**Table S1. Sociodemographic characteristics of the sample upon which normative models were built**

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Typically Developing** |  | **NDCs (n=1298)** |
| **Autism** | **ADHD** | **OCD** | **Other** |
|  | **(n=338)** | **(n=516)** | **(n=543)** | **(n=206)** | **(n=33)** |
| Mean age in years (sd) | 10.64 (3.11) | 11.38 (3.27) | 9.78 (2.76) | 12.09 (2.74) | 10.18 (3.30) |
| N Males (sex assigned at birth) (%) | 201(59.47%) | 401 (77.71%) | 401 (73.84%) | 106 (51.45%) | 24 (72.73%) |
| N Females (sex assigned at birth) (%) | 137 (40.53%) | 115 (22.29%) | 142 (26.15%) | 100 (48.54%) | 9 (27.27%) |
| Mean FSIQ (sd) | 108.64 (12.75) | 96.05 (19.79) | 99.08 (15.30) | 111.11 (10.76) | 74.30 (23.50) |
| **N of individuals with co-occurring conditions (%)** (Autism, ADHD, OCD, Communication Disorders, Down Syndrome, ID, Learning Disorders, Motor Disorders, Anxiety Disorders) |
| 0 | 338 | 290 (56.20%) | 404 (74.40%) | 148 (71.84%) | 26 (78.79%) |
| 1 | 0 | 119 (23.06%) | 72 (13.25%) | 33 (16.02%) | 5 (15.15%) |
| 2 | 0 | 67 (12.98%) | 52 (9.58%) | 16 (7.77%) | 1 (3.03%) |
| 3 | 0 | 22 (4.26%) | 3 (0.56%) | 7(3.40%) | 1 (3.03%) |
| 4 | 0 | 10 (1.94%) | 10 (1.84%) | 2 (0.97%) | 0 |
| 5 | 0 | 8 (0.16%) | 2 (0.4%) | 0 | 0 |
| **Race and Ethnicity in %** |
| Latin American/Hispanic | 2.66 | 3.43 | 1.68 | 1.51 | 0 |
| White | 87.94 | 83.82 | 93.82 | 95.45 | 100 |
| Black | 2.97 | 3.17 | 3.37 | 1.51 | 0 |
| Asian | 7.19 | 11.37 | 1.68 | 0 | 0 |
| Jewish | 3.12 | 3.70 | 2.24 | 0 | 0 |
| Arab | 0.93 | 2.24 | 1.12 | 0 | 0 |
| Aboriginal | 7.84 | 6.61 | 12.92 | 1.51 | 0 |

*Note*. NDCs = Neurodevelopmental Conditions, ADHD = Attention-Deficit/Hyperactivity Disorder, ID = Intellectual Disability, OCD = Obsessive-Compulsive Disorder, sd = standard deviation, FSIQ = full-scale intelligence quotient. Typically developing sample includes siblings (n = 4), sub-threshold OCD (n = 4) and subthreshold ADHD (n = 111). Other NDCs comprise Tourette syndrome (n = 7), Intellectual Disability (n = 10), Fragile X syndrome (n = 2), Down syndrome (n = 1), and non-specified NDCs (n = 13). Race and ethnicity were collected in line with the way how the Canadian Census data were collected. FSIQ and race-ethnicity data were only available in a reduced number of participants (n = 1156): 312 typically developing participants, 386 autistic participants, 336 ADHD participants, 90 OCD participants and 32 participants with other NDCs. Co-occurring conditions are operationalised as the count of participants with a given number of co-occurring conditions within each diagnostic group.

**Table S2. STROBE Statement**

|  |  |  |  |
| --- | --- | --- | --- |
|  | Item No | Recommendation | PageNo |
| **Title and abstract** | 1 | (*a*) Indicate the study’s design with a commonly used term in the title or the abstract | 1-2 |
| (*b*) Provide in the abstract an informative and balanced summary of what was done and what was found | 2 |
| Introduction |
| Background/rationale | 2 | Explain the scientific background and rationale for the investigation being reported | 4-6 |
| Objectives | 3 | State specific objectives, including any prespecified hypotheses | 5-6 |
| Methods |
| Study design | 4 | Present key elements of study design early in the paper | 6-9, Figure 1 |
| Setting | 5 | Describe the setting, locations, and relevant dates, including periods of recruitment, exposure, follow-up, and data collection | 6-7 |
| Participants | 6 | (*a*) Give the eligibility criteria, and the sources and methods of selection of participants | 6-7 |
| Variables | 7 | Clearly define all outcomes, exposures, predictors, potential confounders, and effect modifiers. Give diagnostic criteria, if applicable | 7-9 |
| Data sources/ measurement | 8\* | For each variable of interest, give sources of data and details of methods of assessment (measurement). Describe comparability of assessment methods if there is more than one group | 6-10 |
| Bias | 9 | Describe any efforts to address potential sources of bias | 9-12 |
| Study size | 10 | Explain how the study size was arrived at | 6-7 |
| Quantitative variables | 11 | Explain how quantitative variables were handled in the analyses. If applicable, describe which groupings were chosen and why | 9-12 |
| Statistical methods | 12 | (*a*) Describe all statistical methods, including those used to control for confounding | 9-12 |
| (*b*) Describe any methods used to examine subgroups and interactions | 9-12 |
| (*c*) Explain how missing data were addressed | 9-12 |
| (*d*) If applicable, describe analytical methods taking account of sampling strategy | N/A |
| (*e*) Describe any sensitivity analyses | 12 |
| Results |
| Participants | 13\* | (a) Report numbers of individuals at each stage of study—eg numbers potentially eligible, examined for eligibility, confirmed eligible, included in the study, completing follow-up, and analysed | 12-14 |
| (b) Give reasons for non-participation at each stage | 9-12 |
| (c) Consider use of a flow diagram | Figure 1 |
| Descriptive data | 14\* | (a) Give characteristics of study participants (eg demographic, clinical, social) and information on exposures and potential confounders | Table 1; Table S1 |
| (b) Indicate number of participants with missing data for each variable of interest | 6-7, 9-12 |
| Outcome data | 15\* | Report numbers of outcome events or summary measures | 12-14 |
| Main results | 16 | (*a*) Give unadjusted estimates and, if applicable, confounder-adjusted estimates and their precision (eg, 95% confidence interval). Make clear which confounders were adjusted for and why they were included | 12-14 |
| (*b*) Report category boundaries when continuous variables were categorized | N/A |
| (*c*) If relevant, consider translating estimates of relative risk into absolute risk for a meaningful time period | N/A |
| Other analyses | 17 | Report other analyses done—eg analyses of subgroups and interactions, and sensitivity analyses | 14 |
| Discussion |
| Key results | 18 | Summarise key results with reference to study objectives | 14-15 |
| Limitations | 19 | Discuss limitations of the study, taking into account sources of potential bias or imprecision. Discuss both direction and magnitude of any potential bias | 17-18 |
| Interpretation | 20 | Give a cautious overall interpretation of results considering objectives, limitations, multiplicity of analyses, results from similar studies, and other relevant evidence | 14-18 |
| Generalisability | 21 | Discuss the generalisability (external validity) of the study results | 14-19 |
| Other information |
| Funding | 22 | Give the source of funding and the role of the funders for the present study and, if applicable, for the original study on which the present article is based | 21 |

  **Table S3. Key bibliography guiding statistical analyses and relevant R packages**

|  |  |  |
| --- | --- | --- |
| **Analysis performed** | **Reference** | **Package** |
| Normative modelling | Marquand AF, Rezek I, Buitelaar J, Beckmann CF. Understanding Heterogeneity in Clinical Cohorts Using Normative Models: Beyond Case-Control Studies. *Biological Psychiatry*. 2016;80(7):552-561.  | Not applicable |
| Child Behavior Checklist Dysregulation Profile calculation | Ayer L, Althoff R, Ivanova M, Rettew D, Waxler E, Sulman J, et al. Child Behavior Checklist Juvenile Bipolar Disorder (CBCL-JBD) and CBCL Posttraumatic Stress Problems (CBCL-PTSP) scales are measures of a single dysregulatory syndrome. Journal of Child Psychology and Psychiatry. 2009 Oct 1;50(10):1291–300. | Not applicable |
| Stratified sampling of the training and test sets | Kuhn M. The caret package. *R Foundation for Statistical Computing, Vienna, Austria URL https://cran r-project org/package= caret*. Published online 2012.  | caret |
| Principal component regression | Mevik BH, Wehrens R. Introduction to the pls Package. *Help section of the “Pls” package of R studio software*. Published online 2015:1-23. | pls |
| Selection of optimal number of principal components: one-sigma heuristic  | Hastie T, Tibshirani R, Friedman JH, Friedman JH. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. Vol 2. Springer; 2009. | Not applicable |
| Selection of optimal number of principal components: permutation approach  | van der Voet H. Comparing the predictive accuracy of models using a simple randomization test. *Chemometrics and intelligent laboratory systems*. 1994;25(2):313-323. | Not applicable |
| Principal component loading significance | Hair JF, Anderson RE, Tatham RL, Black WC. Multivariate Data Analysis With Readings , Englewood Cliffs, NJ: Prentice Hall. Published online 1998. | Not applicable |
| Mediation | Tingley D, Yamamoto T, Hirose K, Keele L, Imai K. Mediation: R package for causal mediation analysis. Published online 2014.  | mediation |
| Aikake Information Criterion, Bayesian Information Criterion | Vrieze SI. Model selection and psychological theory: a discussion of the differences between the Akaike information criterion (AIC) and the Bayesian information criterion (BIC). *Psychological methods*. 2012;17(2):228. | Not applicable |
| Monte Carlo Power Analysis for indirect effects | Schoemann AM, Boulton AJ, Short SD. *Monte Carlo Power Analysis for Indirect Effects*.; 2020. | Shiny, MASS |
| Temporal bias assessment for cross-sectional mediation analysis | Georgeson AR, Alvarez-Bartolo D, MacKinnon DP. A sensitivity analysis for temporal bias in cross-sectional mediation. Psychol Methods. 2023 Dec 21. | phantSEM |
|  |  |  |

 **Table S4. Spearman correlations between T-scores based on the population norm (where available) and z-scores derived from normative modelling based on our sample**

|  |  |  |
| --- | --- | --- |
| **Measure** | **Males** | **Females** |
| ABAS-II-Social | 0.976 | 0.978 |
| CBCL Anxiety/Depression | 0.976 | 0.994 |
| CBCL Attention | 0.970 | 0.982 |
| CBCL Aggression | 0.966 | 0.984 |

*Note.* ABAS-II = Adaptive Behavior Assessment System 2nd Edition. **Table S5. Sociodemographic characteristics of participants in the training (n=324) and test (n=322) sets**

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Training set (n=324)** | **Test set (n=322)** | **Statistics** |
| Mean age in years (sd) | 10.39 (3.03) | 10.61 (2.93) | t = -0.91  |
| N Males (sex assigned at birth) (%) | 224 (69.35%) | 228 (70.81%) | X2 = 0.01  |
| N Females (sex assigned at birth) (%) | 100 (30.86%) | 94 (29.19%) | X2 = 0.01 |
| Mean FSIQ (sd) | 105.85 (15.88) | 102.10 (15.72) | t = 1.01 |
| **Social Cognition** |  |  |  |
| Mean RMET total (sd) | -0.33 (1.26) | -0.35 (1.21) | t = -0.26 |
| Mean RMET positive (sd) | -0.16 (1.02) | -0.09 (1.00) | t = 0.84 |
| Mean RMET negative (sd) | -0.26 (1.06) | -0.19 (1.03) | t = 0.74 |
| Mean RMET neutral (sd) | -0.26 (1.14) | -0.35 (1.11) | t = -1.09 |
| Mean NEPSY-II-AR total (sd) | -0.20 (1.09) | -0.31(1.15) | t = -1.28 |
| Mean NEPSY-II-AR happy (sd) | -0.22(1.28) | -0.30 (1.45) | t = 0.76 |
| Mean NEPSY-II-AR sad (sd) | -0.15 (0.95) | -0.1 (0.91) | **t = -2.19 \*** |
| Mean NEPSY-II-AR neutral (sd) | -0.21 (1.11) | -0.11 (1.14) | t = -1.15 |
| Mean NEPSY-II-AR angry (sd) | -0.11 (1.02) | -0.11(1.00) | t = -0.09 |
| Mean NEPSY-II-AR fear (sd) | -0.02 (1.08) | -0.38 (1.12) | t = 0.27 |
| Mean NEPSY-II-AR disgust (sd) | 0.09 (1.01) | 0.14 (0.13) | t = -0.54 |
| Mean NEPSY-II-ToM (sd) | -0.55 (1.31) | -0.77 (1.52) | t = -1.94  |
| Mean NEPSY-II-ToM-Verbal | -0.49 (1.23) | -0.74 (1.47) | **t = -2.34 \*** |
| (sd) |
| Mean NEPSY-II-ToM-Context (sd) | -0.29 (1.05) | -0.27 (1.17) | t = 0.13 |
| Mean Sandbox Egocentric Bias (sd) | -0.04 (1.09) | -0.03 (0.98) | t = -0.06 |
| **Social Behaviours** |  |  |  |
| Mean ABAS-II-Social (sd) | -1.81 (1.98) | -1.69 (1.97) | t = 0.77 |
| **Dysregulation** |  |  |  |
| Mean CBCL-DP (sd) | 6.18 (6.20) | 5.58 (5.75) | t = 1.28 |
| **Diagnosis (%)** |  |  |  |
| Autism | 107 (33.02%) | 107 (33.22%) | X2 = 0.00 |
| ADHD | 112 (34.57%) | 112 (34.78%) | X2 = 0.00 |
| OCD | 25 (7.72%) | 25 (7.76%) | X2 = 0.00 |
| Other NDCs | 4 (1.23%) | 3 (0.93%) | X2 = 0.11 |
| TD | 76 (23.46%) | 75 (23.60%) | X2 = 0.00 |
| **N of individuals with co-occurring conditions (%)** (Autism, ADHD, OCD, Communication Disorders, Down Syndrome, ID, Learning Disorders, Motor Disorders, Anxiety) |
| 0 | 215 (66.36%) | 223 (69.25%) | X2 = 0.45 |
| 1 | 48 (14.81%) | 37 (11.49%) | X2 = 1.25 |
| 2 | 33 (10.19%) | 45 (13.97%) | X2 = 1.88 |
| 3 | 19 (5.86%) | 11 (3.41%) | X2 = 1.64 |
| 4 | 5 (1.54%) | 3 (0.93%) | X2 = 0.11 |
| 5 | 4 (1.23%) | 3 (0.93%) | X2 = 0.00 |

*Note.* TD = Typically Developing, sd = standard deviation, FSIQ = Full-scale intelligence quotient, RMET = Reading the Mind in the Eyes Test (child version), NEPSY-II-AR = Neuropsychological Assessment Affect Recognition subscale, NEPSY-II-ToM = Neuropsychological Assessment Theory of Mind subscale, CBCL-DP = Child Behavior Checklist Dysregulation Profile, ABAS-II = Adaptive Behavior Assessment System 2nd Edition, ADHD = Attention-Deficit/Hyperactivity Disorder, OCD = Obsessive-Compulsive Disorder, ID = Intellectual Disability. Other NDCs comprise Tourette syndrome, Intellectual Disability, and non-specified NDCs. \*\* indicates a p-value < 0.01, \* indicates a p-value < 0.05. Significant effects appear in bold.

**Table S6. Correlation matrix of data from the training set (n=324)**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | RMET positive | RMET negative | RMET neutral | NEPSY-II-AR happy | NEPSY-II-AR sad | NEPSY-II-AR neutral | NEPSY-II-AR fear | NEPSY-II-AR angry | NEPSY-II-AR disgust | NEPSY-II-ToM-Verbal | NEPSY-II ToM- Contextual | Sandbox Egocentric Bias | CBCL-DP | ABAS-II-Social | Age | FSIQ |
| RMET positive | 1.000 | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** |
| RMET negative | 0.219 | 1.000 | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** |
| RMET neutral | 0.224 | 0.317 | 1.000 | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** |
| NEPSY-II-AR happy | 0.060 | 0.013 | -0.034 | 1.000 | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** |
| NEPSY-II-AR sad | -0.098 | -0.093 | -0.058 | -0.049 | 1.000 | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** |
| NEPSY-II-AR neutral | 0.000 | 0.006 | -0.023 | -0.047 | 0.174 | 1.000 | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** |
| NEPSY-II-AR fear | 0.086 | 0.045 | 0.065 | 0.083 | 0.054 | 0.163 | 1.000 | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** | **-** |
| NEPSY-II-AR angry | 0.006 | -0.087 | -0.110 | -0.064 | 0.292 | 0.115 | 0.171 | 1.000 | - | - | - | - | - | - | - | - |
| NEPSY-II-AR disgust | -0.027 | -0.051 | -0.108 | -0.104 | 0.197 | 0.015 | -0.031 | 0.166 | 1.000 | - | - | - | - | - | - | - |
| NEPSY-II-ToM-Verbal | 0.013 | -0.024 | 0.080 | 0.200 | 0.045 | -0.009 | 0.040 | 0.109 | 0.090 | 1.000 | - | - | - | - | - | - |
| NEPSY-II-ToM-Contextual | -0.098 | -0.147 | -0.067 | 0.182 | 0.093 | -0.010 | 0.034 | 0.178 | 0.116 | 0.349 | 1.000 | - | - | - | - | - |
| Sandbox Egocentric Bias | 0.034 | 0.005 | 0.048 | -0.077 | 0.005 | 0.107 | -0.017 | 0.010 | -0.021 | 0.049 | -0.004 | 1.000 | - | - | - | - |
| CBCL-DP | -0.072 | -0.185 | -0.307 | -0.020 | 0.005 | 0.058 | 0.045 | 0.025 | -0.032 | -0.081 | -0.026 | -0.064 | 1.000 | - | - | - |
| ABAS-II-Social | 0.137 | 0.197 | 0.274 | -0.011 | -0.052 | -0.005 | 0.031 | 0.028 | 0.058 | 0.183 | 0.040 | 0.124 | -0.598 | 1.000 | - | - |
| Age | -0.041 | -0.078 | -0.67 | -0.024 | -0.004 | -0.006 | -0.016 | -0.099 | 0.032 | 0.025 | 0.002 | 0.014 | 0.052 | -0.042 | 1.000 | - |
| FSIQ | -0.020 | -0.16 | 0.046 | 0.011 | -0.101 | -0.054 | 0.039 | 0.007 | 0.031 | 0.013 | 0.013 | 0.094 | -0.081 | 0.066 | -0.001 | 1.000 |

*Note.*RMET = Reading the Mind in the Eyes Test (child version), NEPSY-II-AR = Neuropsychological Assessment Affect Recognition subscale, NEPSY-II-ToM = Neuropsychological Assessment Theory of Mind subscale, CBCL-DP = Child Behavior Checklist Dysregulation Profile, ABAS-II = Adaptive Behavior Assessment System 2nd Edition, FSIQ = full-scale intelligence quotient.

**Table S7. Effects of dysregulation (CBCL-DP) as a partial mediator of the association between social cognition (Social Cognition Component 2) and social behaviours (ABAS-II-Social), controlling for NDC diagnosis**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Estimate | Lower CI | Upper CI | p-value |
| **Training set (n=324)** |
| ACME | 0.147 | 0.056 | 0.235 | 0.002 |
| ADE | 0.397 | 0.240 | 0.547 | < 2e-16 |
| Total effect | 0.544 | 0.370 | 0.695 | < 2e-16 |
| Proportion mediated | 0.271 | 0.112 | 0.434 | 0.002 |
| **Test set (n=322)** |
| ACME | 0.139 | 0.065 | 0.217 | < 2e-16 |
| ADE | 0.264 | 0.123 | 0.406 | 0.002 |
| Total effect | 0.403 | 0.266 | 0.551 | < 2e-16 |
| Proportion mediated | 0.345 | 0.167 | 0.597 | < 2e-16 |

*Note*. CI = confidence interval, ACME = Average Causal Mediation Effect, ADE = Average Direct Effect.

**Table S8. Comparison of hierarchical regression Step 2 statistics between the main analysis and sensitivity analyses in the subset aged 16 years and younger and with FSIQ ≥70**

|  |  |  |
| --- | --- | --- |
|  | Main analysis | Sensitivity analysis |
| Adjusted R2 | 0.414 | 0.432 |
| MSE | 2.248 | 1.500 |
| AIC | 1015.360 | 966.764 |
| BIC | 1051.636 | 1002.448 |

*Note.* MSE = mean standard error, AIC = Akaike Information Criterion, BIC = Bayesian Information Criterion.

**Table S9. Effects of dysregulation (CBCL-DP) as a partial mediator of the association between social cognition (Social Cognition Component 2) and social behaviours (ABAS-II-Social), controlling for full-scale intelligence quotient (FSIQ) and NDC diagnosis, in participants aged 16 years or younger and with FSIQ ≥70**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|   | **Estimate** | **Lower CI** | **Upper CI** | **p-value** |
| **Training subset (n=262)** |
| ACME | 0.113 | 0.006 | 0.215 | 0.034 |
| ADE | 0.409 | 0.241 | 0.552 | < 2e-16 |
| Total effect | 0.522 | 0.321 | 0.696 | < 2e-16 |
| Proportion mediated | 0.216 | 0.013 | 0.382 | 0.034 |
| **Test subset (n=264)** |
| ACME | 0.168 | 0.073 | 0.258 | 0.002 |
| ADE | 0.248 | 0.089 | 0.410 | < 2e-16 |
| Total effect | 0.411 | 0.253 | 0.590 | < 2e-16 |
| Proportion mediated | 0.395 | 0.191 | 0.670 | 0.002 |

*Note.* CI = confidence interval, ACME = Average Causal Mediation Effect, ADE = Average Direct Effect.

**Table S10. Stability of hierarchical regression findings when alternating the training and test sets**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Coefficients** | **Estimate** | **Std. Error** | **t value** | **Pr (>|t|)** |   |   |
| **Step 1** |
| (Intercept) | -1.347 | 0.219 | -6.152 | **2.32e-09** |  |  |
| SC Comp 1 | 0.115 | 0.085 | 1.363 | 0.1739 |  |  |
| SC Comp 2 | 0.415 | 0.082 | 5.072 | **6.74e-07** |  |  |
| Autism | -0.674 | 0.285 | -2.362 | **0.018** |  |  |
| ADHD |  -0.237 | 0.283 | -0.834 | 0.405 | R2 | 0.097 |
| OCD | -0.293 | 0.438 | -0.670 | 0.503 | Adj R2 | 0.080 |
| Other NDC |  0.793 | 1.121 | 0.708 | 0.479 | F | **5.686 \*** |
| **Step 2** |
| (Intercept) | -0.647 | 0.205 | -3.150 | **0.001** |  |  |
| SC Comp 1 | 0.119 | 0.074 | 1.599 | 0.110 |  |  |
| SC Comp 2 | 0.276 | 0.073 | 3.771 | **0.001** |  |  |
| CBCL-DP | -0.165 | 0.017 | -9.706 | **< 2e-16** |  |  |
| Autism | -0.301 | 0.253 | -1.185 | 0.237 |  |  |
| ADHD | -0.123 | 0.249 | -0.496 | 0.620 | R2 | 0.306 |
| OCD | 0.433 | 0.392 | 1.105 | 0.269 | Adj R2 | 0.290 |
| Other NDC | 0.207 | 0.987 | 0.210 | 0.834 |  F |  **19.77 \*** |

*Note.* SC Comp = Social Cognition Component, CBCL-DP = Child Behavior Checklist Dysregulation Profile, ADHD = Attention-Deficit/Hyperactivity Disorder, OCD = Obsessive-Compulsive Disorder, NDC = Neurodevelopmental Conditions. \* indicates a p-value < 0.001. Significant effects appear in bold.

**Figure S1. Selection of the optimal number of social cognition principal components**  *Note.* RMSEP = predicted root mean standard error, MSE = mean standard error, ABAS-II = Adaptive Behavior Assessment System 2nd Edition. **A**: The optimal number of components (n = 2) informed by the one-sigma heuristic. **B**: The optimal number of components (n = 2) informed by the permutation approach. **C**: ABAS-II-Social variance (R2) explained by each component. **D**: Regression coefficients for each social cognition metric vary with the number of components kept to model ABAS-II-Social variance. **E**: PCR model derived from the training set (n = 324) fitted to the test set (n = 322). **Figure S2.** Multicollinearity between independent variables in the hierarchical regression *Note.* CBCL-DP = Child Behavior Checklist Dysregulation Profile, NDCs = Neurodevelopmental Conditions, ADHD = Attention-Deficit/Hyperactivity Disorder, OCD = Obsessive-Compulsive Disorder.