	100	3	1
i1(5I)	3	3	100	1
PHENIX/Parrot	1	1	1	100

Table 4. *Structure completeness comparison for the models generated from the 52 synthetic HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	5	0	3
ARP(B 5I)	8	0	0	4
i1(5I)	93	93	0	86
PHENIX/Parrot	93	92	5	0

Table 5. *Structure completeness comparison for the models generated from the 52 synthetic HA-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	20	1	1
ARP(B 5I)	17	0	0	0
i1(5I)	3	3	0	3
PHENIX/Parrot	2	2	5	0

Table 6. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	24	95	97
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	60	0	100	100
ARP(B 5I) $_{R-free}$	-	0	40	39
i1(5I) $_{R-work}$	4	0	0	45
i1(5I) $_{R-free}$	-	58	0	48
PHENIX/Parrot $_{R-work}$	2	0	49	0
PHENIX/Parrot $_{R-free}$	-	60	48	0

Table 7. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	100	16	1	0
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	16	100	0	0
ARP(B 5I) $_{R-free}$	-	100	2	0
i1(5I) $_{R-work}$	1	0	100	7
i1(5I) $_{R-free}$	-	2	100	4
PHENIX/Parrot $_{R-work}$	0	0	7	100
PHENIX/Parrot $_{R-free}$	-	0	4	100

Table 8. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	2	89	96
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	22	0	97	100
ARP(B 5I) $_{R-free}$	-	0	35	37
i1(5I) $_{R-work}$	2	0	0	22
i1(5I) $_{R-free}$	-	47	0	20
PHENIX/Parrot $_{R-work}$	1	0	28	0
PHENIX/Parrot $_{R-free}$	-	53	23	0

Table 9. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic HA-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	22	6	2
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	38	0	3	0
ARP(B 5I) $_{R-free}$	-	0	5	2
i1(5I) $_{R-work}$	2	0	0	22
i1(5I) $_{R-free}$	-	11	0	28
PHENIX/Parrot $_{R-work}$	1	0	20	0
PHENIX/Parrot $_{R-free}$	-	7	25	0

Table 10. *Structure completeness comparison for the models generated from the 52 synthetic MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	27	1	4
ARP(B 5I)	25	0	0	3
i1(5I)	97	97	0	88
PHENIX/Parrot	95	96	10	0

Table 11. *Structure completeness comparison for the models generated from the 52 synthetic MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	100	49	3	1
ARP(B 5I)	49	100	3	1
i1(5I)	3	3	100	1
PHENIX/Parrot	1	1	1	100

Table 12. *Structure completeness comparison for the models generated from the 52 synthetic MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	6	0	3
ARP(B 5I)	8	0	0	3
i1(5I)	93	93	0	85
PHENIX/Parrot	92	92	4	0

Table 13. *Structure completeness comparison for the models generated from the 52 synthetic MR-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP	0	20	1	1
ARP(B 5I)	16	0	0	0
i1(5I)	4	3	0	4
PHENIX/Parrot	3	4	6	0

Table 14. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	23	95	98
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	63	0	100	100
ARP(B 5I) $_{R-free}$	-	0	39	38
i1(5I) $_{R-work}$	4	0	0	46
i1(5I) $_{R-free}$	-	59	0	48
PHENIX/Parrot $_{R-work}$	2	0	49	0
PHENIX/Parrot $_{R-free}$	-	61	45	0

Table 15. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	100	14	1	0
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	14	100	0	0
ARP(B 5I) $_{R-free}$	-	100	2	1
i1(5I) $_{R-work}$	1	0	100	4
i1(5I) $_{R-free}$	-	2	100	7
PHENIX/Parrot $_{R-work}$	0	0	4	100
PHENIX/Parrot $_{R-free}$	-	1	7	100

Table 16. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	3	90	96
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	18	0	96	100
ARP(B 5I) $_{R-free}$	-	0	35	37
i1(5I) $_{R-work}$	2	0	0	18
i1(5I) $_{R-free}$	-	48	0	19
PHENIX/Parrot $_{R-work}$	1	0	27	0
PHENIX/Parrot $_{R-free}$	-	54	23	0

Table 17. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic MR-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot
ARP $_{R-work}$	0	20	5	2
ARP $_{R-free}$	-	-	-	-
ARP(B 5I) $_{R-work}$	45	0	3	0
ARP(B 5I) $_{R-free}$	-	0	4	1
i1(5I) $_{R-work}$	2	0	0	28
i1(5I) $_{R-free}$	-	10	0	30
PHENIX/Parrot $_{R-work}$	1	0	23	0
PHENIX/Parrot $_{R-free}$	-	7	22	0

Table 18. *Structure completeness comparison for the models generated from the 52 synthetic NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP	0	23	1	4	3
ARP(B 5I)	22	0	0	3	3
i1(5I)	95	96	0	81	82
PHENIX/Parrot	96	96	17	0	45
PHENIX	97	97	16	42	0

Table 19. *Structure completeness comparison for the models generated from the 52 synthetic NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with equal structure completeness to each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP	100	55	3	0	0
ARP(B 5I)	55	100	4	1	0
i1(5I)	3	4	100	2	2
PHENIX/Parrot	0	1	2	100	13
PHENIX	0	0	2	13	100

Table 20. *Structure completeness comparison for the models generated from the 52 synthetic NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with at least 5% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP	0	4	0	3	3
ARP(B 5I)	8	0	0	3	3
i1(5I)	90	90	0	77	76
PHENIX/Parrot	94	93	9	0	12
PHENIX	93	93	10	14	0

Table 21. *Structure completeness comparison for the models generated from the 52 synthetic NO-NCS datasets. Each row corresponds to a pipeline variant, and shows the percentage(rounded to the nearest integer) of models that the pipeline variant built with between 1% and 4% higher structure completeness than each of the other pipeline variants.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP	0	19	1	1	0
ARP(B 5I)	14	0	0	0	0
i1(5I)	6	6	0	4	7
PHENIX/Parrot	2	2	8	0	34
PHENIX	4	4	6	28	0

Table 22. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with lower R-work or R-free than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP $_{R-work}$	0	29	95	97	97
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	56	0	100	100	100
ARP(B 5I) $_{R-free}$	-	0	40	39	38
i1(5I) $_{R-work}$	4	0	0	37	37
i1(5I) $_{R-free}$	-	58	0	36	34
PHENIX/Parrot $_{R-work}$	2	0	57	0	33
PHENIX/Parrot $_{R-free}$	-	60	60	0	38
PHENIX $_{R-work}$	2	0	57	31	0
PHENIX $_{R-free}$	-	61	61	44	0

Table 23. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with equal R-work or R-free to each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP $_{R-work}$	100	16	2	0	1
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	16	100	0	0	0
ARP(B 5I) $_{R-free}$	-	100	2	0	0
i1(5I) $_{R-work}$	2	0	100	6	6
i1(5I) $_{R-free}$	-	2	100	4	5
PHENIX/Parrot $_{R-work}$	0	0	6	100	36
PHENIX/Parrot $_{R-free}$	-	0	4	100	19
PHENIX $_{R-work}$	1	0	6	36	100
PHENIX $_{R-free}$	-	0	5	19	100

Table 24. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free at least 5% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP $_{R-work}$	0	3	89	96	95
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	17	0	96	100	100
ARP(B 5I) $_{R-free}$	-	0	36	37	36
i1(5I) $_{R-work}$	2	0	0	18	17
i1(5I) $_{R-free}$	-	43	0	16	17
PHENIX/Parrot $_{R-work}$	1	0	43	0	0
PHENIX/Parrot $_{R-free}$	-	55	34	0	2
PHENIX $_{R-work}$	1	0	40	0	0
PHENIX $_{R-free}$	-	57	39	5	0

Table 25. *Comparison of R-work/R-free (rounded to two decimal places) for the models generated from the 52 synthetic NO-NCS datasets. Each row shows the percentage of models that a pipeline variant built with R-work or R-free between 1% and 4% lower than each other pipeline variant.*

Pipeline variant	ARP	ARP(B 5I)	i1(5I)	PHENIX/Parrot	PHENIX
ARP $_{R-work}$	0	25	6	2	2
ARP $_{R-free}$	-	-	-	-	-
ARP(B 5I) $_{R-work}$	38	0	3	0	0
ARP(B 5I) $_{R-free}$	-	0	5	2	2
i1(5I) $_{R-work}$	2	0	0	19	20
i1(5I) $_{R-free}$	-	15	0	20	17
PHENIX/Parrot $_{R-work}$	1	0	14	0	33
PHENIX/Parrot $_{R-free}$	-	6	25	0	36
PHENIX $_{R-work}$	1	0	17	31	0
PHENIX $_{R-free}$	-	4	22	39	0

S5. Reproducibility of the Comparison Experiment

The results of this comparison are reproducible, excluding the execution times that the pipeline variants required to build the protein models, which might be affected by certain factors and differ in each run. Tables 1, 2, 3 and 4 compare the mean of completeness, R-work/R-free and the execution times for original and synthetic. It is clear from these tables that completeness and R-work/R-free can be reproduced, while execution times can vary across different runs, as happens in Phenix Autobuild.

Table 1. *The mean of the three comparative factors, completeness(%), R-work/R-free and the execution times in minutes for the reproducibility experiment for the original NO-NCS datasets.*

Pipeline variant	Completeness	R-work/R-free	Execution time
ARP	94	0.24/0.24	32
ARP(B 5I)	93	0.23/0.26	32
i1(5I)	95	0.26/0.29	4
PHENIX	92	0.24/0.26	71
SHELXE	90	0.45/0.44	66
PHENIX/Parrot	93	0.24/0.26	91
SHELXE/Parrot	92	0.44/0.44	59

Table 2. *The mean of the three comparative factors, completeness(%), R-work/R-free and the execution times in minutes for the main experiment for the original NO-NCS datasets.*

Pipeline variant	Completeness	R-work/R-free	Execution time
ARP	94	0.24/0.24	28
ARP(B 5I)	93	0.23/0.26	40
i1(5I)	95	0.26/0.29	4
PHENIX	92	0.24/0.26	101
SHELXE	90	0.45/0.44	65
PHENIX/Parrot	93	0.24/0.26	92
SHELXE/Parrot	92	0.44/0.44	65

Table 3. *The mean of the three comparative factors, completeness(%), R-work/R-free and the execution times in minutes for the reproducibility experiment for the synthetic NO-NCS datasets.*

Pipeline variant	Completeness	R-work/R-free	Execution time
ARP	2	0.21/0.2	30
ARP(B 5I)	1	0.19/0.4	32
i1(5I)	62	0.32/0.4	5
PHENIX	45	0.29/0.37	49
PHENIX/Parrot	43	0.29/0.38	77

Table 4. *The mean of the three comparative factors, completeness(%), R-work/R-free and the execution times in minutes for the main experiment for the synthetic NO-NCS datasets.*

Pipeline variant	Completeness	R-work/R-free	Execution time
ARP	2	0.21/0.2	24
ARP(B 5I)	0	0.19/0.39	45
i1(5I)	63	0.32/0.4	5
PHENIX	45	0.29/0.37	92
PHENIX/Parrot	43	0.29/0.38	95